ABSTRACT

Jorge Vásquez-Kool. Gene family evolution of monolignol biosynthetic genes in loblolly pine (*Pinus taeda* L.) (Under the direction of David M. O'Malley).

Gene family organization in a genome is an important area in the study of genomics because it provides a structured basis to approach larger, more complex problems like gene expression, biochemical pathways and metabolism. Genes control and mediate biological activities of the cell. Although some genes are single copy, a large proportion of genes belong to larger gene families. Members of a gene family are related by homology and share significant sequence identity, modular structure, and their products display similarity in biochemical function and a common structural fold. To gain an understanding of the importance of grouping and characterizing genes into families, Chapter 1 provides an overview of gene family organization in genomes, presenting current delineation schemes to recognize members of a family, concepts of current use in this area of study, and a summary of different computational methods to characterize gene families. The ability to recognize patterns that allow the distinction of genes and the formation of discrete family groups requires the generation and use of multiple classes of information. For any given family, these classes of knowledge include (1) the sequence properties of the genes and its corresponding proteins, including defined motifs; (2) the phylogenetic history and pattern of conservation of the gene and the gene product; and (3) the structual features of the gene product. In order to gather this information and furnish

the data needed to advance inferences on gene families of the monolignol biosynthetic pathway, Chaper 2 describes the three-dimensional structural models of 4-coumarate:CoA ligase, cinnamoyl-CoA reductase and cinnamyl alcohol dehydrogenase, that were built using a comparative modelling approach. The three proteins show a Rossman fold domain, but they were evolutionarily unrelated. The comparison of the modular structure of the gene (exons) and the protein (domains) provided no clear patterns to relate the uni-dimensional gene structure to the three-dimensional structure of its protein product. The 3D structural models served to map conserved and variable sites and to identify active site or positions involved with cofactor or substrate recognition. At present, a major challenge facing the study of gene families is how to characterize sequence features that distinghish subfamilies. The ability to detect positions in a multiple sequence alignment where amino acid composition distinguishes subfamilies provide a basis to pursue studies on functional differences. Chapter 3 tackles this problem by determing a minimal set of homologous positions whose amino acid configuration is associated to subfamily groups. Two measures, the Gu's criterion of divergence and the mutual information criterion, detected aligned positions where molecular evolution differed by subfamily. Some of these positions were found in the substrate binding site, others related with the active site. The specific role of other discriminant positions could not be elucidated at present. The great benefit of recognizing homologous positions with discriminant capability poses the question whether these positions have a predictive ability. Could these signature positions that effectively distinguish subfamilies be applied to predict subfamily structure in loblolly pine DNA sequences? Does loblolly pine subfamily

structure for a given gene have an similar organization similar to other plant species? Chapter 4 describes the application of the signature using loblolly pine expressed sequence tag (EST) data. The rationale of the method involves using an alignment and phylogeny of translated sequences of known genes to detect the signature positions (scaffold alignment). Then, the scaffold is used to align translated EST sequences (obtained from a tBLASTn report). This EST-scaffold alignment allowed determination of the amino acid occupancy in the corresponding signature position in the EST. This operation will allocate ESTs into the different subfamilies. This knowledge-based approach revealed that loblolly pine contained only one type of 4-coumarate:CoA ligase, whereas coumaroyl-CoA reductase and cinnamyl alcohol dehydrogenase had each members of two different classes. One by-product of the method was the assembly of full-length, biologically-meaningful contigs from the same subfamily. This study revealed that the integrated use of phylogenetic, informatic and structural techniques and the use of pertinent biological sequence data could provide a sound basis to extent our capability to study gene family structure in the loblolly pine genome.

Gene family evolution of monolignol biosynthetic genes in loblolly pine (*Pinus taeda L.*)

by

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BIOGRAPHY

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From 1980 to 1985, he went to study forestry in the National Agricultural University at La Molina, near Lima, and graduated with a Bachelor of Science degree in 1986.

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CHAPTER 1

Gene Family Structure and Evolution: A Literature Review

Overview of the Thesis

Lignin: importance in nature and industry

Lignin is a natural product that has far-reaching impacts on agriculture, industry and the environment. The phenylpropanoid metabolism that produces lignin is an important part of plant biochemistry (reviewed by Baucher et al., 1998). As the second most abundant polymer on earth, surpassed only by cellulose, lignin is a major carbon sink in the biosphere, accounting for about 30% of the carbon sequestered into terrestrial plant material each year (reviewed by Lewis et al. 1999). Lignin is an integral cell wall component of all vascular plants. It plays an important role in plant cell walls, enhancing its rigidity, conferring resistance toward pathogens and mechanical stress, and enabling solute transport in the xylem (reviewed by Lewis and Yamamoto 1990). The many functions of lignin and related products in resistance to biotic and abiotic stress make the phenylpropanoid pathway vital to the health and survival of plants.

As a major polymer of plant cell walls, lignin also has a direct impact on wood characteristics, including the ease with which the undesirable lignin polymer can be removed from cellulose fibers during the pulping process (reviewed by Roberts 1996). Lignin reduces the quality and digestibility of forage crops such as alfalfa, which in turn impacts the livestock industry (Jung and Vogel 1986).

Lignins are biopolymers of monolignols

Lignins are heterogeneous polymers derived from *p*-coumaryl, coniferyl, and sinapyl alcohol, i.e. monolignols (Figure 1). In general, woody gymnosperm lignins

are predominantly derived from coniferyl alcohol, together with smaller amounts of p-coumaryl alcohol. In woody angiosperms, sinapyl alcohol is incorporated as well. In grasses and other herbaceous plants, hydroxycinnamic acids are incorporated into the lignin polymer (Higuchi 1985). Lignin monomer composition can also vary markedly between and within different tissues and subcellular compartments (e.g., middle lamella, secondary wall). The processes that accompany cell wall maturation and lignification in woody species is further complicated because cells differ markedly in wall development (e.g., thickness, polymer composition). For example, both lignin content and monomer composition differ in a gradient extending inward from the cambial zone to fully differentiated xylem (reviewed by Campbell and Sederoff 1996).

How this heterogeneity is controlled at the molecular level is unknown. The mechanism of lignin monomer transport from the cytoplasm through the plasma membrane and into the lignifying cell wall still has not been elucidated. Furthermore, it is not clear if the moieties undergoing transport are the free monolignols, their corresponding glucosides, or both (reviewed by Matsui et al. 1994, Donaldson 2001).

Lignin biosynthesis: formation of units and polymerization

The biochemical pathways leading to the formation of monolignols involve successive hydroxylation and O-methylation of the aromatic ring and conversion of the side chain carboxyl to an alcohol functional group (reviewed by Hahlbrock and Scheel 1989, Figure 2). The general phenylpropanoid pathway involves the conversion of

L-phenylalanine to activated cinnamic acids, and include a minimum of three enzymatic steps: deamination of phenylalanine by phenylalanine ammonia-lyase (PAL), hydroxylation of cinnamate by cinnamate 4-hydroxylase (C4H), and the esterification of the *p*-hydroxycinnamate and coenzyme A by 4-coumarate:coenzyme A ligase (4CL), respectively (Grisebach 1977). Activated cinnamic acids (*p*-hydroxycinnamoyl CoA esters) can then enter one of several different biosynthetic pathways, including the one that produces monolignols. Monolignol biosynthetic CoA esters undergo two successive reductive steps. The first is carried out by cinnamoyl-CoA reductase (CCR) which catalyzes the NADPH-dependent reduction of *p*-hydroxycinnamoyl CoA esters to the *p*-hydroxycinnamaldehydes. The second reduces these *p*-hydroxycinnamaldehydes to their corresponding alcohols or monolignols through the NADPH-dependent activity of cinnamyl alcohol dehydrogenase (CAD, reviewed by van Rensburg et al. 1999). Lignin is a complex polymer formed by the oxidative polymerization of hydroxycinnamyl alcohol derivatives. The monolignol units in lignin are joined through five common types of linkages (Davin and Lewis,1992; Figure 3). The mechanisms that determine the relative proportions of these linkage types in a particular lignin polymer are unknown. It has become increasingly apparent that lignin is not simply a random polymer of monolignol units, and that lignin composition is developmentally programmed, both temporally and spatially (Terashima et al.,1993).

The metabolic grid model of monolignol synthesis

A metabolic grid model has been postulated to explain the monolignol biosynthetic pathway (Dixon et al. 2001). This model states that the metabolic flux is governed by cellular concentration of the intermediates and the affinities of the various enzymes for their substrates. However, the enzymatic data do not fullysupport the operation of such a metabolic grid. Some of the enzymes upstream in the pathway display higher affinity for the aldehydes produced downstream. Recent enzyme specificity studies suggest that, if operational, the metabolic grid to monolignols could theoretically involve ring substitution at most, or all, levels of modification of the monolignol side chain, but that there may also be kinetically favored paths through the resultant "grid". Thus, the enzyme designated as F5H has a higher affinity for coniferyl aldehyde than for ferulic acid, at least in sweet gum (Osakabe et al., 1999) and *Arabidopsis* (Humphreys et al., 1999). Likewise, COMT from aspen and alfalfa has a significantly higher affinity for 5-hydroxyconiferyl aldehyde than for caffeic or 5-hydroxyferulic acids. Inhibition of COMT-mediated methylation of caffeic acid *in vitro* by 5-hydroxyconiferyl aldehyde could prevent flux from caffeic acid to ferulic acid *in vivo* (Li et al., 2000).

Downregulation of enzymatic steps in the monolignol pathway

Several studies have been published on the modification of lignin content and composition following transgenic up- or down-regulation of the enzymes, and

naturally occurring mutants in the monolignol pathway have been characterized in loblolly pine *CAD* (MacKay et al.,1997) and *Arabidopsis CCR* (Jones et al., 2001). New insights into lignin biosynthesis have also come through antisense regulation of cinnamoyl CoA reductase (CCR) and cinnamyl alcohol dehydrogenase (CAD). Downregulation of CCR results in a 50% reduction in Klason lignin in tobacco, as well as in stunted growth, reduced apical dominance, abnormal leaf shape, and chlorosis (Piquemal et al.,1998). When CCR expression is reduced, the amount of lignin deposited can be insufficient to support normal development. Transgenic tobacco plants with downregulated expression of CAD show only a slight reduction in Klason lignin and discolored xylem tissue, but otherwise have a wild-type morphology (Halpin et al. 1994). One explanation for these results is that lignification is sufficiently plastic to allow CAD-downregulated plants to form lignin directly from cinnamyl aldehydes (Kim et al., 2000, Yahiaoui et al.,1998). The data confirm that CCR and CAD are indeed critical for normal wild-type lignin biosynthesis in the various species investigated. Furthermore, a sinapyl alcohol dehydrogenase (SAD) in poplar has been identified that is co-expressed with F5H and COMT, and that co-localizes with syringyl lignin formation (Li et al., 2001). This implies that SAD is the primary enzyme responsible for the final step in syringyl monolignol biosynthesis, and that as a result, CAD downregulation has limited effects on this metabolic route. Downregulation experiments have also failed to entirely suppress CCR or CAD activity, indicating that these catalytic steps may be governed by more than one locus.

Gene families provide an structured view of the genome

Monolignol genes may not exist as single copies but instead as multigene families. Sequencing and database searches have revealed the existence of genes with significant sequence identity to known 4CL, CCR and CAD genes in many plant species (Harding et al. 2002, Lauvergeat et al. 2001, Wyrambik and Grisebach 1975).

Several whole-genome sequencing projects, including *Arabidopsis* have revealed the widespread organization of related genes into families (Arabidopsis Genome Initiative 2000). Conceptually, a gene family is a group of related sequences within the genome of a single species. Conventionally, a gene family has been defined as a group of genes whose members have >40% pairwise amino acid identity (reviewed by Graur and Li 2000). Functional and non-functional members of a gene family may reside in close proximity to one another on the same chromosome, or may be located on different chromosomes. The term “paranome” has been coined to refer to the complete set of gene families present in a genome (Friedman and Hughes 2001). Analysis of the *Arabidopsis thaliana* genome shows that 65% of its 11601 gene families contain at least two members. The sizes of the gene families ranges widely by genome. It is remarkable that *Drosophila*, a complex metazoan, has a paranome only twice the size of the yeast paranome. The proportion of genes belonging to families of more than five members is substantially higher in *Arabidopsis* (37.4%) than in *Drosophila* (12.1%) or *C. elegans* (24.0%), possibly due to extensive segmental duplications in *Arabidopsis*. The proportion of gene families with more than two members is considerably more pronounced in *Arabidopsis* than in other eukaryotes. The charac-

terization of the paranome facilitates a structured view of the genome, as well as provides a framework to study the relationship between gene sequence, expression and metabolism.

Gene families are composed of homologous genes. Homologous genes are those derived from the same gene in a common ancestor (Fitch 2000). All members of a gene family are homologs whether they are sampled from a single genome or from genomes of different species. Two basic types of relationship exist between any two homologous genes in a multigene family. If the event that generated the two genes was a duplication event, then the two genes are paralogs (i.e., genes coexisting within the same genome and belonging to a gene family, Fitch 1970). Orthologs are genes in different species that descended from a single gene in a common ancestor. Under a orthologous relationship two genes from different organisms are considered as ‘versions of the same gene in different species’ (Gogarten 1994). The characterization of homology in genes provides the basis to understand the expansion of a gene family, and sets a proper context to study the evolution of functional divergence of a gene family.

Finding paralog members of a gene family in a genome

One strategy for gene family analysis is to detect all the paralogous genes in one genome with a gene prediction method, such as Genscan (Burge and Karlin 1997), Genie (Kulp et al. 1996), or FGENES (Solovyev and Salamov 1997). Other strategies use translated genes to find gene families at the protein level using a similarity search

on protein motif databases, such as BLOCKS (Henikoff et al.1999), Pfam (Bateman et al. 1999), ProDom (Corpet et al. 1999), PRINTS (Attwood et al. 1999), PROSITE (Hofmann et al.1999), InterPro (Apweiler et al. 2001). However, protein motifs can only be used to search for known proteins, and some proteins remain undiscovered by existing experimental or theoretical methods. Xuan et al. (2002) developed GFS-can (Gene Family Scan), a tool that identifies members of a gene family by searching genomic DNA sequences with genomic DNA motifs (or matrices) that are representative of the family. The representative genomic DNA motif is constructed based on protein motifs in PROSITE and the genomic structure of known members of the family. The tBLASTn program of the BLAST package can align protein sequences with translated DNA sequence directly to find genes belonging to a gene family.

Finding orthologs: comparing corresponding genes across species

Orthologous genes are likely to have similar functions due to their phylogenetically close relationships of orthology. However, function is not formally part of the definition. Orthology is not necessarily a one-to-one relationship. In case of one or multiple duplication events subsequent to the speciation event, it can be one to many relationship. The relationship can become complex when assigning orthology to genes of more than two species because orthology is non-transitive. This means that two genes in different species that are both orthologous to a gene in a third species are not necessarily orthologous to each other (Fitch 2000).

Standard methods for finding orthologs start with searching a sequence database. A sequence of interest is compared to all other potentially related sequences that are already known. Search algorithms calculate the probability that the observed match with the most similar sequence in the database would occur by chance, and rank the results in the order of the estimated probability (Altschul et al.,1990). This procedure enables a prediction that the sequence and its best match (generally around an *e* value < 10^{-20}) are likely to be related. Current molecular databases are affected by sampling effects. The search for ortholog sequences in molecular databases is limited by the sampling of genes and organisms, gene loss in specific lineages, and genes that have diverged so greatly that search algorithms fail to detect them. Orthologous relationships may be further complicated by horizontal gene transfer or gene conversion (Gogarten and Olendzenski 1999).

Phylogeny and the clustering of orthologs

The subfamily structure of a gene family can be delineated based on the relationships among sequences represented in a phylogenetic tree. A phylogenetic tree of genes belonging to a family will establish clusters of closely related genes from different species (i.e., a subfamily). This phylogeny serves as a guide in identifying potential orthologues. Such an approach has been taken in the characterization of clusters of orthologous sequences (Tatusov et al., 2000). A variation of this method uses reconciled trees. A new tree is constructed that reconciles the sequence tree with the species tree by postulating missing sequences (e.g., due to gene loss; Yuan et al.

1998, Goodman et al. 1979, Page 1994). A method proposed by Retief et al. (1999) uses an stringent substitution matrix that places greater weight on more closely related sequences than on more distantly related ones. However, choice of substitution matrix alone does not account for other factors like rate variation or compensate for partial sequences.

Loblolly pine genomics

The large amount of DNA sequences generated in high-throughput genomics projects requires a framework to organize the inventory of genes in an organism's genome. The recognition of gene families furnish such a framework and deliver a system that can be used for comparative studies on pathways and metabolism. This rationale has been applied to the study of the loblolly pine (*Pinus taeda* L.) genome. Loblolly pine is the most widely planted tree species in the USA and an important tree in commercial forestry worldwide. The large genome size is an obstacle to molecular genetic analysis. Partial cDNA sequencing to provide expressed sequence tags (ESTs) has become one of the most direct ways to locate transcribed genes in its genome. This is an effective means of furnishing data on the transcriptome associated with different aspects of pine growth and development.

Expressed sequence tags for loblolly pine amount to 60 226 sequences in the dbEST database (July 2002, www.ncbi.nlm.nih.gov/dbEST/dbEST_summary.html). EST sequencing projects have already started to have a major impact on loblolly pine research, by accelerating the identification of new genes related to wood

formation (Whetten et al., 2001, Allona et al., 1998, Ujino-Ihara et al., 2000). Unlike high quality finished genome sequences, which are double-strand and multiple-pass, EST sequences are mostly single-strand, single-pass sequences, which contain sequencing errors (e.g., nucleotide substitutions, insertions or deletions), vary widely in length, and originate from different parts of the cDNA (Hatzigeorgiou et al., 2001). The analysis of ESTs is further complicated by the fact that the sampling of genes represented in a given unnormalized cDNA library causes rare transcripts to be missed and highly expressed genes to be overly abundant (i.e., redundancy). Computational methods of contig assemblage and DNA sequence quality have been implemented to address these issues. The loblolly pine EST contigs are conventionally assembled from individual ESTs at least 100 bp in length using the PHRED-PHRAP computer application and a minimum PHRED quality score of 20 for the EST base pairs. PHRED is a base-calling program for DNA sequence traces (Ewing et al. 1998, Ewing and Green 1998). After calling bases, the program examines the peaks around each base call to assign a quality score to each base call. Quality scores range from 4 to about 60, with higher values corresponding to higher quality. If PHRED assigns a quality score of 20 to a base, the chances that this base is called incorrectly are just 1 in 100.

Contigs are analyzed for functional homologies against the University of Minnesota/Computational Biology Center PEPTIDES database with BLASTX, and for putative protein-coding regions with Diogenes (U Minn). The contig sequences, contig assembly structures, and the BLASTX results are made publicly available at

web.ahc.umn.edu/biodata/nsfpine/contig_dir6. The pine ESTs have been assembled into 7576 contigs, but the number of genes that correspond with the contigs is probably smaller. Contig assembly artifacts and the allelic variation could inflate the number of contigs.

An approach to gene family analysis

The study of gene families can be approached from two perspectives: similarity and difference. Recognition of family members is generally based on similarity. However, it is not possible to prove that two sequences belong to a gene family based on sequence similarity alone. Divergent evolution of homologous genes could cause their gene products to participate in distinct metabolic processes (Gertl and Babbitt 2000). Rigorous statistical and biological evidence can be used to assess differences. Gu's θ quantifies the divergence level between subfamilies, making it feasible to test the null hypothesis (H_0: $\theta = 0$) that two subfamilies do not differ (Gaucher et al. 2002). If the H_0 is rejected it can be interpreted as an evidence of functional diversification of subfamilies. However, failure to reject the H_0 is not conclusive evidence that the subfamilies compared accomplish the same function. This statistical approach provides a context to integrate amino acid level analysis, pattern recognition of amino acid configurations, and the protein structural model to study gene families within the framework of functional divergence.

There are several reasons to characterize proteins rather than DNA sequences. These include the larger alphabet (20 amino acids versus 4 bases), the higher signal-

to-noise ratio in protein sequence searches, the closeness between protein sequence and function, and the availability of good, well annotated databases of protein sequences and protein sequence signatures (Swofford and Oldsen 1999). Proteins can be characterized at different levels. They perform a biochemical function in a cell, in a particular metabolic context, (i.e., as part of a complex pathway in a defined cellular location). Analysis could be carried out at the protein sequence along its entire length, at the level of single domains or motifs, or at the finest level, single amino acid positions. There is scope for protein characterization on all these levels using the correct tools and resources.

The differences between divergent subfamilies could be established at the sequence level by analyzing homologous positions in a multiple sequence alignment. The levels of conservation and variability in a given position produce a specific amino acid configuration that varies across subfamilies, providing a pattern to distinguish subfamilies. Wang and Gu (2001) defined a pattern recognition scheme for amino acid configuration in a multiple alignment of a family of genes clustered into two subfamilies A and B. Type 0 represents positions having a completely conserved amino acid residue through the whole gene family, implying that these residues may be important for the structural and functional integrity of the protein. Type I amino acid configurations are highly conserved in gene A but highly variable in gene B, or vice versa, implying that these subfamilies may have experienced site-specific rate differences. Type II amino acid configurations are highly conserved and different in both genes. Generally, their physico-chemical properties are different (e.g., polar vs.

hydrophobic), suggesting that these residues could be responsible for functional specification in the different subfamilies. Type U amino acid configurations are unclassified. Type I and Type II configurations are more likely to reveal sequence differences among subfamilies, though only a small portion of positions could be involved in functional divergence.

Several algorithms have been proposed to define these types of amino acid configurations based on phylogenetic information and statistical or informatics models. Type 0 positions contain amino acid residues completely conserved in all sequences belonging to a family. Sequence entropy has been used as a measure of positional variability in an alignment, as was proposed for example by Shenkin et al. (1991) and has been implemented in a number of studies (Sander and Schneider 1991, Mirny and Shakhnovich 1999). Entropy for a position is maximal if all 20 amino acids at this position have equal frequencies (Pei and Grishin 2001). Low entropy for a position indicates ‘evolutionary pressure’ to keep a particular type of residue. Type I functional divergence is a consequence of altered rates of amino acid replacements for a given position between two duplicate genes (Gu 1999). Type I amino acid configuration at a site is caused by different evolutionary rates between duplicate genes. Gu (1999) has proposed a method that computes the posterior probability of Type I configurations for each position in an alignment. Type II functional divergence results from fixation of a specific amino acid distinct in each subfamily and is generally detected using a mutual information criterion. Mutual information is frequently used in computational biology for co-variational analysis in RNA and proteins (Clarke 1995,

Gorodkin et al.,1999). The statistical significance of mutual information is evaluated using non-parametric methods to identify amino acid positions where the subfamilies differ by the amino acid conserved. Mutual information is nonnegative and equals zero if and only if amino acid residues and subfamilies are statistically independent. A large value of mutual information indicates a strong association between amino acid residues and clusters (Cover and Thomas 1991). Both Gu's and mutual information criteria can be influenced by small sample size and a biased composition of each column in the multiple sequence alignment.

The three-dimensional (3D) structure of a protein provides contextual information about the possible function of amino acid positions in a protein, and how structural differences could be associated with functional divergence. An understanding of the arrangement of the secondary structures in space provides insights into the different roles of amino acids in catalysis, folding, molecular recognition and interactions. While protein 3D structure is best determined experimentally, it can sometimes be reliably predicted by matching the sequence of a protein with proteins of known structure. 3D structures have been experimentally determined for only a fraction of proteins by X-ray crystallography or nuclear magnetic resonance (NMR) spectroscopy (Sanchez et al., 2000a). While there are approximately 500 000 protein sequences in the NCBI GenPept database, there are only 10 000 experimentally determined protein structures in the Protein Data Bank, 800 of them from plant origin.

A useful 3D model can frequently be obtained by comparative protein structure modeling, which constructs an all-atom 3D model for those proteins that are related

to at least one known protein structure (reviewed Jones et al. 1992). Structures obtained by comparative modeling will be less reliable than those determined experimentally by X-ray crystallography, but can nevertheless provide valuable information on enzyme fold and function. The number of sequences that can be modeled with useful accuracy by comparative modeling is already more than an order of magnitude larger than the number of experimentally determined protein structures (Sanchez et al. 2000b). Furthermore, the fraction of protein sequences that can be modeled reliably by comparative modeling is increasing rapidly. Globular protein domains cluster in only a few thousand fold families. Approximately 900 of these folds have already been structurally defined (Conte et al. 2002). Application of a comparative modeling approach to proteins encoded by a gene family has significant advantages. Since proteins encoded by a gene family have significant amino acid sequence identity (>40%), they most likely share similar 3D structure.

OVERVIEW OF THE THESIS

The goal of the thesis is to determine the organization of the gene families involved in the monolignol biosynthetic pathway in *Pinus taeda*, by integrating existing biological data and phylogenetic, informatics and structural tools. To accomplish this objective, multiple classes of information for a given gene and its protein product were assembled and analyzed. For example, the sequence properties (motifs, pattern of conservation and variability), the phylogeny, and also prediction of the structural features of the gene product were needed.

Chapter 2 describes the three-dimensional structural models of 4-coumarate:CoA ligase, cinnamoyl-CoA reductase and cinnamyl alcohol dehydrogenase that were built using a comparative modeling approach. Protein three-dimensional structures are important for understanding the functional significance of the pattern of conserved and variable sites in proteins. However, experimental determination by X-ray crystallography or NMR spectroscopy is laborious, time-consuming and expensive. Furthermore, there is only a small number of experimentally determined structures in the PDB database from plant sources. Since function and structure are more evolutionarily conserved than sequence, structures from distantly related species could be used to model the three-dimensional structure of these three monolignol proteins. A comparative modeling approach provided an viable method for structural characterization of the plant 4CL, CCR and CAD proteins.

In Chapter 3, pattern recognition of amino acid configurations characterized distinct subfamilies for plant 4CL, CCR and CAD genes, and provided the basis to explore the relationship between protein structure (modeled in Chapter 2), amino acid configuration and functional divergence. Gu's and mutual information criteria identified distinct amino acid configurations (signatures), thereby, furnishing two distinct views on the pattern of molecular evolution for the CAD subfamily. Subfamilies were distinguished by the nature of the amino acid occupancy in these sites. The structural relevance of the positions detected by these criteria revealed a striking pattern of protein subfamily evolution and structure. Gu's criterion detected positions conserved in one subfamily and variable in the other. These positions were located in loops and

bends on the surface of the protein. Mutual information detected positions in β-strands buried in the protein. The functional context of these positions was related to molecular recognition (substrate and cofactor binding), catalysis, and folding.

In Chapter 4, the subfamily structure of loblolly pine 4CL, CCR and CAD gene families was assessed by classifying ESTs and aligning them according to the gene family structure determined in previously known plant genes. The structure of seed plant gene families was characterized by the signature positions that have the predictive capability to distinguish subfamily classes in a population of uncharacterized ESTs. Only one class of 4CL was found in loblolly pine. Two major subfamilies were found for CCR and CAD gene families in loblolly pine, and in a number of monocot and dicot species. The evolution of the monolignol gene families could reflect a process of expansion and functional diversification.

LITERATURE CITED

Allona, I., Quinn, M., Shoop, E., Swope, K., St Cyr, S., Carlis, J., Riedl, J., Retzel, E., Campbell, M.M., Sederoff, R., and Whetten, R.W. 1998. Analysis of xylem formation in pine by cDNA sequencing. PNAS 95:9693-9698.

Altschul, S.F., Gish, W., Miller, W., Myers, E.W., Lipman, D.J. 1990. Basic local alignment search tool. J. Mol. Biol. 215:403-410.

Apweiler, R., Attwood, T.K., Bairoch, A., Bateman, A., Birney, E., Biswas, M., Bucher, P., Cerutti, L., Corpet, F., Croning, M.D.R., Durbin, R., Falquet, L., Fleischmann, W., Gouzy, J., H.Hermjakob, H., Hulo, N., Jonassen, I., Kahn, D., Kanapin, A., Karavidopoulou, Y., Lopez, R., Marx, B., Mulder, N.J., Oinn, T.M., Pagni, M., Servant, F., Sigrist, C.J.A., Zdobnov, E.M. 2001. The InterPro database, an integrated documentation resource for protein families, domains and functional sites. Nucleic Acids Res. 29:37-40.

Arabidopsis Genome Initiative 2000. Analysis of the genome sequence of the flowering plant *Arabidopsis thaliana*. Nature 408:796-815.

Aravind, L. and Koonin, E.V. 1999. DNA polymerase β-like nucleotidyltransferase superfamily: identification of three new families, classification and evolutionary history. Nucleic Acids Res. 27:1609-1618.

Attwood, T.K., Flower, D.R., Lewis, A.P., Mabey, J.E., Morgan, S.R., Scordis, P., Selley, J.N. and Wright, W. 1999. PRINTS prepares for the millennium. Nucleic Acids Res. 27:220-225.

Baucher, M., Monties, B., Van Montagu, M., Boerjan, W. 1998. Biosynthesis and genetic engineering of lignin. Critical Rev. Plant Sci. 17:125-197.

Bateman, A., Birney, E., Durbin, R., Eddy, S.R., Finn, R.D., and Sonnhammer, E.L.L. 1999. Pfam 3:1:1313 multiple sequence alignments and profile HMMs match the majority of proteins. Nucleic Acids Res. 27:260-262.

Burge, C. and Karlin, S. 1997. Prediction of complete gene structure in human genomic DNA. J. Mol. Biol. 268:78-94.

Campbell, M.M. and Sederoff, R.R. 1996. Variation in lignin content and composition. Plant Physiol. 110:3-13.

Clarke, N.D. 1995. Covariation of residues in the homeodomain sequence family. Protein Sci. 4: 2269-2278.

Conte, L.L., , Brenner, S.E., Hubbard, T.J., Chothia, C., Murzin, A.G. 2002. SCOP database in 2002: refinements accommodate structural genomics. Nucleic Acids Res. 30:264-7.

Corpet, F., Gouzy, J. and Kahn, D. 1999. Recent improvements of the ProDom database of protein domain families. Nucleic Acids Res. 27:263-267.

Cover, T.M. and Thomas, J.A. 1991. Elements of information theory. Wiley, New York.

Gorodkin, J., Staerfeldt, H.H., Lund, O., Brunak, S. 1999. Matrixplot: visualizing sequence constraints. Bioinformatics 15: 769-770.

Davin, L.B. Lewis, N.G. 1992. Phenylpropanoid metabolism: biosynthesis of monolignols, lignans and neolignans, lignins and suberins. Recent Advances in Phytochemistry 26:325-375.

Dixon, R.A., Chen, F., Guo, D., and Parvathi, K. 2001. The biosynthesis of monolignols: a "metabolic grid", or independent pathways to guaiacyl and syringyl units? Phytochem. 57:1069-1084

Donaldson, L.A. 2001. Lignification and lignin topochemistry - an ultrastructural view. Phytochem. 57:859-873.

Ewing, B. and Green, P. 1998. Base-Calling of Automated Sequencer Traces Using PHRED. II. Error Probabilities. Genome Res. 8:186-194

Ewing, B., Hillier, L., Wendl, M.C., Green, P. 1998. Base-calling of automated sequencer traces using phred. I. Accuracy assessment. Genome Res. 8:175-185.

Fitch, W.M. 1970. Distinguishing homologous from analogous proteins. Syst. Zool 19:99-113.

Fitch, W.M. 2000. Homology: A personal view. Trends Genet. 16:227-231.

Friedman, R., Hughes, A.L. 2001. Gene duplication and the structure of eukaryotic genomes. Genome Res. 11:373-381.

Gaucher, E. A., Gu, X., Miyamoto, M.M., and Benner, S.A. 2002. Predicting functional divergence in protein evolution by site-specific rate shifts. Trends Biochem. Sci. 27:315-321

Gerlt, J.A. and Babbitt, P.C. 2000. Can sequence determine function? Genome Biol 2000;1(5):Rewiews0005.

Gogarten, J.P. 1994. Which is the most conserved group of proteins? Homology - orthology, paralogy, xenology and the fusion of independent lineages. J. Mol. Evol. 39:541-543.

Gogarten, J.P. and Olendzenski, L. 1999. Orthologs, paralogs and genome comparisons. Curr. Opin. Genet. Dev. 9:630-636.

Goodman, M., Czelusniak, J., Moore, G.W., Romero-Herrera, A.E. and Matsuda, G. 1979. Fitting the gene lineage into its species lineage: a parsimony strategy illustrated by cladograms constructed from globin sequences. Syst. Zool. 28:132-168.

Graur, D. and Li, W.H. 2000. Fundamentals of Molecular Evolution. Sinauer Assoc., Sunderland, MA. 478p.

Grisebach, H. 1977. Biochemistry of lignification. Naturwissenschaften 64:619-625.

Gu, X. 1999. Statistical methods for testing functional divergence after gene duplication. Mol. Biol. Evol. 16:1664-1674.

Hahlbrock, K. and Scheel, D. 1989. Physiology and molecular biology of phenylpropanoid metabolism. Ann. Rev. Plant Physiol. Plant Mol. Biol. 40:347-369.

Halpin, C., Knight, M.E. , Foxon, G.A. , Campbell, M.M., Boudet, A.M., Boon, J.A., Chabbert, B. , Tollier, M.-T. and Schuch, W. 1994. Manipulation of lignin quality by down-regulation of cinnamyl alcohol dehydrogenase. Plant J. 6:339-350.

Harding, S.A., Leshkevich, J., Chiang, V.L., Tsai, C.J. 2002. Differential substrate inhibition couples kinetically distinct 4-coumarate:coenzyme a ligases with spatially distinct metabolic roles in quaking aspen. Plant Physiol. 128:428-438.

Hatzigeorgiou, A.G., Fiziev, P., Reczko, M. 2001. DIANA-EST: statistical analysis. Bioinformatics 17:913-919.

Henikoff, S., Henikoff, J.G. and Pietrokovski, S. 1999. BLOCKS+: A non-redundant database of protein alignment blocks derived from multiple compilations. Bioinformatics 15:471-479.

Higuchi, T. 1980. Biosynthesis of lignin. In: Lignin Biodegradation: Microbiology, Chemistry, and Potential Applications (Kirk. T. K. and Chane. H. M.. eds) Vol. 1. p. 1-19, CRC , Boca Raton; FL.

Hofmann, K., Bucher, P., Falquet, L., and Bairoch, A. 1999. The PROSITE database, its status in 1999. Nucleic Acids Res. 27:215-219.

Humphreys, J.M. , Hemm, M.R. and Chapple, C. 1999. New routes for lignin biosynthesis defined by biochemical characterization of recombinant ferulate 5-hydroxylase, a multifunctional cytochrome P450-dependent monooxygenase. PNAS 96:10045-10050.

Jones, D.T., Taylor, W.R., Thornton, J.M. 1992. A new approach to protein fold recognition. Nature 358:86-89.

Jones L, Ennos AR, Turner SR. 2001. Cloning and characterization of irregular xylem4 (*irx4*): a severely lignin-deficient mutant of *Arabidopsis*. Plant J. 26:205-216.

Jung, H.G. and Vogel, K.P. 1986. Influence of lignin on digestibility of forage cell wall material. J. Anim. Sci. 62:1703-1712.

Kim, H. , Ralph, J. , Yahiaoui, N. , Pean, M. and Boudet, A.M. 2000. Cross-coupling of hydroxycinnamyl aldehydes into lignins. Org. Lett. 2:2197-2200.

Kulp, D., Haussler, D., Reese, M.G. and Eeckman, F.H. 1996. A generalized hidden Markov model for the recognition of human genes in DNA. In D. States et al. (editors) Proceedings of the Fourth International Conference on Intelligent Systems for Molecular Biology, AAAI Press, Menlo Park, CA. pp. 134-142.

Lauvergeat, V., Lacomme, C., Lacombe, E., Lasserre, E., Roby, D., Grima-Pettenati, J. 2001. Two cinnamoyl-CoA reductase (CCR) genes from *Arabidopsis thaliana* are differentially expressed during development and in response to infection with pathogenic bacteria. Phytochemistry 57:1187-1195.

Lewis, N.G., Davin, L.B., Sarkanen, S. 1999. The nature and function of lignins. In D.H.R. Barton and K. Nakanishi (editors) Comprehensive Natural Products Chemistry. Vol.3, Carbohydrates and their derivatives including tannins, celllulose and related lignins. p. 617-745.

Lewis, N.G. and Yamamoto, E. 1990. Lignin: occurrence, biogenesis, and biodegradation. Ann. Rev. Plant Physiol. Plant Mol. Biol. 41:455-496.

Li, L. , Cheng, X.F. , Leshkevich, J. , Umezawa, T. , Harding, S.A. , Chiang, V.L. 2001. The last step of syringyl monolignol biosynthesis in angiosperms is regulated by a novel gene encoding sinapyl alcohol dehydrogenase. Plant Cell 13:1576-1585

MacKay J.J., O'Malley, D.M., Presnell, T., Booker, F.L., Campbell, M.M., Whetten, R.W., Sederoff, R.R. 1997. Inheritance, gene expression, and lignin characterization in a mutant pine deficient in cinnamyl alcohol dehydrogenase. PNAS 94:8255-8260.

Matsui, N., Fukushima, K., Yasuda, S., Terashima, N. 1994. On the behaviour of monolignol glucosides in lignin biosynthesis. Holzforschung 48:375-380.

Mirny, L.A. and Shakhnovich, E.I. 1999. Universally conserved positions in protein folds: reading evolutionary signals about stability, folding kinetics and function. J. Mol. Biol. 291:177-196.

Osakabe, K., Tsao, C.C., Li, L., Popko, J.L., Umezawa, T., Carraway, D.T., Smeltzer, R.H., Joshi, C.P., Chiang, V.J. 1999. Coniferaldehyde 5-hydroxylation and methylation direct syringyl lignin biosynthesis in angiosperms. PNAS 96:8955-8960.

Page, R.D. 1998. GeneTree: comparing gene and species phylogenies using reconciled trees. Bioinformatics 14:819-820.

Pei, J. and Grishin, N.V. 2001. AL2CO: calculation of positional conservation in a protein sequence alignment. Bioinformatics 17:700-712.

Piquemal, J., Lapierre, C., Myton, K., O'Connell, A., Schuch, W., Grima-Pettenati, J. and Boudet, A.-M. 1998. Down-regulation of cinnamoyl-CoA reductase induces significant changes of lignin profiles in transgenic tobacco plants. Plant J. 13:71-83.

Retief, J.D., Lynch, K.R., Pearson, W.R. 1999. Panning for genes: A visual strategy for identifying novel gene orthologs and paralogs. Genome Res. 9:373-382.

Roberts, J.C. 1996. The Chemistry of Paper. Royal Society of Chemistry, Cambridge, U.K. p. 161-175.

Sanchez, R., Pieper, U., Melo, F., Eswar, N., Marti-Renom, M.A., Madhusudhan, M.S., Mirkovic, N. and Sali, A. 2000a. Protein structure modeling for structural genomics. Nature Struct. Biol. (Suppl. Nov 2000) 986-990.

Sanchez, R., Pieper, U., Mirkovi, N., de Bakker, P., Wittenstein, E. Sali, A. 2000b. MODBASE, a database of annotated comparative protein structure models. Nucl. Acid Res. 28:250-253.

Sander, C., and Schneider, R. 1991. Database of homology-derived protein-structures and the structural meaning of sequence alignment. Proteins 9:56-68.

Shenkin, P.S., Erman, B., Mastrandrea, L.D. 1991. Information theoretical entropy as a measure of sequence variability. Proteins 11:297-313.

Solovyev, V.V. and Salamov, A.A. 1997. The Gene-Finder computer tools for analysis of human and model organism genone sequences. Intell. Syst. Mol. Biol. 5:294-302.

Swofford, D.L. and Oldsen, G.J. 1990. Phylogeny reconstruction. In: D.M. Hillis and C. Moritz (eds), Molecular Systematics. Sinauer Associates, Sunderland, MA pp. 411-501.

Tatusov, R.L., Galperi, M.Y., Natale, D.A., Koonin, E.V. 2000. The COG database: a tool for genome-scale analysis of protein functions and evolution. Nucl. Acids Res. 28:33-36.

Teichmann, S.A., Murzin, A.G., and Chotia, C. 2001. Determination of protein function, evolution and interactions by structural genomics. 11:354-363.

Terashima, N., Fukushima, K., He, L.-F., Takabe, K., 1993 In: Jung, H.G., Buxton, D.R., Hatfield, R.D., Ralph, J. (Eds.), Forage Cell Wall Structure and Digestibility, ASA-CSSA-SSSA, Madison, pp. 247-270.

Thornton, J.W. and DeSalle, R. 2000. Gene family evolution and homology: genomics meets phylogenetics. Annu. Rev. Genomics Hum. Genet. 1:41-73.

Ujino-Ihara, T., Yoshimura, K., Ugawa, Y., Yoshimaru, H., Nagasaka, K., Tsumura, Y. 2000. Expression analysis of ESTs derived from the inner bark of *Cryptomeria japonica*. Plant Mol. Biol. 43:451-457.

Wang, Y., Gu, X. 2001. Functional divergence in the caspase gene family and altered functional constraints: statistical analysis and prediction. Genetics 158:1311-1320.

Whetten R, Sun YH, Zhang Y, Sederoff R. 2001. Functional genomics and cell wall biosynthesis in loblolly pine. Plant Mol. Biol. 47:275-291.

Wyrambik D., Grisebach H.1975. Purification and properties of isoenzymes of cinnamyl-alcohol dehydrogenase from soybean-cell-suspension cultures. Eur J. Biochem. 59:9-15.

Yahiaoui, N. , Marque, C. , Myton, K.E. , Negrel,J., Boudet, A.M. 1998. Impact of different levels of cinnamyl alcohol dehydrogenase down-regulation on lignins of transgenic tobacco plants. Planta 204:8-15.

Yuan, Y.P., Eulenstein, O., Vingron, M. and Bork, P. 1998. Towards detection of orthologues in sequence database. Bioinformatics 14:285-289.

Xuan, Z. McCombie, R. and Zhang, M.Q. 2002. GFScan: A Gene Family Search Tool at Genomic DNA Level. Genome Res. 12:1142-1149.

CHAPTER 2

Comparative Three-Dimensional Structural Modeling of the Loblolly Pine (*Pinus taeda L.*) 4-Coumarate:Coenzyme A Ligase, Cinnamoyl-Coenzyme A Reductase, and Cinnamyl Alcohol Dehydrogenase

INTRODUCTION

Protein structures have been determined experimentally using X-ray crystallography and nuclear magnetic resonance (NMR) methods (reviewed by Burley and Bonanno 2002). In spite of recent technical advances in experimental structural determination, the process is still laborious and time consuming. In the absence of crystal structures for these enzymes, comparative modeling could be a reasonable alternative to study the structural basis of enzyme function (Sali 1995). These models can be very useful in deducing the function of proteins where no structural information exists and in extending patterns observed from the structure of a protein to its protein families. Crystal structures have been determined for very few plant proteins. Since structure is more conserved than sequence, it is possible to use known structures from distantly related organisms to predict the structure of plant proteins (Hrmova and Fincher 2001).

The comparative modeling process begins with the detection and selection of possible three-dimensional templates for a given sequence of unknown structure (i.e., the target protein). Once the template is chosen, and often in parallel to this process, a good alignment between the amino acid sequences of the three-dimensional template and the target protein needs to be generated (3D-1D alignment). The next step is to construct a structural model based on this alignment, including backbone and side chain conformation and loop prediction (Al-Lazikani et al. 2001). This approach relies heavily on the knowledge pool of experimentally-determined structures.

The three-dimensional (3D) structure of a protein provides the functional context whereby the amino acid residues could be related to functional aspects of the protein (e.g., catalysis, folding, molecular recognition and interactions). Molecular structure plays an important role in understanding functional divergence among subfamilies of a gene family. Proteins encoded by subfamilies can be discriminated by the amino acid occupancy in certain homologous positions. This provides a structural basis to explore functional divergence. One of the goals of proteomics is to determine all the structures of the proteome. However, if the genomic basis underlying the proteome is viewed as an structured set of families of related genes, then the work load decreases significantly. Proteins encoded by a gene family share significant sequence identity and therefore have similar structure. The structure determination of one single member of a family could produce reliable structural information for the remaining members of the family.

The goal of this chapter was to construct models of the tertiary structure of 4-coumarate:CoA ligase (4CL), cinnamoyl-CoA reductase (CCR) and cinnamyl alcohol dehydrogenase (CAD) enzymes using a comparative approach. Within the limits of this methodology, such models allowed me to explore (1) whether a relationship exists between exonic sequences of the genes and the domain structure of the encoded peptide, and (2) to map variable positions that discriminate between protein subfamilies. The quality of the structural models showed that the comparative approach is viable for these plant proteins.

MATERIALS AND METHODS

Template search and template-target alignment

Pinus taeda protein target sequences were extracted from the NCBI database using the Entrez search and retrieval system and the 4-coumarate:CoA ligase, cinnamoyl-CoA reductase and cinnamyl alcohol dehydrogenase names as text queries. Potential 3D templates were determined for each sequence by submitting them independently to several different fold recognition softwares, namely Gen-Threader (Jones 1999, bioinf.cs.ucl.ac.uk/psiform.html) which is based on profile sequence alignment and threading; 3D-PSSM (Kelley et al. 2000,www.sbg.bio.ic. ac.uk/~3dpssm/) which uses secondary structure, solvation and accessibility position-specific profiles; and BIOINBGU (Fischer 2000, www.cs. bgu.ac.il/~bioinbgu/) which is based upon a hybrid fold recognition approach. These templates were then structurally aligned with each other to help identify possible structurally conserved regions between them. This was accomplished by retrieving structural alignments from the HOMSTRAD database (Mizuguchi 1998, www-cryst.bioc.cam.ac.uk/~homstrad/).

The 3D template structures and the corresponding 1D *Pinus taeda* target 4CL, CCR and CAD sequences were then aligned (3D-1D alignment) and the resulting alignments were compared to each other. Agreement between them established structurally conserved regions. The initial structural alignment of the templates thus provided a framework to help properly align the target sequences according to outputs provided by different methods used for template search.

Model Building

MODELLER (Sánchez and Sali 2000, guitar.rockefeller.edu/modeller) was used to build three-dimensional model structures of the *Pinus taeda* 4CL, CCR and CAD proteins. Provided a 3D-1D alignment, MODELLER computes a model containing all non-hydrogen atoms by satisfaction of spatial restraints (Sali and Blundell 1993.). Spatial restraints on the target structure are obtained by assuming that the distance and angles among the atoms in the 3D templates are similar to the target atoms to which they are aligned. These restraints and the CHARMM force field terms (to enforce proper stereochemistry) are combined with an objective function. The model is generated by optimizing this function in a Cartesian space (Sánchez and Sali 1997).

Model Evaluation

Model accuracy is evaluated by distinguishing between a mistraced or wrongly folded model, and one that is basically correct, but not adequately refined. This was evaluated using the Verify3D software (Bowie et al. 1991, Lüthy et al. 1992, www.doe-mbi.ucla.edu /Services). Verify3D provides a test of the accuracy of a 3D protein model by comparing the model to its own amino-acid sequence, using a 3D profile computed from the atomic coordinates of the structure 3D profiles of known protein structures. Verify3D calculates three properties for each amino acid in the proposed model structure: the total surface area of the residue that is buried in the protein, the fraction of the side chain area that is covered by polar atoms, and the local secondary

structure. These three parameters are then used to allocate the residue to one of eighteen local environmental classes. Each amino acid is given a score that reflects the compatibility of that amino acid for that environment, based upon the analysis of known protein structures.

The root mean square deviation (RMSD) values in the C^{α} positions between the target protein models and their 3D templates were determined using INSIGHTII (Koehl 2001). PROVE was used for atomic volume exclusion analysis (Pontius et al. 1996, biotech.ebi.ac.uk:8400/doc/prove/prove.html) . The atomic volume check calculates the atomic volume for each atom in the structure, and compares it to pre-computed standard averaged volumes for each atom type, resulting in a Z-value for each buried atom.

Protein domain identification

The identification of domain modules was accomplished by means of a distance matrix plot obtained for each structural model using the MatrixPlot server (Gorodkin et al. 1999, www.cbs.dtu.dk/services/MatrixPlot/distmatr/index.html). This is a graphical method in which the amino acid residues of a protein are listed consecutively on the two axes of a two-dimensional matrix. Given the known tertiary structure of the models, a color is associated with a distance scale in angstroms between two residues. In the ideal case, domains are identified as empty, non-overlapping, right-angle triangles whose hypotenuses are on the diagonal of the matrix plot, and whose sides are defined by distinct triangles containing clusters of neighboring residues (<30 Å).

The domain boundaries present in the template were transferred to the target protein model using the 3D-1D alignment as defined by the CATH hierarchical domain classification, version 2.4, Released Jan 2002 (Orengo et al. 1997, www.biochem.ucl.ac.uk/bsm/cath_new/index.html). The CATH computational scheme establishes fold groups based on the orientation and connectivity of secondary structures. Secondary structure determination of the protein models was carried out using PROMOTIF (Hutchinson and Thornton 1996, sapc34.rdg.ac.uk/~gail).

RESULTS

Three-dimensional templates

Table 1 summarizes the results from the template search and the 3D-1D alignment for each of the loblolly pine target proteins 4CL, CCR and CAD. For 4CL, two structures were found that belonged to the AMP-forming CoA thiol ester synthases. Firefly luciferase, in the presence of Mg(II), ATP and molecular oxygen, oxidizes luciferin, emitting yellow-green light. The second structural template for 4CL was the N-terminal adenylation subunit of gramicidin S synthase 1 (GrsA) of the Gram-positive bacterium *Bacillus brevis*. This enzyme activates the L-phenylalanine carboxylate group with ATP to the corresponding acyl-adenylate and catalyses the inversion of configuration of the amino acid to produce a D-phenylalanine molecule (Conti et al. 1997).

The templates for CCR were dTDP-glucose-4,6-dehydratase and the UDP-galactose-4-epimerase. These enzymes belong to the short chain dehydrogenase/reduc-

tase superfamily, share 25% amino acid sequence identity, have similar three-dimensional structural folds, and use nicotinamide dinucleotides to catalyze redox reactions. They participate in the rhamnose and galactose biosynthetic pathways in bacteria, respectively (Hegeman et al 2001, Thoden et al. 2000).

Cinnamyl alcohol dehydrogenases belongs to the medium chain alcohol zinc-containing dehydrogenases. Available information on the sequence of the protein, knowledge of its quaternary structure, the stereochemistry of catalysis, and requirement for zinc and dinucleotide cofactor was included in the template search. The templates found for CAD were dimeric mammalian alcohol dehydrogenases, that display broad substrate specificities. Class I ADHs (3BTO.pdb) are abundant in the liver and are the major enzymes in the first step of ethanol metabolism (Cho et al., 1997). Class IV ADHs (1D1S.pdb) are extra-hepatically expressed with high retinol metabolizing activity in stomach mucosa. Classes I and IV ADHs share 69% sequence identity between them and show similarity in chemical reaction (i.e., alcohol oxidation/aldehyde reduction) and stereochemistry (A-specific with respect to the dinucleotide cofactor, pro-*R* specific with respect to the substrate), the presence of two divalent zinc cations, and zinc-binding and Rossman fold signatures.

Allignment of template and target protein sequences

The sequence identity between the loblolly pine 4CL and template sequences (32% with luciferase and 21% with the peptide synthase; Figure 2A) covered the whole sequence, assuring positional homology of the alignment. The box motif

GEICIRG in loblolly pine 4CL (residues 386 to 392) was well aligned to the corresponding motif box in the templates. In 4CL, the box motif corresponding to the AMP-binding signature (LPYSSGTTGLPK, residues 186-197) was not properly aligned to the corresponding boxes in luciferase (LUCI_PHOPY, ImnSSGSTGlPK, residues 195-206) or in the gramicidin S synthetase (GRSA_BACBR, ViyTSGTTGnPK, residues 187-198). This anomalous situation could be attributed to structural disjunctions in the templates causing amino acid residues not present in the sequence. Luciferase lacked residues Ser199-Gly203, and the peptide synthetase residues Gly192-Asn196 when compared to the standard alignment of this motif alignment (PROSITE PS00455, www.expasy/org/cgi-bin/ft_aligner? psa=PS00455).

Loblolly pine CCR and the sequences of 4,6-dehydratase (1BXK) and 4-epimerase (1UDC) had a very low level of sequence identity (17%; Figure 2B). The biochemistry of these template proteins is different from CCR, precluding the transfer of functional residue information from the templates. The signature characterizing the short chain dehydrogenase/reductase family (PROSITE PS00061, www.expasy.org/cgi-bin/ft_aligner?psa=PS00061) was not found in either the templates or target sequences. None of them was either listed by name or EC number. Thus, the 3D-1D CCR alignment lacked anchors to ensure positional homology.

The alignment of loblolly pine CAD to the templates showed a moderate sequence identity (23% with 3BTO and 19% with 1D1S; Figure 2C). The alignment was facilitated by the presence of the conserved cysteins (residues 100, 103, 106, 115) acting in the coordination sphere of the structural zinc, the two cysteines

(residues 47, 163) and histidine (69) residues involved in coordinating the catalytic zinc. In addition, the zinc-containing alcohol dehydrogenase signature (PROSITE PS00059, GHEVVGIVTEIGSEV) encompassed positions 68 to 82. The dinucleotide binding signature was located between Lys182 to Ser212. This is an α/β domain consisting of a series of conserved amino acid residues, especially in the the βαβ signature that consists of the first two β-strands (underlined) and the intervening amphipathic α-helix (italics) (KKCGIL*GLGG*VGHMGVKIAKAFGLHVTVISS).

General features of the structural models for *Pinus taeda* monolignol enzymes

4-coumarate-CoA ligase

4CL is a multi-domain protein consisting of 4 distinct modules, namely, two 3-layer αβα sandwiches (Rossman fold; residues Ile21-Lys204 and Gly205-Val355), a β-roll (luciferase domain 3; residues Lys356-Val433), and a 2-layer αβ sandwich (GMP synthetase, subunit A, domain 3; Asp434-Ala536) (Table 3). The β-sheets of the two Rossman fold domains project perpendicular to one another. The β-roll was almost engulfed by the 2-layer αβ sandwich (Figure 3). Although there was significant identity between the loblolly pine 4CL and the templates, the 3D-profile (Table 2) showed two portions of the model in which the amino acid residues had poor compatibility to the environment where they were assigned. Positions Asp18 to His25 formed an external loop, and positions Val210 to Val220 established the C-terminal portion of an α-helix (210-213) with an attached loop. These two substructures were spatially close, and probably interact to some extent. The modeling of the loop

possibly affected the model of the α-helical region. The overall score of 196.2, calculated by the 3D profile method, was positioned between the expected (245.5) and the minimum (110.4) indicating that the model was reliable and had few faulty regions. The RMSD in C^{α} positions between the 4CL model and the template was the lowest when the percentage identity was the highest between template and target, indicating that the luciferase structure is more closely related to the 4CL structure than the peptide synthase structure.

Cinnamoyl CoA reductase

CCR has two α/β domains, one is the 3-layer αβα sandwich (Rossman fold; residues Met1-Ile204 and Pro287-Lys324) in which a parallel β-sheet is extended by a 7th strand, order 3214567 with a left-handed crossover connection between strands 6 and 7. The Rossman fold is the largest domain, occupying two thirds of the protein (Figure 3). The second domain consisted of an αβ-complex (UDP-galactose 4-epimerase, domain 1; residues Gln223-Val254). Given the low level of sequence identity, the demarcation of these domains remain uncertain, confounded by the template structures not aligning well in the central (α/β complex) domain. The graphical method revealed a central domain located between positions Ser126 and Ile200 that apparently acts as a linker between the N-terminal and C-terminal domains. The model structure contained large crevices and clefts, probably to account for the large size of its ligands, NADPH and the CoA ester. The loops located between positions Val285 to Lys294 and Leu255 to Val260 were poorly modeled because their close

proximity produced steric hindrances. Loop 285-294 should be located on the surface of the protein, but instead, its backbone was buried in the model. The 3D-profile did not reveal any anomaly in this region, and the 3D-1D alignments produced by all the methods consistently assigned the Lys289 to Lys294 positions to the same location in the template structural alignment. The overall self-compatibility score for the loblolly pine CCR model was poor (96.9) compared to the expected (147.5) and the minimum (66.4) scores. This indicated that the model contained residues in environments with which they are not compatible or that CCR has marked differences in its structural fold with the templates. The RMSDs and the percentage identity of the templates and target models were very similar, indicating that the use of both templates together did not contribute significantly to model reliability compared to each of them alone.

Cinnamyl alcohol dehydrogenase

CAD consisted of two distinct α/β domains, namely the zinc-binding domain (quinone oxidoreductase, subunit A, domain 1; residues Met1-Ser167 and Gly298-Asn357) and the central NADPH-binding domain (3-layer $\alpha\beta\alpha$ sandwich Rossman fold, Pro168-Ile297) whose parallel β-sheet had 6 strands, with order 321456 (Figure 3). The Rossman fold divides the zinc-binding domain into two parts and plays a role in the subunit-subunit interaction (i.e., dimerization). An anomalous feature was found between positions Glu301 to Lys314 which were composed of solvent-exposed polar or charged residues that formed an α-helical structure “broken” at position

Thr309. Inspection of the alignment at this region showed that a gap was inserted between the N- and C-terminus of the helix. The overall self-compatibility score for the model was 114.9, far from the expected (160.4). Examination of the 3D profile of the loblolly pine CAD model showed that most of the residues are positioned in favorable environments within the structure. The RMSDs of the template and the CAD model structures showed that the horse liver alcohol dehydrogenase (3BTO) template was more closely related to the CAD protein.

Correspondence between gene structure and protein domains

The structural domains of a protein could be contained within an exon or split between adjacent exons (Figure 2). The loblolly pine *4CL* gene (Acc. No. U39405) had four exons and three introns, whereas its protein product has 4 distinct domains. The two Rossman fold domains in 4CL are encoded by exon I and half of exon 2. The another half of exon 2 encoded the β-roll domain. The case in which a single structural domain was encoded by two exons was represented by the clear correspondence between exons 3 and 4 and its encoded 2-layer αβ domain.

The exon-intron structure of the loblolly pine *CCR* cDNA (Acc. No. AY064169) was predicted based on the structure of the *Eucalyptus gunnii CCR* gene (Acc. No. X97433) and assumed to contain 5 exons. The Rossman fold in CCR is encoded by exons 1,2,3 and half of exon 4. The αβ complex domain is encoded by exon 5 and half of exon 4. The correspondence between exons and domains for CCR is still uncertain, though each domain can be said to be encoded by two or more exons.

The loblolly pine CAD gene has 5 exons (Mackay 1996). The Rossman fold was encoded by exon 4. The N-terminal portion of the zinc-binding domain was encoded by exons 1, 2, and 3, and the C-terminal portion the zinc-binding domain is encoded by exon 5. Therefore, CAD has two exons that corresponded to single domains, as well as the case where a single structural domain is encoded by two or more exons. No case was found where an exon encoded two complete domains.

The exon-exon boundaries were all were in buried in 4CL. Similarly, CCR and CAD had all of the exon-exon boundaries buried, with the exception of exon2-exon3 in CCR and exon 4-exon 5 in CAD.

DISCUSSION

The comparative model approach

The structural models of loblolly pine 4-coumarate-CoA ligase, cinnamoyl-CoA reductase and cinnamyl alcohol dehydrogenase proteins were constructed using a comparative modeling approach. The three-dimensional structure of proteins is more evolutionarily conserved than their sequences and that facilitates the comparison of proteins across distantly related sequences and from disparate organismal sources. However, structural similarity does not guarantee functional similarity (Skolnick and Fetrow 2000, Chothia and Lesk 1986). The confidence in the structural models obtained by a comparative modeling approach depends on the diversity of the fold library, the sequence-structure alignment technique and the method for fitting the sequence onto the template structure. This work shows the feasibility of utilizing this

method for plant proteins. The confidence of the model structures is high for CAD and 4CL proteins given the number of features in the sequences and to some extent the biochemistry that they hold in common with the mammalian, insect or bacterial protein templates. Confidence is less certain for CCR structural models, indicating that some structural features could be unique to the CCR protein.

The formation of the adenylate intermediate and the presence of conserved peptide motifs are features shared by 4CL and a number of enzymes with divergent functions that group into the adenylate-forming enzyme superfamily despite their low overall amino acid sequence identity. These proteins include firefly luciferases, peptide synthetases, 4-chlorobenzoate ligases and acyl-CoA synthetases. The substrates of these enzymes differ widely, ranging from 4-hydroxycinnamates (4CL), to amino acids (peptide synthetases), luciferin (luciferases) and long-chain fatty acids (acyl-CoA synthetases). Amino acid sequences that define the substrate specificities of these enzymes are unlikely to be conserved, and have not been defined for 4CL (Ehlting et al. 2001). In addition, the reaction path that follows the formation of an adenylate intermediate differs in these proteins. 4CL-catalyzed CoA ester formation takes place via a two-step ATP and Mg(II) dependent reaction in which 4-hydrocinnamoyl-adenylate is formed as a intermediate (Becker-Andre et al. 1979, Knobloch and Hahlbrock 1975; Figure 1A). The adenylate is esterified with coenzyme A by 4CL, with the CoA phosphopatheteine moiety by peptide syntethases, or oxidized by molecular oxygen in the case of luciferases (Ehlting et al. 2001). A classification of AMP-binding proteins based on sequence similarity made by Fulda

et al. (1994) grouped plant 4CL and luciferases from insects into class IV, whereas gramicidin synthetases belonged to class II. 4CL was more closely related to luciferases (32% identity) than to gramicidin synthetases (21%).

CCR is a monomeric protein that uses NADPH and a CoA ester as a substrate. The template enzymes 4,6-dehydratase and 4-epimerase are homodimers, containing a irreversibly bound NAD^+ cofactor in each subunit, and use nucleotide sugar substrates. For both template enzymes catalysis begins with the same mechanistic step, where a tightly bound NAD^+ oxidizes carbon-4 in the hexopyranose moiety of the nucleotide sugar substrate (Hegeman et al. 2001, Thoden et al 2000). The catalytic reaction carried out by CCR has not been well characterized. The reaction probably involves a nucleophylic attack by the NADPH pro-*S* hydrogen to the carbonyl carbon of the substrate, which destabilizes the C-S bond of the coenzyme A ester, and causes the CoA release and formation of hydroxycinnamaldehyde (Figure 1B). The amino terminal region of the pine CCR between positions 15 and 35 is extremely well conserved among all plant CCR proteins (seven invariant positions V12, C14, V15, T16, G17, A18, and G20). This region corresponds to the αβα-dinucleotide binding fold of NADP(H) dehydrogenases/reductases. The first two β strands and the first α helix are located at similar positions in the sequence of *E. coli* UDP-galactose 4-epimerase. Serine 127 is homologous to serine 124 in the epimerase, which is involved in nucleotide binding (Thoden et al. 2000). The 4,6-dehydratase Cys187 corresponded with the loblolly

pine Cys187. In the dehydratase, this residue forms a thiolate involved in catalysis (Hegeman et al. 2001).

The relationship between CAD and its templates was not only structural but also a phylogenetic and functional one (cf. McKie et al. 1993). Horse liver alcohol dehydrogenase, like CAD, is a dimeric protein with each 40 kDa monomer consisting of a zinc and a dinucleotide binding domains. The active site contains a tetracoordinate zinc cation, and is located at the base of the cleft between the two domains. Three of the zinc ligands are supplied by the enzyme. In the open form of the apoenzyme, the active site is accessible to solvent and the fourth zinc ligand is occupied by water. When cofactor binds, it induces a rotation of the catalytic domain relative to the coenzyme binding domain, resulting in a narrowing of the interdomain cleft and a more hydrophobic environment at the active site. This rearrangement facilitates displacement of water by the substrate as the fourth coordination ligand of the catalytic zinc and places the zinc-bound substrate close to the C4 position of the NADPH nicotinamide ring. Once the enzyme adopts this closed form, the substrate and cofactor are sufficiently close to allow direct transfer of a hydride ion from the C4 position of the nicotinamide ring to the *re*-face of the aldehyde, that would become the pro-*R* hydrogen in the alcohol product (Colby et al. 1998, Xie et al. 1999, Cho et al. 1997). The catalytic reaction path carried out by mammalian ADHs can be safely transferred to CAD (Figure 1C).

Both CCR and CAD have a structurally related Rossman fold and use the phosphorylated coenzyme NADP(H), yet they differ in a number of characteristics. Though

the role of this domain is the binding of the dinucleotide cofactor NADPH, the level of sequence identity between these two domains in CCR and CAD is very low (19%). CAD has a greater subunit molecular weight of about 40 kDa and is zinc-dependent whereas CCR has a smaller subunit of 25-35 kDa and no metal requirements. In regard to the stereochemistry of the hydride transfer from the NADPH, CCR is B-specific, meaning that the hydrogen transferred is in the *si*-face of the nicotinamide ring, while CAD uses the *re*-face hydrogen (Wyrambik and Grisebach 1979). The NADPH use by these enzymes as a reducing factor corroborates their role in anabolic processes of the cell to produce building units for the biopolymer lignin. The equilibrium constants for the enzyme kinetics of CCR and CAD show that the reactions tend towards the formation of *p*-hydroxycinnamyl alcohols, probably driven by the high ratio of NADPH to $NADP^+$.

Gene and protein modular structure

The Rossman fold architecture is a common fold present in 4CL, CCR and CAD proteins. This domain is involved in NADPH binding in CAD and CCR. The role of the Rossman fold in 4CL has not been elucidated, but may be related with binding coenzyme A as well as AMP, due to its affinity for nucleotides. The Rossman fold is found in a diverse group of enzymes (Chu and Hwang 1998). Genes can evolve through internal duplication in the gene sequence. However, no evidence of internal duplication and subsequent modification could be found in the *4CL, CCR* and *CAD* genes. The two consecutive Rossman fold domains in 4CL show low sequence

identity (16%) and probably were independently generated. A structurally repeated domain at the protein level does not necessarily indicate an exon duplication event at the DNA level.

The relationship between exons and protein domains is not consistent. The Rossman fold domain in CAD was encoded by exon 4. In others, no pattern could be discerned for the Rossman fold. Two genomic sequences of *Arabidopsis thaliana* CCR, *AtCCR1* (Acc. No. T24D18.5) and *At CCR2* (Acc. No. F23A5.17) are found on chromosome 1. At the protein level, they share 81.6% sequence identity. The sequence corresponding to the *AtCCR1* gene contained four introns at identical positions to the *Eucalyptus gunnii* CCR gene (*EuCCR*, Acc. No. EGCCR1GEN, Lacombe et al. 1997). Only three introns were found in the genomic sequence of *AtCCR2* corresponded with introns 2, 3 and 4 in the *AtCCR1* and *EuCCR* genes, indicating that the first intron is missing (Lauvergeat et al. 2001). Whether an intron was lost in *AtCCR1* or an intron was inserted in *AtTCCR2* remains to be elucidated. Exon fusions have modified the ancestral structure during the evolution of nuclear genes (Go 1981). The relationships between the intron locations found in different species could be used to construct a tree for the evolution of the gene. Mechanistic models to explain intron-exon evolution are lacking, and results based on intron-exon structure are uncertain (Wada et al. 2002).

Some exons tend to be small, such as 4CL exon 3 which encodes a 15 amino acid peptide. Others are large, like the 4CL exon 1 which is as large as the complete coding region for CCR and CAD. Exon-exon boundaries were mostly found buried in

the protein and only in few cases, exposed to the solvent. This is inconsistent with some models that explain that the formation of a protein results by adding domains, and that the connections of the most recently added modules tend to lie in the surface (Lewin 1994).

LITERATURE CITED

Al-Lazikani, B., Jung, J., Xiang, Z., and Honig, B. 2001. Protein structure prediction. Curr. Opinion Chem. Biol. 5:51-56.

Becker-André, M., Schulze-Lefert, P. and Hahlbrock, K. 1991. Structural comparison, modes of expression, and putative cis-acting elements of the two 4-coumarate:CoA ligase genes in potato. J. Biol. Chem. 266:8559.

Bowie, J., Lüthy, R., and Eisenberg, D. 1991. A method to identify protein sequences that fold into a known three-dimensional structure. Science 253:164-70.

Burley, S.K. and Bonanno, J.B. 2002. Structural genomics of proteins from conserved biochemical pathways and processes. Curr. Opin. Struct. Biol. 12:383-391

Colby TD, Bahnson BJ, Chin JK, Klinman JP, and Goldstein BM. 1998. Active site modifications in a double mutant of liver alcohol dehydrogenase: structural studies of two enzyme-ligand complexes. Biochemistry 37:9295-304

Chothia, C. and Lesk, A.M. 1986. The relation between the divergence of sequence and structure in proteins. EMBO J. 5:823-826.

Cho, H., Ramaswamy, S., and Plapp, B.V. 1997. Flexibility of liver alcohol dehydrogenase in stereoselective binding of 3-butylthiolane 1-oxides. Biochemistry 36:382-389

Chu, P.Y. and Hwang, M.J. 1998. New insights for dinucleotide backbone binding in conserved C5'-H...O hydrogen bonds. J. Mol. Biol. 279:695-701

Conti, E., Stachelhaus, T., Marahiel, M.A. and Brick, P. 1997.Structural basis for the activation of phenylalanine in the non-ribosomal biosynthesis of gramicidin S. EMBO J. 16:4174-83.

Ehlting, J., Shin, J.J. and Douglas, C.J. 2001. Identification of 4-coumarate:coenzyme A ligase (4CL) substrate recognition domains. Plant J. 27:455-465.

Fischer, D. 2000. Hybrid fold recognition: Combining sequence derived properties with evolutionary information. Pacific Symp. Biocomputing, Hawaii, January 2000, World Scientific. p. 119-130.

Fulda, M., Heinz, E., and Wolter, F.P. 1994. The *fadD* gene of Escherichia coli K12 is located close to rnd at 39.6 min of the chromosomal map and is a new member of the AMP-binding protein family. Mol. Gen. Genet. 242:241-249.

Go, M. 1981. Correlation of DNA exonic regions with protein structural units in haemoglobin. Nature 291:90-92.

Gorodkin, J., Stærdeldt, Lund, O. and Brunak, S. 1999. MatrixPlot: visualizing sequence constraints. Bioinformatics 15:769-770

Hegeman, A.D., Gross, Gross, J.W., and Frey, P.A. 2001. Probing catalysis by *Escherichia coli* dTDP-glucose-4,6-dehydratase: identification and preliminary characterization of functional amino acid residues at the active site. Biochemistry 40:6598-6610.

Hrmova, M. and Fincher, G.B. 2001. Plant enzyme structure. Explaining substrate specificity and the evolution of function. Plant Physiol. 125:54-57.

Humphreys, J.M. and Chapple, C. 2002. Rewriting the lignin roadmap. Curr. Opinion Plant Biol. 5:224-229.

Hutchinson, E.G. and Thornton, J. M. 1996. PROMOTIF - A program to identify structural motifs in proteins. Prot Sci 5:212-220.

Jones, D. T. 1999. Protein secondary structure prediction based on position-specific scoring matrices. J. Mol. Biol. 292: 195-202.

Kelley, L.A., MacCallum, R.M. and Sternberg, M.J.E. 2000. Enhanced Genome Annotation using Structural Profiles in the Program 3D-PSSM. J. Mol. Biol. 299:499-520.

Knobloch, K.H. and Hahlbrock, K. 1975. Isoenzymes of p-coumarate:CoA ligase from cell suspension cultures of *Glycine max*. Eur. J. Biochem. 52:311-320.

Koehl, P. 2001. Protein structure similarities. Curr. Opinion Struct. Biol. 11:348-353.

Lacombe, E., Hawkins, S., Van Doorsselaere, J., Piquemal, J., Goffner, D., Poeydomenge, O., Boudet, A.M., and Grima-Pettenati, J. 1997. Cinnamoyl CoA reductase, the first committed enzyme of the lignin branch biosynthetic pathway: cloning, expression and phylogenetic relationships. Plant J. 11:429-441.

Lauvergeat, V., Lacomme, C., Lacombe, E., Lasserre, E., Roby, D., and Grima-Pettenati, J. 2001. Two cinnamoyl-CoA reductase (CCR) genes from *Arabidopsis thaliana* are differentially expressed during development and in response to infection with pathogenic bacteria. Phytochemistry 57:1187-1195.

Lewin, B. 1994. Genes V. Oxford University Press. p. 695-702.

Lüthy, R., Bowie, J.U., and Eisenberg, D. 1992. Assessment of protein models with three-dimensional profiles. Nature 356:83-85

Mackay, J.J. 1996. A mutation in lignin biosynthesis in loblolly pine: genetic, molecular and biochemical analytical. Ph.D. Thesis, North Carolina State University. p. 144.

McKie, J.H., Jaouhari, R., Douglas, K.T., Goffner, D., Feuillet, C., Grima-Pettenati, J., Boudet, A.M., Baltas, M., and Gorrichon, L. 1993. A molecular model for cinnamyl alcohol dehydrogenase, a plant aromatic alcohol dehydrogenase involved in lignification. Biochim. Biophys. Acta. 1202:61-69.

Mizuguchi, K., Deane, C.M., Blundell, T.L., and Overington, J.P. 1998. HOMSTRAD: a database of protein structure alignments for homologous families. Protein Sci. 7:2469-2471.

Orengo, C.A., Bray, J.E., Buchan, D.W., Harrison, A., Lee, D., Pearl, F.M., Sillitoe, I., Todd, A.E., and Thornton, J.M.2002.The CATH protein family database: a resource for structural and functional annotation of genomes. Proteomics 2:11-21. Review.

Pontius, J., Richelle, J., and Wodak, S.J.1996. Deviations from standard atomic volumes as a quality measure for protein crystal structures. J. Mol. Biol. 264:121-136.

Sali, A. 1995. Modelling mutations and homologous proteins. Curr. Opinion Biotech. 6:437-451.

Sali, A. and Blundell, T.L. 1993. Comparative protein modelling by satisfaction of spatial restraints. J. Mol. Biol. 234, 779-815.

Sánchez, R. and Sali, A. 1997. Comparative protein modeling as an optimization problem. J. Mol. Struct. 398:489-496.

Sánchez, R. and Sali, A. 2000. Comparative protein structure modeling: Introduction and practical examples with MODELLER. In Protein Structure Prediction: Methods and Protocols, (Webster, D. M., editor), Humana Press, p. 97-129.

Skolnick, J. and Fetrow, J. 2000. From genes to protein structure and function: novel applications of computational approaches in the genomic era. Trends Biotech.18:34-39.

Thoden, J.B., Wohlers., T.M., Frodovich-Keil, J.L., and Holden, H.M. 2000. Crystallographic evidence for Tyr 157 functioning as the active site base in human UDP-galactose 4-epimerase. Biochemistry 39:5691-5701.

Van Rensburg, H., Anterola, A.M., Levine, L.H., Davin, L.B., and Lewis, N.G. 1999. Monolignol compositional determinants in loblolly pine: aromatic amino acid metabolism and associated rate-limiting steps. In: W.G. Glasser, R.A. Northey, T.P. Shultz (editors) Lignin: Historical, biological and materials perspectives. ACS Symposium Series 742. p. 118-144.

Xie, P.T. and Hurley, T.D. 1999. Methionine-141 directly influences the binding of 4-methylpyrazole in human σσ alcohol dehydrogenase. Prot. Sci. 8:2639-2644.

Wada, H., Kobayashi, M., S ato, R., Satoh, N. Miyasaka, H., and Shirayama, Y. 2002. Dynamic insertion-deletion of introns in deuterostome *EF-1*α genes. J. Mol. Biol. 54:118-128.

Wyrambik, D. and Grisebach, H. 1979. Enzymic synthesis of lignin precursors. Further studies on cinnamyl-alcohol dehydrogenase from soybean cell-suspension cultures. Eur. J. Biochem. 97:503-509.

CHAPTER 2

TABLES AND FIGURES

Table 1. Three-dimensional templates for the *Pinus taeda* target proteins 4CL, CCR and CAD. Alignment of the template protein sequence to their corresponding *Pinus taeda* target proteins 4CL, CCR and CAD (3D-1D alignment)

Pinus taeda target protein				3-dimensional template protein								
NCBI Acc.No	EC	Length aa	MW kDa	PDB code	Protein Acc. No.	Ligands	EC	Organism	Res. Å	R factor	Length aa	PID
4-coumarate-CoA ligase												
T09710	6.2.1.12	537	57	1LCI	Lucifearse	-	1.13.12.7	*Photinus pyralis*	2.0	0.224	523	32
				1AMU	Gramicidin S synthase I	Phe, AMP, SO_4	5.1.1.11	*Bacillus brevis*	1.9	0.213	509	21
Cinnamoyl-CoA reductase												
AAL47684	1.2.1.44	324	35	1BXK	dTDP-glucose 4,6-dehydratase	NAD^+,PIG,EDO,Na	4.2.1.46	*Escherichia coli*	1.9	0.195	341	17
				1UDC	UDP-galactose-4-epimerase	-	5.1.3.2	*Escherichia coli*	2.5	0.184	338	16
Cinnamyl-alcohol dehydrogenase												
S49444	1.1.1.195	357	40	3BTO	Alcohol dehydrogenase	NAD^+,SSB,Zn	1.1.1.1	*Equus caballus*	1.6	0.185	341	23
				1D1S	σ-Alcohol dehydrogenase	NAD^+,ACT,CAC,Zn	1.1.1.1	*Homo sapiens*	2.5	0.217	326	19

Ligands: Phe - Phenylalanine; AMP - Adenosine monophosphate; SO_4 - Sulfate ion SO_4^{+2}; NAD - Nicotinamide-adenine-dinucleotide; SSB - 3-butylthiolane 1-oxide; ACT - Acetate ion; CAC - Cacodylate ion, Zn - divalent cation zinc Zn^{+2}, UFM - Uridine-5'-diphosphate-mannose, PIG - (Hydroxyethyloxy)ethanol; EDO - 1,2-ethanediol [ethylene glycol], Na - soidum cation.
Res. Crystal structure atomic resolution in angstroms (Å).
PID Percentage identity between template and target.

Table 2. General features of the *Pinus taeda* structural models of the 4CL, CCR and CAD proteins

Protein	Secondary structure*				RMSD / Å **		Self-Compatibility			Volume***	Domain structure		
	α helix	3_{10} helix	β strand	Turn	Template I	Template II	S	E(S)	Min(S)	Outliers %	Functional	Fold	
4CL	16	3	23	61	1LCI: 0.52	1AMU: 1.68	196.2	245.5	110.4	6.7	AMP-binding domain	3-α/β	21-204
											Substrate-binding domain	3-α/β	205-355
												β-roll	356-433
												2-αβ	443-537
CCR	11	1	9	32	1BXK: 0.89	1UDC: 0.91	96.9	147.5	66.4	7.2	NADPH-binding (Rossman fold)	3-α/β	1-204,287-324
												α/β-complex	223-254
CAD	10	4	15	45	3BTO: 1.06	1D1S: 1.21	114.9	160.4	72.2	8.3	NADPH-binding (Rossman fold)	3-α/β	168-297
											Zinc-binding	α/β-complex	1-167,298-357

* Secondary structural elements calculated by PROMOTIF (Hutchinson and Thornton 1996)

**Root mean square deviation between the C^{α} positions of the model and the template structures, expressed in angstroms.

***Volume outliers indicate the percentage of buried atoms which deviate more than 3 standard deviations from a standard normal distribution of atomic volumes (by atom type). Data obtained using PROVE (Pontius et al. 1996).

Figure 1. Proposed chemical reaction mechanisms catalyzed by 4CL, CCR and CAD

(A) 4-coumarate:coenzyme A ligase (4CL) activates p-hydroxycinnamates (e.g. ferulate) by esterification with conzyme A. The overall ATP- and Mg(II)-dependent reaction can be divided into two steps. First, the formation of the adenylate intermediate. ATP apprently first binds to the enzyme followed by the substrate with pyrophosphate being released while the p-hydroxycinnamoyl-adenylate intermediate still remains bound. Subsequent binding of coenzyme A (CoA) is followed by release of the *p*-hydroxycinnamoyl-CoA thiol ester and AMP. The carboxylate anion (a nucleophile) in 4-coumarate, caffeate, and ferulate is a non-activated, low energy resonance stabilized anion (the double bond is shared by both oxygens), making it extremely difficult to remove either of them enzymatically or non-enzymatically. The removal can be accomplished by activating the carboxylate group and introducing a good leaving group. The nucleophilic attack of the carboxylate anion to the electrophilic α-phosphorus of ATP generates p-coumaroyl.AMP, a covalent adenylate intermediate, with concomitant release of pyrophosphate. A pentacovalent phospharane adduct is apparently involved in the formation of the adenylate intermediate (a nucleophile), which in turn serves as an activated intermediate for the subsequent reaction. Hydrolytic action of pyro-phosphatases on pyrophosphate ensures functional unidirectionality under *in vivo* conditions, by removing one of the products of the first step.

(B) CCR catalyzes the four electron NADPH-dependent reduction of *p*-hydroxycinnamoyl-CoA ester (e.g., feruoyl-CoA ester) and to form the corresponding *p*-hydroxycinnamaldehydes (e.g., coniferaldehyde). The *si*-face hydride from NADPH carries out a nucleophilic attack on the carboxylate carbon of the coen-zyme A ester which destabilizes the C-S thiol bond. This creates an intermediate where the carboxylate oxygen shares the hydrogen of a protonated acid side chain. This intermediate decomposes to an alde-hyde and protonated CoA.

(C) CAD catalyzes the two electron, NADPH-dependent reduction of *p*-hydroxycinnamaldehydes to *p*-hydroxycinnamic alcohols (e.g., coniferyl alcohol). NADPH first binds the enzyme, causing an allosteric

rotation of domains that creates an interdomain catalytic active site. The aldehyde produced in the previous reaction then displaces the water molecule bound to the catalytic zinc, reestablishing its fourth coordination ligand. The close proximity of the carbon-4 from the nicotinamide ring to aldehyde in conjunction with a proton relay system ensures the hydride transfer of the pro-*R* hydride from NADPH to the *re*-face of the aldehyde, releasing $NADP^+$ and a *p*-hydroxycinnamyl alcohol. This hydrogen becomes the pro-*R* hydrogen in the alcohol group.

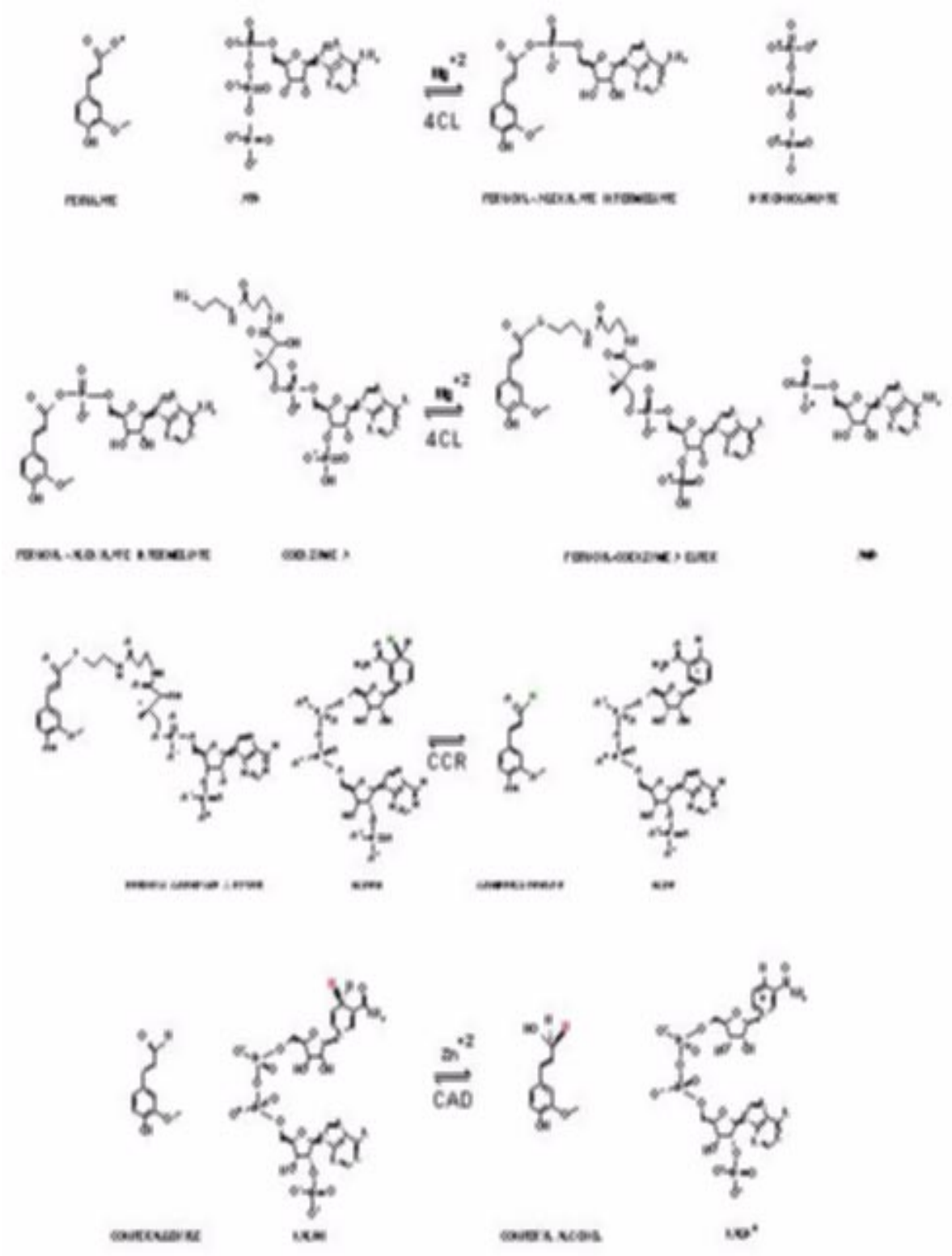

4CL
4CL
CCR
CAD

Figure 2. Template-target alignment, exon-domain structure, 3D-profile evaluation and structural models of loblolly pine 4-coumarate:coenzyme A ligase, coumaroyl-CoA reductase and cinnamyl alcohol dehydrogenase

The threading sequence alignment shows the two three-dimensional (3D) template sequence on top of the pine sequence. Boxed positions in the loblolly pine sequence indicate complete conservation across all orthologous plant sequences. Empty squares in the sequences of the templates indicate missing structural data. Identification of domains in structural models is accomplishd by a two-dimensional distance matrix. The amino acid residues are numbered consecutively on the two axes. Domains are identified unambigously as empty, non-overlapping, right-angle triangles whose hypotenuses are on the diagonal of the plot, and whose sides defined by distinct clusters of spatially neighboring residues. Distances in amgstrons (Å) are color coded. The bar along the diagonal indicates the modular structure of the protein, each color representing a domain. Connected to these domains is a representation of the exon-intron structure of the gene that encodes the protein, where the large rectangles indicate exons. The graphs show the assessment of each position in the structural model by the 3D profile method. Y-axis is the self-compatibility (S) score determined by combining properties of the residues where they occur in th 3-D model. Reliable positions have (S) values above zero, otherwise the model has low confidence. A Rasmol image of a single unit of the model structure is shown for each of the loblolly pine proteins. (A) 4-Coumarate:coenzyme A ligase. (B) Coumaroyl-CoA reductase. (C) Cinnamyl alcohol dehydrogenase.

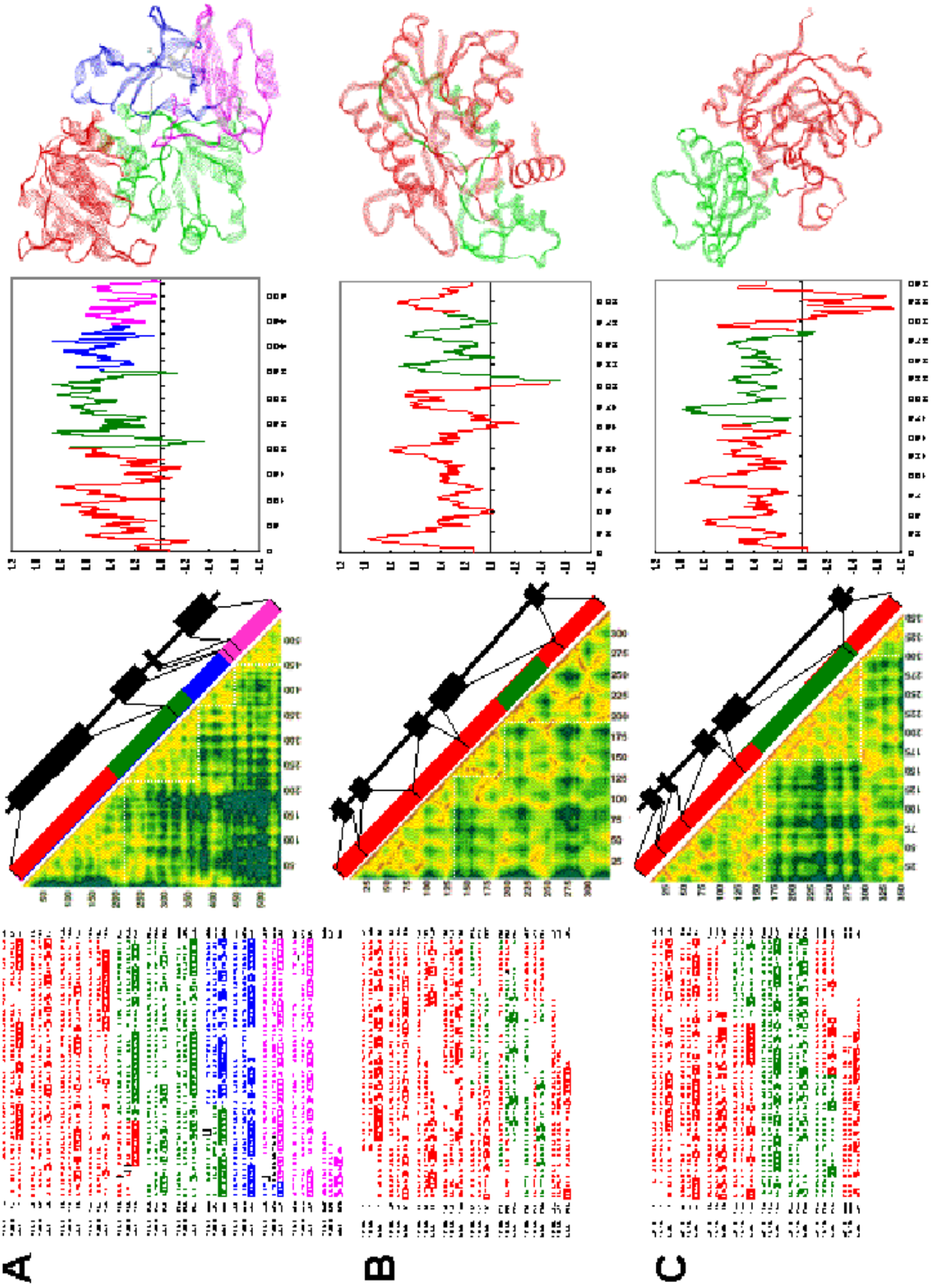
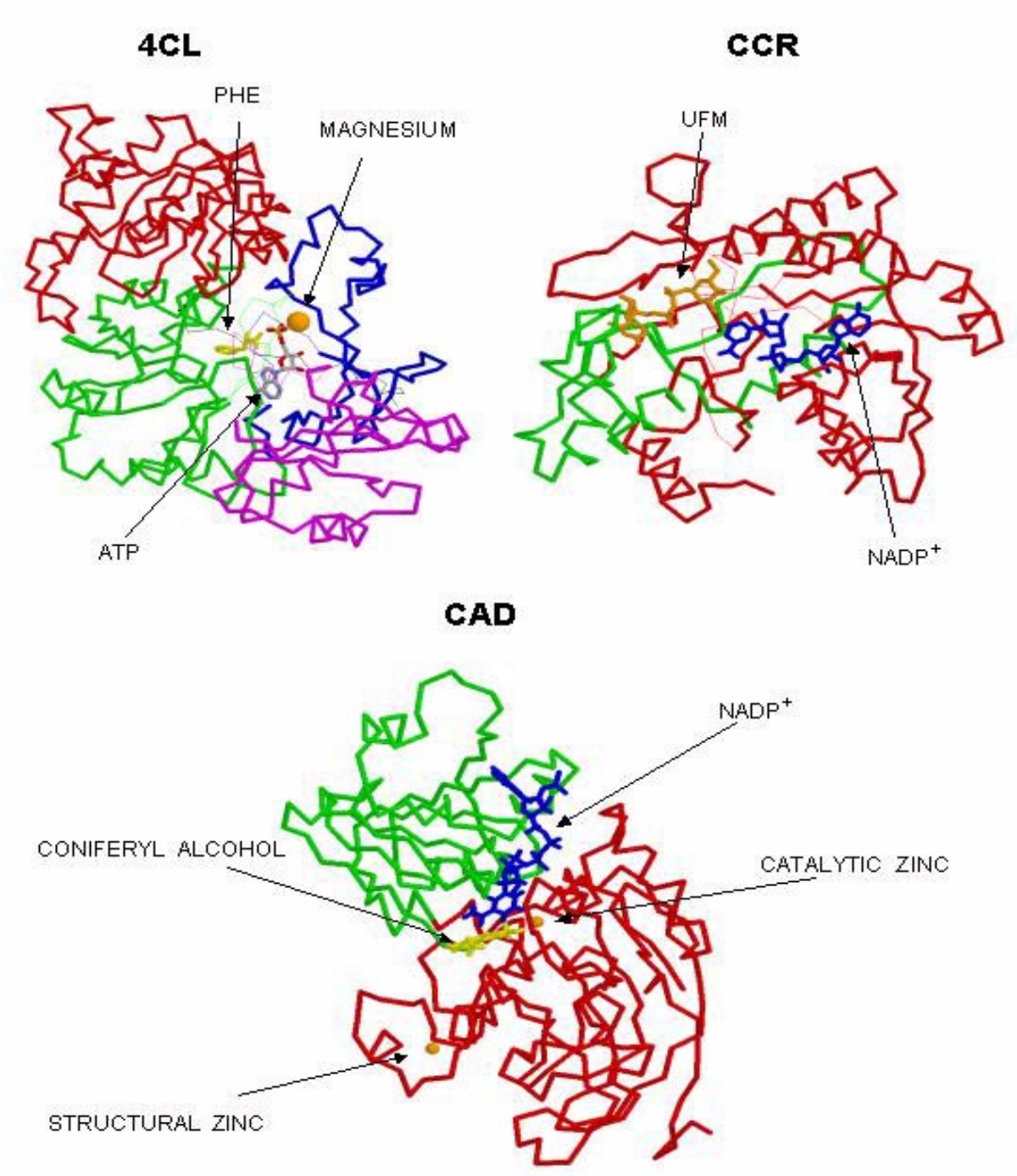

A
B
C

Figure 3. Structural models of loblolly pine 4-coumarate:coenzyme A ligase, coumaroyl-CoA reductase and cinnamyl alcohol dehydrogenase.

Domains indicated by same colors as in Figure 2. Ligands were inserted by superimposition to template structures.


4CL
PHE
MAGNESIUM
ATP
CCR
UFM
NADP+
CAD
NADP+
CONIFERYL ALCOHOL
CATALYTIC ZINC
STRUCTURAL ZINC

CHAPTER 3

Identification of signatures in plant NADP(H)-dependent oxidoreductases with activity towards aromatic substrates

INTRODUCTION

The recognition of amino acid replacement patterns in gene products is a major challenge in properly defining gene families and classifying gene family members. Amino acid replacement pattern recognition is also important for reliable functional assignment of proteins (Busfield et al. 2000) and for the study of functional divergence (Koo 2000). Amino acid differences could reflect changes in the biochemical and cellular role of related proteins (functional divergence), or be associated with their cladistic position (phylogenetic divergence). A pattern of amino acid replacements can be described by specific positions in an alignment and by the identity of amino acid residues occupying those positions (i.e. a 'signature'). Despite its importance to protein family characterization, signatures for discriminating between members of a family have been described in only a few cases [e.g., MAPKs (Kültz 1998), HLH proteins (Chavali et al. 2001), streptococcal M proteins (Hartas et al. 1995), Epstein Barr virus latent membrane protein 1 (Edwards et al. 1999), and Gram-negative bacteria pilins (Girardeau et al. 2000)].

Intense experimental and computational effort has been devoted recently to the determination of amino acid residues directly involved with functional aspects of proteins. Experimental approaches are effective but are time consuming and too laborious for broad application (Sweadner and Rael 2000, Wiebe et al. 2001, Jones et al. 1997, Philpot 1998). Computational methods can predict a reduced set of positions to test hypotheses concerning the structural basis for functional differences. These methods include search algorithms in overlapping frames (Pavesi

2000), covarion-based approaches (Gaucher et al. 2001, Marin et al. 2001), comparison of replacement rates among protein groups (Gu 1999), prediction of physicochemical properties of ancestral sequence common to duplicated genes (Caffrey et al. 2000), and the combination of sequence and structure data to infer the location of functional sites in proteins (evolutionary trace, Sowa 2001, Lichtarge et al. 1996). The complexity of these methods, the intensive computational time or the amount of information required for the application of the methods limit their broad use.

The study of amino acid positional changes also addresses questions about the relationship among the positions undergoing replacements. Do residue pairs at these positions change in a dependent-manner? Do coordinated replacements at certain positions indicate important interactions among the residues involved? One approach to the study of protein evolution is that of Kimura (1985), which assumes that pairs of positions change in a concerted manner, such that the effect of one replacement is compensated by another to preserve the functionality or stability of the protein. These correlating positions have generally been related to close spatial proximity (Afonnikov et al. 2001), and put forward as evidence for compensatory molecular change (Pollock et al. 1999). Experiments have found significant functional correlation among pairs of spatially neighboring residues (Hawko and Francklyn 2001, Debraj et al. 1999, Mateu and Fehrst 1999). This question has also been addressed computationally using statistical methods (Pollock and Taylor 1997, Chelvanayagam et al. 1997) or information theory criteria (Tuffery et al 1999).

Plant alcohol dehydrogenases play important roles in both primary and secondary metabolism. The best characterized proteins belong to a small family of NAD^+-dependent alcohol dehydrogenases (ADH, EC 1.1.1.1) that participate in the glycolytic pathway of oxygen-deprived plant tissues (Richard et al. 1994). Another group, encoded by the aromatic ADH gene family, are the zinc-containing, medium chain, NADP(H)-dependent, aromatic alcohol dehydrogenases/aldehyde reductases. Two subfamilies are recognized in this latter family, CAD or cinnamyl alcohol dehydrogenase (subfamily I) and the elicitor induced ELI3-like proteins (subfamily II). These enzymes are active as dimers with 40 kDa subunits that contain two zinc atoms per subunit. In secondary metabolism, they catalyze the reversible reduction of hydroxycinnaldehydes and other aromatic aldehydes into their corresponding alcohols (Lewis et al. 1999). Genetics and biochemistry established CAD as the last enzymatic step of monolignol biosynthesis in the phenylpropanoid pathway (Boudet et al. 1998, MacKay et al. 1995, 1997). ELI3 proteins were discovered in association with elicitor-induced stress resistance (Kiedrowski et al. 1992).

The goal of this work is to contribute an amino acid positional signature to the current classificiation scheme for CAD/ELI3 proteins, in order to clearly define the common features of the subfamilies, as well as provide positions that clearly distinguish between them. In this study, we used both phylogenetic and informatic methods to analyze amino acid positions in CAD and ELI3 subfamilies in order to determine differences among them. Gu's criterion of divergence (Gu 1999) and the subfamily-determinant mutual information (Mirny and Gefland 2000) rely on a

multiple amino acid sequence alignment and the residue composition of each site. Gu's criterion is used to compare amino acid replacement rates between protein groups to compute a conditional probability for a specific position to be in a state of functional divergence. Mutual information is an information theory criterion in which frequencies of amino acids for each position are used to detect those that are specificity-determinant for the protein clusters. We were able to map the statistically-significant positions found by each criterion onto the predicted tertiary structure of these proteins found in Chapter 2. Our results characterize differences between CAD and ELI3 based upon the identity of the amino acid in these positions. Significant physicochemical correlation was found among positions determined by mutual information but not by Gu's criterion. We used the amino acid signature to classify a *Pinus taeda* EST contig as an ELI3, and also recognized an uncharacterized *Arabidopsis* gene sequence as a member of a new subfamily. This study demonstrates that the application of simple phylogenetics, bioinformatics and structural tools could have broad applications in (1) defining a reduced set of positions that effectively discriminate subfamilies, (2) identifying new sequences for each subfamily, and finally (3) suggest positions in a protein to test hypotheses on the structural basis of functional divergence.

MATERIALS AND METHODS

Databases, sequence compilation and alignment

The non-redundant (NR) database at the National Center for Biotechnology

Information (Bethesda, MD) was used as the source of sequences and for most of the database searches. Gene sequences were extracted from NR using the Entrez search and retrieval system, and the *cinnamyl alcohol dehydrogenase* and *eli3* names as text queries. The tBlastn 2.0.12 program (www.ncbi.nlm.nih.gov/BLAST) was used to compare the loblolly pine (CAD_PINTA, SwissProt P41637) cinnamyl alcohol dehydrogenase protein query against nucleotide databases using BLOSUM62 as scoring matrix and no filtering. Positive hits were retrieved if they had identities >50% and were full length sequences. They were subsequently screened using literature reports to exclude sequences with insufficient annotation. Other sequences annotated as “cinnamyl alcohol dehydrogenase” were also retrieved, including fragments to be used as a validation subset. Deduced amino acid sequences were aligned using CLUSTAL W 1.7 (www2.ebi.ac.uk/clustalw, Thompson et al. 1994]. The resulting alignment was manually inspected, modified and used as a framework to align corresponding codons.The *Pinus taeda* subsections of the NCBI’s dbEST database were searched with tBLASTn using the *Pinus taeda* CAD sequence AI724977 as query to detect related *Pinus taeda* ESTs.

Gene tree

An unrooted topology was determined using a neighbor-joining (NJ) method (Saitou and Nei 1987) and the Jukes-Cantor proportion of non-synonymous nucleotide differences using the MEGA2 (Kumar et al. 2001, www.megasoftware.net). Then, internode lengths for this topology were recalculated on the first and second codon positions using a maximum likelihood approach as implemented on the

baseml module of the PAML software (abacus.gene.ucl.ac.uk/ziheng/paml.html, Yang 1999). Support for the nodes of the topology was assessed by a bootstrap method based on 10^4 pseudosamples (Felsenstein 1985).

Information Content

The variability of a position is quantified by its information content. This score goes to zero as a position strongly retains a particular residue (Schneider et al. 1986). The information content I of position l, (measured in bits), is

$$I(l) = -\sum_{i=1}^{6} P_i(l)\log P_i(l)$$

where $P_i(l)$ is the probability of amino acid residue class i in the l-th position of the alignment. The 20 amino acids were classified into six classes based on their polarity and volume (Miyata et al. 1979): special (C), neutral and small (A,G,P,S,T), polar and relatively large (R,H,K), polar and relatively small (N,D,Q,E), nonpolar and relatively large (F,W,Y), nonpolar and relatively small (I,L,M,V). All amino acid replacements within groups were referred to as conservative and between groups as radical. This classification may not necessarily be correlated with divergence, either phylogenetic or functional. Separate analyses were carried out on the training sets consisting of the 18 CAD and 13 ELI3 amino acid sequences.

Multilevel Consensus Sequence

Multilevel consensus sequence was determined by calculating the probability that each amino acid residue occurs in that position. The MEME algorithm

(meme.sdsc.edu/meme/website/meme.html) used the Bayes' rule to estimate the individual amino acid probabilities for each column (single letter code). The consensus showed the residues at sites where one to three amino acids are found in 80% of the sequences (Bailey and Elkan 1995).

Gu's criterion of divergence

A Hidden Markov model was used to describe which state, divergence (F_D) or constraint (F_C), is more likely at a given position. The posterior probability of state F_D at a position given the number of changes in both clusters, Y_{CAD} and Y_{ELI3}, is calculated as

$$P(F_D|Y_{CAD}, Y_{ELI3}) = \frac{\theta_\lambda P(Y_{CAD}, Y_{ELI3}|F_D)}{(1-\theta_\lambda)P(Y_{CAD}, Y_{ELI3}|F_C) + \theta_\lambda P(Y_{CAD}, Y_{ELI3}|F_D)}$$

where $\theta_\lambda = P(F_D) = 1\text{-}r_\lambda$ is the loss of rate correlation (r_λ) among the replacements rates over sites between a pair of proteins and is equivalent to the probability that a position is in a state of divergence (Gu 1999). Identical replacement rates between the two clusters would suggest constraint and the correlation would be $r_\lambda = 1$. Divergence between the two clusters is indicated by $r_\lambda < 1$. As r_λ increases from 0 to 1, the intensity of divergence increases from weak to strong. θ_λ was estimated by maximizing the likelihood function,

$$L(\theta_\lambda|data) = \prod_{l=1}^{L} [\theta_\lambda P_l(Y_{CAD}, Y_{ELI3}|F_D) + (1-\theta_\lambda)P_l(Y_{CAD}, Y_{ELI3}|F_C)]$$

which is based upon the joint distribution of the number of replacements in site l in each cluster (Y_{CAD}, Y_{ELI3}) conditional on being in either state F_C or F_D. The probabilities are fully formulated in Gu (1999) and calculations were carried out using the Gu99

module of the the DIVERGE software (xgu1.zool.iastate.edu). Positions with probabilities P($F_D|Y_{CAD},Y_{ELI3}$) > 0.9 were taken as part of the signature (Wang and Gu 2001).

Subfamily-determinant mutual information

Mutual information (MI) for position l measures the association between an amino acid residue x and a protein cluster y (Mirny and Gefland 2002), and is calculated as:

$$MI(l) = \sum_{x=1}^{20}\sum_{y=1}^{2} f_l(x,y)\log\frac{f_l(x,y)}{f_l(x)f(y)}$$

where $f_l(x,y)$ is the frequency of amino acid residue x in position l of the multiple alignment of sequences of cluster y (y=1 if CAD or y=2 if ELI3), $f(x)$ is the fraction of cases where a residue is present in position l, and $f(y)$ is the fraction of protein sequences belonging to cluster y. The probability of observing MI_l, P(MI_l), can be computed under the null hypothesis of no association in the l-th position between residue type x and cluster y. Positions where the null hypothesis is rejected due to a low P(MI_l), were taken as specifying cluster differentiation. The distribution of P(MI_l) values under the null hypothesis was obtained by permutation according to the method of Mirny and Gefland (2002). Permutation was carried out by shuffling all the elements irrespective of cluster, but keeping the original cluster size, and then computing mutual information of the shuffled column (10^3 times each position). Permutation was carried out independently in each position using the SEQBOOT module of the PHYLIP software (evolution.genetics.washington.edu/phylip.html). Only positions whose p-values were less than 10^{-6} were chosen as part of the

signature.

Correlation between positions in a multiple sequence alignment

Consider a sample of N aligned sequences (k = 1,..., N) encompassing L positions (l = 1,...,i,...,j,...,L). A physical or chemical characteristic f (e.g. hydrophobicity [Ponnuswamy et al. 1980], solvent accessibility [Rose et al. 1985]) was assigned to each amino acid in the alignment. The elements F_{kl} of the resulting matrix $\mathbf{F}$ are quantities of f for the k-th sequence at the l-th position. Each position or column of this matrix was considered as a set of N realizations of the possible values that physico-chemical property f may have for that position. $\mathbf{F}$ is used to estimate the relationship between these possible values of physico-chemical property f. According to Neher (1994), a linear correlation r_{ij} for each pair of positions i and j can be computed based on the physicochemical characteristic between these positions f_i and f_j, as

$$r_{ij} = \frac{s_{ij}}{\sqrt{s_{ii}s_{jj}}}$$

The covariance (i $\neq$ j) and the variance ($i = j$) can be estimated by the formula:

$$s_{ij} = \frac{1}{N-1}\sum_{k=1}^{N} w_k(f_{ki} - \bar{f}_i)(f_{kj} - \overline{f_j})$$

where $\bar{f}_l = N^{-1}\sum_{k=1}^{N} w_k f_{kl}$ is the mean value of the physical chemical property at position l and w_k is the weight of a sequence, such that $\sum_{k=1}^{N} w_k = \dot{N}$. Weights were calculated based on the method of Altschul et al. (1989) that uses a phylogenetic tree of the sequences analyzed to determine weights for pairs of external nodes. The threshold value r_c is calculated, assuming a Gaussian distribution of the f values throughout the

independent alignment positions. The replacements of residues at positions *i* and *j* can be considered statistically independent when $|r_{ij}|<r_c$ (Kendall and Stuart 1967). The statistic $t = |r_{ij}|\sqrt{(N-2)\left(1-r_{ij}^2\right)^{-1}}$ follows the Student's t-distribution with *N-2* degrees of freedom and provides a nominal P-value for the correlation coefficient. A network of correlated positions clustered all positions i and j having a physicochemical relationship using the distance d_{ij} = 1 - | d_{ij} |. Calculations were carried out using the CRASP server (Afonnikov 2000, www.sgi.sscc.ru/mgs/programs/crasp/pcrasp).

Three-dimensional model prediction of the subunit of CAD protein

The 3D structural models were predicted using a homology-based approach *Pinus taeda* CAD (gi 1076239) as described in Chapter 2.

RESULTS

Sequence and structural features

The CAD and ELI3 proteins share common sequence features that distinguish it from other alcohol dehydrogenases. Sequence alignment encompassing the predicted translations of these genomic and cDNA sequences revealed domains with well conserved blocks of residues extending over the zinc- and NADP(H)-binding core as well as N- and C-terminal region (Figure 1). A general signature sequence for the CAD/ELI3 proteins was determined, comprising the conserved sites present in this family that are absent in other alcohol dehydrogenases (based on the structural alignment of dimeric and tetrameric zinc-containing oxidoreductases, Jörnvall et al.

1987). Table 2 shows those positions and the conserved amino acid occupancy characteristic of members of the CAD/ELI3 proteins. One notable feature is that the side chain in position 212 must be occupied by a polar group Ser or Thr in NADP(H)-dependent enzymes. Overall, the CAD/ELI3 family is characterized by a zinc-containing alcohol dehydrogenase signature (**GHE**xx**G**xxxxx[**G**A]xx[I**V**SAC]) encompassing positions 68 to 82 in the alignment (numbered following the loblolly pine sequence PTCADBMR). The residues involved in the coordination of the catalytic zinc atom were Cys47, His69 and Cys163. The structural zinc atom was coordinated by cysteines 100, 103, 106 and 115. These proteins also have a NADP(H)-binding domain known as the Rossman fold. This α/β-fold consists of a series of conserved amino acid residues at a few crucial positions, whereas other regions of the domain vary considerably (Figure 3A). The conserved part of the motif, the $\beta\alpha\beta$ signature, consists of the first two β-strands (underlined) and the intervening amphipathic α-helix (italics) and contains a few polar (o) and numerous hydrophobic (h) residues (<u>ohxhx</u>**G**x**G**xx ***G****xxxhxxhxxh* xx<u>xhxhxxo</u>) (positions 182 to 212).

Divergence between CAD and ELI3 protein subfamilies

CAD and ELI3 sequences are clearly distinct groups (Figure 2). Conserved sites shared by both CAD and ELI3 proteins had low information content and are distributed throughout the whole length of the protein, accounting for 55% of the aligned positions (Figure 3B). These sites were present in different secondary structures and displayed varying levels of solvent accessibility. To characterize the level of conservation of residues in the entire tree, we modelled the distribution of

replacement rates as a gamma distribution. An α of 0.60 $\pm$0.07 was calculated for the entire tree. In contrast, the α values for both CAD and ELI3 subfamily trees alone were significantly lower [α=0.31 $\pm$ 0.08 and α=0.45 $\pm$ 0.06, respectively]. This shows that replacement rates among sites distribute more uniformly when the two clusters were considered together, rather than separately. The estimated coefficient of divergence between the CAD and ELI3 proteins was $\hat{\theta}_{MLE}$ = 0.39 $\pm$ 0.04 (P>0.0001) implying a significant loss of rate correlation among groups and indicating that the level of sequence separation between them is statistically significant. Therefore, variable positions in one group are not the same as those of another, and presumably some positions are differently constrained.

Signature positions

CAD and ELI3 proteins had positions where amino acid residue identity was distinctive for each group. These positions were identified by using two criteria (Table 2): Gu's criterion computes a correlation of replacement rates between subfamilies to estimate a correlation term that is used to calculate a conditional probability that a position is in a state of functional divergence. The other criterion is the mutual information score, which identified positions that could be specificity-determinants for a family. Positions determined by Gu's criterion were generally found in loops, turns and bends, were mostly positioned on the surface of the protein, and generally involved radical replacements. Mutual information criterion highlighted fifteen positions, mostly buried and located almost exclusively in β-strands. These positions

were mapped onto the 3D structure model of the proteins (Figure 3C,D). Gu's criterion identified positions containing a conserved amino acid residue in one subfamily and a mixture of residues in the another. Important features were positions 116 (a tryptophan conserved in CAD, Trp_{CAD}), 117 (Thr_{ELI3}) and 296 (Phe_{CAD}) that are part of the substrate binding site. Hits obtained by the mutual information criterion were generally located through the Rossman fold and were characterized by positions where both proteins have a different amino acid residue conserved. Most of them occupied buried positions and were located in critical points of the secondary structure (mostly β-strands) and almost exclusively involved conservative replacements. Position 189 (Val_{CAD}, Leu_{ELI3}) is located at one face of the nicotinamide ring and may be critically important for hydrogen tunnelling during catalysis. Position 212 (Ser_{CAD}, Thr_{ELI3}) interacts directly with the phosphate moiety of the NADPH adenine, conferring specificity towards this cofactor.

Some positions determined by mutual information are physicochemically correlated. The locations of the hits suggested that they are not randomly located. Association between pairs of positions was determined by the correlations of their physicochemical properties. Our results on pairwise correlations show that seven positions (out of 15) detected by mutual information were highly correlated using hydrophobicity and solvent accessibility as physicochemical measures (Figure 4). These positions were 27, 29, 192, 229, 253, 283, and 316. Another group consisted of positions 186 and 302. These positions were not generally in close proximity. Positions determined by Gu's method appeared to be more independent with regard

to physical or chemical properties and did not show significant correlations.

Predictive capability of the signature positions

Positions that discriminate the CAD and ELI3 groups are able to distinguish homologs among related sequences. We used the signature to analyze discriminating residues in sequences annotated as cinnamyl alcohol dehydrogenase from several plant species. Our results showed that the *H. vulgare* sequence belonged to CAD. The *Vigna unguiculata* sequence did not present any feature of the CAD/ELI3 proteins and cannot be considered to be a member. The *Brassica napus, B. rapa, and B. oleracea* sequences each had sequences of the CAD and the ELI3-types. Genes annotated in the *Arabidopsis thaliana* genome as “cinnamyl alcohol dehydrogenase” yielded 17 hits. Four of them were used in the analysis, and had genetic and/or biochemical information. Examination of the signatures in the remaining showed that four were new members of the ELI3 group, while one belonged to the CAD group. Six sequences located in chromosome 1 and one in sequence in chromosome 5 were not related to either CAD or ELI3. The other appeared to represent a new group, because it contained most of the conserved amino acids characterizing the family as well as signature positions containing the amino acid residue of CAD or ELI3 groups. In addition, we examined sequences from EST projects of several plant species including loblolly pine. We found that several ESTs from loblolly pine could be assembled into a large contig equivalent to 288 amino acids containing a canonical ELI3-type signature.

DISCUSSION

The purpose of this study was to determine a pattern of amino acid replacements that distinguish CAD and ELI3 based on phylogenetics and informatics criteria, determine the association of the replacements in these positions, and then to map the replacements onto the predicted three-dimensional structure of the proteins to gain a better understanding of the structure-function relationship in CAD and ELI3.

CAD and ELI3 proteins together form a distinct group of plant alcohol dehydrogenases (Shafqat et al. 1986) sharing 55% amino acid identity (Figure 3B). A large proportion of these residues are hydrophobic in character and buried in the central core region of each of the α/β domains (the Rossman fold and the zinc-binding domain; Figure 3A). Twenty-one conserved positions differentiated them from the rest of the zinc-containing alcohol dehydrogenases as described by Jörnvall et al. (1987) (Table 2). Spatial clusters of conserved residues mapped onto the protein structure have been used to predict successfully functional sites of proteins (Aloy et al. 2001) because they play important roles in determining the folding and catalytic features of proteins (Mirny and Shakhnovich 1999, 2001, Cygler et al. 1993), and could also form a lattice of interacting residues in the protein inner core (Poupon and Mornon 1999).

CAD and ELI3 are two divergent group of sequences. The separation of the CAD and ELI3 groups in the tree was clear and unambiguous (Figure 2). The bootstrap support for the CAD and ELI3 nodes was 100%, and the coefficient of sequence divergence θ=0.39 showed that there was a significant divergence in the site-specific

rate profiles of these two protein clusters. The distribution of the amino acid replacement rates, as expressed by the α value, was different for each group. They were lower than the α obtained when both groups were analyzed together. This is an indication that the variable positions of one group are not the same as those of another. Thus, CAD and ELI3 form distinct clusters and differ in the pattern of amino acid replacement.

CAD and ELI3 had sequence features in several homologous sites that discriminate between them. Gu's criterion and mutual information identified, in an alignment of 32 CAD and ELI3 protein sequences from 23 species (Table 1) 26 positions that distinguished these two groups (Figure 1). Some of these positions provide ground to test hypotheses on the structural basis of functional divergence. For example, CAD and ELI3 differ at position 192 (Val in CAD, Leu in ELI3), which is homologous to Val 203 in horse liver alcohol dehydrogenase (*Eq*ADH, Colby et al. 1998). A general feature of oxidoreductases is that this position is occupied by a bulky hydrophobic residue facing the back of the nicotinamide ring of bound cofactor. A mutation Val203Ala caused substantial changes in catalytic efficiency and hydrogen tunneling in *Eq*ADH (Bahnson et al. 1997). Thus, evidence from homologous sites in an alcohol dehydrogenase from horse liver suggests that CAD and ELI3 should show differential reaction kinetics.

Positions 119, 120, 192 and 299 were located in the substrate binding site, suggesting that these protein groups could have different active site geometry. Half of these sites involved amino acid replacements that have different physicochemical characteristics. Even the conservative replacements could confer subtle catalytic

differences leading to qualitative shifts in kinetics driven by substrate specificity (Gertl and Babbitt 2000). These four positions in the binding site could modulate the ability of the enzymes to bind specifically *p*-coumaraldehyde, coniferaldehyde or sinapyl aldehyde, which have different methoxy substitutions in the phenyl ring. CAD is regarded to act preferentially on coniferyl alcohol (Mansell et al. 1974, O'Malley et al. 1992) while ELI3 proteins can be considered more as a substrate specificity-diverse group of enzymes. An ELI3 protein that plays a role in syringyl alcohol biosynthesis in *Populus tremuloides* vascular tissue showed high specificity for sinapaldehyde as opposed to coniferyl aldehyde (Li et al. 2000). Somssich et al. (1996) reported that *At*ELI3-2 catalyzed the $NADP^+$-dependent reduction of various aromatic aldehydes *in vitro*, and that the substrate specificity was different from CAD. In *Petrocelinum crispum*, an $NADP^+$-dependent ELI3-type enzyme efficiently reduced various cinnamyl and benzyl aldehydes, with highest substrate affinities observed for cinnamaldehyde and 4-coumaraldehyde whereas sinapaldehyde was not converted (Logeman et al. 1997).

Correlations among amino acid positions reflect the specific structural and functional features of the protein. Quantitative measures of physical and chemical properties were assigned to each amino acid in a given position. We used a hydrophobicity index and a solvent accessibility score due to their role in protein folding and structural stability (Figure 4). This approach did not include spatial or physicochemical measures derived from the three-dimensional structure, in order that independence of positions and physicochemical values could be assumed.

Among the 26 positions identified by the two criteria, 8 mutual information hits showed significant correlations, while none of the positions identified by Gu's criterion showed any detectable association. Mutual information hits occurred mostly in the interior of the protein where folding and structural stability are more important (Figure 3D). Lack of correlations among Gu's positions could be linked with their consistent location on the protein surface where amino acids are less constrained by folding or stability (Figure 3C). Exterior residues are known to play an important role in the electrostatic distribution of charges, as well as with subunit-subunit interactions (Axe 2000). Physicochemical correlations between distant positions are difficult to explain. Subtle changes in enzyme structure far from the substrate binding site can sometimes alter reaction kinetics (Chin and Klinman 2000). Other interpretations include maintenance of an isoelectric composition (or a macrodipole moment) across the molecule as well as avoidance of self-complementarity of distant secondary structural segments which would interfere with the folding process (Pollock et al. 1999). Correlation might also result if a change in one amino acid site of the protein elicits a compensating change at another site in order to maintain functionality (Crowder et al. 2001). Since these correlations can occur among spatially distant sites, it suggests that Kimura's theory may not necessarily apply to spatially close distant case.

The distinct pattern of replacements detected by the two criteria suggests a link between protein structure and the type of amino acid divergence. Mutual information hits were located in buried β-strands, and mainly involved conservative replacements. Gu's positions were mostly present in loops and bends on the surface of the protein

and featured radical replacements. Adopting the classification by Wang and Gu (2001), Gu's criterion recognized amino acid configurations that were conserved in one group but highly variable in the other (Type I), while mutual information identified amino acid configurations that were conserved and distinct in both groups (Type II). Positions identified by Gu's criterion on the class I α-mannosidase mapped to the periphery of the catalytic domain tertiary structure (Jordan et al. 2001). None of these sites have been directly implicated in the catalytic mechanism of the enzyme nor do they play any structural stabilization of the protein structure, though there is some speculation that they could modulate interactions between members of macromolecular protein assemblies that are endemic to the endoplasmatic reticulum and the Golgi apparatus (Jordan et al. 2001). Positions identified by mutual information on the LacI family of DNA binding proteins were deeply buried in the DNA-binding domain and in the ligand-binding pocket (Mirny and Gelfand 2000). This supports the view that they may serve as determinants for specificity of DNA recognition and ligand binding specificity. Thus, the two criteria are complementary and reveal sites undergoing different types of amino acid replacement in proteins.

CAD and ELI3 are distinct subfamilies belonging to the aromatic plant alcohol dehydrogenases. They encoded oxidoreductases with similar structure and catalytic mechanism, but differing in substrate specificity and expression patterns. *Eli3* mRNA was originally found to rapidly accumulate in *Pseudomonas syringae*-infected leaves of *Arabidopsis thaliana* plants bearing a dominant *RPM1* allele (Kiedrowski et al. 1992). Recently, an *ELI3* homolog (Acc. No. AAF72099, AAF72100) has been identified in tomato plants bearing the *Pto* resistance gene. This homolog is rapidly

induced in plants infected by the avirulent bacteria *Pseudomonas syringae pv. tomato* containing the *avrPto* gene (R. Thilmony and G. Martin, pers. comm.). Differences have also been observed in regard to cell type. In alfalfa, the subfamily II gene, *MsaCad1*, was expressed most actively in stem and floral tissue, whereas *MsaCad2* (subfamily I) was expressed in stem, hypocotyl and root tissue (Brill et al. 1999). Therefore, CAD and ELI3 function in different metabolic contexts. It is expected that the functional diversification of these proteins will often require, besides changes in the coding region, a qualitative shift in their genetic regulation.

Use of amino acid signatures also provides a way to distinguish between putative CAD and ELI3 sequences in EST databases. Observing the presence in conifers of sequences homologous to the ELI3 proteins in conifers has been elusive. The existence of a small CAD gene family within the *Picea abies* genome, consisting of at least two loci has been reported by Schubert et al. (1998). Our results present a contig of 13 *Pinus taeda* EST sequences whose deduced translation had the signature of the ELI3 proteins (Table 3). This discovery now expands the representation of this group to the gymnosperms. In *Arabidopsis thaliana*, Tavares et al. (2000) named LCAD (like-CAD) to a group of 8 expressed genomic sequences with similarity to cinnamyl alcohol dehydrogenase. Parsimony analysis separated these sequences in a tree that is in general agreement with our results (Table 3). Our diagnosis of the signature positions on 13 *Arabidopsis thaliana* genomic sequences showed one sequence had the CAD signature and four had the ELI3 signature. We found a sequence that encodes a protein (Acc. AAG51850) containing mixed features of both CAD and ELI3. That this sequence could represent a new family needs to be

confirmed, yet provides a glimpse of the diverse organization of the *CAD/ELI3* gene family in *Arabidopsis*.

Currently, the Commision on Plant Gene Nomenclature database, Mendel (mbclserver.rutgers.edu/CPGN), recognizes nine plant alcohol dehydrogenase gene families (reviewed by Chase 2000). Among them, the *cad2* gene family encodes cinnamyl alcohol dehydrogenase, dimeric (E.C. 1.1.1195). The *bad1* gene family is represented by the *AtEli3-2* and encodes an $NADP^+$-dependent aryl (or benzyl) alcohol dehydrogenase, dimeric (E.C. 1.1.1.91). A monomeric NAD^+-dependent mannitol dehydrogenase sequence from *Apium graveloens* (*Aq*MTD, Williamson et al. 1995), which has 60% identity with *At*ELI3-2, has also been included in *bad1* (though it appears as a synonym to both *cad2* and *bad1*). However, *Aq*MTD and *At*ELI3-2 differ in a critically important position: *Aq*MTD has an Asp at position 215, which is diagnostic for NAD^+-dependent enzymes, while *At*ELI3 and even other sequences annotated as mannitol dehydrogenase on the basis of sequence similarity contain a polar residue (Thr) at this position, typical of $NADP^+$-dependent enzymes (Table 3). Therefore, we believe that celery MTD is related to ELI3 but establishes a separate group of NAD^+-dependent polyol dehydrogenases. Apart from this, the CPGN classification of sequences agrees with our results. We emphasize that sequence comparison alone is insufficient to classify gene or protein sequences into biologically-meaningful families. The patterns of amino acid conservation and replacements in relation to structure and function is of critical importance to characterize families and associate sequences to families.

Nomenclature for CAD and ELI3 has been made more complex by the recent discovery of an enzyme in *Eucalyptus gunnii* (CAD1, Acc. No. CAA61275, Goffner et al. 1998) with broad specificity for aromatic substrates including unsubstituted and substituted benzaldehydes, and high affinity for 4-coumaraldehyde and coniferaldehyde, but not sinapaldehyde. This enzyme does not have any sequence relationship with the CAD/ELI3 proteins, and apparently belongs to the $NADP^+$-dependent dihydrokaempferol 4-reductase (E.C. 1.1.1.219) family.

The distance between two protein groups can be attributed to the joint effect of two non-stochastic sources of divergence, namely those having a phylogenetic or a functional origin, acting on specific positions in the protein (Wollenberg and Atchley 2000), as well as to random drift (Sala and Wain-Hobson 2000). They highlight cladistic, adaptive and neutral evolution, respectively. For most positions, functional and phylogenetic distinctions are difficult to differentiate computationally. We believe that phylogenetic replacement can now be distinguished at sites with known function *and* where a different but physicochemically similar amino acid is conserved in each protein cluster. For instance, the polar side chain in position 212 (identified by mutual information) establishes hydrogen bonds with the negatively-charged phosphate moiety of $NADP^+$. A mutation Ser212Asp in *Eucalyptus gunnii* CAD caused the cofactor specificity of the enzyme to change from $NADP^+$ to NAD^+ (Lauvergaet et al. 1995). CAD has a Ser and ELI3 a Thr residue at this site. The functional role is the same, so the amino acid replacement could only have phylogenetic relevance. Another example deals with position 215 (identified by Gu's criterion), which is

occupied by Lys in CAD and by residues with polar side chains in ELI3. This position establishes a hydrogen bond with the conserved acidic group Asp234 and brings two surface loops in close proximity. Again given the same function, the differences may be regarded as phylogenetic.

The criteria used in this study successfully identified amino acid replacement patterns “signatures” that can be used to both effectively discriminate between gene subfamilies and suggest specific positions in proteins that may provide a structural basis for functional divergence between subfamilies. No underlying mechanism for these signatures was definitely identified. Thus, these patterns cannot be regarded necessarily as functional. Functional divergence requires (1) a clear definition of function in the context of a functional characterization scheme (Bork et al. 1998), and (2) a causative effect be established between amino acid changes and a qualitative/ quantitative shift in a defined function. Models incorporating structure-function relationships will be needed to help recognize the type of evolution that particular sites are undergoing. Learning to recognize functional divergence in evolving protein families is the next major bioinformatics challenge.

LITERATURE CITED

Afonnikov, D.A. (2000) CRASP: software package for analysis of physicochemcial parameters of aligned sequences of protein families. In *Second International Conference on Bioinformatics of Genome Regulation and Structure*, 7-11 August, 2000., Vol.2, Novosibirsk, Russia, pp. 145-148.

Afonnikov, D.A., Oshchepkov, D.Y. and Kolchanov, N.A. 2001. Detection of conserved physico-chemical characteristics of proteins by analyzing clusters of positions with co-ordinated substitutions. Bioinformatics 17:1035-1046.

Altschul, S.F., Carroll, R.J. and Lipman, D.J. 1989. Weights for data related by a tree. J. Mol. Biol. 207:647-653.

Aloy, P. Querol, E., Aviles, F.X. and Sternberg, M.J.E. 2001. Automated structure-based prediction of functional sites in proteins: applications to assessing the validity of inheriting protein function from homology in genome annotation and protein docking. J. Mol. Biol. 311:395-408.

Axe, D.D. 2000. Extreme functional sensitivity to conservative amino acid changes on enzyme exteriors. J. Mol. Biol. 301:585-595.

Bahnson, B.J., Colby, T.D., Chin, J.K., Goldstein, B.M. and Klinman, J.P. 1997. A link between protein structure and enzyme catalyze hydrogen tunneling. PNAS 94:12797-12802.

Bailey, T.L. and Elkan, C. 1995. The value of prior knowledge in discovering motifs with MEME. Proceedings of the Third International Conference on Intelligent Systems for Molecular Biology, AAAI Press, Menlo Park CA. pp. 21-29.

Bork, P., Dandekar, T., Diaz-Lazcoz, Y., Eisenhaber, F., Huynen, M. and Yuan, Y. 1998. Predicting function: from genes to genomes and back. J. Mol. Biol. 283:707-725.

Boudet, A.M., Goffner, D., Marque, C. and Grima-Pettenati, J. 1998. Genes involved in the final steps of monolignol biosythesis and their manipulation for tailoring new lignins. In: S. Sakanen, N. Lewis (editors) Biosynthesis of lignins and lignans. ACS Symp. Series 697:865-875.

Brill, E.M., Abrahams, S., Hayes, C.M., Jenkins, C.L., and Watson, J.M. 1999. Molecular characterization and expression of a wound-inducible cDNA encoding a novel cinnamyl alcohol dehydrogenase enzyme in lucerne. Plant Mol. Biol. 41:279-291.

Busfield, S.J., Comrack, C.A., Yu, G., Chickering, T.W., Smutko, J.S., Zhou, H., Leiby, K.R., Holmgren, L.M., Gearing, D.P. and Pan, Y. 2000. Identification and gene organization of three novel members of the IL-1 family on human chromosome 2. Genomics 66:213-216.

Caffrey, D.R., O'Neil, L.A.J., and Shields, D.C. 2000. A method to predict residues conferring functional differences between related proteins: Application to MAP kinase pathways. Protein Sci. 9:655-670.

Chase, T. 2000. Alcohol dehyrogenases: Identification and names for gene families. Plant Mol. Biol. Rep. 17:333-350.

Chavali, G.B., Vijayalakshmi, C. and Salunke, D.M. 2001. Analysis of sequence signature defining functional specificity and structural stbility in helix-loop-helix proteins. Prot. Struct. Funct. Genet. 42:471-480.

Chelvanayagam, G., Eggenschwiler, A., Knecht, L., Gonnet, G.H. and Benner, S.A. 1997. An analysis of simulataneous variation in protein structures. Prot. Eng. 10:307-316.

Chin, J.K., and Klinman, J. 2000. Probes of a role for remote binding interactions on hydrogen tunneling in the horse liver alcohol dehydrogenase reaction. Biochemistry 39:1278-1284.

Colby, T.D., Bahnson, B.J., Chin, J.K., Klinman, J.P., Goldstein, B.M. 1998. Active site modifications in a double mutant of liver alcohol dehydrogenase: structural studies of two enzyme-ligand complexes. Biochem. 37:9295-9304.

Crowder, S., Holton, J. and Alber, T. 2001. Covariance analysis of RNA recognition motifs identifies functionally linked amino acids. J. Mol. Biol. 310:793-800.

Cygler, M., Schrag, J.D., Sussman, J.L., Harel, M., Silman, I., Gentry, M.K. and Doctor, B.P. 1993. Relationship between sequence conservation and three-dimensional structure in a large family of esterases, lipases, and related proteins. Protein Sci. 2:366-382.

Debraj, G.T. and Draper, D.E. 1999. Methods protein-RNA sequence covariation in a ribosomal protein-rRNA complex. Biochemistry 38:3633-3640.

Edwards, R.H., Seillier-Moiseiwitsch, F. and Raab-Traub, N. 1999. Signature amino acid changes in latent membrane protein 1 distinguish Epstein-Barr virus strains. Virology 261:79-95.

Eisenberg, D., Luthy, R. and Bo, J.U. 1997. VERIFY3D: assessment of protein models with three-dimensional profiles. Methods Enzymol 277: 396-404.

Felsenstein, J. 1985. Confidence limits on phylogenies: an approach using the bootstrap. Evolution 39:783-791.

Gaucher, E.A. , Miyamoto, M.M. and Benner, S.A. 2001. Function-structure analysis of proteins using covarion-based evolutionary approaches: elongation factors. PNAS 98:548-552.

Gertl, J.A. and Babbitt, P.C. 2000. Can sequence determine function? Genome Biol. 1:reviews0005.1-0005.10.

Girardeau, J.P., Bertin, Y. and Callebaut, I. 2000. Conserved structural features in class I major fimbrial subunits (pilin) in Gram-negative bacteria. Molecular basis of classification in seven subfamilies and identification of intrasubfamily sequence signature motifs which might be implicated in quaternary structure. J. Mol. Evol. 50:424-442.

Goffner, D., Van Doorsselaere J., Yahiaoui, N., Samaj, J., Grima-Pettenati, J. and Boudet, A.M. 1998. A novel aromatic alcohol dehydrogenase in higher plants: molecular cloning and expression. Plant Mol. Biol. 36:755-765.

Gu, X. 1999. Statistical methods for testing functional divergence after gene duplication. Mol. Biol. Evol. 16:1664-1674.

Hartas, J., Goodfellow, A.M., Currie, B.J. and Sriprakash, K.S. 1995. Characterisation of group A streptococcal isolates from tropical Australia with high prevalence of rheumatic fever: probing for signature sequences to identify members of the family of serotype 5. Microb. Pathogen. 18: 345-354

Hawko, S.A. and Francklyn, C.S. 2001. Covariation of a specificity-determining structural motif in an aminoacyl-tRNA synthetase and a tRNA identity element. Biochem. 40:1930-1936.

Jones, M.D., Hunt, J., Liu, J.L., Patterson, S.D., Kohno, T. and Lu, H.S. 1997. Determination of tumor necrosis factor binding protein disulfide structure: deviation of the fourth domain structure from the TNFR/NGFR family cysteine-rich region signature. Biochemistry 36:14914-14923.

Jordan, I.K., Bishop, G.R. and Gonzalez, D.S. 2001. Sequence and structural aspects of functional diversification in class I α-mannosidase evolution. Bioinformatics 17:965-976.

Jörnvall, H., Persson, B. and Jeffrey, J. 1987. Characteristics of alcohol/polyol dehydrogenases. The zinc-containing long-chain alcohol dehydrogenases. Eur. J. Biochem 167:195-201.

Kendall, M.G. and Stuart, A. 1967. The advanced theory of statistics. Vol. 2. Inference and relationship. 2nd edition. Charles Griffin & Co. Ltd., London.

Kiedrowski, S. Kawalleck, P., Halbrock, K., Somssich, I.E. and Dangl, J.L. 1992. Rapid activation of a novel plant defense gene is strictly dependent on the *Arabidopsis RPM1* disease resistance locus. EMBO J. 11:4677-4684.

Kimura, M. 1985. The role of compensatory neutral mutations in molecular evolution. J. Genet. 64:7-19.

Koo, H.M., Choi, S.O., Kim, H.M. and Kim, Y.S. 2000. Identification of active-site residues in *Bradyrhizobium japonicum* malonamidase E2. Biochem. J. 349:501-507.

Kültz, D. 1998. Phylogenetic and functional classification of mitogen- and stress-activated protein kinases. J. Mol. Evol. 46:571-588.

Kumar, S.,Tamura, K., Jakobsen, I.B., and Nei, M. 2001. MEGA2: molecular evolutionary genetics analysis software. Bioinformatics 2001 17: 1244-1245.

Lauvergeat, V., Kennedy, K., Feuillet, C., McKie, J.H., Gorrichon, L., Baltas, M., Boudet, A.M., Grima-Pettenati, J. and Douglas, K.T. 1995. Site-directed mutagenesis of a serine residue in cinnamyl alcohol dehydrogenase, a plant NADPH-dependent dehydrogenase, affects the specificity for the coenzyme. Biochem. 34:12426-12434.

Lewis, N.G., Davin, L.B. and Sarkanen, S. 1999. The nature and function of lignins. In Barton DHR and Nakanishi K (editors) Comprehensive Natural Products Chemistry. Vol. 3. Carbohydrates and their Derivatives including Tannins, Cellulose and Related Lignins. p. 617-745.

Li, L., Cheng, X.F., Leshkevich, J., Umezawa, T., Harding, S.A. and Chiang, V.L. 2001. The last step of syringyl monolignol biosynthesis in angiosperms is regulated by a novel gene encoding sinapyl alcohol dehydrogenase. Plant Cell. 13:1567-1586.

Lichtarge, O., Bourne, H.R. and Cohen, F.E. 1996. The evolutionary trace method defines the binding surfaces common to a protein family. J. Mol. Biol. 257:342-358.

Logeman, E., Reinold, S., Somssich, I.E. and Hahlbrock, K. 1997. A novel type of pathogen defense-related cinnamyl alcohol dehydrogenase. Biol. Chem. 378:909-913.

MacKay, J.J., Liu, W., Whetten, R., Sederoff, R.R. and O'Malley, D.M. 1995. Genetic analysis of cinnamyl alcohol dehydrogenase in loblolly pine: single gene inheritance, molecular characterization and evolution. Mol. Gen. Genet. 247:537-545.

MacKay, J.J., O'Malley, D.M., Presnell, T., Booker, F.L., Campbell, M.M., Whetten, R.W. and Sederoff, R.R. 1997. Inheritance, gene expression, and lignin characterization in a mutant pine deficient in cinnamyl alcohol dehydrogenase. PNAS 94:8255-8260.

Mansell, R.L., Gross, G.G., Stockigt, J., Franke, H. and Zenk, M.H. 1974. Purification and properties of cinnamyl alcohol dehydrogenase from higher plants involved in lignin biosynthesis. Phytochem. 13:2427-2435.

Marin, I., Fares, M.A., Gonzales-Candelas, F., Barrio, E. and Moya, A. 2001. Detecting changes in the functional constraints of paralogous genes. J. Mol. Evol. 52:17-28.

Mateu, M.G. and Fersth, A.R. 1999. Mutually compensatory mutations during evolution of the tetramerization domain of tumor suppressor p53 lead to impaired hetero-oligomerization. PNAS 96:3595-3599.

Mirny, L.A. and Gefland, M.S. 2002. Using orthologous and paralogous proteins to identify specificty determining residues. Genome Biology 3:preprint0002.1-0002.20.

Mirny, L.A. and Shakhnovich, E.I. 1999. Universally conserved positions in protein folds: reading evolutionary signals about stability, folding kinetics and function. J. Mol. Biol. 291:177-196.

Mirny, L.A. and Shakhnovich, E.I. 2001. Evolutionary conservation of the folding nucleus. J. Mol. Biol. 308:123-129.

Miyata, T., Miyazawa, S. and Yasunaga, T. 1979. Two types of amino acid substitutions in protein evolution. J. Mol. Evol. 12:219-36.

Neher, E. 1994. How frequent are correlated changes in families of protein sequences. PNAS 91:98-102.

O'Malley, Porter, S., and Sederoff, R.R. 1992. Purification, characterization, and cloning of cinnamyl alcohol dehydrogenase in loblolly pine (*Pinus taeda* L.) Plant Physiol. 98:1364-1371.

Pavesi, A. 2000. Detection of signature sequences in overlapping genes and prediction of a novel overlapping gene in hepatitis G virus. J. Mol. Evol. 50:284-295.

Philpot, R.M. 1998. Identification of amino acid residues associated with modulation of flavin-containing monooxygenase (FMO) activity by imipramine: structure/function studies with FMO1 from pig and rabbit. Biochemistry 37:5930-5938.

Pollock, D.D. and Taylor, W.R. 1997. Effectiveness of correlation analysis in identifying protein residues undergoing correlated evolution. Prot. Eng. 10:647-657.

Pollock, D.D., Taylor, W.R. and Goldman, N. 1999. Coevolving protein residues: maximum likelihood and relationship to structure. J. Mol. Biol. 287:187-198.

Ponnuswamy, P.K., Prabhakaran, M. and Manalvalan, P. 1980. Hydrophobic packing and spatial arrangement of amino acid residues in globular proteins. Biochim. Biophys. Acta 623:301-316.

Poupon, A. and Mornon, J.P. 1999. Predicting the protein folding nucleous from a sequence. FEBS Lett. 452:283-289.

Richard, B., Couee, I., Raymond, P., Saglio, P.H., Saint-Ges, V. and Pradet, A. 1994. Plant metabolism under hypoxia and anoxia. Plant Physiol. Biochem. 32:1-10.

Rose, G.D., Geselowitz, A.R., Lesser, G.J., Lee, R.H. and Zehfus, M.H. 1985. Hydrophobicity of amino acid residues in globular proteins. Science 229:834-838.

Wang, Y. and Gu, X. 2001. Functional divergence in the caspase gene family and altered functional constraints: statistical analysis and prediction. Genetics 158:1311-1320.

CHAPTER 3

TABLES AND FIGURES

Table 1. CAD and ELI3 sequences analyzed in this study

Taxonomy	Common name	Chrom. 1X	Ploidy level	Generation	Genome (1C) Mbp	pg		NCBI Accession	gi / year
Phyllum Coniferophyta									
Class Coniferopsida									
Order Coniferales									
Family Pinacea									
Pinus taeda L.	Loblolly pine	12	2	perennial	20 000	22.0	01	PTCADBMR	558387 / 1995
Pinus radiata D. Don	Monterrey pine	12	2	perennial	21 000	23.1	02	PRU62394	1465776 / 1996
Picea abies (L.) Karst.	Norway spruce	12	2	perennial	13 500	14.8	03	PACINALDA	393443 / 1993
Phyllum Magnoliophyta									
Class Magnoliopsida (dycotyledons)									
Superorder Myrtanae									
Order Myrtales									
Family Myrtaceae									
Subgenus Symphyomyrtus									
Section Transversaria									
Eucalyptus botryoides Smith	Southern mahogany	11	2	perennial	530	0.6	04	EGCCAD	971397 / 1994
Eucalyptus saligna Smith	Sidney blue gum	11	2	perennial	530	0.6	05	AF294793	10281655 / 2000
Section Maidenaria									
Eucalyptus gunnii Hook.f.	Cider gum	11	2	perennial	640	0.7	06	EGCAD	971397 / 1995
Eucalyptus globulus Labill.	Blue gum	11	2	perennial	530	0.6	07	AF038561	2984652 / 1998
Superorder Violanae									
Order Capparales									
Family Brassicaceae									
Arabidopsis thaliana (L.) Heynh.	Thale cress	5	2	annual	130	0.2	08	ATCIACDE	757535 / 1995
						0.2	09	ATHCAD1B	1168728 / 1995
						0.2	10	AtELI31	16266 / 1992
						0.2	11	AtELI32	16268 / 1992
Order Violales (=Malpighiales)									
Family Salicaceae									
Populus deltoides Bartram ex Marshall	Poplar	19	2	perennial	510	0.6	12	PDCIALDA	288753 / 1995
Populus tremuloides Michx.	Poplar	19	2	perennial	510	0.6	13	AF217957	7239225 / 2000
							14	AAK58693	14279694 / 2001
Superorder Asternaceae									
Order Araliales									
Family Araliaceae									
Aralia cordata Thunb.	Aralia	.	2	perennial	1300	1.5	15	AAICAD	451196 / 1993
Family Apiaceae									
Petroselinum crispum (Miller) A.W. Hill	Parsley	11	2	annual	1900	2.1	16	PCELI3	1168732 / 1992
Order Asterales									
Family Asteraceae									
Zinnia elegans Jacq.	Zinnia	12	2	annual	3 000	3.3	17	D86590	1944403 / 1996
Superorder Rutanae									
Order Sapindales									
Family Fabaceae									
Medicago sativa L.	Alfalfa	8	4	perennial	1 600	1.8	18	MSCIALDHA	19595 / 1995
							19	MSACAD1	3603400 / 1999
Stylosanthes humilis Kunth.	Stylosanthes	10	2	annual	912	1.0	20	SSNCAD1A	556422 / 1995
							21	SSNCAD3	548323 / 1995
Superorder Solanaceae									
Order Solanales									
Family Solanaceae									
Lycopersicon esculentum Miller	Tomato	12	2	annual	1 000	1.1	22	S72477	7430935 / 2000
Nicotiana tabacum L.	Tobbaco	12	4	annual	3 800	5.9	23	NTCAD14MR	19839 / 1992
							24	NTCAD19MR	19841 / 1992
Superorder Caryophyllanaeae									
Order Caryophyllales									
Family Azioaceae									
Mesembryanthemum crystallinum L.	Ice plant	9	2	annual	390	0.4	25	MCU79779	1724109 /1996
Superorder Rosidae									
Order Rosales									
Family Rosaceae									
Fragaria x ananassa Dutch.	Strawberry	7	8	biennial	400	0.4	26	FXU63534	4097521 /1996
Class Liliopsida (monocotyledons)									
Order Poales									
Family Poaceae									
Subfamily Pooideae									
Tribe Poeae									
Lolium perenne L.	Ryegrass	7	2	perennial	1 900	2.1	27	AF010290	2388661 / 1997
Festuca arundinacea Schreb.	Tall fescue	7	4	perennial	3830	4.2	28	AAK97811	15428282 / 2001
Subfamily Panicoideae									
Tribe Andropogoneae									
Saccharum officinarum L.	Sugar cane	10	8	perennial	2 547	3.0	29	SOF231135	3341513 / 1998
Zea mays L.	Maize	10	2	annual	2 400	2.5	30	ZMCADGENE	2239258 / 1997

Note: Tavares et al. (2000) labelled the *Arabidopsis thaliana* sequences ATCIACDE as LCAD-C, and ATHCAD1B as CAD1

Table 2. Amino acid positions that identify protein sequences as members of the cinnamyl alcohol dehydrogenase (CAD/ELI3) family of proteins. These signature positions are linked to the occupancy of a polar group (S or T) in position 212.

Position[a]	Amino Acid		Solvent Accessibility	Secondary structure	Replacement[e]	Comments
CAD/ELI3 family signature						
12	G		5.94	β	-	Zinc-binding domain
17	D		4.26	β	-	Zinc-binding domain
20	G		7.13	L	-	Zinc-binding domain
44	C		1.22	β	-	Zinc-binding domain
56	N		16.97	L	-	Zinc-binding domain
63	Y		21.53	L	-	Zinc-binding domain
67	P		3.84	L	-	Zinc-binding domain
94	G		2.52	β	-	Zinc-binding domain
134	G		3.45	L	-	Zinc-binding domain
170	S		0.00	α	-	Rossman fold
171	P		0.00	α	-	Rossman fold
194	H		2.44	α	-	Rossman fold
208	T		1.55	β	-	Rossman fold
209	V		5.52	β	-	Rossman fold
211	S		7.66	β	-	Rossman fold
220	A		7.96	α	-	Rossman fold
251	T		1.57	β	-	Rossman fold
256	H		6.74	L	-	Rossman fold
265	L		20.74	α	-	Rossman fold
336	R		8.25	π	-	Zinc-binding domain
337	L		25.79	α	-	Zinc-binding domain
346	F		32.79	L	-	Zinc-binding domain
347	V		21.97	L	-	Zinc-binding domain
349	D		2.42	L	-	Zinc-binding domain
Signature positions that discriminate CAD and ELI3 proteins						
Gu's criterion						
104	.	ED	13.08	α	r	Zinc-binding domain
119	W	.	21.35	T	r	Zinc-binding domain substrate specificity
120	.	T	21.60	T	c	Zinc-binding domain substrate specificity
123	D	.	11.96	L	r	Zinc-binding domain
124	V	.	17.95	L	r	Zinc-binding domain
137	.	D	10.54	B	r	Zinc-binding domain
157	Q	.	11.48	α	r	Rossman fold
215	K	.	34.47	π	r	Rossman fold NADPH specificity
259	E	.	37.67	π	r	Rossman fold
290	L	.	49.96	T	c	Rossman fold
299	F	.	10.09	B	r	Rossman fold substrate specificity
Mutual information						
27	Y	F	17.39	β	c	Zinc-binding domain
29	L	R	28.63	β	r	Zinc-binding domain
71	V	I	3.84	β	c	Zinc-binding domain, vdW with Ser138, Leu159, Val93,Cys44
156	E	D	15.90	β	c	Zinc-binding domain
186	I	V	1.03	β	c	Rossman fold, vdW I 207
192	V	L	10.44	β	c	Rossman fold, H tunnelling, catalysis, pyrophosphate stability
206	H	K	45.68	β	c	Rossman fold, stabilizes with D224
212	S	T	6.08	β	c	Rossman fold, NADPH-specificity determinant
229	Y	F	10.30	β	c	Rossman fold, vdW (SCAD,TELI3)209, 215
253	P	S	0.17	β	c	Rossmanfold
254	V	A	3.72	L	c	Rossman fold, β-sheet fold stability, nicotinamide ribose
261	Y	L	5.76	π	r	Rossman fold
283	F	L	34.14	L	c	Rossman fold
302	S	G	0.77	π	r	Zinc-binding domain
316	K	H	6.89	α	c	Zinc-binding domain

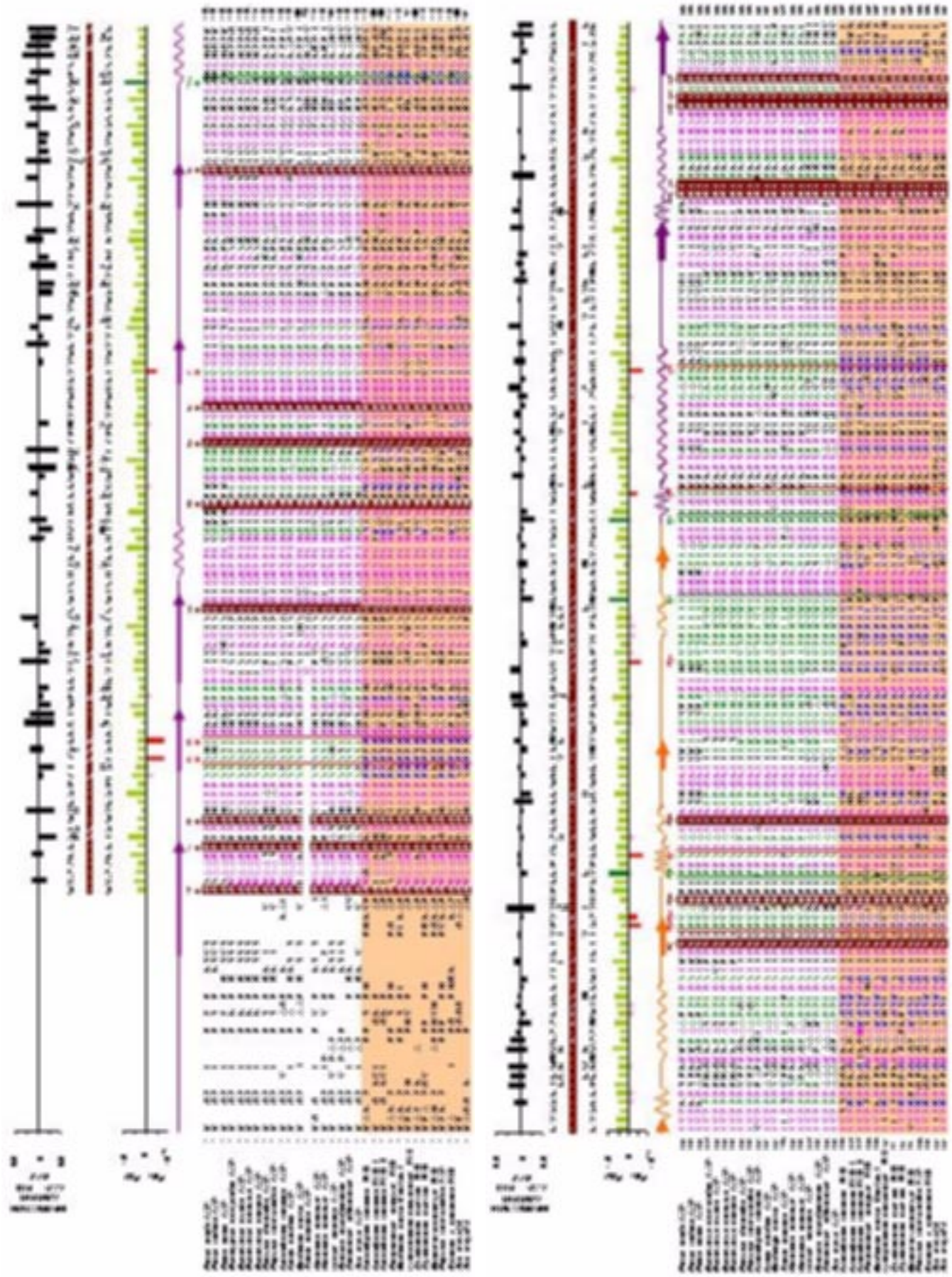
[a]Position number based on pine CAD sequence. [b]For Gu's criterion and mutual information, first amino acid corresponds to CAD and the second to ELI3 groups. [c]Solvent accessible surface in squred angstroms were generated using the WHATIF program (www.cmbi.kun.nl/whatif) assuming a Van der Waals radius of 1.14 Å for the solvent water. [d]Secondary structure based from structural models: α, alpha helix; π, 3_{10} helix; β, beta strand; L, loop. e Raplacement class: r, radical; c, conservative.

Table 3. Diagnosis of genomic and EST sequences annotated as “cinnamyl alcohol dehydrogenase”.

Acc. No.	Project	Clone / Gene	Group	Tissue / Treatment/ Comments
Apium graveloens gene				
AF067082	_	_	ELI3	Mannitol dehydrogenase with signature relating it to ELI3. Asp 215 involved in NAD^+ recognition.
Arabidopsis thaliana genomic sequences				
AAD20406	IGR	At2g21890	ELI3	Chrom. 2 LCAD-F
AAD20393	IGR	At2g21730	ELI3	Chrom. 2 LCAD-E
CAB80462	IBP	At4g37970	ELI3	Chrom. 4, LCAD-A
CAA76419	IBP	*LCAD-B*	ELI3	Chrom. 4, LCAD-B, fragment
CAA17549	IGR	At4g34230	CAD	Chrom. 4 LCAD-D
AAG52618	IGR	F5D21.12	not related	Chrom. 1
AAG60085	IGR	F4N21_7	not related	Chrom. 1
AAC33208	IGR	F14J9.14	not related	Chrom. 1
AAC33209	IGR	F14J9.15	not related	Chrom. 1
AAC33210	IGR	F14J9.16	not related	Chrom. 1
AAC33211	IGR	F14J9.17	not related	Chrom. 1
NP_197445	IGR	At5g19440	not related	Chrom. 5
AAG51850	IGR	F28P22.13	new	Chrom. 1 Probable new subfamily
Eucalyptus gunnii gene				
CAA61275	_	CAD1	not related	
Brassica rapa gene fragments				
AAF23412	_	CADa	CAD	
AAF23416	_	CADb	ELI3	
Brassica napus gene fragments				
AAF23409	INRA	CADa-1	CAD	
AAF23413	INRA	CADb-1	ELI3	
Brassica oleracea gene fragments				
AF207554	INRA	CADa	CAD	
AAF23415	INRA	CADb	ELI3	
Fragaria x ananassa gene				
Q9ZRF1	_	MTD	ELI3	Mannitol dehydrogenase Thr 216 probably involved in NADP(H) recognition
Hordeum vulgare gene fragment				
CAA63410	_	CAD	CAD	
Lotus corniculatus gene				
AAK61495	_	_	ELI3	Leaf tissue
Malus x domestica gene				
T16995	_	_	not related	
Medicago sativa gene				
O82515 recognition	_	MTD	ELI3	Mannitol dehydrogenase Thr 216 probably involved in NADP(H)
Mesembryanthemum crystallinum gene				
P93257 recognition	_	MTD	ELI3	Mannitol dehydrogenase Thr 216 probably involved in NADP(H)
Populus balsamifera subsp. trichocarpa gene				
CAC07423	_	_	CAD	Leaf tissue
Populus deltoides gene fragment				
S31571	_	_	CAD	
Vigna unguiculata gene				
T11610	_	_	Not related	drought - inducible gene - CAD1
Pinus taeda expressed sequence tags				
AA556583	NCSU	2C11E	CAD	Xylem wood
AA740078	IFG	9398M	CAD	Xylem wood
BE643901	NSF	NXCI_048_G10	ELI3	Xylem Compression wood Inclined
BI643894	NSF	NXPV_126_F10	ELI3	Xylem Planings wood Vertical
BG039205	NSF	NXSI_096_B09	ELI3	Xylem Side wood Inclined
AW736795	NSF	NXNV_083_A10	ELI3	Xylem Normal wood Vertical
BG317522	NSF	NXPV_002_G08	ELI3	Xylem Planings wood Vertical
BI076958	NSF	NXPV_085_C05	ELI3	Xylem Planings wood Vertical
BG318121	NSF	NXPV_010_F11	ELI3	Xylem Planings wood Vertical
BF186357	NSF	NXCI_136_H08_F	ELI3	Xylem Compression wood Inclined
BE123786	NSF	NXNV_156_D04	ELI3	Xylem Normal wood Vertical
BF010579	NSF	NXCI_086_D01	ELI3	Xylem Compression wood Inclined
BE996924	NSF	NXCI_102_C08	ELI3	Compr ession wood Incline
BF060645	NSF	NXCI_118_H04	ELI3	Xylem Compression wood InclineD
AI812486	NCSU	11G1	ELI3	Xylem Normal wood Vertical
AA739647	IFG	8695M	ELI3	Xylem wood
AI 725214	IFG	9328R	ELI3	Xylem wood
AI 724977	IFG	8695R	ELI3	Xylem wood
AW010115	DOE	ST02B03	ELI3	Shoot tips

Figure 1

Multiple sequence alignment of plant subfamily I (cad) and subfamily II (eli3) cinnamyl alcohol dehydrogenases. Sequences are ordered by similarity, the top 19 sequences correspond to CAD and the lower 13 are ELI3 proteins. Residues are numbered based on the sequence of *Pinus taeda* CAD. Conserved positions (pink) have information content lower than 0.1. Among them, positions bearing an amino acid residue that are distinguished from other zinc-containing alcohol dehydrogenases are indicated boxed in brown background. Positions that were found significant by Gu's criterion of divergence [having a conditional probability that the site is in a state of divergence $P(F_D|Y_{CAD},Y_{ELI3})>0.9$] are indicated and boxed by a green line across the alignment. Positions found to be significant by the mutual information criterion [$P(MI)<10^{-6}$] are indicated with a line border. Dash (-) indicates gaps in the alignment. Annotations above the alignment indicate the information content of the position, the multiple level consensus residue and a central line that compares the consensus residues as radical replacements if residues belong to different classes, or conservative replacements if residues belong to the same class. The six amino acid classes were: neutral and small (A,G,P, S, T), polar and relatively small (N,D,Q,E), polar and relatively large (R,H,K), non-polar and relatively small (I,L,M.V) and nonpolar and relatively large (F, W,Y), and special (C). The predicted secondary structure of the zinc-binding domain (red) and dinucleotide binding domain (dark yellow). Residues buried (with solvent accessible area < 20% are in depicted in yellow areas. secondary structure: ≈ α-helix, ➜ β-sheet, /\/\/\, π-helix (3_{10}),



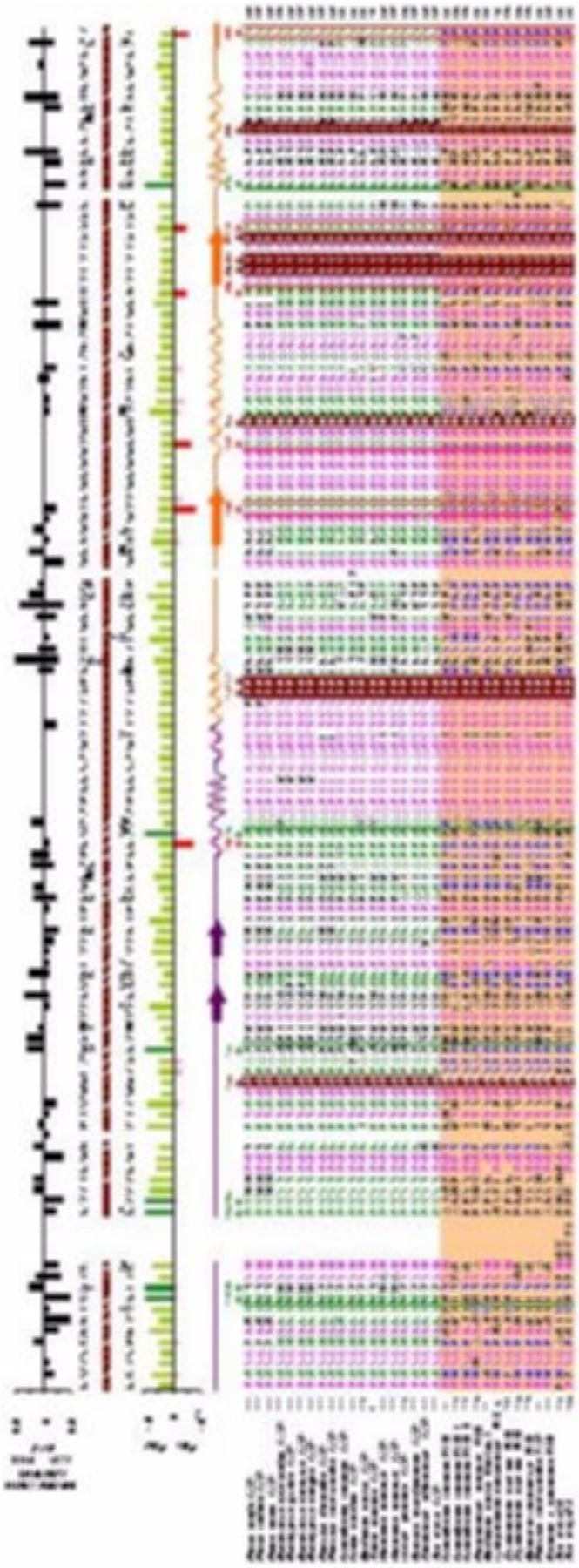


Figure 2

Phylogenetic relationship between cinnamyl alcohol dehydrogenases sequences. The tree topology (unrooted) was determined using a neighbor-joining (NJ) method (Saitou and Nei 1987) based on the Jukes-Cantor proportion of non-synonymous nucleotide differences (MEGA2, Kumar et al. 2001). Internode lengths were recalculated based on first and second codon positions using the baseml module of the PAML software (Yang 1999). The reliability of the topology was evaluated by a bootstrap method based on 10^4 pseudosamples.

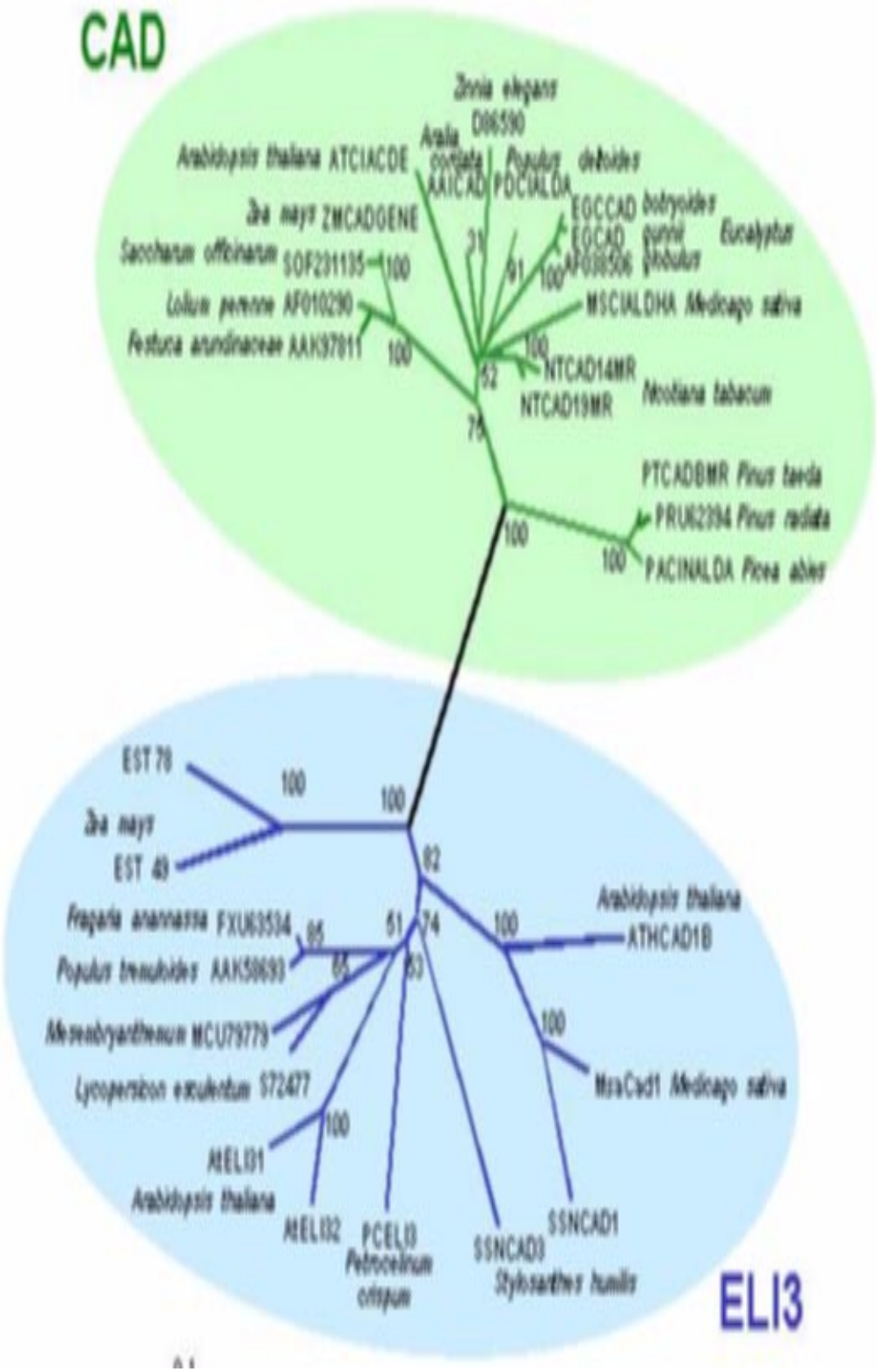

CAD
Zinnia elegans D86590
Arabidopsis thaliana ATCIACDE
Populus deltoides AAICAD
PDCIALDA
Zea mays ZMCADGENE
EGCCAD botryoides
EGCAD gunnii
Eucalyptus globulus AF038506
Saccharum officinarum SOF231135
Lolium perenne AF010290
Festuca arundinacea AAK97011
MSCIALDHA Medicago sativa
NTCAD14MR
NTCAD19MR
Nicotiana tabacum
PTCADBMR Pinus taeda
PRUI2394 Pinus radiata
PACINALDA Picea abies
EST 70
Zea mays
EST 49
Fragaria ananassa FXU63534
Populus tremuloides AAK59693
Mesembryanthemum MCU79779
Lycopersicon esculentum S72477
Arabidopsis thaliana ATHCAD1B
MsaCad1 Medicago sativa
AtELI01
Arabidopsis thaliana
AtELI02
PCELI3
Petroselinum crispum
SSNCAD3
SSNCAD1
Stylosanthes humilis
ELI3

Figure 3

Structural model of the subfamily I cinnamyl alcohol dehydrogenase subunit complexed to $NADP^+$ and coniferyl alcohol. The spatial coordinates used for modelling was a consensus derived from the X-ray structures of human sigma alcohol dehydrogenase (1AGN.pdb, 1D1S.pdb), and horse liver alcohol dehydrogenase (3BTO.pdb). (A) Structure of the α/β-domains of the CAD subunit showing the dinucleotide-binding domain (Rossman fold, green-yellow, upper part), and the zinc-binding domain (blue, lower part). Coniferyl alcohol is bound in the cleft formed by these two domains. Zinc represented as spheres (orange). (B) Conserved positions in both CAD and ELI3 subfamilies. They amount to 55% of the aligned positions. (C) Significant positions detected using Gu's criterion. Green spheres locate the $C\alpha$ of the positions. (D) Significant positions detected by the specificity-determinat mutual information criterion (red).

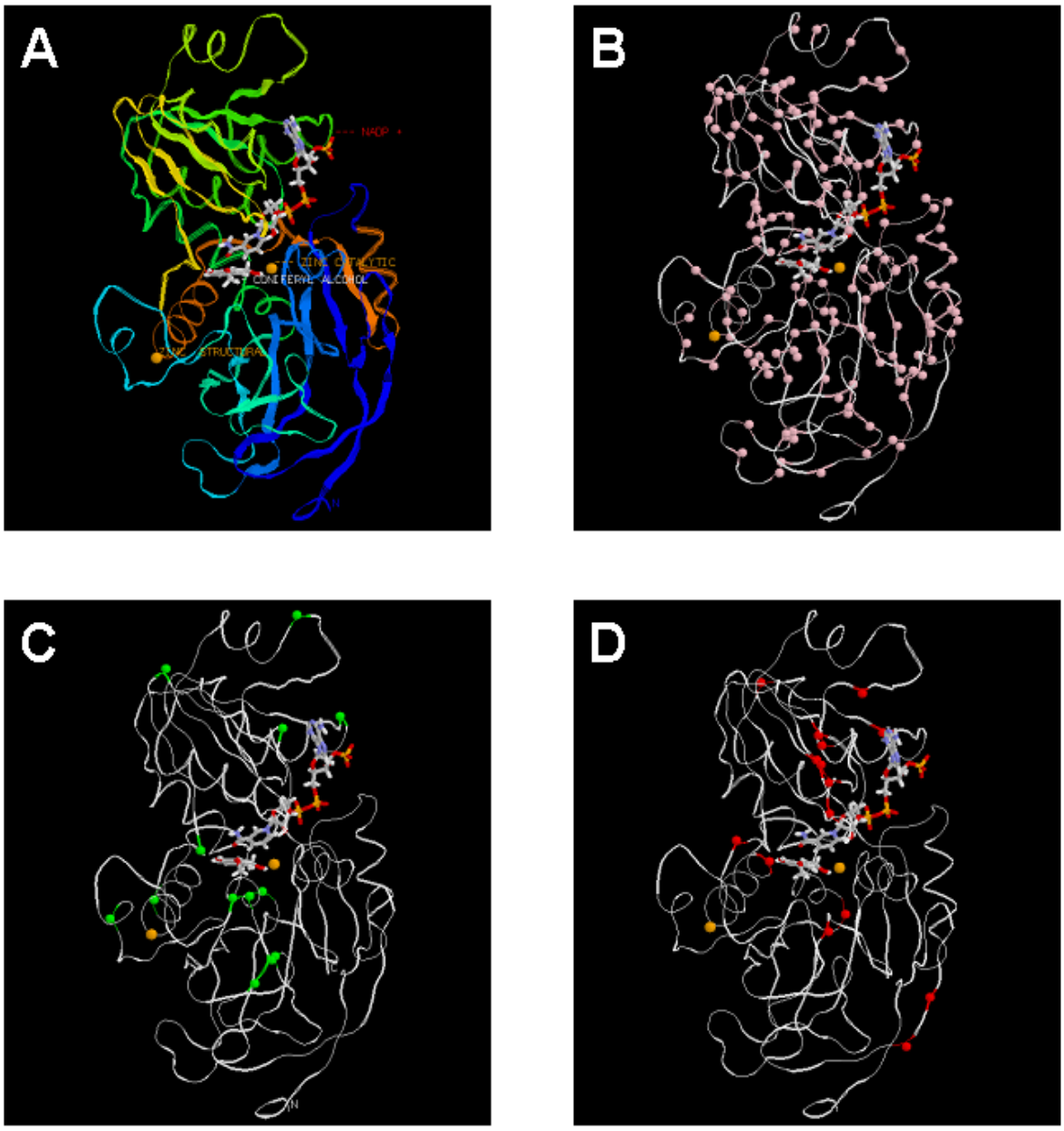
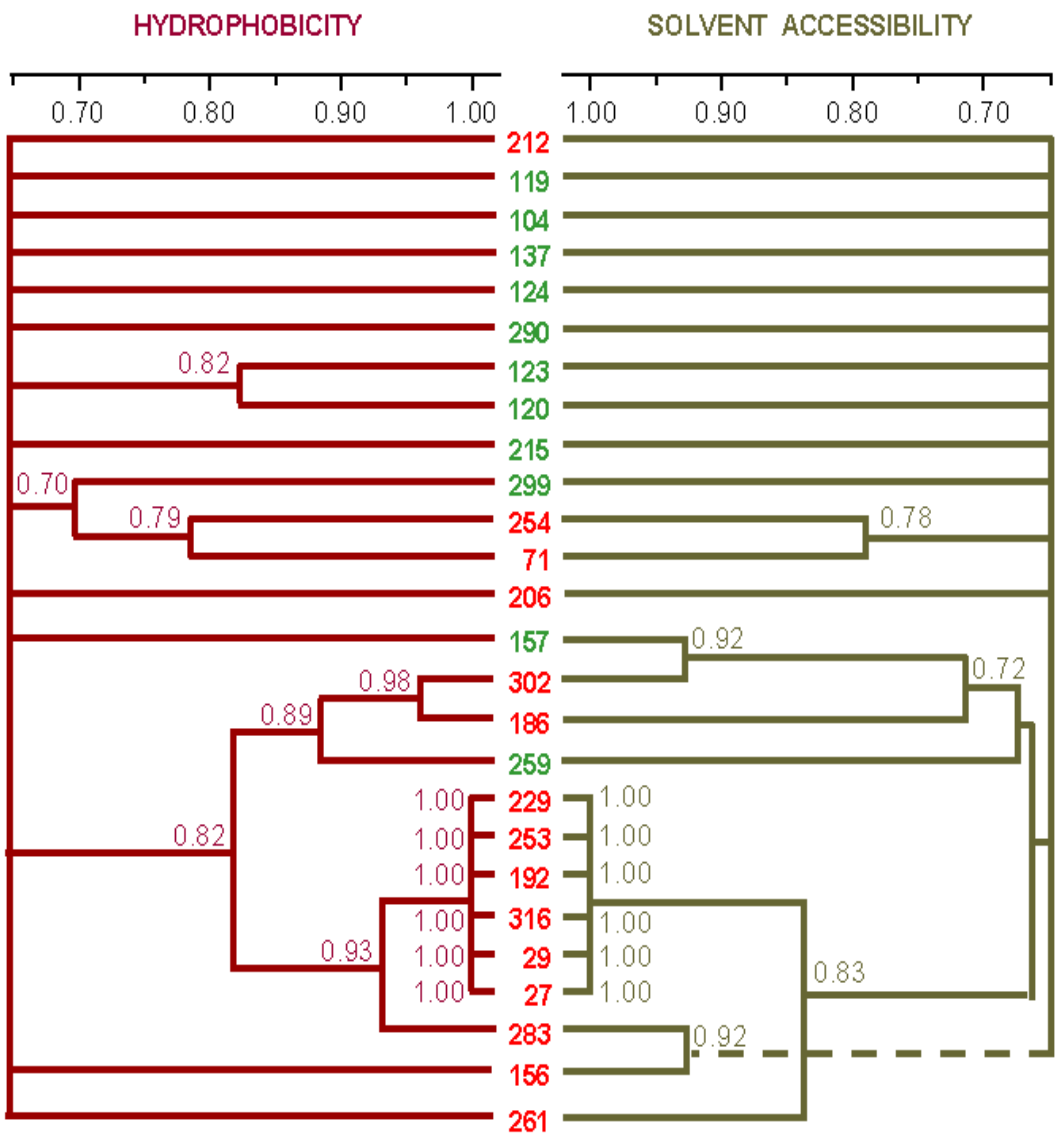

A
B
C
D

Figure 4

Network of correlation distances among positions determined by Gu's criterion (green numbers) and mutual information (red). Numbers at the nodes indicate the correlation coefficient common to a cluster. Only coefficients higher than 0.66 were found to be highly significant.


HYDROPHOBICITY
SOLVENT ACCESSIBILITY
0.70
0.80
0.90
1.00
1.00
0.90
0.80
0.70
212
119
104
137
124
290
123
120
215
299
254
71
206
157
302
186
259
229
253
192
316
29
27
283
156
261
0.82
0.70
0.79
0.78
0.92
0.72
0.98
0.89
0.82
1.00
0.93
0.83
0.92

CHAPTER 4

Diversification of the *4CL, CCR* and *CAD* gene families in loblolly pine (*Pinus taeda*) as revealed by EST data

INTRODUCTION

Lignin plays important roles in plant development and in resistance to biotic and abiotic stress (Lange et al. 1995). It is also important to the paper industry and for animal forage (Jung and Vogel 1986). New insights into the enzymes of the lignin biosynthetic pathway have brought a re-evaluation of the metabolic routes leading to the formation of specific monolignols. Experimental evidence has shown the presence of isozymes for 4CL, CCR and CAD in a number of species (Knobloch and Hahlbrock 1975, Jones et al. 2001, Grima-Pettenati et al. 1994). This suggests that these genes may not exist as single copies but instead as multigene families. Sequencing and database searches have also revealed the existence of genes with significant sequence identity to known 4CL, CCR, and CAD genes in plants. Down-regulation experiments designed specifically to target 4CL, CCR, and CAD genes have failed to entirely suppress enzymatic activity (Kajita et al. 1997, Chabannes et al. 2001, Piquemal et al. 1998, Russell et al. 2000, Ralph et al. 1998), suggesting that these genes encode specific isozymes that have restricted substrate specificity. Isozymes could participate in parallel routes leading to the formation of specific monolignols (Boudet 1998a, b). Understanding gene family structure is critically important for the proper interpretation of experimental data and understanding functional divergence in the lignin pathway.

The conventional way of studying gene families requires extensive cloning and sequencing of genomic DNA, which is time-consuming and laborious (Sambrook et al. 1989). Another way to characterize coding regions of genes is the analysis of

sequences from cDNA libraries. Partial cDNA sequencing to provide expressed sequence tags (ESTs) has become one of the most direct ways to characterize transcribed genes in a genome. ESTs are single-pass sequences of varying length (100-600 bp), which contain sequencing errors (typically 1-5%), originate from different parts of the cDNA, and are affected by alternative splicing or cloning artifacts.

These issues significantly limit utility of individual ESTs in reliably predicting coding regions of genes. Fortunately, the negative effects of these issues can be minimized by aligning overlapping ESTs that originate from the same cDNA and, therefore, from the same transcribed gene. PHRAP (bozeman.mbt.washington.edu/phrap.docs/phrap.html) is a commonly used computer program that assembles individual ESTs into contigs, a consensus cDNA sequence derived from clustered and aligned ESTs based on overlap length, sequence quality, and nucleotide identity criteria of the individual ESTs. The ability to predict the coding region of a gene can be successfully achieved by comparison of the contig against genomic sequences. Genomic sequences provides information on the structure of a gene family (i.e. subfamilies) and thus serves as a context to classify ESTs according to the gene family structure.

a consensus DNA sequence derived from clustered and aligned ESTs).

In the absence of genomic sequences to serve as templates, well annotated gene sequences from other organisms can be used as a scaffold for EST analysis and classification. The use of a multiple sequence alignment of known genes introduces valuable information on the sequence features in the coding region (conserved sites, catalytic sites). The alignment provides the basis to cluster genes into subfamilies

based upon a phylogeny. It permits the detection of signature sites (i.e. positions whose amino acid occupancy distinguish subfamilies). This scaffold alignment is a means to lay out the ESTs, and determine the usable length of each EST based on its alignable translated sequence. It allows ESTs to be classified into subfamilies by assessing the amino acid residue occupancy in the signature positions, and eventually leads to the clustering and alignment of ESTs representing a given subfamily. This approach highlights the use of extrinsic information obtained from known genes to cluster the ESTs, in contrast with methods like PHRAP that cluster ESTs directly.

A critical step in the characterization of the subfamily structure of a gene family is recognition of the signature. Gu (1999) developed a Bayesian approach that used the number of amino acid replacements in a homologous position in two subfamilies to detect sites undergoing differential rates of evolution. Mirny and Gelfand (2002) proposed an informatics method (i.e., mutual information) to identify homologous positions whose amino acid residue is associated with a subfamily. Both criteria detect positions with distinct patterns of molecular evolution.

The goal of this study was to determine the diversity of 4CL, CCR and CAD genes families in the loblolly pine genome. This was done by systematically compiling and classifying loblolly pine EST data into subfamilies. Results showed that all the ESTs of loblolly pine 4CL resolved into one single gene subfamily whereas those for CCR and CAD showed two major divergent subfamilies for each gene. The two-subfamily structure of the CCR and CAD gene families was found to be widespread in a number

of plant species. A concerted duplication and functional diversification of these genes could be related to their sequential participation in the phenylpropanoid pathway.

MATERIALS AND METHODS

Generation of the scaffold alignments

Nucleotide sequences of genes encoding 4-coumarate:coenzyme A ligase (4CL; E.C. 6.2.1.12), cinnamoyl:coenzyme A reductase (CCR, E.C. 1.2.1.44), and cinnamyl alcohol dehydrogenase (CAD, E.C. 1.1.1.195) were compiled from the non-redundant (NR) GenBank database at the National Center for Biotechnology Information (Bethesda, MD) using the Entrez search and retrieval system. For all searches, the full length gene sequences were screened using literature reports to include those with adequate annotation. Deduced amino acid sequences were aligned using CLUSTAL W 1.7 (Thompson et al. 1994, www2.ebi.ac.uk/clustalw). The resulting alignment for each gene (i.e., the scaffold alignment), was manually inspected, modified and used as a framework to align codons.

Gene trees

Gene trees were constructed to determine the relationships between the sequences of a particular gene and to separate major classes of gene family members. Unrooted topologies based on Poisson corrected distances were constructed by the neighbor-joining (NJ) method (Saitou and Nei 1987) and the UPGMA method

(Sneath and Sokal 1973), using the MEGA2 software (Kumar et al. 2001, www.megasoftware.net). Support for the nodes of the topology was assessed by a bootstrap method based on 10^4 pseudosamples (Felsenstein 1985).

Position-specific statistics

Position-specific statistics were used to detect the presence of specific amino acid positions ("signature" sites) at which the amino acid composition at that position is associated with gene cluster differentiation. These statistics (i.e., Gu's criterion of divergence and mutual information) are formulated in Chapter 3. Gu's criterion of divergence (θ) is based on a hidden Markov model to describe which state, divergence or constraint, is more likely at a given position (Gu 1999). A Bayesian approach is used to test the significance of the replacement rate differences in a given position. Mutual information (MI) for a given position measures the association between an amino acid residue and a subfamily using the amino acid frequencies. Statistical testing of mutual information values is based on a permutation test (Mirny and Gefland 2002).

Compilation, screening and cleaning of *Pinus taeda* EST sequences

The "EST_other" subsection of the NCBI's dbEST database was searched with tBLASTn (www.ncbi.nlm.nih.gov/BLAST) using each of the known loblolly pine protein sequences for 4CL (gi 7437871), CCR (gi 17978649) and CAD (gi 1076239) as queries to detect related ESTs. The pine ESTs present in this database are pro-

cessed to ensure that all have at least 200 nucleotides of PHRED 20 quality score (Ewing and Green 1998, Ewing et al. 1998). tBLASTn uses a protein query to search a nucleotide database in all six reading frames and reports the matches by their deduced protein sequence. The search space was the 45112 loblolly pine ESTs as available from the March 2002 release, using the BLOSUM62 as the scoring matrix and no filtering.

A principal component analysis (PCA) was used to identify ESTs that were similarly informative based on normalized bit score, percentage identity to the protein query, and the EST nucleotide length. PCA is a linear procedure that reduces the number of variables by finding new, uncorrelated ones that are linear combinations of the original variables (Jolliffe 1986). The eigenvalues and the eigenvectors were computed using a square symmetric matrix of correlation values (SAS Insight software version 6.12, SAS Institute, 1994). The majority of the data variation is contained in the first principal component. EST sequences with the first principal component equal to or greater than zero were retrieved for further analyses. Each EST was then corrected ("cleaned") by assuming that an EST represents the coding region of transcribed genes. ESTs were translated into the reading frame(s) according to the tBLASTn output using the Expasy translate tool server (www.expasy.ch/tools/dna.html). Sequence variations, gaps, insertions, misincorporations, frameshifts and regions with unusual variability were detected by examination of the alignment of the EST-predicted amino acid sequence with the tBLASTn translated gene alignment .

Subfamily classification of loblolly pine ESTs

The screened EST data, the tBLASTn report, and the scaffold alignment were used to obtain alignments of all of the EST sequences that contributed to the coding region of each gene product. Throughout the analysis, translated genes and ESTs kept codon information of each site. The procedure to classify ESTs into subfamilies is shown in Figure 2. The first step was to lay out the ESTs onto the scaffold using the tBLASTn report alignments of the translated ESTs to the query sequence. The translated EST was aligned using the encoded amino acid sequence of the scaffold as a guide. The second step consisted of classifying ESTs by assessing 'by eye' the amino acid occupancy in signature positions as determined by Gu's and mutual information criteria. For an EST to be classified to a gene subfamily, all signature positions encompassed in the scaffold region aligned to the EST were evaluated. Based on the amino acid occupancy in these signature positions, an EST was assigned to a subfamily. The third step assembled all the ESTs belonging to a specific subfamily and produced an aligned set of ESTs (i.e., a contig), all derived from the same subfamily.

RESULTS

Gene alignment and motifs

Alignments of the amino acid sequences of each gene were performed as the first step in assessing homology. The large proportion of conserved positions both facilitated alignments and assured reliability. Conserved positions in 4CL, CCR and

CAD comprised 54, 52 and 55% of the sites, respectively. 4CL sequences contained the putative AMP-binding signature (LPYSSGTTGLPKG, Prosite PDOC00427) located between amino acid positions 186 and 192 (numbering according to the loblolly pine 4CL sequence Acc. T09710). In addition, a conserved motif apparently involved in ligand binding (GEICIRG), was also present between positions 386 to 392. CCR sequences displayed conservation of the positions involved in cofactor binding (V15, T16, G17, G20, L30 and S127 (numbered following the loblolly pine CCR sequence Acc. AAL47684). Furthermore, conserved residues K158 and K165 flanked a region presumably involved in substrate binding. The CAD sequences were characterized by a zinc-containing alcohol dehydrogenase signature (**GHE**xx**G**xxxxx**G**xx**V**, Prosite PDOC00058) encompassing amino acid positions 68 to 82 in the alignment (numbered following the loblolly pine CAD sequence Acc. PTCADBMR) . The residues involved in the coordination of the catalytic zinc atom were Cys47, His69 and Cys163. The structural zinc atom was coordinated by cysteines 100, 103, 106 and 115. These proteins have an NADP(H)-binding domain known as the Rossman fold. This α/β-fold consists of a series of conserved amino acid residues at a few crucial positions, whereas other regions of the domain vary considerably. The conserved part of the motif, the $\beta\alpha\beta$ signature, consists of the first two β-strands (underlined) and the intervening amphipathic α-helix (italics) and contains a few polar and numerous hydrophobic residues (<u>KCGIL**G**L**G**GV</u>***G****HMGVKI-AKAF*<u>GLHVTVISS</u>; positions 182 to 212).

Subfamily structure and divergence of gene families

4CL, CCR and CAD gene sequences formed two major subfamilies (Figure 3). Divergence statistics showed that these subfamilies had different patterns of replacement rates per site (Table 1). The coefficient of divergence between the two 4CL clusters was $\hat{\theta}_{MLE} = 0.06$, which though statistically non-significant, both clusters contained sequences known to participate in distinct metabolic pathways. The coefficient of divergence for the CCR and CAD were 0.28 ± 0.07 ($P > 0.0002$) and 0.39 ± 0.04 ($P > 0.0001$), respectively, implying a significant loss of rate correlation among subfamilies and indicating that the level of sequence separation between them is statistically significant.

The sequences of the subfamilies consistently clustered together using several tree building algorithms, with large bootstrap support for the internal nodes (data not shown). However, the 4CL clusters were separated by a short internode distance. The bootstrap support for this internal node was 0.58 using a neighbor-joining topology, and 0.70 using a UPGMA tree. The pine 4CL sequences belonged to subfamily I, and constituted a well separated group from the angiosperm members of the subfamily. The trees for both CCR and CAD genes formed two well differentiated clusters with strong bootstrap support (100%).

Signature recognition in gene products

Pattern recognition methods were used to identify homologous positions where the amino acid composition could be associated with cluster differentiation. The distri-

bution of replacement rates was modeled as a gamma distribution to characterize the level of conservation of residues in the entire tree. The values for the shape parameter α for the entire trees were large (0.76 ± 0.09 for 4CL, 1.83 ± 0.13 for CCR, and 0.60 ± 0.07 for CAD) compared to each subfamily I and II individually (0.47 and 0.58 for 4CL, 0.62 and 0.83 for CCR, and 0.31 and 0.45 for CAD). This shows that sites having variable replacement rates are more frequently observed when the two subfamilies were considered together, rather than separately. Therefore, variable positions in one group are not the same as those of another, and presumably some positions are constrained differently in each subfamily. Thus, positions that varied across the alignment could be conserved within subfamily.

Gu's criterion of divergence and the mutual information criterion were used to determine positions where amino acid occupancy could discriminate subfamilies. Gu's criterion recognizes amino acid configurations that are conserved in one group but highly variable in another (Type I, according to Wang and Gu 2001), while mutual information identifies amino acid configurations that are conserved but distinct in both groups (Type II).

Alignment of loblolly pine ESTs onto gene scaffold

The scaffold alignment constituted the alignment of all known sequences of a gene family, ordered according to the phylogeny, and labeled with signature positions. *Pinus taeda* ESTs were aligned on the scaffold alignment constructed from all the non-redundant sequences of a gene. EST sequences were first screened by a princi-

pal component analysis of bit score, percentage identity of the EST to the protein query, and the EST nucleotide length. The final EST data sets contained 78, 28 and 51 ESTs for 4CL, CCR and CAD, respectively. EST data was cleaned of ambiguities and frameshifts, and trimmed using the BLAST output and the scaffold alignment. The scaffold alignment of genes was used to identify conserved and variable sites, and to determine which regions in an EST can be reliably aligned to the scaffold. ESTs covered the full length of the scaffold alignment. In only two cases was the valid reading frame 3'-5' (4CL: NXNV_075_B12_F; CCR: NXCI_106_G05_F).

For a given EST to be classified into a subfamily, all signature positions that could possibly be evaluated in a EST should agree with a given subfamily. ESTs had an average length of 30 alignable amino acid positions, and generally contained 3 to 5 signature positions. In very few cases (<1%) some ESTs contained signatures for both gene classes. These ESTs were assigned to the most similar, as long as there was only a single disagreeing site. In general terms, amino acid positions highlighted by these criteria were distributed throughout the alignment spanning all structural domains. Inspection of the pine EST aligned data showed that all the translated pine EST sequences had the conserved amino acid residues expected to occur on basis of the alignment.

Subfamily representation in loblolly pine ESTs

Signature positions differentiating subfamily were then used to determine whether the pine EST sequences also reflected a similar classification (Table 4). Pine 4CL

ESTs belonged to subfamily I. It had the highest level of conservation, at both the amino acid and nucleotide levels (e.g., 2% of the amino acid sites had a codon variant). Most of the ESTs constituting this subfamily came from xylem tissue of compression wood, and from normal and side wood. This sequence was identical to the fully annotated loblolly pine 4CL gene sequence (Acc. No. PTU12013).

Cinnamoyl coenzyme A reductase ESTs formed two distinct groups, each belonging to a different subfamily, and differing in 44% of the sites. The subfamily I CCR sequence had one fourth of its amino acid positions containing more than one possible codon, half of them constituted by synonymous codons. This sequence, made up mostly of pollen cone ESTs, represented a class of genes identical to a loblolly pine CCR gene (Acc. No. AY064169). A subfamily II CCR was assembled from shoot tip and pollen cone ESTs. The alignment of the subfamily II CCR ESTs contained 73% of the sites displaying alternative codons, two-thirds involving synonymous codons.

Cinnamyl alcohol dehydrogenase genes in loblolly pine were also constituted into two major classes, differing in 38% of the sites. The subfamily I CAD sequence contained ESTs from compression and side wood, and had less than 2% of the sites diplaying codon variants. This sequence was identical to the loblolly pine CAD gene (Acc. No. PTCADBMR). The subfamily II CAD was comparatively more variable, having one third of the positions containing more than one possible codon, half involving synonymous codons. This sequence was mainly composed of ESTs from xylem planing wood, side wood, and compression wood.

Coevolution of CCR and CAD gene families

Classification of EST data from other plant species showed that the two-subfamily structure of CAD and CCR is widespread in plants (Figure 4). Although the topology is affected by the nature of data (i.e., ESTs, consensus sequences), and the inherent differential evolutionary rate of the progenitor genes, each of the subfamilies grouped sequences consistent with their taxonomic position (e.g., leguminosae: *Lotus, Medicago, Glycine*; gramineae: Hordeum, *Sorghum, Zea, Oryza, Triticum*; solananeae: *Lycopersicon, Solanum*).

DISCUSSION

The appropriateness of the bioinformatic approach

The bioinformatics approach used in this study obtained phylogenetic and informatics knowledge from a known system (e.g., annotated genes) to model or classify an uncharacterized system (e.g., ESTs). The exhaustive compilation of non-redundant sequences of a gene yield enough data to resolve differences at the subfamily level. The ability to resolve subfamilies is dependent upon their degree of divergence and representation in the database. The delineation of subfamilies here was carried out using robust phylogenetic methods that establish the relationship among the gene sequences. Bootstrapping provided a confidence estimate for the tree topology, and furnished a statistical support for the reliability of the subfamily clusters. Gu's θ quantified the divergence level between subfamilies and provided a model to test the null hypothesis (Ho: $\theta = 0$) that two subfamilies do not differ. If the

Ho is rejected it can be interpreted as an evidence of diversification of subfamilies. In contrast, failure to reject the Ho is not evidence that the subfamilies compared accomplish the same function. Functional differences may lie, nevertheless, at the regulatory region of the genes (Bonifer 2000). This means that the expression patterns may differ substantially whereas the biochemical role remains unchanged as proposed by the subfunctionalization hypothesis of Lynch and Conery (2000).

The use of known sequences from a variety of organisms provided a broad overview of the sequence features of the gene family in seed plants. The signature positions were not affected by exclusion of any single sequence, suggesting that the signatures are not affected much by sampling of sequences in the database. Therefore, signatures clearly defined a minimal set of positions for subfamily identification. The effectiveness of the scaffold alignment to provide information on the subfamily structure of a gene depends upon the representation of diverse subfamilies and the number of sequences in each subfamily.

The EST data obtained by the tBLASTn searches of the dbEST were screened and trimmed prior to analysis. The screening procedure based on principal component analysis ensured that the ESTs used had comparable length, bit score and percentage identity. The screened ESTs were trimmed by eye based on the expected translation of the sequence and comparison with consensus sequences from alignments. The genetic code was effectively used not only as a data reduction technique but also to increase the signal-to-noise ratio in the analysis, and to associate DNA sequences with their functionally relevant gene product. The clustering and

alignment of ESTs produced by this method represented the sequence of a specific subfamily.

4-Coumarate:Coenzyme A Ligase

Loblolly pine 4CL ESTs belonged to subfamily I. Analyses failed to find any evidence of transcripts belonging to subfamily II. Despite the low bootstrap support and coefficient of divergence, annotation of the sequences found in these clusters showed that they participate in distinct cellular contexts, e.g. flavonoid or monolignol biosynthesis (Allina et al. 1998, Ehlting et al. 1999, Hu et al. 1998). The high level of sequence identity of the 4CL ESTs to the known *4CL* gene in pine showed that the genes do not vary much at the coding region level. Experimental results also showed that loblolly pine appears to contain contain only one class of 4CL (Voo 1995). Zhang and Chiang (1997) found in loblolly pine two three-intron containing 4CL genomic sequences with identical coding region, but with slight difference in the intron 3 sequence. This difference may reflect allelic variation, and their functional contexts remain to be elucidated. Active 4CL isoforms with distinct capacities to convert different substituted 4-hydroxycinnamates have been reported in soybean, petunia and pea (Allina et al. 1998, Stuible and Kombrink 2001). One 4CL isoform belonging to subfamily II in *Arabidopsis thaliana* has been associated with flavonoid formation (*At4CL3*) whereas two others (*At4CL1* and *At4CL2*) belonging to subfamily I are probably involved in lignin production and in metabolic routes leading to the biosynthesis of phenolic compounds other than flavonoids (Ehlting et al. 1999).

Soybean 4CL cDNAs encoding *Gm4CL1* and *Gm4CL3/4*, belonging to subfamily I and II, respectively, were differentially affected after elicitor treatment of soybean cell cultures with a β-glucan elicitor of *Phytophtora sojae*, revealing the down regulation of *Gm4CL1* versus up-regulation of *Gm4CL3/4* transcripts (Lindermayr et al. 2002).

Cinnamoyl-Coenzyme A Reductase

The two seed plant cinnamoyl-CoA reductase subfamilies were represented in the population of expressed genes in loblolly pine. CCR genes have been reported in distinct metabolic contexts in other plants (e.g. development or defense response). There are two distinct subfamilies of CCR represented in both maize (Pinchon et al. 1998) and *Arabidopsis* (Lauvergeat et al. 2001). The maize CCR genes, *ZmCCR1* and *ZmCCR2*, belong to subfamily I and II, respectively. They are 64% identical to each other at the amino acid level, and differ in tissue expression. Northern blot assays showed that *ZmCCR1* was involved in lignification in the stalk whereas the role of *ZmCCR2* was expressed only in roots and at a low level (Pinchon et al. 1998). The characterization of the *Arabidopsis* genes *AtCCR1* and *AtCCR2* (81% identity at the amino acid level) has provided evidence for concluding that they serve different physiological roles despite the fact that both belong to subfamily I (Lauvergeat et al. 2001). Biochemical and *in vivo* expression analyses provided evidence that *AtCCR1* is associated with lignin biosynthesis during development. *AtCCR2* is strongly induced during the incompatible reaction with *Xanthomonas campestris* pv. *campestris* but not in lignifying tissue, suggesting a role for this enzyme in defense

response in *Arabidopsis*. In cell suspension cultures of *Picea abies*, fungal elicitor induced both lignification and a transient increase of CCR activity (Messner and Boll 1993).

Cinnamyl alcohol dehydrogenase

Two distinct cinnamyl alcohol dehydrogenase subfamilies were represented in the loblolly pine ESTs. One belongs to subfamily I, whose role in monolignol biosynthesis is well established (MacKay et al. 1997). The other belongs to subfamily II, represented by the pathogen-stress responsive ELI3 and sinapyl alcohol dehydrogenase (SAD). Subfamilies I and II encode enzymes with similar structure and catalytic mechanism but differ in substrate specificity and expression patterns. The expression of *Eli3* homologs in *Arabidopsis* and tomato has been related to the presence of a resistance genes in these species. *Eli3* mRNA rapidly accumulates in plants having a dominant resistance allele (*RPM1* in Arabidopsis, *AvrPto* in tomato), whereas it has a laggard expression level in the presence of recessive alleles (Kiedrowski et al. 1992, R. Thilmony and G. Martin, pers. comm.). Differences have also been observed with regard to cell type. In alfalfa, the class II-gene, *MsaCad1*, was expressed most actively in stem and floral tissue, whereas *MsaCad2* (class I) was expressed in stem, hypocotyl and root tissue (Brill et al. 1999).

Both CCR and CAD were previously identified and characterized in the context of the formation of lignified vascular tissue during development. However, their expression also occurs in the context of defense response during pathogen attack. In loblolly

pine, cinnamyl alcohol dehydrogenase activity was found in differenting xylem, megagametophyte tissues (O'Malley et al. 1992), and in pollen pine cone (Table 4). The function of CAD activity in non-lignifying tissue is still unknown. The CAD family could support a diversity of functions in plants not related with lignification (Lacombe et al. 1997). Coniferaldehyde and coniferyl alcohol function as phytoalexins in the incompatible interaction between flax and *Melampsora lini* (Keen and Littlefield 1979). Studies have provided experimental evidence concerning the possible involvement of monolignols in oat epidermal cell defense against penetration by appressoria of *Erysiphe graminis* f.sp. *avenae* (Carver et al. 1994) and in *Pinus sylvestris* as a means to control fungal infection by *Ceratocystis bruneociliata* (Daurade-Le Vagueresse et al. 2001). Further research is needed to elucidate the metabolic context (e.g. constitutive, defense) of the distinct members of the gene family.

Coevolution of gene families

The subfamily structure found in CCR and CAD are widespread in plants (Figure 4). The results of analyses made on EST-derived contigs from a number of different plant species show that CCR and CAD are separated into two distinct classes in a number of plants, and that each may have followed distinct patterns of differentiation. In land plants, lignification is a constitutive process carried out in secondary wall of lignifying tissue. Furthermore, induced lignification is one of several plant defense responses to wounding and to pathogen attack. Therefore, the major diversification of these gene

families could be due to the diversification of the pathway into a constitutive role and into a defense response mechanism (Lange et al. 1995).

Genes encoding enzymes involved in sequential chemical transformations could be subject to a common genetic regulation (Finnegan 2001). In addition, the molecular interaction between enzymes (e.g. in enzyme complexes) suggests that changes in their sequences could occur in a coordinated manner (Fryxell et al. 1996). The production of monolignols could involve the formation of enzyme complexes in the endoplasmatic reticulum to facilitate the passage of phenylpropanoid metabolites from the active site of one enzyme to the active site of another enzyme (Dixon et al. 2001).

Finally, this comprehensive study of organization of *4CL, CCR* and *CAD* genes in seed plants provides a basis for genetic and biochemical studies on functional divergence in phenylpropanoid gene families. The isozymes encoded by the different subfamilies of genes in the phenylpropanoid pathway adds new complexity to interpretation of the metabolic network leading to the biosynthesis of hydroxycinnamic alcohols (Dixon et al. 2001). In plants, isozymes of these enzymes may combine to produce versatile routes supplying products for specific metabolic pools.

LITERATURE CITED

Allina, S.M., Pri-Hadash, A., Theilmann, D.A., Ellis, B.E., and Douglas, C.J. 1998. 4-Coumarate:coenzyme A ligase in hybrid poplar. Properties of native enzymes, cDNA cloning, and analysis of recombinant enzymes. Plant Physiol. 116:743-754.

Bonifer, C. 2000. Developmental regulation of eukaryotic gene loci. TIG 16:310-315.

Boudet, A.M. 1998a. A new view of lignification. Trends Plant Sci. 3:67-71.

Boudet, A.M., Goffner, D., Marque, C. and Grima-Pettenati, J. 1998b. Genes involved in the final steps of monolignol biosythesis and their manipulation for tailoring new lignins. In: S. Sakanen, N. Lewis (editors) Biosynthesis of lignins and lignans. ACS Symp. Series 697:865-875.

Brill, E.M., Abrahams, S., Hayes, C.M., Jenkins, C.L., and Watson, J.M. (1999) Molecular characterization and expression of a wound-inducible cDNA encoding a novel cinnamyl alcohol dehydrogenase enzyme in lucerne. Plant Mol. Biol. 41:279-291.

Carver, T.L.W., Zeyen, R.J., Robbins, M.P., Vance, C.P., and Boyles, D.A. 1994. Suppression of host cinnamyl alcohol dehydrogenase and phenylalanine ammonia lyase increases oat epidermal cell susceptibility to powdery mildew penetration. Physiol. Mol. Plant Pathol. 44:243-259.

Chabannes, M; Barakate, A; Lapierre, C; Marita, J M; Ralph, J; Pean, M; Danoun, S; Halpin, C; Grima-Pettenati, J; and Boudet, A. M. 2001. Strong decrease in lignin content without significant alteration of plant development is induced by simultaneous down-regulation of cinnamoyl CoA reductase (CCR) and cinnamyl alcohol dehydrogenase (CAD) in tobacco plants. Plant J. 28:257-270.

Darade-Le Vagueresse, M.H., Romiti, C., Grosclaude, C., and Bounias, M. 2001. Coevolutionary toxicity as suggested by differential coniferyl alcohol inhibition of ceratocystis species growth. Toxicon 39:203-208.

Dixon, R.A., Chen, F., Guo, D. and Parvathi, K. 2001. The biosynthesis of monolignols: a “metabolic grid”, or independent pathways to guaiacyl and syringyl units? Phytochemistry 57:1069-1084.

Ehlting, J., Büttner, D., Wang, Q., Douglas, C.J., Somssich, I.E., and Kombrink, E. 1999. Three 4-coumarate:coenzyme A ligases in *Arabidopsis thaliana* represent two evolutionarily divergent classes in angiosperms. Plant J. 19:9-20.

Ewing, B. and Green, P. 1998. Base-Calling of Automated Sequencer Traces Using PHRED. II. Error Probabilities. Genome Res. 8:186-194

Ewing, B., Hillier, L., Wendl, M.C., and Green, P. 1998. Base-calling of automated sequencer traces using PHRED. I. Accuracy assessment. Genome Res. 8:175-185.

Felsenstein, J. 1985. Confidence limits on phylogenies: an approach using the bootstrap. Evolution 39:783-791.

Finnegan, E.J. 2001. Is plant gene expression regulated globally?. Trends Genet. 17:361-365.

Fryxell, K.J. 1996. The coevolution of gene family trees. Trends Genet. 12:364-369.

Grima-Pettenati, J., Campargue, C., Boudet, A., and Boudet, A.M. 1994. Purification and characterization of cinnamyl alcohol dehydrogenase isoforms from *Phaseolus vulgaris*. Phytochemistry 37:941-947.

Gu, X. (1999) Statistical methods for testing functional divergence after gene duplication. Mol. Biol. Evol. 16:1664-1674.

Jolliffe, I. T. 1986. Principal component analysis. Springer series in statistics. Springer-Verlag, New York, 271 p.

Jones, L., Ennos, A.R., and Turner, S.R. 2001. Cloning and characterization of *irregular xyelm (irx4*): a severly lignin-deficient mutant of Arabidopsis. Plant J. 26:205-216.

Jung, H.G. and Vogel, K.P. 1986. Influence of lignin on digestibility of forage cell wall material. J. Anim. Sci. 62:1703-1712.

Kajita, S., Hishiyama, S., Tomimura, Y., Katayama, Y., and Omori, S. 1997. Structural characterization of modified lignin in transgenic tobacco plants in which the activity of 4-coumarate:coenzyme A ligase is depressed. Plant Physiol. 114:871-879.

Keen, N.T. and Littlefield, L.J. 1979. The possible association of phytoalexins with resistance gene expression in flax to *Melampsora lini*. Physiol. Plant Pathol. 14:265-280.

Kiedrowski, S. Kawalleck, P., Halbrock, K., Somssich, I.E. and Dangl, J.L. (1992) Rapid activation of a novel plant defense gene is strictly dependent on the *Arabidopsis RPM1* disease resistance locus. EMBO J. 11:4677-4684.

Knobloch, K.H. and Hahlbrock, K. 1975. Isoenzymes of p-coumarate:CoA ligase from cell suspension cultures of Glycine max. Eur. J. Biochem. 52:311-320.

Kumar, S.,Tamura, K., Jakobsen, I.B., and Nei, M. (2001) MEGA2: molecular evolutionary genetics analysis software. Bioinformatics 2001 17: 1244-1245.

Lacombe, E., Hawkins, S., Van Doorsselaere, J., Piquemal, J., Goffner, D., Poeydomenge, O., Boudet, A.M., and Grima-Pettenati, J. 1997. Cinnamoyl CoA reductase, the first committed enzyme of the lignin branch biosynthetic pathway: cloning, expression and phylogenetic relationships. Plant J. 11:429-441.

Lange, B.M., Lapierre, C., and Sandermann, H. 1995. Elicitor-induced spruce stress lignin. Plant Physiol. 108:1277-1287.

Lauvergeat, V., Lacomme, C., Lacombe, E., Lasserre, E., Roby, D., and Grima-Pettenati, J. 2001.Two cinnamoyl-CoA reductase (CCR) genes from *Arabidopsis thaliana* are differentially expressed during development and in response to infection with pathogenic bacteria. Phytochemistry 57:1187-1195.

Li, L., Cheng, X.F., Leshkevich, J., Umezawa, T., Harding, S.A. and Chiang, V.L. 2001. The last step of syringyl monolignol biosynthesis in angiosperms is regulated by a novel gene encoding sinapyl alcohol dehydrogenase. Plant Cell. 13:1567-1586.

Lindermayr, C., Mollers, B., Fliegmann, J., Uhlmann, A., Lottspeich, F., Meimberg, H., Ebel, J. 2002. Divergent members of a soybean (*Glycine max* L.) 4-coumarate: coenzyme A ligase gene family. Eur. J. Biochem. 269:1304-15.

Logeman, E., Reinold, S., Somssich, I.E. and Hahlbrock, K. 1997. A novel type of pathogen defense-related cinnamyl alcohol dehydrogenase. Biol. Chem. 378:909-913.

Lynch, M., and Conery, J,S. 2000. The evolutionary fate and consequences of duplicate genes. Science 290:1151-1155.

MacKay, J.J., Liu, W., Whetten, R., Sederoff, R.R. and O'Malley, D.M. 1995a. Genetic analysis of cinnamyl alcohol dehydrogenase in loblolly pine: single gene inheritance, molecular characterization and evolution. Mol. Gen. Genet. 247:537-545.

MacKay, J.J., O'Malley, D.M., Presnell, T., Booker, F.L., Campbell, M.M., Whetten, R.W. and Sederoff, R.R. 1997b. Inheritance, gene expression, and lignin characterization in a mutant pine deficient in cinnamyl alcohol dehydrogenase. PNAS 94:8255-8260.

Messner, B. and Boll, M. 1993. Elicitor-mediated induction of enzymes of lignin biosynthesis and formation of lignin-like material in cell suspension cultures of spruce (*Picea abies*). Plant Cell Tissue Organ Culture 34:261-269.

Mirny, L.A. and Gefland, M.S. (2002) Using orthologous and paralogous proteins to identify specificty determining residues. Genome Biology 3:preprint0002.1-0002.20.

O'Malley, D., Porter, S. and Sederoff, R.R. 1992. Purification, characterization and cloning of cinnamyl alcohol dehydrogenase in loblolly pine (*Pinus taeda* L.) Plant Physiol. 98:1364-1371.

Pinchon, M., Courbou, I., Beckert, M., Boudet, A.M., and Grima-Pettenati, J. 1998. Cloning and characterization of two maize cDNAs encoding cinnamoyl-CoA reductase (CCR) and differential expression of the corresponding genes. Plant Mol. Biol. 38:671-676.

Piquemal, J., Lapierre, C., Myton, K., O'Connell, A., Schuch, W., Grima-Pettenati, J., and Boudet, A.M. 1998. Down-regulation of cinnamoyl-CoA reductases induces significant changes of lignin profiles in trangenic tobacco plants. Plant J. 13:71-83.

Ralph, J., Hatfield, R.D., Piquemal, J., Yahiahoui, N., Pean, M., Lapierre, C., and Boudet, A.M. NMR characterization of altered lignins extracted from tobacco plants down-regulated for lignification enzymes cinnamyl alcohol dehydrogenase and cinnamyl-CoA reductase. PNAS 95:12803-12808.

Russell, W.R., Provan, G.J., Burkitt, M.J., and Chesson, A. 2000. Extent of incorporation of hydroxycinnamaldehydes into lignin in cinnamyl alcohol dehydrogenase-down regulated plants. J. Biotech. 79:73-85.

Saitou, N. and Nei, M. 1987. The neighbor-joining method: a new method for reconstructing phylogenetic trees. Mol. Biol. Evol. 4:406-425.

Sambrook, J., Fritsch, E.F. and Maniatis, T. 1989. Molecular cloning: a laboratory manual. 2nd edition. Cold Spring Harbor, N.Y.

Sneath, P.H.A. and Sokal, R.R. 1973. Numerical Taxonomy. Freeman, San Francisco.

Stuible, H. P., Kombrink, E. 2001 Identification of the substrate specificity-conferring amino acids residues of 4-coumarate:coenzyme A ligase allows the rational design of mutant enzymes with new catalytic properties. J. Biol. Chem. 276:26893-26897.

Thompson, J.D., Higgins D.G. and Gibson T.J. (1994) CLUSTAL W: improving the sensitivity of progressive multiple sequence alignment through sequence weighting, position-specific gap penalties and weight matrix choice. Nucleic Acids Res. 22:4673-4680.

Voo, K.S., Whetten, R.W., O'Malley, D.M., Sederoff, R.R. 1995. 4-coumarate:coenzyme A ligase from loblolly pine xylem. Isolation, characterization, and complementary DNA cloning. Plant Physiol. 108:85-97.

Zhang, X.H., and Chiang, V.L. 1997. Molecular cloning of 4-coumarate:coenzyme A ligase in loblolly pine and the roles of thyis enzyme in the biosynthesis of lignin in compression wood. Plant Physiol. 113:65-74.

CHAPTER 4

TABLES AND FIGURES

Table 1. Divergence between clusters of sequences within the 4CL, CCR and CAD gene families

Gene	α			Θ	SE(Θ)	LRT(Θ)	$P[\chi_1^2 > LRT(\Theta)]$	p-Distance		
	Overall	Class I	Class II					Overall	Class I	Class II
4CL	0.76	0.47	0.58	0.03	0.037855	0.835	0.3607	0.33	0.25	0.36
CCR	1.83	0.62	0.83	0.28	0.076463	14.344	0.0002	0.42	0.28	0.56
CAD	0.60	0.31	0.45	0.39	0.038494	79.859	0.0000	0.30	0.22	0.33

Θ, Coefficient of divergence
α, Gamma parameter alpha of the distribution of replacement rates
p-Distance is the proportion of amino acid positions different

Table 2. Correlation analysis and principal component analysis of EST features

A. Correlation analysis

	4CL		CCR		CAD	
	Bit score	Identity	Bit score	Identity	Bit score	Identity
Identity	0.6852		0.4560		0.8696	
Length	0.3257	-0.2136	-0.1077	-0.3079	0.0115	-0.2695

B. Principal component analysis

Component	Eigenvalue	Proportion	Cumulative	Eigenvectors			Pattern Matrix		
				Bit score	Identity	Length	Bit score	Identity	Length
4CL									
1	1.6958	0.5653	0.5653	0.7263	0.6744	0.1329	0.9458	0.8782	0.1731
2	1.1600	0.3867	0.9520	0.1917	-0.3844	0.9030	0.2064	-0.4141	0.9726
CCR									
1	1.6037	0.5346	0.5346	0.5883	0.6730	-0.4482	0.7451	0.8523	-0.5676
2	0.9007	0.3002	0.8348	0.5462	0.0780	0.8340	0.5184	0.0740	0.7915
CAD									
1	1.9071	0.6357	0.6357	0.6764	0.7083	-0.2018	0.9341	0.9782	-0.2787
2	1.0065	0.3355	0.9712	0.2959	-0.0105	0.9552	0.2969	-0.0105	0.9583

Eigenvalue give the variance of a linear function of variables as defined by the principal component.
Eigenvector define a linear function of the variables with a particular property or characteristic of the EST, namely, bit score, indentity or length.

Table 3. P-Distance between genes and EST-derived sequences assembled for CCR and CAD. Top number indicates comparison with gene, bottom number show comparison to protein. In parenthesis are the standard erors calculated by a bootstrap method involving 10000 pseudosamples. (CCR gene Acc. No 17978648, CCR protein Acc. No 17978649, CAD gene Acc. No 558386, CAD protein Acc. No 558387)

	CCR	CCR subfamily I
CCR subfamily I	0.00000 0.00000	
CCR subfamily II	0.44479 (0.02694) 0.44654 (0.02688)	0.44479 (0.02680) 0.44654 (0.02682)

	CAD	CAD subfamily I
CAD subfamily I	0.00000 0.00000	
CAD subfamily II	0.38553 (0.01513) 0.38554 (0.02595)	0.38353 (0.01507) 0.38554 (0.02563)

Table 4. cDNA library representation of *Pinus taeda* EST clones in different contigs for 4CL, CCR and CAD. (Size of each library is also shown)

Contig	NXRV	NXLV	NXPV	NXSI	NXCI	NXNV	Pine TriplEx		Loblolly Pine		PtIFG2	
Pine Class							Pollen Cone	Shoot Tip	C	NA		
Lambda	2257	5220	4844	8342	7169	4488	1507	5642	774		Zap 1277	3592
4CL												
I	0	0	7	11	32	15	1	2	2	1	3	4
CCR												
I	1	0	0	0	1	2	5	1	0	0	0	0
II	0	0	1	3	2	0	4	8	0	0	0	0
CAD												
I	2	2	2	8	9	4	1	0	1	0	1	0
II	1	0	4	2	4	4	0	3	0	0	2	1

NXRV=xylem root wood vertical, The library is from primary xylem scraped from the roots of a twelve year old tree in the transitional phase from juvenile wood to mature wood production. **NXLV**=xylem late wood vertical, The library is from late (summer-August) wood, taken from below the crown of a 20 year old tree. The harvested xylem tissue was on the the cusp between transitional and mature wood. **NXPV**=xylem planings wood vertical, The library is from early (spring) secondary wood, taken from a ten year old tree in the transitional phase. The tree is a kind gift of the Westvaco Corporation. Secondary xylem was harvested from the tree by peeling back the bark and primary xylem and then removing the underlying tissue with a block plane. **NXSI**=xylem side wood inclined, The library is from early (spring) wood, taken from three six-year old trees (three different genotypes), in the juvenile phase. These trees were induced to form side wood by bending to a 45 degree angle and tying them to the ground. Differentiating xylem was harvested from the sides of the inclined stems, and a mixture of all three genotypes was used for the library. **NXCI**=xylem compression wood inclined, The library is from early (spring) wood, taken from three six-year old trees (three different genotypes), in the juvenile phase. These trees were induced to form compression wood by bending to a 45 degree angle and tying them to the ground. Differentiating xylem was harvested from the bottoms of the inclined stems, and a mixture of all three genotypes was used for the library. **NXNV**=Xylem normal wood vertical. **Pine Triplex pollen cone**, Immature pollen cones were collected in the early spring, frozen and used for mRNA isolation. **Pine TriplEx shoot tips**, Shoot tips (approx. 2 cm from apex) were collected during the spring, frozen and used for mRNA isolation. **Loblolly pine C**, The library was made from immature xylem from the underside of inclined stems of differentiating wood. A mixture of four genotypes were used. **Loblolly pine NA**, The result of subtraction of library N with library C. Immature xylem from the side of inclined stems of differentiating wood was subtracted with immature xylem from underside of inclined stems of differentiating compression wood. **PtIFG2**, The tissue source for this library is xylem. The xylem tissue was harvested in spring and summer from branches of seed orchard trees which are clones of the same genotype. Branches were 4-6 inches in diameter. **Pine Lambda Zap xylem**, Differentiating xylem was collected from the main stem of a 35-year old loblolly pine tree harvested during the growing season.

Figure 1. The monolignol biosynthetic pathway. The general phenylpropanoid pathway involves a minimum of three enzymatic steps, catalyzed by the actions of phenylalanine ammonia-lyase (PAL), cinnamate 4-hydroxylase (C4H), and 4-coumarate:coenzyme A ligase (4CL). The formation of CoA thiol esters of 4-coumarate and other hydroxycinnamates by 4CL serve as substrates for entry into various branchways. Activated acids, namely *p*-Hydroxycinnamoyl CoA esters, enter the monolignol biosynthetic pathway by undergoing two successive reductive steps. The first carried out by cinnamoyl-CoA reductase (CCR) which catalyzes the NADPH-dependent reduction of *p*-Hydroxycinnamoyl CoA esters to *p*-Hydroxycinnamaldehydes. This product is taken by cinnamyl alcohol dehydrogenase (CAD) to produce the *p*-Hydroxycinnamic alcohols or monolignols (viz. *p*-coumaryl, coniferyl, and sinapyl alcohol). Notice the diversity of phenylpropanoid metabolites that each enzyme can take as a substrate. Not all metabolites are present in all plant groups.

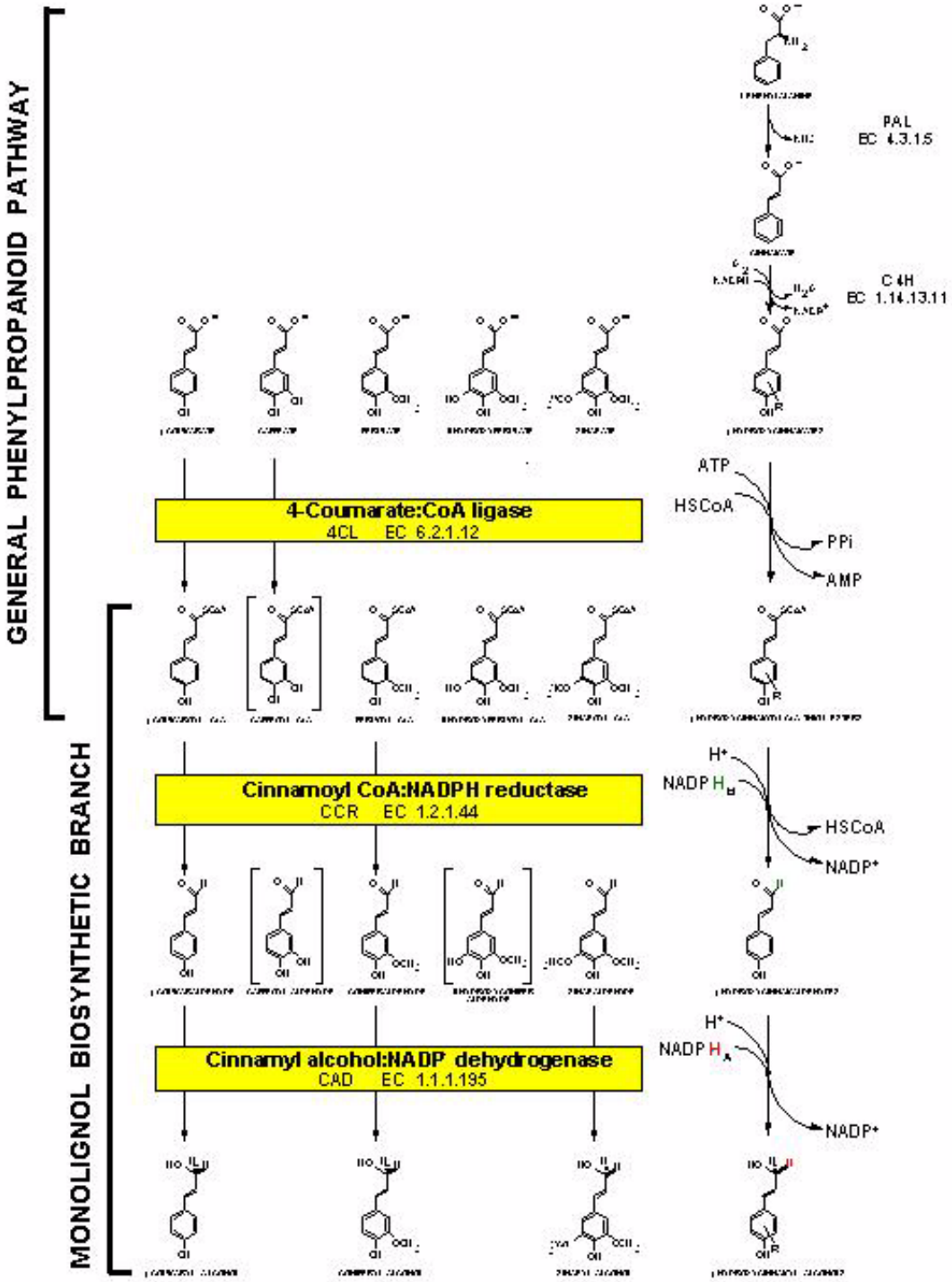

GENERAL PHENYLPROPANOID PATHWAY
MONOLIGNOL BIOSYNTHETIC BRANCH
PAL
EC 4.3.1.5
C4H
EC 1.14.13.11
4-Coumarate:CoA ligase
4CL EC 6.2.1.12
ATP
HSCoA
PPi
AMP
Cinnamoyl CoA:NADPH reductase
CCR EC 1.2.1.44
H+
NADPH
HSCoA
NADP+
Cinnamyl alcohol:NADP dehydrogenase
CAD EC 1.1.1.195
H+
NADPH
NADP+

Figure 2. Sequential steps taken to assemble *Pinus taeda* ESTs into subfamilies based upon the family structure of the gene. Database searches create two separate lists, one of nucleotide sequences of the gene (Entrez search), another of EST nucleotide sequences with similarity to a protein product from one of the canonical sequences of the gene (tBLASTn). Gene sequences are translated and the gene products aligned, guiding the subsequent alignment of codons (Scaffold). The tree clusters the sequences into groups that are used as a surrogate for gene family structure. Position-specific statistics provide a means to determine those sites that are relevant discriminators of the clusters. On the other hand, the list of EST nucleotide sequences contained each EST sequenced translated and aligned to the protein query. In the same way, we associate the codons to each amino acid residue for each of the ESTs. The next step is the alignment of the ESTs onto the scaffold. The assembly of EST sequences into subfamilies is guided by those signature positions.

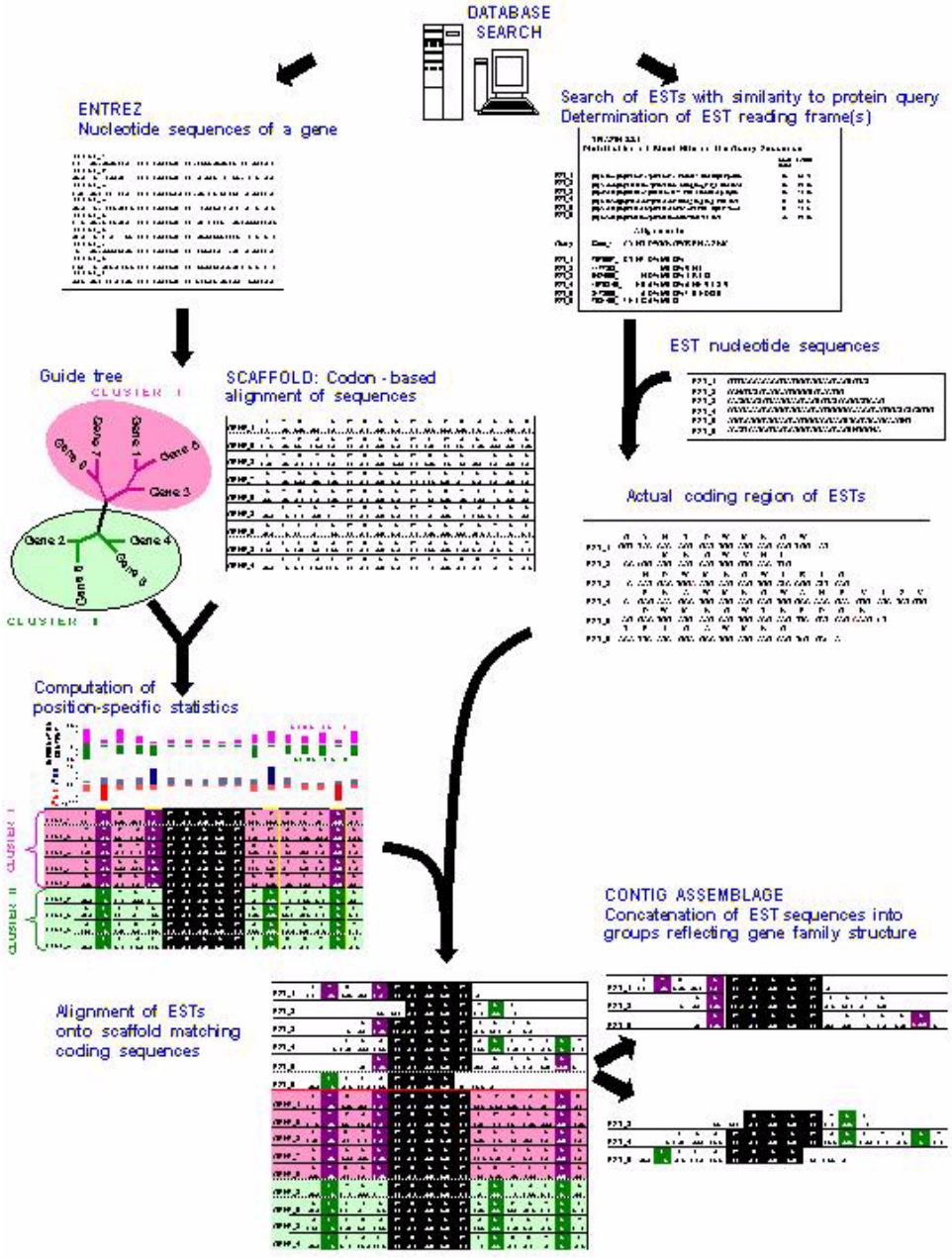

DATABASE
SEARCH
ENTREZ
Nucleotide sequences of a gene
Search of ESTs with similarity to protein query
Determination of EST reading frame(s)
EST nucleotide sequences
Guide tree
SCAFFOLD: Codon - based
alignment of sequences
Actual coding region of ESTs
Computation of
position-specific statistics
CONTIG ASSEMBLAGE
Concatenation of EST sequences into
groups reflecting gene family structure
Alignment of ESTs
onto scaffold matching
coding sequences

Figure 3. Hypothesis of relationship among 4CL, CCR and CAD sequences. Relationship between the unrooted topology was determined using a neighbor-joining method based on the Kimura distances. Numbers indicate the percent occurrence of that cluster in 10^4 bootstrap pseudosamples. The position of consensus sequences for 4CL, CCR, and CAD are shown. (A) 4-Coumarate:coenzyme A ligase reveals two large, distinct classes, Class I and Class II. Class I in Arabidopsis, poplar, and soybean are more associated with biosynthesis of lignins and other phenylpropanoids whereas class II 4CLs have been generally associated with flavonoid biosynthesis. (B) CCR shows two distinct subfamilies. Sequences belonging to subfamily I are related to the production of monolignols for lignin biosynthesis. Subfamily II contain sequences mostly related to CCR based on similarity. (C) CAD contain two subfamilies. Subfamily I has sequences involved in lignin biosynthesis during development. Subfamily II are ELI3-related proteins, mostly known by their involvement to pathogen stress resistance.

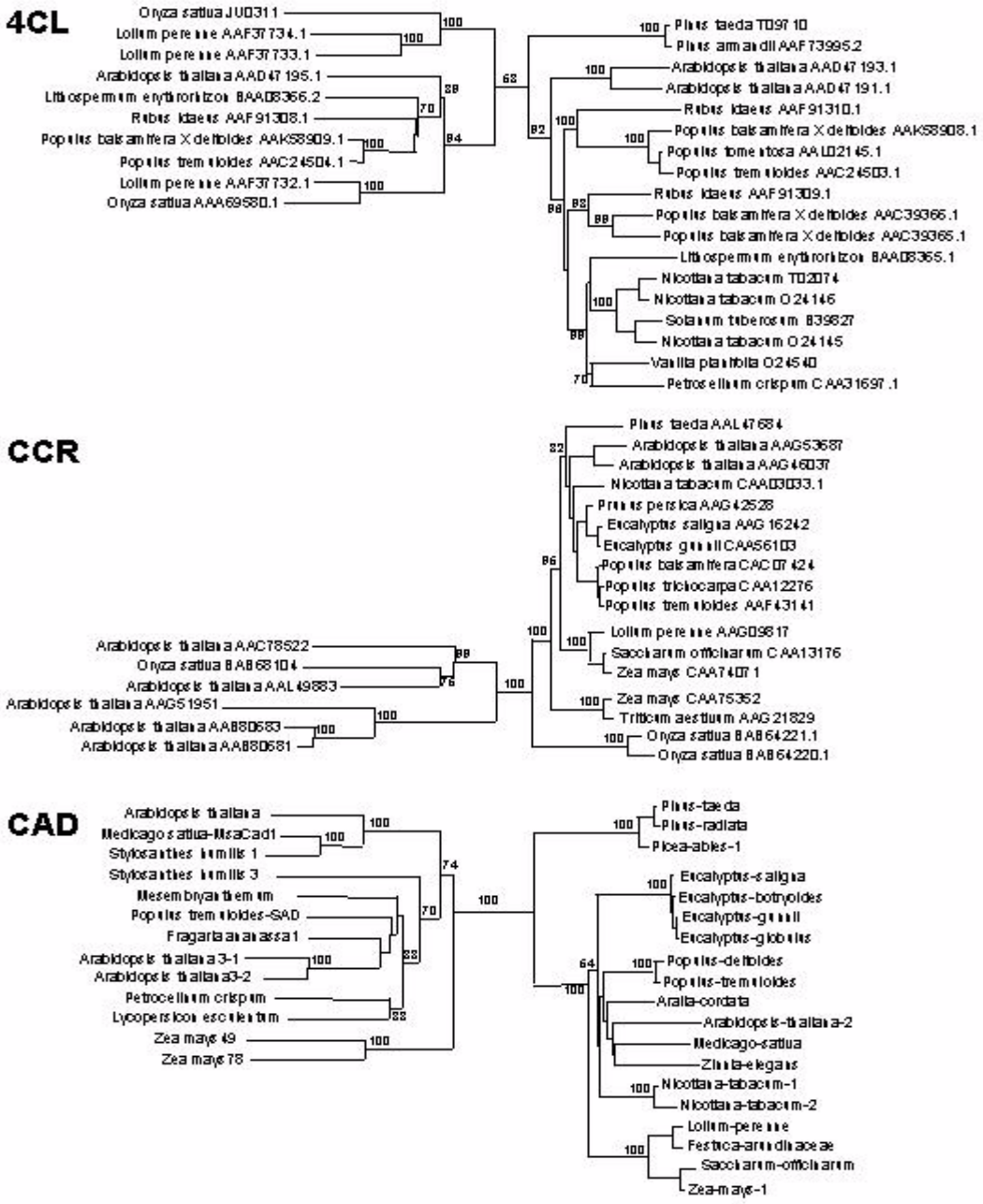
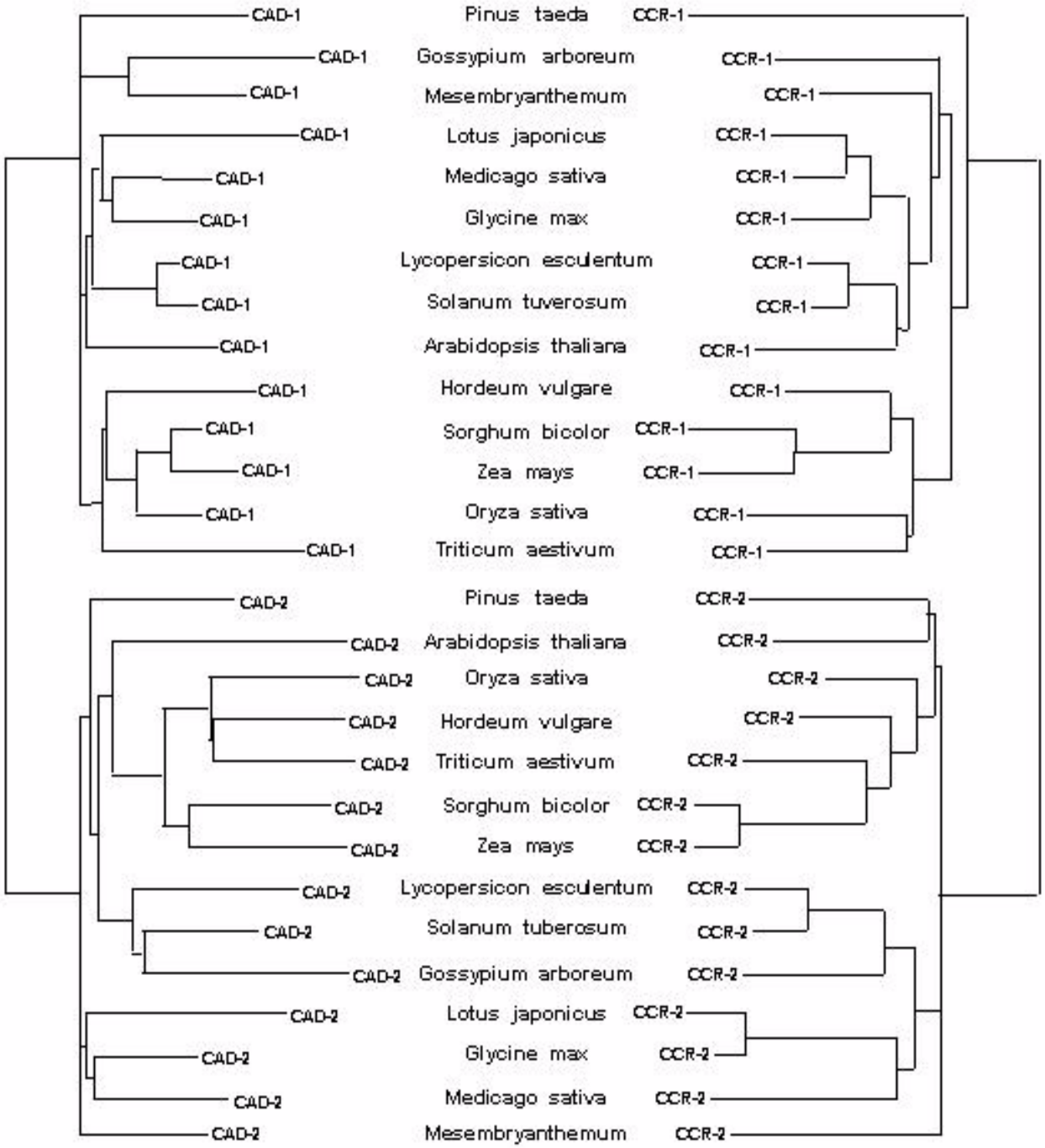

4CL
Oryza sativa JU0311
Lolium perenne AAF37734.1
Lolium perenne AAF37733.1
Arabidopsis thaliana AAD47195.1
Lithospermum erythrorhizon BAA08366.2
Ribes idaeus AAF91308.1
Populus balsamifera X deltoides AAK58909.1
Populus tremuloides AAC24504.1
Lolium perenne AAF37732.1
Oryza sativa AAA69580.1
Pinus taeda T09710
Pinus armandii AAF73995.2
Arabidopsis thaliana AAD47193.1
Arabidopsis thaliana AAD47191.1
Ribes idaeus AAF91310.1
Populus balsamifera X deltoides AAK58908.1
Populus tomentosa AAL02145.1
Populus tremuloides AAC24503.1
Ribes idaeus AAF91309.1
Populus balsamifera X deltoides AAC39366.1
Populus balsamifera X deltoides AAC39365.1
Lithospermum erythrorhizon BAA08365.1
Nicotiana tabacum T02074
Nicotiana tabacum O24146
Solanum tuberosum B39827
Nicotiana tabacum O24145
Vanilla planifolia O24540
Petroselinum crispum CAA31697.1
CCR
Pinus taeda AAL47684
Arabidopsis thaliana AAG53687
Arabidopsis thaliana AAG46037
Nicotiana tabacum CAA03033.1
Prunus persica AAG42528
Eucalyptus saligna AAG16242
Eucalyptus gunnii CAA56103
Populus balsamifera CAC07424
Populus trichocarpa CAA12276
Populus tremuloides AAF43141
Arabidopsis thaliana AAC78522
Oryza sativa BAB68104
Arabidopsis thaliana AAL49883
Arabidopsis thaliana AAG51951
Arabidopsis thaliana AAB80683
Arabidopsis thaliana AAB80681
Lolium perenne AAG09817
Saccharum officinarum CAA13176
Zea mays CAA74071
Zea mays CAA75352
Triticum aestivum AAG21829
Oryza sativa BAB64221.1
Oryza sativa BAB64220.1
CAD
Arabidopsis thaliana
Medicago sativa-MsaCad1
Stylosanthes humilis 1
Stylosanthes humilis 3
Mesembryanthemum
Populus tremuloides-SAD
Fragaria ananassa1
Arabidopsis thaliana 3-1
Arabidopsis thaliana3-2
Petroselinum crispum
Lycopersicon esculentum
Zea mays 49
Zea mays 78
Pinus-taeda
Pinus-radiata
Picea-abies-1
Eucalyptus-saligna
Eucalyptus-botryoides
Eucalyptus-gunnii
Eucalyptus-globulus
Populus-deltoides
Populus-tremuloides
Aralia-cordata
Arabidopsis-thaliana-2
Medicago-sativa
Zinnia-elegans
Nicotiana-tabacum-1
Nicotiana-tabacum-2
Lolium-perenne
Festuca-arundinaceae
Saccharum-officinarum
Zea-mays-1

Figure 4. Analysis of the cinnamyl alcohol dehydrogenase (*CAD*) and coumaroyl:CoA reductase (*CCR*) genes in plants. All sequences are assembled from EST data, and were characterized using discriminant signature positions. These signature positions were derived from the alignment of CAD and CCR genes, respectively.


CAD-1
Pinus taeda
CCR-1
CAD-1
Gossypium arboreum
CCR-1
CAD-1
Mesembryanthemum
CCR-1
CAD-1
Lotus japonicus
CCR-1
CAD-1
Medicago sativa
CCR-1
CAD-1
Glycine max
CCR-1
CAD-1
Lycopersicon esculentum
CCR-1
CAD-1
Solanum tuverosum
CCR-1
CAD-1
Arabidopsis thaliana
CCR-1
CAD-1
Hordeum vulgare
CCR-1
CAD-1
Sorghum bicolor
CCR-1
CAD-1
Zea mays
CCR-1
CAD-1
Oryza sativa
CCR-1
CAD-1
Triticum aestivum
CCR-1
CAD-2
Pinus taeda
CCR-2
CAD-2
Arabidopsis thaliana
CCR-2
CAD-2
Oryza sativa
CCR-2
CAD-2
Hordeum vulgare
CCR-2
CAD-2
Triticum aestivum
CCR-2
CAD-2
Sorghum bicolor
CCR-2
CAD-2
Zea mays
CCR-2
CAD-2
Lycopersicon esculentum
CCR-2
CAD-2
Solanum tuberosum
CCR-2
CAD-2
Gossypium arboreum
CCR-2
CAD-2
Lotus japonicus
CCR-2
CAD-2
Glycine max
CCR-2
CAD-2
Medicago sativa
CCR-2
CAD-2
Mesembryanthemum
CCR-2
0.1

Appendices

Appendix 1. PDB files of the structural model for *Pinus taeda* 4CL, CCR and CAD proteins.

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Pinus taeda 4-Coumarate:Coenzyme A ligase

REMARK       4CL  Pinus taeda  molecular  model
REMARK       4CL PINE COMPLIES WITH FORMAT V. 2.0, 23-MAY-2002
ATOM     78  N   LEU    11      28.839 100.842  53.683  1.00  0.00           N
ATOM     79  CA  LEU    11      28.373 100.271  52.460  1.00  0.00           C
ATOM     80  CB  LEU    11      28.387 101.318  51.316  1.00  0.00           C
ATOM     81  CG  LEU    11      27.604 100.979  50.021  1.00  0.00           C
ATOM     82  CD2 LEU    11      26.227 100.403  50.379  1.00  0.00           C
ATOM     83  CD1 LEU    11      28.359 100.079  49.030  1.00  0.00           C
ATOM     84  C   LEU    11      29.356  99.174  52.197  1.00  0.00           C
ATOM     85  O   LEU    11      29.641  98.808  51.063  1.00  0.00           O
ATOM     86  N   TYR    12      29.906  98.586  53.272  1.00  0.00           N
ATOM     87  CA  TYR    12      30.749  97.447  53.086  1.00  0.00           C
ATOM     88  CB  TYR    12      31.847  97.414  54.176  1.00  0.00           C
ATOM     89  CG  TYR    12      32.645  96.152  54.159  1.00  0.00           C
ATOM     90  CD1 TYR    12      33.617  95.919  53.214  1.00  0.00           C
ATOM     91  CD2 TYR    12      32.422  95.203  55.130  1.00  0.00           C
ATOM     92  CE1 TYR    12      34.341  94.748  53.234  1.00  0.00           C
ATOM     93  CE2 TYR    12      33.139  94.032  55.156  1.00  0.00           C
ATOM     94  CZ  TYR    12      34.102  93.803  54.205  1.00  0.00           C
ATOM     95  OH  TYR    12      34.839  92.601  54.233  1.00  0.00           O
ATOM     96  C   TYR    12      29.770  96.337  53.298  1.00  0.00           C
ATOM     97  O   TYR    12      30.148  95.201  53.594  1.00  0.00           O
ATOM     98  N   ARG    13      28.459  96.642  53.071  1.00  0.00           N
ATOM     99  CA  ARG    13      27.527  95.581  53.253  1.00  0.00           C
ATOM    100  CB  ARG    13      26.056  95.977  53.076  1.00  0.00           C
ATOM    101  CG  ARG    13      25.510  96.770  54.264  1.00  0.00           C
ATOM    102  CD  ARG    13      25.423  95.949  55.555  1.00  0.00           C
ATOM    103  NE  ARG    13      24.482  94.817  55.314  1.00  0.00           N
ATOM    104  CZ  ARG    13      24.952  93.615  54.868  1.00  0.00           C
ATOM    105  NH1 ARG    13      26.291  93.426  54.686  1.00  0.00           N
ATOM    106  NH2 ARG    13      24.081  92.595  54.613  1.00  0.00           N
ATOM    107  C   ARG    13      27.867  94.549  52.237  1.00  0.00           C
ATOM    108  O   ARG    13      27.827  93.346  52.498  1.00  0.00           O
ATOM    109  N   SER    14      28.294  95.016  51.054  1.00  0.00           N
ATOM    110  CA  SER    14      28.480  94.105  49.974  1.00  0.00           C
ATOM    111  CB  SER    14      28.124  94.752  48.630  1.00  0.00           C
ATOM    112  OG  SER    14      28.914  95.913  48.415  1.00  0.00           O
ATOM    113  C   SER    14      29.883  93.630  49.858  1.00  0.00           C
ATOM    114  O   SER    14      30.706  94.224  49.167  1.00  0.00           O
ATOM    115  N   LYS    15      30.209  92.514  50.524  1.00  0.00           N
ATOM    116  CA  LYS    15      31.477  91.951  50.205  1.00  0.00           C
ATOM    117  CB  LYS    15      32.599  92.271  51.208  1.00  0.00           C
ATOM    118  CG  LYS    15      33.949  91.701  50.764  1.00  0.00           C
ATOM    119  CD  LYS    15      35.155  92.305  51.484  1.00  0.00           C
ATOM    120  CE  LYS    15      36.496  91.723  51.030  1.00  0.00           C
ATOM    121  NZ  LYS    15      37.605  92.362  51.774  1.00  0.00           N
ATOM    122  C   LYS    15      31.289  90.479  50.197  1.00  0.00           C
ATOM    123  O   LYS    15      31.598  89.804  51.176  1.00  0.00           O
ATOM    124  N   LEU    16      30.743  89.927  49.097  1.00  0.00           N
ATOM    125  CA  LEU    16      30.650  88.499  49.082  1.00  0.00           C
ATOM    126  CB  LEU    16      29.290  87.937  49.527  1.00  0.00           C
ATOM    127  CG  LEU    16      28.134  88.226  48.554  1.00  0.00           C
ATOM    128  CD2 LEU    16      28.022  89.726  48.237  1.00  0.00           C
ATOM    129  CD1 LEU    16      26.825  87.625  49.082  1.00  0.00           C
ATOM    130  C   LEU    16      30.890  88.030  47.687  1.00  0.00           C
ATOM    131  O   LEU    16      30.187  88.395  46.746  1.00  0.00           O
ATOM    132  N   PRO    17      31.898  87.224  47.541  1.00  0.00           N
ATOM    133  CA  PRO    17      32.175  86.668  46.247  1.00  0.00           C
ATOM    134  CD  PRO    17      33.108  87.391  48.326  1.00  0.00           C
ATOM    135  CB  PRO    17      33.653  86.270  46.254  1.00  0.00           C
ATOM    136  CG  PRO    17      34.077  86.360  47.731  1.00  0.00           C
ATOM    137  C   PRO    17      31.234  85.534  46.000  1.00  0.00           C
ATOM    138  O   PRO    17      30.761  84.935  46.965  1.00  0.00           O
ATOM    139  N   ASP    18      30.946  85.233  44.720  1.00  0.00           N
ATOM    140  CA  ASP    18      30.050  84.163  44.385  1.00  0.00           C
ATOM    141  CB  ASP    18      29.201  84.477  43.137  1.00  0.00           C
ATOM    142  CG  ASP    18      28.023  83.514  43.054  1.00  0.00           C
ATOM    143  OD1 ASP    18      28.252  82.276  43.019  1.00  0.00           O
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ATOM    144  OD2 ASP    18      26.867  84.014  43.007  1.00  0.00           O
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ATOM    146  O   ASP    18      32.010  83.045  43.630  1.00  0.00           O
ATOM    147  N   ILE    19      30.367  81.763  44.472  1.00  0.00           N
ATOM    148  CA  ILE    19      31.070  80.545  44.199  1.00  0.00           C
ATOM    149  CB  ILE    19      30.463  79.353  44.892  1.00  0.00           C
ATOM    150  CG2 ILE    19      29.010  79.179  44.420  1.00  0.00           C
ATOM    151  CG1 ILE    19      31.351  78.114  44.693  1.00  0.00           C
ATOM    152  CD1 ILE    19      30.970  76.939  45.593  1.00  0.00           C
ATOM    153  C   ILE    19      31.076  80.281  42.719  1.00  0.00           C
ATOM    154  O   ILE    19      32.098  79.908  42.146  1.00  0.00           O
ATOM    155  N   GLU    20      29.907  80.473  42.080  1.00  0.00           N
ATOM    156  CA  GLU    20      29.606  80.160  40.710  1.00  0.00           C
ATOM    157  CB  GLU    20      28.096  80.179  40.416  1.00  0.00           C
ATOM    158  CG  GLU    20      27.753  79.685  39.009  1.00  0.00           C
ATOM    159  CD  GLU    20      26.239  79.696  38.856  1.00  0.00           C
ATOM    160  OE1 GLU    20      25.550  79.164  39.766  1.00  0.00           O
ATOM    161  OE2 GLU    20      25.753  80.239  37.829  1.00  0.00           O
ATOM    162  C   GLU    20      30.259  81.044  39.693  1.00  0.00           C
ATOM    163  O   GLU    20      30.521  80.575  38.593  1.00  0.00           O
ATOM    164  N   ILE    21      30.492  82.338  39.977  1.00  0.00           N
ATOM    165  CA  ILE    21      31.056  83.222  38.991  1.00  0.00           C
ATOM    166  CB  ILE    21      32.326  82.717  38.370  1.00  0.00           C
ATOM    167  CG2 ILE    21      32.705  83.670  37.224  1.00  0.00           C
ATOM    168  CG1 ILE    21      33.423  82.571  39.438  1.00  0.00           C
ATOM    169  CD1 ILE    21      34.652  81.805  38.950  1.00  0.00           C
ATOM    170  C   ILE    21      30.050  83.436  37.901  1.00  0.00           C
ATOM    171  O   ILE    21      29.505  82.500  37.321  1.00  0.00           O
ATOM    172  N   SER    22      29.772  84.714  37.588  1.00  0.00           N
ATOM    173  CA  SER    22      28.804  84.981  36.572  1.00  0.00           C
ATOM    174  CB  SER    22      28.442  86.470  36.442  1.00  0.00           C
ATOM    175  OG  SER    22      27.476  86.650  35.417  1.00  0.00           O
ATOM    176  C   SER    22      29.396  84.538  35.276  1.00  0.00           C
ATOM    177  O   SER    22      30.602  84.648  35.058  1.00  0.00           O
ATOM    178  N   ASP    23      28.545  83.995  34.386  1.00  0.00           N
ATOM    179  CA  ASP    23      29.012  83.555  33.106  1.00  0.00           C
ATOM    180  CB  ASP    23      28.403  82.220  32.650  1.00  0.00           C
ATOM    181  CG  ASP    23      28.963  81.122  33.540  1.00  0.00           C
ATOM    182  OD1 ASP    23      29.954  81.398  34.268  1.00  0.00           O
ATOM    183  OD2 ASP    23      28.406  79.992  33.508  1.00  0.00           O
ATOM    184  C   ASP    23      28.587  84.600  32.124  1.00  0.00           C
ATOM    185  O   ASP    23      27.559  85.245  32.316  1.00  0.00           O
ATOM    186  N   HIS    24      29.371  84.816  31.050  1.00  0.00           N
ATOM    187  CA  HIS    24      28.988  85.829  30.107  1.00  0.00           C
ATOM    188  ND1 HIS    24      31.919  86.943  31.306  1.00  0.00           N
ATOM    189  CG  HIS    24      30.925  87.420  30.481  1.00  0.00           C
ATOM    190  NE2 HIS    24      31.697  89.107  31.766  1.00  0.00           N
ATOM    191  CD2 HIS    24      30.802  88.743  30.775  1.00  0.00           C
ATOM    192  CE1 HIS    24      32.345  87.993  32.053  1.00  0.00           C
ATOM    193  CB  HIS    24      30.179  86.581  29.487  1.00  0.00           C
ATOM    194  C   HIS    24      28.251  85.172  28.992  1.00  0.00           C
ATOM    195  O   HIS    24      28.853  84.606  28.084  1.00  0.00           O
ATOM    196  N   LEU    25      26.910  85.211  29.057  1.00  0.00           N
ATOM    197  CA  LEU    25      26.061  84.638  28.058  1.00  0.00           C
ATOM    198  CB  LEU    25      25.875  83.112  28.198  1.00  0.00           C
ATOM    199  CG  LEU    25      27.124  82.226  28.009  1.00  0.00           C
ATOM    200  CD2 LEU    25      28.057  82.246  29.230  1.00  0.00           C
ATOM    201  CD1 LEU    25      27.813  82.500  26.662  1.00  0.00           C
ATOM    202  C   LEU    25      24.715  85.234  28.326  1.00  0.00           C
ATOM    203  O   LEU    25      24.493  85.802  29.393  1.00  0.00           O
ATOM    204  N   PRO    26      23.818  85.154  27.386  1.00  0.00           N
ATOM    205  CA  PRO    26      22.483  85.604  27.659  1.00  0.00           C
ATOM    206  CD  PRO    26      24.182  85.393  26.002  1.00  0.00           C
ATOM    207  CB  PRO    26      21.823  85.865  26.299  1.00  0.00           C
ATOM    208  CG  PRO    26      22.838  85.337  25.264  1.00  0.00           C
ATOM    209  C   PRO    26      21.827  84.556  28.505  1.00  0.00           C
ATOM    210  O   PRO    26      22.385  83.468  28.644  1.00  0.00           O
ATOM    211  N   LEU    27      20.663  84.866  29.103  1.00  0.00           N
ATOM    212  CA  LEU    27      19.977  83.930  29.951  1.00  0.00           C
ATOM    213  CB  LEU    27      18.656  84.541  30.482  1.00  0.00           C
ATOM    214  CG  LEU    27      17.709  83.643  31.320  1.00  0.00           C
ATOM    215  CD2 LEU    27      18.392  83.088  32.576  1.00  0.00           C
ATOM    216  CD1 LEU    27      17.029  82.550  30.476  1.00  0.00           C
ATOM    217  C   LEU    27      19.638  82.726  29.136  1.00  0.00           C
ATOM    218  O   LEU    27      19.832  81.589  29.563  1.00  0.00           O
ATOM    219  N   HIS    28      19.123  82.932  27.918  1.00  0.00           N
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ATOM    220  CA  HIS    28      18.718  81.780  27.175  1.00  0.00           C
ATOM    221  ND1 HIS    28      19.761  82.128  24.150  1.00  0.00           N
ATOM    222  CG  HIS    28      18.943  82.779  25.028  1.00  0.00           C
ATOM    223  NE2 HIS    28      20.381  84.256  24.158  1.00  0.00           N
ATOM    224  CD2 HIS    28      19.323  84.077  25.020  1.00  0.00           C
ATOM    225  CE1 HIS    28      20.609  83.052  23.660  1.00  0.00           C
ATOM    226  CB  HIS    28      17.993  82.071  25.896  1.00  0.00           C
ATOM    227  C   HIS    28      19.895  80.960  26.766  1.00  0.00           C
ATOM    228  O   HIS    28      19.756  79.751  26.605  1.00  0.00           O
ATOM    229  N   SER    29      21.058  81.591  26.499  1.00  0.00           N
ATOM    230  CA  SER    29      22.180  80.830  26.049  1.00  0.00           C
ATOM    231  CB  SER    29      23.335  81.710  25.561  1.00  0.00           C
ATOM    232  OG  SER    29      23.682  82.631  26.577  1.00  0.00           O
ATOM    233  C   SER    29      22.638  79.964  27.168  1.00  0.00           C
ATOM    234  O   SER    29      22.978  78.797  26.975  1.00  0.00           O
ATOM    235  N   TYR    30      22.634  80.517  28.389  1.00  0.00           N
ATOM    236  CA  TYR    30      23.078  79.742  29.507  1.00  0.00           C
ATOM    237  CB  TYR    30      23.126  80.548  30.812  1.00  0.00           C
ATOM    238  CG  TYR    30      23.742  79.698  31.868  1.00  0.00           C
ATOM    239  CD1 TYR    30      25.109  79.678  32.029  1.00  0.00           C
ATOM    240  CD2 TYR    30      22.963  78.922  32.694  1.00  0.00           C
ATOM    241  CE1 TYR    30      25.688  78.900  33.003  1.00  0.00           C
ATOM    242  CE2 TYR    30      23.537  78.142  33.670  1.00  0.00           C
ATOM    243  CZ  TYR    30      24.901  78.131  33.825  1.00  0.00           C
ATOM    244  OH  TYR    30      25.495  77.333  34.827  1.00  0.00           O
ATOM    245  C   TYR    30      22.115  78.607  29.690  1.00  0.00           C
ATOM    246  O   TYR    30      22.521  77.479  29.965  1.00  0.00           O
ATOM    247  N   CYS    31      20.805  78.888  29.552  1.00  0.00           N
ATOM    248  CA  CYS    31      19.793  77.886  29.737  1.00  0.00           C
ATOM    249  CB  CYS    31      18.365  78.448  29.643  1.00  0.00           C
ATOM    250  SG  CYS    31      17.972  79.593  30.997  1.00  0.00           S
ATOM    251  C   CYS    31      19.905  76.832  28.683  1.00  0.00           C
ATOM    252  O   CYS    31      19.820  75.642  28.981  1.00  0.00           O
ATOM    253  N   PHE    32      20.113  77.222  27.411  1.00  0.00           N
ATOM    254  CA  PHE    32      20.096  76.182  26.425  1.00  0.00           C
ATOM    255  CB  PHE    32      20.135  76.613  24.939  1.00  0.00           C
ATOM    256  CG  PHE    32      21.500  77.033  24.513  1.00  0.00           C
ATOM    257  CD1 PHE    32      22.423  76.100  24.096  1.00  0.00           C
ATOM    258  CD2 PHE    32      21.856  78.354  24.511  1.00  0.00           C
ATOM    259  CE1 PHE    32      23.681  76.484  23.698  1.00  0.00           C
ATOM    260  CE2 PHE    32      23.112  78.749  24.114  1.00  0.00           C
ATOM    261  CZ  PHE    32      24.031  77.811  23.708  1.00  0.00           C
ATOM    262  C   PHE    32      21.251  75.271  26.669  1.00  0.00           C
ATOM    263  O   PHE    32      21.132  74.058  26.508  1.00  0.00           O
ATOM    264  N   GLU    33      22.410  75.830  27.059  1.00  0.00           N
ATOM    265  CA  GLU    33      23.569  75.007  27.241  1.00  0.00           C
ATOM    266  CB  GLU    33      24.802  75.821  27.669  1.00  0.00           C
ATOM    267  CG  GLU    33      25.289  76.790  26.589  1.00  0.00           C
ATOM    268  CD  GLU    33      26.503  77.533  27.128  1.00  0.00           C
ATOM    269  OE1 GLU    33      26.867  77.293  28.310  1.00  0.00           O
ATOM    270  OE2 GLU    33      27.081  78.352  26.365  1.00  0.00           O
ATOM    271  C   GLU    33      23.297  73.995  28.308  1.00  0.00           C
ATOM    272  O   GLU    33      23.579  72.810  28.132  1.00  0.00           O
ATOM    273  N   ARG    34      22.725  74.429  29.444  1.00  0.00           N
ATOM    274  CA  ARG    34      22.491  73.512  30.522  1.00  0.00           C
ATOM    275  CB  ARG    34      21.969  74.195  31.797  1.00  0.00           C
ATOM    276  CG  ARG    34      23.066  74.936  32.561  1.00  0.00           C
ATOM    277  CD  ARG    34      24.002  73.986  33.313  1.00  0.00           C
ATOM    278  NE  ARG    34      25.057  74.807  33.969  1.00  0.00           N
ATOM    279  CZ  ARG    34      25.938  74.218  34.828  1.00  0.00           C
ATOM    280  NH1 ARG    34      25.846  72.882  35.091  1.00  0.00           N
ATOM    281  NH2 ARG    34      26.915  74.964  35.423  1.00  0.00           N
ATOM    282  C   ARG    34      21.495  72.466  30.126  1.00  0.00           C
ATOM    283  O   ARG    34      21.721  71.278  30.351  1.00  0.00           O
ATOM    284  N   VAL    35      20.378  72.876  29.496  1.00  0.00           N
ATOM    285  CA  VAL    35      19.320  71.961  29.166  1.00  0.00           C
ATOM    286  CB  VAL    35      18.090  72.617  28.609  1.00  0.00           C
ATOM    287  CG1 VAL    35      17.456  73.486  29.705  1.00  0.00           C
ATOM    288  CG2 VAL    35      18.476  73.394  27.344  1.00  0.00           C
ATOM    289  C   VAL    35      19.777  70.943  28.171  1.00  0.00           C
ATOM    290  O   VAL    35      19.348  69.792  28.218  1.00  0.00           O
ATOM    291  N   ALA    36      20.644  71.338  27.226  1.00  0.00           N
ATOM    292  CA  ALA    36      21.072  70.420  26.213  1.00  0.00           C
ATOM    293  CB  ALA    36      22.038  71.061  25.201  1.00  0.00           C
ATOM    294  C   ALA    36      21.790  69.274  26.856  1.00  0.00           C
ATOM    295  O   ALA    36      21.609  68.122  26.464  1.00  0.00           O
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ATOM    296  N   GLU    37      22.630  69.560  27.866  1.00  0.00           N
ATOM    297  CA  GLU    37      23.412  68.536  28.500  1.00  0.00           C
ATOM    298  CB  GLU    37      24.376  69.098  29.559  1.00  0.00           C
ATOM    299  CG  GLU    37      25.491  69.964  28.970  1.00  0.00           C
ATOM    300  CD  GLU    37      26.446  69.053  28.213  1.00  0.00           C
ATOM    301  OE1 GLU    37      26.731  67.938  28.726  1.00  0.00           O
ATOM    302  OE2 GLU    37      26.899  69.457  27.109  1.00  0.00           O
ATOM    303  C   GLU    37      22.509  67.565  29.191  1.00  0.00           C
ATOM    304  O   GLU    37      22.703  66.353  29.102  1.00  0.00           O
ATOM    305  N   PHE    38      21.491  68.083  29.897  1.00  0.00           N
ATOM    306  CA  PHE    38      20.578  67.267  30.639  1.00  0.00           C
ATOM    307  CB  PHE    38      19.597  68.069  31.510  1.00  0.00           C
ATOM    308  CG  PHE    38      20.395  68.750  32.566  1.00  0.00           C
ATOM    309  CD1 PHE    38      20.964  68.025  33.588  1.00  0.00           C
ATOM    310  CD2 PHE    38      20.557  70.115  32.546  1.00  0.00           C
ATOM    311  CE1 PHE    38      21.699  68.654  34.565  1.00  0.00           C
ATOM    312  CE2 PHE    38      21.290  70.748  33.520  1.00  0.00           C
ATOM    313  CZ  PHE    38      21.866  70.017  34.531  1.00  0.00           C
ATOM    314  C   PHE    38      19.772  66.456  29.693  1.00  0.00           C
ATOM    315  O   PHE    38      19.473  65.308  29.984  1.00  0.00           O
ATOM    316  N   ALA    39      19.421  67.040  28.535  1.00  0.00           N
ATOM    317  CA  ALA    39      18.593  66.482  27.501  1.00  0.00           C
ATOM    318  CB  ALA    39      18.411  67.428  26.304  1.00  0.00           C
ATOM    319  C   ALA    39      19.198  65.217  26.978  1.00  0.00           C
ATOM    320  O   ALA    39      18.494  64.377  26.421  1.00  0.00           O
ATOM    321  N   ASP    40      20.531  65.078  27.018  1.00  0.00           N
ATOM    322  CA  ASP    40      21.054  63.827  26.551  1.00  0.00           C
ATOM    323  CB  ASP    40      22.592  63.806  26.537  1.00  0.00           C
ATOM    324  CG  ASP    40      23.065  64.788  25.476  1.00  0.00           C
ATOM    325  OD1 ASP    40      22.206  65.270  24.691  1.00  0.00           O
ATOM    326  OD2 ASP    40      24.292  65.073  25.439  1.00  0.00           O
ATOM    327  C   ASP    40      20.597  62.705  27.459  1.00  0.00           C
ATOM    328  O   ASP    40      20.057  61.701  26.999  1.00  0.00           O
ATOM    329  N   ARG    41      20.845  62.852  28.778  1.00  0.00           N
ATOM    330  CA  ARG    41      20.549  61.923  29.852  1.00  0.00           C
ATOM    331  CB  ARG    41      21.475  62.134  31.062  1.00  0.00           C
ATOM    332  CG  ARG    41      21.383  63.535  31.673  1.00  0.00           C
ATOM    333  CD  ARG    41      20.102  63.785  32.473  1.00  0.00           C
ATOM    334  NE  ARG    41      20.371  63.386  33.885  1.00  0.00           N
ATOM    335  CZ  ARG    41      20.139  62.106  34.296  1.00  0.00           C
ATOM    336  NH1 ARG    41      19.657  61.181  33.416  1.00  0.00           N
ATOM    337  NH2 ARG    41      20.388  61.750  35.590  1.00  0.00           N
ATOM    338  C   ARG    41      19.132  61.938  30.387  1.00  0.00           C
ATOM    339  O   ARG    41      18.654  60.968  30.958  1.00  0.00           O
ATOM    340  N   PRO    42      18.429  62.988  30.224  1.00  0.00           N
ATOM    341  CA  PRO    42      17.306  63.254  31.062  1.00  0.00           C
ATOM    342  CD  PRO    42      17.974  63.204  28.880  1.00  0.00           C
ATOM    343  CB  PRO    42      16.744  64.546  30.496  1.00  0.00           C
ATOM    344  CG  PRO    42      16.997  64.384  28.984  1.00  0.00           C
ATOM    345  C   PRO    42      16.236  62.237  31.183  1.00  0.00           C
ATOM    346  O   PRO    42      15.703  61.762  30.181  1.00  0.00           O
ATOM    347  N   CYS    43      15.923  61.926  32.446  1.00  0.00           N
ATOM    348  CA  CYS    43      14.778  61.186  32.829  1.00  0.00           C
ATOM    349  CB  CYS    43      15.117  59.918  33.631  1.00  0.00           C
ATOM    350  SG  CYS    43      15.977  60.291  35.188  1.00  0.00           S
ATOM    351  C   CYS    43      14.151  62.159  33.773  1.00  0.00           C
ATOM    352  O   CYS    43      13.233  61.824  34.517  1.00  0.00           O
ATOM    353  N   LEU    44      14.658  63.417  33.740  1.00  0.00           N
ATOM    354  CA  LEU    44      14.211  64.449  34.645  1.00  0.00           C
ATOM    355  CB  LEU    44      15.200  65.616  34.790  1.00  0.00           C
ATOM    356  CG  LEU    44      16.557  65.203  35.387  1.00  0.00           C
ATOM    357  CD2 LEU    44      17.283  64.195  34.480  1.00  0.00           C
ATOM    358  CD1 LEU    44      16.406  64.708  36.833  1.00  0.00           C
ATOM    359  C   LEU    44      12.882  65.007  34.197  1.00  0.00           C
ATOM    360  O   LEU    44      12.725  65.277  33.007  1.00  0.00           O
ATOM    361  N   ILE    45      11.929  65.241  35.158  1.00  0.00           N
ATOM    362  CA  ILE    45      10.539  65.596  34.859  1.00  0.00           C
ATOM    363  CB  ILE    45       9.707  64.374  34.622  1.00  0.00           C
ATOM    364  CG2 ILE    45      10.272  63.684  33.369  1.00  0.00           C
ATOM    365  CG1 ILE    45       9.668  63.447  35.855  1.00  0.00           C
ATOM    366  CD1 ILE    45       8.801  63.932  37.018  1.00  0.00           C
ATOM    367  C   ILE    45       9.802  66.468  35.920  1.00  0.00           C
ATOM    368  O   ILE    45      10.494  67.150  36.680  1.00  0.00           O
ATOM    369  N   ASP    46       8.386  66.510  35.900  1.00  0.00           N
ATOM    370  CA  ASP    46       7.370  67.208  36.753  1.00  0.00           C
ATOM    371  CB  ASP    46       6.953  68.572  36.171  1.00  0.00           C
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ATOM    372  CG  ASP    46       5.992  69.258  37.133  1.00  0.00           C
ATOM    373  OD1 ASP    46       5.997  68.898  38.339  1.00  0.00           O
ATOM    374  OD2 ASP    46       5.239  70.156  36.670  1.00  0.00           O
ATOM    375  C   ASP    46       6.057  66.395  36.875  1.00  0.00           C
ATOM    376  O   ASP    46       5.723  65.690  35.928  1.00  0.00           O
ATOM    377  N   GLY    47       5.254  66.416  38.006  1.00  0.00           N
ATOM    378  CA  GLY    47       3.987  65.699  37.865  1.00  0.00           C
ATOM    379  C   GLY    47       3.028  65.594  39.053  1.00  0.00           C
ATOM    380  O   GLY    47       3.260  64.839  39.998  1.00  0.00           O
ATOM    381  N   ALA    48       1.913  66.383  39.037  1.00  0.00           N
ATOM    382  CA  ALA    48       0.745  66.195  39.880  1.00  0.00           C
ATOM    383  CB  ALA    48      -0.204  67.405  39.856  1.00  0.00           C
ATOM    384  C   ALA    48       0.012  65.034  39.302  1.00  0.00           C
ATOM    385  O   ALA    48      -0.456  64.128  39.990  1.00  0.00           O
ATOM    386  N   THR    49      -0.091  65.087  37.964  1.00  0.00           N
ATOM    387  CA  THR    49      -0.686  64.116  37.103  1.00  0.00           C
ATOM    388  CB  THR    49      -0.855  64.618  35.698  1.00  0.00           C
ATOM    389  OG1 THR    49      -1.485  63.630  34.895  1.00  0.00           O
ATOM    390  CG2 THR    49       0.522  64.987  35.124  1.00  0.00           C
ATOM    391  C   THR    49       0.253  62.964  37.096  1.00  0.00           C
ATOM    392  O   THR    49      -0.117  61.836  36.777  1.00  0.00           O
ATOM    393  N   ASP    50       1.516  63.244  37.467  1.00  0.00           N
ATOM    394  CA  ASP    50       2.547  62.259  37.432  1.00  0.00           C
ATOM    395  CB  ASP    50       2.133  60.911  38.049  1.00  0.00           C
ATOM    396  CG  ASP    50       1.977  61.103  39.551  1.00  0.00           C
ATOM    397  OD1 ASP    50       2.272  62.228  40.037  1.00  0.00           O
ATOM    398  OD2 ASP    50       1.565  60.127  40.232  1.00  0.00           O
ATOM    399  C   ASP    50       2.872  62.026  35.996  1.00  0.00           C
ATOM    400  O   ASP    50       3.418  60.986  35.629  1.00  0.00           O
ATOM    401  N   ARG    51       2.550  63.022  35.149  1.00  0.00           N
ATOM    402  CA  ARG    51       2.916  62.965  33.768  1.00  0.00           C
ATOM    403  CB  ARG    51       1.930  63.689  32.837  1.00  0.00           C
ATOM    404  CG  ARG    51       0.554  63.021  32.786  1.00  0.00           C
ATOM    405  CD  ARG    51      -0.447  63.726  31.868  1.00  0.00           C
ATOM    406  NE  ARG    51      -1.721  62.956  31.929  1.00  0.00           N
ATOM    407  CZ  ARG    51      -2.881  63.512  31.472  1.00  0.00           C
ATOM    408  NH1 ARG    51      -2.876  64.778  30.960  1.00  0.00           N
ATOM    409  NH2 ARG    51      -4.045  62.801  31.526  1.00  0.00           N
ATOM    410  C   ARG    51       4.211  63.689  33.719  1.00  0.00           C
ATOM    411  O   ARG    51       4.277  64.877  34.026  1.00  0.00           O
ATOM    412  N   THR    52       5.279  62.991  33.301  1.00  0.00           N
ATOM    413  CA  THR    52       6.590  63.546  33.428  1.00  0.00           C
ATOM    414  CB  THR    52       7.584  62.503  33.841  1.00  0.00           C
ATOM    415  OG1 THR    52       7.678  61.495  32.844  1.00  0.00           O
ATOM    416  CG2 THR    52       7.126  61.888  35.174  1.00  0.00           C
ATOM    417  C   THR    52       7.052  64.098  32.122  1.00  0.00           C
ATOM    418  O   THR    52       6.743  63.565  31.056  1.00  0.00           O
ATOM    419  N   TYR    53       7.786  65.229  32.200  1.00  0.00           N
ATOM    420  CA  TYR    53       8.382  65.833  31.049  1.00  0.00           C
ATOM    421  CB  TYR    53       7.860  67.245  30.754  1.00  0.00           C
ATOM    422  CG  TYR    53       6.458  67.062  30.288  1.00  0.00           C
ATOM    423  CD1 TYR    53       5.452  66.769  31.180  1.00  0.00           C
ATOM    424  CD2 TYR    53       6.147  67.184  28.952  1.00  0.00           C
ATOM    425  CE1 TYR    53       4.158  66.599  30.747  1.00  0.00           C
ATOM    426  CE2 TYR    53       4.855  67.015  28.513  1.00  0.00           C
ATOM    427  CZ  TYR    53       3.859  66.722  29.411  1.00  0.00           C
ATOM    428  OH  TYR    53       2.532  66.549  28.963  1.00  0.00           O
ATOM    429  C   TYR    53       9.849  65.891  31.302  1.00  0.00           C
ATOM    430  O   TYR    53      10.329  66.479  32.270  1.00  0.00           O
ATOM    431  N   CYS    54      10.579  65.252  30.385  1.00  0.00           N
ATOM    432  CA  CYS    54      11.987  65.029  30.379  1.00  0.00           C
ATOM    433  CB  CYS    54      12.239  63.896  29.382  1.00  0.00           C
ATOM    434  SG  CYS    54      13.956  63.642  28.946  1.00  0.00           S
ATOM    435  C   CYS    54      12.711  66.273  29.954  1.00  0.00           C
ATOM    436  O   CYS    54      12.135  67.150  29.314  1.00  0.00           O
ATOM    437  N   PHE    55      14.006  66.392  30.333  1.00  0.00           N
ATOM    438  CA  PHE    55      14.788  67.506  29.868  1.00  0.00           C
ATOM    439  CB  PHE    55      16.242  67.576  30.375  1.00  0.00           C
ATOM    440  CG  PHE    55      16.283  68.310  31.669  1.00  0.00           C
ATOM    441  CD1 PHE    55      16.030  67.675  32.859  1.00  0.00           C
ATOM    442  CD2 PHE    55      16.590  69.651  31.682  1.00  0.00           C
ATOM    443  CE1 PHE    55      16.076  68.368  34.046  1.00  0.00           C
ATOM    444  CE2 PHE    55      16.637  70.351  32.865  1.00  0.00           C
ATOM    445  CZ  PHE    55      16.378  69.709  34.052  1.00  0.00           C
ATOM    446  C   PHE    55      14.876  67.403  28.386  1.00  0.00           C
ATOM    447  O   PHE    55      14.854  68.413  27.687  1.00  0.00           O
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ATOM    448  N   SER    56      15.007  66.175  27.859  1.00  0.00           N
ATOM    449  CA  SER    56      15.129  66.061  26.434  1.00  0.00           C
ATOM    450  CB  SER    56      15.304  64.616  25.937  1.00  0.00           C
ATOM    451  OG  SER    56      14.084  63.900  26.056  1.00  0.00           O
ATOM    452  C   SER    56      13.880  66.594  25.810  1.00  0.00           C
ATOM    453  O   SER    56      13.931  67.377  24.865  1.00  0.00           O
ATOM    454  N   GLU    57      12.711  66.202  26.341  1.00  0.00           N
ATOM    455  CA  GLU    57      11.486  66.625  25.732  1.00  0.00           C
ATOM    456  CB  GLU    57      10.260  66.024  26.440  1.00  0.00           C
ATOM    457  CG  GLU    57      10.184  64.502  26.310  1.00  0.00           C
ATOM    458  CD  GLU    57       9.068  64.003  27.216  1.00  0.00           C
ATOM    459  OE1 GLU    57       9.084  64.361  28.424  1.00  0.00           O
ATOM    460  OE2 GLU    57       8.184  63.261  26.712  1.00  0.00           O
ATOM    461  C   GLU    57      11.384  68.114  25.821  1.00  0.00           C
ATOM    462  O   GLU    57      11.038  68.778  24.845  1.00  0.00           O
ATOM    463  N   VAL    58      11.703  68.681  27.000  1.00  0.00           N
ATOM    464  CA  VAL    58      11.564  70.095  27.203  1.00  0.00           C
ATOM    465  CB  VAL    58      11.804  70.518  28.625  1.00  0.00           C
ATOM    466  CG1 VAL    58      10.758  69.832  29.521  1.00  0.00           C
ATOM    467  CG2 VAL    58      13.258  70.208  29.007  1.00  0.00           C
ATOM    468  C   VAL    58      12.515  70.854  26.334  1.00  0.00           C
ATOM    469  O   VAL    58      12.143  71.873  25.754  1.00  0.00           O
ATOM    470  N   GLU    59      13.775  70.392  26.223  1.00  0.00           N
ATOM    471  CA  GLU    59      14.712  71.152  25.443  1.00  0.00           C
ATOM    472  CB  GLU    59      16.159  70.638  25.483  1.00  0.00           C
ATOM    473  CG  GLU    59      17.087  71.567  24.693  1.00  0.00           C
ATOM    474  CD  GLU    59      18.512  71.040  24.746  1.00  0.00           C
ATOM    475  OE1 GLU    59      18.688  69.819  24.990  1.00  0.00           O
ATOM    476  OE2 GLU    59      19.446  71.860  24.535  1.00  0.00           O
ATOM    477  C   GLU    59      14.305  71.165  24.003  1.00  0.00           C
ATOM    478  O   GLU    59      14.344  72.210  23.355  1.00  0.00           O
ATOM    479  N   LEU    60      13.889  70.002  23.465  1.00  0.00           N
ATOM    480  CA  LEU    60      13.555  69.930  22.070  1.00  0.00           C
ATOM    481  CB  LEU    60      13.191  68.505  21.609  1.00  0.00           C
ATOM    482  CG  LEU    60      14.401  67.577  21.371  1.00  0.00           C
ATOM    483  CD2 LEU    60      15.378  67.585  22.555  1.00  0.00           C
ATOM    484  CD1 LEU    60      15.113  67.922  20.056  1.00  0.00           C
ATOM    485  C   LEU    60      12.394  70.822  21.767  1.00  0.00           C
ATOM    486  O   LEU    60      12.417  71.556  20.780  1.00  0.00           O
ATOM    487  N   ILE    61      11.351  70.794  22.613  1.00  0.00           N
ATOM    488  CA  ILE    61      10.176  71.576  22.361  1.00  0.00           C
ATOM    489  CB  ILE    61       9.074  71.270  23.328  1.00  0.00           C
ATOM    490  CG2 ILE    61       9.620  71.513  24.739  1.00  0.00           C
ATOM    491  CG1 ILE    61       7.797  72.050  22.976  1.00  0.00           C
ATOM    492  CD1 ILE    61       6.561  71.567  23.732  1.00  0.00           C
ATOM    493  C   ILE    61      10.499  73.038  22.435  1.00  0.00           C
ATOM    494  O   ILE    61      10.009  73.828  21.631  1.00  0.00           O
ATOM    495  N   SER    62      11.315  73.448  23.422  1.00  0.00           N
ATOM    496  CA  SER    62      11.654  74.835  23.581  1.00  0.00           C
ATOM    497  CB  SER    62      12.490  75.095  24.845  1.00  0.00           C
ATOM    498  OG  SER    62      11.737  74.758  26.000  1.00  0.00           O
ATOM    499  C   SER    62      12.462  75.297  22.404  1.00  0.00           C
ATOM    500  O   SER    62      12.287  76.414  21.921  1.00  0.00           O
ATOM    501  N   ARG    63      13.387  74.452  21.920  1.00  0.00           N
ATOM    502  CA  ARG    63      14.225  74.824  20.816  1.00  0.00           C
ATOM    503  CB  ARG    63      15.302  73.766  20.517  1.00  0.00           C
ATOM    504  CG  ARG    63      16.217  73.512  21.717  1.00  0.00           C
ATOM    505  CD  ARG    63      17.439  72.647  21.407  1.00  0.00           C
ATOM    506  NE  ARG    63      18.563  73.568  21.080  1.00  0.00           N
ATOM    507  CZ  ARG    63      19.851  73.167  21.287  1.00  0.00           C
ATOM    508  NH1 ARG    63      20.106  71.927  21.799  1.00  0.00           N
ATOM    509  NH2 ARG    63      20.885  74.007  20.987  1.00  0.00           N
ATOM    510  C   ARG    63      13.382  74.999  19.590  1.00  0.00           C
ATOM    511  O   ARG    63      13.568  75.950  18.832  1.00  0.00           O
ATOM    512  N   LYS    64      12.425  74.080  19.363  1.00  0.00           N
ATOM    513  CA  LYS    64      11.578  74.142  18.209  1.00  0.00           C
ATOM    514  CB  LYS    64      10.715  72.878  18.026  1.00  0.00           C
ATOM    515  CG  LYS    64       9.877  72.485  19.243  1.00  0.00           C
ATOM    516  CD  LYS    64       8.895  71.347  18.961  1.00  0.00           C
ATOM    517  CE  LYS    64       9.573  70.020  18.618  1.00  0.00           C
ATOM    518  NZ  LYS    64      10.234  69.463  19.820  1.00  0.00           N
ATOM    519  C   LYS    64      10.709  75.362  18.271  1.00  0.00           C
ATOM    520  O   LYS    64      10.480  76.007  17.250  1.00  0.00           O
ATOM    521  N   VAL    65      10.190  75.712  19.464  1.00  0.00           N
ATOM    522  CA  VAL    65       9.351  76.872  19.566  1.00  0.00           C
ATOM    523  CB  VAL    65       8.682  77.032  20.903  1.00  0.00           C
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ATOM    524  CG1 VAL    65       9.732  77.394  21.963  1.00  0.00           C
ATOM    525  CG2 VAL    65       7.568  78.082  20.759  1.00  0.00           C
ATOM    526  C   VAL    65      10.164  78.105  19.294  1.00  0.00           C
ATOM    527  O   VAL    65       9.679  79.052  18.680  1.00  0.00           O
ATOM    528  N   ALA    66      11.428  78.143  19.759  1.00  0.00           N
ATOM    529  CA  ALA    66      12.235  79.311  19.543  1.00  0.00           C
ATOM    530  CB  ALA    66      13.631  79.196  20.177  1.00  0.00           C
ATOM    531  C   ALA    66      12.426  79.505  18.068  1.00  0.00           C
ATOM    532  O   ALA    66      12.253  80.609  17.552  1.00  0.00           O
ATOM    533  N   ALA    67      12.757  78.421  17.343  1.00  0.00           N
ATOM    534  CA  ALA    67      13.023  78.505  15.936  1.00  0.00           C
ATOM    535  CB  ALA    67      13.475  77.163  15.337  1.00  0.00           C
ATOM    536  C   ALA    67      11.783  78.923  15.210  1.00  0.00           C
ATOM    537  O   ALA    67      11.844  79.746  14.298  1.00  0.00           O
ATOM    538  N   GLY    68      10.623  78.359  15.599  1.00  0.00           N
ATOM    539  CA  GLY    68       9.376  78.643  14.944  1.00  0.00           C
ATOM    540  C   GLY    68       9.033  80.089  15.107  1.00  0.00           C
ATOM    541  O   GLY    68       8.564  80.730  14.168  1.00  0.00           O
ATOM    542  N   LEU    69       9.234  80.638  16.318  1.00  0.00           N
ATOM    543  CA  LEU    69       8.908  82.016  16.544  1.00  0.00           C
ATOM    544  CB  LEU    69       8.968  82.427  18.024  1.00  0.00           C
ATOM    545  CG  LEU    69       7.860  81.740  18.849  1.00  0.00           C
ATOM    546  CD2 LEU    69       6.514  81.786  18.107  1.00  0.00           C
ATOM    547  CD1 LEU    69       7.767  82.303  20.274  1.00  0.00           C
ATOM    548  C   LEU    69       9.825  82.881  15.734  1.00  0.00           C
ATOM    549  O   LEU    69       9.406  83.911  15.206  1.00  0.00           O
ATOM    550  N   ALA    70      11.108  82.489  15.621  1.00  0.00           N
ATOM    551  CA  ALA    70      12.056  83.251  14.855  1.00  0.00           C
ATOM    552  CB  ALA    70      13.475  82.659  14.906  1.00  0.00           C
ATOM    553  C   ALA    70      11.622  83.260  13.418  1.00  0.00           C
ATOM    554  O   ALA    70      11.677  84.294  12.754  1.00  0.00           O
ATOM    555  N   LYS    71      11.168  82.096  12.908  1.00  0.00           N
ATOM    556  CA  LYS    71      10.741  81.951  11.543  1.00  0.00           C
ATOM    557  CB  LYS    71      10.319  80.510  11.207  1.00  0.00           C
ATOM    558  CG  LYS    71      11.453  79.491  11.348  1.00  0.00           C
ATOM    559  CD  LYS    71      12.636  79.737  10.410  1.00  0.00           C
ATOM    560  CE  LYS    71      12.428  79.176   9.002  1.00  0.00           C
ATOM    561  NZ  LYS    71      13.617  79.455   8.165  1.00  0.00           N
ATOM    562  C   LYS    71       9.546  82.825  11.345  1.00  0.00           C
ATOM    563  O   LYS    71       9.368  83.429  10.289  1.00  0.00           O
ATOM    564  N   LEU    72       8.694  82.906  12.383  1.00  0.00           N
ATOM    565  CA  LEU    72       7.509  83.715  12.357  1.00  0.00           C
ATOM    566  CB  LEU    72       6.680  83.618  13.651  1.00  0.00           C
ATOM    567  CG  LEU    72       5.927  82.287  13.798  1.00  0.00           C
ATOM    568  CD2 LEU    72       5.053  82.028  12.559  1.00  0.00           C
ATOM    569  CD1 LEU    72       5.112  82.243  15.101  1.00  0.00           C
ATOM    570  C   LEU    72       7.927  85.145  12.192  1.00  0.00           C
ATOM    571  O   LEU    72       7.211  85.926  11.570  1.00  0.00           O
ATOM    572  N   GLY    73       9.106  85.532  12.728  1.00  0.00           N
ATOM    573  CA  GLY    73       9.521  86.901  12.570  1.00  0.00           C
ATOM    574  C   GLY    73       9.682  87.575  13.898  1.00  0.00           C
ATOM    575  O   GLY    73      10.016  88.756  13.970  1.00  0.00           O
ATOM    576  N   LEU    74       9.437  86.842  14.992  1.00  0.00           N
ATOM    577  CA  LEU    74       9.593  87.383  16.307  1.00  0.00           C
ATOM    578  CB  LEU    74       8.914  86.434  17.300  1.00  0.00           C
ATOM    579  CG  LEU    74       7.392  86.328  17.097  1.00  0.00           C
ATOM    580  CD2 LEU    74       6.744  87.718  16.992  1.00  0.00           C
ATOM    581  CD1 LEU    74       6.742  85.444  18.172  1.00  0.00           C
ATOM    582  C   LEU    74      11.077  87.510  16.596  1.00  0.00           C
ATOM    583  O   LEU    74      11.862  86.640  16.226  1.00  0.00           O
ATOM    584  N   GLN    75      11.515  88.618  17.244  1.00  0.00           N
ATOM    585  CA  GLN    75      12.915  88.815  17.545  1.00  0.00           C
ATOM    586  CB  GLN    75      13.726  89.411  16.382  1.00  0.00           C
ATOM    587  CG  GLN    75      13.309  90.830  15.984  1.00  0.00           C
ATOM    588  CD  GLN    75      11.996  90.751  15.218  1.00  0.00           C
ATOM    589  OE1 GLN    75      10.914  90.723  15.803  1.00  0.00           O
ATOM    590  NE2 GLN    75      12.092  90.713  13.863  1.00  0.00           N
ATOM    591  C   GLN    75      13.000  89.783  18.681  1.00  0.00           C
ATOM    592  O   GLN    75      12.005  90.041  19.348  1.00  0.00           O
ATOM    593  N   GLN    76      14.202  90.315  18.984  1.00  0.00           N
ATOM    594  CA  GLN    76      14.213  91.340  19.988  1.00  0.00           C
ATOM    595  CB  GLN    76      15.613  91.915  20.270  1.00  0.00           C
ATOM    596  CG  GLN    76      15.626  93.008  21.341  1.00  0.00           C
ATOM    597  CD  GLN    76      17.065  93.478  21.504  1.00  0.00           C
ATOM    598  OE1 GLN    76      17.975  92.965  20.857  1.00  0.00           O
ATOM    599  NE2 GLN    76      17.281  94.471  22.408  1.00  0.00           N
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ATOM    600  C   GLN    76      13.388  92.395  19.340  1.00  0.00           C
ATOM    601  O   GLN    76      13.488  92.578  18.137  1.00  0.00           O
ATOM    602  N   GLY    77      12.534  93.113  20.079  1.00  0.00           N
ATOM    603  CA  GLY    77      11.644  94.018  19.415  1.00  0.00           C
ATOM    604  C   GLY    77      10.285  93.404  19.515  1.00  0.00           C
ATOM    605  O   GLY    77       9.281  94.054  19.226  1.00  0.00           O
ATOM    606  N   GLN    78      10.221  92.127  19.950  1.00  0.00           N
ATOM    607  CA  GLN    78       8.952  91.463  20.062  1.00  0.00           C
ATOM    608  CB  GLN    78       8.889  90.064  19.445  1.00  0.00           C
ATOM    609  CG  GLN    78       9.653  89.098  20.350  1.00  0.00           C
ATOM    610  CD  GLN    78       9.504  87.680  19.879  1.00  0.00           C
ATOM    611  OE1 GLN    78       8.411  87.114  19.903  1.00  0.00           O
ATOM    612  NE2 GLN    78      10.650  87.072  19.468  1.00  0.00           N
ATOM    613  C   GLN    78       8.732  91.119  21.499  1.00  0.00           C
ATOM    614  O   GLN    78       9.663  91.008  22.298  1.00  0.00           O
ATOM    615  N   VAL    79       7.449  90.930  21.848  1.00  0.00           N
ATOM    616  CA  VAL    79       7.097  90.500  23.163  1.00  0.00           C
ATOM    617  CB  VAL    79       6.516  91.604  23.998  1.00  0.00           C
ATOM    618  CG1 VAL    79       5.365  92.258  23.226  1.00  0.00           C
ATOM    619  CG2 VAL    79       6.106  91.019  25.361  1.00  0.00           C
ATOM    620  C   VAL    79       6.058  89.437  22.999  1.00  0.00           C
ATOM    621  O   VAL    79       5.247  89.470  22.076  1.00  0.00           O
ATOM    622  N   VAL    80       6.086  88.433  23.890  1.00  0.00           N
ATOM    623  CA  VAL    80       5.116  87.380  23.882  1.00  0.00           C
ATOM    624  CB  VAL    80       5.726  86.025  23.705  1.00  0.00           C
ATOM    625  CG1 VAL    80       6.256  85.889  22.277  1.00  0.00           C
ATOM    626  CG2 VAL    80       6.844  85.894  24.747  1.00  0.00           C
ATOM    627  C   VAL    80       4.509  87.378  25.238  1.00  0.00           C
ATOM    628  O   VAL    80       5.130  87.801  26.210  1.00  0.00           O
ATOM    629  N   MET    81       3.252  86.928  25.343  1.00  0.00           N
ATOM    630  CA  MET    81       2.670  86.863  26.647  1.00  0.00           C
ATOM    631  CB  MET    81       1.321  87.592  26.749  1.00  0.00           C
ATOM    632  CG  MET    81       1.433  89.096  26.496  1.00  0.00           C
ATOM    633  SD  MET    81      -0.135  90.009  26.604  1.00  0.00           S
ATOM    634  CE  MET    81       0.576  91.595  26.078  1.00  0.00           C
ATOM    635  C   MET    81       2.421  85.414  26.900  1.00  0.00           C
ATOM    636  O   MET    81       2.100  84.668  25.976  1.00  0.00           O
ATOM    637  N   LEU    82       2.630  84.969  28.155  1.00  0.00           N
ATOM    638  CA  LEU    82       2.327  83.613  28.512  1.00  0.00           C
ATOM    639  CB  LEU    82       3.556  82.803  28.951  1.00  0.00           C
ATOM    640  CG  LEU    82       4.528  82.518  27.789  1.00  0.00           C
ATOM    641  CD2 LEU    82       5.648  81.554  28.217  1.00  0.00           C
ATOM    642  CD1 LEU    82       5.062  83.821  27.173  1.00  0.00           C
ATOM    643  C   LEU    82       1.363  83.687  29.650  1.00  0.00           C
ATOM    644  O   LEU    82       1.665  84.254  30.699  1.00  0.00           O
ATOM    645  N   LEU    83       0.145  83.144  29.456  1.00  0.00           N
ATOM    646  CA  LEU    83      -0.805  83.179  30.529  1.00  0.00           C
ATOM    647  CB  LEU    83      -1.996  84.142  30.330  1.00  0.00           C
ATOM    648  CG  LEU    83      -2.611  84.191  28.919  1.00  0.00           C
ATOM    649  CD2 LEU    83      -1.600  84.674  27.865  1.00  0.00           C
ATOM    650  CD1 LEU    83      -3.876  85.063  28.901  1.00  0.00           C
ATOM    651  C   LEU    83      -1.327  81.799  30.766  1.00  0.00           C
ATOM    652  O   LEU    83      -2.136  81.281  29.993  1.00  0.00           O
ATOM    653  N   LEU    84      -0.848  81.157  31.853  1.00  0.00           N
ATOM    654  CA  LEU    84      -1.298  79.837  32.187  1.00  0.00           C
ATOM    655  CB  LEU    84      -0.551  78.691  31.475  1.00  0.00           C
ATOM    656  CG  LEU    84      -0.658  78.652  29.938  1.00  0.00           C
ATOM    657  CD2 LEU    84      -0.322  77.251  29.407  1.00  0.00           C
ATOM    658  CD1 LEU    84       0.174  79.757  29.270  1.00  0.00           C
ATOM    659  C   LEU    84      -1.057  79.589  33.648  1.00  0.00           C
ATOM    660  O   LEU    84      -0.258  80.247  34.311  1.00  0.00           O
ATOM    661  N   PRO    85      -1.784  78.622  34.143  1.00  0.00           N
ATOM    662  CA  PRO    85      -1.596  78.170  35.495  1.00  0.00           C
ATOM    663  CD  PRO    85      -3.164  78.467  33.709  1.00  0.00           C
ATOM    664  CB  PRO    85      -2.843  77.365  35.848  1.00  0.00           C
ATOM    665  CG  PRO    85      -3.932  77.969  34.944  1.00  0.00           C
ATOM    666  C   PRO    85      -0.344  77.361  35.494  1.00  0.00           C
ATOM    667  O   PRO    85       0.131  77.017  34.413  1.00  0.00           O
ATOM    668  N   ASN    86       0.218  77.053  36.675  1.00  0.00           N
ATOM    669  CA  ASN    86       1.433  76.299  36.678  1.00  0.00           C
ATOM    670  CB  ASN    86       1.933  75.973  38.095  1.00  0.00           C
ATOM    671  CG  ASN    86       2.275  77.290  38.779  1.00  0.00           C
ATOM    672  OD1 ASN    86       2.652  78.261  38.126  1.00  0.00           O
ATOM    673  ND2 ASN    86       2.135  77.326  40.131  1.00  0.00           N
ATOM    674  C   ASN    86       1.171  75.009  35.969  1.00  0.00           C
ATOM    675  O   ASN    86       0.235  74.279  36.291  1.00  0.00           O
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ATOM    676  N   CYS    87       1.999  74.698  34.956  1.00  0.00           N
ATOM    677  CA  CYS    87       1.773  73.482  34.236  1.00  0.00           C
ATOM    678  CB  CYS    87       0.736  73.625  33.108  1.00  0.00           C
ATOM    679  SG  CYS    87       0.194  72.022  32.440  1.00  0.00           S
ATOM    680  C   CYS    87       3.072  73.083  33.623  1.00  0.00           C
ATOM    681  O   CYS    87       4.070  73.797  33.713  1.00  0.00           O
ATOM    682  N   ILE    88       3.085  71.897  32.996  1.00  0.00           N
ATOM    683  CA  ILE    88       4.261  71.386  32.366  1.00  0.00           C
ATOM    684  CB  ILE    88       4.085  70.003  31.819  1.00  0.00           C
ATOM    685  CG2 ILE    88       5.310  69.701  30.941  1.00  0.00           C
ATOM    686  CG1 ILE    88       3.868  68.993  32.960  1.00  0.00           C
ATOM    687  CD1 ILE    88       2.545  69.178  33.703  1.00  0.00           C
ATOM    688  C   ILE    88       4.644  72.271  31.221  1.00  0.00           C
ATOM    689  O   ILE    88       5.827  72.491  30.983  1.00  0.00           O
ATOM    690  N   GLU    89       3.638  72.763  30.472  1.00  0.00           N
ATOM    691  CA  GLU    89       3.771  73.554  29.276  1.00  0.00           C
ATOM    692  CB  GLU    89       2.454  73.679  28.491  1.00  0.00           C
ATOM    693  CG  GLU    89       2.066  72.395  27.753  1.00  0.00           C
ATOM    694  CD  GLU    89       1.621  71.367  28.781  1.00  0.00           C
ATOM    695  OE1 GLU    89       0.790  71.733  29.652  1.00  0.00           O
ATOM    696  OE2 GLU    89       2.110  70.208  28.712  1.00  0.00           O
ATOM    697  C   GLU    89       4.292  74.944  29.512  1.00  0.00           C
ATOM    698  O   GLU    89       4.878  75.537  28.607  1.00  0.00           O
ATOM    699  N   PHE    90       4.120  75.500  30.724  1.00  0.00           N
ATOM    700  CA  PHE    90       4.337  76.905  30.959  1.00  0.00           C
ATOM    701  CB  PHE    90       4.196  77.259  32.448  1.00  0.00           C
ATOM    702  CG  PHE    90       3.996  78.730  32.559  1.00  0.00           C
ATOM    703  CD1 PHE    90       5.061  79.600  32.538  1.00  0.00           C
ATOM    704  CD2 PHE    90       2.723  79.236  32.690  1.00  0.00           C
ATOM    705  CE1 PHE    90       4.851  80.956  32.643  1.00  0.00           C
ATOM    706  CE2 PHE    90       2.508  80.590  32.794  1.00  0.00           C
ATOM    707  CZ  PHE    90       3.576  81.451  32.772  1.00  0.00           C
ATOM    708  C   PHE    90       5.697  77.358  30.496  1.00  0.00           C
ATOM    709  O   PHE    90       5.818  78.348  29.776  1.00  0.00           O
ATOM    710  N   ALA    91       6.760  76.642  30.882  1.00  0.00           N
ATOM    711  CA  ALA    91       8.122  76.990  30.592  1.00  0.00           C
ATOM    712  CB  ALA    91       9.121  76.083  31.319  1.00  0.00           C
ATOM    713  C   ALA    91       8.475  76.942  29.129  1.00  0.00           C
ATOM    714  O   ALA    91       9.408  77.617  28.702  1.00  0.00           O
ATOM    715  N   PHE    92       7.803  76.111  28.317  1.00  0.00           N
ATOM    716  CA  PHE    92       8.257  75.909  26.967  1.00  0.00           C
ATOM    717  CB  PHE    92       7.358  74.949  26.173  1.00  0.00           C
ATOM    718  CG  PHE    92       7.318  73.671  26.936  1.00  0.00           C
ATOM    719  CD1 PHE    92       8.443  72.891  27.052  1.00  0.00           C
ATOM    720  CD2 PHE    92       6.170  73.275  27.580  1.00  0.00           C
ATOM    721  CE1 PHE    92       8.420  71.714  27.760  1.00  0.00           C
ATOM    722  CE2 PHE    92       6.139  72.098  28.290  1.00  0.00           C
ATOM    723  CZ  PHE    92       7.262  71.311  28.379  1.00  0.00           C
ATOM    724  C   PHE    92       8.325  77.198  26.208  1.00  0.00           C
ATOM    725  O   PHE    92       9.344  77.500  25.587  1.00  0.00           O
ATOM    726  N   VAL    93       7.247  77.997  26.227  1.00  0.00           N
ATOM    727  CA  VAL    93       7.243  79.238  25.514  1.00  0.00           C
ATOM    728  CB  VAL    93       5.909  79.926  25.550  1.00  0.00           C
ATOM    729  CG1 VAL    93       6.044  81.293  24.859  1.00  0.00           C
ATOM    730  CG2 VAL    93       4.865  79.001  24.905  1.00  0.00           C
ATOM    731  C   VAL    93       8.244  80.168  26.134  1.00  0.00           C
ATOM    732  O   VAL    93       8.890  80.929  25.415  1.00  0.00           O
ATOM    733  N   PHE    94       8.396  80.165  27.481  1.00  0.00           N
ATOM    734  CA  PHE    94       9.290  81.144  28.035  1.00  0.00           C
ATOM    735  CB  PHE    94       9.318  81.341  29.573  1.00  0.00           C
ATOM    736  CG  PHE    94      10.306  80.462  30.265  1.00  0.00           C
ATOM    737  CD1 PHE    94      11.621  80.857  30.383  1.00  0.00           C
ATOM    738  CD2 PHE    94       9.940  79.269  30.824  1.00  0.00           C
ATOM    739  CE1 PHE    94      12.546  80.067  31.024  1.00  0.00           C
ATOM    740  CE2 PHE    94      10.853  78.468  31.466  1.00  0.00           C
ATOM    741  CZ  PHE    94      12.163  78.865  31.567  1.00  0.00           C
ATOM    742  C   PHE    94      10.683  80.834  27.595  1.00  0.00           C
ATOM    743  O   PHE    94      11.417  81.729  27.182  1.00  0.00           O
ATOM    744  N   MET    95      11.085  79.550  27.664  1.00  0.00           N
ATOM    745  CA  MET    95      12.413  79.161  27.277  1.00  0.00           C
ATOM    746  CB  MET    95      12.671  77.658  27.475  1.00  0.00           C
ATOM    747  CG  MET    95      14.083  77.219  27.081  1.00  0.00           C
ATOM    748  SD  MET    95      14.409  75.445  27.307  1.00  0.00           S
ATOM    749  CE  MET    95      14.500  75.529  29.120  1.00  0.00           C
ATOM    750  C   MET    95      12.607  79.472  25.826  1.00  0.00           C
ATOM    751  O   MET    95      13.640  80.006  25.429  1.00  0.00           O
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ATOM    752  N   GLY    96      11.596  79.179  24.987  1.00  0.00           N
ATOM    753  CA  GLY    96      11.743  79.380  23.573  1.00  0.00           C
ATOM    754  C   GLY    96      12.002  80.832  23.293  1.00  0.00           C
ATOM    755  O   GLY    96      12.846  81.163  22.461  1.00  0.00           O
ATOM    756  N   ALA    97      11.261  81.734  23.968  1.00  0.00           N
ATOM    757  CA  ALA    97      11.385  83.150  23.762  1.00  0.00           C
ATOM    758  CB  ALA    97      10.325  83.952  24.532  1.00  0.00           C
ATOM    759  C   ALA    97      12.727  83.643  24.207  1.00  0.00           C
ATOM    760  O   ALA    97      13.352  84.453  23.528  1.00  0.00           O
ATOM    761  N   SER    98      13.212  83.164  25.367  1.00  0.00           N
ATOM    762  CA  SER    98      14.464  83.624  25.890  1.00  0.00           C
ATOM    763  CB  SER    98      14.832  82.970  27.232  1.00  0.00           C
ATOM    764  OG  SER    98      13.881  83.327  28.226  1.00  0.00           O
ATOM    765  C   SER    98      15.541  83.284  24.922  1.00  0.00           C
ATOM    766  O   SER    98      16.495  84.041  24.760  1.00  0.00           O
ATOM    767  N   VAL    99      15.420  82.118  24.263  1.00  0.00           N
ATOM    768  CA  VAL    99      16.397  81.567  23.363  1.00  0.00           C
ATOM    769  CB  VAL    99      15.993  80.233  22.805  1.00  0.00           C
ATOM    770  CG1 VAL    99      17.038  79.803  21.761  1.00  0.00           C
ATOM    771  CG2 VAL    99      15.836  79.243  23.969  1.00  0.00           C
ATOM    772  C   VAL    99      16.586  82.491  22.207  1.00  0.00           C
ATOM    773  O   VAL    99      17.666  82.528  21.619  1.00  0.00           O
ATOM    774  N   ARG   100      15.532  83.228  21.811  1.00  0.00           N
ATOM    775  CA  ARG   100      15.696  84.055  20.652  1.00  0.00           C
ATOM    776  CB  ARG   100      14.609  83.814  19.592  1.00  0.00           C
ATOM    777  CG  ARG   100      13.209  84.178  20.085  1.00  0.00           C
ATOM    778  CD  ARG   100      12.094  83.833  19.097  1.00  0.00           C
ATOM    779  NE  ARG   100      11.634  82.456  19.424  1.00  0.00           N
ATOM    780  CZ  ARG   100      10.733  82.283  20.433  1.00  0.00           C
ATOM    781  NH1 ARG   100      10.285  83.372  21.125  1.00  0.00           N
ATOM    782  NH2 ARG   100      10.292  81.033  20.759  1.00  0.00           N
ATOM    783  C   ARG   100      15.600  85.513  21.010  1.00  0.00           C
ATOM    784  O   ARG   100      15.522  86.354  20.116  1.00  0.00           O
ATOM    785  N   GLY   101      15.627  85.870  22.311  1.00  0.00           N
ATOM    786  CA  GLY   101      15.662  87.260  22.683  1.00  0.00           C
ATOM    787  C   GLY   101      14.328  87.937  22.650  1.00  0.00           C
ATOM    788  O   GLY   101      14.258  89.164  22.596  1.00  0.00           O
ATOM    789  N   ALA   102      13.233  87.166  22.663  1.00  0.00           N
ATOM    790  CA  ALA   102      11.916  87.728  22.713  1.00  0.00           C
ATOM    791  CB  ALA   102      10.844  86.716  22.298  1.00  0.00           C
ATOM    792  C   ALA   102      11.616  88.000  24.153  1.00  0.00           C
ATOM    793  O   ALA   102      11.951  87.196  25.020  1.00  0.00           O
ATOM    794  N   ILE   103      10.933  89.120  24.453  1.00  0.00           N
ATOM    795  CA  ILE   103      10.621  89.385  25.828  1.00  0.00           C
ATOM    796  CB  ILE   103      10.352  90.840  26.117  1.00  0.00           C
ATOM    797  CG2 ILE   103      11.553  91.660  25.629  1.00  0.00           C
ATOM    798  CG1 ILE   103       9.060  91.300  25.436  1.00  0.00           C
ATOM    799  CD1 ILE   103       8.573  92.667  25.913  1.00  0.00           C
ATOM    800  C   ILE   103       9.350  88.635  26.136  1.00  0.00           C
ATOM    801  O   ILE   103       8.406  88.640  25.350  1.00  0.00           O
ATOM    802  N   VAL   104       9.305  87.936  27.288  1.00  0.00           N
ATOM    803  CA  VAL   104       8.154  87.184  27.700  1.00  0.00           C
ATOM    804  CB  VAL   104       8.498  85.805  28.181  1.00  0.00           C
ATOM    805  CG1 VAL   104       7.221  85.128  28.701  1.00  0.00           C
ATOM    806  CG2 VAL   104       9.185  85.046  27.032  1.00  0.00           C
ATOM    807  C   VAL   104       7.492  87.895  28.836  1.00  0.00           C
ATOM    808  O   VAL   104       8.138  88.268  29.815  1.00  0.00           O
ATOM    809  N   THR   105       6.162  88.101  28.719  1.00  0.00           N
ATOM    810  CA  THR   105       5.430  88.744  29.773  1.00  0.00           C
ATOM    811  CB  THR   105       4.617  89.916  29.305  1.00  0.00           C
ATOM    812  OG1 THR   105       5.463  90.888  28.704  1.00  0.00           O
ATOM    813  CG2 THR   105       3.887  90.525  30.514  1.00  0.00           C
ATOM    814  C   THR   105       4.473  87.730  30.307  1.00  0.00           C
ATOM    815  O   THR   105       3.490  87.394  29.649  1.00  0.00           O
ATOM    816  N   THR   106       4.737  87.211  31.523  1.00  0.00           N
ATOM    817  CA  THR   106       3.855  86.224  32.064  1.00  0.00           C
ATOM    818  CB  THR   106       4.494  85.372  33.129  1.00  0.00           C
ATOM    819  OG1 THR   106       3.747  84.180  33.288  1.00  0.00           O
ATOM    820  CG2 THR   106       4.569  86.148  34.457  1.00  0.00           C
ATOM    821  C   THR   106       2.679  86.959  32.620  1.00  0.00           C
ATOM    822  O   THR   106       2.822  87.937  33.351  1.00  0.00           O
ATOM    823  N   ALA   107       1.460  86.514  32.270  1.00  0.00           N
ATOM    824  CA  ALA   107       0.313  87.216  32.763  1.00  0.00           C
ATOM    825  CB  ALA   107      -0.726  87.532  31.673  1.00  0.00           C
ATOM    826  C   ALA   107      -0.347  86.332  33.760  1.00  0.00           C
ATOM    827  O   ALA   107      -0.531  85.138  33.527  1.00  0.00           O
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ATOM    828  N   ASN   108      -0.726  86.912  34.914  1.00  0.00           N
ATOM    829  CA  ASN   108      -1.319  86.124  35.948  1.00  0.00           C
ATOM    830  CB  ASN   108      -1.535  86.921  37.250  1.00  0.00           C
ATOM    831  CG  ASN   108      -1.698  85.974  38.424  1.00  0.00           C
ATOM    832  OD1 ASN   108      -2.527  85.067  38.417  1.00  0.00           O
ATOM    833  ND2 ASN   108      -0.865  86.190  39.477  1.00  0.00           N
ATOM    834  C   ASN   108      -2.628  85.614  35.432  1.00  0.00           C
ATOM    835  O   ASN   108      -3.484  86.364  34.965  1.00  0.00           O
ATOM    836  N   PRO   109      -2.758  84.316  35.500  1.00  0.00           N
ATOM    837  CA  PRO   109      -3.917  83.626  35.002  1.00  0.00           C
ATOM    838  CD  PRO   109      -1.594  83.452  35.561  1.00  0.00           C
ATOM    839  CB  PRO   109      -3.521  82.146  34.909  1.00  0.00           C
ATOM    840  CG  PRO   109      -2.191  82.042  35.679  1.00  0.00           C
ATOM    841  C   PRO   109      -5.138  83.877  35.812  1.00  0.00           C
ATOM    842  O   PRO   109      -6.225  83.566  35.345  1.00  0.00           O
ATOM    843  N   PHE   110      -4.983  84.345  37.058  1.00  0.00           N
ATOM    844  CA  PHE   110      -6.100  84.616  37.910  1.00  0.00           C
ATOM    845  CB  PHE   110      -5.664  84.576  39.385  1.00  0.00           C
ATOM    846  CG  PHE   110      -6.798  84.066  40.206  1.00  0.00           C
ATOM    847  CD1 PHE   110      -7.361  82.846  39.894  1.00  0.00           C
ATOM    848  CD2 PHE   110      -7.260  84.745  41.310  1.00  0.00           C
ATOM    849  CE1 PHE   110      -8.393  82.330  40.639  1.00  0.00           C
ATOM    850  CE2 PHE   110      -8.295  84.232  42.060  1.00  0.00           C
ATOM    851  CZ  PHE   110      -8.868  83.030  41.721  1.00  0.00           C
ATOM    852  C   PHE   110      -6.687  85.957  37.542  1.00  0.00           C
ATOM    853  O   PHE   110      -7.886  86.178  37.697  1.00  0.00           O
ATOM    854  N   TYR   111      -5.846  86.900  37.057  1.00  0.00           N
ATOM    855  CA  TYR   111      -6.286  88.242  36.775  1.00  0.00           C
ATOM    856  CB  TYR   111      -5.283  89.205  36.112  1.00  0.00           C
ATOM    857  CG  TYR   111      -4.271  89.661  37.106  1.00  0.00           C
ATOM    858  CD1 TYR   111      -4.659  90.249  38.287  1.00  0.00           C
ATOM    859  CD2 TYR   111      -2.934  89.473  36.876  1.00  0.00           C
ATOM    860  CE1 TYR   111      -3.725  90.663  39.208  1.00  0.00           C
ATOM    861  CE2 TYR   111      -1.992  89.885  37.790  1.00  0.00           C
ATOM    862  CZ  TYR   111      -2.386  90.485  38.959  1.00  0.00           C
ATOM    863  OH  TYR   111      -1.419  90.907  39.895  1.00  0.00           O
ATOM    864  C   TYR   111      -7.523  88.292  35.946  1.00  0.00           C
ATOM    865  O   TYR   111      -7.787  87.438  35.104  1.00  0.00           O
ATOM    866  N   LYS   112      -8.324  89.341  36.218  1.00  0.00           N
ATOM    867  CA  LYS   112      -9.533  89.637  35.512  1.00  0.00           C
ATOM    868  CB  LYS   112     -10.322  90.849  36.049  1.00  0.00           C
ATOM    869  CG  LYS   112     -10.875  90.750  37.471  1.00  0.00           C
ATOM    870  CD  LYS   112      -9.825  90.918  38.569  1.00  0.00           C
ATOM    871  CE  LYS   112      -9.522  89.625  39.319  1.00  0.00           C
ATOM    872  NZ  LYS   112     -10.657  89.298  40.211  1.00  0.00           N
ATOM    873  C   LYS   112      -9.096  90.077  34.158  1.00  0.00           C
ATOM    874  O   LYS   112      -7.903  90.137  33.866  1.00  0.00           O
ATOM    875  N   PRO   113     -10.040  90.338  33.303  1.00  0.00           N
ATOM    876  CA  PRO   113      -9.710  90.803  31.990  1.00  0.00           C
ATOM    877  CD  PRO   113     -11.326  89.663  33.345  1.00  0.00           C
ATOM    878  CB  PRO   113     -11.021  90.793  31.208  1.00  0.00           C
ATOM    879  CG  PRO   113     -11.839  89.684  31.894  1.00  0.00           C
ATOM    880  C   PRO   113      -9.024  92.136  32.007  1.00  0.00           C
ATOM    881  O   PRO   113      -8.252  92.405  31.088  1.00  0.00           O
ATOM    882  N   GLY   114      -9.321  93.003  32.997  1.00  0.00           N
ATOM    883  CA  GLY   114      -8.713  94.308  33.082  1.00  0.00           C
ATOM    884  C   GLY   114      -7.258  94.216  33.436  1.00  0.00           C
ATOM    885  O   GLY   114      -6.416  94.905  32.862  1.00  0.00           O
ATOM    886  N   GLU   115      -6.929  93.366  34.423  1.00  0.00           N
ATOM    887  CA  GLU   115      -5.570  93.241  34.857  1.00  0.00           C
ATOM    888  CB  GLU   115      -5.402  92.226  35.999  1.00  0.00           C
ATOM    889  CG  GLU   115      -6.081  92.634  37.305  1.00  0.00           C
ATOM    890  CD  GLU   115      -5.407  93.908  37.776  1.00  0.00           C
ATOM    891  OE1 GLU   115      -5.512  94.923  37.041  1.00  0.00           O
ATOM    892  OE2 GLU   115      -4.777  93.884  38.866  1.00  0.00           O
ATOM    893  C   GLU   115      -4.811  92.695  33.706  1.00  0.00           C
ATOM    894  O   GLU   115      -3.683  93.099  33.422  1.00  0.00           O
ATOM    895  N   ILE   116      -5.450  91.740  33.014  1.00  0.00           N
ATOM    896  CA  ILE   116      -4.826  91.125  31.895  1.00  0.00           C
ATOM    897  CB  ILE   116      -5.635  90.005  31.308  1.00  0.00           C
ATOM    898  CG2 ILE   116      -4.945  89.548  30.012  1.00  0.00           C
ATOM    899  CG1 ILE   116      -5.805  88.877  32.341  1.00  0.00           C
ATOM    900  CD1 ILE   116      -6.837  87.824  31.938  1.00  0.00           C
ATOM    901  C   ILE   116      -4.629  92.172  30.848  1.00  0.00           C
ATOM    902  O   ILE   116      -3.570  92.252  30.231  1.00  0.00           O
ATOM    903  N   ALA   117      -5.651  93.017  30.631  1.00  0.00           N
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ATOM    904  CA  ALA   117      -5.578  94.030  29.622  1.00  0.00           C
ATOM    905  CB  ALA   117      -6.882  94.835  29.494  1.00  0.00           C
ATOM    906  C   ALA   117      -4.481  94.998  29.940  1.00  0.00           C
ATOM    907  O   ALA   117      -3.730  95.390  29.056  1.00  0.00           O
ATOM    908  N   LYS   118      -4.356  95.428  31.208  1.00  0.00           N
ATOM    909  CA  LYS   118      -3.366  96.407  31.561  1.00  0.00           C
ATOM    910  CB  LYS   118      -3.553  96.914  32.998  1.00  0.00           C
ATOM    911  CG  LYS   118      -4.903  97.619  33.158  1.00  0.00           C
ATOM    912  CD  LYS   118      -5.325  97.883  34.603  1.00  0.00           C
ATOM    913  CE  LYS   118      -6.728  98.487  34.709  1.00  0.00           C
ATOM    914  NZ  LYS   118      -6.816  99.709  33.879  1.00  0.00           N
ATOM    915  C   LYS   118      -1.998  95.827  31.408  1.00  0.00           C
ATOM    916  O   LYS   118      -1.083  96.473  30.894  1.00  0.00           O
ATOM    917  N   GLN   119      -1.823  94.570  31.839  1.00  0.00           N
ATOM    918  CA  GLN   119      -0.529  93.980  31.746  1.00  0.00           C
ATOM    919  CB  GLN   119      -0.528  92.526  32.251  1.00  0.00           C
ATOM    920  CG  GLN   119       0.854  91.870  32.303  1.00  0.00           C
ATOM    921  CD  GLN   119       1.495  92.242  33.634  1.00  0.00           C
ATOM    922  OE1 GLN   119       1.826  93.401  33.885  1.00  0.00           O
ATOM    923  NE2 GLN   119       1.670  91.227  34.521  1.00  0.00           N
ATOM    924  C   GLN   119      -0.185  93.950  30.292  1.00  0.00           C
ATOM    925  O   GLN   119       0.892  94.384  29.890  1.00  0.00           O
ATOM    926  N   ALA   120      -1.140  93.477  29.470  1.00  0.00           N
ATOM    927  CA  ALA   120      -1.001  93.299  28.051  1.00  0.00           C
ATOM    928  CB  ALA   120      -2.225  92.615  27.415  1.00  0.00           C
ATOM    929  C   ALA   120      -0.806  94.606  27.342  1.00  0.00           C
ATOM    930  O   ALA   120      -0.081  94.680  26.354  1.00  0.00           O
ATOM    931  N   LYS   121      -1.480  95.672  27.793  1.00  0.00           N
ATOM    932  CA  LYS   121      -1.401  96.939  27.131  1.00  0.00           C
ATOM    933  CB  LYS   121      -2.256  98.012  27.830  1.00  0.00           C
ATOM    934  CG  LYS   121      -2.360  99.344  27.080  1.00  0.00           C
ATOM    935  CD  LYS   121      -3.250  99.291  25.836  1.00  0.00           C
ATOM    936  CE  LYS   121      -3.480 100.662  25.196  1.00  0.00           C
ATOM    937  NZ  LYS   121      -4.413 100.540  24.054  1.00  0.00           N
ATOM    938  C   LYS   121       0.016  97.389  27.198  1.00  0.00           C
ATOM    939  O   LYS   121       0.579  97.858  26.210  1.00  0.00           O
ATOM    940  N   ALA   122       0.634  97.260  28.384  1.00  0.00           N
ATOM    941  CA  ALA   122       1.986  97.704  28.510  1.00  0.00           C
ATOM    942  CB  ALA   122       2.513  97.601  29.952  1.00  0.00           C
ATOM    943  C   ALA   122       2.859  96.848  27.652  1.00  0.00           C
ATOM    944  O   ALA   122       3.691  97.353  26.898  1.00  0.00           O
ATOM    945  N   ALA   123       2.651  95.521  27.745  1.00  0.00           N
ATOM    946  CA  ALA   123       3.455  94.523  27.100  1.00  0.00           C
ATOM    947  CB  ALA   123       3.057  93.094  27.509  1.00  0.00           C
ATOM    948  C   ALA   123       3.375  94.595  25.601  1.00  0.00           C
ATOM    949  O   ALA   123       4.389  94.423  24.925  1.00  0.00           O
ATOM    950  N   GLY   124       2.171  94.807  25.033  1.00  0.00           N
ATOM    951  CA  GLY   124       2.045  94.926  23.605  1.00  0.00           C
ATOM    952  C   GLY   124       2.578  93.689  22.932  1.00  0.00           C
ATOM    953  O   GLY   124       3.421  93.789  22.041  1.00  0.00           O
ATOM    954  N   ALA   125       2.120  92.486  23.344  1.00  0.00           N
ATOM    955  CA  ALA   125       2.635  91.260  22.791  1.00  0.00           C
ATOM    956  CB  ALA   125       2.355  90.030  23.673  1.00  0.00           C
ATOM    957  C   ALA   125       2.084  90.962  21.426  1.00  0.00           C
ATOM    958  O   ALA   125       0.899  91.151  21.153  1.00  0.00           O
ATOM    959  N   ARG   126       2.976  90.506  20.518  1.00  0.00           N
ATOM    960  CA  ARG   126       2.622  90.082  19.191  1.00  0.00           C
ATOM    961  CB  ARG   126       3.840  89.902  18.273  1.00  0.00           C
ATOM    962  CG  ARG   126       4.571  91.206  17.961  1.00  0.00           C
ATOM    963  CD  ARG   126       5.722  91.028  16.971  1.00  0.00           C
ATOM    964  NE  ARG   126       5.127  90.620  15.667  1.00  0.00           N
ATOM    965  CZ  ARG   126       5.842  90.762  14.514  1.00  0.00           C
ATOM    966  NH1 ARG   126       7.104  91.283  14.552  1.00  0.00           N
ATOM    967  NH2 ARG   126       5.294  90.388  13.322  1.00  0.00           N
ATOM    968  C   ARG   126       1.931  88.754  19.244  1.00  0.00           C
ATOM    969  O   ARG   126       0.942  88.525  18.550  1.00  0.00           O
ATOM    970  N   ILE   127       2.455  87.823  20.068  1.00  0.00           N
ATOM    971  CA  ILE   127       1.870  86.513  20.123  1.00  0.00           C
ATOM    972  CB  ILE   127       2.767  85.432  19.595  1.00  0.00           C
ATOM    973  CG2 ILE   127       3.088  85.761  18.127  1.00  0.00           C
ATOM    974  CG1 ILE   127       4.018  85.290  20.466  1.00  0.00           C
ATOM    975  CD1 ILE   127       4.837  84.037  20.159  1.00  0.00           C
ATOM    976  C   ILE   127       1.573  86.197  21.551  1.00  0.00           C
ATOM    977  O   ILE   127       2.323  86.571  22.451  1.00  0.00           O
ATOM    978  N   ILE   128       0.440  85.515  21.803  1.00  0.00           N
ATOM    979  CA  ILE   128       0.126  85.188  23.160  1.00  0.00           C
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ATOM    980  CB  ILE   128      -1.042  85.951  23.719  1.00  0.00           C
ATOM    981  CG2 ILE   128      -0.622  87.427  23.818  1.00  0.00           C
ATOM    982  CG1 ILE   128      -2.305  85.740  22.878  1.00  0.00           C
ATOM    983  CD1 ILE   128      -2.260  86.428  21.519  1.00  0.00           C
ATOM    984  C   ILE   128      -0.106  83.718  23.304  1.00  0.00           C
ATOM    985  O   ILE   128      -0.877  83.102  22.567  1.00  0.00           O
ATOM    986  N   VAL   129       0.588  83.114  24.286  1.00  0.00           N
ATOM    987  CA  VAL   129       0.427  81.715  24.536  1.00  0.00           C
ATOM    988  CB  VAL   129       1.711  81.030  24.899  1.00  0.00           C
ATOM    989  CG1 VAL   129       1.403  79.568  25.261  1.00  0.00           C
ATOM    990  CG2 VAL   129       2.699  81.195  23.732  1.00  0.00           C
ATOM    991  C   VAL   129      -0.495  81.592  25.708  1.00  0.00           C
ATOM    992  O   VAL   129      -0.250  82.187  26.758  1.00  0.00           O
ATOM    993  N   THR   130      -1.601  80.828  25.555  1.00  0.00           N
ATOM    994  CA  THR   130      -2.508  80.694  26.662  1.00  0.00           C
ATOM    995  CB  THR   130      -3.799  81.447  26.555  1.00  0.00           C
ATOM    996  OG1 THR   130      -4.563  80.980  25.455  1.00  0.00           O
ATOM    997  CG2 THR   130      -3.493  82.933  26.416  1.00  0.00           C
ATOM    998  C   THR   130      -2.931  79.276  26.808  1.00  0.00           C
ATOM    999  O   THR   130      -2.852  78.470  25.884  1.00  0.00           O
ATOM   1000  N   LEU   131      -3.414  78.970  28.024  1.00  0.00           N
ATOM   1001  CA  LEU   131      -3.932  77.696  28.403  1.00  0.00           C
ATOM   1002  CB  LEU   131      -4.017  77.560  29.937  1.00  0.00           C
ATOM   1003  CG  LEU   131      -4.369  76.163  30.485  1.00  0.00           C
ATOM   1004  CD2 LEU   131      -4.921  76.247  31.916  1.00  0.00           C
ATOM   1005  CD1 LEU   131      -3.172  75.205  30.379  1.00  0.00           C
ATOM   1006  C   LEU   131      -5.333  77.674  27.881  1.00  0.00           C
ATOM   1007  O   LEU   131      -5.930  78.717  27.612  1.00  0.00           O
ATOM   1008  N   ALA   132      -5.897  76.466  27.734  1.00  0.00           N
ATOM   1009  CA  ALA   132      -7.226  76.317  27.226  1.00  0.00           C
ATOM   1010  CB  ALA   132      -7.672  74.847  27.151  1.00  0.00           C
ATOM   1011  C   ALA   132      -8.159  77.031  28.147  1.00  0.00           C
ATOM   1012  O   ALA   132      -9.163  77.585  27.698  1.00  0.00           O
ATOM   1013  N   ALA   133      -7.843  77.043  29.461  1.00  0.00           N
ATOM   1014  CA  ALA   133      -8.762  77.580  30.420  1.00  0.00           C
ATOM   1015  CB  ALA   133      -8.186  77.609  31.847  1.00  0.00           C
ATOM   1016  C   ALA   133      -9.117  78.972  30.055  1.00  0.00           C
ATOM   1017  O   ALA   133     -10.307  79.248  29.908  1.00  0.00           O
ATOM   1018  N   TYR   134      -8.184  79.929  29.862  1.00  0.00           N
ATOM   1019  CA  TYR   134      -8.978  81.005  29.381  1.00  0.00           C
ATOM   1020  CB  TYR   134      -9.770  81.897  30.354  1.00  0.00           C
ATOM   1021  CG  TYR   134      -8.993  82.796  31.218  1.00  0.00           C
ATOM   1022  CD1 TYR   134      -8.632  84.035  30.759  1.00  0.00           C
ATOM   1023  CD2 TYR   134      -8.661  82.412  32.488  1.00  0.00           C
ATOM   1024  CE1 TYR   134      -7.927  84.904  31.551  1.00  0.00           C
ATOM   1025  CE2 TYR   134      -7.960  83.278  33.278  1.00  0.00           C
ATOM   1026  CZ  TYR   134      -7.588  84.518  32.822  1.00  0.00           C
ATOM   1027  OH  TYR   134      -6.869  85.401  33.650  1.00  0.00           O
ATOM   1028  C   TYR   134      -8.481  81.749  28.210  1.00  0.00           C
ATOM   1029  O   TYR   134      -7.936  82.851  28.286  1.00  0.00           O
ATOM   1030  N   VAL   135      -8.779  81.130  27.062  1.00  0.00           N
ATOM   1031  CA  VAL   135      -8.555  81.701  25.786  1.00  0.00           C
ATOM   1032  CB  VAL   135      -8.726  80.726  24.661  1.00  0.00           C
ATOM   1033  CG1 VAL   135     -10.220  80.420  24.479  1.00  0.00           C
ATOM   1034  CG2 VAL   135      -8.043  81.318  23.421  1.00  0.00           C
ATOM   1035  C   VAL   135      -9.566  82.792  25.648  1.00  0.00           C
ATOM   1036  O   VAL   135      -9.336  83.787  24.966  1.00  0.00           O
ATOM   1037  N   GLU   136     -10.737  82.616  26.293  1.00  0.00           N
ATOM   1038  CA  GLU   136     -11.791  83.580  26.160  1.00  0.00           C
ATOM   1039  CB  GLU   136     -13.082  83.186  26.892  1.00  0.00           C
ATOM   1040  CG  GLU   136     -13.816  82.028  26.218  1.00  0.00           C
ATOM   1041  CD  GLU   136     -14.386  82.525  24.893  1.00  0.00           C
ATOM   1042  OE1 GLU   136     -13.740  83.391  24.246  1.00  0.00           O
ATOM   1043  OE2 GLU   136     -15.483  82.037  24.513  1.00  0.00           O
ATOM   1044  C   GLU   136     -11.364  84.922  26.664  1.00  0.00           C
ATOM   1045  O   GLU   136     -11.581  85.925  25.987  1.00  0.00           O
ATOM   1046  N   LYS   137     -10.736  85.005  27.852  1.00  0.00           N
ATOM   1047  CA  LYS   137     -10.383  86.328  28.278  1.00  0.00           C
ATOM   1048  CB  LYS   137      -9.909  86.470  29.729  1.00  0.00           C
ATOM   1049  CG  LYS   137     -11.077  86.403  30.713  1.00  0.00           C
ATOM   1050  CD  LYS   137     -10.668  86.534  32.180  1.00  0.00           C
ATOM   1051  CE  LYS   137     -11.861  86.666  33.129  1.00  0.00           C
ATOM   1052  NZ  LYS   137     -11.383  86.880  34.511  1.00  0.00           N
ATOM   1053  C   LYS   137      -9.356  86.877  27.352  1.00  0.00           C
ATOM   1054  O   LYS   137      -9.318  88.080  27.099  1.00  0.00           O
ATOM   1055  N   LEU   138      -8.483  86.002  26.825  1.00  0.00           N
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ATOM   1056  CA  LEU   138      -7.457  86.431  25.922  1.00  0.00           C
ATOM   1057  CB  LEU   138      -6.504  85.289  25.563  1.00  0.00           C
ATOM   1058  CG  LEU   138      -5.387  85.702  24.600  1.00  0.00           C
ATOM   1059  CD2 LEU   138      -4.604  84.462  24.175  1.00  0.00           C
ATOM   1060  CD1 LEU   138      -4.481  86.791  25.197  1.00  0.00           C
ATOM   1061  C   LEU   138      -8.089  86.951  24.667  1.00  0.00           C
ATOM   1062  O   LEU   138      -7.626  87.936  24.091  1.00  0.00           O
ATOM   1063  N   ALA   139      -9.165  86.293  24.203  1.00  0.00           N
ATOM   1064  CA  ALA   139      -9.831  86.724  23.006  1.00  0.00           C
ATOM   1065  CB  ALA   139     -11.012  85.819  22.621  1.00  0.00           C
ATOM   1066  C   ALA   139     -10.377  88.093  23.256  1.00  0.00           C
ATOM   1067  O   ALA   139     -10.344  88.955  22.381  1.00  0.00           O
ATOM   1068  N   ASP   140     -10.908  88.314  24.472  1.00  0.00           N
ATOM   1069  CA  ASP   140     -11.500  89.572  24.822  1.00  0.00           C
ATOM   1070  CB  ASP   140     -12.133  89.550  26.220  1.00  0.00           C
ATOM   1071  CG  ASP   140     -13.019  90.777  26.319  1.00  0.00           C
ATOM   1072  OD1 ASP   140     -13.100  91.517  25.304  1.00  0.00           O
ATOM   1073  OD2 ASP   140     -13.625  90.990  27.403  1.00  0.00           O
ATOM   1074  C   ASP   140     -10.450  90.636  24.811  1.00  0.00           C
ATOM   1075  O   ASP   140     -10.691  91.758  24.369  1.00  0.00           O
ATOM   1076  N   LEU   141      -9.251  90.316  25.323  1.00  0.00           N
ATOM   1077  CA  LEU   141      -8.174  91.263  25.351  1.00  0.00           C
ATOM   1078  CB  LEU   141      -6.954  90.725  26.129  1.00  0.00           C
ATOM   1079  CG  LEU   141      -5.729  91.664  26.190  1.00  0.00           C
ATOM   1080  CD2 LEU   141      -6.123  93.063  26.687  1.00  0.00           C
ATOM   1081  CD1 LEU   141      -4.961  91.706  24.857  1.00  0.00           C
ATOM   1082  C   LEU   141      -7.752  91.548  23.944  1.00  0.00           C
ATOM   1083  O   LEU   141      -7.430  92.682  23.591  1.00  0.00           O
ATOM   1084  N   GLN   142      -7.753  90.503  23.099  1.00  0.00           N
ATOM   1085  CA  GLN   142      -7.287  90.585  21.746  1.00  0.00           C
ATOM   1086  CB  GLN   142      -7.402  89.221  21.036  1.00  0.00           C
ATOM   1087  CG  GLN   142      -6.824  89.164  19.620  1.00  0.00           C
ATOM   1088  CD  GLN   142      -6.917  87.715  19.154  1.00  0.00           C
ATOM   1089  OE1 GLN   142      -7.890  87.018  19.438  1.00  0.00           O
ATOM   1090  NE2 GLN   142      -5.870  87.241  18.427  1.00  0.00           N
ATOM   1091  C   GLN   142      -8.107  91.593  21.004  1.00  0.00           C
ATOM   1092  O   GLN   142      -7.577  92.354  20.195  1.00  0.00           O
ATOM   1093  N   SER   143      -9.424  91.646  21.271  1.00  0.00           N
ATOM   1094  CA  SER   143     -10.252  92.581  20.567  1.00  0.00           C
ATOM   1095  CB  SER   143     -11.713  92.562  21.047  1.00  0.00           C
ATOM   1096  OG  SER   143     -12.478  93.507  20.312  1.00  0.00           O
ATOM   1097  C   SER   143      -9.713  93.959  20.811  1.00  0.00           C
ATOM   1098  O   SER   143      -9.665  94.782  19.897  1.00  0.00           O
ATOM   1099  N   HIS   144      -9.306  94.246  22.065  1.00  0.00           N
ATOM   1100  CA  HIS   144      -8.762  95.526  22.428  1.00  0.00           C
ATOM   1101  ND1 HIS   144     -10.948  95.497  24.965  1.00  0.00           N
ATOM   1102  CG  HIS   144      -9.862  96.259  24.600  1.00  0.00           C
ATOM   1103  NE2 HIS   144     -11.419  97.594  25.542  1.00  0.00           N
ATOM   1104  CD2 HIS   144     -10.165  97.536  24.960  1.00  0.00           C
ATOM   1105  CE1 HIS   144     -11.849  96.345  25.524  1.00  0.00           C
ATOM   1106  CB  HIS   144      -8.620  95.733  23.945  1.00  0.00           C
ATOM   1107  C   HIS   144      -7.409  95.764  21.834  1.00  0.00           C
ATOM   1108  O   HIS   144      -7.113  96.879  21.413  1.00  0.00           O
ATOM   1109  N   ASP   145      -6.525  94.748  21.811  1.00  0.00           N
ATOM   1110  CA  ASP   145      -5.198  95.025  21.334  1.00  0.00           C
ATOM   1111  CB  ASP   145      -4.081  94.552  22.280  1.00  0.00           C
ATOM   1112  CG  ASP   145      -4.043  95.519  23.456  1.00  0.00           C
ATOM   1113  OD1 ASP   145      -4.779  96.541  23.403  1.00  0.00           O
ATOM   1114  OD2 ASP   145      -3.276  95.253  24.420  1.00  0.00           O
ATOM   1115  C   ASP   145      -4.961  94.407  19.989  1.00  0.00           C
ATOM   1116  O   ASP   145      -4.888  93.189  19.842  1.00  0.00           O
ATOM   1117  N   VAL   146      -4.797  95.278  18.974  1.00  0.00           N
ATOM   1118  CA  VAL   146      -4.591  94.933  17.595  1.00  0.00           C
ATOM   1119  CB  VAL   146      -4.560  96.133  16.696  1.00  0.00           C
ATOM   1120  CG1 VAL   146      -4.210  95.670  15.272  1.00  0.00           C
ATOM   1121  CG2 VAL   146      -5.911  96.859  16.802  1.00  0.00           C
ATOM   1122  C   VAL   146      -3.282  94.229  17.422  1.00  0.00           C
ATOM   1123  O   VAL   146      -3.133  93.402  16.522  1.00  0.00           O
ATOM   1124  N   LEU   147      -2.294  94.551  18.273  1.00  0.00           N
ATOM   1125  CA  LEU   147      -0.967  94.019  18.152  1.00  0.00           C
ATOM   1126  CB  LEU   147      -0.013  94.523  19.249  1.00  0.00           C
ATOM   1127  CG  LEU   147       0.301  96.027  19.155  1.00  0.00           C
ATOM   1128  CD2 LEU   147      -0.970  96.878  19.311  1.00  0.00           C
ATOM   1129  CD1 LEU   147       1.085  96.352  17.873  1.00  0.00           C
ATOM   1130  C   LEU   147      -0.997  92.523  18.245  1.00  0.00           C
ATOM   1131  O   LEU   147      -0.168  91.856  17.627  1.00  0.00           O
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ATOM   1132  N   VAL   148      -1.927  91.946  19.032  1.00  0.00           N
ATOM   1133  CA  VAL   148      -1.920  90.516  19.175  1.00  0.00           C
ATOM   1134  CB  VAL   148      -2.808  90.022  20.286  1.00  0.00           C
ATOM   1135  CG1 VAL   148      -2.212  90.505  21.620  1.00  0.00           C
ATOM   1136  CG2 VAL   148      -4.245  90.528  20.061  1.00  0.00           C
ATOM   1137  C   VAL   148      -2.322  89.865  17.886  1.00  0.00           C
ATOM   1138  O   VAL   148      -3.501  89.758  17.543  1.00  0.00           O
ATOM   1139  N   ILE   149      -1.296  89.446  17.118  1.00  0.00           N
ATOM   1140  CA  ILE   149      -1.443  88.777  15.862  1.00  0.00           C
ATOM   1141  CB  ILE   149      -0.166  88.762  15.069  1.00  0.00           C
ATOM   1142  CG2 ILE   149       0.216  90.217  14.754  1.00  0.00           C
ATOM   1143  CG1 ILE   149       0.931  87.985  15.817  1.00  0.00           C
ATOM   1144  CD1 ILE   149       2.158  87.679  14.959  1.00  0.00           C
ATOM   1145  C   ILE   149      -1.885  87.354  16.025  1.00  0.00           C
ATOM   1146  O   ILE   149      -2.790  86.902  15.326  1.00  0.00           O
ATOM   1147  N   THR   150      -1.252  86.592  16.944  1.00  0.00           N
ATOM   1148  CA  THR   150      -1.594  85.199  16.983  1.00  0.00           C
ATOM   1149  CB  THR   150      -0.566  84.313  16.343  1.00  0.00           C
ATOM   1150  OG1 THR   150      -1.076  82.996  16.196  1.00  0.00           O
ATOM   1151  CG2 THR   150       0.693  84.296  17.226  1.00  0.00           C
ATOM   1152  C   THR   150      -1.771  84.727  18.387  1.00  0.00           C
ATOM   1153  O   THR   150      -1.155  85.235  19.321  1.00  0.00           O
ATOM   1154  N   ILE   151      -2.638  83.709  18.546  1.00  0.00           N
ATOM   1155  CA  ILE   151      -2.954  83.136  19.819  1.00  0.00           C
ATOM   1156  CB  ILE   151      -4.426  83.310  20.108  1.00  0.00           C
ATOM   1157  CG2 ILE   151      -5.255  82.425  19.168  1.00  0.00           C
ATOM   1158  CG1 ILE   151      -4.767  83.094  21.575  1.00  0.00           C
ATOM   1159  CD1 ILE   151      -6.198  83.539  21.880  1.00  0.00           C
ATOM   1160  C   ILE   151      -2.597  81.676  19.729  1.00  0.00           C
ATOM   1161  O   ILE   151      -2.973  80.995  18.777  1.00  0.00           O
ATOM   1162  N   ASP   152      -1.811  81.149  20.694  1.00  0.00           N
ATOM   1163  CA  ASP   152      -1.470  79.752  20.615  1.00  0.00           C
ATOM   1164  CB  ASP   152       0.023  79.465  20.352  1.00  0.00           C
ATOM   1165  CG  ASP   152       0.855  80.014  21.497  1.00  0.00           C
ATOM   1166  OD1 ASP   152       0.652  81.205  21.850  1.00  0.00           O
ATOM   1167  OD2 ASP   152       1.703  79.253  22.035  1.00  0.00           O
ATOM   1168  C   ASP   152      -1.872  79.066  21.887  1.00  0.00           C
ATOM   1169  O   ASP   152      -1.713  79.621  22.973  1.00  0.00           O
ATOM   1170  N   ASP   153      -2.416  77.829  21.778  1.00  0.00           N
ATOM   1171  CA  ASP   153      -2.884  77.111  22.938  1.00  0.00           C
ATOM   1172  CB  ASP   153      -4.148  76.273  22.685  1.00  0.00           C
ATOM   1173  CG  ASP   153      -4.697  75.860  24.040  1.00  0.00           C
ATOM   1174  OD1 ASP   153      -4.153  76.351  25.065  1.00  0.00           O
ATOM   1175  OD2 ASP   153      -5.671  75.061  24.071  1.00  0.00           O
ATOM   1176  C   ASP   153      -1.812  76.185  23.446  1.00  0.00           C
ATOM   1177  O   ASP   153      -1.302  75.331  22.723  1.00  0.00           O
ATOM   1178  N   ALA   154      -1.407  76.385  24.717  1.00  0.00           N
ATOM   1179  CA  ALA   154      -0.369  75.623  25.368  1.00  0.00           C
ATOM   1180  CB  ALA   154       0.136  76.297  26.656  1.00  0.00           C
ATOM   1181  C   ALA   154      -0.720  74.194  25.712  1.00  0.00           C
ATOM   1182  O   ALA   154       0.085  73.295  25.481  1.00  0.00           O
ATOM   1183  N   PRO   155      -1.868  73.948  26.280  1.00  0.00           N
ATOM   1184  CA  PRO   155      -2.256  72.634  26.755  1.00  0.00           C
ATOM   1185  CD  PRO   155      -2.579  75.001  26.985  1.00  0.00           C
ATOM   1186  CB  PRO   155      -3.328  72.874  27.820  1.00  0.00           C
ATOM   1187  CG  PRO   155      -3.814  74.308  27.565  1.00  0.00           C
ATOM   1188  C   PRO   155      -2.746  71.620  25.762  1.00  0.00           C
ATOM   1189  O   PRO   155      -3.086  70.521  26.196  1.00  0.00           O
ATOM   1190  N   LYS   156      -2.858  71.934  24.461  1.00  0.00           N
ATOM   1191  CA  LYS   156      -3.500  70.996  23.574  1.00  0.00           C
ATOM   1192  CB  LYS   156      -4.533  71.708  22.693  1.00  0.00           C
ATOM   1193  CG  LYS   156      -3.901  72.845  21.885  1.00  0.00           C
ATOM   1194  CD  LYS   156      -4.881  73.595  20.984  1.00  0.00           C
ATOM   1195  CE  LYS   156      -4.234  74.724  20.184  1.00  0.00           C
ATOM   1196  NZ  LYS   156      -5.232  75.779  19.906  1.00  0.00           N
ATOM   1197  C   LYS   156      -2.496  70.367  22.686  1.00  0.00           C
ATOM   1198  O   LYS   156      -1.454  70.950  22.482  1.00  0.00           O
ATOM   1199  N   GLU   157      -2.698  69.124  22.209  1.00  0.00           N
ATOM   1200  CA  GLU   157      -1.767  68.574  21.253  1.00  0.00           C
ATOM   1201  CB  GLU   157      -1.846  67.040  21.170  1.00  0.00           C
ATOM   1202  CG  GLU   157      -0.785  66.417  20.259  1.00  0.00           C
ATOM   1203  CD  GLU   157       0.550  66.488  20.984  1.00  0.00           C
ATOM   1204  OE1 GLU   157       0.703  67.387  21.852  1.00  0.00           O
ATOM   1205  OE2 GLU   157       1.434  65.643  20.680  1.00  0.00           O
ATOM   1206  C   GLU   157      -2.087  69.108  19.887  1.00  0.00           C
ATOM   1207  O   GLU   157      -1.215  69.567  19.150  1.00  0.00           O
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ATOM   1208  N   GLY   158      -3.383  69.055  19.516  1.00  0.00           N
ATOM   1209  CA  GLY   158      -3.799  69.482  18.212  1.00  0.00           C
ATOM   1210  C   GLY   158      -4.274  70.888  18.322  1.00  0.00           C
ATOM   1211  O   GLY   158      -4.141  71.514  19.370  1.00  0.00           O
ATOM   1212  N   CYS   159      -4.856  71.420  17.230  1.00  0.00           N
ATOM   1213  CA  CYS   159      -5.365  72.757  17.271  1.00  0.00           C
ATOM   1214  CB  CYS   159      -5.793  73.302  15.897  1.00  0.00           C
ATOM   1215  SG  CYS   159      -4.399  73.462  14.741  1.00  0.00           S
ATOM   1216  C   CYS   159      -6.580  72.714  18.134  1.00  0.00           C
ATOM   1217  O   CYS   159      -7.236  71.678  18.225  1.00  0.00           O
ATOM   1218  N   GLN   160      -6.901  73.827  18.826  1.00  0.00           N
ATOM   1219  CA  GLN   160      -8.079  73.780  19.640  1.00  0.00           C
ATOM   1220  CB  GLN   160      -7.816  73.740  21.153  1.00  0.00           C
ATOM   1221  CG  GLN   160      -9.092  73.518  21.966  1.00  0.00           C
ATOM   1222  CD  GLN   160      -9.599  72.119  21.645  1.00  0.00           C
ATOM   1223  OE1 GLN   160      -8.915  71.332  20.991  1.00  0.00           O
ATOM   1224  NE2 GLN   160     -10.835  71.796  22.111  1.00  0.00           N
ATOM   1225  C   GLN   160      -8.919  74.988  19.371  1.00  0.00           C
ATOM   1226  O   GLN   160      -8.433  76.120  19.393  1.00  0.00           O
ATOM   1227  N   HIS   161     -10.221  74.751  19.106  1.00  0.00           N
ATOM   1228  CA  HIS   161     -11.187  75.790  18.876  1.00  0.00           C
ATOM   1229  ND1 HIS   161     -11.949  74.883  22.031  1.00  0.00           N
ATOM   1230  CG  HIS   161     -12.445  75.719  21.057  1.00  0.00           C
ATOM   1231  NE2 HIS   161     -14.164  74.701  22.107  1.00  0.00           N
ATOM   1232  CD2 HIS   161     -13.800  75.597  21.117  1.00  0.00           C
ATOM   1233  CE1 HIS   161     -13.019  74.299  22.628  1.00  0.00           C
ATOM   1234  CB  HIS   161     -11.597  76.554  20.145  1.00  0.00           C
ATOM   1235  C   HIS   161     -10.639  76.748  17.884  1.00  0.00           C
ATOM   1236  O   HIS   161     -10.626  77.953  18.127  1.00  0.00           O
ATOM   1237  N   ILE   162     -10.215  76.206  16.728  1.00  0.00           N
ATOM   1238  CA  ILE   162      -9.516  76.913  15.700  1.00  0.00           C
ATOM   1239  CB  ILE   162     -10.408  77.685  14.759  1.00  0.00           C
ATOM   1240  CG2 ILE   162     -11.270  78.677  15.561  1.00  0.00           C
ATOM   1241  CG1 ILE   162      -9.573  78.320  13.635  1.00  0.00           C
ATOM   1242  CD1 ILE   162     -10.412  78.867  12.481  1.00  0.00           C
ATOM   1243  C   ILE   162      -8.542  77.815  16.379  1.00  0.00           C
ATOM   1244  O   ILE   162      -8.795  78.972  16.694  1.00  0.00           O
ATOM   1245  N   SER   163      -7.353  77.260  16.605  1.00  0.00           N
ATOM   1246  CA  SER   163      -6.256  77.923  17.221  1.00  0.00           C
ATOM   1247  CB  SER   163      -6.471  78.264  18.702  1.00  0.00           C
ATOM   1248  OG  SER   163      -5.327  78.924  19.223  1.00  0.00           O
ATOM   1249  C   SER   163      -5.209  76.882  17.156  1.00  0.00           C
ATOM   1250  O   SER   163      -5.513  75.693  17.223  1.00  0.00           O
ATOM   1251  N   VAL   164      -3.944  77.281  17.015  1.00  0.00           N
ATOM   1252  CA  VAL   164      -2.957  76.255  16.920  1.00  0.00           C
ATOM   1253  CB  VAL   164      -1.817  76.605  16.007  1.00  0.00           C
ATOM   1254  CG1 VAL   164      -2.366  76.783  14.582  1.00  0.00           C
ATOM   1255  CG2 VAL   164      -1.112  77.852  16.566  1.00  0.00           C
ATOM   1256  C   VAL   164      -2.377  76.028  18.278  1.00  0.00           C
ATOM   1257  O   VAL   164      -2.351  76.929  19.113  1.00  0.00           O
ATOM   1258  N   LEU   165      -1.945  74.777  18.530  1.00  0.00           N
ATOM   1259  CA  LEU   165      -1.192  74.433  19.706  1.00  0.00           C
ATOM   1260  CB  LEU   165      -1.090  72.891  19.985  1.00  0.00           C
ATOM   1261  CG  LEU   165       0.144  72.444  20.847  1.00  0.00           C
ATOM   1262  CD2 LEU   165       0.554  70.971  20.697  1.00  0.00           C
ATOM   1263  CD1 LEU   165       0.176  73.063  22.266  1.00  0.00           C
ATOM   1264  C   LEU   165       0.195  74.893  19.386  1.00  0.00           C
ATOM   1265  O   LEU   165       0.499  75.218  18.243  1.00  0.00           O
ATOM   1266  N   THR   166       1.065  74.953  20.403  1.00  0.00           N
ATOM   1267  CA  THR   166       2.446  75.178  20.214  1.00  0.00           C
ATOM   1268  CB  THR   166       3.229  75.077  21.489  1.00  0.00           C
ATOM   1269  OG1 THR   166       4.570  75.491  21.275  1.00  0.00           O
ATOM   1270  CG2 THR   166       3.191  73.619  21.977  1.00  0.00           C
ATOM   1271  C   THR   166       2.967  74.118  19.268  1.00  0.00           C
ATOM   1272  O   THR   166       3.868  74.409  18.485  1.00  0.00           O
ATOM   1273  N   GLU   167       2.471  72.855  19.317  1.00  0.00           N
ATOM   1274  CA  GLU   167       3.007  71.859  18.413  1.00  0.00           C
ATOM   1275  CB  GLU   167       2.580  70.394  18.641  1.00  0.00           C
ATOM   1276  CG  GLU   167       1.239  70.011  18.006  1.00  0.00           C
ATOM   1277  CD  GLU   167       1.105  68.495  18.061  1.00  0.00           C
ATOM   1278  OE1 GLU   167       2.065  67.835  18.538  1.00  0.00           O
ATOM   1279  OE2 GLU   167       0.045  67.976  17.620  1.00  0.00           O
ATOM   1280  C   GLU   167       2.628  72.155  16.992  1.00  0.00           C
ATOM   1281  O   GLU   167       3.452  72.020  16.091  1.00  0.00           O
ATOM   1282  N   ALA   168       1.358  72.528  16.738  1.00  0.00           N
ATOM   1283  CA  ALA   168       0.928  72.787  15.391  1.00  0.00           C
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ATOM   1284  CB  ALA   168      -0.580  73.067  15.289  1.00  0.00           C
ATOM   1285  C   ALA   168       1.644  73.992  14.873  1.00  0.00           C
ATOM   1286  O   ALA   168       2.079  74.023  13.724  1.00  0.00           O
ATOM   1287  N   ASP   169       1.791  75.034  15.711  1.00  0.00           N
ATOM   1288  CA  ASP   169       2.431  76.219  15.225  1.00  0.00           C
ATOM   1289  CB  ASP   169       2.344  77.432  16.183  1.00  0.00           C
ATOM   1290  CG  ASP   169       3.025  77.184  17.524  1.00  0.00           C
ATOM   1291  OD1 ASP   169       4.235  76.836  17.549  1.00  0.00           O
ATOM   1292  OD2 ASP   169       2.325  77.360  18.557  1.00  0.00           O
ATOM   1293  C   ASP   169       3.854  75.914  14.873  1.00  0.00           C
ATOM   1294  O   ASP   169       4.377  76.427  13.885  1.00  0.00           O
ATOM   1295  N   GLU   170       4.516  75.053  15.666  1.00  0.00           N
ATOM   1296  CA  GLU   170       5.877  74.691  15.420  1.00  0.00           C
ATOM   1297  CB  GLU   170       6.434  73.775  16.521  1.00  0.00           C
ATOM   1298  CG  GLU   170       6.543  74.490  17.871  1.00  0.00           C
ATOM   1299  CD  GLU   170       6.828  73.450  18.943  1.00  0.00           C
ATOM   1300  OE1 GLU   170       6.324  72.304  18.804  1.00  0.00           O
ATOM   1301  OE2 GLU   170       7.555  73.787  19.916  1.00  0.00           O
ATOM   1302  C   GLU   170       5.915  73.954  14.116  1.00  0.00           C
ATOM   1303  O   GLU   170       6.819  74.121  13.311  1.00  0.00           O
ATOM   1304  N   THR   171       4.922  73.113  13.823  1.00  0.00           N
ATOM   1305  CA  THR   171       5.024  72.390  12.592  1.00  0.00           C
ATOM   1306  CB  THR   171       3.970  71.334  12.395  1.00  0.00           C
ATOM   1307  OG1 THR   171       4.380  70.441  11.372  1.00  0.00           O
ATOM   1308  CG2 THR   171       2.643  71.991  11.985  1.00  0.00           C
ATOM   1309  C   THR   171       4.964  73.340  11.434  1.00  0.00           C
ATOM   1310  O   THR   171       5.565  73.078  10.393  1.00  0.00           O
ATOM   1311  N   GLN   172       4.222  74.462  11.544  1.00  0.00           N
ATOM   1312  CA  GLN   172       4.160  75.263  10.357  1.00  0.00           C
ATOM   1313  CB  GLN   172       2.770  75.856  10.053  1.00  0.00           C
ATOM   1314  CG  GLN   172       2.235  76.832  11.102  1.00  0.00           C
ATOM   1315  CD  GLN   172       1.220  76.084  11.954  1.00  0.00           C
ATOM   1316  OE1 GLN   172       0.891  74.933  11.674  1.00  0.00           O
ATOM   1317  NE2 GLN   172       0.693  76.761  13.009  1.00  0.00           N
ATOM   1318  C   GLN   172       5.132  76.407  10.364  1.00  0.00           C
ATOM   1319  O   GLN   172       4.866  77.425   9.727  1.00  0.00           O
ATOM   1320  N   CYS   173       6.308  76.280  11.015  1.00  0.00           N
ATOM   1321  CA  CYS   173       7.216  77.396  10.958  1.00  0.00           C
ATOM   1322  CB  CYS   173       7.099  78.331  12.179  1.00  0.00           C
ATOM   1323  SG  CYS   173       5.418  78.987  12.374  1.00  0.00           S
ATOM   1324  C   CYS   173       8.627  76.879  10.846  1.00  0.00           C
ATOM   1325  O   CYS   173       9.457  77.476  10.168  1.00  0.00           O
ATOM   1326  N   PRO   174       8.953  75.822  11.533  1.00  0.00           N
ATOM   1327  CA  PRO   174      10.252  75.265  11.310  1.00  0.00           C
ATOM   1328  CD  PRO   174       8.810  75.986  12.973  1.00  0.00           C
ATOM   1329  CB  PRO   174      10.521  74.335  12.482  1.00  0.00           C
ATOM   1330  CG  PRO   174       9.905  75.133  13.640  1.00  0.00           C
ATOM   1331  C   PRO   174      10.610  74.731   9.975  1.00  0.00           C
ATOM   1332  O   PRO   174       9.758  74.408   9.149  1.00  0.00           O
ATOM   1333  N   ALA   175      11.936  74.672   9.798  1.00  0.00           N
ATOM   1334  CA  ALA   175      12.673  74.371   8.620  1.00  0.00           C
ATOM   1335  CB  ALA   175      14.190  74.461   8.844  1.00  0.00           C
ATOM   1336  C   ALA   175      12.398  73.024   8.043  1.00  0.00           C
ATOM   1337  O   ALA   175      12.451  72.972   6.835  1.00  0.00           O
ATOM   1338  N   VAL   176      12.183  71.919   8.799  1.00  0.00           N
ATOM   1339  CA  VAL   176      11.927  70.576   8.281  1.00  0.00           C
ATOM   1340  CB  VAL   176      11.776  70.362   6.796  1.00  0.00           C
ATOM   1341  CG1 VAL   176      11.725  68.848   6.528  1.00  0.00           C
ATOM   1342  CG2 VAL   176      10.514  71.103   6.317  1.00  0.00           C
ATOM   1343  C   VAL   176      13.068  69.740   8.726  1.00  0.00           C
ATOM   1344  O   VAL   176      12.972  68.964   9.673  1.00  0.00           O
ATOM   1345  N   LYS   177      14.191  69.890   8.006  1.00  0.00           N
ATOM   1346  CA  LYS   177      15.400  69.192   8.301  1.00  0.00           C
ATOM   1347  CB  LYS   177      16.556  69.543   7.347  1.00  0.00           C
ATOM   1348  CG  LYS   177      16.357  69.048   5.913  1.00  0.00           C
ATOM   1349  CD  LYS   177      17.372  69.633   4.928  1.00  0.00           C
ATOM   1350  CE  LYS   177      17.210  69.117   3.497  1.00  0.00           C
ATOM   1351  NZ  LYS   177      18.230  69.736   2.620  1.00  0.00           N
ATOM   1352  C   LYS   177      15.822  69.616   9.668  1.00  0.00           C
ATOM   1353  O   LYS   177      16.537  68.869  10.334  1.00  0.00           O
ATOM   1354  N   ILE   178      15.400  70.836  10.088  1.00  0.00           N
ATOM   1355  CA  ILE   178      15.776  71.451  11.341  1.00  0.00           C
ATOM   1356  CB  ILE   178      14.815  72.508  11.808  1.00  0.00           C
ATOM   1357  CG2 ILE   178      13.477  71.821  12.130  1.00  0.00           C
ATOM   1358  CG1 ILE   178      15.411  73.292  12.989  1.00  0.00           C
ATOM   1359  CD1 ILE   178      16.631  74.131  12.610  1.00  0.00           C
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ATOM   1360  C   ILE   178      15.927  70.452  12.450  1.00  0.00           C
ATOM   1361  O   ILE   178      15.111  69.552  12.639  1.00  0.00           O
ATOM   1362  N   HIS   179      17.045  70.558  13.194  1.00  0.00           N
ATOM   1363  CA  HIS   179      17.207  69.679  14.315  1.00  0.00           C
ATOM   1364  ND1 HIS   179      20.628  68.698  14.748  1.00  0.00           N
ATOM   1365  CG  HIS   179      19.616  68.818  13.822  1.00  0.00           C
ATOM   1366  NE2 HIS   179      21.585  69.306  12.836  1.00  0.00           N
ATOM   1367  CD2 HIS   179      20.217  69.195  12.661  1.00  0.00           C
ATOM   1368  CE1 HIS   179      21.783  68.997  14.105  1.00  0.00           C
ATOM   1369  CB  HIS   179      18.183  68.499  14.113  1.00  0.00           C
ATOM   1370  C   HIS   179      17.578  70.510  15.503  1.00  0.00           C
ATOM   1371  O   HIS   179      18.427  71.399  15.452  1.00  0.00           O
ATOM   1372  N   PRO   180      16.915  70.217  16.583  1.00  0.00           N
ATOM   1373  CA  PRO   180      17.083  70.975  17.792  1.00  0.00           C
ATOM   1374  CD  PRO   180      15.594  69.614  16.500  1.00  0.00           C
ATOM   1375  CB  PRO   180      15.978  70.505  18.732  1.00  0.00           C
ATOM   1376  CG  PRO   180      14.857  70.063  17.772  1.00  0.00           C
ATOM   1377  C   PRO   180      18.459  70.878  18.356  1.00  0.00           C
ATOM   1378  O   PRO   180      18.811  71.717  19.184  1.00  0.00           O
ATOM   1379  N   ASP   181      19.225  69.848  17.963  1.00  0.00           N
ATOM   1380  CA  ASP   181      20.566  69.627  18.422  1.00  0.00           C
ATOM   1381  CB  ASP   181      21.103  68.239  18.030  1.00  0.00           C
ATOM   1382  CG  ASP   181      20.327  67.195  18.820  1.00  0.00           C
ATOM   1383  OD1 ASP   181      19.545  67.597  19.723  1.00  0.00           O
ATOM   1384  OD2 ASP   181      20.503  65.981  18.529  1.00  0.00           O
ATOM   1385  C   ASP   181      21.519  70.644  17.853  1.00  0.00           C
ATOM   1386  O   ASP   181      22.529  70.957  18.484  1.00  0.00           O
ATOM   1387  N   ASP   182      21.279  71.156  16.624  1.00  0.00           N
ATOM   1388  CA  ASP   182      22.262  72.080  16.121  1.00  0.00           C
ATOM   1389  CB  ASP   182      22.737  71.808  14.678  1.00  0.00           C
ATOM   1390  CG  ASP   182      21.601  72.003  13.681  1.00  0.00           C
ATOM   1391  OD1 ASP   182      20.433  72.175  14.115  1.00  0.00           O
ATOM   1392  OD2 ASP   182      21.894  71.975  12.456  1.00  0.00           O
ATOM   1393  C   ASP   182      21.725  73.476  16.152  1.00  0.00           C
ATOM   1394  O   ASP   182      22.344  74.393  15.612  1.00  0.00           O
ATOM   1395  N   VAL   183      20.576  73.694  16.812  1.00  0.00           N
ATOM   1396  CA  VAL   183      20.072  75.032  16.878  1.00  0.00           C
ATOM   1397  CB  VAL   183      18.698  75.126  17.474  1.00  0.00           C
ATOM   1398  CG1 VAL   183      18.314  76.611  17.591  1.00  0.00           C
ATOM   1399  CG2 VAL   183      17.731  74.297  16.610  1.00  0.00           C
ATOM   1400  C   VAL   183      20.997  75.817  17.749  1.00  0.00           C
ATOM   1401  O   VAL   183      21.544  75.293  18.719  1.00  0.00           O
ATOM   1402  N   VAL   184      21.222  77.100  17.392  1.00  0.00           N
ATOM   1403  CA  VAL   184      22.060  77.955  18.177  1.00  0.00           C
ATOM   1404  CB  VAL   184      23.202  78.547  17.402  1.00  0.00           C
ATOM   1405  CG1 VAL   184      23.970  79.517  18.315  1.00  0.00           C
ATOM   1406  CG2 VAL   184      24.061  77.399  16.847  1.00  0.00           C
ATOM   1407  C   VAL   184      21.189  79.084  18.628  1.00  0.00           C
ATOM   1408  O   VAL   184      20.461  79.674  17.831  1.00  0.00           O
ATOM   1409  N   ALA   185      21.242  79.406  19.933  1.00  0.00           N
ATOM   1410  CA  ALA   185      20.435  80.440  20.508  1.00  0.00           C
ATOM   1411  CB  ALA   185      20.458  80.375  22.032  1.00  0.00           C
ATOM   1412  C   ALA   185      20.976  81.771  20.056  1.00  0.00           C
ATOM   1413  O   ALA   185      22.133  81.860  19.647  1.00  0.00           O
ATOM   1414  N   LEU   186      20.134  82.834  20.084  1.00  0.00           N
ATOM   1415  CA  LEU   186      20.509  84.145  19.603  1.00  0.00           C
ATOM   1416  CB  LEU   186      19.303  85.044  19.278  1.00  0.00           C
ATOM   1417  CG  LEU   186      18.422  84.504  18.137  1.00  0.00           C
ATOM   1418  CD2 LEU   186      17.392  85.551  17.682  1.00  0.00           C
ATOM   1419  CD1 LEU   186      17.778  83.162  18.516  1.00  0.00           C
ATOM   1420  C   LEU   186      21.360  84.890  20.599  1.00  0.00           C
ATOM   1421  O   LEU   186      21.021  85.045  21.763  1.00  0.00           O
ATOM   1422  N   PRO   187      22.469  85.372  20.131  1.00  0.00           N
ATOM   1423  CA  PRO   187      23.424  86.093  20.955  1.00  0.00           C
ATOM   1424  CD  PRO   187      23.149  84.554  19.136  1.00  0.00           C
ATOM   1425  CB  PRO   187      24.794  85.866  20.315  1.00  0.00           C
ATOM   1426  CG  PRO   187      24.632  84.563  19.522  1.00  0.00           C
ATOM   1427  C   PRO   187      23.209  87.570  21.205  1.00  0.00           C
ATOM   1428  O   PRO   187      24.202  88.251  21.409  1.00  0.00           O
ATOM   1429  N   TYR   188      22.005  88.148  21.163  1.00  0.00           N
ATOM   1430  CA  TYR   188      21.944  89.588  21.130  1.00  0.00           C
ATOM   1431  CB  TYR   188      20.472  90.017  21.112  1.00  0.00           C
ATOM   1432  CG  TYR   188      19.762  89.069  22.024  1.00  0.00           C
ATOM   1433  CD1 TYR   188      19.646  89.287  23.379  1.00  0.00           C
ATOM   1434  CD2 TYR   188      19.219  87.921  21.496  1.00  0.00           C
ATOM   1435  CE1 TYR   188      18.984  88.395  24.190  1.00  0.00           C
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ATOM   1436  CE2 TYR   188      18.561  87.026  22.295  1.00  0.00           C
ATOM   1437  CZ  TYR   188      18.443  87.262  23.642  1.00  0.00           C
ATOM   1438  OH  TYR   188      17.756  86.340  24.454  1.00  0.00           O
ATOM   1439  C   TYR   188      22.661  90.388  22.189  1.00  0.00           C
ATOM   1440  O   TYR   188      23.768  90.841  21.934  1.00  0.00           O
ATOM   1441  N   SER   189      22.164  90.546  23.424  1.00  0.00           N
ATOM   1442  CA  SER   189      22.887  91.410  24.323  1.00  0.00           C
ATOM   1443  CB  SER   189      22.891  92.887  23.895  1.00  0.00           C
ATOM   1444  OG  SER   189      23.619  93.666  24.832  1.00  0.00           O
ATOM   1445  C   SER   189      22.149  91.334  25.608  1.00  0.00           C
ATOM   1446  O   SER   189      20.970  91.668  25.677  1.00  0.00           O
ATOM   1447  N   SER   190      22.848  90.914  26.667  1.00  0.00           N
ATOM   1448  CA  SER   190      22.218  90.641  27.919  1.00  0.00           C
ATOM   1449  CB  SER   190      23.193  89.972  28.901  1.00  0.00           C
ATOM   1450  OG  SER   190      22.547  89.711  30.137  1.00  0.00           O
ATOM   1451  C   SER   190      21.681  91.868  28.584  1.00  0.00           C
ATOM   1452  O   SER   190      20.605  91.826  29.181  1.00  0.00           O
ATOM   1453  N   GLY   191      22.450  92.973  28.565  1.00  0.00           N
ATOM   1454  CA  GLY   191      22.016  94.162  29.246  1.00  0.00           C
ATOM   1455  C   GLY   191      20.862  94.820  28.565  1.00  0.00           C
ATOM   1456  O   GLY   191      19.896  95.221  29.210  1.00  0.00           O
ATOM   1457  N   THR   192      20.962  95.002  27.238  1.00  0.00           N
ATOM   1458  CA  THR   192      19.955  95.711  26.509  1.00  0.00           C
ATOM   1459  CB  THR   192      20.397  96.076  25.123  1.00  0.00           C
ATOM   1460  OG1 THR   192      20.646  94.903  24.363  1.00  0.00           O
ATOM   1461  CG2 THR   192      21.675  96.925  25.223  1.00  0.00           C
ATOM   1462  C   THR   192      18.706  94.906  26.371  1.00  0.00           C
ATOM   1463  O   THR   192      17.604  95.428  26.528  1.00  0.00           O
ATOM   1464  N   THR   193      18.838  93.603  26.064  1.00  0.00           N
ATOM   1465  CA  THR   193      17.641  92.870  25.788  1.00  0.00           C
ATOM   1466  CB  THR   193      17.830  91.619  24.995  1.00  0.00           C
ATOM   1467  OG1 THR   193      18.599  90.682  25.727  1.00  0.00           O
ATOM   1468  CG2 THR   193      18.530  91.995  23.682  1.00  0.00           C
ATOM   1469  C   THR   193      16.958  92.513  27.051  1.00  0.00           C
ATOM   1470  O   THR   193      17.587  92.149  28.045  1.00  0.00           O
ATOM   1471  N   GLY   194      15.616  92.589  27.019  1.00  0.00           N
ATOM   1472  CA  GLY   194      14.906  92.366  28.234  1.00  0.00           C
ATOM   1473  C   GLY   194      14.071  91.145  28.156  1.00  0.00           C
ATOM   1474  O   GLY   194      13.651  90.702  27.091  1.00  0.00           O
ATOM   1475  N   LEU   195      13.917  90.508  29.325  1.00  0.00           N
ATOM   1476  CA  LEU   195      13.017  89.425  29.511  1.00  0.00           C
ATOM   1477  CB  LEU   195      13.434  88.490  30.652  1.00  0.00           C
ATOM   1478  CG  LEU   195      14.704  87.708  30.281  1.00  0.00           C
ATOM   1479  CD2 LEU   195      14.580  87.095  28.877  1.00  0.00           C
ATOM   1480  CD1 LEU   195      15.057  86.668  31.346  1.00  0.00           C
ATOM   1481  C   LEU   195      11.521  89.863  29.688  1.00  0.00           C
ATOM   1482  O   LEU   195      10.769  89.167  29.023  1.00  0.00           O
ATOM   1483  N   PRO   196      11.024  90.866  30.522  1.00  0.00           N
ATOM   1484  CA  PRO   196       9.590  91.261  30.789  1.00  0.00           C
ATOM   1485  CD  PRO   196      11.732  90.852  31.792  1.00  0.00           C
ATOM   1486  CB  PRO   196       9.383  91.102  32.298  1.00  0.00           C
ATOM   1487  CG  PRO   196      10.672  90.455  32.826  1.00  0.00           C
ATOM   1488  C   PRO   196       9.015  92.639  30.383  1.00  0.00           C
ATOM   1489  O   PRO   196       9.211  93.099  29.264  1.00  0.00           O
ATOM   1490  N   LYS   197       8.166  93.239  31.288  1.00  0.00           N
ATOM   1491  CA  LYS   197       7.652  94.614  31.344  1.00  0.00           C
ATOM   1492  CB  LYS   197       6.516  95.103  30.427  1.00  0.00           C
ATOM   1493  CG  LYS   197       6.580  96.614  30.046  1.00  0.00           C
ATOM   1494  CD  LYS   197       6.746  97.723  31.114  1.00  0.00           C
ATOM   1495  CE  LYS   197       5.453  98.216  31.770  1.00  0.00           C
ATOM   1496  NZ  LYS   197       5.773  99.184  32.843  1.00  0.00           N
ATOM   1497  C   LYS   197       7.039  94.716  32.695  1.00  0.00           C
ATOM   1498  O   LYS   197       7.278  93.867  33.550  1.00  0.00           O
ATOM   1499  N   GLY   198       6.170  95.728  32.893  1.00  0.00           N
ATOM   1500  CA  GLY   198       5.829  96.066  34.206  1.00  0.00           C
ATOM   1501  C   GLY   198       7.222  96.409  34.553  1.00  0.00           C
ATOM   1502  O   GLY   198       7.787  97.350  33.995  1.00  0.00           O
ATOM   1503  N   VAL   199       7.834  95.574  35.396  1.00  0.00           N
ATOM   1504  CA  VAL   199       9.231  95.700  35.625  1.00  0.00           C
ATOM   1505  CB  VAL   199       9.646  95.046  36.911  1.00  0.00           C
ATOM   1506  CG1 VAL   199      11.173  95.128  37.055  1.00  0.00           C
ATOM   1507  CG2 VAL   199       8.863  95.701  38.058  1.00  0.00           C
ATOM   1508  C   VAL   199       9.944  94.976  34.514  1.00  0.00           C
ATOM   1509  O   VAL   199       9.717  93.788  34.288  1.00  0.00           O
ATOM   1510  N   MET   200      10.841  95.688  33.796  1.00  0.00           N
ATOM   1511  CA  MET   200      11.598  95.122  32.709  1.00  0.00           C
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ATOM   1512  CB  MET   200      12.068  96.181  31.699  1.00  0.00           C
ATOM   1513  CG  MET   200      10.969  96.741  30.802  1.00  0.00           C
ATOM   1514  SD  MET   200      10.581  95.675  29.387  1.00  0.00           S
ATOM   1515  CE  MET   200      12.153  96.011  28.540  1.00  0.00           C
ATOM   1516  C   MET   200      12.845  94.540  33.288  1.00  0.00           C
ATOM   1517  O   MET   200      13.602  95.228  33.972  1.00  0.00           O
ATOM   1518  N   LEU   201      13.096  93.242  33.025  1.00  0.00           N
ATOM   1519  CA  LEU   201      14.282  92.642  33.563  1.00  0.00           C
ATOM   1520  CB  LEU   201      13.985  91.440  34.475  1.00  0.00           C
ATOM   1521  CG  LEU   201      13.105  91.792  35.690  1.00  0.00           C
ATOM   1522  CD2 LEU   201      13.681  92.976  36.484  1.00  0.00           C
ATOM   1523  CD1 LEU   201      12.845  90.558  36.566  1.00  0.00           C
ATOM   1524  C   LEU   201      15.086  92.134  32.415  1.00  0.00           C
ATOM   1525  O   LEU   201      14.665  91.218  31.715  1.00  0.00           O
ATOM   1526  N   THR   202      16.287  92.702  32.212  1.00  0.00           N
ATOM   1527  CA  THR   202      17.125  92.310  31.121  1.00  0.00           C
ATOM   1528  CB  THR   202      18.284  93.237  30.929  1.00  0.00           C
ATOM   1529  OG1 THR   202      19.145  93.190  32.057  1.00  0.00           O
ATOM   1530  CG2 THR   202      17.714  94.657  30.768  1.00  0.00           C
ATOM   1531  C   THR   202      17.644  90.946  31.427  1.00  0.00           C
ATOM   1532  O   THR   202      17.478  90.434  32.532  1.00  0.00           O
ATOM   1533  N   HIS   203      18.288  90.318  30.431  1.00  0.00           N
ATOM   1534  CA  HIS   203      18.776  88.978  30.576  1.00  0.00           C
ATOM   1535  ND1 HIS   203      18.009  86.616  28.192  1.00  0.00           N
ATOM   1536  CG  HIS   203      18.385  87.936  28.307  1.00  0.00           C
ATOM   1537  NE2 HIS   203      16.807  87.750  26.706  1.00  0.00           N
ATOM   1538  CD2 HIS   203      17.640  88.614  27.392  1.00  0.00           C
ATOM   1539  CE1 HIS   203      17.064  86.561  27.221  1.00  0.00           C
ATOM   1540  CB  HIS   203      19.409  88.419  29.290  1.00  0.00           C
ATOM   1541  C   HIS   203      19.796  88.903  31.670  1.00  0.00           C
ATOM   1542  O   HIS   203      19.909  87.884  32.347  1.00  0.00           O
ATOM   1543  N   LYS   204      20.562  89.984  31.883  1.00  0.00           N
ATOM   1544  CA  LYS   204      21.644  89.958  32.829  1.00  0.00           C
ATOM   1545  CB  LYS   204      22.382  91.305  32.921  1.00  0.00           C
ATOM   1546  CG  LYS   204      21.492  92.463  33.368  1.00  0.00           C
ATOM   1547  CD  LYS   204      22.263  93.731  33.731  1.00  0.00           C
ATOM   1548  CE  LYS   204      21.352  94.876  34.176  1.00  0.00           C
ATOM   1549  NZ  LYS   204      22.163  96.067  34.509  1.00  0.00           N
ATOM   1550  C   LYS   204      21.166  89.595  34.207  1.00  0.00           C
ATOM   1551  O   LYS   204      21.859  88.889  34.936  1.00  0.00           O
ATOM   1552  N   GLY   205      19.977  90.058  34.623  1.00  0.00           N
ATOM   1553  CA  GLY   205      19.534  89.781  35.966  1.00  0.00           C
ATOM   1554  C   GLY   205      19.408  88.301  36.163  1.00  0.00           C
ATOM   1555  O   GLY   205      19.746  87.779  37.225  1.00  0.00           O
ATOM   1556  N   LEU   206      18.881  87.586  35.154  1.00  0.00           N
ATOM   1557  CA  LEU   206      18.737  86.168  35.291  1.00  0.00           C
ATOM   1558  CB  LEU   206      17.901  85.502  34.191  1.00  0.00           C
ATOM   1559  CG  LEU   206      16.397  85.791  34.341  1.00  0.00           C
ATOM   1560  CD2 LEU   206      15.553  84.781  33.547  1.00  0.00           C
ATOM   1561  CD1 LEU   206      16.071  87.264  34.050  1.00  0.00           C
ATOM   1562  C   LEU   206      20.082  85.514  35.345  1.00  0.00           C
ATOM   1563  O   LEU   206      20.264  84.547  36.084  1.00  0.00           O
ATOM   1564  N   VAL   207      21.066  86.013  34.567  1.00  0.00           N
ATOM   1565  CA  VAL   207      22.357  85.377  34.573  1.00  0.00           C
ATOM   1566  CB  VAL   207      23.348  85.940  33.588  1.00  0.00           C
ATOM   1567  CG1 VAL   207      23.902  87.273  34.110  1.00  0.00           C
ATOM   1568  CG2 VAL   207      24.437  84.879  33.355  1.00  0.00           C
ATOM   1569  C   VAL   207      22.941  85.501  35.946  1.00  0.00           C
ATOM   1570  O   VAL   207      23.626  84.601  36.422  1.00  0.00           O
ATOM   1571  N   SER   208      22.713  86.639  36.625  1.00  0.00           N
ATOM   1572  CA  SER   208      23.226  86.793  37.956  1.00  0.00           C
ATOM   1573  CB  SER   208      22.967  88.195  38.536  1.00  0.00           C
ATOM   1574  OG  SER   208      23.665  89.174  37.778  1.00  0.00           O
ATOM   1575  C   SER   208      22.536  85.801  38.845  1.00  0.00           C
ATOM   1576  O   SER   208      23.160  85.188  39.709  1.00  0.00           O
ATOM   1577  N   SER   209      21.218  85.610  38.638  1.00  0.00           N
ATOM   1578  CA  SER   209      20.433  84.721  39.450  1.00  0.00           C
ATOM   1579  CB  SER   209      18.948  84.711  39.055  1.00  0.00           C
ATOM   1580  OG  SER   209      18.227  83.817  39.889  1.00  0.00           O
ATOM   1581  C   SER   209      20.945  83.315  39.300  1.00  0.00           C
ATOM   1582  O   SER   209      20.890  82.534  40.249  1.00  0.00           O
ATOM   1583  N   VAL   210      21.458  82.940  38.113  1.00  0.00           N
ATOM   1584  CA  VAL   210      21.916  81.582  37.964  1.00  0.00           C
ATOM   1585  CB  VAL   210      22.401  81.162  36.608  1.00  0.00           C
ATOM   1586  CG1 VAL   210      23.713  81.880  36.274  1.00  0.00           C
ATOM   1587  CG2 VAL   210      22.602  79.638  36.673  1.00  0.00           C
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ATOM   1588  C   VAL   210      23.063  81.341  38.886  1.00  0.00           C
ATOM   1589  O   VAL   210      23.250  80.230  39.373  1.00  0.00           O
ATOM   1590  N   ALA   211      23.907  82.358  39.115  1.00  0.00           N
ATOM   1591  CA  ALA   211      25.014  82.146  40.003  1.00  0.00           C
ATOM   1592  CB  ALA   211      25.933  83.376  40.108  1.00  0.00           C
ATOM   1593  C   ALA   211      24.470  81.870  41.371  1.00  0.00           C
ATOM   1594  O   ALA   211      24.940  80.986  42.088  1.00  0.00           O
ATOM   1595  N   GLN   212      23.431  82.635  41.743  1.00  0.00           N
ATOM   1596  CA  GLN   212      22.795  82.580  43.023  1.00  0.00           C
ATOM   1597  CB  GLN   212      21.639  83.602  43.027  1.00  0.00           C
ATOM   1598  CG  GLN   212      20.977  83.907  44.366  1.00  0.00           C
ATOM   1599  CD  GLN   212      19.876  84.928  44.114  1.00  0.00           C
ATOM   1600  OE1 GLN   212      19.022  85.166  44.966  1.00  0.00           O
ATOM   1601  NE2 GLN   212      19.893  85.547  42.903  1.00  0.00           N
ATOM   1602  C   GLN   212      22.231  81.202  43.216  1.00  0.00           C
ATOM   1603  O   GLN   212      22.436  80.592  44.264  1.00  0.00           O
ATOM   1604  N   GLN   213      21.592  80.635  42.172  1.00  0.00           N
ATOM   1605  CA  GLN   213      20.838  79.414  42.301  1.00  0.00           C
ATOM   1606  CB  GLN   213      20.349  78.860  40.951  1.00  0.00           C
ATOM   1607  CG  GLN   213      21.466  78.292  40.076  1.00  0.00           C
ATOM   1608  CD  GLN   213      20.960  78.149  38.649  1.00  0.00           C
ATOM   1609  OE1 GLN   213      20.250  79.015  38.141  1.00  0.00           O
ATOM   1610  NE2 GLN   213      21.351  77.036  37.974  1.00  0.00           N
ATOM   1611  C   GLN   213      21.669  78.338  42.919  1.00  0.00           C
ATOM   1612  O   GLN   213      21.180  77.636  43.801  1.00  0.00           O
ATOM   1613  N   VAL   214      22.928  78.132  42.487  1.00  0.00           N
ATOM   1614  CA  VAL   214      23.656  77.188  43.286  1.00  0.00           C
ATOM   1615  CB  VAL   214      24.036  75.887  42.635  1.00  0.00           C
ATOM   1616  CG1 VAL   214      25.148  75.167  43.412  1.00  0.00           C
ATOM   1617  CG2 VAL   214      22.803  75.012  42.814  1.00  0.00           C
ATOM   1618  C   VAL   214      24.846  77.848  43.890  1.00  0.00           C
ATOM   1619  O   VAL   214      25.970  77.738  43.407  1.00  0.00           O
ATOM   1620  N   ASP   215      24.644  78.554  45.013  1.00  0.00           N
ATOM   1621  CA  ASP   215      25.823  79.098  45.604  1.00  0.00           C
ATOM   1622  CB  ASP   215      26.046  80.589  45.288  1.00  0.00           C
ATOM   1623  CG  ASP   215      24.862  81.373  45.806  1.00  0.00           C
ATOM   1624  OD1 ASP   215      23.925  80.722  46.343  1.00  0.00           O
ATOM   1625  OD2 ASP   215      24.879  82.625  45.665  1.00  0.00           O
ATOM   1626  C   ASP   215      25.835  78.909  47.098  1.00  0.00           C
ATOM   1627  O   ASP   215      25.921  79.884  47.835  1.00  0.00           O
ATOM   1628  N   GLY   216      25.765  77.651  47.585  1.00  0.00           N
ATOM   1629  CA  GLY   216      25.912  77.288  48.978  1.00  0.00           C
ATOM   1630  C   GLY   216      25.097  78.122  49.926  1.00  0.00           C
ATOM   1631  O   GLY   216      24.009  77.744  50.367  1.00  0.00           O
ATOM   1632  N   GLU   217      25.696  79.249  50.347  1.00  0.00           N
ATOM   1633  CA  GLU   217      25.140  80.149  51.304  1.00  0.00           C
ATOM   1634  CB  GLU   217      26.090  81.303  51.670  1.00  0.00           C
ATOM   1635  CG  GLU   217      27.346  80.861  52.425  1.00  0.00           C
ATOM   1636  CD  GLU   217      28.361  80.342  51.415  1.00  0.00           C
ATOM   1637  OE1 GLU   217      28.056  80.380  50.193  1.00  0.00           O
ATOM   1638  OE2 GLU   217      29.458  79.906  51.853  1.00  0.00           O
ATOM   1639  C   GLU   217      23.902  80.772  50.758  1.00  0.00           C
ATOM   1640  O   GLU   217      22.920  80.930  51.481  1.00  0.00           O
ATOM   1641  N   ASN   218      23.912  81.128  49.462  1.00  0.00           N
ATOM   1642  CA  ASN   218      22.800  81.830  48.904  1.00  0.00           C
ATOM   1643  CB  ASN   218      23.286  82.878  47.881  1.00  0.00           C
ATOM   1644  CG  ASN   218      24.202  83.851  48.615  1.00  0.00           C
ATOM   1645  OD1 ASN   218      25.339  83.515  48.944  1.00  0.00           O
ATOM   1646  ND2 ASN   218      23.708  85.091  48.877  1.00  0.00           N
ATOM   1647  C   ASN   218      21.804  80.793  48.410  1.00  0.00           C
ATOM   1648  O   ASN   218      21.161  80.218  49.280  1.00  0.00           O
ATOM   1649  N   PRO   219      21.477  80.548  47.162  1.00  0.00           N
ATOM   1650  CA  PRO   219      20.594  79.428  46.920  1.00  0.00           C
ATOM   1651  CD  PRO   219      20.988  81.679  46.390  1.00  0.00           C
ATOM   1652  CB  PRO   219      20.052  79.614  45.509  1.00  0.00           C
ATOM   1653  CG  PRO   219      19.917  81.141  45.425  1.00  0.00           C
ATOM   1654  C   PRO   219      20.835  78.001  47.312  1.00  0.00           C
ATOM   1655  O   PRO   219      20.263  77.582  48.312  1.00  0.00           O
ATOM   1656  N   ASN   220      21.657  77.207  46.609  1.00  0.00           N
ATOM   1657  CA  ASN   220      21.730  75.866  47.116  1.00  0.00           C
ATOM   1658  CB  ASN   220      20.551  74.952  46.725  1.00  0.00           C
ATOM   1659  CG  ASN   220      20.528  74.733  45.223  1.00  0.00           C
ATOM   1660  OD1 ASN   220      21.211  73.847  44.715  1.00  0.00           O
ATOM   1661  ND2 ASN   220      19.702  75.535  44.500  1.00  0.00           N
ATOM   1662  C   ASN   220      23.000  75.257  46.662  1.00  0.00           C
ATOM   1663  O   ASN   220      23.411  75.426  45.516  1.00  0.00           O
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ATOM   1664  N   LEU   221      23.623  74.489  47.573  1.00  0.00           N
ATOM   1665  CA  LEU   221      24.897  73.893  47.334  1.00  0.00           C
ATOM   1666  CB  LEU   221      25.365  72.953  48.465  1.00  0.00           C
ATOM   1667  CG  LEU   221      24.353  71.859  48.868  1.00  0.00           C
ATOM   1668  CD2 LEU   221      24.743  71.220  50.212  1.00  0.00           C
ATOM   1669  CD1 LEU   221      24.144  70.815  47.759  1.00  0.00           C
ATOM   1670  C   LEU   221      24.804  73.138  46.078  1.00  0.00           C
ATOM   1671  O   LEU   221      23.709  72.666  45.755  1.00  0.00           O
ATOM   1672  N   TYR   222      25.984  73.084  45.389  1.00  0.00           N
ATOM   1673  CA  TYR   222      26.267  72.544  44.085  1.00  0.00           C
ATOM   1674  CB  TYR   222      27.570  71.728  44.010  1.00  0.00           C
ATOM   1675  CG  TYR   222      27.712  71.245  42.607  1.00  0.00           C
ATOM   1676  CD1 TYR   222      27.094  70.086  42.196  1.00  0.00           C
ATOM   1677  CD2 TYR   222      28.463  71.956  41.700  1.00  0.00           C
ATOM   1678  CE1 TYR   222      27.225  69.643  40.902  1.00  0.00           C
ATOM   1679  CE2 TYR   222      28.598  71.518  40.403  1.00  0.00           C
ATOM   1680  CZ  TYR   222      27.978  70.359  40.003  1.00  0.00           C
ATOM   1681  OH  TYR   222      28.113  69.905  38.673  1.00  0.00           O
ATOM   1682  C   TYR   222      25.144  71.673  43.741  1.00  0.00           C
ATOM   1683  O   TYR   222      24.839  70.763  44.514  1.00  0.00           O
ATOM   1684  N   PHE   223      24.470  71.994  42.617  1.00  0.00           N
ATOM   1685  CA  PHE   223      23.279  71.283  42.287  1.00  0.00           C
ATOM   1686  CB  PHE   223      22.666  71.595  40.910  1.00  0.00           C
ATOM   1687  CG  PHE   223      21.958  72.911  40.922  1.00  0.00           C
ATOM   1688  CD1 PHE   223      20.845  73.101  41.713  1.00  0.00           C
ATOM   1689  CD2 PHE   223      22.380  73.940  40.108  1.00  0.00           C
ATOM   1690  CE1 PHE   223      20.171  74.303  41.706  1.00  0.00           C
ATOM   1691  CE2 PHE   223      21.710  75.144  40.095  1.00  0.00           C
ATOM   1692  CZ  PHE   223      20.605  75.330  40.897  1.00  0.00           C
ATOM   1693  C   PHE   223      23.590  69.838  42.309  1.00  0.00           C
ATOM   1694  O   PHE   223      24.292  69.309  41.450  1.00  0.00           O
ATOM   1695  N   HIS   224      23.064  69.185  43.355  1.00  0.00           N
ATOM   1696  CA  HIS   224      23.308  67.799  43.548  1.00  0.00           C
ATOM   1697  ND1 HIS   224      24.605  65.521  45.616  1.00  0.00           N
ATOM   1698  CG  HIS   224      23.340  65.869  45.196  1.00  0.00           C
ATOM   1699  NE2 HIS   224      23.455  63.627  45.425  1.00  0.00           N
ATOM   1700  CD2 HIS   224      22.651  64.701  45.085  1.00  0.00           C
ATOM   1701  CE1 HIS   224      24.618  64.170  45.737  1.00  0.00           C
ATOM   1702  CB  HIS   224      22.902  67.282  44.938  1.00  0.00           C
ATOM   1703  C   HIS   224      22.490  67.094  42.535  1.00  0.00           C
ATOM   1704  O   HIS   224      21.450  67.591  42.101  1.00  0.00           O
ATOM   1705  N   SER   225      22.967  65.917  42.115  1.00  0.00           N
ATOM   1706  CA  SER   225      22.221  65.205  41.137  1.00  0.00           C
ATOM   1707  CB  SER   225      22.905  63.914  40.655  1.00  0.00           C
ATOM   1708  OG  SER   225      22.096  63.268  39.682  1.00  0.00           O
ATOM   1709  C   SER   225      20.929  64.834  41.767  1.00  0.00           C
ATOM   1710  O   SER   225      20.859  64.540  42.959  1.00  0.00           O
ATOM   1711  N   ASP   226      19.866  64.845  40.951  1.00  0.00           N
ATOM   1712  CA  ASP   226      18.566  64.469  41.403  1.00  0.00           C
ATOM   1713  CB  ASP   226      18.500  63.017  41.908  1.00  0.00           C
ATOM   1714  CG  ASP   226      18.670  62.095  40.708  1.00  0.00           C
ATOM   1715  OD1 ASP   226      18.650  62.611  39.558  1.00  0.00           O
ATOM   1716  OD2 ASP   226      18.826  60.864  40.926  1.00  0.00           O
ATOM   1717  C   ASP   226      18.094  65.361  42.506  1.00  0.00           C
ATOM   1718  O   ASP   226      17.383  64.905  43.400  1.00  0.00           O
ATOM   1719  N   ASP   227      18.462  66.655  42.486  1.00  0.00           N
ATOM   1720  CA  ASP   227      17.885  67.520  43.472  1.00  0.00           C
ATOM   1721  CB  ASP   227      18.591  68.883  43.574  1.00  0.00           C
ATOM   1722  CG  ASP   227      18.136  69.583  44.844  1.00  0.00           C
ATOM   1723  OD1 ASP   227      16.921  69.511  45.172  1.00  0.00           O
ATOM   1724  OD2 ASP   227      19.010  70.197  45.512  1.00  0.00           O
ATOM   1725  C   ASP   227      16.486  67.749  42.991  1.00  0.00           C
ATOM   1726  O   ASP   227      16.266  67.944  41.798  1.00  0.00           O
ATOM   1727  N   VAL   228      15.496  67.715  43.900  1.00  0.00           N
ATOM   1728  CA  VAL   228      14.136  67.897  43.481  1.00  0.00           C
ATOM   1729  CB  VAL   228      13.309  66.665  43.690  1.00  0.00           C
ATOM   1730  CG1 VAL   228      13.491  66.202  45.142  1.00  0.00           C
ATOM   1731  CG2 VAL   228      11.852  66.987  43.336  1.00  0.00           C
ATOM   1732  C   VAL   228      13.540  69.003  44.291  1.00  0.00           C
ATOM   1733  O   VAL   228      13.755  69.082  45.497  1.00  0.00           O
ATOM   1734  N   ILE   229      12.772  69.897  43.629  1.00  0.00           N
ATOM   1735  CA  ILE   229      12.156  71.010  44.302  1.00  0.00           C
ATOM   1736  CB  ILE   229      12.594  72.351  43.755  1.00  0.00           C
ATOM   1737  CG2 ILE   229      11.722  73.444  44.392  1.00  0.00           C
ATOM   1738  CG1 ILE   229      14.098  72.593  43.978  1.00  0.00           C
ATOM   1739  CD1 ILE   229      15.012  71.731  43.115  1.00  0.00           C
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ATOM   1740  C   ILE   229      10.665  70.921  44.109  1.00  0.00           C
ATOM   1741  O   ILE   229      10.184  70.608  43.023  1.00  0.00           O
ATOM   1742  N   LEU   230       9.886  71.180  45.180  1.00  0.00           N
ATOM   1743  CA  LEU   230       8.447  71.172  45.112  1.00  0.00           C
ATOM   1744  CB  LEU   230       7.826  70.498  46.357  1.00  0.00           C
ATOM   1745  CG  LEU   230       6.284  70.405  46.428  1.00  0.00           C
ATOM   1746  CD2 LEU   230       5.713  69.567  45.283  1.00  0.00           C
ATOM   1747  CD1 LEU   230       5.614  71.778  46.550  1.00  0.00           C
ATOM   1748  C   LEU   230       8.034  72.616  45.099  1.00  0.00           C
ATOM   1749  O   LEU   230       8.169  73.304  46.109  1.00  0.00           O
ATOM   1750  N   CYS   231       7.513  73.121  43.958  1.00  0.00           N
ATOM   1751  CA  CYS   231       7.196  74.524  43.873  1.00  0.00           C
ATOM   1752  CB  CYS   231       7.804  75.212  42.638  1.00  0.00           C
ATOM   1753  SG  CYS   231       7.205  74.516  41.069  1.00  0.00           S
ATOM   1754  C   CYS   231       5.711  74.720  43.820  1.00  0.00           C
ATOM   1755  O   CYS   231       5.025  74.153  42.969  1.00  0.00           O
ATOM   1756  N   VAL   232       5.184  75.560  44.742  1.00  0.00           N
ATOM   1757  CA  VAL   232       3.767  75.782  44.770  1.00  0.00           C
ATOM   1758  CB  VAL   232       3.201  75.520  46.142  1.00  0.00           C
ATOM   1759  CG1 VAL   232       1.685  75.784  46.137  1.00  0.00           C
ATOM   1760  CG2 VAL   232       3.594  74.096  46.557  1.00  0.00           C
ATOM   1761  C   VAL   232       3.494  77.228  44.426  1.00  0.00           C
ATOM   1762  O   VAL   232       2.347  77.614  44.208  1.00  0.00           O
ATOM   1763  N   LEU   233       4.550  78.066  44.313  1.00  0.00           N
ATOM   1764  CA  LEU   233       4.360  79.469  44.038  1.00  0.00           C
ATOM   1765  CB  LEU   233       5.606  80.332  44.327  1.00  0.00           C
ATOM   1766  CG  LEU   233       6.043  80.321  45.803  1.00  0.00           C
ATOM   1767  CD2 LEU   233       4.842  80.520  46.740  1.00  0.00           C
ATOM   1768  CD1 LEU   233       7.173  81.329  46.058  1.00  0.00           C
ATOM   1769  C   LEU   233       3.995  79.675  42.588  1.00  0.00           C
ATOM   1770  O   LEU   233       4.291  78.828  41.747  1.00  0.00           O
ATOM   1771  N   PRO   234       3.374  80.789  42.255  1.00  0.00           N
ATOM   1772  CA  PRO   234       3.017  81.043  40.873  1.00  0.00           C
ATOM   1773  CD  PRO   234       2.429  81.406  43.172  1.00  0.00           C
ATOM   1774  CB  PRO   234       1.989  82.172  40.898  1.00  0.00           C
ATOM   1775  CG  PRO   234       1.331  82.022  42.283  1.00  0.00           C
ATOM   1776  C   PRO   234       4.191  81.316  39.975  1.00  0.00           C
ATOM   1777  O   PRO   234       4.994  82.186  40.302  1.00  0.00           O
ATOM   1778  N   LEU   235       4.249  80.632  38.807  1.00  0.00           N
ATOM   1779  CA  LEU   235       5.304  80.680  37.822  1.00  0.00           C
ATOM   1780  CB  LEU   235       5.087  79.685  36.666  1.00  0.00           C
ATOM   1781  CG  LEU   235       5.194  78.205  37.084  1.00  0.00           C
ATOM   1782  CD2 LEU   235       6.526  77.922  37.799  1.00  0.00           C
ATOM   1783  CD1 LEU   235       4.965  77.276  35.881  1.00  0.00           C
ATOM   1784  C   LEU   235       5.388  82.035  37.209  1.00  0.00           C
ATOM   1785  O   LEU   235       6.462  82.472  36.790  1.00  0.00           O
ATOM   1786  N   PHE   236       4.233  82.705  37.086  1.00  0.00           N
ATOM   1787  CA  PHE   236       4.173  84.005  36.490  1.00  0.00           C
ATOM   1788  CB  PHE   236       2.778  84.247  35.882  1.00  0.00           C
ATOM   1789  CG  PHE   236       1.772  83.579  36.762  1.00  0.00           C
ATOM   1790  CD1 PHE   236       1.262  84.171  37.892  1.00  0.00           C
ATOM   1791  CD2 PHE   236       1.341  82.317  36.422  1.00  0.00           C
ATOM   1792  CE1 PHE   236       0.337  83.504  38.668  1.00  0.00           C
ATOM   1793  CE2 PHE   236       0.417  81.646  37.188  1.00  0.00           C
ATOM   1794  CZ  PHE   236      -0.085  82.243  38.316  1.00  0.00           C
ATOM   1795  C   PHE   236       4.493  85.057  37.507  1.00  0.00           C
ATOM   1796  O   PHE   236       4.217  86.239  37.302  1.00  0.00           O
ATOM   1797  N   HIS   237       5.170  84.655  38.600  1.00  0.00           N
ATOM   1798  CA  HIS   237       5.572  85.575  39.625  1.00  0.00           C
ATOM   1799  ND1 HIS   237       6.312  86.120  42.946  1.00  0.00           N
ATOM   1800  CG  HIS   237       5.263  86.266  42.063  1.00  0.00           C
ATOM   1801  NE2 HIS   237       5.315  88.041  43.460  1.00  0.00           N
ATOM   1802  CD2 HIS   237       4.667  87.443  42.391  1.00  0.00           C
ATOM   1803  CE1 HIS   237       6.296  87.207  43.757  1.00  0.00           C
ATOM   1804  CB  HIS   237       4.925  85.273  40.992  1.00  0.00           C
ATOM   1805  C   HIS   237       7.052  85.414  39.754  1.00  0.00           C
ATOM   1806  O   HIS   237       7.610  84.401  39.337  1.00  0.00           O
ATOM   1807  N   ILE   238       7.732  86.419  40.337  1.00  0.00           N
ATOM   1808  CA  ILE   238       9.164  86.405  40.444  1.00  0.00           C
ATOM   1809  CB  ILE   238       9.727  87.631  41.067  1.00  0.00           C
ATOM   1810  CG2 ILE   238      10.868  87.194  41.996  1.00  0.00           C
ATOM   1811  CG1 ILE   238      10.022  88.674  39.983  1.00  0.00           C
ATOM   1812  CD1 ILE   238      10.602  89.967  40.528  1.00  0.00           C
ATOM   1813  C   ILE   238       9.705  85.261  41.226  1.00  0.00           C
ATOM   1814  O   ILE   238      10.738  84.714  40.841  1.00  0.00           O
ATOM   1815  N   TYR   239       9.083  84.883  42.357  1.00  0.00           N
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ATOM   1816  CA  TYR   239       9.718  83.823  43.086  1.00  0.00           C
ATOM   1817  CB  TYR   239       9.063  83.427  44.417  1.00  0.00           C
ATOM   1818  CG  TYR   239      10.007  82.403  44.958  1.00  0.00           C
ATOM   1819  CD1 TYR   239      11.124  82.802  45.655  1.00  0.00           C
ATOM   1820  CD2 TYR   239       9.802  81.056  44.754  1.00  0.00           C
ATOM   1821  CE1 TYR   239      12.013  81.877  46.150  1.00  0.00           C
ATOM   1822  CE2 TYR   239      10.687  80.127  45.245  1.00  0.00           C
ATOM   1823  CZ  TYR   239      11.797  80.537  45.941  1.00  0.00           C
ATOM   1824  OH  TYR   239      12.711  79.587  46.445  1.00  0.00           O
ATOM   1825  C   TYR   239       9.725  82.593  42.240  1.00  0.00           C
ATOM   1826  O   TYR   239      10.750  81.925  42.119  1.00  0.00           O
ATOM   1827  N   SER   240       8.578  82.246  41.630  1.00  0.00           N
ATOM   1828  CA  SER   240       8.563  81.047  40.850  1.00  0.00           C
ATOM   1829  CB  SER   240       7.183  80.581  40.462  1.00  0.00           C
ATOM   1830  OG  SER   240       6.487  80.375  41.670  1.00  0.00           O
ATOM   1831  C   SER   240       9.325  81.205  39.592  1.00  0.00           C
ATOM   1832  O   SER   240      10.014  80.281  39.174  1.00  0.00           O
ATOM   1833  N   LEU   241       9.225  82.371  38.940  1.00  0.00           N
ATOM   1834  CA  LEU   241       9.848  82.477  37.657  1.00  0.00           C
ATOM   1835  CB  LEU   241       9.554  83.841  37.002  1.00  0.00           C
ATOM   1836  CG  LEU   241       9.907  83.930  35.505  1.00  0.00           C
ATOM   1837  CD2 LEU   241       9.097  82.911  34.687  1.00  0.00           C
ATOM   1838  CD1 LEU   241      11.414  83.822  35.262  1.00  0.00           C
ATOM   1839  C   LEU   241      11.335  82.296  37.785  1.00  0.00           C
ATOM   1840  O   LEU   241      11.933  81.498  37.064  1.00  0.00           O
ATOM   1841  N   ASN   242      11.969  83.023  38.724  1.00  0.00           N
ATOM   1842  CA  ASN   242      13.399  82.981  38.860  1.00  0.00           C
ATOM   1843  CB  ASN   242      13.941  84.118  39.742  1.00  0.00           C
ATOM   1844  CG  ASN   242      13.785  85.408  38.947  1.00  0.00           C
ATOM   1845  OD1 ASN   242      13.566  85.379  37.736  1.00  0.00           O
ATOM   1846  ND2 ASN   242      13.907  86.572  39.638  1.00  0.00           N
ATOM   1847  C   ASN   242      13.895  81.678  39.402  1.00  0.00           C
ATOM   1848  O   ASN   242      14.946  81.191  38.986  1.00  0.00           O
ATOM   1849  N   SER   243      13.178  81.107  40.385  1.00  0.00           N
ATOM   1850  CA  SER   243      13.601  79.895  41.020  1.00  0.00           C
ATOM   1851  CB  SER   243      12.799  79.595  42.298  1.00  0.00           C
ATOM   1852  OG  SER   243      13.013  80.622  43.252  1.00  0.00           O
ATOM   1853  C   SER   243      13.434  78.697  40.127  1.00  0.00           C
ATOM   1854  O   SER   243      14.290  77.817  40.124  1.00  0.00           O
ATOM   1855  N   VAL   244      12.352  78.646  39.321  1.00  0.00           N
ATOM   1856  CA  VAL   244      11.954  77.449  38.619  1.00  0.00           C
ATOM   1857  CB  VAL   244      10.549  77.493  38.051  1.00  0.00           C
ATOM   1858  CG1 VAL   244       9.581  77.578  39.242  1.00  0.00           C
ATOM   1859  CG2 VAL   244      10.374  78.640  37.031  1.00  0.00           C
ATOM   1860  C   VAL   244      12.898  77.002  37.583  1.00  0.00           C
ATOM   1861  O   VAL   244      14.079  76.785  37.827  1.00  0.00           O
ATOM   1862  N   LEU   245      12.381  76.815  36.367  1.00  0.00           N
ATOM   1863  CA  LEU   245      13.189  76.358  35.303  1.00  0.00           C
ATOM   1864  CB  LEU   245      12.419  76.194  33.985  1.00  0.00           C
ATOM   1865  CG  LEU   245      11.427  75.019  34.085  1.00  0.00           C
ATOM   1866  CD2 LEU   245      11.097  74.416  32.713  1.00  0.00           C
ATOM   1867  CD1 LEU   245      10.201  75.386  34.937  1.00  0.00           C
ATOM   1868  C   LEU   245      14.300  77.333  35.170  1.00  0.00           C
ATOM   1869  O   LEU   245      15.342  76.993  34.615  1.00  0.00           O
ATOM   1870  N   LEU   246      14.123  78.588  35.640  1.00  0.00           N
ATOM   1871  CA  LEU   246      15.284  79.394  35.508  1.00  0.00           C
ATOM   1872  CB  LEU   246      15.117  80.832  36.021  1.00  0.00           C
ATOM   1873  CG  LEU   246      14.153  81.704  35.203  1.00  0.00           C
ATOM   1874  CD2 LEU   246      14.364  81.521  33.692  1.00  0.00           C
ATOM   1875  CD1 LEU   246      14.256  83.170  35.652  1.00  0.00           C
ATOM   1876  C   LEU   246      16.444  78.827  36.289  1.00  0.00           C
ATOM   1877  O   LEU   246      17.368  78.271  35.698  1.00  0.00           O
ATOM   1878  N   CYS   247      16.411  78.874  37.635  1.00  0.00           N
ATOM   1879  CA  CYS   247      17.580  78.425  38.345  1.00  0.00           C
ATOM   1880  CB  CYS   247      17.627  78.839  39.838  1.00  0.00           C
ATOM   1881  SG  CYS   247      16.983  77.632  41.043  1.00  0.00           S
ATOM   1882  C   CYS   247      17.690  76.936  38.288  1.00  0.00           C
ATOM   1883  O   CYS   247      18.771  76.384  38.088  1.00  0.00           O
ATOM   1884  N   ALA   248      16.545  76.258  38.482  1.00  0.00           N
ATOM   1885  CA  ALA   248      16.457  74.832  38.566  1.00  0.00           C
ATOM   1886  CB  ALA   248      15.039  74.344  38.913  1.00  0.00           C
ATOM   1887  C   ALA   248      16.844  74.204  37.267  1.00  0.00           C
ATOM   1888  O   ALA   248      17.573  73.214  37.265  1.00  0.00           O
ATOM   1889  N   LEU   249      16.374  74.743  36.123  1.00  0.00           N
ATOM   1890  CA  LEU   249      16.737  74.093  34.893  1.00  0.00           C
ATOM   1891  CB  LEU   249      16.042  74.566  33.606  1.00  0.00           C
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ATOM   1892  CG  LEU   249      14.548  74.214  33.529  1.00  0.00           C
ATOM   1893  CD2 LEU   249      14.277  72.771  33.981  1.00  0.00           C
ATOM   1894  CD1 LEU   249      13.987  74.522  32.131  1.00  0.00           C
ATOM   1895  C   LEU   249      18.204  74.225  34.656  1.00  0.00           C
ATOM   1896  O   LEU   249      18.826  73.320  34.104  1.00  0.00           O
ATOM   1897  N   ARG   250      18.798  75.368  35.040  1.00  0.00           N
ATOM   1898  CA  ARG   250      20.206  75.523  34.828  1.00  0.00           C
ATOM   1899  CB  ARG   250      20.698  76.935  35.184  1.00  0.00           C
ATOM   1900  CG  ARG   250      20.209  77.980  34.172  1.00  0.00           C
ATOM   1901  CD  ARG   250      20.666  79.406  34.475  1.00  0.00           C
ATOM   1902  NE  ARG   250      20.381  80.258  33.285  1.00  0.00           N
ATOM   1903  CZ  ARG   250      21.226  81.290  32.988  1.00  0.00           C
ATOM   1904  NH1 ARG   250      22.325  81.516  33.764  1.00  0.00           N
ATOM   1905  NH2 ARG   250      20.985  82.092  31.911  1.00  0.00           N
ATOM   1906  C   ARG   250      20.880  74.480  35.661  1.00  0.00           C
ATOM   1907  O   ARG   250      21.910  73.917  35.289  1.00  0.00           O
ATOM   1908  N   ALA   251      20.276  74.214  36.828  1.00  0.00           N
ATOM   1909  CA  ALA   251      20.694  73.254  37.804  1.00  0.00           C
ATOM   1910  CB  ALA   251      19.739  73.250  38.997  1.00  0.00           C
ATOM   1911  C   ALA   251      20.617  71.860  37.267  1.00  0.00           C
ATOM   1912  O   ALA   251      21.497  71.041  37.532  1.00  0.00           O
ATOM   1913  N   GLY   252      19.542  71.548  36.518  1.00  0.00           N
ATOM   1914  CA  GLY   252      19.341  70.211  36.045  1.00  0.00           C
ATOM   1915  C   GLY   252      18.434  69.534  37.022  1.00  0.00           C
ATOM   1916  O   GLY   252      18.128  68.350  36.891  1.00  0.00           O
ATOM   1917  N   ALA   253      17.979  70.298  38.035  1.00  0.00           N
ATOM   1918  CA  ALA   253      17.126  69.785  39.064  1.00  0.00           C
ATOM   1919  CB  ALA   253      17.011  70.706  40.292  1.00  0.00           C
ATOM   1920  C   ALA   253      15.759  69.603  38.509  1.00  0.00           C
ATOM   1921  O   ALA   253      15.407  70.167  37.473  1.00  0.00           O
ATOM   1922  N   ALA   254      14.959  68.769  39.199  1.00  0.00           N
ATOM   1923  CA  ALA   254      13.622  68.535  38.771  1.00  0.00           C
ATOM   1924  CB  ALA   254      13.126  67.101  39.030  1.00  0.00           C
ATOM   1925  C   ALA   254      12.759  69.462  39.547  1.00  0.00           C
ATOM   1926  O   ALA   254      12.884  69.577  40.767  1.00  0.00           O
ATOM   1927  N   THR   255      11.866  70.174  38.839  1.00  0.00           N
ATOM   1928  CA  THR   255      10.988  71.057  39.529  1.00  0.00           C
ATOM   1929  CB  THR   255      10.923  72.438  38.932  1.00  0.00           C
ATOM   1930  OG1 THR   255      10.041  73.255  39.689  1.00  0.00           O
ATOM   1931  CG2 THR   255      10.470  72.361  37.464  1.00  0.00           C
ATOM   1932  C   THR   255       9.636  70.429  39.497  1.00  0.00           C
ATOM   1933  O   THR   255       9.045  70.236  38.436  1.00  0.00           O
ATOM   1934  N   LEU   256       9.122  70.070  40.688  1.00  0.00           N
ATOM   1935  CA  LEU   256       7.822  69.484  40.801  1.00  0.00           C
ATOM   1936  CB  LEU   256       7.701  68.490  41.954  1.00  0.00           C
ATOM   1937  CG  LEU   256       8.412  67.173  41.629  1.00  0.00           C
ATOM   1938  CD2 LEU   256       8.292  66.218  42.813  1.00  0.00           C
ATOM   1939  CD1 LEU   256       9.869  67.394  41.199  1.00  0.00           C
ATOM   1940  C   LEU   256       6.894  70.613  41.047  1.00  0.00           C
ATOM   1941  O   LEU   256       7.120  71.432  41.934  1.00  0.00           O
ATOM   1942  N   ILE   257       5.816  70.679  40.249  1.00  0.00           N
ATOM   1943  CA  ILE   257       4.937  71.799  40.334  1.00  0.00           C
ATOM   1944  CB  ILE   257       4.677  72.468  39.006  1.00  0.00           C
ATOM   1945  CG2 ILE   257       3.607  73.552  39.214  1.00  0.00           C
ATOM   1946  CG1 ILE   257       5.968  73.029  38.391  1.00  0.00           C
ATOM   1947  CD1 ILE   257       6.925  71.956  37.883  1.00  0.00           C
ATOM   1948  C   ILE   257       3.612  71.352  40.839  1.00  0.00           C
ATOM   1949  O   ILE   257       3.155  70.241  40.570  1.00  0.00           O
ATOM   1950  N   MET   258       2.985  72.238  41.635  1.00  0.00           N
ATOM   1951  CA  MET   258       1.678  71.991  42.145  1.00  0.00           C
ATOM   1952  CB  MET   258       1.686  71.803  43.668  1.00  0.00           C
ATOM   1953  CG  MET   258       0.412  71.184  44.235  1.00  0.00           C
ATOM   1954  SD  MET   258       0.534  70.752  45.996  1.00  0.00           S
ATOM   1955  CE  MET   258       1.615  69.317  45.731  1.00  0.00           C
ATOM   1956  C   MET   258       0.859  73.201  41.815  1.00  0.00           C
ATOM   1957  O   MET   258       1.204  74.326  42.178  1.00  0.00           O
ATOM   1958  N   GLN   259      -0.219  72.994  41.039  1.00  0.00           N
ATOM   1959  CA  GLN   259      -1.136  74.029  40.660  1.00  0.00           C
ATOM   1960  CB  GLN   259      -2.068  73.590  39.518  1.00  0.00           C
ATOM   1961  CG  GLN   259      -3.064  74.664  39.079  1.00  0.00           C
ATOM   1962  CD  GLN   259      -3.903  74.082  37.950  1.00  0.00           C
ATOM   1963  OE1 GLN   259      -4.771  74.753  37.394  1.00  0.00           O
ATOM   1964  NE2 GLN   259      -3.639  72.795  37.601  1.00  0.00           N
ATOM   1965  C   GLN   259      -2.006  74.381  41.836  1.00  0.00           C
ATOM   1966  O   GLN   259      -2.393  75.539  41.993  1.00  0.00           O
ATOM   1967  N   LYS   260      -2.361  73.373  42.672  1.00  0.00           N
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ATOM   1968  CA  LYS   260      -3.296  73.564  43.755  1.00  0.00           C
ATOM   1969  CB  LYS   260      -4.484  72.583  43.705  1.00  0.00           C
ATOM   1970  CG  LYS   260      -5.525  72.822  44.800  1.00  0.00           C
ATOM   1971  CD  LYS   260      -6.282  74.143  44.646  1.00  0.00           C
ATOM   1972  CE  LYS   260      -7.325  74.384  45.739  1.00  0.00           C
ATOM   1973  NZ  LYS   260      -8.412  73.386  45.632  1.00  0.00           N
ATOM   1974  C   LYS   260      -2.635  73.396  45.103  1.00  0.00           C
ATOM   1975  O   LYS   260      -1.566  72.804  45.232  1.00  0.00           O
ATOM   1976  N   PHE   261      -3.308  73.943  46.144  1.00  0.00           N
ATOM   1977  CA  PHE   261      -2.915  74.096  47.527  1.00  0.00           C
ATOM   1978  CB  PHE   261      -3.884  75.005  48.305  1.00  0.00           C
ATOM   1979  CG  PHE   261      -3.774  76.378  47.738  1.00  0.00           C
ATOM   1980  CD1 PHE   261      -4.497  76.733  46.622  1.00  0.00           C
ATOM   1981  CD2 PHE   261      -2.949  77.312  48.321  1.00  0.00           C
ATOM   1982  CE1 PHE   261      -4.398  78.000  46.096  1.00  0.00           C
ATOM   1983  CE2 PHE   261      -2.847  78.580  47.800  1.00  0.00           C
ATOM   1984  CZ  PHE   261      -3.571  78.926  46.685  1.00  0.00           C
ATOM   1985  C   PHE   261      -2.759  72.845  48.363  1.00  0.00           C
ATOM   1986  O   PHE   261      -1.837  72.791  49.176  1.00  0.00           O
ATOM   1987  N   ASN   262      -3.640  71.834  48.200  1.00  0.00           N
ATOM   1988  CA  ASN   262      -3.822  70.659  49.038  1.00  0.00           C
ATOM   1989  CB  ASN   262      -4.251  69.416  48.234  1.00  0.00           C
ATOM   1990  CG  ASN   262      -4.763  68.351  49.196  1.00  0.00           C
ATOM   1991  OD1 ASN   262      -4.728  68.508  50.415  1.00  0.00           O
ATOM   1992  ND2 ASN   262      -5.257  67.218  48.626  1.00  0.00           N
ATOM   1993  C   ASN   262      -2.628  70.275  49.873  1.00  0.00           C
ATOM   1994  O   ASN   262      -1.516  70.089  49.380  1.00  0.00           O
ATOM   1995  N   LEU   263      -2.869  70.174  51.203  1.00  0.00           N
ATOM   1996  CA  LEU   263      -1.896  69.835  52.211  1.00  0.00           C
ATOM   1997  CB  LEU   263      -2.449  69.995  53.638  1.00  0.00           C
ATOM   1998  CG  LEU   263      -2.819  71.446  53.997  1.00  0.00           C
ATOM   1999  CD2 LEU   263      -1.645  72.405  53.733  1.00  0.00           C
ATOM   2000  CD1 LEU   263      -3.360  71.549  55.432  1.00  0.00           C
ATOM   2001  C   LEU   263      -1.431  68.416  52.077  1.00  0.00           C
ATOM   2002  O   LEU   263      -0.232  68.150  52.122  1.00  0.00           O
ATOM   2003  N   THR   264      -2.364  67.460  51.913  1.00  0.00           N
ATOM   2004  CA  THR   264      -1.980  66.077  51.860  1.00  0.00           C
ATOM   2005  CB  THR   264      -3.154  65.146  51.784  1.00  0.00           C
ATOM   2006  OG1 THR   264      -3.995  65.326  52.912  1.00  0.00           O
ATOM   2007  CG2 THR   264      -2.628  63.701  51.743  1.00  0.00           C
ATOM   2008  C   THR   264      -1.143  65.844  50.647  1.00  0.00           C
ATOM   2009  O   THR   264      -0.114  65.173  50.710  1.00  0.00           O
ATOM   2010  N   THR   265      -1.562  66.411  49.503  1.00  0.00           N
ATOM   2011  CA  THR   265      -0.838  66.202  48.287  1.00  0.00           C
ATOM   2012  CB  THR   265      -1.485  66.845  47.093  1.00  0.00           C
ATOM   2013  OG1 THR   265      -0.825  66.439  45.903  1.00  0.00           O
ATOM   2014  CG2 THR   265      -1.422  68.374  47.240  1.00  0.00           C
ATOM   2015  C   THR   265       0.523  66.787  48.462  1.00  0.00           C
ATOM   2016  O   THR   265       1.510  66.234  47.979  1.00  0.00           O
ATOM   2017  N   CYS   266       0.609  67.936  49.157  1.00  0.00           N
ATOM   2018  CA  CYS   266       1.881  68.571  49.324  1.00  0.00           C
ATOM   2019  CB  CYS   266       1.819  69.901  50.090  1.00  0.00           C
ATOM   2020  SG  CYS   266       1.098  71.239  49.104  1.00  0.00           S
ATOM   2021  C   CYS   266       2.816  67.691  50.089  1.00  0.00           C
ATOM   2022  O   CYS   266       3.940  67.461  49.647  1.00  0.00           O
ATOM   2023  N   LEU   267       2.384  67.171  51.255  1.00  0.00           N
ATOM   2024  CA  LEU   267       3.275  66.375  52.052  1.00  0.00           C
ATOM   2025  CB  LEU   267       2.759  66.018  53.458  1.00  0.00           C
ATOM   2026  CG  LEU   267       2.755  67.207  54.438  1.00  0.00           C
ATOM   2027  CD2 LEU   267       2.731  66.733  55.896  1.00  0.00           C
ATOM   2028  CD1 LEU   267       1.646  68.216  54.117  1.00  0.00           C
ATOM   2029  C   LEU   267       3.606  65.100  51.347  1.00  0.00           C
ATOM   2030  O   LEU   267       4.741  64.634  51.410  1.00  0.00           O
ATOM   2031  N   GLU   268       2.621  64.492  50.666  1.00  0.00           N
ATOM   2032  CA  GLU   268       2.856  63.243  50.007  1.00  0.00           C
ATOM   2033  CB  GLU   268       1.583  62.639  49.388  1.00  0.00           C
ATOM   2034  CG  GLU   268       0.915  63.528  48.338  1.00  0.00           C
ATOM   2035  CD  GLU   268      -0.319  62.796  47.831  1.00  0.00           C
ATOM   2036  OE1 GLU   268      -0.542  61.639  48.274  1.00  0.00           O
ATOM   2037  OE2 GLU   268      -1.054  63.385  46.993  1.00  0.00           O
ATOM   2038  C   GLU   268       3.869  63.429  48.914  1.00  0.00           C
ATOM   2039  O   GLU   268       4.702  62.554  48.683  1.00  0.00           O
ATOM   2040  N   LEU   269       3.813  64.568  48.194  1.00  0.00           N
ATOM   2041  CA  LEU   269       4.723  64.814  47.107  1.00  0.00           C
ATOM   2042  CB  LEU   269       4.307  66.021  46.237  1.00  0.00           C
ATOM   2043  CG  LEU   269       5.112  66.200  44.931  1.00  0.00           C
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ATOM   2044  CD2 LEU   269       6.585  66.555  45.196  1.00  0.00           C
ATOM   2045  CD1 LEU   269       4.440  67.235  44.015  1.00  0.00           C
ATOM   2046  C   LEU   269       6.110  64.993  47.640  1.00  0.00           C
ATOM   2047  O   LEU   269       7.081  64.563  47.018  1.00  0.00           O
ATOM   2048  N   ILE   270       6.243  65.629  48.818  1.00  0.00           N
ATOM   2049  CA  ILE   270       7.536  65.850  49.400  1.00  0.00           C
ATOM   2050  CB  ILE   270       7.434  66.527  50.738  1.00  0.00           C
ATOM   2051  CG2 ILE   270       8.830  66.542  51.383  1.00  0.00           C
ATOM   2052  CG1 ILE   270       6.782  67.914  50.591  1.00  0.00           C
ATOM   2053  CD1 ILE   270       7.554  68.867  49.679  1.00  0.00           C
ATOM   2054  C   ILE   270       8.143  64.500  49.622  1.00  0.00           C
ATOM   2055  O   ILE   270       9.332  64.285  49.386  1.00  0.00           O
ATOM   2056  N   GLN   271       7.310  63.567  50.112  1.00  0.00           N
ATOM   2057  CA  GLN   271       7.663  62.215  50.435  1.00  0.00           C
ATOM   2058  CB  GLN   271       6.404  61.446  50.847  1.00  0.00           C
ATOM   2059  CG  GLN   271       5.848  61.970  52.139  1.00  0.00           C
ATOM   2060  CD  GLN   271       7.074  61.738  52.953  1.00  0.00           C
ATOM   2061  OE1 GLN   271       7.541  62.612  53.679  1.00  0.00           O
ATOM   2062  NE2 GLN   271       7.631  60.515  52.744  1.00  0.00           N
ATOM   2063  C   GLN   271       8.073  61.429  49.245  1.00  0.00           C
ATOM   2064  O   GLN   271       9.186  60.911  49.157  1.00  0.00           O
ATOM   2065  N   LYS   272       7.130  61.334  48.297  1.00  0.00           N
ATOM   2066  CA  LYS   272       7.256  60.464  47.171  1.00  0.00           C
ATOM   2067  CB  LYS   272       5.976  60.418  46.317  1.00  0.00           C
ATOM   2068  CG  LYS   272       4.780  59.808  47.053  1.00  0.00           C
ATOM   2069  CD  LYS   272       3.439  60.042  46.354  1.00  0.00           C
ATOM   2070  CE  LYS   272       2.250  59.427  47.096  1.00  0.00           C
ATOM   2071  NZ  LYS   272       0.997  59.697  46.356  1.00  0.00           N
ATOM   2072  C   LYS   272       8.365  60.906  46.294  1.00  0.00           C
ATOM   2073  O   LYS   272       9.138  60.086  45.801  1.00  0.00           O
ATOM   2074  N   TYR   273       8.487  62.223  46.075  1.00  0.00           N
ATOM   2075  CA  TYR   273       9.478  62.584  45.119  1.00  0.00           C
ATOM   2076  CB  TYR   273       9.039  63.789  44.286  1.00  0.00           C
ATOM   2077  CG  TYR   273       7.733  63.455  43.646  1.00  0.00           C
ATOM   2078  CD1 TYR   273       6.560  63.583  44.355  1.00  0.00           C
ATOM   2079  CD2 TYR   273       7.673  63.035  42.339  1.00  0.00           C
ATOM   2080  CE1 TYR   273       5.349  63.286  43.775  1.00  0.00           C
ATOM   2081  CE2 TYR   273       6.465  62.736  41.753  1.00  0.00           C
ATOM   2082  CZ  TYR   273       5.301  62.859  42.471  1.00  0.00           C
ATOM   2083  OH  TYR   273       4.062  62.552  41.869  1.00  0.00           O
ATOM   2084  C   TYR   273      10.726  62.987  45.829  1.00  0.00           C
ATOM   2085  O   TYR   273      11.607  63.580  45.208  1.00  0.00           O
ATOM   2086  N   LYS   274      10.847  62.624  47.123  1.00  0.00           N
ATOM   2087  CA  LYS   274      12.018  62.894  47.915  1.00  0.00           C
ATOM   2088  CB  LYS   274      13.149  61.863  47.705  1.00  0.00           C
ATOM   2089  CG  LYS   274      13.451  61.501  46.247  1.00  0.00           C
ATOM   2090  CD  LYS   274      14.167  62.589  45.447  1.00  0.00           C
ATOM   2091  CE  LYS   274      14.451  62.188  43.998  1.00  0.00           C
ATOM   2092  NZ  LYS   274      15.141  63.290  43.293  1.00  0.00           N
ATOM   2093  C   LYS   274      12.503  64.296  47.683  1.00  0.00           C
ATOM   2094  O   LYS   274      13.660  64.517  47.330  1.00  0.00           O
ATOM   2095  N   VAL   275      11.613  65.287  47.885  1.00  0.00           N
ATOM   2096  CA  VAL   275      11.952  66.654  47.612  1.00  0.00           C
ATOM   2097  CB  VAL   275      10.769  67.576  47.593  1.00  0.00           C
ATOM   2098  CG1 VAL   275      10.179  67.644  49.008  1.00  0.00           C
ATOM   2099  CG2 VAL   275      11.225  68.940  47.048  1.00  0.00           C
ATOM   2100  C   VAL   275      12.926  67.181  48.615  1.00  0.00           C
ATOM   2101  O   VAL   275      12.780  66.991  49.822  1.00  0.00           O
ATOM   2102  N   THR   276      13.998  67.808  48.088  1.00  0.00           N
ATOM   2103  CA  THR   276      15.029  68.441  48.853  1.00  0.00           C
ATOM   2104  CB  THR   276      16.271  68.645  48.049  1.00  0.00           C
ATOM   2105  OG1 THR   276      16.716  67.411  47.506  1.00  0.00           O
ATOM   2106  CG2 THR   276      17.343  69.200  48.993  1.00  0.00           C
ATOM   2107  C   THR   276      14.594  69.806  49.324  1.00  0.00           C
ATOM   2108  O   THR   276      14.920  70.211  50.437  1.00  0.00           O
ATOM   2109  N   VAL   277      13.870  70.570  48.472  1.00  0.00           N
ATOM   2110  CA  VAL   277      13.563  71.928  48.848  1.00  0.00           C
ATOM   2111  CB  VAL   277      14.442  72.911  48.122  1.00  0.00           C
ATOM   2112  CG1 VAL   277      14.066  74.338  48.549  1.00  0.00           C
ATOM   2113  CG2 VAL   277      15.911  72.527  48.357  1.00  0.00           C
ATOM   2114  C   VAL   277      12.144  72.260  48.457  1.00  0.00           C
ATOM   2115  O   VAL   277      11.666  71.818  47.414  1.00  0.00           O
ATOM   2116  N   ALA   278      11.425  73.066  49.285  1.00  0.00           N
ATOM   2117  CA  ALA   278      10.071  73.415  48.938  1.00  0.00           C
ATOM   2118  CB  ALA   278       9.020  72.730  49.828  1.00  0.00           C
ATOM   2119  C   ALA   278       9.843  74.906  49.055  1.00  0.00           C
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ATOM   2120  O   ALA   278      10.170  75.515  50.074  1.00  0.00           O
ATOM   2121  N   PRO   279       9.367  75.510  47.977  1.00  0.00           N
ATOM   2122  CA  PRO   279       8.953  76.903  48.024  1.00  0.00           C
ATOM   2123  CD  PRO   279      10.099  75.243  46.746  1.00  0.00           C
ATOM   2124  CB  PRO   279       9.210  77.488  46.639  1.00  0.00           C
ATOM   2125  CG  PRO   279      10.326  76.602  46.069  1.00  0.00           C
ATOM   2126  C   PRO   279       7.540  77.116  48.475  1.00  0.00           C
ATOM   2127  O   PRO   279       6.646  76.402  48.017  1.00  0.00           O
ATOM   2128  N   ILE   280       7.308  78.145  49.316  1.00  0.00           N
ATOM   2129  CA  ILE   280       6.006  78.351  49.875  1.00  0.00           C
ATOM   2130  CB  ILE   280       5.958  77.784  51.273  1.00  0.00           C
ATOM   2131  CG2 ILE   280       4.645  78.184  51.925  1.00  0.00           C
ATOM   2132  CG1 ILE   280       6.195  76.262  51.287  1.00  0.00           C
ATOM   2133  CD1 ILE   280       7.656  75.846  51.125  1.00  0.00           C
ATOM   2134  C   ILE   280       5.721  79.820  49.972  1.00  0.00           C
ATOM   2135  O   ILE   280       6.627  80.645  50.066  1.00  0.00           O
ATOM   2136  N   VAL   281       4.420  80.176  49.940  1.00  0.00           N
ATOM   2137  CA  VAL   281       3.973  81.526  50.135  1.00  0.00           C
ATOM   2138  CB  VAL   281       2.550  81.708  49.695  1.00  0.00           C
ATOM   2139  CG1 VAL   281       2.137  83.160  49.940  1.00  0.00           C
ATOM   2140  CG2 VAL   281       2.410  81.254  48.240  1.00  0.00           C
ATOM   2141  C   VAL   281       3.977  81.715  51.634  1.00  0.00           C
ATOM   2142  O   VAL   281       3.788  80.743  52.364  1.00  0.00           O
ATOM   2143  N   PRO   282       4.181  82.898  52.149  1.00  0.00           N
ATOM   2144  CA  PRO   282       4.231  83.081  53.577  1.00  0.00           C
ATOM   2145  CD  PRO   282       4.926  83.923  51.438  1.00  0.00           C
ATOM   2146  CB  PRO   282       4.665  84.528  53.786  1.00  0.00           C
ATOM   2147  CG  PRO   282       5.509  84.833  52.533  1.00  0.00           C
ATOM   2148  C   PRO   282       2.960  82.718  54.279  1.00  0.00           C
ATOM   2149  O   PRO   282       3.030  82.276  55.424  1.00  0.00           O
ATOM   2150  N   PRO   283       1.827  82.903  53.672  1.00  0.00           N
ATOM   2151  CA  PRO   283       0.612  82.535  54.335  1.00  0.00           C
ATOM   2152  CD  PRO   283       1.633  84.044  52.791  1.00  0.00           C
ATOM   2153  CB  PRO   283      -0.512  83.144  53.503  1.00  0.00           C
ATOM   2154  CG  PRO   283       0.141  84.399  52.896  1.00  0.00           C
ATOM   2155  C   PRO   283       0.543  81.057  54.513  1.00  0.00           C
ATOM   2156  O   PRO   283      -0.174  80.611  55.406  1.00  0.00           O
ATOM   2157  N   ILE   284       1.227  80.293  53.641  1.00  0.00           N
ATOM   2158  CA  ILE   284       1.308  78.860  53.713  1.00  0.00           C
ATOM   2159  CB  ILE   284       1.766  78.226  52.437  1.00  0.00           C
ATOM   2160  CG2 ILE   284       1.958  76.721  52.694  1.00  0.00           C
ATOM   2161  CG1 ILE   284       0.780  78.537  51.299  1.00  0.00           C
ATOM   2162  CD1 ILE   284       1.316  78.178  49.914  1.00  0.00           C
ATOM   2163  C   ILE   284       2.203  78.447  54.855  1.00  0.00           C
ATOM   2164  O   ILE   284       1.999  77.398  55.462  1.00  0.00           O
ATOM   2165  N   VAL   285       3.259  79.239  55.146  1.00  0.00           N
ATOM   2166  CA  VAL   285       4.191  78.939  56.204  1.00  0.00           C
ATOM   2167  CB  VAL   285       5.259  79.985  56.342  1.00  0.00           C
ATOM   2168  CG1 VAL   285       6.115  79.656  57.577  1.00  0.00           C
ATOM   2169  CG2 VAL   285       6.055  80.046  55.026  1.00  0.00           C
ATOM   2170  C   VAL   285       3.433  78.900  57.489  1.00  0.00           C
ATOM   2171  O   VAL   285       3.667  78.039  58.337  1.00  0.00           O
ATOM   2172  N   LEU   286       2.500  79.850  57.666  1.00  0.00           N
ATOM   2173  CA  LEU   286       1.704  79.875  58.855  1.00  0.00           C
ATOM   2174  CB  LEU   286       0.753  81.084  58.941  1.00  0.00           C
ATOM   2175  CG  LEU   286       1.464  82.427  59.197  1.00  0.00           C
ATOM   2176  CD2 LEU   286       0.451  83.534  59.532  1.00  0.00           C
ATOM   2177  CD1 LEU   286       2.397  82.807  58.039  1.00  0.00           C
ATOM   2178  C   LEU   286       0.865  78.644  58.884  1.00  0.00           C
ATOM   2179  O   LEU   286       0.623  78.071  59.943  1.00  0.00           O
ATOM   2180  N   ASP   287       0.383  78.208  57.708  1.00  0.00           N
ATOM   2181  CA  ASP   287      -0.452  77.047  57.663  1.00  0.00           C
ATOM   2182  CB  ASP   287      -0.927  76.719  56.238  1.00  0.00           C
ATOM   2183  CG  ASP   287      -1.910  77.802  55.816  1.00  0.00           C
ATOM   2184  OD1 ASP   287      -2.399  78.539  56.713  1.00  0.00           O
ATOM   2185  OD2 ASP   287      -2.186  77.906  54.591  1.00  0.00           O
ATOM   2186  C   ASP   287       0.332  75.869  58.167  1.00  0.00           C
ATOM   2187  O   ASP   287      -0.178  75.064  58.942  1.00  0.00           O
ATOM   2188  N   ILE   288       1.607  75.760  57.747  1.00  0.00           N
ATOM   2189  CA  ILE   288       2.499  74.678  58.075  1.00  0.00           C
ATOM   2190  CB  ILE   288       3.831  74.816  57.404  1.00  0.00           C
ATOM   2191  CG2 ILE   288       4.758  73.751  58.004  1.00  0.00           C
ATOM   2192  CG1 ILE   288       3.686  74.746  55.875  1.00  0.00           C
ATOM   2193  CD1 ILE   288       3.099  73.426  55.375  1.00  0.00           C
ATOM   2194  C   ILE   288       2.766  74.641  59.546  1.00  0.00           C
ATOM   2195  O   ILE   288       2.963  73.573  60.120  1.00  0.00           O
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ATOM   2196  N   THR   289       2.835  75.807  60.204  1.00  0.00           N
ATOM   2197  CA  THR   289       3.130  75.787  61.606  1.00  0.00           C
ATOM   2198  CB  THR   289       3.155  77.150  62.233  1.00  0.00           C
ATOM   2199  OG1 THR   289       1.870  77.748  62.177  1.00  0.00           O
ATOM   2200  CG2 THR   289       4.179  78.017  61.479  1.00  0.00           C
ATOM   2201  C   THR   289       2.055  74.994  62.284  1.00  0.00           C
ATOM   2202  O   THR   289       2.310  74.309  63.273  1.00  0.00           O
ATOM   2203  N   LYS   290       0.810  75.116  61.790  1.00  0.00           N
ATOM   2204  CA  LYS   290      -0.340  74.444  62.333  1.00  0.00           C
ATOM   2205  CB  LYS   290      -1.661  74.999  61.776  1.00  0.00           C
ATOM   2206  CG  LYS   290      -1.953  76.430  62.232  1.00  0.00           C
ATOM   2207  CD  LYS   290      -2.065  76.570  63.751  1.00  0.00           C
ATOM   2208  CE  LYS   290      -3.268  75.837  64.346  1.00  0.00           C
ATOM   2209  NZ  LYS   290      -3.255  75.958  65.821  1.00  0.00           N
ATOM   2210  C   LYS   290      -0.353  72.954  62.092  1.00  0.00           C
ATOM   2211  O   LYS   290      -0.801  72.210  62.963  1.00  0.00           O
ATOM   2212  N   SER   291       0.110  72.479  60.912  1.00  0.00           N
ATOM   2213  CA  SER   291      -0.080  71.102  60.510  1.00  0.00           C
ATOM   2214  CB  SER   291       0.426  70.788  59.090  1.00  0.00           C
ATOM   2215  OG  SER   291       1.842  70.697  59.080  1.00  0.00           O
ATOM   2216  C   SER   291       0.560  70.094  61.425  1.00  0.00           C
ATOM   2217  O   SER   291       1.744  70.168  61.747  1.00  0.00           O
ATOM   2218  N   PRO   292      -0.276  69.201  61.915  1.00  0.00           N
ATOM   2219  CA  PRO   292       0.140  68.041  62.675  1.00  0.00           C
ATOM   2220  CD  PRO   292      -1.630  69.607  62.254  1.00  0.00           C
ATOM   2221  CB  PRO   292      -1.011  67.725  63.630  1.00  0.00           C
ATOM   2222  CG  PRO   292      -2.233  68.405  62.995  1.00  0.00           C
ATOM   2223  C   PRO   292       0.501  66.849  61.823  1.00  0.00           C
ATOM   2224  O   PRO   292       1.033  65.879  62.360  1.00  0.00           O
ATOM   2225  N   ILE   293       0.168  66.892  60.519  1.00  0.00           N
ATOM   2226  CA  ILE   293       0.280  65.843  59.537  1.00  0.00           C
ATOM   2227  CB  ILE   293      -0.351  66.225  58.230  1.00  0.00           C
ATOM   2228  CG2 ILE   293       0.445  67.400  57.641  1.00  0.00           C
ATOM   2229  CG1 ILE   293      -0.453  65.003  57.303  1.00  0.00           C
ATOM   2230  CD1 ILE   293      -1.344  65.238  56.083  1.00  0.00           C
ATOM   2231  C   ILE   293       1.699  65.450  59.235  1.00  0.00           C
ATOM   2232  O   ILE   293       1.963  64.298  58.892  1.00  0.00           O
ATOM   2233  N   VAL   294       2.643  66.399  59.328  1.00  0.00           N
ATOM   2234  CA  VAL   294       3.989  66.244  58.848  1.00  0.00           C
ATOM   2235  CB  VAL   294       4.869  67.394  59.236  1.00  0.00           C
ATOM   2236  CG1 VAL   294       5.003  67.411  60.768  1.00  0.00           C
ATOM   2237  CG2 VAL   294       6.210  67.252  58.497  1.00  0.00           C
ATOM   2238  C   VAL   294       4.674  64.993  59.330  1.00  0.00           C
ATOM   2239  O   VAL   294       5.372  64.356  58.544  1.00  0.00           O
ATOM   2240  N   SER   295       4.517  64.596  60.605  1.00  0.00           N
ATOM   2241  CA  SER   295       5.231  63.466  61.143  1.00  0.00           C
ATOM   2242  CB  SER   295       4.975  63.265  62.646  1.00  0.00           C
ATOM   2243  OG  SER   295       5.700  62.139  63.120  1.00  0.00           O
ATOM   2244  C   SER   295       4.840  62.190  60.452  1.00  0.00           C
ATOM   2245  O   SER   295       5.545  61.187  60.541  1.00  0.00           O
ATOM   2246  N   GLN   296       3.694  62.192  59.758  1.00  0.00           N
ATOM   2247  CA  GLN   296       3.159  61.040  59.084  1.00  0.00           C
ATOM   2248  CB  GLN   296       1.755  61.294  58.515  1.00  0.00           C
ATOM   2249  CG  GLN   296       0.713  61.607  59.593  1.00  0.00           C
ATOM   2250  CD  GLN   296      -0.626  61.839  58.907  1.00  0.00           C
ATOM   2251  OE1 GLN   296      -1.408  62.696  59.321  1.00  0.00           O
ATOM   2252  NE2 GLN   296      -0.909  61.049  57.838  1.00  0.00           N
ATOM   2253  C   GLN   296       4.046  60.639  57.939  1.00  0.00           C
ATOM   2254  O   GLN   296       4.027  59.483  57.519  1.00  0.00           O
ATOM   2255  N   TYR   297       4.820  61.585  57.374  1.00  0.00           N
ATOM   2256  CA  TYR   297       5.521  61.327  56.147  1.00  0.00           C
ATOM   2257  CB  TYR   297       5.233  62.439  55.131  1.00  0.00           C
ATOM   2258  CG  TYR   297       3.773  62.481  54.837  1.00  0.00           C
ATOM   2259  CD1 TYR   297       2.921  63.186  55.655  1.00  0.00           C
ATOM   2260  CD2 TYR   297       3.260  61.823  53.744  1.00  0.00           C
ATOM   2261  CE1 TYR   297       1.573  63.235  55.388  1.00  0.00           C
ATOM   2262  CE2 TYR   297       1.914  61.868  53.471  1.00  0.00           C
ATOM   2263  CZ  TYR   297       1.068  62.575  54.294  1.00  0.00           C
ATOM   2264  OH  TYR   297      -0.314  62.624  54.016  1.00  0.00           O
ATOM   2265  C   TYR   297       7.019  61.275  56.339  1.00  0.00           C
ATOM   2266  O   TYR   297       7.574  61.892  57.246  1.00  0.00           O
ATOM   2267  N   ASP   298       7.705  60.498  55.462  1.00  0.00           N
ATOM   2268  CA  ASP   298       9.138  60.300  55.437  1.00  0.00           C
ATOM   2269  CB  ASP   298       9.552  58.964  54.796  1.00  0.00           C
ATOM   2270  CG  ASP   298      11.043  58.751  55.030  1.00  0.00           C
ATOM   2271  OD1 ASP   298      11.703  59.681  55.564  1.00  0.00           O
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ATOM   2272  OD2 ASP   298      11.540  57.650  54.675  1.00  0.00           O
ATOM   2273  C   ASP   298       9.779  61.401  54.633  1.00  0.00           C
ATOM   2274  O   ASP   298      10.065  61.279  53.442  1.00  0.00           O
ATOM   2275  N   VAL   299       9.980  62.527  55.326  1.00  0.00           N
ATOM   2276  CA  VAL   299      10.499  63.821  54.988  1.00  0.00           C
ATOM   2277  CB  VAL   299      10.029  64.790  56.042  1.00  0.00           C
ATOM   2278  CG1 VAL   299      10.527  66.213  55.774  1.00  0.00           C
ATOM   2279  CG2 VAL   299       8.497  64.683  56.113  1.00  0.00           C
ATOM   2280  C   VAL   299      12.011  63.799  54.916  1.00  0.00           C
ATOM   2281  O   VAL   299      12.637  64.838  54.721  1.00  0.00           O
ATOM   2282  N   SER   300      12.652  62.638  55.144  1.00  0.00           N
ATOM   2283  CA  SER   300      14.083  62.548  55.299  1.00  0.00           C
ATOM   2284  CB  SER   300      14.589  61.096  55.268  1.00  0.00           C
ATOM   2285  OG  SER   300      14.060  60.372  56.367  1.00  0.00           O
ATOM   2286  C   SER   300      14.843  63.292  54.233  1.00  0.00           C
ATOM   2287  O   SER   300      15.937  63.789  54.495  1.00  0.00           O
ATOM   2288  N   SER   301      14.318  63.371  53.001  1.00  0.00           N
ATOM   2289  CA  SER   301      15.012  64.044  51.937  1.00  0.00           C
ATOM   2290  CB  SER   301      14.415  63.709  50.558  1.00  0.00           C
ATOM   2291  OG  SER   301      13.078  64.184  50.479  1.00  0.00           O
ATOM   2292  C   SER   301      14.980  65.548  52.066  1.00  0.00           C
ATOM   2293  O   SER   301      15.880  66.217  51.561  1.00  0.00           O
ATOM   2294  N   VAL   302      13.959  66.141  52.726  1.00  0.00           N
ATOM   2295  CA  VAL   302      13.846  67.577  52.633  1.00  0.00           C
ATOM   2296  CB  VAL   302      12.497  68.140  52.994  1.00  0.00           C
ATOM   2297  CG1 VAL   302      12.327  68.155  54.518  1.00  0.00           C
ATOM   2298  CG2 VAL   302      12.377  69.532  52.352  1.00  0.00           C
ATOM   2299  C   VAL   302      14.888  68.312  53.415  1.00  0.00           C
ATOM   2300  O   VAL   302      15.056  68.138  54.621  1.00  0.00           O
ATOM   2301  N   ARG   303      15.697  69.093  52.674  1.00  0.00           N
ATOM   2302  CA  ARG   303      16.676  69.993  53.202  1.00  0.00           C
ATOM   2303  CB  ARG   303      17.825  70.246  52.213  1.00  0.00           C
ATOM   2304  CG  ARG   303      18.643  68.997  51.873  1.00  0.00           C
ATOM   2305  CD  ARG   303      19.784  69.273  50.890  1.00  0.00           C
ATOM   2306  NE  ARG   303      20.496  67.987  50.643  1.00  0.00           N
ATOM   2307  CZ  ARG   303      21.619  67.970  49.867  1.00  0.00           C
ATOM   2308  NH1 ARG   303      22.094  69.133  49.331  1.00  0.00           N
ATOM   2309  NH2 ARG   303      22.268  66.794  49.627  1.00  0.00           N
ATOM   2310  C   ARG   303      16.115  71.349  53.550  1.00  0.00           C
ATOM   2311  O   ARG   303      16.478  71.928  54.571  1.00  0.00           O
ATOM   2312  N   ILE   304      15.242  71.936  52.696  1.00  0.00           N
ATOM   2313  CA  ILE   304      14.940  73.318  52.979  1.00  0.00           C
ATOM   2314  CB  ILE   304      15.924  74.236  52.285  1.00  0.00           C
ATOM   2315  CG2 ILE   304      15.584  75.704  52.592  1.00  0.00           C
ATOM   2316  CG1 ILE   304      17.361  73.882  52.704  1.00  0.00           C
ATOM   2317  CD1 ILE   304      18.429  74.535  51.828  1.00  0.00           C
ATOM   2318  C   ILE   304      13.557  73.707  52.533  1.00  0.00           C
ATOM   2319  O   ILE   304      12.973  73.095  51.641  1.00  0.00           O
ATOM   2320  N   ILE   305      13.004  74.758  53.182  1.00  0.00           N
ATOM   2321  CA  ILE   305      11.754  75.380  52.845  1.00  0.00           C
ATOM   2322  CB  ILE   305      10.715  75.220  53.916  1.00  0.00           C
ATOM   2323  CG2 ILE   305       9.493  76.078  53.547  1.00  0.00           C
ATOM   2324  CG1 ILE   305      10.395  73.722  54.081  1.00  0.00           C
ATOM   2325  CD1 ILE   305       9.565  73.386  55.317  1.00  0.00           C
ATOM   2326  C   ILE   305      12.079  76.844  52.658  1.00  0.00           C
ATOM   2327  O   ILE   305      12.797  77.421  53.475  1.00  0.00           O
ATOM   2328  N   MET   306      11.588  77.488  51.568  1.00  0.00           N
ATOM   2329  CA  MET   306      11.995  78.853  51.306  1.00  0.00           C
ATOM   2330  CB  MET   306      12.914  78.980  50.076  1.00  0.00           C
ATOM   2331  CG  MET   306      14.356  78.516  50.286  1.00  0.00           C
ATOM   2332  SD  MET   306      15.401  79.715  51.166  1.00  0.00           S
ATOM   2333  CE  MET   306      16.967  78.844  50.875  1.00  0.00           C
ATOM   2334  C   MET   306      10.834  79.781  51.032  1.00  0.00           C
ATOM   2335  O   MET   306       9.825  79.383  50.449  1.00  0.00           O
ATOM   2336  N   SER   307      10.958  81.044  51.521  1.00  0.00           N
ATOM   2337  CA  SER   307      10.041  82.158  51.374  1.00  0.00           C
ATOM   2338  CB  SER   307      10.077  83.114  52.574  1.00  0.00           C
ATOM   2339  OG  SER   307       9.665  82.443  53.749  1.00  0.00           O
ATOM   2340  C   SER   307      10.319  83.042  50.183  1.00  0.00           C
ATOM   2341  O   SER   307       9.477  83.850  49.785  1.00  0.00           O
ATOM   2342  N   GLY   308      11.529  82.990  49.608  1.00  0.00           N
ATOM   2343  CA  GLY   308      11.798  83.892  48.522  1.00  0.00           C
ATOM   2344  C   GLY   308      11.934  85.301  49.050  1.00  0.00           C
ATOM   2345  O   GLY   308      12.671  85.582  49.990  1.00  0.00           O
ATOM   2346  N   ALA   309      11.250  86.241  48.381  1.00  0.00           N
ATOM   2347  CA  ALA   309      11.207  87.670  48.592  1.00  0.00           C
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ATOM   2348  CB  ALA   309      10.521  88.408  47.429  1.00  0.00           C
ATOM   2349  C   ALA   309      10.506  88.109  49.860  1.00  0.00           C
ATOM   2350  O   ALA   309      10.663  89.268  50.239  1.00  0.00           O
ATOM   2351  N   ALA   310       9.618  87.288  50.472  1.00  0.00           N
ATOM   2352  CA  ALA   310       8.817  87.749  51.599  1.00  0.00           C
ATOM   2353  CB  ALA   310       7.429  87.094  51.631  1.00  0.00           C
ATOM   2354  C   ALA   310       9.433  87.444  52.944  1.00  0.00           C
ATOM   2355  O   ALA   310       9.920  86.341  53.197  1.00  0.00           O
ATOM   2356  N   PRO   311       9.409  88.465  53.795  1.00  0.00           N
ATOM   2357  CA  PRO   311       9.840  88.342  55.172  1.00  0.00           C
ATOM   2358  CD  PRO   311       9.710  89.791  53.273  1.00  0.00           C
ATOM   2359  CB  PRO   311      10.123  89.760  55.664  1.00  0.00           C
ATOM   2360  CG  PRO   311      10.498  90.516  54.377  1.00  0.00           C
ATOM   2361  C   PRO   311       8.855  87.583  56.008  1.00  0.00           C
ATOM   2362  O   PRO   311       7.648  87.688  55.781  1.00  0.00           O
ATOM   2363  N   LEU   312       9.358  86.811  56.987  1.00  0.00           N
ATOM   2364  CA  LEU   312       8.512  86.039  57.846  1.00  0.00           C
ATOM   2365  CB  LEU   312       8.623  84.515  57.679  1.00  0.00           C
ATOM   2366  CG  LEU   312       8.072  84.012  56.336  1.00  0.00           C
ATOM   2367  CD2 LEU   312       6.675  84.585  56.057  1.00  0.00           C
ATOM   2368  CD1 LEU   312       8.111  82.480  56.268  1.00  0.00           C
ATOM   2369  C   LEU   312       8.866  86.365  59.250  1.00  0.00           C
ATOM   2370  O   LEU   312       9.872  87.013  59.520  1.00  0.00           O
ATOM   2371  N   GLY   313       8.019  85.958  60.203  1.00  0.00           N
ATOM   2372  CA  GLY   313       8.340  86.280  61.554  1.00  0.00           C
ATOM   2373  C   GLY   313       9.284  85.266  62.081  1.00  0.00           C
ATOM   2374  O   GLY   313       9.423  84.163  61.553  1.00  0.00           O
ATOM   2375  N   LYS   314       9.942  85.636  63.188  1.00  0.00           N
ATOM   2376  CA  LYS   314      10.860  84.762  63.837  1.00  0.00           C
ATOM   2377  CB  LYS   314      11.481  85.445  65.073  1.00  0.00           C
ATOM   2378  CG  LYS   314      12.186  84.547  66.094  1.00  0.00           C
ATOM   2379  CD  LYS   314      11.234  83.721  66.965  1.00  0.00           C
ATOM   2380  CE  LYS   314      11.898  83.106  68.200  1.00  0.00           C
ATOM   2381  NZ  LYS   314      10.890  82.392  69.016  1.00  0.00           N
ATOM   2382  C   LYS   314      10.082  83.559  64.266  1.00  0.00           C
ATOM   2383  O   LYS   314      10.534  82.427  64.102  1.00  0.00           O
ATOM   2384  N   GLU   315       8.872  83.785  64.813  1.00  0.00           N
ATOM   2385  CA  GLU   315       8.062  82.719  65.330  1.00  0.00           C
ATOM   2386  CB  GLU   315       6.772  83.230  65.994  1.00  0.00           C
ATOM   2387  CG  GLU   315       5.930  82.124  66.634  1.00  0.00           C
ATOM   2388  CD  GLU   315       6.611  81.702  67.929  1.00  0.00           C
ATOM   2389  OE1 GLU   315       7.815  81.336  67.870  1.00  0.00           O
ATOM   2390  OE2 GLU   315       5.937  81.745  68.992  1.00  0.00           O
ATOM   2391  C   GLU   315       7.658  81.785  64.231  1.00  0.00           C
ATOM   2392  O   GLU   315       7.732  80.570  64.402  1.00  0.00           O
ATOM   2393  N   LEU   316       7.219  82.318  63.074  1.00  0.00           N
ATOM   2394  CA  LEU   316       6.751  81.478  62.007  1.00  0.00           C
ATOM   2395  CB  LEU   316       6.289  82.269  60.769  1.00  0.00           C
ATOM   2396  CG  LEU   316       5.004  83.081  60.968  1.00  0.00           C
ATOM   2397  CD2 LEU   316       3.864  82.184  61.465  1.00  0.00           C
ATOM   2398  CD1 LEU   316       4.625  83.837  59.686  1.00  0.00           C
ATOM   2399  C   LEU   316       7.870  80.644  61.520  1.00  0.00           C
ATOM   2400  O   LEU   316       7.717  79.440  61.326  1.00  0.00           O
ATOM   2401  N   GLU   317       9.030  81.280  61.307  1.00  0.00           N
ATOM   2402  CA  GLU   317      10.138  80.552  60.771  1.00  0.00           C
ATOM   2403  CB  GLU   317      11.374  81.424  60.496  1.00  0.00           C
ATOM   2404  CG  GLU   317      11.989  82.028  61.757  1.00  0.00           C
ATOM   2405  CD  GLU   317      13.254  82.762  61.339  1.00  0.00           C
ATOM   2406  OE1 GLU   317      14.175  82.094  60.801  1.00  0.00           O
ATOM   2407  OE2 GLU   317      13.315  84.001  61.551  1.00  0.00           O
ATOM   2408  C   GLU   317      10.542  79.513  61.756  1.00  0.00           C
ATOM   2409  O   GLU   317      10.870  78.388  61.384  1.00  0.00           O
ATOM   2410  N   ASP   318      10.538  79.879  63.049  1.00  0.00           N
ATOM   2411  CA  ASP   318      10.954  78.965  64.067  1.00  0.00           C
ATOM   2412  CB  ASP   318      11.001  79.640  65.449  1.00  0.00           C
ATOM   2413  CG  ASP   318      11.847  78.787  66.379  1.00  0.00           C
ATOM   2414  OD1 ASP   318      12.294  77.696  65.940  1.00  0.00           O
ATOM   2415  OD2 ASP   318      12.060  79.219  67.544  1.00  0.00           O
ATOM   2416  C   ASP   318       9.983  77.831  64.139  1.00  0.00           C
ATOM   2417  O   ASP   318      10.377  76.671  64.247  1.00  0.00           O
ATOM   2418  N   ALA   319       8.674  78.140  64.078  1.00  0.00           N
ATOM   2419  CA  ALA   319       7.693  77.103  64.201  1.00  0.00           C
ATOM   2420  CB  ALA   319       6.255  77.646  64.183  1.00  0.00           C
ATOM   2421  C   ALA   319       7.828  76.150  63.059  1.00  0.00           C
ATOM   2422  O   ALA   319       7.787  74.936  63.245  1.00  0.00           O
ATOM   2423  N   LEU   320       7.987  76.685  61.835  1.00  0.00           N
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ATOM   2424  CA  LEU   320       8.056  75.841  60.681  1.00  0.00           C
ATOM   2425  CB  LEU   320       7.970  76.639  59.360  1.00  0.00           C
ATOM   2426  CG  LEU   320       7.729  75.798  58.083  1.00  0.00           C
ATOM   2427  CD2 LEU   320       8.836  74.764  57.821  1.00  0.00           C
ATOM   2428  CD1 LEU   320       7.521  76.708  56.864  1.00  0.00           C
ATOM   2429  C   LEU   320       9.315  75.023  60.700  1.00  0.00           C
ATOM   2430  O   LEU   320       9.282  73.838  60.370  1.00  0.00           O
ATOM   2431  N   ARG   321      10.464  75.618  61.077  1.00  0.00           N
ATOM   2432  CA  ARG   321      11.687  74.863  61.024  1.00  0.00           C
ATOM   2433  CB  ARG   321      12.958  75.688  61.307  1.00  0.00           C
ATOM   2434  CG  ARG   321      13.102  76.261  62.715  1.00  0.00           C
ATOM   2435  CD  ARG   321      13.634  75.235  63.717  1.00  0.00           C
ATOM   2436  NE  ARG   321      14.062  75.977  64.934  1.00  0.00           N
ATOM   2437  CZ  ARG   321      14.933  75.404  65.815  1.00  0.00           C
ATOM   2438  NH1 ARG   321      15.392  74.138  65.595  1.00  0.00           N
ATOM   2439  NH2 ARG   321      15.349  76.100  66.913  1.00  0.00           N
ATOM   2440  C   ARG   321      11.583  73.733  61.997  1.00  0.00           C
ATOM   2441  O   ARG   321      12.084  72.641  61.740  1.00  0.00           O
ATOM   2442  N   GLU   322      10.940  73.976  63.154  1.00  0.00           N
ATOM   2443  CA  GLU   322      10.773  72.962  64.152  1.00  0.00           C
ATOM   2444  CB  GLU   322      10.195  73.510  65.468  1.00  0.00           C
ATOM   2445  CG  GLU   322      11.132  74.488  66.178  1.00  0.00           C
ATOM   2446  CD  GLU   322      10.444  74.947  67.455  1.00  0.00           C
ATOM   2447  OE1 GLU   322       9.371  74.374  67.787  1.00  0.00           O
ATOM   2448  OE2 GLU   322      10.981  75.875  68.117  1.00  0.00           O
ATOM   2449  C   GLU   322       9.832  71.893  63.667  1.00  0.00           C
ATOM   2450  O   GLU   322      10.061  70.706  63.897  1.00  0.00           O
ATOM   2451  N   ARG   323       8.742  72.288  62.979  1.00  0.00           N
ATOM   2452  CA  ARG   323       7.723  71.361  62.571  1.00  0.00           C
ATOM   2453  CB  ARG   323       6.497  72.035  61.937  1.00  0.00           C
ATOM   2454  CG  ARG   323       5.288  71.101  61.951  1.00  0.00           C
ATOM   2455  CD  ARG   323       4.853  70.743  63.376  1.00  0.00           C
ATOM   2456  NE  ARG   323       3.845  69.650  63.289  1.00  0.00           N
ATOM   2457  CZ  ARG   323       3.508  68.946  64.410  1.00  0.00           C
ATOM   2458  NH1 ARG   323       4.102  69.238  65.603  1.00  0.00           N
ATOM   2459  NH2 ARG   323       2.577  67.951  64.338  1.00  0.00           N
ATOM   2460  C   ARG   323       8.268  70.366  61.602  1.00  0.00           C
ATOM   2461  O   ARG   323       7.863  69.203  61.627  1.00  0.00           O
ATOM   2462  N   PHE   324       9.170  70.792  60.695  1.00  0.00           N
ATOM   2463  CA  PHE   324       9.718  69.821  59.790  1.00  0.00           C
ATOM   2464  CB  PHE   324       9.898  70.331  58.349  1.00  0.00           C
ATOM   2465  CG  PHE   324       8.579  70.495  57.680  1.00  0.00           C
ATOM   2466  CD1 PHE   324       7.941  69.412  57.121  1.00  0.00           C
ATOM   2467  CD2 PHE   324       7.991  71.735  57.591  1.00  0.00           C
ATOM   2468  CE1 PHE   324       6.725  69.556  56.493  1.00  0.00           C
ATOM   2469  CE2 PHE   324       6.778  71.882  56.965  1.00  0.00           C
ATOM   2470  CZ  PHE   324       6.141  70.795  56.415  1.00  0.00           C
ATOM   2471  C   PHE   324      11.100  69.532  60.244  1.00  0.00           C
ATOM   2472  O   PHE   324      11.951  69.282  59.394  1.00  0.00           O
ATOM   2473  N   PRO   325      11.234  69.273  61.522  1.00  0.00           N
ATOM   2474  CA  PRO   325      12.477  69.443  62.228  1.00  0.00           C
ATOM   2475  CD  PRO   325      10.448  68.192  62.097  1.00  0.00           C
ATOM   2476  CB  PRO   325      12.569  68.306  63.244  1.00  0.00           C
ATOM   2477  CG  PRO   325      11.110  67.870  63.447  1.00  0.00           C
ATOM   2478  C   PRO   325      13.707  69.588  61.416  1.00  0.00           C
ATOM   2479  O   PRO   325      14.409  68.619  61.136  1.00  0.00           O
ATOM   2480  N   LYS   326      13.955  70.856  61.047  1.00  0.00           N
ATOM   2481  CA  LYS   326      15.154  71.253  60.410  1.00  0.00           C
ATOM   2482  CB  LYS   326      15.144  71.461  58.889  1.00  0.00           C
ATOM   2483  CG  LYS   326      15.266  70.112  58.179  1.00  0.00           C
ATOM   2484  CD  LYS   326      15.657  70.202  56.707  1.00  0.00           C
ATOM   2485  CE  LYS   326      17.179  70.153  56.528  1.00  0.00           C
ATOM   2486  NZ  LYS   326      17.723  68.886  57.066  1.00  0.00           N
ATOM   2487  C   LYS   326      15.558  72.497  61.111  1.00  0.00           C
ATOM   2488  O   LYS   326      14.745  73.176  61.730  1.00  0.00           O
ATOM   2489  N   ALA   327      16.859  72.779  61.107  1.00  0.00           N
ATOM   2490  CA  ALA   327      17.365  73.939  61.763  1.00  0.00           C
ATOM   2491  CB  ALA   327      18.903  73.976  61.801  1.00  0.00           C
ATOM   2492  C   ALA   327      16.904  75.176  61.033  1.00  0.00           C
ATOM   2493  O   ALA   327      16.797  76.250  61.631  1.00  0.00           O
ATOM   2494  N   ILE   328      16.660  75.032  59.709  1.00  0.00           N
ATOM   2495  CA  ILE   328      16.543  76.102  58.743  1.00  0.00           C
ATOM   2496  CB  ILE   328      17.360  75.769  57.528  1.00  0.00           C
ATOM   2497  CG2 ILE   328      16.825  74.431  56.984  1.00  0.00           C
ATOM   2498  CG1 ILE   328      17.340  76.894  56.483  1.00  0.00           C
ATOM   2499  CD1 ILE   328      18.238  76.605  55.280  1.00  0.00           C
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ATOM   2500  C   ILE   328      15.194  76.407  58.165  1.00  0.00           C
ATOM   2501  O   ILE   328      14.368  75.526  57.927  1.00  0.00           O
ATOM   2502  N   PHE   329      15.006  77.729  57.904  1.00  0.00           N
ATOM   2503  CA  PHE   329      13.926  78.326  57.181  1.00  0.00           C
ATOM   2504  CB  PHE   329      12.977  79.098  58.106  1.00  0.00           C
ATOM   2505  CG  PHE   329      11.768  79.397  57.313  1.00  0.00           C
ATOM   2506  CD1 PHE   329      11.738  80.496  56.493  1.00  0.00           C
ATOM   2507  CD2 PHE   329      10.678  78.568  57.396  1.00  0.00           C
ATOM   2508  CE1 PHE   329      10.613  80.765  55.754  1.00  0.00           C
ATOM   2509  CE2 PHE   329       9.552  78.836  56.657  1.00  0.00           C
ATOM   2510  CZ  PHE   329       9.524  79.933  55.836  1.00  0.00           C
ATOM   2511  C   PHE   329      14.639  79.314  56.298  1.00  0.00           C
ATOM   2512  O   PHE   329      15.470  80.088  56.778  1.00  0.00           O
ATOM   2513  N   GLY   330      14.361  79.327  54.979  1.00  0.00           N
ATOM   2514  CA  GLY   330      15.112  80.244  54.175  1.00  0.00           C
ATOM   2515  C   GLY   330      14.212  81.371  53.827  1.00  0.00           C
ATOM   2516  O   GLY   330      13.190  81.189  53.169  1.00  0.00           O
ATOM   2517  N   GLN   331      14.591  82.590  54.248  1.00  0.00           N
ATOM   2518  CA  GLN   331      13.743  83.700  53.955  1.00  0.00           C
ATOM   2519  CB  GLN   331      13.157  84.346  55.216  1.00  0.00           C
ATOM   2520  CG  GLN   331      12.347  83.347  56.039  1.00  0.00           C
ATOM   2521  CD  GLN   331      11.810  84.063  57.259  1.00  0.00           C
ATOM   2522  OE1 GLN   331      11.413  85.221  57.158  1.00  0.00           O
ATOM   2523  NE2 GLN   331      11.799  83.373  58.432  1.00  0.00           N
ATOM   2524  C   GLN   331      14.564  84.708  53.243  1.00  0.00           C
ATOM   2525  O   GLN   331      15.732  84.477  52.935  1.00  0.00           O
ATOM   2526  N   GLY   332      13.953  85.856  52.923  1.00  0.00           N
ATOM   2527  CA  GLY   332      14.717  86.828  52.215  1.00  0.00           C
ATOM   2528  C   GLY   332      13.853  87.986  51.903  1.00  0.00           C
ATOM   2529  O   GLY   332      12.662  88.022  52.213  1.00  0.00           O
ATOM   2530  N   TYR   333      14.486  88.985  51.278  1.00  0.00           N
ATOM   2531  CA  TYR   333      13.822  90.189  50.925  1.00  0.00           C
ATOM   2532  CB  TYR   333      14.274  91.308  51.880  1.00  0.00           C
ATOM   2533  CG  TYR   333      13.890  92.656  51.410  1.00  0.00           C
ATOM   2534  CD1 TYR   333      12.588  92.983  51.128  1.00  0.00           C
ATOM   2535  CD2 TYR   333      14.861  93.620  51.319  1.00  0.00           C
ATOM   2536  CE1 TYR   333      12.274  94.253  50.711  1.00  0.00           C
ATOM   2537  CE2 TYR   333      14.552  94.889  50.905  1.00  0.00           C
ATOM   2538  CZ  TYR   333      13.256  95.204  50.592  1.00  0.00           C
ATOM   2539  OH  TYR   333      12.934  96.510  50.163  1.00  0.00           O
ATOM   2540  C   TYR   333      14.148  90.479  49.500  1.00  0.00           C
ATOM   2541  O   TYR   333      15.310  90.480  49.095  1.00  0.00           O
ATOM   2542  N   GLY   334      13.103  90.714  48.687  1.00  0.00           N
ATOM   2543  CA  GLY   334      13.328  90.978  47.297  1.00  0.00           C
ATOM   2544  C   GLY   334      12.124  91.685  46.788  1.00  0.00           C
ATOM   2545  O   GLY   334      11.043  91.588  47.365  1.00  0.00           O
ATOM   2546  N   MET   335      12.299  92.409  45.667  1.00  0.00           N
ATOM   2547  CA  MET   335      11.218  93.135  45.079  1.00  0.00           C
ATOM   2548  CB  MET   335      11.432  94.656  45.118  1.00  0.00           C
ATOM   2549  CG  MET   335      10.152  95.457  44.904  1.00  0.00           C
ATOM   2550  SD  MET   335       9.001  95.430  46.305  1.00  0.00           S
ATOM   2551  CE  MET   335      10.052  96.472  47.357  1.00  0.00           C
ATOM   2552  C   MET   335      11.147  92.701  43.650  1.00  0.00           C
ATOM   2553  O   MET   335      12.073  92.075  43.139  1.00  0.00           O
ATOM   2554  N   THR   336      10.028  93.008  42.967  1.00  0.00           N
ATOM   2555  CA  THR   336       9.909  92.608  41.599  1.00  0.00           C
ATOM   2556  CB  THR   336       8.591  92.973  40.982  1.00  0.00           C
ATOM   2557  OG1 THR   336       8.466  92.364  39.706  1.00  0.00           O
ATOM   2558  CG2 THR   336       8.490  94.499  40.855  1.00  0.00           C
ATOM   2559  C   THR   336      11.013  93.296  40.858  1.00  0.00           C
ATOM   2560  O   THR   336      11.634  92.728  39.961  1.00  0.00           O
ATOM   2561  N   GLU   337      11.301  94.545  41.259  1.00  0.00           N
ATOM   2562  CA  GLU   337      12.296  95.375  40.638  1.00  0.00           C
ATOM   2563  CB  GLU   337      12.315  96.813  41.188  1.00  0.00           C
ATOM   2564  CG  GLU   337      11.148  97.667  40.683  1.00  0.00           C
ATOM   2565  CD  GLU   337       9.869  97.129  41.292  1.00  0.00           C
ATOM   2566  OE1 GLU   337       9.935  96.618  42.440  1.00  0.00           O
ATOM   2567  OE2 GLU   337       8.808  97.212  40.621  1.00  0.00           O
ATOM   2568  C   GLU   337      13.675  94.794  40.781  1.00  0.00           C
ATOM   2569  O   GLU   337      14.560  95.087  39.982  1.00  0.00           O
ATOM   2570  N   ALA   338      13.914  94.057  41.874  1.00  0.00           N
ATOM   2571  CA  ALA   338      15.130  93.370  42.226  1.00  0.00           C
ATOM   2572  CB  ALA   338      15.208  93.025  43.726  1.00  0.00           C
ATOM   2573  C   ALA   338      15.357  92.105  41.446  1.00  0.00           C
ATOM   2574  O   ALA   338      16.448  91.542  41.501  1.00  0.00           O
ATOM   2575  N   GLY   339      14.309  91.541  40.813  1.00  0.00           N
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ATOM   2576  CA  GLY   339      14.439  90.263  40.169  1.00  0.00           C
ATOM   2577  C   GLY   339      14.088  89.236  41.208  1.00  0.00           C
ATOM   2578  O   GLY   339      12.961  88.753  41.235  1.00  0.00           O
ATOM   2579  N   PRO   340      15.071  88.774  41.932  1.00  0.00           N
ATOM   2580  CA  PRO   340      14.819  87.871  43.041  1.00  0.00           C
ATOM   2581  CD  PRO   340      16.211  88.320  41.153  1.00  0.00           C
ATOM   2582  CB  PRO   340      15.728  86.660  42.825  1.00  0.00           C
ATOM   2583  CG  PRO   340      16.265  86.809  41.394  1.00  0.00           C
ATOM   2584  C   PRO   340      15.190  88.539  44.334  1.00  0.00           C
ATOM   2585  O   PRO   340      15.415  89.747  44.348  1.00  0.00           O
ATOM   2586  N   VAL   341      15.317  87.749  45.429  1.00  0.00           N
ATOM   2587  CA  VAL   341      15.718  88.300  46.693  1.00  0.00           C
ATOM   2588  CB  VAL   341      15.539  87.359  47.846  1.00  0.00           C
ATOM   2589  CG1 VAL   341      14.037  87.075  47.999  1.00  0.00           C
ATOM   2590  CG2 VAL   341      16.392  86.103  47.602  1.00  0.00           C
ATOM   2591  C   VAL   341      17.165  88.715  46.640  1.00  0.00           C
ATOM   2592  O   VAL   341      18.028  88.012  46.112  1.00  0.00           O
ATOM   2593  N   LEU   342      17.406  89.960  47.105  1.00  0.00           N
ATOM   2594  CA  LEU   342      18.664  90.645  47.269  1.00  0.00           C
ATOM   2595  CB  LEU   342      18.435  92.169  47.336  1.00  0.00           C
ATOM   2596  CG  LEU   342      19.696  93.054  47.384  1.00  0.00           C
ATOM   2597  CD2 LEU   342      20.570  92.823  46.144  1.00  0.00           C
ATOM   2598  CD1 LEU   342      20.467  92.919  48.706  1.00  0.00           C
ATOM   2599  C   LEU   342      19.325  90.215  48.539  1.00  0.00           C
ATOM   2600  O   LEU   342      20.551  90.185  48.646  1.00  0.00           O
ATOM   2601  N   ALA   343      18.505  89.958  49.573  1.00  0.00           N
ATOM   2602  CA  ALA   343      19.030  89.547  50.835  1.00  0.00           C
ATOM   2603  CB  ALA   343      18.700  90.515  51.984  1.00  0.00           C
ATOM   2604  C   ALA   343      18.365  88.254  51.142  1.00  0.00           C
ATOM   2605  O   ALA   343      17.147  88.127  51.022  1.00  0.00           O
ATOM   2606  N   MET   344      19.165  87.245  51.523  1.00  0.00           N
ATOM   2607  CA  MET   344      18.573  86.002  51.893  1.00  0.00           C
ATOM   2608  CB  MET   344      18.272  85.039  50.727  1.00  0.00           C
ATOM   2609  CG  MET   344      19.160  85.184  49.495  1.00  0.00           C
ATOM   2610  SD  MET   344      20.856  84.562  49.610  1.00  0.00           S
ATOM   2611  CE  MET   344      21.060  84.798  47.821  1.00  0.00           C
ATOM   2612  C   MET   344      19.393  85.361  52.956  1.00  0.00           C
ATOM   2613  O   MET   344      20.590  85.615  53.071  1.00  0.00           O
ATOM   2614  N   ASN   345      18.752  84.545  53.817  1.00  0.00           N
ATOM   2615  CA  ASN   345      19.562  83.941  54.828  1.00  0.00           C
ATOM   2616  CB  ASN   345      19.661  84.759  56.127  1.00  0.00           C
ATOM   2617  CG  ASN   345      20.856  84.305  56.962  1.00  0.00           C
ATOM   2618  OD1 ASN   345      20.786  83.354  57.737  1.00  0.00           O
ATOM   2619  ND2 ASN   345      21.997  85.028  56.810  1.00  0.00           N
ATOM   2620  C   ASN   345      19.052  82.574  55.127  1.00  0.00           C
ATOM   2621  O   ASN   345      17.974  82.185  54.681  1.00  0.00           O
ATOM   2622  N   LEU   346      19.857  81.784  55.864  1.00  0.00           N
ATOM   2623  CA  LEU   346      19.441  80.456  56.216  1.00  0.00           C
ATOM   2624  CB  LEU   346      20.466  79.369  55.849  1.00  0.00           C
ATOM   2625  CG  LEU   346      20.683  79.213  54.333  1.00  0.00           C
ATOM   2626  CD2 LEU   346      19.346  79.018  53.599  1.00  0.00           C
ATOM   2627  CD1 LEU   346      21.702  78.104  54.024  1.00  0.00           C
ATOM   2628  C   LEU   346      19.259  80.412  57.701  1.00  0.00           C
ATOM   2629  O   LEU   346      20.078  80.947  58.449  1.00  0.00           O
ATOM   2630  N   ALA   347      18.160  79.769  58.154  1.00  0.00           N
ATOM   2631  CA  ALA   347      17.846  79.697  59.554  1.00  0.00           C
ATOM   2632  CB  ALA   347      16.404  79.242  59.844  1.00  0.00           C
ATOM   2633  C   ALA   347      18.763  78.717  60.199  1.00  0.00           C
ATOM   2634  O   ALA   347      19.079  77.673  59.629  1.00  0.00           O
ATOM   2635  N   PHE   348      19.196  79.038  61.433  1.00  0.00           N
ATOM   2636  CA  PHE   348      20.074  78.180  62.165  1.00  0.00           C
ATOM   2637  CB  PHE   348      21.290  78.917  62.756  1.00  0.00           C
ATOM   2638  CG  PHE   348      22.267  77.900  63.238  1.00  0.00           C
ATOM   2639  CD1 PHE   348      23.103  77.258  62.353  1.00  0.00           C
ATOM   2640  CD2 PHE   348      22.362  77.592  64.574  1.00  0.00           C
ATOM   2641  CE1 PHE   348      24.007  76.320  62.797  1.00  0.00           C
ATOM   2642  CE2 PHE   348      23.262  76.658  65.025  1.00  0.00           C
ATOM   2643  CZ  PHE   348      24.087  76.017  64.135  1.00  0.00           C
ATOM   2644  C   PHE   348      19.269  77.598  63.294  1.00  0.00           C
ATOM   2645  O   PHE   348      18.209  78.108  63.652  1.00  0.00           O
ATOM   2646  N   ALA   349      19.758  76.483  63.868  1.00  0.00           N
ATOM   2647  CA  ALA   349      19.113  75.810  64.960  1.00  0.00           C
ATOM   2648  CB  ALA   349      19.892  74.574  65.440  1.00  0.00           C
ATOM   2649  C   ALA   349      19.048  76.772  66.105  1.00  0.00           C
ATOM   2650  O   ALA   349      18.108  76.747  66.897  1.00  0.00           O
ATOM   2651  N   LYS   350      20.069  77.641  66.213  1.00  0.00           N
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ATOM   2652  CA  LYS   350      20.219  78.593  67.279  1.00  0.00           C
ATOM   2653  CB  LYS   350      21.422  79.538  67.102  1.00  0.00           C
ATOM   2654  CG  LYS   350      22.781  78.842  67.214  1.00  0.00           C
ATOM   2655  CD  LYS   350      23.953  79.710  66.749  1.00  0.00           C
ATOM   2656  CE  LYS   350      25.314  79.020  66.861  1.00  0.00           C
ATOM   2657  NZ  LYS   350      26.385  79.936  66.410  1.00  0.00           N
ATOM   2658  C   LYS   350      18.992  79.441  67.394  1.00  0.00           C
ATOM   2659  O   LYS   350      18.149  79.471  66.498  1.00  0.00           O
ATOM   2660  N   ASN   351      18.865  80.133  68.552  1.00  0.00           N
ATOM   2661  CA  ASN   351      17.716  80.932  68.878  1.00  0.00           C
ATOM   2662  CB  ASN   351      17.767  81.564  70.282  1.00  0.00           C
ATOM   2663  CG  ASN   351      18.906  82.574  70.308  1.00  0.00           C
ATOM   2664  OD1 ASN   351      20.042  82.263  69.956  1.00  0.00           O
ATOM   2665  ND2 ASN   351      18.590  83.829  70.730  1.00  0.00           N
ATOM   2666  C   ASN   351      17.577  82.047  67.899  1.00  0.00           C
ATOM   2667  O   ASN   351      18.530  82.728  67.525  1.00  0.00           O
ATOM   2668  N   PRO   352      16.361  82.188  67.454  1.00  0.00           N
ATOM   2669  CA  PRO   352      16.024  83.194  66.490  1.00  0.00           C
ATOM   2670  CD  PRO   352      15.464  81.049  67.382  1.00  0.00           C
ATOM   2671  CB  PRO   352      14.657  82.799  65.921  1.00  0.00           C
ATOM   2672  CG  PRO   352      14.169  81.649  66.821  1.00  0.00           C
ATOM   2673  C   PRO   352      16.147  84.634  66.883  1.00  0.00           C
ATOM   2674  O   PRO   352      16.685  85.374  66.065  1.00  0.00           O
ATOM   2675  N   PHE   353      15.666  85.038  68.088  1.00  0.00           N
ATOM   2676  CA  PHE   353      15.680  86.392  68.605  1.00  0.00           C
ATOM   2677  CB  PHE   353      16.661  87.365  67.900  1.00  0.00           C
ATOM   2678  CG  PHE   353      16.817  88.629  68.671  1.00  0.00           C
ATOM   2679  CD1 PHE   353      17.710  88.703  69.716  1.00  0.00           C
ATOM   2680  CD2 PHE   353      16.071  89.741  68.354  1.00  0.00           C
ATOM   2681  CE1 PHE   353      17.857  89.867  70.432  1.00  0.00           C
ATOM   2682  CE2 PHE   353      16.214  90.908  69.068  1.00  0.00           C
ATOM   2683  CZ  PHE   353      17.108  90.973  70.109  1.00  0.00           C
ATOM   2684  C   PHE   353      14.275  86.910  68.462  1.00  0.00           C
ATOM   2685  O   PHE   353      13.448  86.268  67.819  1.00  0.00           O
ATOM   2686  N   PRO   354      13.945  88.027  69.059  1.00  0.00           N
ATOM   2687  CA  PRO   354      12.631  88.566  68.840  1.00  0.00           C
ATOM   2688  CD  PRO   354      14.389  88.284  70.423  1.00  0.00           C
ATOM   2689  CB  PRO   354      12.453  89.660  69.888  1.00  0.00           C
ATOM   2690  CG  PRO   354      13.287  89.140  71.072  1.00  0.00           C
ATOM   2691  C   PRO   354      12.504  89.004  67.426  1.00  0.00           C
ATOM   2692  O   PRO   354      11.403  89.341  66.992  1.00  0.00           O
ATOM   2693  N   VAL   355      13.630  89.021  66.696  1.00  0.00           N
ATOM   2694  CA  VAL   355      13.582  89.446  65.338  1.00  0.00           C
ATOM   2695  CB  VAL   355      14.437  90.650  65.063  1.00  0.00           C
ATOM   2696  CG1 VAL   355      15.909  90.254  65.259  1.00  0.00           C
ATOM   2697  CG2 VAL   355      14.113  91.189  63.659  1.00  0.00           C
ATOM   2698  C   VAL   355      14.085  88.328  64.498  1.00  0.00           C
ATOM   2699  O   VAL   355      14.672  87.359  64.973  1.00  0.00           O
ATOM   2700  N   LYS   356      13.810  88.422  63.195  1.00  0.00           N
ATOM   2701  CA  LYS   356      14.247  87.420  62.294  1.00  0.00           C
ATOM   2702  CB  LYS   356      13.060  86.730  61.606  1.00  0.00           C
ATOM   2703  CG  LYS   356      11.950  87.695  61.166  1.00  0.00           C
ATOM   2704  CD  LYS   356      11.144  88.346  62.295  1.00  0.00           C
ATOM   2705  CE  LYS   356      10.068  89.315  61.798  1.00  0.00           C
ATOM   2706  NZ  LYS   356       9.351  89.915  62.946  1.00  0.00           N
ATOM   2707  C   LYS   356      15.073  88.109  61.260  1.00  0.00           C
ATOM   2708  O   LYS   356      14.574  88.945  60.510  1.00  0.00           O
ATOM   2709  N   SER   357      16.383  87.811  61.244  1.00  0.00           N
ATOM   2710  CA  SER   357      17.232  88.227  60.171  1.00  0.00           C
ATOM   2711  CB  SER   357      18.707  88.392  60.566  1.00  0.00           C
ATOM   2712  OG  SER   357      19.466  88.803  59.439  1.00  0.00           O
ATOM   2713  C   SER   357      17.116  86.991  59.353  1.00  0.00           C
ATOM   2714  O   SER   357      16.558  86.013  59.827  1.00  0.00           O
ATOM   2715  N   GLY   358      17.517  86.923  58.087  1.00  0.00           N
ATOM   2716  CA  GLY   358      17.244  85.629  57.515  1.00  0.00           C
ATOM   2717  C   GLY   358      15.872  85.722  56.953  1.00  0.00           C
ATOM   2718  O   GLY   358      15.624  85.381  55.798  1.00  0.00           O
ATOM   2719  N   SER   359      14.945  86.234  57.790  1.00  0.00           N
ATOM   2720  CA  SER   359      13.704  86.695  57.307  1.00  0.00           C
ATOM   2721  CB  SER   359      12.834  87.337  58.388  1.00  0.00           C
ATOM   2722  OG  SER   359      11.655  87.877  57.811  1.00  0.00           O
ATOM   2723  C   SER   359      14.269  87.773  56.492  1.00  0.00           C
ATOM   2724  O   SER   359      13.882  87.988  55.344  1.00  0.00           O
ATOM   2725  N   CYS   360      15.279  88.458  57.074  1.00  0.00           N
ATOM   2726  CA  CYS   360      15.920  89.221  56.098  1.00  0.00           C
ATOM   2727  CB  CYS   360      16.504  90.545  56.586  1.00  0.00           C
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ATOM   2728  SG  CYS   360      17.228  91.509  55.228  1.00  0.00           S
ATOM   2729  C   CYS   360      16.998  88.327  55.585  1.00  0.00           C
ATOM   2730  O   CYS   360      16.727  87.429  54.788  1.00  0.00           O
ATOM   2731  N   GLY   361      18.248  88.529  56.037  1.00  0.00           N
ATOM   2732  CA  GLY   361      19.303  87.685  55.562  1.00  0.00           C
ATOM   2733  C   GLY   361      20.499  88.553  55.331  1.00  0.00           C
ATOM   2734  O   GLY   361      20.698  89.550  56.023  1.00  0.00           O
ATOM   2735  N   THR   362      21.340  88.179  54.347  1.00  0.00           N
ATOM   2736  CA  THR   362      22.513  88.948  54.046  1.00  0.00           C
ATOM   2737  CB  THR   362      23.792  88.199  54.279  1.00  0.00           C
ATOM   2738  OG1 THR   362      23.857  87.064  53.429  1.00  0.00           O
ATOM   2739  CG2 THR   362      23.842  87.762  55.753  1.00  0.00           C
ATOM   2740  C   THR   362      22.460  89.300  52.592  1.00  0.00           C
ATOM   2741  O   THR   362      21.679  88.734  51.830  1.00  0.00           O
ATOM   2742  N   VAL   363      23.297  90.270  52.173  1.00  0.00           N
ATOM   2743  CA  VAL   363      23.292  90.701  50.808  1.00  0.00           C
ATOM   2744  CB  VAL   363      24.154  91.909  50.573  1.00  0.00           C
ATOM   2745  CG1 VAL   363      24.089  92.287  49.086  1.00  0.00           C
ATOM   2746  CG2 VAL   363      23.696  93.027  51.525  1.00  0.00           C
ATOM   2747  C   VAL   363      23.821  89.587  49.974  1.00  0.00           C
ATOM   2748  O   VAL   363      24.766  88.902  50.357  1.00  0.00           O
ATOM   2749  N   VAL   364      23.195  89.376  48.803  1.00  0.00           N
ATOM   2750  CA  VAL   364      23.567  88.332  47.895  1.00  0.00           C
ATOM   2751  CB  VAL   364      22.501  88.043  46.876  1.00  0.00           C
ATOM   2752  CG1 VAL   364      22.976  86.919  45.947  1.00  0.00           C
ATOM   2753  CG2 VAL   364      21.193  87.734  47.607  1.00  0.00           C
ATOM   2754  C   VAL   364      24.777  88.809  47.146  1.00  0.00           C
ATOM   2755  O   VAL   364      25.042  90.008  47.080  1.00  0.00           O
ATOM   2756  N   ARG   365      25.556  87.877  46.569  1.00  0.00           N
ATOM   2757  CA  ARG   365      26.733  88.265  45.850  1.00  0.00           C
ATOM   2758  CB  ARG   365      27.506  87.083  45.237  1.00  0.00           C
ATOM   2759  CG  ARG   365      28.058  86.092  46.264  1.00  0.00           C
ATOM   2760  CD  ARG   365      26.978  85.240  46.935  1.00  0.00           C
ATOM   2761  NE  ARG   365      27.665  84.297  47.862  1.00  0.00           N
ATOM   2762  CZ  ARG   365      28.111  83.091  47.399  1.00  0.00           C
ATOM   2763  NH1 ARG   365      27.932  82.754  46.089  1.00  0.00           N
ATOM   2764  NH2 ARG   365      28.737  82.225  48.247  1.00  0.00           N
ATOM   2765  C   ARG   365      26.309  89.149  44.720  1.00  0.00           C
ATOM   2766  O   ARG   365      25.188  89.046  44.221  1.00  0.00           O
ATOM   2767  N   ASN   366      27.223  90.049  44.301  1.00  0.00           N
ATOM   2768  CA  ASN   366      27.034  90.983  43.225  1.00  0.00           C
ATOM   2769  CB  ASN   366      26.537  90.306  41.935  1.00  0.00           C
ATOM   2770  CG  ASN   366      27.633  89.357  41.462  1.00  0.00           C
ATOM   2771  OD1 ASN   366      28.812  89.710  41.443  1.00  0.00           O
ATOM   2772  ND2 ASN   366      27.239  88.113  41.081  1.00  0.00           N
ATOM   2773  C   ASN   366      26.044  92.023  43.627  1.00  0.00           C
ATOM   2774  O   ASN   366      25.567  92.789  42.791  1.00  0.00           O
ATOM   2775  N   ALA   367      25.746  92.124  44.933  1.00  0.00           N
ATOM   2776  CA  ALA   367      24.799  93.113  45.347  1.00  0.00           C
ATOM   2777  CB  ALA   367      23.488  92.513  45.881  1.00  0.00           C
ATOM   2778  C   ALA   367      25.407  93.878  46.460  1.00  0.00           C
ATOM   2779  O   ALA   367      26.287  93.376  47.155  1.00  0.00           O
ATOM   2780  N   GLN   368      24.949  95.133  46.628  1.00  0.00           N
ATOM   2781  CA  GLN   368      25.432  96.020  47.645  1.00  0.00           C
ATOM   2782  CB  GLN   368      26.171  97.204  47.016  1.00  0.00           C
ATOM   2783  CG  GLN   368      27.390  96.733  46.233  1.00  0.00           C
ATOM   2784  CD  GLN   368      27.652  97.691  45.093  1.00  0.00           C
ATOM   2785  OE1 GLN   368      27.975  98.863  45.273  1.00  0.00           O
ATOM   2786  NE2 GLN   368      27.495  97.143  43.857  1.00  0.00           N
ATOM   2787  C   GLN   368      24.220  96.577  48.312  1.00  0.00           C
ATOM   2788  O   GLN   368      23.238  96.903  47.648  1.00  0.00           O
ATOM   2789  N   ILE   369      24.253  96.685  49.654  1.00  0.00           N
ATOM   2790  CA  ILE   369      23.141  97.212  50.387  1.00  0.00           C
ATOM   2791  CB  ILE   369      22.454  96.178  51.227  1.00  0.00           C
ATOM   2792  CG2 ILE   369      21.448  96.885  52.151  1.00  0.00           C
ATOM   2793  CG1 ILE   369      21.818  95.124  50.319  1.00  0.00           C
ATOM   2794  CD1 ILE   369      20.827  95.762  49.355  1.00  0.00           C
ATOM   2795  C   ILE   369      23.635  98.250  51.345  1.00  0.00           C
ATOM   2796  O   ILE   369      24.661  98.075  52.002  1.00  0.00           O
ATOM   2797  N   LYS   370      22.892  99.372  51.440  1.00  0.00           N
ATOM   2798  CA  LYS   370      23.209 100.399  52.386  1.00  0.00           C
ATOM   2799  CB  LYS   370      23.933 101.612  51.779  1.00  0.00           C
ATOM   2800  CG  LYS   370      23.131 102.348  50.704  1.00  0.00           C
ATOM   2801  CD  LYS   370      23.751 103.690  50.312  1.00  0.00           C
ATOM   2802  CE  LYS   370      22.960 104.437  49.238  1.00  0.00           C
ATOM   2803  NZ  LYS   370      23.625 105.720  48.919  1.00  0.00           N
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ATOM   2804  C   LYS   370      21.906 100.875  52.938  1.00  0.00           C
ATOM   2805  O   LYS   370      20.860 100.685  52.322  1.00  0.00           O
ATOM   2806  N   ILE   371      21.949 101.493  54.132  1.00  0.00           N
ATOM   2807  CA  ILE   371      20.784 101.998  54.795  1.00  0.00           C
ATOM   2808  CB  ILE   371      20.674 101.421  56.174  1.00  0.00           C
ATOM   2809  CG2 ILE   371      19.557 102.142  56.930  1.00  0.00           C
ATOM   2810  CG1 ILE   371      20.480  99.898  56.075  1.00  0.00           C
ATOM   2811  CD1 ILE   371      20.673  99.153  57.395  1.00  0.00           C
ATOM   2812  C   ILE   371      20.987 103.479  54.871  1.00  0.00           C
ATOM   2813  O   ILE   371      22.071 103.939  55.224  1.00  0.00           O
ATOM   2814  N   LEU   372      19.950 104.264  54.512  1.00  0.00           N
ATOM   2815  CA  LEU   372      20.117 105.683  54.372  1.00  0.00           C
ATOM   2816  CB  LEU   372      19.798 106.044  52.918  1.00  0.00           C
ATOM   2817  CG  LEU   372      20.475 107.313  52.431  1.00  0.00           C
ATOM   2818  CD2 LEU   372      19.864 107.826  51.117  1.00  0.00           C
ATOM   2819  CD1 LEU   372      21.990 107.059  52.334  1.00  0.00           C
ATOM   2820  C   LEU   372      19.115 106.383  55.264  1.00  0.00           C
ATOM   2821  O   LEU   372      18.060 105.832  55.571  1.00  0.00           O
ATOM   2822  N   ASP   373      19.417 107.626  55.707  1.00  0.00           N
ATOM   2823  CA  ASP   373      18.516 108.368  56.558  1.00  0.00           C
ATOM   2824  CB  ASP   373      19.076 109.728  57.018  1.00  0.00           C
ATOM   2825  CG  ASP   373      18.072 110.397  57.951  1.00  0.00           C
ATOM   2826  OD1 ASP   373      16.945 110.725  57.490  1.00  0.00           O
ATOM   2827  OD2 ASP   373      18.421 110.582  59.146  1.00  0.00           O
ATOM   2828  C   ASP   373      17.267 108.611  55.770  1.00  0.00           C
ATOM   2829  O   ASP   373      17.316 109.010  54.608  1.00  0.00           O
ATOM   2830  N   THR   374      16.098 108.371  56.392  1.00  0.00           N
ATOM   2831  CA  THR   374      14.874 108.437  55.648  1.00  0.00           C
ATOM   2832  CB  THR   374      13.676 108.083  56.480  1.00  0.00           C
ATOM   2833  OG1 THR   374      13.816 106.773  57.008  1.00  0.00           O
ATOM   2834  CG2 THR   374      12.422 108.165  55.593  1.00  0.00           C
ATOM   2835  C   THR   374      14.634 109.788  55.089  1.00  0.00           C
ATOM   2836  O   THR   374      14.478 109.977  53.884  1.00  0.00           O
ATOM   2837  N   GLU   375      14.565 110.791  55.960  1.00  0.00           N
ATOM   2838  CA  GLU   375      14.281 112.052  55.378  1.00  0.00           C
ATOM   2839  CB  GLU   375      13.927 113.103  56.436  1.00  0.00           C
ATOM   2840  CG  GLU   375      12.666 112.762  57.231  1.00  0.00           C
ATOM   2841  CD  GLU   375      12.437 113.880  58.237  1.00  0.00           C
ATOM   2842  OE1 GLU   375      13.273 114.823  58.272  1.00  0.00           O
ATOM   2843  OE2 GLU   375      11.427 113.807  58.985  1.00  0.00           O
ATOM   2844  C   GLU   375      15.538 112.561  54.678  1.00  0.00           C
ATOM   2845  O   GLU   375      15.483 112.993  53.527  1.00  0.00           O
ATOM   2846  N   THR   376      16.704 112.525  55.383  1.00  0.00           N
ATOM   2847  CA  THR   376      17.981 113.089  54.969  1.00  0.00           C
ATOM   2848  CB  THR   376      19.016 113.030  56.049  1.00  0.00           C
ATOM   2849  OG1 THR   376      18.548 113.665  57.225  1.00  0.00           O
ATOM   2850  CG2 THR   376      20.277 113.745  55.540  1.00  0.00           C
ATOM   2851  C   THR   376      18.630 112.393  53.806  1.00  0.00           C
ATOM   2852  O   THR   376      19.033 113.035  52.837  1.00  0.00           O
ATOM   2853  N   GLY   377      18.764 111.055  53.864  1.00  0.00           N
ATOM   2854  CA  GLY   377      19.424 110.354  52.796  1.00  0.00           C
ATOM   2855  C   GLY   377      20.886 110.152  53.102  1.00  0.00           C
ATOM   2856  O   GLY   377      21.649 109.764  52.220  1.00  0.00           O
ATOM   2857  N   GLU   378      21.343 110.409  54.343  1.00  0.00           N
ATOM   2858  CA  GLU   378      22.730 110.160  54.647  1.00  0.00           C
ATOM   2859  CB  GLU   378      23.197 110.891  55.915  1.00  0.00           C
ATOM   2860  CG  GLU   378      23.179 112.413  55.764  1.00  0.00           C
ATOM   2861  CD  GLU   378      23.477 113.018  57.126  1.00  0.00           C
ATOM   2862  OE1 GLU   378      22.794 112.618  58.106  1.00  0.00           O
ATOM   2863  OE2 GLU   378      24.391 113.882  57.208  1.00  0.00           O
ATOM   2864  C   GLU   378      22.887 108.682  54.880  1.00  0.00           C
ATOM   2865  O   GLU   378      21.979 108.042  55.401  1.00  0.00           O
ATOM   2866  N   SER   379      24.043 108.090  54.501  1.00  0.00           N
ATOM   2867  CA  SER   379      24.210 106.668  54.669  1.00  0.00           C
ATOM   2868  CB  SER   379      25.357 106.091  53.822  1.00  0.00           C
ATOM   2869  OG  SER   379      25.382 104.677  53.934  1.00  0.00           O
ATOM   2870  C   SER   379      24.491 106.379  56.116  1.00  0.00           C
ATOM   2871  O   SER   379      25.431 106.917  56.699  1.00  0.00           O
ATOM   2872  N   LEU   380      23.668 105.497  56.722  1.00  0.00           N
ATOM   2873  CA  LEU   380      23.742 105.175  58.124  1.00  0.00           C
ATOM   2874  CB  LEU   380      22.375 104.800  58.720  1.00  0.00           C
ATOM   2875  CG  LEU   380      21.330 105.926  58.590  1.00  0.00           C
ATOM   2876  CD2 LEU   380      21.858 107.259  59.146  1.00  0.00           C
ATOM   2877  CD1 LEU   380      19.984 105.514  59.204  1.00  0.00           C
ATOM   2878  C   LEU   380      24.694 104.037  58.394  1.00  0.00           C
ATOM   2879  O   LEU   380      25.039 103.219  57.542  1.00  0.00           O
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ATOM   2880  N   PRO   381      25.128 104.060  59.628  1.00  0.00           N
ATOM   2881  CA  PRO   381      26.033 103.088  60.205  1.00  0.00           C
ATOM   2882  CD  PRO   381      25.277 105.360  60.263  1.00  0.00           C
ATOM   2883  CB  PRO   381      26.801 103.820  61.308  1.00  0.00           C
ATOM   2884  CG  PRO   381      25.965 105.074  61.602  1.00  0.00           C
ATOM   2885  C   PRO   381      25.365 101.849  60.725  1.00  0.00           C
ATOM   2886  O   PRO   381      24.162 101.671  60.543  1.00  0.00           O
ATOM   2887  N   HIS   382      26.159 100.977  61.383  1.00  0.00           N
ATOM   2888  CA  HIS   382      25.692  99.732  61.921  1.00  0.00           C
ATOM   2889  ND1 HIS   382      26.715  99.415  65.108  1.00  0.00           N
ATOM   2890  CG  HIS   382      27.303  99.559  63.870  1.00  0.00           C
ATOM   2891  NE2 HIS   382      28.473 100.745  65.392  1.00  0.00           N
ATOM   2892  CD2 HIS   382      28.376 100.374  64.063  1.00  0.00           C
ATOM   2893  CE1 HIS   382      27.455 100.145  65.980  1.00  0.00           C
ATOM   2894  CB  HIS   382      26.791  98.911  62.618  1.00  0.00           C
ATOM   2895  C   HIS   382      24.609  99.967  62.925  1.00  0.00           C
ATOM   2896  O   HIS   382      24.612 100.948  63.666  1.00  0.00           O
ATOM   2897  N   ASN   383      23.630  99.041  62.930  1.00  0.00           N
ATOM   2898  CA  ASN   383      22.538  99.009  63.857  1.00  0.00           C
ATOM   2899  CB  ASN   383      22.982  98.743  65.306  1.00  0.00           C
ATOM   2900  CG  ASN   383      23.443  97.295  65.395  1.00  0.00           C
ATOM   2901  OD1 ASN   383      22.701  96.373  65.060  1.00  0.00           O
ATOM   2902  ND2 ASN   383      24.706  97.087  65.853  1.00  0.00           N
ATOM   2903  C   ASN   383      21.782 100.294  63.830  1.00  0.00           C
ATOM   2904  O   ASN   383      21.133 100.651  64.810  1.00  0.00           O
ATOM   2905  N   GLN   384      21.810 101.017  62.698  1.00  0.00           N
ATOM   2906  CA  GLN   384      21.027 102.214  62.662  1.00  0.00           C
ATOM   2907  CB  GLN   384      21.825 103.467  62.260  1.00  0.00           C
ATOM   2908  CG  GLN   384      20.999 104.751  62.349  1.00  0.00           C
ATOM   2909  CD  GLN   384      21.917 105.939  62.106  1.00  0.00           C
ATOM   2910  OE1 GLN   384      23.137 105.796  62.053  1.00  0.00           O
ATOM   2911  NE2 GLN   384      21.316 107.151  61.961  1.00  0.00           N
ATOM   2912  C   GLN   384      19.954 101.976  61.651  1.00  0.00           C
ATOM   2913  O   GLN   384      20.225 101.512  60.545  1.00  0.00           O
ATOM   2914  N   ALA   385      18.691 102.256  62.027  1.00  0.00           N
ATOM   2915  CA  ALA   385      17.592 102.021  61.133  1.00  0.00           C
ATOM   2916  CB  ALA   385      16.220 102.032  61.828  1.00  0.00           C
ATOM   2917  C   ALA   385      17.577 103.089  60.089  1.00  0.00           C
ATOM   2918  O   ALA   385      17.841 104.256  60.374  1.00  0.00           O
ATOM   2919  N   GLY   386      17.244 102.703  58.843  1.00  0.00           N
ATOM   2920  CA  GLY   386      17.175 103.640  57.760  1.00  0.00           C
ATOM   2921  C   GLY   386      16.596 102.907  56.585  1.00  0.00           C
ATOM   2922  O   GLY   386      16.254 101.730  56.681  1.00  0.00           O
ATOM   2923  N   GLU   387      16.462 103.598  55.434  1.00  0.00           N
ATOM   2924  CA  GLU   387      15.893 102.975  54.274  1.00  0.00           C
ATOM   2925  CB  GLU   387      15.442 103.973  53.194  1.00  0.00           C
ATOM   2926  CG  GLU   387      14.688 103.312  52.039  1.00  0.00           C
ATOM   2927  CD  GLU   387      14.300 104.394  51.043  1.00  0.00           C
ATOM   2928  OE1 GLU   387      14.873 105.512  51.133  1.00  0.00           O
ATOM   2929  OE2 GLU   387      13.426 104.118  50.179  1.00  0.00           O
ATOM   2930  C   GLU   387      16.906 102.074  53.655  1.00  0.00           C
ATOM   2931  O   GLU   387      18.084 102.417  53.560  1.00  0.00           O
ATOM   2932  N   ILE   388      16.476 100.882  53.193  1.00  0.00           N
ATOM   2933  CA  ILE   388      17.474 100.063  52.583  1.00  0.00           C
ATOM   2934  CB  ILE   388      17.370  98.574  52.773  1.00  0.00           C
ATOM   2935  CG2 ILE   388      17.507  98.286  54.277  1.00  0.00           C
ATOM   2936  CG1 ILE   388      16.087  98.024  52.163  1.00  0.00           C
ATOM   2937  CD1 ILE   388      14.880  98.531  52.921  1.00  0.00           C
ATOM   2938  C   ILE   388      17.496 100.361  51.127  1.00  0.00           C
ATOM   2939  O   ILE   388      16.468 100.417  50.451  1.00  0.00           O
ATOM   2940  N   CYS   389      18.717 100.614  50.629  1.00  0.00           N
ATOM   2941  CA  CYS   389      18.927 100.883  49.246  1.00  0.00           C
ATOM   2942  CB  CYS   389      19.673 102.202  48.986  1.00  0.00           C
ATOM   2943  SG  CYS   389      18.697 103.648  49.497  1.00  0.00           S
ATOM   2944  C   CYS   389      19.770  99.761  48.751  1.00  0.00           C
ATOM   2945  O   CYS   389      20.673  99.291  49.447  1.00  0.00           O
ATOM   2946  N   ILE   390      19.468  99.293  47.528  1.00  0.00           N
ATOM   2947  CA  ILE   390      20.156  98.155  47.008  1.00  0.00           C
ATOM   2948  CB  ILE   390      19.206  97.023  46.720  1.00  0.00           C
ATOM   2949  CG2 ILE   390      20.009  95.847  46.138  1.00  0.00           C
ATOM   2950  CG1 ILE   390      18.389  96.661  47.973  1.00  0.00           C
ATOM   2951  CD1 ILE   390      17.191  95.754  47.690  1.00  0.00           C
ATOM   2952  C   ILE   390      20.731  98.544  45.687  1.00  0.00           C
ATOM   2953  O   ILE   390      20.142  99.327  44.945  1.00  0.00           O
ATOM   2954  N   ARG   391      21.924  98.017  45.366  1.00  0.00           N
ATOM   2955  CA  ARG   391      22.507  98.289  44.089  1.00  0.00           C
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ATOM   2956  CB  ARG   391      23.625  99.346  44.144  1.00  0.00           C
ATOM   2957  CG  ARG   391      24.256  99.648  42.785  1.00  0.00           C
ATOM   2958  CD  ARG   391      25.032 100.967  42.756  1.00  0.00           C
ATOM   2959  NE  ARG   391      26.180 100.850  43.699  1.00  0.00           N
ATOM   2960  CZ  ARG   391      27.145 101.816  43.704  1.00  0.00           C
ATOM   2961  NH1 ARG   391      27.050 102.877  42.850  1.00  0.00           N
ATOM   2962  NH2 ARG   391      28.203 101.721  44.560  1.00  0.00           N
ATOM   2963  C   ARG   391      23.090  97.000  43.620  1.00  0.00           C
ATOM   2964  O   ARG   391      23.769  96.312  44.381  1.00  0.00           O
ATOM   2965  N   GLY   392      22.829  96.624  42.353  1.00  0.00           N
ATOM   2966  CA  GLY   392      23.368  95.382  41.882  1.00  0.00           C
ATOM   2967  C   GLY   392      22.836  95.108  40.507  1.00  0.00           C
ATOM   2968  O   GLY   392      21.964  95.801  39.988  1.00  0.00           O
ATOM   2969  N   PRO   393      23.369  94.070  39.926  1.00  0.00           N
ATOM   2970  CA  PRO   393      23.016  93.686  38.581  1.00  0.00           C
ATOM   2971  CD  PRO   393      24.737  93.694  40.248  1.00  0.00           C
ATOM   2972  CB  PRO   393      24.077  92.679  38.145  1.00  0.00           C
ATOM   2973  CG  PRO   393      25.314  93.073  38.967  1.00  0.00           C
ATOM   2974  C   PRO   393      21.616  93.178  38.388  1.00  0.00           C
ATOM   2975  O   PRO   393      21.194  93.055  37.240  1.00  0.00           O
ATOM   2976  N   GLU   394      20.920  92.800  39.473  1.00  0.00           N
ATOM   2977  CA  GLU   394      19.574  92.281  39.461  1.00  0.00           C
ATOM   2978  CB  GLU   394      19.215  91.580  40.783  1.00  0.00           C
ATOM   2979  CG  GLU   394      20.039  90.319  41.046  1.00  0.00           C
ATOM   2980  CD  GLU   394      19.645  89.772  42.410  1.00  0.00           C
ATOM   2981  OE1 GLU   394      18.452  89.403  42.579  1.00  0.00           O
ATOM   2982  OE2 GLU   394      20.532  89.719  43.304  1.00  0.00           O
ATOM   2983  C   GLU   394      18.568  93.375  39.255  1.00  0.00           C
ATOM   2984  O   GLU   394      17.439  93.123  38.834  1.00  0.00           O
ATOM   2985  N   ILE   395      18.924  94.617  39.625  1.00  0.00           N
ATOM   2986  CA  ILE   395      17.997  95.710  39.543  1.00  0.00           C
ATOM   2987  CB  ILE   395      18.593  97.034  39.931  1.00  0.00           C
ATOM   2988  CG2 ILE   395      17.538  98.128  39.690  1.00  0.00           C
ATOM   2989  CG1 ILE   395      19.092  96.979  41.385  1.00  0.00           C
ATOM   2990  CD1 ILE   395      17.987  96.666  42.394  1.00  0.00           C
ATOM   2991  C   ILE   395      17.489  95.811  38.142  1.00  0.00           C
ATOM   2992  O   ILE   395      18.224  95.630  37.174  1.00  0.00           O
ATOM   2993  N   MET   396      16.180  96.092  38.017  1.00  0.00           N
ATOM   2994  CA  MET   396      15.515  96.150  36.753  1.00  0.00           C
ATOM   2995  CB  MET   396      13.996  96.365  36.877  1.00  0.00           C
ATOM   2996  CG  MET   396      13.623  97.717  37.497  1.00  0.00           C
ATOM   2997  SD  MET   396      11.844  98.099  37.460  1.00  0.00           S
ATOM   2998  CE  MET   396      11.965  99.717  38.275  1.00  0.00           C
ATOM   2999  C   MET   396      16.037  97.288  35.935  1.00  0.00           C
ATOM   3000  O   MET   396      16.696  98.197  36.436  1.00  0.00           O
ATOM   3001  N   LYS   397      15.770  97.213  34.617  1.00  0.00           N
ATOM   3002  CA  LYS   397      16.118  98.221  33.659  1.00  0.00           C
ATOM   3003  CB  LYS   397      15.763  97.789  32.225  1.00  0.00           C
ATOM   3004  CG  LYS   397      16.111  98.822  31.152  1.00  0.00           C
ATOM   3005  CD  LYS   397      16.018  98.276  29.726  1.00  0.00           C
ATOM   3006  CE  LYS   397      16.362  99.311  28.653  1.00  0.00           C
ATOM   3007  NZ  LYS   397      17.801  99.654  28.727  1.00  0.00           N
ATOM   3008  C   LYS   397      15.295  99.430  33.972  1.00  0.00           C
ATOM   3009  O   LYS   397      15.758 100.562  33.844  1.00  0.00           O
ATOM   3010  N   GLY   398      14.031  99.203  34.378  1.00  0.00           N
ATOM   3011  CA  GLY   398      13.116 100.261  34.699  1.00  0.00           C
ATOM   3012  C   GLY   398      11.768  99.762  34.292  1.00  0.00           C
ATOM   3013  O   GLY   398      11.622  98.598  33.930  1.00  0.00           O
ATOM   3014  N   TYR   399      10.736 100.625  34.348  1.00  0.00           N
ATOM   3015  CA  TYR   399       9.441 100.214  33.884  1.00  0.00           C
ATOM   3016  CB  TYR   399       8.246 100.967  34.467  1.00  0.00           C
ATOM   3017  CG  TYR   399       7.968 100.408  35.803  1.00  0.00           C
ATOM   3018  CD1 TYR   399       7.281  99.226  35.911  1.00  0.00           C
ATOM   3019  CD2 TYR   399       8.374 101.066  36.934  1.00  0.00           C
ATOM   3020  CE1 TYR   399       6.998  98.685  37.135  1.00  0.00           C
ATOM   3021  CE2 TYR   399       8.094 100.535  38.167  1.00  0.00           C
ATOM   3022  CZ  TYR   399       7.408  99.349  38.262  1.00  0.00           C
ATOM   3023  OH  TYR   399       7.122  98.813  39.531  1.00  0.00           O
ATOM   3024  C   TYR   399       9.390 100.486  32.418  1.00  0.00           C
ATOM   3025  O   TYR   399       9.884 101.517  31.964  1.00  0.00           O
ATOM   3026  N   ILE   400       8.799  99.579  31.610  1.00  0.00           N
ATOM   3027  CA  ILE   400       8.851  99.934  30.222  1.00  0.00           C
ATOM   3028  CB  ILE   400       8.614  98.886  29.159  1.00  0.00           C
ATOM   3029  CG2 ILE   400       7.202  99.083  28.569  1.00  0.00           C
ATOM   3030  CG1 ILE   400       9.600  99.141  28.006  1.00  0.00           C
ATOM   3031  CD1 ILE   400      11.060  98.895  28.386  1.00  0.00           C
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ATOM   3032  C   ILE   400       7.835 100.995  30.025  1.00  0.00           C
ATOM   3033  O   ILE   400       6.718 100.917  30.539  1.00  0.00           O
ATOM   3034  N   ASN   401       8.245 102.044  29.294  1.00  0.00           N
ATOM   3035  CA  ASN   401       7.394 103.154  29.013  1.00  0.00           C
ATOM   3036  CB  ASN   401       6.205 102.793  28.107  1.00  0.00           C
ATOM   3037  CG  ASN   401       6.760 102.491  26.722  1.00  0.00           C
ATOM   3038  OD1 ASN   401       7.869 102.903  26.386  1.00  0.00           O
ATOM   3039  ND2 ASN   401       5.970 101.758  25.894  1.00  0.00           N
ATOM   3040  C   ASN   401       6.877 103.702  30.301  1.00  0.00           C
ATOM   3041  O   ASN   401       5.710 104.077  30.392  1.00  0.00           O
ATOM   3042  N   ASP   402       7.733 103.754  31.340  1.00  0.00           N
ATOM   3043  CA  ASP   402       7.286 104.322  32.579  1.00  0.00           C
ATOM   3044  CB  ASP   402       6.652 103.264  33.496  1.00  0.00           C
ATOM   3045  CG  ASP   402       5.932 103.949  34.645  1.00  0.00           C
ATOM   3046  OD1 ASP   402       6.151 105.171  34.855  1.00  0.00           O
ATOM   3047  OD2 ASP   402       5.145 103.241  35.330  1.00  0.00           O
ATOM   3048  C   ASP   402       8.491 104.872  33.280  1.00  0.00           C
ATOM   3049  O   ASP   402       8.798 104.481  34.405  1.00  0.00           O
ATOM   3050  N   PRO   403       9.173 105.776  32.632  1.00  0.00           N
ATOM   3051  CA  PRO   403      10.383 106.370  33.134  1.00  0.00           C
ATOM   3052  CD  PRO   403       8.598 106.538  31.536  1.00  0.00           C
ATOM   3053  CB  PRO   403      10.825 107.346  32.047  1.00  0.00           C
ATOM   3054  CG  PRO   403       9.495 107.781  31.405  1.00  0.00           C
ATOM   3055  C   PRO   403      10.199 107.084  34.439  1.00  0.00           C
ATOM   3056  O   PRO   403      11.137 107.107  35.235  1.00  0.00           O
ATOM   3057  N   GLU   404       9.030 107.705  34.671  1.00  0.00           N
ATOM   3058  CA  GLU   404       8.862 108.464  35.875  1.00  0.00           C
ATOM   3059  CB  GLU   404       7.518 109.207  35.928  1.00  0.00           C
ATOM   3060  CG  GLU   404       7.394 110.138  37.133  1.00  0.00           C
ATOM   3061  CD  GLU   404       8.374 111.284  36.927  1.00  0.00           C
ATOM   3062  OE1 GLU   404       9.091 111.267  35.890  1.00  0.00           O
ATOM   3063  OE2 GLU   404       8.419 112.190  37.800  1.00  0.00           O
ATOM   3064  C   GLU   404       8.914 107.547  37.052  1.00  0.00           C
ATOM   3065  O   GLU   404       9.607 107.815  38.033  1.00  0.00           O
ATOM   3066  N   SER   405       8.193 106.417  36.969  1.00  0.00           N
ATOM   3067  CA  SER   405       8.155 105.497  38.064  1.00  0.00           C
ATOM   3068  CB  SER   405       7.243 104.288  37.791  1.00  0.00           C
ATOM   3069  OG  SER   405       7.241 103.414  38.911  1.00  0.00           O
ATOM   3070  C   SER   405       9.535 104.977  38.277  1.00  0.00           C
ATOM   3071  O   SER   405       9.968 104.772  39.410  1.00  0.00           O
ATOM   3072  N   THR   406      10.264 104.754  37.173  1.00  0.00           N
ATOM   3073  CA  THR   406      11.589 104.214  37.261  1.00  0.00           C
ATOM   3074  CB  THR   406      12.188 103.967  35.910  1.00  0.00           C
ATOM   3075  OG1 THR   406      11.369 103.076  35.169  1.00  0.00           O
ATOM   3076  CG2 THR   406      13.591 103.365  36.094  1.00  0.00           C
ATOM   3077  C   THR   406      12.482 105.177  37.982  1.00  0.00           C
ATOM   3078  O   THR   406      13.237 104.792  38.873  1.00  0.00           O
ATOM   3079  N   ALA   407      12.405 106.471  37.627  1.00  0.00           N
ATOM   3080  CA  ALA   407      13.289 107.454  38.187  1.00  0.00           C
ATOM   3081  CB  ALA   407      13.055 108.859  37.607  1.00  0.00           C
ATOM   3082  C   ALA   407      13.093 107.542  39.663  1.00  0.00           C
ATOM   3083  O   ALA   407      14.055 107.702  40.412  1.00  0.00           O
ATOM   3084  N   ALA   408      11.834 107.467  40.127  1.00  0.00           N
ATOM   3085  CA  ALA   408      11.582 107.607  41.529  1.00  0.00           C
ATOM   3086  CB  ALA   408      10.082 107.578  41.869  1.00  0.00           C
ATOM   3087  C   ALA   408      12.232 106.490  42.287  1.00  0.00           C
ATOM   3088  O   ALA   408      12.830 106.720  43.337  1.00  0.00           O
ATOM   3089  N   THR   409      12.105 105.246  41.786  1.00  0.00           N
ATOM   3090  CA  THR   409      12.631 104.090  42.461  1.00  0.00           C
ATOM   3091  CB  THR   409      12.150 102.806  41.842  1.00  0.00           C
ATOM   3092  OG1 THR   409      12.608 102.705  40.501  1.00  0.00           O
ATOM   3093  CG2 THR   409      10.612 102.786  41.881  1.00  0.00           C
ATOM   3094  C   THR   409      14.130 104.057  42.460  1.00  0.00           C
ATOM   3095  O   THR   409      14.748 103.854  43.506  1.00  0.00           O
ATOM   3096  N   ILE   410      14.773 104.263  41.291  1.00  0.00           N
ATOM   3097  CA  ILE   410      16.205 104.165  41.280  1.00  0.00           C
ATOM   3098  CB  ILE   410      16.811 103.109  40.386  1.00  0.00           C
ATOM   3099  CG2 ILE   410      16.659 101.752  41.079  1.00  0.00           C
ATOM   3100  CG1 ILE   410      16.268 103.151  38.954  1.00  0.00           C
ATOM   3101  CD1 ILE   410      14.855 102.583  38.834  1.00  0.00           C
ATOM   3102  C   ILE   410      16.869 105.474  41.021  1.00  0.00           C
ATOM   3103  O   ILE   410      16.457 106.283  40.192  1.00  0.00           O
ATOM   3104  N   ASP   411      17.943 105.672  41.803  1.00  0.00           N
ATOM   3105  CA  ASP   411      18.814 106.804  41.904  1.00  0.00           C
ATOM   3106  CB  ASP   411      19.647 106.616  43.195  1.00  0.00           C
ATOM   3107  CG  ASP   411      20.539 107.782  43.587  1.00  0.00           C
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ATOM   3108  OD1 ASP   411      21.480 108.123  42.825  1.00  0.00           O
ATOM   3109  OD2 ASP   411      20.307 108.327  44.698  1.00  0.00           O
ATOM   3110  C   ASP   411      19.724 106.815  40.708  1.00  0.00           C
ATOM   3111  O   ASP   411      19.851 105.824  39.991  1.00  0.00           O
ATOM   3112  N   GLU   412      20.375 107.971  40.466  1.00  0.00           N
ATOM   3113  CA  GLU   412      21.293 108.176  39.380  1.00  0.00           C
ATOM   3114  CB  GLU   412      21.813 109.623  39.327  1.00  0.00           C
ATOM   3115  CG  GLU   412      20.711 110.640  39.016  1.00  0.00           C
ATOM   3116  CD  GLU   412      21.330 112.030  39.003  1.00  0.00           C
ATOM   3117  OE1 GLU   412      22.577 112.127  39.160  1.00  0.00           O
ATOM   3118  OE2 GLU   412      20.562 113.015  38.837  1.00  0.00           O
ATOM   3119  C   GLU   412      22.465 107.263  39.582  1.00  0.00           C
ATOM   3120  O   GLU   412      23.060 106.774  38.622  1.00  0.00           O
ATOM   3121  N   GLU   413      22.830 107.038  40.859  1.00  0.00           N
ATOM   3122  CA  GLU   413      23.917 106.195  41.270  1.00  0.00           C
ATOM   3123  CB  GLU   413      24.196 106.276  42.781  1.00  0.00           C
ATOM   3124  CG  GLU   413      25.462 105.533  43.210  1.00  0.00           C
ATOM   3125  CD  GLU   413      26.659 106.376  42.795  1.00  0.00           C
ATOM   3126  OE1 GLU   413      26.437 107.462  42.195  1.00  0.00           O
ATOM   3127  OE2 GLU   413      27.811 105.948  43.073  1.00  0.00           O
ATOM   3128  C   GLU   413      23.575 104.774  40.935  1.00  0.00           C
ATOM   3129  O   GLU   413      24.461 103.942  40.748  1.00  0.00           O
ATOM   3130  N   GLY   414      22.272 104.440  40.873  1.00  0.00           N
ATOM   3131  CA  GLY   414      21.913 103.086  40.551  1.00  0.00           C
ATOM   3132  C   GLY   414      21.349 102.426  41.765  1.00  0.00           C
ATOM   3133  O   GLY   414      20.927 101.272  41.715  1.00  0.00           O
ATOM   3134  N   TRP   415      21.330 103.143  42.901  1.00  0.00           N
ATOM   3135  CA  TRP   415      20.786 102.566  44.089  1.00  0.00           C
ATOM   3136  CB  TRP   415      21.118 103.385  45.346  1.00  0.00           C
ATOM   3137  CG  TRP   415      22.596 103.438  45.647  1.00  0.00           C
ATOM   3138  CD2 TRP   415      23.303 102.433  46.391  1.00  0.00           C
ATOM   3139  CD1 TRP   415      23.520 104.373  45.284  1.00  0.00           C
ATOM   3140  NE1 TRP   415      24.761 104.014  45.755  1.00  0.00           N
ATOM   3141  CE2 TRP   415      24.642 102.822  46.438  1.00  0.00           C
ATOM   3142  CE3 TRP   415      22.874 101.280  46.984  1.00  0.00           C
ATOM   3143  CZ2 TRP   415      25.575 102.059  47.082  1.00  0.00           C
ATOM   3144  CZ3 TRP   415      23.817 100.515  47.634  1.00  0.00           C
ATOM   3145  CH2 TRP   415      25.141 100.898  47.681  1.00  0.00           C
ATOM   3146  C   TRP   415      19.297 102.550  43.945  1.00  0.00           C
ATOM   3147  O   TRP   415      18.682 103.555  43.589  1.00  0.00           O
ATOM   3148  N   LEU   416      18.678 101.388  44.230  1.00  0.00           N
ATOM   3149  CA  LEU   416      17.252 101.308  44.194  1.00  0.00           C
ATOM   3150  CB  LEU   416      16.706  99.888  43.969  1.00  0.00           C
ATOM   3151  CG  LEU   416      15.166  99.825  43.935  1.00  0.00           C
ATOM   3152  CD2 LEU   416      14.638  98.469  44.421  1.00  0.00           C
ATOM   3153  CD1 LEU   416      14.598 100.275  42.576  1.00  0.00           C
ATOM   3154  C   LEU   416      16.835 101.670  45.575  1.00  0.00           C
ATOM   3155  O   LEU   416      17.401 101.180  46.553  1.00  0.00           O
ATOM   3156  N   HIS   417      15.839 102.561  45.695  1.00  0.00           N
ATOM   3157  CA  HIS   417      15.373 102.934  46.992  1.00  0.00           C
ATOM   3158  ND1 HIS   417      16.811 105.948  47.826  1.00  0.00           N
ATOM   3159  CG  HIS   417      16.082 105.350  46.822  1.00  0.00           C
ATOM   3160  NE2 HIS   417      17.689 106.643  45.904  1.00  0.00           N
ATOM   3161  CD2 HIS   417      16.633 105.784  45.655  1.00  0.00           C
ATOM   3162  CE1 HIS   417      17.758 106.710  47.222  1.00  0.00           C
ATOM   3163  CB  HIS   417      14.938 104.407  47.060  1.00  0.00           C
ATOM   3164  C   HIS   417      14.187 102.064  47.231  1.00  0.00           C
ATOM   3165  O   HIS   417      13.128 102.255  46.636  1.00  0.00           O
ATOM   3166  N   THR   418      14.355 101.061  48.110  1.00  0.00           N
ATOM   3167  CA  THR   418      13.329 100.094  48.348  1.00  0.00           C
ATOM   3168  CB  THR   418      13.761  99.045  49.309  1.00  0.00           C
ATOM   3169  OG1 THR   418      13.984  99.660  50.563  1.00  0.00           O
ATOM   3170  CG2 THR   418      15.059  98.392  48.802  1.00  0.00           C
ATOM   3171  C   THR   418      12.149 100.760  48.956  1.00  0.00           C
ATOM   3172  O   THR   418      11.008 100.441  48.631  1.00  0.00           O
ATOM   3173  N   GLY   419      12.397 101.706  49.874  1.00  0.00           N
ATOM   3174  CA  GLY   419      11.311 102.348  50.540  1.00  0.00           C
ATOM   3175  C   GLY   419      11.104 101.609  51.822  1.00  0.00           C
ATOM   3176  O   GLY   419      10.265 101.990  52.635  1.00  0.00           O
ATOM   3177  N   ASP   420      11.873 100.521  52.034  1.00  0.00           N
ATOM   3178  CA  ASP   420      11.737  99.751  53.236  1.00  0.00           C
ATOM   3179  CB  ASP   420      11.957  98.240  53.041  1.00  0.00           C
ATOM   3180  CG  ASP   420      10.827  97.682  52.197  1.00  0.00           C
ATOM   3181  OD1 ASP   420       9.847  98.431  51.936  1.00  0.00           O
ATOM   3182  OD2 ASP   420      10.930  96.492  51.796  1.00  0.00           O
ATOM   3183  C   ASP   420      12.734 100.229  54.246  1.00  0.00           C
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ATOM   3184  O   ASP   420      13.755 100.821  53.904  1.00  0.00           O
ATOM   3185  N   VAL   421      12.441  99.989  55.542  1.00  0.00           N
ATOM   3186  CA  VAL   421      13.361 100.390  56.566  1.00  0.00           C
ATOM   3187  CB  VAL   421      12.736 101.142  57.704  1.00  0.00           C
ATOM   3188  CG1 VAL   421      11.742 100.218  58.421  1.00  0.00           C
ATOM   3189  CG2 VAL   421      13.862 101.664  58.613  1.00  0.00           C
ATOM   3190  C   VAL   421      13.969  99.146  57.126  1.00  0.00           C
ATOM   3191  O   VAL   421      13.275  98.170  57.404  1.00  0.00           O
ATOM   3192  N   GLU   422      15.304  99.148  57.275  1.00  0.00           N
ATOM   3193  CA  GLU   422      16.005  98.014  57.797  1.00  0.00           C
ATOM   3194  CB  GLU   422      16.457  96.983  56.739  1.00  0.00           C
ATOM   3195  CG  GLU   422      15.394  95.983  56.272  1.00  0.00           C
ATOM   3196  CD  GLU   422      14.718  96.455  54.997  1.00  0.00           C
ATOM   3197  OE1 GLU   422      13.767  97.277  55.085  1.00  0.00           O
ATOM   3198  OE2 GLU   422      15.149  95.985  53.910  1.00  0.00           O
ATOM   3199  C   GLU   422      17.266  98.506  58.427  1.00  0.00           C
ATOM   3200  O   GLU   422      17.600  99.685  58.339  1.00  0.00           O
ATOM   3201  N   TYR   423      17.979  97.601  59.128  1.00  0.00           N
ATOM   3202  CA  TYR   423      19.263  97.927  59.677  1.00  0.00           C
ATOM   3203  CB  TYR   423      19.227  98.487  61.115  1.00  0.00           C
ATOM   3204  CG  TYR   423      18.585  97.512  62.039  1.00  0.00           C
ATOM   3205  CD1 TYR   423      19.322  96.519  62.641  1.00  0.00           C
ATOM   3206  CD2 TYR   423      17.239  97.603  62.314  1.00  0.00           C
ATOM   3207  CE1 TYR   423      18.724  95.625  63.498  1.00  0.00           C
ATOM   3208  CE2 TYR   423      16.635  96.714  63.170  1.00  0.00           C
ATOM   3209  CZ  TYR   423      17.379  95.722  63.762  1.00  0.00           C
ATOM   3210  OH  TYR   423      16.762  94.807  64.642  1.00  0.00           O
ATOM   3211  C   TYR   423      20.091  96.678  59.631  1.00  0.00           C
ATOM   3212  O   TYR   423      19.556  95.581  59.480  1.00  0.00           O
ATOM   3213  N   ILE   424      21.431  96.813  59.730  1.00  0.00           N
ATOM   3214  CA  ILE   424      22.280  95.655  59.680  1.00  0.00           C
ATOM   3215  CB  ILE   424      23.279  95.675  58.556  1.00  0.00           C
ATOM   3216  CG2 ILE   424      22.494  95.702  57.234  1.00  0.00           C
ATOM   3217  CG1 ILE   424      24.271  96.841  58.714  1.00  0.00           C
ATOM   3218  CD1 ILE   424      23.626  98.225  58.648  1.00  0.00           C
ATOM   3219  C   ILE   424      23.052  95.591  60.958  1.00  0.00           C
ATOM   3220  O   ILE   424      23.524  96.607  61.462  1.00  0.00           O
ATOM   3221  N   ASP   425      23.184  94.380  61.529  1.00  0.00           N
ATOM   3222  CA  ASP   425      23.902  94.229  62.759  1.00  0.00           C
ATOM   3223  CB  ASP   425      23.432  93.035  63.602  1.00  0.00           C
ATOM   3224  CG  ASP   425      23.670  91.779  62.788  1.00  0.00           C
ATOM   3225  OD1 ASP   425      23.179  91.713  61.630  1.00  0.00           O
ATOM   3226  OD2 ASP   425      24.345  90.863  63.322  1.00  0.00           O
ATOM   3227  C   ASP   425      25.357  94.061  62.442  1.00  0.00           C
ATOM   3228  O   ASP   425      25.789  94.255  61.306  1.00  0.00           O
ATOM   3229  N   ASP   426      26.155  93.717  63.473  1.00  0.00           N
ATOM   3230  CA  ASP   426      27.577  93.546  63.357  1.00  0.00           C
ATOM   3231  CB  ASP   426      28.253  93.222  64.700  1.00  0.00           C
ATOM   3232  CG  ASP   426      28.206  94.472  65.569  1.00  0.00           C
ATOM   3233  OD1 ASP   426      27.815  95.547  65.039  1.00  0.00           O
ATOM   3234  OD2 ASP   426      28.557  94.368  66.774  1.00  0.00           O
ATOM   3235  C   ASP   426      27.855  92.402  62.431  1.00  0.00           C
ATOM   3236  O   ASP   426      28.858  92.397  61.717  1.00  0.00           O
ATOM   3237  N   ASP   427      26.968  91.392  62.446  1.00  0.00           N
ATOM   3238  CA  ASP   427      27.061  90.205  61.639  1.00  0.00           C
ATOM   3239  CB  ASP   427      26.021  89.136  62.008  1.00  0.00           C
ATOM   3240  CG  ASP   427      26.371  88.604  63.390  1.00  0.00           C
ATOM   3241  OD1 ASP   427      27.583  88.585  63.733  1.00  0.00           O
ATOM   3242  OD2 ASP   427      25.424  88.216  64.125  1.00  0.00           O
ATOM   3243  C   ASP   427      26.846  90.585  60.206  1.00  0.00           C
ATOM   3244  O   ASP   427      27.169  89.820  59.297  1.00  0.00           O
ATOM   3245  N   GLU   428      26.280  91.784  59.972  1.00  0.00           N
ATOM   3246  CA  GLU   428      25.938  92.234  58.653  1.00  0.00           C
ATOM   3247  CB  GLU   428      27.027  91.985  57.594  1.00  0.00           C
ATOM   3248  CG  GLU   428      28.255  92.879  57.768  1.00  0.00           C
ATOM   3249  CD  GLU   428      29.227  92.564  56.642  1.00  0.00           C
ATOM   3250  OE1 GLU   428      29.464  91.354  56.384  1.00  0.00           O
ATOM   3251  OE2 GLU   428      29.739  93.530  56.017  1.00  0.00           O
ATOM   3252  C   GLU   428      24.706  91.515  58.237  1.00  0.00           C
ATOM   3253  O   GLU   428      24.371  91.440  57.055  1.00  0.00           O
ATOM   3254  N   GLU   429      23.979  90.985  59.236  1.00  0.00           N
ATOM   3255  CA  GLU   429      22.708  90.399  58.972  1.00  0.00           C
ATOM   3256  CB  GLU   429      22.211  89.500  60.118  1.00  0.00           C
ATOM   3257  CG  GLU   429      23.090  88.267  60.334  1.00  0.00           C
ATOM   3258  CD  GLU   429      22.627  87.564  61.602  1.00  0.00           C
ATOM   3259  OE1 GLU   429      22.625  88.225  62.675  1.00  0.00           O
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ATOM   3260  OE2 GLU   429      22.272  86.358  61.516  1.00  0.00           O
ATOM   3261  C   GLU   429      21.793  91.568  58.864  1.00  0.00           C
ATOM   3262  O   GLU   429      21.995  92.580  59.534  1.00  0.00           O
ATOM   3263  N   ILE   430      20.758  91.475  58.015  1.00  0.00           N
ATOM   3264  CA  ILE   430      19.898  92.607  57.888  1.00  0.00           C
ATOM   3265  CB  ILE   430      19.604  93.012  56.469  1.00  0.00           C
ATOM   3266  CG2 ILE   430      18.560  94.141  56.506  1.00  0.00           C
ATOM   3267  CG1 ILE   430      20.900  93.421  55.745  1.00  0.00           C
ATOM   3268  CD1 ILE   430      20.733  93.597  54.235  1.00  0.00           C
ATOM   3269  C   ILE   430      18.617  92.248  58.549  1.00  0.00           C
ATOM   3270  O   ILE   430      18.236  91.082  58.620  1.00  0.00           O
ATOM   3271  N   PHE   431      17.959  93.260  59.130  1.00  0.00           N
ATOM   3272  CA  PHE   431      16.697  93.044  59.758  1.00  0.00           C
ATOM   3273  CB  PHE   431      16.683  93.439  61.243  1.00  0.00           C
ATOM   3274  CG  PHE   431      17.645  92.538  61.936  1.00  0.00           C
ATOM   3275  CD1 PHE   431      18.996  92.778  61.855  1.00  0.00           C
ATOM   3276  CD2 PHE   431      17.199  91.463  62.669  1.00  0.00           C
ATOM   3277  CE1 PHE   431      19.893  91.953  62.491  1.00  0.00           C
ATOM   3278  CE2 PHE   431      18.091  90.636  63.308  1.00  0.00           C
ATOM   3279  CZ  PHE   431      19.441  90.879  63.220  1.00  0.00           C
ATOM   3280  C   PHE   431      15.779  93.964  59.047  1.00  0.00           C
ATOM   3281  O   PHE   431      16.136  95.106  58.759  1.00  0.00           O
ATOM   3282  N   ILE   432      14.565  93.488  58.738  1.00  0.00           N
ATOM   3283  CA  ILE   432      13.685  94.340  58.011  1.00  0.00           C
ATOM   3284  CB  ILE   432      12.975  93.646  56.887  1.00  0.00           C
ATOM   3285  CG2 ILE   432      12.005  94.647  56.236  1.00  0.00           C
ATOM   3286  CG1 ILE   432      14.005  93.080  55.897  1.00  0.00           C
ATOM   3287  CD1 ILE   432      13.403  92.113  54.885  1.00  0.00           C
ATOM   3288  C   ILE   432      12.677  94.839  58.977  1.00  0.00           C
ATOM   3289  O   ILE   432      12.101  94.066  59.743  1.00  0.00           O
ATOM   3290  N   VAL   433      12.492  96.175  58.992  1.00  0.00           N
ATOM   3291  CA  VAL   433      11.573  96.745  59.922  1.00  0.00           C
ATOM   3292  CB  VAL   433      12.259  97.776  60.787  1.00  0.00           C
ATOM   3293  CG1 VAL   433      11.302  98.316  61.866  1.00  0.00           C
ATOM   3294  CG2 VAL   433      13.536  97.138  61.354  1.00  0.00           C
ATOM   3295  C   VAL   433      10.460  97.404  59.131  1.00  0.00           C
ATOM   3296  O   VAL   433       9.949  98.455  59.508  1.00  0.00           O
ATOM   3297  N   ASP   434      10.018  96.770  58.024  1.00  0.00           N
ATOM   3298  CA  ASP   434       8.860  97.191  57.271  1.00  0.00           C
ATOM   3299  CB  ASP   434       7.643  97.514  58.149  1.00  0.00           C
ATOM   3300  CG  ASP   434       6.372  97.271  57.341  1.00  0.00           C
ATOM   3301  OD1 ASP   434       6.477  96.722  56.211  1.00  0.00           O
ATOM   3302  OD2 ASP   434       5.275  97.618  57.855  1.00  0.00           O
ATOM   3303  C   ASP   434       9.098  98.372  56.381  1.00  0.00           C
ATOM   3304  O   ASP   434      10.173  98.967  56.360  1.00  0.00           O
ATOM   3305  N   ARG   435       8.054  98.715  55.589  1.00  0.00           N
ATOM   3306  CA  ARG   435       8.074  99.786  54.632  1.00  0.00           C
ATOM   3307  CB  ARG   435       6.946  99.714  53.589  1.00  0.00           C
ATOM   3308  CG  ARG   435       7.168  98.606  52.565  1.00  0.00           C
ATOM   3309  CD  ARG   435       6.943  97.197  53.110  1.00  0.00           C
ATOM   3310  NE  ARG   435       7.701  96.287  52.211  1.00  0.00           N
ATOM   3311  CZ  ARG   435       7.226  96.001  50.964  1.00  0.00           C
ATOM   3312  NH1 ARG   435       6.017  96.488  50.561  1.00  0.00           N
ATOM   3313  NH2 ARG   435       7.981  95.245  50.115  1.00  0.00           N
ATOM   3314  C   ARG   435       7.949 101.108  55.318  1.00  0.00           C
ATOM   3315  O   ARG   435       7.339 101.236  56.377  1.00  0.00           O
ATOM   3316  N   VAL   436       8.564 102.134  54.704  1.00  0.00           N
ATOM   3317  CA  VAL   436       8.554 103.484  55.191  1.00  0.00           C
ATOM   3318  CB  VAL   436       9.456 104.391  54.406  1.00  0.00           C
ATOM   3319  CG1 VAL   436       8.937 104.475  52.960  1.00  0.00           C
ATOM   3320  CG2 VAL   436       9.522 105.751  55.121  1.00  0.00           C
ATOM   3321  C   VAL   436       7.166 104.032  55.092  1.00  0.00           C
ATOM   3322  O   VAL   436       6.726 104.794  55.950  1.00  0.00           O
ATOM   3323  N   LYS   437       6.448 103.651  54.022  1.00  0.00           N
ATOM   3324  CA  LYS   437       5.112 104.101  53.764  1.00  0.00           C
ATOM   3325  CB  LYS   437       4.532 103.503  52.471  1.00  0.00           C
ATOM   3326  CG  LYS   437       5.283 103.938  51.210  1.00  0.00           C
ATOM   3327  CD  LYS   437       4.949 103.093  49.979  1.00  0.00           C
ATOM   3328  CE  LYS   437       5.526 101.676  50.034  1.00  0.00           C
ATOM   3329  NZ  LYS   437       7.003 101.725  49.961  1.00  0.00           N
ATOM   3330  C   LYS   437       4.277 103.613  54.898  1.00  0.00           C
ATOM   3331  O   LYS   437       3.279 104.226  55.272  1.00  0.00           O
ATOM   3332  N   GLU   438       4.707 102.480  55.471  1.00  0.00           N
ATOM   3333  CA  GLU   438       4.057 101.782  56.534  1.00  0.00           C
ATOM   3334  CB  GLU   438       4.772 100.480  56.921  1.00  0.00           C
ATOM   3335  CG  GLU   438       4.674  99.392  55.849  1.00  0.00           C
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ATOM   3336  CD  GLU   438       3.254  98.846  55.870  1.00  0.00           C
ATOM   3337  OE1 GLU   438       2.313  99.656  56.087  1.00  0.00           O
ATOM   3338  OE2 GLU   438       3.091  97.612  55.675  1.00  0.00           O
ATOM   3339  C   GLU   438       3.978 102.657  57.735  1.00  0.00           C
ATOM   3340  O   GLU   438       3.197 102.380  58.637  1.00  0.00           O
ATOM   3341  N   ILE   439       4.816 103.700  57.831  1.00  0.00           N
ATOM   3342  CA  ILE   439       4.724 104.539  58.988  1.00  0.00           C
ATOM   3343  CB  ILE   439       5.707 105.682  58.941  1.00  0.00           C
ATOM   3344  CG2 ILE   439       5.338 106.585  57.753  1.00  0.00           C
ATOM   3345  CG1 ILE   439       5.809 106.424  60.286  1.00  0.00           C
ATOM   3346  CD1 ILE   439       4.558 107.190  60.714  1.00  0.00           C
ATOM   3347  C   ILE   439       3.324 105.087  59.075  1.00  0.00           C
ATOM   3348  O   ILE   439       2.792 105.636  58.111  1.00  0.00           O
ATOM   3349  N   ILE   440       2.693 104.934  60.265  1.00  0.00           N
ATOM   3350  CA  ILE   440       1.382 105.456  60.549  1.00  0.00           C
ATOM   3351  CB  ILE   440       0.456 104.490  61.250  1.00  0.00           C
ATOM   3352  CG2 ILE   440       1.087 104.039  62.571  1.00  0.00           C
ATOM   3353  CG1 ILE   440      -0.920 105.132  61.475  1.00  0.00           C
ATOM   3354  CD1 ILE   440      -1.906 104.200  62.181  1.00  0.00           C
ATOM   3355  C   ILE   440       1.620 106.583  61.503  1.00  0.00           C
ATOM   3356  O   ILE   440       2.396 106.445  62.448  1.00  0.00           O
ATOM   3357  N   LYS   441       0.986 107.748  61.266  1.00  0.00           N
ATOM   3358  CA  LYS   441       1.231 108.875  62.117  1.00  0.00           C
ATOM   3359  CB  LYS   441       1.460 110.173  61.324  1.00  0.00           C
ATOM   3360  CG  LYS   441       1.843 111.383  62.177  1.00  0.00           C
ATOM   3361  CD  LYS   441       2.345 112.565  61.342  1.00  0.00           C
ATOM   3362  CE  LYS   441       2.735 113.792  62.169  1.00  0.00           C
ATOM   3363  NZ  LYS   441       4.088 113.609  62.738  1.00  0.00           N
ATOM   3364  C   LYS   441       0.029 109.086  62.970  1.00  0.00           C
ATOM   3365  O   LYS   441      -1.055 109.383  62.473  1.00  0.00           O
ATOM   3366  N   TYR   442       0.199 108.941  64.299  1.00  0.00           N
ATOM   3367  CA  TYR   442      -0.901 109.157  65.184  1.00  0.00           C
ATOM   3368  CB  TYR   442      -1.181 107.957  66.109  1.00  0.00           C
ATOM   3369  CG  TYR   442      -2.297 108.331  67.023  1.00  0.00           C
ATOM   3370  CD1 TYR   442      -3.606 108.113  66.662  1.00  0.00           C
ATOM   3371  CD2 TYR   442      -2.034 108.908  68.244  1.00  0.00           C
ATOM   3372  CE1 TYR   442      -4.634 108.458  67.507  1.00  0.00           C
ATOM   3373  CE2 TYR   442      -3.057 109.255  69.094  1.00  0.00           C
ATOM   3374  CZ  TYR   442      -4.360 109.030  68.726  1.00  0.00           C
ATOM   3375  OH  TYR   442      -5.413 109.384  69.597  1.00  0.00           O
ATOM   3376  C   TYR   442      -0.557 110.328  66.043  1.00  0.00           C
ATOM   3377  O   TYR   442       0.377 110.279  66.843  1.00  0.00           O
ATOM   3378  N   LYS   443      -1.320 111.423  65.884  1.00  0.00           N
ATOM   3379  CA  LYS   443      -1.116 112.606  66.661  1.00  0.00           C
ATOM   3380  CB  LYS   443      -1.403 112.393  68.156  1.00  0.00           C
ATOM   3381  CG  LYS   443      -1.519 113.696  68.945  1.00  0.00           C
ATOM   3382  CD  LYS   443      -2.156 113.516  70.323  1.00  0.00           C
ATOM   3383  CE  LYS   443      -2.275 114.818  71.116  1.00  0.00           C
ATOM   3384  NZ  LYS   443      -2.908 114.557  72.427  1.00  0.00           N
ATOM   3385  C   LYS   443       0.299 113.061  66.492  1.00  0.00           C
ATOM   3386  O   LYS   443       0.892 113.631  67.406  1.00  0.00           O
ATOM   3387  N   GLY   444       0.876 112.827  65.299  1.00  0.00           N
ATOM   3388  CA  GLY   444       2.206 113.293  65.028  1.00  0.00           C
ATOM   3389  C   GLY   444       3.196 112.254  65.451  1.00  0.00           C
ATOM   3390  O   GLY   444       4.374 112.341  65.110  1.00  0.00           O
ATOM   3391  N   PHE   445       2.747 111.236  66.207  1.00  0.00           N
ATOM   3392  CA  PHE   445       3.664 110.223  66.643  1.00  0.00           C
ATOM   3393  CB  PHE   445       3.228 109.511  67.936  1.00  0.00           C
ATOM   3394  CG  PHE   445       3.324 110.506  69.041  1.00  0.00           C
ATOM   3395  CD1 PHE   445       2.301 111.397  69.270  1.00  0.00           C
ATOM   3396  CD2 PHE   445       4.437 110.548  69.847  1.00  0.00           C
ATOM   3397  CE1 PHE   445       2.389 112.316  70.290  1.00  0.00           C
ATOM   3398  CE2 PHE   445       4.531 111.463  70.868  1.00  0.00           C
ATOM   3399  CZ  PHE   445       3.505 112.350  71.091  1.00  0.00           C
ATOM   3400  C   PHE   445       3.780 109.195  65.562  1.00  0.00           C
ATOM   3401  O   PHE   445       2.828 108.927  64.832  1.00  0.00           O
ATOM   3402  N   GLN   446       4.975 108.587  65.441  1.00  0.00           N
ATOM   3403  CA  GLN   446       5.239 107.632  64.402  1.00  0.00           C
ATOM   3404  CB  GLN   446       6.689 107.718  63.896  1.00  0.00           C
ATOM   3405  CG  GLN   446       7.082 106.601  62.933  1.00  0.00           C
ATOM   3406  CD  GLN   446       8.531 106.820  62.525  1.00  0.00           C
ATOM   3407  OE1 GLN   446       9.164 107.793  62.931  1.00  0.00           O
ATOM   3408  NE2 GLN   446       9.075 105.892  61.694  1.00  0.00           N
ATOM   3409  C   GLN   446       5.050 106.241  64.920  1.00  0.00           C
ATOM   3410  O   GLN   446       5.580 105.883  65.971  1.00  0.00           O
ATOM   3411  N   VAL   447       4.277 105.417  64.178  1.00  0.00           N
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ATOM   3412  CA  VAL   447       4.085 104.045  64.553  1.00  0.00           C
ATOM   3413  CB  VAL   447       2.687 103.762  65.030  1.00  0.00           C
ATOM   3414  CG1 VAL   447       2.559 102.263  65.349  1.00  0.00           C
ATOM   3415  CG2 VAL   447       2.375 104.690  66.216  1.00  0.00           C
ATOM   3416  C   VAL   447       4.335 103.192  63.338  1.00  0.00           C
ATOM   3417  O   VAL   447       3.720 103.377  62.290  1.00  0.00           O
ATOM   3418  N   ALA   448       5.247 102.207  63.440  1.00  0.00           N
ATOM   3419  CA  ALA   448       5.488 101.373  62.296  1.00  0.00           C
ATOM   3420  CB  ALA   448       6.946 100.894  62.178  1.00  0.00           C
ATOM   3421  C   ALA   448       4.626 100.165  62.470  1.00  0.00           C
ATOM   3422  O   ALA   448       4.719  99.452  63.467  1.00  0.00           O
ATOM   3423  N   PRO   449       3.789  99.935  61.499  1.00  0.00           N
ATOM   3424  CA  PRO   449       2.831  98.865  61.551  1.00  0.00           C
ATOM   3425  CD  PRO   449       4.170 100.222  60.133  1.00  0.00           C
ATOM   3426  CB  PRO   449       2.140  98.882  60.199  1.00  0.00           C
ATOM   3427  CG  PRO   449       3.287  99.299  59.268  1.00  0.00           C
ATOM   3428  C   PRO   449       3.493  97.541  61.751  1.00  0.00           C
ATOM   3429  O   PRO   449       2.935  96.698  62.451  1.00  0.00           O
ATOM   3430  N   ALA   450       4.670  97.330  61.139  1.00  0.00           N
ATOM   3431  CA  ALA   450       5.323  96.054  61.211  1.00  0.00           C
ATOM   3432  CB  ALA   450       6.653  95.992  60.453  1.00  0.00           C
ATOM   3433  C   ALA   450       5.642  95.763  62.636  1.00  0.00           C
ATOM   3434  O   ALA   450       5.589  94.611  63.061  1.00  0.00           O
ATOM   3435  N   GLU   451       6.018  96.805  63.399  1.00  0.00           N
ATOM   3436  CA  GLU   451       6.385  96.637  64.774  1.00  0.00           C
ATOM   3437  CB  GLU   451       6.813  97.956  65.440  1.00  0.00           C
ATOM   3438  CG  GLU   451       7.204  97.795  66.910  1.00  0.00           C
ATOM   3439  CD  GLU   451       7.461  99.180  67.487  1.00  0.00           C
ATOM   3440  OE1 GLU   451       7.471 100.161  66.697  1.00  0.00           O
ATOM   3441  OE2 GLU   451       7.649  99.276  68.730  1.00  0.00           O
ATOM   3442  C   GLU   451       5.202  96.138  65.544  1.00  0.00           C
ATOM   3443  O   GLU   451       5.338  95.275  66.409  1.00  0.00           O
ATOM   3444  N   LEU   452       4.007  96.698  65.277  1.00  0.00           N
ATOM   3445  CA  LEU   452       2.827  96.266  65.963  1.00  0.00           C
ATOM   3446  CB  LEU   452       1.607  97.154  65.674  1.00  0.00           C
ATOM   3447  CG  LEU   452       1.766  98.591  66.206  1.00  0.00           C
ATOM   3448  CD2 LEU   452       2.146  98.596  67.694  1.00  0.00           C
ATOM   3449  CD1 LEU   452       0.521  99.439  65.905  1.00  0.00           C
ATOM   3450  C   LEU   452       2.497  94.871  65.533  1.00  0.00           C
ATOM   3451  O   LEU   452       2.086  94.046  66.347  1.00  0.00           O
ATOM   3452  N   GLU   453       2.654  94.577  64.226  1.00  0.00           N
ATOM   3453  CA  GLU   453       2.315  93.272  63.734  1.00  0.00           C
ATOM   3454  CB  GLU   453       2.181  93.204  62.195  1.00  0.00           C
ATOM   3455  CG  GLU   453       3.263  93.916  61.385  1.00  0.00           C
ATOM   3456  CD  GLU   453       2.728  94.090  59.964  1.00  0.00           C
ATOM   3457  OE1 GLU   453       1.796  94.917  59.772  1.00  0.00           O
ATOM   3458  OE2 GLU   453       3.247  93.392  59.052  1.00  0.00           O
ATOM   3459  C   GLU   453       3.239  92.239  64.301  1.00  0.00           C
ATOM   3460  O   GLU   453       2.803  91.140  64.636  1.00  0.00           O
ATOM   3461  N   ALA   454       4.536  92.561  64.453  1.00  0.00           N
ATOM   3462  CA  ALA   454       5.455  91.616  65.020  1.00  0.00           C
ATOM   3463  CB  ALA   454       6.899  92.141  65.065  1.00  0.00           C
ATOM   3464  C   ALA   454       5.033  91.333  66.436  1.00  0.00           C
ATOM   3465  O   ALA   454       5.114  90.200  66.905  1.00  0.00           O
ATOM   3466  N   LEU   455       4.590  92.369  67.170  1.00  0.00           N
ATOM   3467  CA  LEU   455       4.173  92.208  68.536  1.00  0.00           C
ATOM   3468  CB  LEU   455       3.771  93.541  69.182  1.00  0.00           C
ATOM   3469  CG  LEU   455       3.321  93.404  70.647  1.00  0.00           C
ATOM   3470  CD2 LEU   455       2.611  94.683  71.126  1.00  0.00           C
ATOM   3471  CD1 LEU   455       4.479  92.972  71.553  1.00  0.00           C
ATOM   3472  C   LEU   455       2.966  91.318  68.607  1.00  0.00           C
ATOM   3473  O   LEU   455       2.890  90.434  69.458  1.00  0.00           O
ATOM   3474  N   LEU   456       1.983  91.543  67.713  1.00  0.00           N
ATOM   3475  CA  LEU   456       0.753  90.793  67.716  1.00  0.00           C
ATOM   3476  CB  LEU   456      -0.291  91.335  66.725  1.00  0.00           C
ATOM   3477  CG  LEU   456      -0.877  92.694  67.149  1.00  0.00           C
ATOM   3478  CD2 LEU   456      -1.427  92.632  68.584  1.00  0.00           C
ATOM   3479  CD1 LEU   456      -1.917  93.195  66.135  1.00  0.00           C
ATOM   3480  C   LEU   456       1.018  89.367  67.372  1.00  0.00           C
ATOM   3481  O   LEU   456       0.408  88.460  67.938  1.00  0.00           O
ATOM   3482  N   VAL   457       1.945  89.116  66.438  1.00  0.00           N
ATOM   3483  CA  VAL   457       2.162  87.760  66.042  1.00  0.00           C
ATOM   3484  CB  VAL   457       3.158  87.590  64.930  1.00  0.00           C
ATOM   3485  CG1 VAL   457       2.669  88.387  63.710  1.00  0.00           C
ATOM   3486  CG2 VAL   457       4.561  87.964  65.429  1.00  0.00           C
ATOM   3487  C   VAL   457       2.652  86.981  67.225  1.00  0.00           C
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ATOM   3488  O   VAL   457       2.407  85.781  67.328  1.00  0.00           O
ATOM   3489  N   ALA   458       3.365  87.648  68.148  1.00  0.00           N
ATOM   3490  CA  ALA   458       3.956  87.015  69.295  1.00  0.00           C
ATOM   3491  CB  ALA   458       4.721  88.004  70.194  1.00  0.00           C
ATOM   3492  C   ALA   458       2.907  86.358  70.143  1.00  0.00           C
ATOM   3493  O   ALA   458       3.176  85.328  70.755  1.00  0.00           O
ATOM   3494  N   HIS   459       1.699  86.945  70.235  1.00  0.00           N
ATOM   3495  CA  HIS   459       0.652  86.405  71.062  1.00  0.00           C
ATOM   3496  ND1 HIS   459      -2.548  85.935  71.994  1.00  0.00           N
ATOM   3497  CG  HIS   459      -1.653  86.980  72.033  1.00  0.00           C
ATOM   3498  NE2 HIS   459      -2.983  87.076  73.852  1.00  0.00           N
ATOM   3499  CD2 HIS   459      -1.931  87.667  73.174  1.00  0.00           C
ATOM   3500  CE1 HIS   459      -3.320  86.040  73.105  1.00  0.00           C
ATOM   3501  CB  HIS   459      -0.626  87.260  70.977  1.00  0.00           C
ATOM   3502  C   HIS   459       0.352  85.016  70.579  1.00  0.00           C
ATOM   3503  O   HIS   459       0.188  84.770  69.384  1.00  0.00           O
ATOM   3504  N   PRO   460       0.254  84.094  71.497  1.00  0.00           N
ATOM   3505  CA  PRO   460       0.082  82.715  71.129  1.00  0.00           C
ATOM   3506  CD  PRO   460       0.901  84.238  72.791  1.00  0.00           C
ATOM   3507  CB  PRO   460       0.245  81.922  72.424  1.00  0.00           C
ATOM   3508  CG  PRO   460       1.185  82.802  73.268  1.00  0.00           C
ATOM   3509  C   PRO   460      -1.184  82.428  70.393  1.00  0.00           C
ATOM   3510  O   PRO   460      -1.205  81.477  69.612  1.00  0.00           O
ATOM   3511  N   SER   461      -2.254  83.196  70.657  1.00  0.00           N
ATOM   3512  CA  SER   461      -3.517  82.954  70.030  1.00  0.00           C
ATOM   3513  CB  SER   461      -4.680  83.587  70.796  1.00  0.00           C
ATOM   3514  OG  SER   461      -4.788  83.005  72.087  1.00  0.00           O
ATOM   3515  C   SER   461      -3.562  83.456  68.617  1.00  0.00           C
ATOM   3516  O   SER   461      -4.301  82.913  67.797  1.00  0.00           O
ATOM   3517  N   ILE   462      -2.792  84.506  68.269  1.00  0.00           N
ATOM   3518  CA  ILE   462      -2.946  85.020  66.937  1.00  0.00           C
ATOM   3519  CB  ILE   462      -3.137  86.510  66.850  1.00  0.00           C
ATOM   3520  CG2 ILE   462      -4.605  86.830  67.145  1.00  0.00           C
ATOM   3521  CG1 ILE   462      -2.107  87.273  67.687  1.00  0.00           C
ATOM   3522  CD1 ILE   462      -2.292  88.788  67.611  1.00  0.00           C
ATOM   3523  C   ILE   462      -1.899  84.541  65.980  1.00  0.00           C
ATOM   3524  O   ILE   462      -0.695  84.659  66.202  1.00  0.00           O
ATOM   3525  N   ALA   463      -2.403  83.879  64.914  1.00  0.00           N
ATOM   3526  CA  ALA   463      -1.644  83.325  63.827  1.00  0.00           C
ATOM   3527  CB  ALA   463      -2.471  82.352  62.972  1.00  0.00           C
ATOM   3528  C   ALA   463      -1.088  84.368  62.895  1.00  0.00           C
ATOM   3529  O   ALA   463       0.079  84.299  62.513  1.00  0.00           O
ATOM   3530  N   ASP   464      -1.911  85.353  62.476  1.00  0.00           N
ATOM   3531  CA  ASP   464      -1.445  86.298  61.496  1.00  0.00           C
ATOM   3532  CB  ASP   464      -1.913  85.938  60.064  1.00  0.00           C
ATOM   3533  CG  ASP   464      -1.055  86.625  58.998  1.00  0.00           C
ATOM   3534  OD1 ASP   464      -0.094  87.350  59.368  1.00  0.00           O
ATOM   3535  OD2 ASP   464      -1.348  86.426  57.787  1.00  0.00           O
ATOM   3536  C   ASP   464      -2.018  87.629  61.850  1.00  0.00           C
ATOM   3537  O   ASP   464      -3.106  87.712  62.419  1.00  0.00           O
ATOM   3538  N   ALA   465      -1.283  88.714  61.538  1.00  0.00           N
ATOM   3539  CA  ALA   465      -1.810  90.002  61.869  1.00  0.00           C
ATOM   3540  CB  ALA   465      -1.313  90.539  63.224  1.00  0.00           C
ATOM   3541  C   ALA   465      -1.388  90.975  60.823  1.00  0.00           C
ATOM   3542  O   ALA   465      -0.353  90.814  60.175  1.00  0.00           O
ATOM   3543  N   ALA   466      -2.219  92.015  60.623  1.00  0.00           N
ATOM   3544  CA  ALA   466      -1.887  93.038  59.679  1.00  0.00           C
ATOM   3545  CB  ALA   466      -2.658  92.930  58.354  1.00  0.00           C
ATOM   3546  C   ALA   466      -2.296  94.326  60.321  1.00  0.00           C
ATOM   3547  O   ALA   466      -3.373  94.418  60.910  1.00  0.00           O
ATOM   3548  N   VAL   467      -1.445  95.366  60.217  1.00  0.00           N
ATOM   3549  CA  VAL   467      -1.761  96.610  60.861  1.00  0.00           C
ATOM   3550  CB  VAL   467      -0.690  97.066  61.808  1.00  0.00           C
ATOM   3551  CG1 VAL   467      -1.086  98.438  62.377  1.00  0.00           C
ATOM   3552  CG2 VAL   467      -0.486  95.979  62.877  1.00  0.00           C
ATOM   3553  C   VAL   467      -1.906  97.670  59.813  1.00  0.00           C
ATOM   3554  O   VAL   467      -1.151  97.699  58.843  1.00  0.00           O
ATOM   3555  N   VAL   468      -2.904  98.564  59.989  1.00  0.00           N
ATOM   3556  CA  VAL   468      -3.133  99.635  59.058  1.00  0.00           C
ATOM   3557  CB  VAL   468      -4.225  99.334  58.076  1.00  0.00           C
ATOM   3558  CG1 VAL   468      -5.531  99.138  58.865  1.00  0.00           C
ATOM   3559  CG2 VAL   468      -4.310 100.486  57.062  1.00  0.00           C
ATOM   3560  C   VAL   468      -3.610 100.819  59.834  1.00  0.00           C
ATOM   3561  O   VAL   468      -4.107 100.693  60.951  1.00  0.00           O
ATOM   3562  N   PRO   469      -3.381 101.978  59.285  1.00  0.00           N
ATOM   3563  CA  PRO   469      -3.878 103.176  59.900  1.00  0.00           C
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ATOM   3564  CD  PRO   469      -2.121 102.201  58.594  1.00  0.00           C
ATOM   3565  CB  PRO   469      -3.013 104.317  59.369  1.00  0.00           C
ATOM   3566  CG  PRO   469      -1.698 103.630  58.963  1.00  0.00           C
ATOM   3567  C   PRO   469      -5.312 103.375  59.555  1.00  0.00           C
ATOM   3568  O   PRO   469      -5.610 103.510  58.369  1.00  0.00           O
ATOM   3569  N   GLN   470      -6.213 103.470  60.546  1.00  0.00           N
ATOM   3570  CA  GLN   470      -7.544 103.828  60.187  1.00  0.00           C
ATOM   3571  CB  GLN   470      -8.643 103.263  61.100  1.00  0.00           C
ATOM   3572  CG  GLN   470      -8.865 101.763  60.890  1.00  0.00           C
ATOM   3573  CD  GLN   470     -10.059 101.349  61.732  1.00  0.00           C
ATOM   3574  OE1 GLN   470     -10.423 102.058  62.669  1.00  0.00           O
ATOM   3575  NE2 GLN   470     -10.676 100.184  61.403  1.00  0.00           N
ATOM   3576  C   GLN   470      -7.567 105.325  60.253  1.00  0.00           C
ATOM   3577  O   GLN   470      -7.014 105.921  61.177  1.00  0.00           O
ATOM   3578  N   LYS   471      -8.187 105.979  59.249  1.00  0.00           N
ATOM   3579  CA  LYS   471      -8.169 107.414  59.210  1.00  0.00           C
ATOM   3580  CB  LYS   471      -8.636 107.999  57.866  1.00  0.00           C
ATOM   3581  CG  LYS   471      -8.567 109.527  57.814  1.00  0.00           C
ATOM   3582  CD  LYS   471      -8.703 110.099  56.401  1.00  0.00           C
ATOM   3583  CE  LYS   471      -8.634 111.626  56.349  1.00  0.00           C
ATOM   3584  NZ  LYS   471      -8.774 112.092  54.951  1.00  0.00           N
ATOM   3585  C   LYS   471      -9.048 107.984  60.282  1.00  0.00           C
ATOM   3586  O   LYS   471     -10.229 107.657  60.394  1.00  0.00           O
ATOM   3587  N   HIS   472      -8.458 108.872  61.104  1.00  0.00           N
ATOM   3588  CA  HIS   472      -9.139 109.590  62.143  1.00  0.00           C
ATOM   3589  ND1 HIS   472     -10.942 109.375  64.965  1.00  0.00           N
ATOM   3590  CG  HIS   472      -9.641 109.693  64.642  1.00  0.00           C
ATOM   3591  NE2 HIS   472     -10.311 110.974  66.374  1.00  0.00           N
ATOM   3592  CD2 HIS   472      -9.272 110.673  65.513  1.00  0.00           C
ATOM   3593  CE1 HIS   472     -11.293 110.171  66.007  1.00  0.00           C
ATOM   3594  CB  HIS   472      -8.859 109.028  63.548  1.00  0.00           C
ATOM   3595  C   HIS   472      -8.561 110.970  62.087  1.00  0.00           C
ATOM   3596  O   HIS   472      -7.454 111.217  62.562  1.00  0.00           O
ATOM   3597  N   GLU   473      -9.324 111.926  61.536  1.00  0.00           N
ATOM   3598  CA  GLU   473      -8.796 113.238  61.289  1.00  0.00           C
ATOM   3599  CB  GLU   473      -9.825 114.183  60.646  1.00  0.00           C
ATOM   3600  CG  GLU   473      -9.251 115.559  60.302  1.00  0.00           C
ATOM   3601  CD  GLU   473     -10.354 116.383  59.653  1.00  0.00           C
ATOM   3602  OE1 GLU   473     -11.467 115.827  59.451  1.00  0.00           O
ATOM   3603  OE2 GLU   473     -10.097 117.578  59.347  1.00  0.00           O
ATOM   3604  C   GLU   473      -8.322 113.876  62.554  1.00  0.00           C
ATOM   3605  O   GLU   473      -7.305 114.568  62.553  1.00  0.00           O
ATOM   3606  N   GLU   474      -9.034 113.666  63.673  1.00  0.00           N
ATOM   3607  CA  GLU   474      -8.642 114.331  64.879  1.00  0.00           C
ATOM   3608  CB  GLU   474      -9.547 113.978  66.069  1.00  0.00           C
ATOM   3609  CG  GLU   474     -10.961 114.549  65.934  1.00  0.00           C
ATOM   3610  CD  GLU   474     -11.705 113.750  64.872  1.00  0.00           C
ATOM   3611  OE1 GLU   474     -11.263 112.613  64.562  1.00  0.00           O
ATOM   3612  OE2 GLU   474     -12.730 114.269  64.356  1.00  0.00           O
ATOM   3613  C   GLU   474      -7.242 113.942  65.225  1.00  0.00           C
ATOM   3614  O   GLU   474      -6.423 114.812  65.519  1.00  0.00           O
ATOM   3615  N   ALA   475      -6.898 112.638  65.193  1.00  0.00           N
ATOM   3616  CA  ALA   475      -5.533 112.380  65.539  1.00  0.00           C
ATOM   3617  CB  ALA   475      -5.374 111.294  66.616  1.00  0.00           C
ATOM   3618  C   ALA   475      -4.796 111.905  64.336  1.00  0.00           C
ATOM   3619  O   ALA   475      -3.836 111.149  64.474  1.00  0.00           O
ATOM   3620  N   GLY   476      -5.138 112.424  63.140  1.00  0.00           N
ATOM   3621  CA  GLY   476      -4.458 111.993  61.951  1.00  0.00           C
ATOM   3622  C   GLY   476      -4.876 110.590  61.627  1.00  0.00           C
ATOM   3623  O   GLY   476      -5.803 110.371  60.850  1.00  0.00           O
ATOM   3624  N   GLU   477      -4.160 109.580  62.154  1.00  0.00           N
ATOM   3625  CA  GLU   477      -4.580 108.242  61.866  1.00  0.00           C
ATOM   3626  CB  GLU   477      -3.841 107.602  60.678  1.00  0.00           C
ATOM   3627  CG  GLU   477      -2.319 107.629  60.777  1.00  0.00           C
ATOM   3628  CD  GLU   477      -1.791 107.154  59.429  1.00  0.00           C
ATOM   3629  OE1 GLU   477      -2.628 106.981  58.504  1.00  0.00           O
ATOM   3630  OE2 GLU   477      -0.553 106.961  59.299  1.00  0.00           O
ATOM   3631  C   GLU   477      -4.434 107.404  63.096  1.00  0.00           C
ATOM   3632  O   GLU   477      -3.565 107.645  63.931  1.00  0.00           O
ATOM   3633  N   VAL   478      -5.322 106.397  63.243  1.00  0.00           N
ATOM   3634  CA  VAL   478      -5.301 105.568  64.412  1.00  0.00           C
ATOM   3635  CB  VAL   478      -6.648 105.435  65.061  1.00  0.00           C
ATOM   3636  CG1 VAL   478      -7.096 106.824  65.546  1.00  0.00           C
ATOM   3637  CG2 VAL   478      -7.612 104.782  64.056  1.00  0.00           C
ATOM   3638  C   VAL   478      -4.873 104.201  63.997  1.00  0.00           C
ATOM   3639  O   VAL   478      -5.305 103.700  62.964  1.00  0.00           O
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ATOM   3640  N   PRO   479      -4.018 103.570  64.745  1.00  0.00           N
ATOM   3641  CA  PRO   479      -3.610 102.254  64.337  1.00  0.00           C
ATOM   3642  CD  PRO   479      -2.937 104.294  65.395  1.00  0.00           C
ATOM   3643  CB  PRO   479      -2.320 101.959  65.098  1.00  0.00           C
ATOM   3644  CG  PRO   479      -1.717 103.357  65.334  1.00  0.00           C
ATOM   3645  C   PRO   479      -4.699 101.252  64.553  1.00  0.00           C
ATOM   3646  O   PRO   479      -5.324 101.269  65.612  1.00  0.00           O
ATOM   3647  N   VAL   480      -4.930 100.355  63.574  1.00  0.00           N
ATOM   3648  CA  VAL   480      -5.944  99.354  63.728  1.00  0.00           C
ATOM   3649  CB  VAL   480      -7.189  99.654  62.956  1.00  0.00           C
ATOM   3650  CG1 VAL   480      -8.160  98.469  63.088  1.00  0.00           C
ATOM   3651  CG2 VAL   480      -7.741 100.980  63.503  1.00  0.00           C
ATOM   3652  C   VAL   480      -5.367  98.071  63.235  1.00  0.00           C
ATOM   3653  O   VAL   480      -4.523  98.060  62.341  1.00  0.00           O
ATOM   3654  N   ALA   481      -5.793  96.939  63.823  1.00  0.00           N
ATOM   3655  CA  ALA   481      -5.180  95.720  63.403  1.00  0.00           C
ATOM   3656  CB  ALA   481      -4.266  95.093  64.471  1.00  0.00           C
ATOM   3657  C   ALA   481      -6.213  94.705  63.076  1.00  0.00           C
ATOM   3658  O   ALA   481      -7.280  94.645  63.685  1.00  0.00           O
ATOM   3659  N   PHE   482      -5.891  93.871  62.072  1.00  0.00           N
ATOM   3660  CA  PHE   482      -6.763  92.825  61.651  1.00  0.00           C
ATOM   3661  CB  PHE   482      -6.978  92.852  60.136  1.00  0.00           C
ATOM   3662  CG  PHE   482      -7.249  94.293  59.873  1.00  0.00           C
ATOM   3663  CD1 PHE   482      -8.399  94.899  60.322  1.00  0.00           C
ATOM   3664  CD2 PHE   482      -6.332  95.047  59.180  1.00  0.00           C
ATOM   3665  CE1 PHE   482      -8.636  96.232  60.084  1.00  0.00           C
ATOM   3666  CE2 PHE   482      -6.564  96.379  58.938  1.00  0.00           C
ATOM   3667  CZ  PHE   482      -7.715  96.974  59.390  1.00  0.00           C
ATOM   3668  C   PHE   482      -6.019  91.593  62.027  1.00  0.00           C
ATOM   3669  O   PHE   482      -4.801  91.527  61.862  1.00  0.00           O
ATOM   3670  N   VAL   483      -6.711  90.584  62.582  1.00  0.00           N
ATOM   3671  CA  VAL   483      -5.919  89.484  63.030  1.00  0.00           C
ATOM   3672  CB  VAL   483      -5.691  89.544  64.514  1.00  0.00           C
ATOM   3673  CG1 VAL   483      -6.825  88.798  65.233  1.00  0.00           C
ATOM   3674  CG2 VAL   483      -4.266  89.082  64.831  1.00  0.00           C
ATOM   3675  C   VAL   483      -6.630  88.210  62.712  1.00  0.00           C
ATOM   3676  O   VAL   483      -7.855  88.175  62.602  1.00  0.00           O
ATOM   3677  N   VAL   484      -5.848  87.126  62.539  1.00  0.00           N
ATOM   3678  CA  VAL   484      -6.389  85.823  62.286  1.00  0.00           C
ATOM   3679  CB  VAL   484      -5.706  85.098  61.165  1.00  0.00           C
ATOM   3680  CG1 VAL   484      -6.285  83.676  61.074  1.00  0.00           C
ATOM   3681  CG2 VAL   484      -5.877  85.923  59.879  1.00  0.00           C
ATOM   3682  C   VAL   484      -6.146  85.044  63.540  1.00  0.00           C
ATOM   3683  O   VAL   484      -5.086  85.160  64.152  1.00  0.00           O
ATOM   3684  N   LYS   485      -7.147  84.245  63.962  1.00  0.00           N
ATOM   3685  CA  LYS   485      -7.074  83.548  65.215  1.00  0.00           C
ATOM   3686  CB  LYS   485      -7.576  84.476  66.322  1.00  0.00           C
ATOM   3687  CG  LYS   485      -8.880  85.110  65.835  1.00  0.00           C
ATOM   3688  CD  LYS   485      -9.681  85.925  66.843  1.00  0.00           C
ATOM   3689  CE  LYS   485     -11.044  86.333  66.277  1.00  0.00           C
ATOM   3690  NZ  LYS   485     -11.900  85.137  66.107  1.00  0.00           N
ATOM   3691  C   LYS   485      -8.045  82.404  65.160  1.00  0.00           C
ATOM   3692  O   LYS   485      -9.168  82.556  64.682  1.00  0.00           O
ATOM   3693  N   SER   486      -7.641  81.217  65.656  1.00  0.00           N
ATOM   3694  CA  SER   486      -8.538  80.097  65.676  1.00  0.00           C
ATOM   3695  CB  SER   486      -7.862  78.804  66.163  1.00  0.00           C
ATOM   3696  OG  SER   486      -8.796  77.733  66.160  1.00  0.00           O
ATOM   3697  C   SER   486      -9.645  80.414  66.633  1.00  0.00           C
ATOM   3698  O   SER   486     -10.821  80.214  66.330  1.00  0.00           O
ATOM   3699  N   SER   487      -9.276  80.923  67.824  1.00  0.00           N
ATOM   3700  CA  SER   487     -10.225  81.265  68.847  1.00  0.00           C
ATOM   3701  CB  SER   487      -9.660  81.145  70.271  1.00  0.00           C
ATOM   3702  OG  SER   487     -10.655  81.493  71.224  1.00  0.00           O
ATOM   3703  C   SER   487     -10.640  82.685  68.645  1.00  0.00           C
ATOM   3704  O   SER   487     -10.048  83.403  67.845  1.00  0.00           O
ATOM   3705  N   GLU   488     -11.686  83.115  69.378  1.00  0.00           N
ATOM   3706  CA  GLU   488     -12.266  84.424  69.256  1.00  0.00           C
ATOM   3707  CB  GLU   488     -13.556  84.580  70.084  1.00  0.00           C
ATOM   3708  CG  GLU   488     -13.345  84.402  71.588  1.00  0.00           C
ATOM   3709  CD  GLU   488     -14.694  84.583  72.271  1.00  0.00           C
ATOM   3710  OE1 GLU   488     -15.691  84.854  71.549  1.00  0.00           O
ATOM   3711  OE2 GLU   488     -14.746  84.456  73.524  1.00  0.00           O
ATOM   3712  C   GLU   488     -11.335  85.526  69.676  1.00  0.00           C
ATOM   3713  O   GLU   488     -11.266  86.545  68.996  1.00  0.00           O
ATOM   3714  N   ILE   489     -10.592  85.370  70.791  1.00  0.00           N
ATOM   3715  CA  ILE   489      -9.744  86.423  71.299  1.00  0.00           C
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ATOM   3716  CB  ILE   489      -8.756  86.956  70.296  1.00  0.00           C
ATOM   3717  CG2 ILE   489      -8.121  88.223  70.896  1.00  0.00           C
ATOM   3718  CG1 ILE   489      -7.705  85.902  69.937  1.00  0.00           C
ATOM   3719  CD1 ILE   489      -6.783  85.608  71.114  1.00  0.00           C
ATOM   3720  C   ILE   489     -10.588  87.589  71.722  1.00  0.00           C
ATOM   3721  O   ILE   489     -11.311  88.180  70.922  1.00  0.00           O
ATOM   3722  N   SER   490     -10.497  87.972  73.014  1.00  0.00           N
ATOM   3723  CA  SER   490     -11.257  89.095  73.484  1.00  0.00           C
ATOM   3724  CB  SER   490     -11.289  89.242  75.014  1.00  0.00           C
ATOM   3725  OG  SER   490     -11.938  88.130  75.606  1.00  0.00           O
ATOM   3726  C   SER   490     -10.583  90.323  72.975  1.00  0.00           C
ATOM   3727  O   SER   490      -9.357  90.392  72.920  1.00  0.00           O
ATOM   3728  N   GLU   491     -11.379  91.341  72.604  1.00  0.00           N
ATOM   3729  CA  GLU   491     -10.790  92.540  72.091  1.00  0.00           C
ATOM   3730  CB  GLU   491     -11.809  93.569  71.571  1.00  0.00           C
ATOM   3731  CG  GLU   491     -12.781  94.091  72.626  1.00  0.00           C
ATOM   3732  CD  GLU   491     -13.704  95.089  71.941  1.00  0.00           C
ATOM   3733  OE1 GLU   491     -13.177  96.057  71.330  1.00  0.00           O
ATOM   3734  OE2 GLU   491     -14.946  94.893  72.013  1.00  0.00           O
ATOM   3735  C   GLU   491     -10.012  93.174  73.186  1.00  0.00           C
ATOM   3736  O   GLU   491      -8.948  93.745  72.960  1.00  0.00           O
ATOM   3737  N   GLN   492     -10.521  93.065  74.423  1.00  0.00           N
ATOM   3738  CA  GLN   492      -9.869  93.704  75.519  1.00  0.00           C
ATOM   3739  CB  GLN   492     -10.550  93.384  76.858  1.00  0.00           C
ATOM   3740  CG  GLN   492     -12.015  93.817  76.898  1.00  0.00           C
ATOM   3741  CD  GLN   492     -12.579  93.450  78.264  1.00  0.00           C
ATOM   3742  OE1 GLN   492     -13.748  93.696  78.552  1.00  0.00           O
ATOM   3743  NE2 GLN   492     -11.724  92.845  79.131  1.00  0.00           N
ATOM   3744  C   GLN   492      -8.487  93.151  75.597  1.00  0.00           C
ATOM   3745  O   GLN   492      -7.525  93.885  75.818  1.00  0.00           O
ATOM   3746  N   GLU   493      -8.354  91.830  75.400  1.00  0.00           N
ATOM   3747  CA  GLU   493      -7.075  91.204  75.535  1.00  0.00           C
ATOM   3748  CB  GLU   493      -7.156  89.674  75.394  1.00  0.00           C
ATOM   3749  CG  GLU   493      -7.906  89.000  76.547  1.00  0.00           C
ATOM   3750  CD  GLU   493      -7.914  87.499  76.296  1.00  0.00           C
ATOM   3751  OE1 GLU   493      -7.522  87.085  75.172  1.00  0.00           O
ATOM   3752  OE2 GLU   493      -8.318  86.746  77.221  1.00  0.00           O
ATOM   3753  C   GLU   493      -6.100  91.703  74.506  1.00  0.00           C
ATOM   3754  O   GLU   493      -4.965  92.025  74.851  1.00  0.00           O
ATOM   3755  N   ILE   494      -6.494  91.780  73.217  1.00  0.00           N
ATOM   3756  CA  ILE   494      -5.543  92.163  72.202  1.00  0.00           C
ATOM   3757  CB  ILE   494      -6.033  91.982  70.792  1.00  0.00           C
ATOM   3758  CG2 ILE   494      -4.996  92.608  69.842  1.00  0.00           C
ATOM   3759  CG1 ILE   494      -6.279  90.493  70.498  1.00  0.00           C
ATOM   3760  CD1 ILE   494      -6.899  90.241  69.124  1.00  0.00           C
ATOM   3761  C   ILE   494      -5.103  93.587  72.355  1.00  0.00           C
ATOM   3762  O   ILE   494      -3.909  93.878  72.305  1.00  0.00           O
ATOM   3763  N   LYS   495      -6.051  94.522  72.540  1.00  0.00           N
ATOM   3764  CA  LYS   495      -5.672  95.901  72.638  1.00  0.00           C
ATOM   3765  CB  LYS   495      -6.885  96.858  72.641  1.00  0.00           C
ATOM   3766  CG  LYS   495      -7.986  96.536  73.656  1.00  0.00           C
ATOM   3767  CD  LYS   495      -7.652  96.899  75.103  1.00  0.00           C
ATOM   3768  CE  LYS   495      -8.777  96.562  76.084  1.00  0.00           C
ATOM   3769  NZ  LYS   495      -9.992  97.336  75.745  1.00  0.00           N
ATOM   3770  C   LYS   495      -4.848  96.092  73.876  1.00  0.00           C
ATOM   3771  O   LYS   495      -3.849  96.809  73.856  1.00  0.00           O
ATOM   3772  N   GLU   496      -5.241  95.438  74.986  1.00  0.00           N
ATOM   3773  CA  GLU   496      -4.537  95.570  76.228  1.00  0.00           C
ATOM   3774  CB  GLU   496      -5.227  94.831  77.386  1.00  0.00           C
ATOM   3775  CG  GLU   496      -4.499  94.989  78.722  1.00  0.00           C
ATOM   3776  CD  GLU   496      -4.719  96.412  79.216  1.00  0.00           C
ATOM   3777  OE1 GLU   496      -5.500  97.153  78.560  1.00  0.00           O
ATOM   3778  OE2 GLU   496      -4.109  96.776  80.255  1.00  0.00           O
ATOM   3779  C   GLU   496      -3.167  94.989  76.072  1.00  0.00           C
ATOM   3780  O   GLU   496      -2.186  95.543  76.565  1.00  0.00           O
ATOM   3781  N   PHE   497      -3.070  93.854  75.357  1.00  0.00           N
ATOM   3782  CA  PHE   497      -1.821  93.180  75.160  1.00  0.00           C
ATOM   3783  CB  PHE   497      -1.987  91.944  74.256  1.00  0.00           C
ATOM   3784  CG  PHE   497      -0.645  91.370  73.955  1.00  0.00           C
ATOM   3785  CD1 PHE   497       0.069  91.795  72.860  1.00  0.00           C
ATOM   3786  CD2 PHE   497      -0.098  90.406  74.766  1.00  0.00           C
ATOM   3787  CE1 PHE   497       1.306  91.270  72.572  1.00  0.00           C
ATOM   3788  CE2 PHE   497       1.139  89.878  74.484  1.00  0.00           C
ATOM   3789  CZ  PHE   497       1.846  90.306  73.388  1.00  0.00           C
ATOM   3790  C   PHE   497      -0.887  94.123  74.483  1.00  0.00           C
ATOM   3791  O   PHE   497       0.259  94.279  74.902  1.00  0.00           O
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ATOM   3792  N   VAL   498      -1.361  94.792  73.418  1.00  0.00           N
ATOM   3793  CA  VAL   498      -0.507  95.689  72.701  1.00  0.00           C
ATOM   3794  CB  VAL   498      -1.164  96.340  71.526  1.00  0.00           C
ATOM   3795  CG1 VAL   498      -0.169  97.361  70.954  1.00  0.00           C
ATOM   3796  CG2 VAL   498      -1.595  95.254  70.524  1.00  0.00           C
ATOM   3797  C   VAL   498      -0.075  96.798  73.607  1.00  0.00           C
ATOM   3798  O   VAL   498       1.098  97.163  73.635  1.00  0.00           O
ATOM   3799  N   ALA   499      -1.012  97.346  74.399  1.00  0.00           N
ATOM   3800  CA  ALA   499      -0.719  98.492  75.212  1.00  0.00           C
ATOM   3801  CB  ALA   499      -1.920  98.938  76.064  1.00  0.00           C
ATOM   3802  C   ALA   499       0.402  98.174  76.151  1.00  0.00           C
ATOM   3803  O   ALA   499       1.280  99.003  76.380  1.00  0.00           O
ATOM   3804  N   LYS   500       0.419  96.962  76.726  1.00  0.00           N
ATOM   3805  CA  LYS   500       1.452  96.653  77.670  1.00  0.00           C
ATOM   3806  CB  LYS   500       1.300  95.239  78.262  1.00  0.00           C
ATOM   3807  CG  LYS   500       2.213  94.941  79.457  1.00  0.00           C
ATOM   3808  CD  LYS   500       3.710  94.958  79.137  1.00  0.00           C
ATOM   3809  CE  LYS   500       4.599  94.660  80.346  1.00  0.00           C
ATOM   3810  NZ  LYS   500       6.023  94.695  79.946  1.00  0.00           N
ATOM   3811  C   LYS   500       2.776  96.729  76.974  1.00  0.00           C
ATOM   3812  O   LYS   500       3.764  97.193  77.541  1.00  0.00           O
ATOM   3813  N   GLN   501       2.826  96.235  75.726  1.00  0.00           N
ATOM   3814  CA  GLN   501       4.027  96.144  74.949  1.00  0.00           C
ATOM   3815  CB  GLN   501       3.855  95.207  73.746  1.00  0.00           C
ATOM   3816  CG  GLN   501       3.382  93.811  74.160  1.00  0.00           C
ATOM   3817  CD  GLN   501       4.395  93.226  75.135  1.00  0.00           C
ATOM   3818  OE1 GLN   501       4.090  92.301  75.886  1.00  0.00           O
ATOM   3819  NE2 GLN   501       5.635  93.780  75.129  1.00  0.00           N
ATOM   3820  C   GLN   501       4.546  97.464  74.440  1.00  0.00           C
ATOM   3821  O   GLN   501       5.759  97.636  74.337  1.00  0.00           O
ATOM   3822  N   VAL   502       3.673  98.426  74.069  1.00  0.00           N
ATOM   3823  CA  VAL   502       4.201  99.602  73.430  1.00  0.00           C
ATOM   3824  CB  VAL   502       3.787  99.714  71.992  1.00  0.00           C
ATOM   3825  CG1 VAL   502       4.421  98.556  71.203  1.00  0.00           C
ATOM   3826  CG2 VAL   502       2.249  99.726  71.930  1.00  0.00           C
ATOM   3827  C   VAL   502       3.774 100.871  74.110  1.00  0.00           C
ATOM   3828  O   VAL   502       2.891 100.898  74.965  1.00  0.00           O
ATOM   3829  N   ILE   503       4.450 101.969  73.715  1.00  0.00           N
ATOM   3830  CA  ILE   503       4.237 103.310  74.180  1.00  0.00           C
ATOM   3831  CB  ILE   503       5.283 104.279  73.691  1.00  0.00           C
ATOM   3832  CG2 ILE   503       6.604 103.916  74.390  1.00  0.00           C
ATOM   3833  CG1 ILE   503       5.387 104.276  72.159  1.00  0.00           C
ATOM   3834  CD1 ILE   503       4.167 104.836  71.449  1.00  0.00           C
ATOM   3835  C   ILE   503       2.847 103.753  73.827  1.00  0.00           C
ATOM   3836  O   ILE   503       2.205 103.194  72.941  1.00  0.00           O
ATOM   3837  N   PHE   504       2.349 104.783  74.538  1.00  0.00           N
ATOM   3838  CA  PHE   504       0.985 105.224  74.457  1.00  0.00           C
ATOM   3839  CB  PHE   504       0.734 106.495  75.291  1.00  0.00           C
ATOM   3840  CG  PHE   504      -0.707 106.862  75.170  1.00  0.00           C
ATOM   3841  CD1 PHE   504      -1.151 107.644  74.128  1.00  0.00           C
ATOM   3842  CD2 PHE   504      -1.614 106.425  76.106  1.00  0.00           C
ATOM   3843  CE1 PHE   504      -2.480 107.981  74.022  1.00  0.00           C
ATOM   3844  CE2 PHE   504      -2.945 106.758  76.006  1.00  0.00           C
ATOM   3845  CZ  PHE   504      -3.380 107.538  74.962  1.00  0.00           C
ATOM   3846  C   PHE   504       0.580 105.518  73.043  1.00  0.00           C
ATOM   3847  O   PHE   504      -0.501 105.111  72.619  1.00  0.00           O
ATOM   3848  N   TYR   505       1.408 106.229  72.261  1.00  0.00           N
ATOM   3849  CA  TYR   505       0.976 106.551  70.929  1.00  0.00           C
ATOM   3850  CB  TYR   505       1.803 107.643  70.205  1.00  0.00           C
ATOM   3851  CG  TYR   505       3.248 107.299  70.126  1.00  0.00           C
ATOM   3852  CD1 TYR   505       3.738 106.541  69.087  1.00  0.00           C
ATOM   3853  CD2 TYR   505       4.116 107.758  71.090  1.00  0.00           C
ATOM   3854  CE1 TYR   505       5.078 106.236  69.018  1.00  0.00           C
ATOM   3855  CE2 TYR   505       5.456 107.456  71.027  1.00  0.00           C
ATOM   3856  CZ  TYR   505       5.936 106.690  69.991  1.00  0.00           C
ATOM   3857  OH  TYR   505       7.310 106.376  69.924  1.00  0.00           O
ATOM   3858  C   TYR   505       0.818 105.314  70.082  1.00  0.00           C
ATOM   3859  O   TYR   505      -0.010 105.291  69.173  1.00  0.00           O
ATOM   3860  N   LYS   506       1.634 104.274  70.337  1.00  0.00           N
ATOM   3861  CA  LYS   506       1.662 103.018  69.624  1.00  0.00           C
ATOM   3862  CB  LYS   506       2.848 102.118  70.020  1.00  0.00           C
ATOM   3863  CG  LYS   506       4.213 102.608  69.530  1.00  0.00           C
ATOM   3864  CD  LYS   506       4.377 102.628  68.011  1.00  0.00           C
ATOM   3865  CE  LYS   506       5.687 103.269  67.550  1.00  0.00           C
ATOM   3866  NZ  LYS   506       6.838 102.454  67.995  1.00  0.00           N
ATOM   3867  C   LYS   506       0.412 102.192  69.824  1.00  0.00           C
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ATOM   3868  O   LYS   506       0.156 101.287  69.032  1.00  0.00           O
ATOM   3869  N   LYS   507      -0.367 102.418  70.903  1.00  0.00           N
ATOM   3870  CA  LYS   507      -1.513 101.585  71.199  1.00  0.00           C
ATOM   3871  CB  LYS   507      -2.406 102.107  72.342  1.00  0.00           C
ATOM   3872  CG  LYS   507      -1.841 101.913  73.751  1.00  0.00           C
ATOM   3873  CD  LYS   507      -0.628 102.784  74.070  1.00  0.00           C
ATOM   3874  CE  LYS   507      -0.265 102.791  75.556  1.00  0.00           C
ATOM   3875  NZ  LYS   507       0.279 101.476  75.952  1.00  0.00           N
ATOM   3876  C   LYS   507      -2.403 101.435  70.000  1.00  0.00           C
ATOM   3877  O   LYS   507      -2.455 102.305  69.134  1.00  0.00           O
ATOM   3878  N   ILE   508      -3.124 100.291  69.921  1.00  0.00           N
ATOM   3879  CA  ILE   508      -3.995 100.030  68.805  1.00  0.00           C
ATOM   3880  CB  ILE   508      -4.000  98.602  68.343  1.00  0.00           C
ATOM   3881  CG2 ILE   508      -5.237  98.398  67.454  1.00  0.00           C
ATOM   3882  CG1 ILE   508      -2.678  98.272  67.629  1.00  0.00           C
ATOM   3883  CD1 ILE   508      -1.446  98.403  68.515  1.00  0.00           C
ATOM   3884  C   ILE   508      -5.399 100.406  69.153  1.00  0.00           C
ATOM   3885  O   ILE   508      -6.019  99.852  70.053  1.00  0.00           O
ATOM   3886  N   HIS   509      -5.942 101.376  68.401  1.00  0.00           N
ATOM   3887  CA  HIS   509      -7.262 101.902  68.603  1.00  0.00           C
ATOM   3888  ND1 HIS   509      -7.103 105.288  68.883  1.00  0.00           N
ATOM   3889  CG  HIS   509      -6.708 104.276  68.036  1.00  0.00           C
ATOM   3890  NE2 HIS   509      -5.024 105.761  68.251  1.00  0.00           N
ATOM   3891  CD2 HIS   509      -5.437 104.582  67.658  1.00  0.00           C
ATOM   3892  CE1 HIS   509      -6.058 106.149  68.976  1.00  0.00           C
ATOM   3893  CB  HIS   509      -7.560 103.095  67.684  1.00  0.00           C
ATOM   3894  C   HIS   509      -8.303 100.841  68.379  1.00  0.00           C
ATOM   3895  O   HIS   509      -9.288 100.813  69.112  1.00  0.00           O
ATOM   3896  N   ARG   510      -8.168  99.961  67.359  1.00  0.00           N
ATOM   3897  CA  ARG   510      -9.184  98.942  67.255  1.00  0.00           C
ATOM   3898  CB  ARG   510     -10.465  99.383  66.524  1.00  0.00           C
ATOM   3899  CG  ARG   510     -10.259  99.883  65.096  1.00  0.00           C
ATOM   3900  CD  ARG   510     -11.573 100.303  64.433  1.00  0.00           C
ATOM   3901  NE  ARG   510     -12.380 101.025  65.459  1.00  0.00           N
ATOM   3902  CZ  ARG   510     -12.175 102.354  65.698  1.00  0.00           C
ATOM   3903  NH1 ARG   510     -11.209 103.035  65.017  1.00  0.00           N
ATOM   3904  NH2 ARG   510     -12.937 103.002  66.627  1.00  0.00           N
ATOM   3905  C   ARG   510      -8.653  97.707  66.596  1.00  0.00           C
ATOM   3906  O   ARG   510      -7.618  97.726  65.929  1.00  0.00           O
ATOM   3907  N   VAL   511      -9.370  96.578  66.797  1.00  0.00           N
ATOM   3908  CA  VAL   511      -8.965  95.311  66.252  1.00  0.00           C
ATOM   3909  CB  VAL   511      -8.594  94.305  67.304  1.00  0.00           C
ATOM   3910  CG1 VAL   511      -8.312  92.960  66.613  1.00  0.00           C
ATOM   3911  CG2 VAL   511      -7.411  94.849  68.120  1.00  0.00           C
ATOM   3912  C   VAL   511     -10.121  94.725  65.503  1.00  0.00           C
ATOM   3913  O   VAL   511     -11.270  94.829  65.929  1.00  0.00           O
ATOM   3914  N   TYR   512      -9.828  94.087  64.350  1.00  0.00           N
ATOM   3915  CA  TYR   512     -10.834  93.448  63.551  1.00  0.00           C
ATOM   3916  CB  TYR   512     -11.011  94.097  62.167  1.00  0.00           C
ATOM   3917  CG  TYR   512     -12.073  93.337  61.448  1.00  0.00           C
ATOM   3918  CD1 TYR   512     -13.404  93.601  61.676  1.00  0.00           C
ATOM   3919  CD2 TYR   512     -11.733  92.360  60.540  1.00  0.00           C
ATOM   3920  CE1 TYR   512     -14.380  92.898  61.010  1.00  0.00           C
ATOM   3921  CE2 TYR   512     -12.704  91.655  59.871  1.00  0.00           C
ATOM   3922  CZ  TYR   512     -14.031  91.924  60.107  1.00  0.00           C
ATOM   3923  OH  TYR   512     -15.032  91.202  59.421  1.00  0.00           O
ATOM   3924  C   TYR   512     -10.371  92.045  63.321  1.00  0.00           C
ATOM   3925  O   TYR   512      -9.219  91.811  62.957  1.00  0.00           O
ATOM   3926  N   PHE   513     -11.262  91.056  63.519  1.00  0.00           N
ATOM   3927  CA  PHE   513     -10.837  89.699  63.348  1.00  0.00           C
ATOM   3928  CB  PHE   513     -11.433  88.746  64.395  1.00  0.00           C
ATOM   3929  CG  PHE   513     -10.953  89.226  65.722  1.00  0.00           C
ATOM   3930  CD1 PHE   513      -9.677  88.943  66.151  1.00  0.00           C
ATOM   3931  CD2 PHE   513     -11.783  89.957  66.542  1.00  0.00           C
ATOM   3932  CE1 PHE   513      -9.234  89.385  67.376  1.00  0.00           C
ATOM   3933  CE2 PHE   513     -11.346  90.401  67.767  1.00  0.00           C
ATOM   3934  CZ  PHE   513     -10.069  90.116  68.186  1.00  0.00           C
ATOM   3935  C   PHE   513     -11.286  89.254  61.998  1.00  0.00           C
ATOM   3936  O   PHE   513     -12.458  89.382  61.647  1.00  0.00           O
ATOM   3937  N   VAL   514     -10.342  88.724  61.194  1.00  0.00           N
ATOM   3938  CA  VAL   514     -10.674  88.276  59.875  1.00  0.00           C
ATOM   3939  CB  VAL   514      -9.809  88.874  58.805  1.00  0.00           C
ATOM   3940  CG1 VAL   514     -10.030  90.396  58.791  1.00  0.00           C
ATOM   3941  CG2 VAL   514      -8.350  88.458  59.060  1.00  0.00           C
ATOM   3942  C   VAL   514     -10.469  86.799  59.835  1.00  0.00           C
ATOM   3943  O   VAL   514      -9.568  86.264  60.480  1.00  0.00           O
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ATOM   3944  N   ASP   515     -11.338  86.096  59.087  1.00  0.00           N
ATOM   3945  CA  ASP   515     -11.211  84.676  58.981  1.00  0.00           C
ATOM   3946  CB  ASP   515     -12.338  84.034  58.154  1.00  0.00           C
ATOM   3947  CG  ASP   515     -13.631  84.135  58.951  1.00  0.00           C
ATOM   3948  OD1 ASP   515     -13.559  84.504  60.155  1.00  0.00           O
ATOM   3949  OD2 ASP   515     -14.708  83.840  58.369  1.00  0.00           O
ATOM   3950  C   ASP   515      -9.923  84.396  58.279  1.00  0.00           C
ATOM   3951  O   ASP   515      -9.153  83.531  58.694  1.00  0.00           O
ATOM   3952  N   ALA   516      -9.653  85.143  57.191  1.00  0.00           N
ATOM   3953  CA  ALA   516      -8.441  84.928  56.460  1.00  0.00           C
ATOM   3954  CB  ALA   516      -8.629  84.077  55.193  1.00  0.00           C
ATOM   3955  C   ALA   516      -7.931  86.263  56.022  1.00  0.00           C
ATOM   3956  O   ALA   516      -8.694  87.215  55.862  1.00  0.00           O
ATOM   3957  N   ILE   517      -6.603  86.357  55.820  1.00  0.00           N
ATOM   3958  CA  ILE   517      -5.996  87.591  55.410  1.00  0.00           C
ATOM   3959  CB  ILE   517      -4.548  87.699  55.787  1.00  0.00           C
ATOM   3960  CG2 ILE   517      -3.776  86.621  55.008  1.00  0.00           C
ATOM   3961  CG1 ILE   517      -4.035  89.129  55.550  1.00  0.00           C
ATOM   3962  CD1 ILE   517      -4.668  90.166  56.477  1.00  0.00           C
ATOM   3963  C   ILE   517      -6.085  87.690  53.922  1.00  0.00           C
ATOM   3964  O   ILE   517      -5.932  86.697  53.217  1.00  0.00           O
ATOM   3965  N   PRO   518      -6.395  88.852  53.415  1.00  0.00           N
ATOM   3966  CA  PRO   518      -6.420  89.033  51.990  1.00  0.00           C
ATOM   3967  CD  PRO   518      -7.246  89.804  54.103  1.00  0.00           C
ATOM   3968  CB  PRO   518      -7.186  90.335  51.737  1.00  0.00           C
ATOM   3969  CG  PRO   518      -7.316  90.990  53.127  1.00  0.00           C
ATOM   3970  C   PRO   518      -5.019  89.007  51.465  1.00  0.00           C
ATOM   3971  O   PRO   518      -4.162  89.697  52.017  1.00  0.00           O
ATOM   3972  N   LYS   519      -4.769  88.243  50.384  1.00  0.00           N
ATOM   3973  CA  LYS   519      -3.437  88.134  49.863  1.00  0.00           C
ATOM   3974  CB  LYS   519      -2.908  86.689  49.795  1.00  0.00           C
ATOM   3975  CG  LYS   519      -2.673  85.990  51.133  1.00  0.00           C
ATOM   3976  CD  LYS   519      -3.949  85.473  51.789  1.00  0.00           C
ATOM   3977  CE  LYS   519      -4.610  84.322  51.026  1.00  0.00           C
ATOM   3978  NZ  LYS   519      -5.837  83.885  51.729  1.00  0.00           N
ATOM   3979  C   LYS   519      -3.451  88.589  48.443  1.00  0.00           C
ATOM   3980  O   LYS   519      -4.445  88.431  47.739  1.00  0.00           O
ATOM   3981  N   SER   520      -2.331  89.183  47.986  1.00  0.00           N
ATOM   3982  CA  SER   520      -2.246  89.554  46.606  1.00  0.00           C
ATOM   3983  CB  SER   520      -1.240  90.679  46.314  1.00  0.00           C
ATOM   3984  OG  SER   520      -1.623  91.867  46.988  1.00  0.00           O
ATOM   3985  C   SER   520      -1.746  88.336  45.903  1.00  0.00           C
ATOM   3986  O   SER   520      -1.323  87.390  46.564  1.00  0.00           O
ATOM   3987  N   PRO   521      -1.802  88.265  44.602  1.00  0.00           N
ATOM   3988  CA  PRO   521      -1.206  87.128  43.974  1.00  0.00           C
ATOM   3989  CD  PRO   521      -2.856  88.847  43.797  1.00  0.00           C
ATOM   3990  CB  PRO   521      -1.657  87.166  42.510  1.00  0.00           C
ATOM   3991  CG  PRO   521      -2.403  88.512  42.365  1.00  0.00           C
ATOM   3992  C   PRO   521       0.249  87.286  44.225  1.00  0.00           C
ATOM   3993  O   PRO   521       0.874  88.159  43.634  1.00  0.00           O
ATOM   3994  N   SER   522       0.833  86.430  45.066  1.00  0.00           N
ATOM   3995  CA  SER   522       2.190  86.677  45.425  1.00  0.00           C
ATOM   3996  CB  SER   522       2.453  88.127  45.875  1.00  0.00           C
ATOM   3997  OG  SER   522       3.835  88.323  46.137  1.00  0.00           O
ATOM   3998  C   SER   522       2.380  85.863  46.648  1.00  0.00           C
ATOM   3999  O   SER   522       2.242  84.646  46.641  1.00  0.00           O
ATOM   4000  N   GLY   523       2.710  86.540  47.754  1.00  0.00           N
ATOM   4001  CA  GLY   523       2.913  85.823  48.965  1.00  0.00           C
ATOM   4002  C   GLY   523       3.230  86.838  49.989  1.00  0.00           C
ATOM   4003  O   GLY   523       2.562  86.918  51.018  1.00  0.00           O
ATOM   4004  N   LYS   524       4.255  87.676  49.725  1.00  0.00           N
ATOM   4005  CA  LYS   524       4.530  88.748  50.638  1.00  0.00           C
ATOM   4006  CB  LYS   524       5.938  89.349  50.477  1.00  0.00           C
ATOM   4007  CG  LYS   524       6.453  90.103  51.711  1.00  0.00           C
ATOM   4008  CD  LYS   524       5.607  91.305  52.139  1.00  0.00           C
ATOM   4009  CE  LYS   524       5.804  92.539  51.255  1.00  0.00           C
ATOM   4010  NZ  LYS   524       4.932  93.641  51.721  1.00  0.00           N
ATOM   4011  C   LYS   524       3.569  89.821  50.247  1.00  0.00           C
ATOM   4012  O   LYS   524       3.938  90.967  49.995  1.00  0.00           O
ATOM   4013  N   ILE   525       2.287  89.438  50.169  1.00  0.00           N
ATOM   4014  CA  ILE   525       1.221  90.301  49.826  1.00  0.00           C
ATOM   4015  CB  ILE   525       0.668  90.008  48.457  1.00  0.00           C
ATOM   4016  CG2 ILE   525       1.521  90.793  47.448  1.00  0.00           C
ATOM   4017  CG1 ILE   525       0.623  88.493  48.158  1.00  0.00           C
ATOM   4018  CD1 ILE   525      -0.220  87.614  49.066  1.00  0.00           C
ATOM   4019  C   ILE   525       0.203  90.302  50.909  1.00  0.00           C
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ATOM   4020  O   ILE   525      -0.695  89.470  50.998  1.00  0.00           O
ATOM   4021  N   LEU   526       0.351  91.295  51.788  1.00  0.00           N
ATOM   4022  CA  LEU   526      -0.532  91.509  52.887  1.00  0.00           C
ATOM   4023  CB  LEU   526       0.060  92.549  53.871  1.00  0.00           C
ATOM   4024  CG  LEU   526      -0.724  92.826  55.176  1.00  0.00           C
ATOM   4025  CD2 LEU   526      -2.117  93.415  54.908  1.00  0.00           C
ATOM   4026  CD1 LEU   526       0.089  93.737  56.113  1.00  0.00           C
ATOM   4027  C   LEU   526      -1.849  91.982  52.345  1.00  0.00           C
ATOM   4028  O   LEU   526      -2.893  91.703  52.920  1.00  0.00           O
ATOM   4029  N   ARG   527      -1.841  92.702  51.209  1.00  0.00           N
ATOM   4030  CA  ARG   527      -3.022  93.340  50.682  1.00  0.00           C
ATOM   4031  CB  ARG   527      -4.149  92.383  50.262  1.00  0.00           C
ATOM   4032  CG  ARG   527      -3.840  91.583  48.997  1.00  0.00           C
ATOM   4033  CD  ARG   527      -5.094  91.034  48.314  1.00  0.00           C
ATOM   4034  NE  ARG   527      -5.638  92.118  47.450  1.00  0.00           N
ATOM   4035  CZ  ARG   527      -6.639  91.849  46.563  1.00  0.00           C
ATOM   4036  NH1 ARG   527      -7.149  90.587  46.469  1.00  0.00           N
ATOM   4037  NH2 ARG   527      -7.129  92.845  45.767  1.00  0.00           N
ATOM   4038  C   ARG   527      -3.535  94.224  51.775  1.00  0.00           C
ATOM   4039  O   ARG   527      -4.618  94.024  52.323  1.00  0.00           O
ATOM   4040  N   LYS   528      -2.719  95.245  52.091  1.00  0.00           N
ATOM   4041  CA  LYS   528      -2.882  96.227  53.125  1.00  0.00           C
ATOM   4042  CB  LYS   528      -1.581  97.044  53.243  1.00  0.00           C
ATOM   4043  CG  LYS   528      -1.384  97.886  54.502  1.00  0.00           C
ATOM   4044  CD  LYS   528      -2.337  99.068  54.651  1.00  0.00           C
ATOM   4045  CE  LYS   528      -1.778 100.133  55.596  1.00  0.00           C
ATOM   4046  NZ  LYS   528      -1.268  99.496  56.829  1.00  0.00           N
ATOM   4047  C   LYS   528      -4.017  97.155  52.834  1.00  0.00           C
ATOM   4048  O   LYS   528      -4.832  97.453  53.705  1.00  0.00           O
ATOM   4049  N   ASP   529      -4.104  97.636  51.585  1.00  0.00           N
ATOM   4050  CA  ASP   529      -5.144  98.563  51.260  1.00  0.00           C
ATOM   4051  CB  ASP   529      -5.046  99.125  49.830  1.00  0.00           C
ATOM   4052  CG  ASP   529      -5.094  97.971  48.843  1.00  0.00           C
ATOM   4053  OD1 ASP   529      -4.119  97.173  48.833  1.00  0.00           O
ATOM   4054  OD2 ASP   529      -6.089  97.880  48.075  1.00  0.00           O
ATOM   4055  C   ASP   529      -6.434  97.825  51.412  1.00  0.00           C
ATOM   4056  O   ASP   529      -7.464  98.414  51.731  1.00  0.00           O
ATOM   4057  N   LEU   530      -6.378  96.494  51.206  1.00  0.00           N
ATOM   4058  CA  LEU   530      -7.496  95.594  51.204  1.00  0.00           C
ATOM   4059  CB  LEU   530      -7.118  94.147  50.842  1.00  0.00           C
ATOM   4060  CG  LEU   530      -6.683  93.967  49.378  1.00  0.00           C
ATOM   4061  CD2 LEU   530      -5.409  94.765  49.065  1.00  0.00           C
ATOM   4062  CD1 LEU   530      -7.837  94.274  48.412  1.00  0.00           C
ATOM   4063  C   LEU   530      -8.215  95.536  52.515  1.00  0.00           C
ATOM   4064  O   LEU   530      -9.416  95.270  52.533  1.00  0.00           O
ATOM   4065  N   ARG   531      -7.518  95.725  53.649  1.00  0.00           N
ATOM   4066  CA  ARG   531      -8.186  95.632  54.917  1.00  0.00           C
ATOM   4067  CB  ARG   531      -7.249  95.925  56.106  1.00  0.00           C
ATOM   4068  CG  ARG   531      -6.413  97.212  56.001  1.00  0.00           C
ATOM   4069  CD  ARG   531      -7.179  98.533  55.894  1.00  0.00           C
ATOM   4070  NE  ARG   531      -7.976  98.717  57.136  1.00  0.00           N
ATOM   4071  CZ  ARG   531      -8.500  99.941  57.438  1.00  0.00           C
ATOM   4072  NH1 ARG   531      -8.291 100.999  56.602  1.00  0.00           N
ATOM   4073  NH2 ARG   531      -9.232 100.104  58.578  1.00  0.00           N
ATOM   4074  C   ARG   531      -9.385  96.533  54.964  1.00  0.00           C
ATOM   4075  O   ARG   531      -9.357  97.667  54.494  1.00  0.00           O
END
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Pinus taeda Cinnamoyl-Coenzyme A Reductase

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REMARK     CCR  Pinus taeda   molecular  model
REMARK   CCR COMPLIES WITH FORMAT V. 2.0, 28-MAY-2002
ATOM     72  N   GLN    11      38.410 -17.347  39.017  1.00  0.00           N
ATOM     73  CA  GLN    11      37.825 -16.438  38.089  1.00  0.00           C
ATOM     74  CB  GLN    11      36.366 -16.103  38.430  1.00  0.00           C
ATOM     75  CG  GLN    11      35.906 -14.761  37.865  1.00  0.00           C
ATOM     76  CD  GLN    11      36.189 -13.730  38.954  1.00  0.00           C
ATOM     77  OE1 GLN    11      35.677 -13.848  40.067  1.00  0.00           O
ATOM     78  NE2 GLN    11      37.035 -12.711  38.646  1.00  0.00           N
ATOM     79  C   GLN    11      38.590 -15.170  38.034  1.00  0.00           C
ATOM     80  O   GLN    11      38.912 -14.559  39.052  1.00  0.00           O
ATOM     81  N   THR    12      38.907 -14.762  36.793  1.00  0.00           N
ATOM     82  CA  THR    12      39.544 -13.511  36.552  1.00  0.00           C
ATOM     83  CB  THR    12      40.774 -13.617  35.701  1.00  0.00           C
ATOM     84  OG1 THR    12      41.724 -14.478  36.312  1.00  0.00           O
ATOM     85  CG2 THR    12      41.371 -12.211  35.527  1.00  0.00           C
ATOM     86  C   THR    12      38.531 -12.737  35.786  1.00  0.00           C
ATOM     87  O   THR    12      38.100 -13.158  34.714  1.00  0.00           O
ATOM     88  N   VAL    13      38.096 -11.586  36.324  1.00  0.00           N
ATOM     89  CA  VAL    13      37.096 -10.874  35.597  1.00  0.00           C
ATOM     90  CB  VAL    13      35.832 -10.599  36.360  1.00  0.00           C
ATOM     91  CG1 VAL    13      35.131 -11.935  36.655  1.00  0.00           C
ATOM     92  CG2 VAL    13      36.177  -9.776  37.610  1.00  0.00           C
ATOM     93  C   VAL    13      37.650  -9.567  35.162  1.00  0.00           C
ATOM     94  O   VAL    13      38.369  -8.892  35.896  1.00  0.00           O
ATOM     95  N   CYS    14      37.333  -9.185  33.915  1.00  0.00           N
ATOM     96  CA  CYS    14      37.800  -7.920  33.463  1.00  0.00           C
ATOM     97  CB  CYS    14      38.330  -7.918  32.019  1.00  0.00           C
ATOM     98  SG  CYS    14      37.127  -8.532  30.812  1.00  0.00           S
ATOM     99  C   CYS    14      36.667  -6.967  33.603  1.00  0.00           C
ATOM    100  O   CYS    14      35.558  -7.209  33.125  1.00  0.00           O
ATOM    101  N   VAL    15      36.929  -5.857  34.314  1.00  0.00           N
ATOM    102  CA  VAL    15      35.903  -4.895  34.540  1.00  0.00           C
ATOM    103  CB  VAL    15      35.744  -4.538  35.995  1.00  0.00           C
ATOM    104  CG1 VAL    15      37.079  -3.994  36.530  1.00  0.00           C
ATOM    105  CG2 VAL    15      34.577  -3.550  36.139  1.00  0.00           C
ATOM    106  C   VAL    15      36.251  -3.662  33.782  1.00  0.00           C
ATOM    107  O   VAL    15      37.306  -3.059  33.966  1.00  0.00           O
ATOM    108  N   THR    16      35.360  -3.266  32.864  1.00  0.00           N
ATOM    109  CA  THR    16      35.595  -2.057  32.150  1.00  0.00           C
ATOM    110  CB  THR    16      35.108  -2.141  30.735  1.00  0.00           C
ATOM    111  OG1 THR    16      33.787  -2.657  30.716  1.00  0.00           O
ATOM    112  CG2 THR    16      36.046  -3.071  29.945  1.00  0.00           C
ATOM    113  C   THR    16      34.928  -0.965  32.923  1.00  0.00           C
ATOM    114  O   THR    16      33.913  -1.186  33.581  1.00  0.00           O
ATOM    115  N   GLY    17      35.521   0.243  32.906  1.00  0.00           N
ATOM    116  CA  GLY    17      34.956   1.348  33.627  1.00  0.00           C
ATOM    117  C   GLY    17      35.203   1.134  35.089  1.00  0.00           C
ATOM    118  O   GLY    17      34.545   1.749  35.925  1.00  0.00           O
ATOM    119  N   ALA    18      36.209   0.297  35.420  1.00  0.00           N
ATOM    120  CA  ALA    18      36.529  -0.121  36.763  1.00  0.00           C
ATOM    121  CB  ALA    18      37.689  -1.121  36.828  1.00  0.00           C
ATOM    122  C   ALA    18      36.875   1.051  37.633  1.00  0.00           C
ATOM    123  O   ALA    18      36.653   1.018  38.842  1.00  0.00           O
ATOM    124  N   GLY    19      37.500   2.083  37.047  1.00  0.00           N
ATOM    125  CA  GLY    19      37.903   3.302  37.699  1.00  0.00           C
ATOM    126  C   GLY    19      36.707   4.117  38.107  1.00  0.00           C
ATOM    127  O   GLY    19      36.823   5.011  38.945  1.00  0.00           O
ATOM    128  N   GLY    20      35.551   3.896  37.450  1.00  0.00           N
ATOM    129  CA  GLY    20      34.374   4.686  37.695  1.00  0.00           C
ATOM    130  C   GLY    20      33.829   4.385  39.055  1.00  0.00           C
ATOM    131  O   GLY    20      34.343   3.539  39.784  1.00  0.00           O
ATOM    132  N   PHE    21      32.757   5.109  39.435  1.00  0.00           N
ATOM    133  CA  PHE    21      32.212   4.982  40.755  1.00  0.00           C
ATOM    134  CB  PHE    21      31.093   6.004  41.032  1.00  0.00           C
ATOM    135  CG  PHE    21      30.380   5.591  42.273  1.00  0.00           C
ATOM    136  CD1 PHE    21      31.066   5.370  43.445  1.00  0.00           C
ATOM    137  CD2 PHE    21      29.009   5.467  42.272  1.00  0.00           C
ATOM    138  CE1 PHE    21      30.391   4.995  44.582  1.00  0.00           C
ATOM    139  CE2 PHE    21      28.331   5.095  43.409  1.00  0.00           C
ATOM    140  CZ  PHE    21      29.025   4.856  44.569  1.00  0.00           C
ATOM    141  C   PHE    21      31.701   3.603  41.038  1.00  0.00           C
ATOM    142  O   PHE    21      32.119   2.986  42.016  1.00  0.00           O
ATOM    143  N   ILE    22      30.803   3.059  40.196  1.00  0.00           N
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ATOM    144  CA  ILE    22      30.273   1.760  40.508  1.00  0.00           C
ATOM    145  CB  ILE    22      29.133   1.332  39.625  1.00  0.00           C
ATOM    146  CG2 ILE    22      27.954   2.282  39.880  1.00  0.00           C
ATOM    147  CG1 ILE    22      29.564   1.249  38.153  1.00  0.00           C
ATOM    148  CD1 ILE    22      29.950   2.596  37.543  1.00  0.00           C
ATOM    149  C   ILE    22      31.340   0.731  40.393  1.00  0.00           C
ATOM    150  O   ILE    22      31.502  -0.129  41.258  1.00  0.00           O
ATOM    151  N   ALA    23      32.120   0.800  39.309  1.00  0.00           N
ATOM    152  CA  ALA    23      33.099  -0.214  39.098  1.00  0.00           C
ATOM    153  CB  ALA    23      33.768  -0.129  37.736  1.00  0.00           C
ATOM    154  C   ALA    23      34.133  -0.199  40.184  1.00  0.00           C
ATOM    155  O   ALA    23      34.620  -1.256  40.579  1.00  0.00           O
ATOM    156  N   SER    24      34.513   0.989  40.697  1.00  0.00           N
ATOM    157  CA  SER    24      35.538   1.041  41.708  1.00  0.00           C
ATOM    158  CB  SER    24      35.881   2.477  42.155  1.00  0.00           C
ATOM    159  OG  SER    24      34.760   3.080  42.784  1.00  0.00           O
ATOM    160  C   SER    24      35.078   0.283  42.921  1.00  0.00           C
ATOM    161  O   SER    24      35.838  -0.492  43.500  1.00  0.00           O
ATOM    162  N   TRP    25      33.815   0.473  43.348  1.00  0.00           N
ATOM    163  CA  TRP    25      33.344  -0.256  44.495  1.00  0.00           C
ATOM    164  CB  TRP    25      31.954   0.155  45.010  1.00  0.00           C
ATOM    165  CG  TRP    25      31.996   1.277  46.020  1.00  0.00           C
ATOM    166  CD2 TRP    25      32.136   1.031  47.428  1.00  0.00           C
ATOM    167  CD1 TRP    25      31.929   2.630  45.867  1.00  0.00           C
ATOM    168  NE1 TRP    25      32.021   3.244  47.098  1.00  0.00           N
ATOM    169  CE2 TRP    25      32.146   2.268  48.066  1.00  0.00           C
ATOM    170  CE3 TRP    25      32.246  -0.136  48.132  1.00  0.00           C
ATOM    171  CZ2 TRP    25      32.267   2.358  49.425  1.00  0.00           C
ATOM    172  CZ3 TRP    25      32.368  -0.044  49.501  1.00  0.00           C
ATOM    173  CH2 TRP    25      32.377   1.181  50.136  1.00  0.00           C
ATOM    174  C   TRP    25      33.328  -1.724  44.206  1.00  0.00           C
ATOM    175  O   TRP    25      33.621  -2.533  45.085  1.00  0.00           O
ATOM    176  N   LEU    26      32.971  -2.117  42.971  1.00  0.00           N
ATOM    177  CA  LEU    26      32.899  -3.511  42.626  1.00  0.00           C
ATOM    178  CB  LEU    26      32.446  -3.728  41.175  1.00  0.00           C
ATOM    179  CG  LEU    26      32.366  -5.211  40.773  1.00  0.00           C
ATOM    180  CD2 LEU    26      32.191  -5.372  39.253  1.00  0.00           C
ATOM    181  CD1 LEU    26      31.290  -5.950  41.584  1.00  0.00           C
ATOM    182  C   LEU    26      34.259  -4.127  42.743  1.00  0.00           C
ATOM    183  O   LEU    26      34.406  -5.227  43.275  1.00  0.00           O
ATOM    184  N   VAL    27      35.296  -3.430  42.241  1.00  0.00           N
ATOM    185  CA  VAL    27      36.612  -3.995  42.270  1.00  0.00           C
ATOM    186  CB  VAL    27      37.649  -3.197  41.526  1.00  0.00           C
ATOM    187  CG1 VAL    27      37.254  -3.134  40.046  1.00  0.00           C
ATOM    188  CG2 VAL    27      37.829  -1.823  42.180  1.00  0.00           C
ATOM    189  C   VAL    27      37.061  -4.154  43.688  1.00  0.00           C
ATOM    190  O   VAL    27      37.692  -5.150  44.038  1.00  0.00           O
ATOM    191  N   LYS    28      36.738  -3.175  44.551  1.00  0.00           N
ATOM    192  CA  LYS    28      37.178  -3.255  45.912  1.00  0.00           C
ATOM    193  CB  LYS    28      36.700  -2.058  46.750  1.00  0.00           C
ATOM    194  CG  LYS    28      37.240  -0.714  46.256  1.00  0.00           C
ATOM    195  CD  LYS    28      36.494   0.492  46.829  1.00  0.00           C
ATOM    196  CE  LYS    28      36.965   1.829  46.257  1.00  0.00           C
ATOM    197  NZ  LYS    28      36.116   2.928  46.770  1.00  0.00           N
ATOM    198  C   LYS    28      36.596  -4.484  46.538  1.00  0.00           C
ATOM    199  O   LYS    28      37.300  -5.240  47.208  1.00  0.00           O
ATOM    200  N   LEU    29      35.292  -4.728  46.308  1.00  0.00           N
ATOM    201  CA  LEU    29      34.602  -5.823  46.932  1.00  0.00           C
ATOM    202  CB  LEU    29      33.099  -5.835  46.578  1.00  0.00           C
ATOM    203  CG  LEU    29      32.248  -6.927  47.267  1.00  0.00           C
ATOM    204  CD2 LEU    29      32.355  -6.819  48.795  1.00  0.00           C
ATOM    205  CD1 LEU    29      32.553  -8.340  46.743  1.00  0.00           C
ATOM    206  C   LEU    29      35.211  -7.108  46.471  1.00  0.00           C
ATOM    207  O   LEU    29      35.453  -8.017  47.264  1.00  0.00           O
ATOM    208  N   LEU    30      35.495  -7.200  45.166  1.00  0.00           N
ATOM    209  CA  LEU    30      35.998  -8.406  44.585  1.00  0.00           C
ATOM    210  CB  LEU    30      36.179  -8.197  43.069  1.00  0.00           C
ATOM    211  CG  LEU    30      36.578  -9.442  42.273  1.00  0.00           C
ATOM    212  CD2 LEU    30      35.525 -10.548  42.454  1.00  0.00           C
ATOM    213  CD1 LEU    30      38.019  -9.864  42.593  1.00  0.00           C
ATOM    214  C   LEU    30      37.315  -8.733  45.221  1.00  0.00           C
ATOM    215  O   LEU    30      37.565  -9.873  45.608  1.00  0.00           O
ATOM    216  N   LEU    31      38.200  -7.731  45.356  1.00  0.00           N
ATOM    217  CA  LEU    31      39.490  -8.009  45.916  1.00  0.00           C
ATOM    218  CB  LEU    31      40.439  -6.804  45.815  1.00  0.00           C
ATOM    219  CG  LEU    31      40.722  -6.378  44.361  1.00  0.00           C
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ATOM    220  CD2 LEU    31      41.211  -7.565  43.510  1.00  0.00           C
ATOM    221  CD1 LEU    31      41.674  -5.173  44.306  1.00  0.00           C
ATOM    222  C   LEU    31      39.366  -8.379  47.360  1.00  0.00           C
ATOM    223  O   LEU    31      39.932  -9.379  47.800  1.00  0.00           O
ATOM    224  N   GLU    32      38.628  -7.582  48.154  1.00  0.00           N
ATOM    225  CA  GLU    32      38.591  -7.888  49.555  1.00  0.00           C
ATOM    226  CB  GLU    32      37.944  -6.787  50.410  1.00  0.00           C
ATOM    227  CG  GLU    32      38.000  -7.103  51.907  1.00  0.00           C
ATOM    228  CD  GLU    32      37.246  -6.020  52.666  1.00  0.00           C
ATOM    229  OE1 GLU    32      36.037  -5.823  52.363  1.00  0.00           O
ATOM    230  OE2 GLU    32      37.863  -5.379  53.555  1.00  0.00           O
ATOM    231  C   GLU    32      37.816  -9.139  49.832  1.00  0.00           C
ATOM    232  O   GLU    32      38.308 -10.049  50.497  1.00  0.00           O
ATOM    233  N   ARG    33      36.572  -9.203  49.319  1.00  0.00           N
ATOM    234  CA  ARG    33      35.667 -10.283  49.605  1.00  0.00           C
ATOM    235  CB  ARG    33      34.217 -10.010  49.160  1.00  0.00           C
ATOM    236  CG  ARG    33      33.413  -9.202  50.177  1.00  0.00           C
ATOM    237  CD  ARG    33      32.453 -10.070  50.996  1.00  0.00           C
ATOM    238  NE  ARG    33      33.237 -11.212  51.549  1.00  0.00           N
ATOM    239  CZ  ARG    33      33.374 -12.363  50.826  1.00  0.00           C
ATOM    240  NH1 ARG    33      32.799 -12.467  49.593  1.00  0.00           N
ATOM    241  NH2 ARG    33      34.085 -13.412  51.336  1.00  0.00           N
ATOM    242  C   ARG    33      36.067 -11.575  48.987  1.00  0.00           C
ATOM    243  O   ARG    33      35.970 -12.622  49.624  1.00  0.00           O
ATOM    244  N   GLY    34      36.541 -11.561  47.731  1.00  0.00           N
ATOM    245  CA  GLY    34      36.722 -12.844  47.129  1.00  0.00           C
ATOM    246  C   GLY    34      38.152 -13.098  46.840  1.00  0.00           C
ATOM    247  O   GLY    34      39.017 -12.247  47.041  1.00  0.00           O
ATOM    248  N   TYR    35      38.430 -14.335  46.395  1.00  0.00           N
ATOM    249  CA  TYR    35      39.761 -14.659  46.009  1.00  0.00           C
ATOM    250  CB  TYR    35      40.242 -15.989  46.613  1.00  0.00           C
ATOM    251  CG  TYR    35      41.675 -16.194  46.259  1.00  0.00           C
ATOM    252  CD1 TYR    35      42.656 -15.534  46.961  1.00  0.00           C
ATOM    253  CD2 TYR    35      42.043 -17.053  45.248  1.00  0.00           C
ATOM    254  CE1 TYR    35      43.983 -15.715  46.654  1.00  0.00           C
ATOM    255  CE2 TYR    35      43.368 -17.237  44.934  1.00  0.00           C
ATOM    256  CZ  TYR    35      44.340 -16.567  45.636  1.00  0.00           C
ATOM    257  OH  TYR    35      45.701 -16.757  45.317  1.00  0.00           O
ATOM    258  C   TYR    35      39.701 -14.827  44.530  1.00  0.00           C
ATOM    259  O   TYR    35      39.883 -15.921  44.002  1.00  0.00           O
ATOM    260  N   THR    36      39.434 -13.725  43.815  1.00  0.00           N
ATOM    261  CA  THR    36      39.432 -13.793  42.392  1.00  0.00           C
ATOM    262  CB  THR    36      38.078 -13.742  41.747  1.00  0.00           C
ATOM    263  OG1 THR    36      37.429 -12.525  42.056  1.00  0.00           O
ATOM    264  CG2 THR    36      37.249 -14.936  42.250  1.00  0.00           C
ATOM    265  C   THR    36      40.248 -12.629  41.958  1.00  0.00           C
ATOM    266  O   THR    36      40.579 -11.762  42.764  1.00  0.00           O
ATOM    267  N   VAL    37      40.614 -12.596  40.667  1.00  0.00           N
ATOM    268  CA  VAL    37      41.478 -11.559  40.194  1.00  0.00           C
ATOM    269  CB  VAL    37      42.623 -12.086  39.379  1.00  0.00           C
ATOM    270  CG1 VAL    37      43.498 -10.909  38.910  1.00  0.00           C
ATOM    271  CG2 VAL    37      43.380 -13.123  40.226  1.00  0.00           C
ATOM    272  C   VAL    37      40.673 -10.657  39.320  1.00  0.00           C
ATOM    273  O   VAL    37      39.632 -11.046  38.800  1.00  0.00           O
ATOM    274  N   ARG    38      41.130  -9.398  39.179  1.00  0.00           N
ATOM    275  CA  ARG    38      40.402  -8.474  38.369  1.00  0.00           C
ATOM    276  CB  ARG    38      39.698  -7.386  39.204  1.00  0.00           C
ATOM    277  CG  ARG    38      38.773  -6.471  38.400  1.00  0.00           C
ATOM    278  CD  ARG    38      37.462  -7.146  37.988  1.00  0.00           C
ATOM    279  NE  ARG    38      36.668  -7.375  39.230  1.00  0.00           N
ATOM    280  CZ  ARG    38      35.824  -6.409  39.693  1.00  0.00           C
ATOM    281  NH1 ARG    38      35.660  -5.256  38.983  1.00  0.00           N
ATOM    282  NH2 ARG    38      35.137  -6.599  40.857  1.00  0.00           N
ATOM    283  C   ARG    38      41.367  -7.776  37.468  1.00  0.00           C
ATOM    284  O   ARG    38      42.535  -7.580  37.801  1.00  0.00           O
ATOM    285  N   GLY    39      40.883  -7.402  36.272  1.00  0.00           N
ATOM    286  CA  GLY    39      41.666  -6.649  35.344  1.00  0.00           C
ATOM    287  C   GLY    39      40.814  -5.472  35.017  1.00  0.00           C
ATOM    288  O   GLY    39      39.697  -5.621  34.524  1.00  0.00           O
ATOM    289  N   THR    40      41.341  -4.264  35.275  1.00  0.00           N
ATOM    290  CA  THR    40      40.604  -3.052  35.071  1.00  0.00           C
ATOM    291  CB  THR    40      40.972  -1.983  36.058  1.00  0.00           C
ATOM    292  OG1 THR    40      40.601  -2.366  37.373  1.00  0.00           O
ATOM    293  CG2 THR    40      40.332  -0.649  35.644  1.00  0.00           C
ATOM    294  C   THR    40      40.952  -2.498  33.736  1.00  0.00           C
ATOM    295  O   THR    40      42.125  -2.370  33.388  1.00  0.00           O
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ATOM    296  N   VAL    41      39.915  -2.175  32.942  1.00  0.00           N
ATOM    297  CA  VAL    41      40.157  -1.556  31.677  1.00  0.00           C
ATOM    298  CB  VAL    41      39.613  -2.351  30.524  1.00  0.00           C
ATOM    299  CG1 VAL    41      39.871  -1.585  29.216  1.00  0.00           C
ATOM    300  CG2 VAL    41      40.234  -3.758  30.560  1.00  0.00           C
ATOM    301  C   VAL    41      39.422  -0.258  31.709  1.00  0.00           C
ATOM    302  O   VAL    41      38.191  -0.237  31.733  1.00  0.00           O
ATOM    303  N   ARG    42      40.149   0.877  31.736  1.00  0.00           N
ATOM    304  CA  ARG    42      39.410   2.101  31.703  1.00  0.00           C
ATOM    305  CB  ARG    42      39.142   2.742  33.073  1.00  0.00           C
ATOM    306  CG  ARG    42      40.396   3.336  33.711  1.00  0.00           C
ATOM    307  CD  ARG    42      40.144   3.992  35.069  1.00  0.00           C
ATOM    308  NE  ARG    42      41.164   5.068  35.226  1.00  0.00           N
ATOM    309  CZ  ARG    42      42.464   4.756  35.491  1.00  0.00           C
ATOM    310  NH1 ARG    42      42.838   3.449  35.594  1.00  0.00           N
ATOM    311  NH2 ARG    42      43.393   5.747  35.625  1.00  0.00           N
ATOM    312  C   ARG    42      40.246   3.096  30.974  1.00  0.00           C
ATOM    313  O   ARG    42      41.465   3.139  31.132  1.00  0.00           O
ATOM    314  N   ASN    43      39.597   3.917  30.131  1.00  0.00           N
ATOM    315  CA  ASN    43      40.289   4.982  29.477  1.00  0.00           C
ATOM    316  CB  ASN    43      39.901   5.120  27.987  1.00  0.00           C
ATOM    317  CG  ASN    43      38.383   5.241  27.838  1.00  0.00           C
ATOM    318  OD1 ASN    43      37.618   4.601  28.557  1.00  0.00           O
ATOM    319  ND2 ASN    43      37.934   6.101  26.885  1.00  0.00           N
ATOM    320  C   ASN    43      39.889   6.199  30.242  1.00  0.00           C
ATOM    321  O   ASN    43      38.967   6.928  29.888  1.00  0.00           O
ATOM    322  N   PRO    44      40.660   6.427  31.268  1.00  0.00           N
ATOM    323  CA  PRO    44      40.398   7.418  32.282  1.00  0.00           C
ATOM    324  CD  PRO    44      42.048   6.003  31.246  1.00  0.00           C
ATOM    325  CB  PRO    44      41.737   7.629  32.996  1.00  0.00           C
ATOM    326  CG  PRO    44      42.591   6.408  32.620  1.00  0.00           C
ATOM    327  C   PRO    44      39.862   8.704  31.739  1.00  0.00           C
ATOM    328  O   PRO    44      40.598   9.435  31.084  1.00  0.00           O
ATOM    329  N   GLU    45      38.588   9.017  32.043  1.00  0.00           N
ATOM    330  CA  GLU    45      37.997  10.232  31.566  1.00  0.00           C
ATOM    331  CB  GLU    45      36.691  10.056  30.765  1.00  0.00           C
ATOM    332  CG  GLU    45      35.509   9.516  31.572  1.00  0.00           C
ATOM    333  CD  GLU    45      34.294   9.462  30.652  1.00  0.00           C
ATOM    334  OE1 GLU    45      34.303   8.635  29.703  1.00  0.00           O
ATOM    335  OE2 GLU    45      33.340  10.253  30.885  1.00  0.00           O
ATOM    336  C   GLU    45      37.681  11.032  32.786  1.00  0.00           C
ATOM    337  O   GLU    45      38.214  10.770  33.861  1.00  0.00           O
ATOM    338  N   ASP    46      36.797  12.034  32.649  1.00  0.00           N
ATOM    339  CA  ASP    46      36.473  12.893  33.750  1.00  0.00           C
ATOM    340  CB  ASP    46      35.373  13.911  33.395  1.00  0.00           C
ATOM    341  CG  ASP    46      35.230  14.907  34.539  1.00  0.00           C
ATOM    342  OD1 ASP    46      35.967  14.768  35.550  1.00  0.00           O
ATOM    343  OD2 ASP    46      34.374  15.824  34.411  1.00  0.00           O
ATOM    344  C   ASP    46      35.949  12.033  34.855  1.00  0.00           C
ATOM    345  O   ASP    46      36.201  12.288  36.032  1.00  0.00           O
ATOM    346  N   GLN    47      35.199  10.982  34.491  1.00  0.00           N
ATOM    347  CA  GLN    47      34.582  10.108  35.445  1.00  0.00           C
ATOM    348  CB  GLN    47      33.607   9.111  34.794  1.00  0.00           C
ATOM    349  CG  GLN    47      34.269   8.111  33.849  1.00  0.00           C
ATOM    350  CD  GLN    47      33.179   7.203  33.291  1.00  0.00           C
ATOM    351  OE1 GLN    47      33.443   6.358  32.437  1.00  0.00           O
ATOM    352  NE2 GLN    47      31.923   7.383  33.778  1.00  0.00           N
ATOM    353  C   GLN    47      35.603   9.322  36.217  1.00  0.00           C
ATOM    354  O   GLN    47      35.389   9.016  37.388  1.00  0.00           O
ATOM    355  N   LYS    48      36.735   8.962  35.577  1.00  0.00           N
ATOM    356  CA  LYS    48      37.722   8.089  36.161  1.00  0.00           C
ATOM    357  CB  LYS    48      38.856   7.747  35.181  1.00  0.00           C
ATOM    358  CG  LYS    48      39.869   8.883  34.996  1.00  0.00           C
ATOM    359  CD  LYS    48      40.982   8.928  36.053  1.00  0.00           C
ATOM    360  CE  LYS    48      41.977  10.076  35.870  1.00  0.00           C
ATOM    361  NZ  LYS    48      42.849   9.822  34.702  1.00  0.00           N
ATOM    362  C   LYS    48      38.362   8.716  37.354  1.00  0.00           C
ATOM    363  O   LYS    48      38.538   9.932  37.407  1.00  0.00           O
ATOM    364  N   ASN    49      38.718   7.876  38.355  1.00  0.00           N
ATOM    365  CA  ASN    49      39.415   8.364  39.511  1.00  0.00           C
ATOM    366  CB  ASN    49      38.471   8.660  40.690  1.00  0.00           C
ATOM    367  CG  ASN    49      39.218   9.482  41.730  1.00  0.00           C
ATOM    368  OD1 ASN    49      40.351   9.174  42.094  1.00  0.00           O
ATOM    369  ND2 ASN    49      38.566  10.569  42.221  1.00  0.00           N
ATOM    370  C   ASN    49      40.372   7.293  39.959  1.00  0.00           C
ATOM    371  O   ASN    49      39.967   6.266  40.499  1.00  0.00           O
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ATOM    372  N   ALA    50      41.685   7.534  39.784  1.00  0.00           N
ATOM    373  CA  ALA    50      42.707   6.588  40.143  1.00  0.00           C
ATOM    374  CB  ALA    50      44.118   7.067  39.762  1.00  0.00           C
ATOM    375  C   ALA    50      42.689   6.381  41.627  1.00  0.00           C
ATOM    376  O   ALA    50      42.949   5.284  42.120  1.00  0.00           O
ATOM    377  N   HIS    51      42.366   7.448  42.375  1.00  0.00           N
ATOM    378  CA  HIS    51      42.410   7.457  43.810  1.00  0.00           C
ATOM    379  ND1 HIS    51      42.645  10.693  42.826  1.00  0.00           N
ATOM    380  CG  HIS    51      42.868   9.938  43.955  1.00  0.00           C
ATOM    381  NE2 HIS    51      44.504  11.479  43.759  1.00  0.00           N
ATOM    382  CD2 HIS    51      44.007  10.431  44.514  1.00  0.00           C
ATOM    383  CE1 HIS    51      43.652  11.601  42.757  1.00  0.00           C
ATOM    384  CB  HIS    51      41.982   8.811  44.398  1.00  0.00           C
ATOM    385  C   HIS    51      41.486   6.411  44.362  1.00  0.00           C
ATOM    386  O   HIS    51      41.763   5.829  45.409  1.00  0.00           O
ATOM    387  N   LEU    52      40.359   6.158  43.677  1.00  0.00           N
ATOM    388  CA  LEU    52      39.360   5.225  44.125  1.00  0.00           C
ATOM    389  CB  LEU    52      38.165   5.154  43.159  1.00  0.00           C
ATOM    390  CG  LEU    52      37.419   6.491  42.987  1.00  0.00           C
ATOM    391  CD2 LEU    52      36.996   7.078  44.343  1.00  0.00           C
ATOM    392  CD1 LEU    52      36.242   6.346  42.008  1.00  0.00           C
ATOM    393  C   LEU    52      39.949   3.839  44.201  1.00  0.00           C
ATOM    394  O   LEU    52      39.560   3.038  45.050  1.00  0.00           O
ATOM    395  N   LYS    53      40.849   3.511  43.256  1.00  0.00           N
ATOM    396  CA  LYS    53      41.526   2.248  43.124  1.00  0.00           C
ATOM    397  CB  LYS    53      42.275   2.120  41.789  1.00  0.00           C
ATOM    398  CG  LYS    53      41.359   1.999  40.572  1.00  0.00           C
ATOM    399  CD  LYS    53      40.477   0.750  40.609  1.00  0.00           C
ATOM    400  CE  LYS    53      39.570   0.599  39.387  1.00  0.00           C
ATOM    401  NZ  LYS    53      38.827  -0.677  39.471  1.00  0.00           N
ATOM    402  C   LYS    53      42.553   2.041  44.199  1.00  0.00           C
ATOM    403  O   LYS    53      42.857   0.905  44.558  1.00  0.00           O
ATOM    404  N   GLN    54      43.106   3.135  44.752  1.00  0.00           N
ATOM    405  CA  GLN    54      44.265   3.076  45.601  1.00  0.00           C
ATOM    406  CB  GLN    54      44.586   4.442  46.232  1.00  0.00           C
ATOM    407  CG  GLN    54      45.654   4.381  47.326  1.00  0.00           C
ATOM    408  CD  GLN    54      46.983   4.008  46.688  1.00  0.00           C
ATOM    409  OE1 GLN    54      47.094   3.901  45.468  1.00  0.00           O
ATOM    410  NE2 GLN    54      48.027   3.808  47.537  1.00  0.00           N
ATOM    411  C   GLN    54      44.110   2.108  46.730  1.00  0.00           C
ATOM    412  O   GLN    54      45.037   1.345  47.005  1.00  0.00           O
ATOM    413  N   LEU    55      42.953   2.079  47.409  1.00  0.00           N
ATOM    414  CA  LEU    55      42.878   1.237  48.568  1.00  0.00           C
ATOM    415  CB  LEU    55      41.523   1.342  49.292  1.00  0.00           C
ATOM    416  CG  LEU    55      41.468   0.540  50.605  1.00  0.00           C
ATOM    417  CD2 LEU    55      40.039   0.491  51.171  1.00  0.00           C
ATOM    418  CD1 LEU    55      42.488   1.074  51.625  1.00  0.00           C
ATOM    419  C   LEU    55      43.098  -0.198  48.173  1.00  0.00           C
ATOM    420  O   LEU    55      43.906  -0.902  48.774  1.00  0.00           O
ATOM    421  N   GLU    56      42.388  -0.666  47.134  1.00  0.00           N
ATOM    422  CA  GLU    56      42.469  -2.018  46.649  1.00  0.00           C
ATOM    423  CB  GLU    56      41.304  -2.393  45.713  1.00  0.00           C
ATOM    424  CG  GLU    56      41.163  -1.499  44.479  1.00  0.00           C
ATOM    425  CD  GLU    56      40.199  -0.364  44.808  1.00  0.00           C
ATOM    426  OE1 GLU    56      40.149   0.060  45.992  1.00  0.00           O
ATOM    427  OE2 GLU    56      39.497   0.096  43.868  1.00  0.00           O
ATOM    428  C   GLU    56      43.748  -2.256  45.917  1.00  0.00           C
ATOM    429  O   GLU    56      44.257  -3.377  45.885  1.00  0.00           O
ATOM    430  N   GLY    57      44.295  -1.206  45.284  1.00  0.00           N
ATOM    431  CA  GLY    57      45.490  -1.368  44.515  1.00  0.00           C
ATOM    432  C   GLY    57      46.534  -1.890  45.439  1.00  0.00           C
ATOM    433  O   GLY    57      47.381  -2.686  45.037  1.00  0.00           O
ATOM    434  N   ALA    58      46.525  -1.427  46.700  1.00  0.00           N
ATOM    435  CA  ALA    58      47.472  -1.943  47.638  1.00  0.00           C
ATOM    436  CB  ALA    58      47.457  -1.229  49.001  1.00  0.00           C
ATOM    437  C   ALA    58      47.086  -3.365  47.861  1.00  0.00           C
ATOM    438  O   ALA    58      45.916  -3.726  47.760  1.00  0.00           O
ATOM    439  N   GLU    59      48.060  -4.223  48.195  1.00  0.00           N
ATOM    440  CA  GLU    59      47.737  -5.611  48.312  1.00  0.00           C
ATOM    441  CB  GLU    59      46.615  -5.868  49.332  1.00  0.00           C
ATOM    442  CG  GLU    59      47.004  -5.476  50.758  1.00  0.00           C
ATOM    443  CD  GLU    59      45.756  -5.568  51.624  1.00  0.00           C
ATOM    444  OE1 GLU    59      44.732  -6.108  51.127  1.00  0.00           O
ATOM    445  OE2 GLU    59      45.808  -5.092  52.790  1.00  0.00           O
ATOM    446  C   GLU    59      47.249  -5.985  46.965  1.00  0.00           C
ATOM    447  O   GLU    59      46.359  -6.821  46.840  1.00  0.00           O
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ATOM    448  N   GLU    60      47.915  -5.391  45.949  1.00  0.00           N
ATOM    449  CA  GLU    60      47.600  -5.363  44.547  1.00  0.00           C
ATOM    450  CB  GLU    60      48.797  -4.937  43.683  1.00  0.00           C
ATOM    451  CG  GLU    60      48.487  -4.900  42.186  1.00  0.00           C
ATOM    452  CD  GLU    60      49.705  -4.329  41.478  1.00  0.00           C
ATOM    453  OE1 GLU    60      49.960  -3.106  41.647  1.00  0.00           O
ATOM    454  OE2 GLU    60      50.396  -5.100  40.760  1.00  0.00           O
ATOM    455  C   GLU    60      47.118  -6.657  44.012  1.00  0.00           C
ATOM    456  O   GLU    60      47.854  -7.379  43.341  1.00  0.00           O
ATOM    457  N   ARG    61      45.852  -6.994  44.310  1.00  0.00           N
ATOM    458  CA  ARG    61      45.306  -8.145  43.684  1.00  0.00           C
ATOM    459  CB  ARG    61      44.098  -8.746  44.422  1.00  0.00           C
ATOM    460  CG  ARG    61      44.544  -9.610  45.608  1.00  0.00           C
ATOM    461  CD  ARG    61      43.406 -10.305  46.359  1.00  0.00           C
ATOM    462  NE  ARG    61      42.813  -9.320  47.303  1.00  0.00           N
ATOM    463  CZ  ARG    61      43.270  -9.258  48.588  1.00  0.00           C
ATOM    464  NH1 ARG    61      44.265 -10.098  48.999  1.00  0.00           N
ATOM    465  NH2 ARG    61      42.731  -8.359  49.462  1.00  0.00           N
ATOM    466  C   ARG    61      44.937  -7.744  42.297  1.00  0.00           C
ATOM    467  O   ARG    61      45.116  -8.495  41.340  1.00  0.00           O
ATOM    468  N   LEU    62      44.435  -6.501  42.170  1.00  0.00           N
ATOM    469  CA  LEU    62      43.920  -5.987  40.935  1.00  0.00           C
ATOM    470  CB  LEU    62      42.906  -4.851  41.147  1.00  0.00           C
ATOM    471  CG  LEU    62      42.415  -4.200  39.842  1.00  0.00           C
ATOM    472  CD2 LEU    62      41.591  -2.937  40.132  1.00  0.00           C
ATOM    473  CD1 LEU    62      41.672  -5.207  38.950  1.00  0.00           C
ATOM    474  C   LEU    62      45.001  -5.448  40.059  1.00  0.00           C
ATOM    475  O   LEU    62      46.009  -4.939  40.548  1.00  0.00           O
ATOM    476  N   THR    63      44.772  -5.547  38.725  1.00  0.00           N
ATOM    477  CA  THR    63      45.658  -5.065  37.700  1.00  0.00           C
ATOM    478  CB  THR    63      46.073  -6.117  36.716  1.00  0.00           C
ATOM    479  OG1 THR    63      47.106  -5.620  35.876  1.00  0.00           O
ATOM    480  CG2 THR    63      44.849  -6.519  35.877  1.00  0.00           C
ATOM    481  C   THR    63      44.917  -4.008  36.936  1.00  0.00           C
ATOM    482  O   THR    63      43.687  -4.033  36.857  1.00  0.00           O
ATOM    483  N   LEU    64      45.652  -3.034  36.360  1.00  0.00           N
ATOM    484  CA  LEU    64      45.002  -1.942  35.690  1.00  0.00           C
ATOM    485  CB  LEU    64      45.242  -0.609  36.414  1.00  0.00           C
ATOM    486  CG  LEU    64      44.589   0.615  35.756  1.00  0.00           C
ATOM    487  CD2 LEU    64      45.116   1.909  36.395  1.00  0.00           C
ATOM    488  CD1 LEU    64      43.053   0.513  35.776  1.00  0.00           C
ATOM    489  C   LEU    64      45.547  -1.793  34.304  1.00  0.00           C
ATOM    490  O   LEU    64      46.751  -1.918  34.081  1.00  0.00           O
ATOM    491  N   VAL    65      44.651  -1.532  33.327  1.00  0.00           N
ATOM    492  CA  VAL    65      45.080  -1.290  31.980  1.00  0.00           C
ATOM    493  CB  VAL    65      44.799  -2.434  31.052  1.00  0.00           C
ATOM    494  CG1 VAL    65      45.213  -2.026  29.630  1.00  0.00           C
ATOM    495  CG2 VAL    65      45.526  -3.683  31.580  1.00  0.00           C
ATOM    496  C   VAL    65      44.299  -0.115  31.474  1.00  0.00           C
ATOM    497  O   VAL    65      43.081  -0.057  31.634  1.00  0.00           O
ATOM    498  N   LYS    66      44.981   0.864  30.846  1.00  0.00           N
ATOM    499  CA  LYS    66      44.252   1.977  30.312  1.00  0.00           C
ATOM    500  CB  LYS    66      45.025   3.307  30.289  1.00  0.00           C
ATOM    501  CG  LYS    66      44.196   4.456  29.705  1.00  0.00           C
ATOM    502  CD  LYS    66      44.846   5.838  29.812  1.00  0.00           C
ATOM    503  CE  LYS    66      44.061   6.925  29.071  1.00  0.00           C
ATOM    504  NZ  LYS    66      44.739   8.235  29.206  1.00  0.00           N
ATOM    505  C   LYS    66      43.961   1.637  28.890  1.00  0.00           C
ATOM    506  O   LYS    66      44.874   1.519  28.074  1.00  0.00           O
ATOM    507  N   ALA    67      42.671   1.461  28.555  1.00  0.00           N
ATOM    508  CA  ALA    67      42.346   1.114  27.205  1.00  0.00           C
ATOM    509  CB  ALA    67      42.385  -0.401  26.938  1.00  0.00           C
ATOM    510  C   ALA    67      40.947   1.567  26.950  1.00  0.00           C
ATOM    511  O   ALA    67      40.168   1.773  27.880  1.00  0.00           O
ATOM    512  N   ASP    68      40.604   1.758  25.664  1.00  0.00           N
ATOM    513  CA  ASP    68      39.275   2.165  25.320  1.00  0.00           C
ATOM    514  CB  ASP    68      39.243   3.240  24.213  1.00  0.00           C
ATOM    515  CG  ASP    68      37.865   3.895  24.158  1.00  0.00           C
ATOM    516  OD1 ASP    68      36.839   3.172  24.264  1.00  0.00           O
ATOM    517  OD2 ASP    68      37.823   5.146  24.015  1.00  0.00           O
ATOM    518  C   ASP    68      38.583   0.939  24.808  1.00  0.00           C
ATOM    519  O   ASP    68      39.177   0.131  24.096  1.00  0.00           O
ATOM    520  N   LEU    69      37.298   0.762  25.172  1.00  0.00           N
ATOM    521  CA  LEU    69      36.555  -0.383  24.726  1.00  0.00           C
ATOM    522  CB  LEU    69      35.116  -0.517  25.252  1.00  0.00           C
ATOM    523  CG  LEU    69      34.974  -0.972  26.713  1.00  0.00           C
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ATOM    524  CD2 LEU    69      36.013  -2.044  27.083  1.00  0.00           C
ATOM    525  CD1 LEU    69      33.529  -1.425  26.977  1.00  0.00           C
ATOM    526  C   LEU    69      36.432  -0.335  23.245  1.00  0.00           C
ATOM    527  O   LEU    69      36.302  -1.372  22.599  1.00  0.00           O
ATOM    528  N   MET    70      36.428   0.875  22.663  1.00  0.00           N
ATOM    529  CA  MET    70      36.247   0.987  21.248  1.00  0.00           C
ATOM    530  CB  MET    70      36.206   2.443  20.754  1.00  0.00           C
ATOM    531  CG  MET    70      34.939   3.188  21.188  1.00  0.00           C
ATOM    532  SD  MET    70      34.853   4.922  20.650  1.00  0.00           S
ATOM    533  CE  MET    70      36.139   5.483  21.803  1.00  0.00           C
ATOM    534  C   MET    70      37.366   0.280  20.547  1.00  0.00           C
ATOM    535  O   MET    70      37.145  -0.325  19.499  1.00  0.00           O
ATOM    536  N   ASP    71      38.597   0.337  21.091  1.00  0.00           N
ATOM    537  CA  ASP    71      39.702  -0.297  20.425  1.00  0.00           C
ATOM    538  CB  ASP    71      41.067   0.084  21.031  1.00  0.00           C
ATOM    539  CG  ASP    71      42.167  -0.340  20.066  1.00  0.00           C
ATOM    540  OD1 ASP    71      42.047  -1.444  19.471  1.00  0.00           O
ATOM    541  OD2 ASP    71      43.139   0.443  19.900  1.00  0.00           O
ATOM    542  C   ASP    71      39.538  -1.788  20.521  1.00  0.00           C
ATOM    543  O   ASP    71      39.835  -2.397  21.548  1.00  0.00           O
ATOM    544  N   TYR    72      39.073  -2.407  19.415  1.00  0.00           N
ATOM    545  CA  TYR    72      38.815  -3.817  19.326  1.00  0.00           C
ATOM    546  CB  TYR    72      38.158  -4.197  17.985  1.00  0.00           C
ATOM    547  CG  TYR    72      38.171  -5.680  17.850  1.00  0.00           C
ATOM    548  CD1 TYR    72      37.145  -6.441  18.359  1.00  0.00           C
ATOM    549  CD2 TYR    72      39.220  -6.309  17.220  1.00  0.00           C
ATOM    550  CE1 TYR    72      37.165  -7.810  18.232  1.00  0.00           C
ATOM    551  CE2 TYR    72      39.244  -7.676  17.089  1.00  0.00           C
ATOM    552  CZ  TYR    72      38.215  -8.428  17.598  1.00  0.00           C
ATOM    553  OH  TYR    72      38.235  -9.833  17.466  1.00  0.00           O
ATOM    554  C   TYR    72      40.082  -4.598  19.459  1.00  0.00           C
ATOM    555  O   TYR    72      40.137  -5.579  20.200  1.00  0.00           O
ATOM    556  N   ASN    73      41.144  -4.172  18.754  1.00  0.00           N
ATOM    557  CA  ASN    73      42.364  -4.922  18.758  1.00  0.00           C
ATOM    558  CB  ASN    73      43.441  -4.308  17.849  1.00  0.00           C
ATOM    559  CG  ASN    73      44.590  -5.300  17.743  1.00  0.00           C
ATOM    560  OD1 ASN    73      44.471  -4.117  18.059  1.00  0.00           O
ATOM    561  ND2 ASN    73      43.783  -6.316  17.336  1.00  0.00           N
ATOM    562  C   ASN    73      42.910  -4.967  20.148  1.00  0.00           C
ATOM    563  O   ASN    73      43.341  -6.018  20.617  1.00  0.00           O
ATOM    564  N   SER    74      42.890  -3.822  20.852  1.00  0.00           N
ATOM    565  CA  SER    74      43.445  -3.764  22.173  1.00  0.00           C
ATOM    566  CB  SER    74      43.393  -2.349  22.774  1.00  0.00           C
ATOM    567  OG  SER    74      44.158  -1.451  21.984  1.00  0.00           O
ATOM    568  C   SER    74      42.655  -4.662  23.069  1.00  0.00           C
ATOM    569  O   SER    74      43.213  -5.371  23.904  1.00  0.00           O
ATOM    570  N   LEU    75      41.321  -4.662  22.911  1.00  0.00           N
ATOM    571  CA  LEU    75      40.494  -5.456  23.764  1.00  0.00           C
ATOM    572  CB  LEU    75      38.995  -5.273  23.483  1.00  0.00           C
ATOM    573  CG  LEU    75      38.096  -6.074  24.441  1.00  0.00           C
ATOM    574  CD2 LEU    75      36.642  -6.110  23.951  1.00  0.00           C
ATOM    575  CD1 LEU    75      38.218  -5.549  25.880  1.00  0.00           C
ATOM    576  C   LEU    75      40.827  -6.891  23.526  1.00  0.00           C
ATOM    577  O   LEU    75      40.912  -7.686  24.461  1.00  0.00           O
ATOM    578  N   LEU    76      41.047  -7.258  22.253  1.00  0.00           N
ATOM    579  CA  LEU    76      41.312  -8.626  21.928  1.00  0.00           C
ATOM    580  CB  LEU    76      41.497  -8.835  20.409  1.00  0.00           C
ATOM    581  CG  LEU    76      41.707 -10.297  19.952  1.00  0.00           C
ATOM    582  CD2 LEU    76      40.525 -11.182  20.381  1.00  0.00           C
ATOM    583  CD1 LEU    76      43.069 -10.867  20.380  1.00  0.00           C
ATOM    584  C   LEU    76      42.572  -9.031  22.620  1.00  0.00           C
ATOM    585  O   LEU    76      42.651 -10.119  23.190  1.00  0.00           O
ATOM    586  N   ASN    77      43.596  -8.160  22.597  1.00  0.00           N
ATOM    587  CA  ASN    77      44.863  -8.508  23.172  1.00  0.00           C
ATOM    588  CB  ASN    77      45.946  -7.446  22.916  1.00  0.00           C
ATOM    589  CG  ASN    77      47.293  -8.038  23.308  1.00  0.00           C
ATOM    590  OD1 ASN    77      48.062  -8.491  22.459  1.00  0.00           O
ATOM    591  ND2 ASN    77      47.589  -8.040  24.635  1.00  0.00           N
ATOM    592  C   ASN    77      44.735  -8.690  24.652  1.00  0.00           C
ATOM    593  O   ASN    77      45.258  -9.653  25.210  1.00  0.00           O
ATOM    594  N   ALA    78      44.016  -7.777  25.332  1.00  0.00           N
ATOM    595  CA  ALA    78      43.915  -7.845  26.762  1.00  0.00           C
ATOM    596  CB  ALA    78      43.094  -6.686  27.352  1.00  0.00           C
ATOM    597  C   ALA    78      43.234  -9.117  27.145  1.00  0.00           C
ATOM    598  O   ALA    78      43.658  -9.806  28.072  1.00  0.00           O
ATOM    599  N   ILE    79      42.163  -9.473  26.417  1.00  0.00           N
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ATOM    600  CA  ILE    79      41.394 -10.633  26.753  1.00  0.00           C
ATOM    601  CB  ILE    79      40.178 -10.793  25.887  1.00  0.00           C
ATOM    602  CG2 ILE    79      39.497 -12.118  26.269  1.00  0.00           C
ATOM    603  CG1 ILE    79      39.254  -9.572  26.028  1.00  0.00           C
ATOM    604  CD1 ILE    79      38.129  -9.536  24.995  1.00  0.00           C
ATOM    605  C   ILE    79      42.227 -11.862  26.596  1.00  0.00           C
ATOM    606  O   ILE    79      42.203 -12.747  27.450  1.00  0.00           O
ATOM    607  N   ASN    80      42.988 -11.964  25.494  1.00  0.00           N
ATOM    608  CA  ASN    80      43.736 -13.169  25.295  1.00  0.00           C
ATOM    609  CB  ASN    80      44.458 -13.220  23.937  1.00  0.00           C
ATOM    610  CG  ASN    80      44.819 -14.673  23.652  1.00  0.00           C
ATOM    611  OD1 ASN    80      43.940 -15.514  23.468  1.00  0.00           O
ATOM    612  ND2 ASN    80      46.144 -14.979  23.605  1.00  0.00           N
ATOM    613  C   ASN    80      44.765 -13.294  26.374  1.00  0.00           C
ATOM    614  O   ASN    80      44.914 -14.354  26.979  1.00  0.00           O
ATOM    615  N   GLY    81      45.492 -12.196  26.661  1.00  0.00           N
ATOM    616  CA  GLY    81      46.555 -12.261  27.623  1.00  0.00           C
ATOM    617  C   GLY    81      46.023 -12.577  28.989  1.00  0.00           C
ATOM    618  O   GLY    81      46.563 -13.433  29.688  1.00  0.00           O
ATOM    619  N   CYS    82      44.959 -11.868  29.406  1.00  0.00           N
ATOM    620  CA  CYS    82      44.361 -12.012  30.705  1.00  0.00           C
ATOM    621  CB  CYS    82      43.355 -10.894  31.028  1.00  0.00           C
ATOM    622  SG  CYS    82      41.871 -10.975  29.984  1.00  0.00           S
ATOM    623  C   CYS    82      43.631 -13.315  30.819  1.00  0.00           C
ATOM    624  O   CYS    82      43.569 -13.897  31.900  1.00  0.00           O
ATOM    625  N   GLN    83      43.051 -13.806  29.705  1.00  0.00           N
ATOM    626  CA  GLN    83      42.278 -15.017  29.745  1.00  0.00           C
ATOM    627  CB  GLN    83      43.102 -16.237  30.178  1.00  0.00           C
ATOM    628  CG  GLN    83      44.243 -16.567  29.218  1.00  0.00           C
ATOM    629  CD  GLN    83      44.970 -17.784  29.766  1.00  0.00           C
ATOM    630  OE1 GLN    83      46.095 -18.076  29.363  1.00  0.00           O
ATOM    631  NE2 GLN    83      44.319 -18.509  30.714  1.00  0.00           N
ATOM    632  C   GLN    83      41.169 -14.848  30.734  1.00  0.00           C
ATOM    633  O   GLN    83      40.928 -15.722  31.563  1.00  0.00           O
ATOM    634  N   GLY    84      40.456 -13.707  30.665  1.00  0.00           N
ATOM    635  CA  GLY    84      39.389 -13.458  31.594  1.00  0.00           C
ATOM    636  C   GLY    84      38.248 -14.387  31.316  1.00  0.00           C
ATOM    637  O   GLY    84      37.920 -14.675  30.164  1.00  0.00           O
ATOM    638  N   VAL    85      37.656 -14.925  32.403  1.00  0.00           N
ATOM    639  CA  VAL    85      36.504 -15.779  32.343  1.00  0.00           C
ATOM    640  CB  VAL    85      36.296 -16.557  33.610  1.00  0.00           C
ATOM    641  CG1 VAL    85      36.052 -15.573  34.766  1.00  0.00           C
ATOM    642  CG2 VAL    85      35.141 -17.544  33.385  1.00  0.00           C
ATOM    643  C   VAL    85      35.263 -14.974  32.084  1.00  0.00           C
ATOM    644  O   VAL    85      34.403 -15.368  31.295  1.00  0.00           O
ATOM    645  N   PHE    86      35.149 -13.806  32.749  1.00  0.00           N
ATOM    646  CA  PHE    86      33.939 -13.034  32.689  1.00  0.00           C
ATOM    647  CB  PHE    86      33.125 -13.192  33.989  1.00  0.00           C
ATOM    648  CG  PHE    86      31.980 -12.246  33.974  1.00  0.00           C
ATOM    649  CD1 PHE    86      30.803 -12.577  33.350  1.00  0.00           C
ATOM    650  CD2 PHE    86      32.101 -11.012  34.571  1.00  0.00           C
ATOM    651  CE1 PHE    86      29.758 -11.688  33.340  1.00  0.00           C
ATOM    652  CE2 PHE    86      31.056 -10.120  34.564  1.00  0.00           C
ATOM    653  CZ  PHE    86      29.880 -10.460  33.943  1.00  0.00           C
ATOM    654  C   PHE    86      34.275 -11.582  32.505  1.00  0.00           C
ATOM    655  O   PHE    86      35.379 -11.142  32.814  1.00  0.00           O
ATOM    656  N   HIS    87      33.311 -10.801  31.968  1.00  0.00           N
ATOM    657  CA  HIS    87      33.500  -9.400  31.734  1.00  0.00           C
ATOM    658  ND1 HIS    87      34.921  -7.072  29.432  1.00  0.00           N
ATOM    659  CG  HIS    87      33.750  -7.622  29.905  1.00  0.00           C
ATOM    660  NE2 HIS    87      33.447  -5.414  29.556  1.00  0.00           N
ATOM    661  CD2 HIS    87      32.862  -6.594  29.977  1.00  0.00           C
ATOM    662  CE1 HIS    87      34.685  -5.750  29.240  1.00  0.00           C
ATOM    663  CB  HIS    87      33.554  -9.074  30.232  1.00  0.00           C
ATOM    664  C   HIS    87      32.332  -8.653  32.291  1.00  0.00           C
ATOM    665  O   HIS    87      31.178  -8.989  32.026  1.00  0.00           O
ATOM    666  N   VAL    88      32.614  -7.612  33.099  1.00  0.00           N
ATOM    667  CA  VAL    88      31.568  -6.769  33.591  1.00  0.00           C
ATOM    668  CB  VAL    88      31.642  -6.539  35.077  1.00  0.00           C
ATOM    669  CG1 VAL    88      33.012  -5.943  35.429  1.00  0.00           C
ATOM    670  CG2 VAL    88      30.454  -5.661  35.500  1.00  0.00           C
ATOM    671  C   VAL    88      31.753  -5.467  32.869  1.00  0.00           C
ATOM    672  O   VAL    88      32.837  -4.884  32.908  1.00  0.00           O
ATOM    673  N   ALA    89      30.710  -4.971  32.171  1.00  0.00           N
ATOM    674  CA  ALA    89      30.968  -3.790  31.399  1.00  0.00           C
ATOM    675  CB  ALA    89      30.571  -3.932  29.918  1.00  0.00           C
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ATOM    676  C   ALA    89      30.237  -2.604  31.928  1.00  0.00           C
ATOM    677  O   ALA    89      29.074  -2.370  31.603  1.00  0.00           O
ATOM    678  N   SER    90      30.927  -1.834  32.787  1.00  0.00           N
ATOM    679  CA  SER    90      30.452  -0.569  33.262  1.00  0.00           C
ATOM    680  CB  SER    90      30.984  -0.238  34.666  1.00  0.00           C
ATOM    681  OG  SER    90      30.489   1.023  35.091  1.00  0.00           O
ATOM    682  C   SER    90      30.830   0.603  32.369  1.00  0.00           C
ATOM    683  O   SER    90      30.162   1.630  32.483  1.00  0.00           O
ATOM    684  N   PRO    91      31.843   0.586  31.518  1.00  0.00           N
ATOM    685  CA  PRO    91      32.240   1.817  30.894  1.00  0.00           C
ATOM    686  CD  PRO    91      31.993  -0.460  30.525  1.00  0.00           C
ATOM    687  CB  PRO    91      33.460   1.445  30.080  1.00  0.00           C
ATOM    688  CG  PRO    91      33.106   0.033  29.580  1.00  0.00           C
ATOM    689  C   PRO    91      31.179   2.363  29.994  1.00  0.00           C
ATOM    690  O   PRO    91      30.685   1.626  29.146  1.00  0.00           O
ATOM    691  N   VAL    92      30.869   3.668  30.123  1.00  0.00           N
ATOM    692  CA  VAL    92      29.904   4.309  29.281  1.00  0.00           C
ATOM    693  CB  VAL    92      28.460   4.030  29.683  1.00  0.00           C
ATOM    694  CG1 VAL    92      27.503   4.766  28.728  1.00  0.00           C
ATOM    695  CG2 VAL    92      28.187   2.519  29.763  1.00  0.00           C
ATOM    696  C   VAL    92      30.094   5.777  29.530  1.00  0.00           C
ATOM    697  O   VAL    92      30.711   6.168  30.519  1.00  0.00           O
ATOM    698  N   THR    93      29.599   6.629  28.612  1.00  0.00           N
ATOM    699  CA  THR    93      29.550   8.033  28.886  1.00  0.00           C
ATOM    700  CB  THR    93      29.585   8.890  27.656  1.00  0.00           C
ATOM    701  OG1 THR    93      29.655  10.263  28.013  1.00  0.00           O
ATOM    702  CG2 THR    93      28.317   8.616  26.829  1.00  0.00           C
ATOM    703  C   THR    93      28.201   8.182  29.504  1.00  0.00           C
ATOM    704  O   THR    93      27.269   7.487  29.101  1.00  0.00           O
ATOM    705  N   ASP    94      28.027   9.050  30.518  1.00  0.00           N
ATOM    706  CA  ASP    94      26.704   9.006  31.063  1.00  0.00           C
ATOM    707  CB  ASP    94      26.610   8.160  32.344  1.00  0.00           C
ATOM    708  CG  ASP    94      27.453   8.833  33.422  1.00  0.00           C
ATOM    709  OD1 ASP    94      28.397   9.582  33.058  1.00  0.00           O
ATOM    710  OD2 ASP    94      27.164   8.604  34.628  1.00  0.00           O
ATOM    711  C   ASP    94      26.199  10.357  31.439  1.00  0.00           C
ATOM    712  O   ASP    94      25.399  10.453  32.366  1.00  0.00           O
ATOM    713  N   ASP    95      26.606  11.428  30.737  1.00  0.00           N
ATOM    714  CA  ASP    95      26.073  12.720  31.071  1.00  0.00           C
ATOM    715  CB  ASP    95      27.139  13.834  31.018  1.00  0.00           C
ATOM    716  CG  ASP    95      27.938  13.734  29.725  1.00  0.00           C
ATOM    717  OD1 ASP    95      27.535  12.968  28.810  1.00  0.00           O
ATOM    718  OD2 ASP    95      28.999  14.413  29.656  1.00  0.00           O
ATOM    719  C   ASP    95      24.893  13.013  30.188  1.00  0.00           C
ATOM    720  O   ASP    95      25.015  13.130  28.970  1.00  0.00           O
ATOM    721  N   PRO    96      23.725  13.090  30.782  1.00  0.00           N
ATOM    722  CA  PRO    96      22.514  13.296  30.032  1.00  0.00           C
ATOM    723  CD  PRO    96      23.473  12.482  32.077  1.00  0.00           C
ATOM    724  CB  PRO    96      21.368  13.088  31.019  1.00  0.00           C
ATOM    725  CG  PRO    96      21.971  12.157  32.088  1.00  0.00           C
ATOM    726  C   PRO    96      22.435  14.598  29.302  1.00  0.00           C
ATOM    727  O   PRO    96      21.994  14.604  28.153  1.00  0.00           O
ATOM    728  N   GLU    97      22.847  15.708  29.941  1.00  0.00           N
ATOM    729  CA  GLU    97      22.764  16.989  29.305  1.00  0.00           C
ATOM    730  CB  GLU    97      23.193  18.134  30.234  1.00  0.00           C
ATOM    731  CG  GLU    97      24.632  17.990  30.730  1.00  0.00           C
ATOM    732  CD  GLU    97      24.975  19.228  31.542  1.00  0.00           C
ATOM    733  OE1 GLU    97      24.036  19.823  32.134  1.00  0.00           O
ATOM    734  OE2 GLU    97      26.179  19.600  31.581  1.00  0.00           O
ATOM    735  C   GLU    97      23.696  17.003  28.143  1.00  0.00           C
ATOM    736  O   GLU    97      23.345  17.447  27.051  1.00  0.00           O
ATOM    737  N   GLU    98      24.915  16.482  28.360  1.00  0.00           N
ATOM    738  CA  GLU    98      25.923  16.462  27.345  1.00  0.00           C
ATOM    739  CB  GLU    98      27.259  15.903  27.845  1.00  0.00           C
ATOM    740  CG  GLU    98      27.888  16.801  28.907  1.00  0.00           C
ATOM    741  CD  GLU    98      28.254  18.115  28.240  1.00  0.00           C
ATOM    742  OE1 GLU    98      28.291  18.146  26.981  1.00  0.00           O
ATOM    743  OE2 GLU    98      28.501  19.105  28.979  1.00  0.00           O
ATOM    744  C   GLU    98      25.422  15.582  26.255  1.00  0.00           C
ATOM    745  O   GLU    98      25.648  15.833  25.074  1.00  0.00           O
ATOM    746  N   MET    99      24.682  14.531  26.630  1.00  0.00           N
ATOM    747  CA  MET    99      24.156  13.631  25.653  1.00  0.00           C
ATOM    748  CB  MET    99      23.271  12.552  26.297  1.00  0.00           C
ATOM    749  CG  MET    99      22.092  12.153  25.410  1.00  0.00           C
ATOM    750  SD  MET    99      20.636  13.217  25.683  1.00  0.00           S
ATOM    751  CE  MET    99      20.219  13.416  23.926  1.00  0.00           C
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ATOM    752  C   MET    99      23.312  14.402  24.705  1.00  0.00           C
ATOM    753  O   MET    99      23.325  14.139  23.503  1.00  0.00           O
ATOM    754  N   VAL   100      22.546  15.378  25.220  1.00  0.00           N
ATOM    755  CA  VAL   100      21.663  16.070  24.342  1.00  0.00           C
ATOM    756  CB  VAL   100      20.844  17.111  25.053  1.00  0.00           C
ATOM    757  CG1 VAL   100      20.050  17.921  24.012  1.00  0.00           C
ATOM    758  CG2 VAL   100      19.967  16.403  26.100  1.00  0.00           C
ATOM    759  C   VAL   100      22.464  16.759  23.293  1.00  0.00           C
ATOM    760  O   VAL   100      22.201  16.593  22.103  1.00  0.00           O
ATOM    761  N   GLU   101      23.461  17.572  23.687  1.00  0.00           N
ATOM    762  CA  GLU   101      24.115  18.233  22.605  1.00  0.00           C
ATOM    763  CB  GLU   101      24.882  19.503  23.015  1.00  0.00           C
ATOM    764  CG  GLU   101      25.276  20.342  21.802  1.00  0.00           C
ATOM    765  CD  GLU   101      23.986  20.809  21.138  1.00  0.00           C
ATOM    766  OE1 GLU   101      22.934  20.819  21.831  1.00  0.00           O
ATOM    767  OE2 GLU   101      24.035  21.157  19.927  1.00  0.00           O
ATOM    768  C   GLU   101      24.980  17.290  21.805  1.00  0.00           C
ATOM    769  O   GLU   101      24.716  17.158  20.611  1.00  0.00           O
ATOM    770  N   PRO   102      25.998  16.631  22.336  1.00  0.00           N
ATOM    771  CA  PRO   102      26.661  15.685  21.470  1.00  0.00           C
ATOM    772  CD  PRO   102      26.985  17.356  23.128  1.00  0.00           C
ATOM    773  CB  PRO   102      28.157  15.735  21.790  1.00  0.00           C
ATOM    774  CG  PRO   102      28.234  16.467  23.137  1.00  0.00           C
ATOM    775  C   PRO   102      26.100  14.297  21.506  1.00  0.00           C
ATOM    776  O   PRO   102      26.418  13.554  22.431  1.00  0.00           O
ATOM    777  N   ALA   103      25.335  13.896  20.480  1.00  0.00           N
ATOM    778  CA  ALA   103      24.817  12.565  20.393  1.00  0.00           C
ATOM    779  CB  ALA   103      23.779  12.408  19.272  1.00  0.00           C
ATOM    780  C   ALA   103      25.938  11.617  20.094  1.00  0.00           C
ATOM    781  O   ALA   103      25.974  10.502  20.608  1.00  0.00           O
ATOM    782  N   VAL   104      26.882  12.062  19.240  1.00  0.00           N
ATOM    783  CA  VAL   104      27.926  11.243  18.686  1.00  0.00           C
ATOM    784  CB  VAL   104      28.825  12.007  17.756  1.00  0.00           C
ATOM    785  CG1 VAL   104      27.982  12.490  16.562  1.00  0.00           C
ATOM    786  CG2 VAL   104      29.505  13.142  18.540  1.00  0.00           C
ATOM    787  C   VAL   104      28.792  10.614  19.733  1.00  0.00           C
ATOM    788  O   VAL   104      29.063   9.417  19.662  1.00  0.00           O
ATOM    789  N   ASN   105      29.252  11.379  20.737  1.00  0.00           N
ATOM    790  CA  ASN   105      30.150  10.798  21.698  1.00  0.00           C
ATOM    791  CB  ASN   105      30.617  11.810  22.759  1.00  0.00           C
ATOM    792  CG  ASN   105      31.692  11.146  23.607  1.00  0.00           C
ATOM    793  OD1 ASN   105      32.606  10.513  23.080  1.00  0.00           O
ATOM    794  ND2 ASN   105      31.581  11.285  24.955  1.00  0.00           N
ATOM    795  C   ASN   105      29.446   9.686  22.404  1.00  0.00           C
ATOM    796  O   ASN   105      30.020   8.621  22.635  1.00  0.00           O
ATOM    797  N   GLY   106      28.169   9.911  22.762  1.00  0.00           N
ATOM    798  CA  GLY   106      27.424   8.925  23.483  1.00  0.00           C
ATOM    799  C   GLY   106      27.260   7.698  22.645  1.00  0.00           C
ATOM    800  O   GLY   106      27.388   6.580  23.139  1.00  0.00           O
ATOM    801  N   THR   107      26.959   7.874  21.345  1.00  0.00           N
ATOM    802  CA  THR   107      26.744   6.746  20.484  1.00  0.00           C
ATOM    803  CB  THR   107      26.415   7.140  19.070  1.00  0.00           C
ATOM    804  OG1 THR   107      25.244   7.939  19.028  1.00  0.00           O
ATOM    805  CG2 THR   107      26.210   5.863  18.236  1.00  0.00           C
ATOM    806  C   THR   107      28.009   5.961  20.394  1.00  0.00           C
ATOM    807  O   THR   107      28.000   4.735  20.495  1.00  0.00           O
ATOM    808  N   LYS   108      29.140   6.662  20.201  1.00  0.00           N
ATOM    809  CA  LYS   108      30.387   5.991  19.998  1.00  0.00           C
ATOM    810  CB  LYS   108      31.563   6.972  19.852  1.00  0.00           C
ATOM    811  CG  LYS   108      31.477   7.933  18.662  1.00  0.00           C
ATOM    812  CD  LYS   108      31.542   7.258  17.291  1.00  0.00           C
ATOM    813  CE  LYS   108      31.494   8.258  16.133  1.00  0.00           C
ATOM    814  NZ  LYS   108      31.731   7.568  14.847  1.00  0.00           N
ATOM    815  C   LYS   108      30.711   5.157  21.195  1.00  0.00           C
ATOM    816  O   LYS   108      30.955   3.958  21.077  1.00  0.00           O
ATOM    817  N   ASN   109      30.724   5.779  22.387  1.00  0.00           N
ATOM    818  CA  ASN   109      31.108   5.054  23.560  1.00  0.00           C
ATOM    819  CB  ASN   109      31.264   5.951  24.802  1.00  0.00           C
ATOM    820  CG  ASN   109      32.505   6.820  24.656  1.00  0.00           C
ATOM    821  OD1 ASN   109      32.918   7.462  25.620  1.00  0.00           O
ATOM    822  ND2 ASN   109      33.119   6.844  23.442  1.00  0.00           N
ATOM    823  C   ASN   109      30.085   4.022  23.917  1.00  0.00           C
ATOM    824  O   ASN   109      30.415   2.873  24.185  1.00  0.00           O
ATOM    825  N   VAL   110      28.804   4.404  23.984  1.00  0.00           N
ATOM    826  CA  VAL   110      27.845   3.438  24.429  1.00  0.00           C
ATOM    827  CB  VAL   110      26.512   4.059  24.718  1.00  0.00           C
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ATOM    828  CG1 VAL   110      25.534   2.952  25.151  1.00  0.00           C
ATOM    829  CG2 VAL   110      26.712   5.167  25.765  1.00  0.00           C
ATOM    830  C   VAL   110      27.604   2.353  23.426  1.00  0.00           C
ATOM    831  O   VAL   110      27.777   1.172  23.722  1.00  0.00           O
ATOM    832  N   LEU   111      27.158   2.738  22.214  1.00  0.00           N
ATOM    833  CA  LEU   111      26.799   1.780  21.207  1.00  0.00           C
ATOM    834  CB  LEU   111      26.071   2.438  20.023  1.00  0.00           C
ATOM    835  CG  LEU   111      25.784   1.471  18.860  1.00  0.00           C
ATOM    836  CD2 LEU   111      25.278   2.231  17.623  1.00  0.00           C
ATOM    837  CD1 LEU   111      24.851   0.329  19.289  1.00  0.00           C
ATOM    838  C   LEU   111      27.978   1.070  20.631  1.00  0.00           C
ATOM    839  O   LEU   111      28.061  -0.157  20.668  1.00  0.00           O
ATOM    840  N   ASP   112      28.936   1.844  20.093  1.00  0.00           N
ATOM    841  CA  ASP   112      30.042   1.252  19.404  1.00  0.00           C
ATOM    842  CB  ASP   112      30.954   2.296  18.732  1.00  0.00           C
ATOM    843  CG  ASP   112      31.950   1.557  17.849  1.00  0.00           C
ATOM    844  OD1 ASP   112      31.888   0.300  17.809  1.00  0.00           O
ATOM    845  OD2 ASP   112      32.789   2.239  17.202  1.00  0.00           O
ATOM    846  C   ASP   112      30.878   0.480  20.363  1.00  0.00           C
ATOM    847  O   ASP   112      31.279  -0.650  20.084  1.00  0.00           O
ATOM    848  N   ALA   113      31.159   1.066  21.538  1.00  0.00           N
ATOM    849  CA  ALA   113      32.037   0.374  22.428  1.00  0.00           C
ATOM    850  CB  ALA   113      32.454   1.148  23.686  1.00  0.00           C
ATOM    851  C   ALA   113      31.422  -0.913  22.863  1.00  0.00           C
ATOM    852  O   ALA   113      32.113  -1.915  23.029  1.00  0.00           O
ATOM    853  N   CYS   114      30.103  -0.934  23.092  1.00  0.00           N
ATOM    854  CA  CYS   114      29.540  -2.168  23.543  1.00  0.00           C
ATOM    855  CB  CYS   114      28.034  -2.062  23.830  1.00  0.00           C
ATOM    856  SG  CYS   114      27.336  -3.637  24.401  1.00  0.00           S
ATOM    857  C   CYS   114      29.738  -3.212  22.489  1.00  0.00           C
ATOM    858  O   CYS   114      30.120  -4.344  22.784  1.00  0.00           O
ATOM    859  N   ALA   115      29.495  -2.850  21.216  1.00  0.00           N
ATOM    860  CA  ALA   115      29.596  -3.808  20.152  1.00  0.00           C
ATOM    861  CB  ALA   115      29.231  -3.213  18.783  1.00  0.00           C
ATOM    862  C   ALA   115      31.001  -4.313  20.050  1.00  0.00           C
ATOM    863  O   ALA   115      31.226  -5.515  19.911  1.00  0.00           O
ATOM    864  N   VAL   116      31.988  -3.403  20.127  1.00  0.00           N
ATOM    865  CA  VAL   116      33.360  -3.788  19.973  1.00  0.00           C
ATOM    866  CB  VAL   116      34.306  -2.620  19.915  1.00  0.00           C
ATOM    867  CG1 VAL   116      34.036  -1.687  21.099  1.00  0.00           C
ATOM    868  CG2 VAL   116      35.744  -3.161  19.867  1.00  0.00           C
ATOM    869  C   VAL   116      33.759  -4.713  21.077  1.00  0.00           C
ATOM    870  O   VAL   116      34.504  -5.665  20.842  1.00  0.00           O
ATOM    871  N   ALA   117      33.262  -4.476  22.306  1.00  0.00           N
ATOM    872  CA  ALA   117      33.626  -5.333  23.397  1.00  0.00           C
ATOM    873  CB  ALA   117      32.918  -4.966  24.712  1.00  0.00           C
ATOM    874  C   ALA   117      33.191  -6.705  23.008  1.00  0.00           C
ATOM    875  O   ALA   117      33.930  -7.675  23.168  1.00  0.00           O
ATOM    876  N   GLY   118      31.979  -6.810  22.442  1.00  0.00           N
ATOM    877  CA  GLY   118      31.567  -8.067  21.904  1.00  0.00           C
ATOM    878  C   GLY   118      31.270  -9.063  22.959  1.00  0.00           C
ATOM    879  O   GLY   118      30.432  -8.830  23.824  1.00  0.00           O
ATOM    880  N   VAL   119      31.941 -10.230  22.909  1.00  0.00           N
ATOM    881  CA  VAL   119      31.411 -11.261  23.755  1.00  0.00           C
ATOM    882  CB  VAL   119      30.694 -12.328  22.977  1.00  0.00           C
ATOM    883  CG1 VAL   119      29.516 -11.687  22.221  1.00  0.00           C
ATOM    884  CG2 VAL   119      31.711 -13.038  22.068  1.00  0.00           C
ATOM    885  C   VAL   119      32.389 -11.987  24.641  1.00  0.00           C
ATOM    886  O   VAL   119      33.606 -11.832  24.536  1.00  0.00           O
ATOM    887  N   ARG   120      31.786 -12.788  25.573  1.00  0.00           N
ATOM    888  CA  ARG   120      32.341 -13.666  26.575  1.00  0.00           C
ATOM    889  CB  ARG   120      33.503 -13.025  27.359  1.00  0.00           C
ATOM    890  CG  ARG   120      34.252 -13.986  28.285  1.00  0.00           C
ATOM    891  CD  ARG   120      35.286 -14.860  27.568  1.00  0.00           C
ATOM    892  NE  ARG   120      34.568 -15.721  26.586  1.00  0.00           N
ATOM    893  CZ  ARG   120      35.247 -16.704  25.924  1.00  0.00           C
ATOM    894  NH1 ARG   120      36.574 -16.906  26.175  1.00  0.00           N
ATOM    895  NH2 ARG   120      34.596 -17.491  25.019  1.00  0.00           N
ATOM    896  C   ARG   120      31.212 -13.876  27.552  1.00  0.00           C
ATOM    897  O   ARG   120      30.052 -13.630  27.227  1.00  0.00           O
ATOM    898  N   ARG   121      31.490 -14.368  28.777  1.00  0.00           N
ATOM    899  CA  ARG   121      30.394 -14.385  29.703  1.00  0.00           C
ATOM    900  CB  ARG   121      30.706 -15.142  31.005  1.00  0.00           C
ATOM    901  CG  ARG   121      29.475 -15.813  31.619  1.00  0.00           C
ATOM    902  CD  ARG   121      28.231 -14.931  31.697  1.00  0.00           C
ATOM    903  NE  ARG   121      28.315 -14.130  32.945  1.00  0.00           N
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ATOM    904  CZ  ARG   121      27.276 -13.309  33.274  1.00  0.00           C
ATOM    905  NH1 ARG   121      26.212 -13.196  32.426  1.00  0.00           N
ATOM    906  NH2 ARG   121      27.288 -12.618  34.452  1.00  0.00           N
ATOM    907  C   ARG   121      30.284 -12.926  30.006  1.00  0.00           C
ATOM    908  O   ARG   121      31.291 -12.304  30.344  1.00  0.00           O
ATOM    909  N   VAL   122      29.093 -12.312  29.868  1.00  0.00           N
ATOM    910  CA  VAL   122      29.139 -10.886  30.008  1.00  0.00           C
ATOM    911  CB  VAL   122      29.034 -10.176  28.688  1.00  0.00           C
ATOM    912  CG1 VAL   122      28.958  -8.661  28.932  1.00  0.00           C
ATOM    913  CG2 VAL   122      30.213 -10.607  27.802  1.00  0.00           C
ATOM    914  C   VAL   122      28.033 -10.367  30.859  1.00  0.00           C
ATOM    915  O   VAL   122      26.919 -10.888  30.860  1.00  0.00           O
ATOM    916  N   VAL   123      28.342  -9.293  31.615  1.00  0.00           N
ATOM    917  CA  VAL   123      27.342  -8.616  32.376  1.00  0.00           C
ATOM    918  CB  VAL   123      27.593  -8.574  33.858  1.00  0.00           C
ATOM    919  CG1 VAL   123      28.830  -7.711  34.147  1.00  0.00           C
ATOM    920  CG2 VAL   123      26.317  -8.061  34.544  1.00  0.00           C
ATOM    921  C   VAL   123      27.345  -7.216  31.855  1.00  0.00           C
ATOM    922  O   VAL   123      28.398  -6.605  31.682  1.00  0.00           O
ATOM    923  N   PHE   124      26.149  -6.678  31.560  1.00  0.00           N
ATOM    924  CA  PHE   124      26.076  -5.370  30.986  1.00  0.00           C
ATOM    925  CB  PHE   124      25.326  -5.381  29.639  1.00  0.00           C
ATOM    926  CG  PHE   124      25.115  -3.993  29.146  1.00  0.00           C
ATOM    927  CD1 PHE   124      26.156  -3.254  28.632  1.00  0.00           C
ATOM    928  CD2 PHE   124      23.855  -3.441  29.172  1.00  0.00           C
ATOM    929  CE1 PHE   124      25.942  -1.977  28.168  1.00  0.00           C
ATOM    930  CE2 PHE   124      23.634  -2.167  28.708  1.00  0.00           C
ATOM    931  CZ  PHE   124      24.682  -1.430  28.213  1.00  0.00           C
ATOM    932  C   PHE   124      25.359  -4.471  31.934  1.00  0.00           C
ATOM    933  O   PHE   124      24.344  -4.845  32.518  1.00  0.00           O
ATOM    934  N   THR   125      25.882  -3.241  32.109  1.00  0.00           N
ATOM    935  CA  THR   125      25.256  -2.330  33.016  1.00  0.00           C
ATOM    936  CB  THR   125      26.214  -1.352  33.640  1.00  0.00           C
ATOM    937  OG1 THR   125      26.828  -0.543  32.645  1.00  0.00           O
ATOM    938  CG2 THR   125      27.282  -2.148  34.405  1.00  0.00           C
ATOM    939  C   THR   125      24.249  -1.553  32.234  1.00  0.00           C
ATOM    940  O   THR   125      24.596  -0.751  31.370  1.00  0.00           O
ATOM    941  N   SER   126      22.957  -1.804  32.513  1.00  0.00           N
ATOM    942  CA  SER   126      21.889  -1.129  31.837  1.00  0.00           C
ATOM    943  CB  SER   126      20.745  -2.071  31.423  1.00  0.00           C
ATOM    944  OG  SER   126      19.799  -1.382  30.618  1.00  0.00           O
ATOM    945  C   SER   126      21.338  -0.082  32.759  1.00  0.00           C
ATOM    946  O   SER   126      21.904   0.169  33.821  1.00  0.00           O
ATOM    947  N   SER   127      20.227   0.578  32.360  1.00  0.00           N
ATOM    948  CA  SER   127      19.672   1.604  33.196  1.00  0.00           C
ATOM    949  CB  SER   127      20.032   3.026  32.726  1.00  0.00           C
ATOM    950  OG  SER   127      19.454   3.993  33.592  1.00  0.00           O
ATOM    951  C   SER   127      18.172   1.514  33.196  1.00  0.00           C
ATOM    952  O   SER   127      17.545   0.977  32.285  1.00  0.00           O
ATOM    953  N   ILE   128      17.573   2.079  34.261  1.00  0.00           N
ATOM    954  CA  ILE   128      16.169   2.150  34.545  1.00  0.00           C
ATOM    955  CB  ILE   128      15.883   2.792  35.870  1.00  0.00           C
ATOM    956  CG2 ILE   128      14.356   2.898  36.022  1.00  0.00           C
ATOM    957  CG1 ILE   128      16.563   2.009  37.005  1.00  0.00           C
ATOM    958  CD1 ILE   128      16.119   0.551  37.085  1.00  0.00           C
ATOM    959  C   ILE   128      15.515   2.993  33.501  1.00  0.00           C
ATOM    960  O   ILE   128      14.322   2.858  33.238  1.00  0.00           O
ATOM    961  N   GLY   129      16.289   3.924  32.918  1.00  0.00           N
ATOM    962  CA  GLY   129      15.830   4.890  31.961  1.00  0.00           C
ATOM    963  C   GLY   129      15.189   4.196  30.802  1.00  0.00           C
ATOM    964  O   GLY   129      14.337   4.771  30.126  1.00  0.00           O
ATOM    965  N   ALA   130      15.603   2.952  30.517  1.00  0.00           N
ATOM    966  CA  ALA   130      15.090   2.259  29.371  1.00  0.00           C
ATOM    967  CB  ALA   130      15.648   0.833  29.233  1.00  0.00           C
ATOM    968  C   ALA   130      13.595   2.150  29.457  1.00  0.00           C
ATOM    969  O   ALA   130      12.908   2.333  28.452  1.00  0.00           O
ATOM    970  N   VAL   131      13.032   1.847  30.643  1.00  0.00           N
ATOM    971  CA  VAL   131      11.599   1.738  30.700  1.00  0.00           C
ATOM    972  CB  VAL   131      11.071   1.325  32.046  1.00  0.00           C
ATOM    973  CG1 VAL   131      11.555   2.315  33.118  1.00  0.00           C
ATOM    974  CG2 VAL   131       9.539   1.222  31.945  1.00  0.00           C
ATOM    975  C   VAL   131      11.009   3.067  30.339  1.00  0.00           C
ATOM    976  O   VAL   131      10.077   3.156  29.544  1.00  0.00           O
ATOM    977  N   TYR   132      11.539   4.129  30.961  1.00  0.00           N
ATOM    978  CA  TYR   132      11.260   5.515  30.736  1.00  0.00           C
ATOM    979  CB  TYR   132      11.758   6.029  29.369  1.00  0.00           C
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ATOM    980  CG  TYR   132      11.745   7.517  29.454  1.00  0.00           C
ATOM    981  CD1 TYR   132      12.724   8.168  30.171  1.00  0.00           C
ATOM    982  CD2 TYR   132      10.779   8.259  28.816  1.00  0.00           C
ATOM    983  CE1 TYR   132      12.729   9.538  30.273  1.00  0.00           C
ATOM    984  CE2 TYR   132      10.779   9.630  28.916  1.00  0.00           C
ATOM    985  CZ  TYR   132      11.752  10.272  29.645  1.00  0.00           C
ATOM    986  OH  TYR   132      11.750  11.680  29.749  1.00  0.00           O
ATOM    987  C   TYR   132       9.809   5.841  30.920  1.00  0.00           C
ATOM    988  O   TYR   132       9.439   7.007  30.847  1.00  0.00           O
ATOM    989  N   MET   133       8.929   4.879  31.244  1.00  0.00           N
ATOM    990  CA  MET   133       7.570   5.321  31.383  1.00  0.00           C
ATOM    991  CB  MET   133       6.500   4.337  30.877  1.00  0.00           C
ATOM    992  CG  MET   133       5.073   4.875  31.045  1.00  0.00           C
ATOM    993  SD  MET   133       3.748   3.773  30.457  1.00  0.00           S
ATOM    994  CE  MET   133       3.827   4.325  28.729  1.00  0.00           C
ATOM    995  C   MET   133       7.324   5.545  32.829  1.00  0.00           C
ATOM    996  O   MET   133       7.755   4.762  33.672  1.00  0.00           O
ATOM    997  N   ASP   134       6.626   6.645  33.153  1.00  0.00           N
ATOM    998  CA  ASP   134       6.409   6.928  34.535  1.00  0.00           C
ATOM    999  CB  ASP   134       6.549   8.420  34.896  1.00  0.00           C
ATOM   1000  CG  ASP   134       5.481   9.199  34.142  1.00  0.00           C
ATOM   1001  OD1 ASP   134       5.338   8.961  32.911  1.00  0.00           O
ATOM   1002  OD2 ASP   134       4.784  10.027  34.786  1.00  0.00           O
ATOM   1003  C   ASP   134       5.038   6.511  34.922  1.00  0.00           C
ATOM   1004  O   ASP   134       4.028   6.875  34.319  1.00  0.00           O
ATOM   1005  N   PRO   135       5.024   5.700  35.926  1.00  0.00           N
ATOM   1006  CA  PRO   135       3.778   5.314  36.509  1.00  0.00           C
ATOM   1007  CD  PRO   135       6.014   4.637  36.011  1.00  0.00           C
ATOM   1008  CB  PRO   135       4.059   4.054  37.322  1.00  0.00           C
ATOM   1009  CG  PRO   135       5.276   3.433  36.618  1.00  0.00           C
ATOM   1010  C   PRO   135       3.388   6.479  37.346  1.00  0.00           C
ATOM   1011  O   PRO   135       4.131   7.459  37.390  1.00  0.00           O
ATOM   1012  N   SER   136       2.233   6.400  38.019  1.00  0.00           N
ATOM   1013  CA  SER   136       1.789   7.478  38.846  1.00  0.00           C
ATOM   1014  CB  SER   136       0.379   7.267  39.419  1.00  0.00           C
ATOM   1015  OG  SER   136      -0.568   7.182  38.366  1.00  0.00           O
ATOM   1016  C   SER   136       2.714   7.567  40.013  1.00  0.00           C
ATOM   1017  O   SER   136       3.876   7.166  39.949  1.00  0.00           O
ATOM   1018  N   ARG   137       2.213   8.146  41.119  1.00  0.00           N
ATOM   1019  CA  ARG   137       3.013   8.289  42.294  1.00  0.00           C
ATOM   1020  CB  ARG   137       2.251   8.885  43.490  1.00  0.00           C
ATOM   1021  CG  ARG   137       1.831  10.344  43.316  1.00  0.00           C
ATOM   1022  CD  ARG   137       1.114  10.911  44.543  1.00  0.00           C
ATOM   1023  NE  ARG   137       0.770  12.330  44.250  1.00  0.00           N
ATOM   1024  CZ  ARG   137       0.264  13.123  45.238  1.00  0.00           C
ATOM   1025  NH1 ARG   137       0.065  12.611  46.487  1.00  0.00           N
ATOM   1026  NH2 ARG   137      -0.025  14.432  44.983  1.00  0.00           N
ATOM   1027  C   ARG   137       3.400   6.912  42.687  1.00  0.00           C
ATOM   1028  O   ARG   137       4.530   6.683  43.119  1.00  0.00           O
ATOM   1029  N   ASP   138       2.457   5.957  42.547  1.00  0.00           N
ATOM   1030  CA  ASP   138       2.800   4.605  42.855  1.00  0.00           C
ATOM   1031  CB  ASP   138       1.664   3.592  42.616  1.00  0.00           C
ATOM   1032  CG  ASP   138       1.302   3.587  41.136  1.00  0.00           C
ATOM   1033  OD1 ASP   138       1.340   4.681  40.516  1.00  0.00           O
ATOM   1034  OD2 ASP   138       0.991   2.489  40.600  1.00  0.00           O
ATOM   1035  C   ASP   138       3.934   4.284  41.947  1.00  0.00           C
ATOM   1036  O   ASP   138       3.870   4.510  40.741  1.00  0.00           O
ATOM   1037  N   TYR   139       5.026   3.781  42.535  1.00  0.00           N
ATOM   1038  CA  TYR   139       6.231   3.526  41.817  1.00  0.00           C
ATOM   1039  CB  TYR   139       7.358   4.455  42.298  1.00  0.00           C
ATOM   1040  CG  TYR   139       7.530   4.210  43.763  1.00  0.00           C
ATOM   1041  CD1 TYR   139       6.803   4.931  44.683  1.00  0.00           C
ATOM   1042  CD2 TYR   139       8.406   3.256  44.225  1.00  0.00           C
ATOM   1043  CE1 TYR   139       6.951   4.710  46.031  1.00  0.00           C
ATOM   1044  CE2 TYR   139       8.562   3.027  45.573  1.00  0.00           C
ATOM   1045  CZ  TYR   139       7.833   3.759  46.478  1.00  0.00           C
ATOM   1046  OH  TYR   139       7.984   3.535  47.863  1.00  0.00           O
ATOM   1047  C   TYR   139       6.625   2.136  42.158  1.00  0.00           C
ATOM   1048  O   TYR   139       6.149   1.588  43.149  1.00  0.00           O
ATOM   1049  N   ASP   140       7.489   1.506  41.337  1.00  0.00           N
ATOM   1050  CA  ASP   140       8.008   2.086  40.135  1.00  0.00           C
ATOM   1051  CB  ASP   140       9.095   3.133  40.336  1.00  0.00           C
ATOM   1052  CG  ASP   140       9.521   3.636  38.964  1.00  0.00           C
ATOM   1053  OD1 ASP   140       8.753   3.422  37.989  1.00  0.00           O
ATOM   1054  OD2 ASP   140      10.629   4.228  38.874  1.00  0.00           O
ATOM   1055  C   ASP   140       8.752   1.007  39.450  1.00  0.00           C
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ATOM   1056  O   ASP   140       9.838   0.652  39.904  1.00  0.00           O
ATOM   1057  N   ALA   141       8.215   0.493  38.330  1.00  0.00           N
ATOM   1058  CA  ALA   141       8.887  -0.567  37.651  1.00  0.00           C
ATOM   1059  CB  ALA   141      10.248  -0.133  37.085  1.00  0.00           C
ATOM   1060  C   ALA   141       9.099  -1.645  38.663  1.00  0.00           C
ATOM   1061  O   ALA   141      10.178  -2.231  38.739  1.00  0.00           O
ATOM   1062  N   LEU   142       8.064  -1.904  39.493  1.00  0.00           N
ATOM   1063  CA  LEU   142       8.200  -2.917  40.498  1.00  0.00           C
ATOM   1064  CB  LEU   142       6.905  -3.153  41.289  1.00  0.00           C
ATOM   1065  CG  LEU   142       7.034  -4.244  42.367  1.00  0.00           C
ATOM   1066  CD2 LEU   142       5.656  -4.608  42.940  1.00  0.00           C
ATOM   1067  CD1 LEU   142       8.055  -3.861  43.452  1.00  0.00           C
ATOM   1068  C   LEU   142       8.502  -4.158  39.746  1.00  0.00           C
ATOM   1069  O   LEU   142       9.479  -4.850  40.030  1.00  0.00           O
ATOM   1070  N   VAL   143       7.676  -4.447  38.730  1.00  0.00           N
ATOM   1071  CA  VAL   143       8.032  -5.510  37.855  1.00  0.00           C
ATOM   1072  CB  VAL   143       6.854  -6.341  37.428  1.00  0.00           C
ATOM   1073  CG1 VAL   143       6.376  -7.143  38.652  1.00  0.00           C
ATOM   1074  CG2 VAL   143       5.755  -5.412  36.881  1.00  0.00           C
ATOM   1075  C   VAL   143       8.605  -4.775  36.695  1.00  0.00           C
ATOM   1076  O   VAL   143       8.079  -4.785  35.584  1.00  0.00           O
ATOM   1077  N   ASP   144       9.741  -4.104  36.956  1.00  0.00           N
ATOM   1078  CA  ASP   144      10.364  -3.307  35.955  1.00  0.00           C
ATOM   1079  CB  ASP   144      11.655  -2.636  36.428  1.00  0.00           C
ATOM   1080  CG  ASP   144      12.131  -1.716  35.316  1.00  0.00           C
ATOM   1081  OD1 ASP   144      11.388  -1.590  34.307  1.00  0.00           O
ATOM   1082  OD2 ASP   144      13.235  -1.125  35.455  1.00  0.00           O
ATOM   1083  C   ASP   144      10.760  -4.216  34.857  1.00  0.00           C
ATOM   1084  O   ASP   144      10.574  -3.909  33.682  1.00  0.00           O
ATOM   1085  N   GLU   145      11.294  -5.390  35.225  1.00  0.00           N
ATOM   1086  CA  GLU   145      11.720  -6.299  34.210  1.00  0.00           C
ATOM   1087  CB  GLU   145      12.342  -7.594  34.764  1.00  0.00           C
ATOM   1088  CG  GLU   145      11.506  -8.280  35.844  1.00  0.00           C
ATOM   1089  CD  GLU   145      11.808  -7.566  37.153  1.00  0.00           C
ATOM   1090  OE1 GLU   145      12.781  -6.765  37.176  1.00  0.00           O
ATOM   1091  OE2 GLU   145      11.078  -7.814  38.149  1.00  0.00           O
ATOM   1092  C   GLU   145      10.518  -6.636  33.403  1.00  0.00           C
ATOM   1093  O   GLU   145      10.600  -6.764  32.183  1.00  0.00           O
ATOM   1094  N   ASN   146       9.359  -6.769  34.070  1.00  0.00           N
ATOM   1095  CA  ASN   146       8.151  -7.080  33.369  1.00  0.00           C
ATOM   1096  CB  ASN   146       6.927  -7.200  34.297  1.00  0.00           C
ATOM   1097  CG  ASN   146       5.748  -7.721  33.484  1.00  0.00           C
ATOM   1098  OD1 ASN   146       5.432  -7.216  32.408  1.00  0.00           O
ATOM   1099  ND2 ASN   146       5.070  -8.773  34.019  1.00  0.00           N
ATOM   1100  C   ASN   146       7.872  -5.962  32.418  1.00  0.00           C
ATOM   1101  O   ASN   146       7.529  -6.197  31.259  1.00  0.00           O
ATOM   1102  N   CYS   147       8.029  -4.707  32.880  1.00  0.00           N
ATOM   1103  CA  CYS   147       7.752  -3.610  32.003  1.00  0.00           C
ATOM   1104  CB  CYS   147       7.973  -2.230  32.643  1.00  0.00           C
ATOM   1105  SG  CYS   147       6.841  -1.923  34.032  1.00  0.00           S
ATOM   1106  C   CYS   147       8.698  -3.736  30.862  1.00  0.00           C
ATOM   1107  O   CYS   147       9.875  -4.038  31.044  1.00  0.00           O
ATOM   1108  N   TRP   148       8.195  -3.520  29.634  1.00  0.00           N
ATOM   1109  CA  TRP   148       9.057  -3.679  28.508  1.00  0.00           C
ATOM   1110  CB  TRP   148       8.453  -4.527  27.374  1.00  0.00           C
ATOM   1111  CG  TRP   148       8.274  -5.992  27.696  1.00  0.00           C
ATOM   1112  CD2 TRP   148       7.101  -6.543  28.311  1.00  0.00           C
ATOM   1113  CD1 TRP   148       9.124  -7.036  27.477  1.00  0.00           C
ATOM   1114  NE1 TRP   148       8.554  -8.205  27.920  1.00  0.00           N
ATOM   1115  CE2 TRP   148       7.308  -7.917  28.436  1.00  0.00           C
ATOM   1116  CE3 TRP   148       5.947  -5.954  28.738  1.00  0.00           C
ATOM   1117  CZ2 TRP   148       6.357  -8.726  28.991  1.00  0.00           C
ATOM   1118  CZ3 TRP   148       4.991  -6.771  29.297  1.00  0.00           C
ATOM   1119  CH2 TRP   148       5.191  -8.130  29.421  1.00  0.00           C
ATOM   1120  C   TRP   148       9.334  -2.334  27.935  1.00  0.00           C
ATOM   1121  O   TRP   148       8.491  -1.438  27.978  1.00  0.00           O
ATOM   1122  N   SER   149      10.554  -2.156  27.399  1.00  0.00           N
ATOM   1123  CA  SER   149      10.882  -0.931  26.743  1.00  0.00           C
ATOM   1124  CB  SER   149      12.344  -0.498  26.937  1.00  0.00           C
ATOM   1125  OG  SER   149      12.609  -0.292  28.315  1.00  0.00           O
ATOM   1126  C   SER   149      10.713  -1.255  25.296  1.00  0.00           C
ATOM   1127  O   SER   149      11.234  -2.261  24.823  1.00  0.00           O
ATOM   1128  N   ASN   150       9.960  -0.426  24.555  1.00  0.00           N
ATOM   1129  CA  ASN   150       9.730  -0.699  23.171  1.00  0.00           C
ATOM   1130  CB  ASN   150       8.253  -0.998  22.845  1.00  0.00           C
ATOM   1131  CG  ASN   150       8.192  -1.749  21.520  1.00  0.00           C
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ATOM   1132  OD1 ASN   150       7.115  -2.011  20.985  1.00  0.00           O
ATOM   1133  ND2 ASN   150       9.382  -2.129  20.981  1.00  0.00           N
ATOM   1134  C   ASN   150      10.103   0.547  22.449  1.00  0.00           C
ATOM   1135  O   ASN   150      10.244   1.606  23.059  1.00  0.00           O
ATOM   1136  N   LEU   151      10.302   0.454  21.123  1.00  0.00           N
ATOM   1137  CA  LEU   151      10.676   1.632  20.404  1.00  0.00           C
ATOM   1138  CB  LEU   151      11.459   1.320  19.121  1.00  0.00           C
ATOM   1139  CG  LEU   151      11.873   2.572  18.333  1.00  0.00           C
ATOM   1140  CD2 LEU   151      12.414   2.202  16.943  1.00  0.00           C
ATOM   1141  CD1 LEU   151      12.847   3.440  19.142  1.00  0.00           C
ATOM   1142  C   LEU   151       9.425   2.338  20.011  1.00  0.00           C
ATOM   1143  O   LEU   151       8.945   2.192  18.889  1.00  0.00           O
ATOM   1144  N   ASP   152       8.867   3.127  20.946  1.00  0.00           N
ATOM   1145  CA  ASP   152       7.686   3.885  20.675  1.00  0.00           C
ATOM   1146  CB  ASP   152       6.378   3.145  21.014  1.00  0.00           C
ATOM   1147  CG  ASP   152       6.163   2.080  19.940  1.00  0.00           C
ATOM   1148  OD1 ASP   152       6.243   2.434  18.732  1.00  0.00           O
ATOM   1149  OD2 ASP   152       5.906   0.903  20.311  1.00  0.00           O
ATOM   1150  C   ASP   152       7.774   5.132  21.493  1.00  0.00           C
ATOM   1151  O   ASP   152       8.861   5.565  21.868  1.00  0.00           O
ATOM   1152  N   TYR   153       6.616   5.756  21.778  1.00  0.00           N
ATOM   1153  CA  TYR   153       6.619   6.973  22.531  1.00  0.00           C
ATOM   1154  CB  TYR   153       5.204   7.533  22.753  1.00  0.00           C
ATOM   1155  CG  TYR   153       4.627   7.865  21.419  1.00  0.00           C
ATOM   1156  CD1 TYR   153       4.114   6.870  20.619  1.00  0.00           C
ATOM   1157  CD2 TYR   153       4.586   9.166  20.971  1.00  0.00           C
ATOM   1158  CE1 TYR   153       3.575   7.163  19.388  1.00  0.00           C
ATOM   1159  CE2 TYR   153       4.049   9.466  19.741  1.00  0.00           C
ATOM   1160  CZ  TYR   153       3.544   8.463  18.947  1.00  0.00           C
ATOM   1161  OH  TYR   153       2.991   8.763  17.684  1.00  0.00           O
ATOM   1162  C   TYR   153       7.196   6.677  23.876  1.00  0.00           C
ATOM   1163  O   TYR   153       8.051   7.413  24.368  1.00  0.00           O
ATOM   1164  N   CYS   154       6.753   5.571  24.507  1.00  0.00           N
ATOM   1165  CA  CYS   154       7.247   5.261  25.817  1.00  0.00           C
ATOM   1166  CB  CYS   154       6.139   5.062  26.862  1.00  0.00           C
ATOM   1167  SG  CYS   154       5.219   6.596  27.181  1.00  0.00           S
ATOM   1168  C   CYS   154       8.025   3.989  25.745  1.00  0.00           C
ATOM   1169  O   CYS   154       8.073   3.325  24.712  1.00  0.00           O
ATOM   1170  N   LYS   155       8.675   3.634  26.875  1.00  0.00           N
ATOM   1171  CA  LYS   155       9.495   2.468  26.956  1.00  0.00           C
ATOM   1172  CB  LYS   155       8.749   1.217  26.487  1.00  0.00           C
ATOM   1173  CG  LYS   155       7.441   1.025  27.251  1.00  0.00           C
ATOM   1174  CD  LYS   155       7.623   1.039  28.770  1.00  0.00           C
ATOM   1175  CE  LYS   155       6.311   0.956  29.548  1.00  0.00           C
ATOM   1176  NZ  LYS   155       6.590   0.933  31.001  1.00  0.00           N
ATOM   1177  C   LYS   155      10.666   2.747  26.084  1.00  0.00           C
ATOM   1178  O   LYS   155      11.422   1.861  25.685  1.00  0.00           O
ATOM   1179  N   GLU   156      10.832   4.048  25.807  1.00  0.00           N
ATOM   1180  CA  GLU   156      11.914   4.587  25.066  1.00  0.00           C
ATOM   1181  CB  GLU   156      11.532   5.016  23.641  1.00  0.00           C
ATOM   1182  CG  GLU   156      12.735   5.377  22.771  1.00  0.00           C
ATOM   1183  CD  GLU   156      12.249   5.535  21.337  1.00  0.00           C
ATOM   1184  OE1 GLU   156      11.292   4.810  20.951  1.00  0.00           O
ATOM   1185  OE2 GLU   156      12.833   6.377  20.606  1.00  0.00           O
ATOM   1186  C   GLU   156      12.292   5.796  25.847  1.00  0.00           C
ATOM   1187  O   GLU   156      11.436   6.447  26.444  1.00  0.00           O
ATOM   1188  N   THR   157      13.592   6.112  25.905  1.00  0.00           N
ATOM   1189  CA  THR   157      13.967   7.226  26.717  1.00  0.00           C
ATOM   1190  CB  THR   157      15.308   7.100  27.310  1.00  0.00           C
ATOM   1191  OG1 THR   157      15.502   8.093  28.308  1.00  0.00           O
ATOM   1192  CG2 THR   157      16.290   7.316  26.153  1.00  0.00           C
ATOM   1193  C   THR   157      14.053   8.445  25.869  1.00  0.00           C
ATOM   1194  O   THR   157      14.195   8.364  24.651  1.00  0.00           O
ATOM   1195  N   LYS   158      13.932   9.621  26.516  1.00  0.00           N
ATOM   1196  CA  LYS   158      14.055  10.872  25.829  1.00  0.00           C
ATOM   1197  CB  LYS   158      13.569  12.087  26.640  1.00  0.00           C
ATOM   1198  CG  LYS   158      13.680  13.395  25.850  1.00  0.00           C
ATOM   1199  CD  LYS   158      12.956  14.587  26.481  1.00  0.00           C
ATOM   1200  CE  LYS   158      13.865  15.471  27.337  1.00  0.00           C
ATOM   1201  NZ  LYS   158      13.119  16.660  27.805  1.00  0.00           N
ATOM   1202  C   LYS   158      15.482  11.155  25.472  1.00  0.00           C
ATOM   1203  O   LYS   158      15.767  11.663  24.390  1.00  0.00           O
ATOM   1204  N   ASN   159      16.420  10.849  26.393  1.00  0.00           N
ATOM   1205  CA  ASN   159      17.796  11.218  26.205  1.00  0.00           C
ATOM   1206  CB  ASN   159      18.610  11.231  27.511  1.00  0.00           C
ATOM   1207  CG  ASN   159      18.042  12.305  28.429  1.00  0.00           C
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ATOM   1208  OD1 ASN   159      17.470  13.296  27.981  1.00  0.00           O
ATOM   1209  ND2 ASN   159      18.212  12.102  29.764  1.00  0.00           N
ATOM   1210  C   ASN   159      18.479  10.264  25.282  1.00  0.00           C
ATOM   1211  O   ASN   159      18.143   9.087  25.190  1.00  0.00           O
ATOM   1212  N   TRP   160      19.488  10.773  24.561  1.00  0.00           N
ATOM   1213  CA  TRP   160      20.268   9.979  23.672  1.00  0.00           C
ATOM   1214  CB  TRP   160      21.274  10.781  22.833  1.00  0.00           C
ATOM   1215  CG  TRP   160      22.051   9.890  21.901  1.00  0.00           C
ATOM   1216  CD2 TRP   160      21.498   9.343  20.694  1.00  0.00           C
ATOM   1217  CD1 TRP   160      23.316   9.391  22.010  1.00  0.00           C
ATOM   1218  NE1 TRP   160      23.582   8.564  20.946  1.00  0.00           N
ATOM   1219  CE2 TRP   160      22.472   8.522  20.128  1.00  0.00           C
ATOM   1220  CE3 TRP   160      20.273   9.501  20.112  1.00  0.00           C
ATOM   1221  CZ2 TRP   160      22.234   7.845  18.965  1.00  0.00           C
ATOM   1222  CZ3 TRP   160      20.040   8.825  18.935  1.00  0.00           C
ATOM   1223  CH2 TRP   160      21.002   8.011  18.373  1.00  0.00           C
ATOM   1224  C   TRP   160      21.011   9.006  24.524  1.00  0.00           C
ATOM   1225  O   TRP   160      21.271   7.878  24.111  1.00  0.00           O
ATOM   1226  N   TYR   161      21.391   9.436  25.743  1.00  0.00           N
ATOM   1227  CA  TYR   161      22.110   8.586  26.643  1.00  0.00           C
ATOM   1228  CB  TYR   161      22.441   9.299  27.968  1.00  0.00           C
ATOM   1229  CG  TYR   161      22.823   8.269  28.977  1.00  0.00           C
ATOM   1230  CD1 TYR   161      24.027   7.611  28.901  1.00  0.00           C
ATOM   1231  CD2 TYR   161      21.972   7.980  30.020  1.00  0.00           C
ATOM   1232  CE1 TYR   161      24.368   6.669  29.843  1.00  0.00           C
ATOM   1233  CE2 TYR   161      22.307   7.039  30.966  1.00  0.00           C
ATOM   1234  CZ  TYR   161      23.508   6.379  30.876  1.00  0.00           C
ATOM   1235  OH  TYR   161      23.856   5.411  31.842  1.00  0.00           O
ATOM   1236  C   TYR   161      21.281   7.392  26.981  1.00  0.00           C
ATOM   1237  O   TYR   161      21.733   6.256  26.858  1.00  0.00           O
ATOM   1238  N   CYS   162      20.025   7.606  27.402  1.00  0.00           N
ATOM   1239  CA  CYS   162      19.243   6.465  27.762  1.00  0.00           C
ATOM   1240  CB  CYS   162      17.962   6.815  28.520  1.00  0.00           C
ATOM   1241  SG  CYS   162      18.296   7.575  30.137  1.00  0.00           S
ATOM   1242  C   CYS   162      18.945   5.673  26.527  1.00  0.00           C
ATOM   1243  O   CYS   162      18.819   4.451  26.573  1.00  0.00           O
ATOM   1244  N   TYR   163      18.824   6.360  25.379  1.00  0.00           N
ATOM   1245  CA  TYR   163      18.525   5.717  24.131  1.00  0.00           C
ATOM   1246  CB  TYR   163      18.381   6.736  22.986  1.00  0.00           C
ATOM   1247  CG  TYR   163      17.968   6.015  21.749  1.00  0.00           C
ATOM   1248  CD1 TYR   163      16.651   5.658  21.563  1.00  0.00           C
ATOM   1249  CD2 TYR   163      18.886   5.706  20.772  1.00  0.00           C
ATOM   1250  CE1 TYR   163      16.255   4.996  20.425  1.00  0.00           C
ATOM   1251  CE2 TYR   163      18.497   5.044  19.631  1.00  0.00           C
ATOM   1252  CZ  TYR   163      17.182   4.689  19.457  1.00  0.00           C
ATOM   1253  OH  TYR   163      16.782   4.010  18.287  1.00  0.00           O
ATOM   1254  C   TYR   163      19.667   4.801  23.812  1.00  0.00           C
ATOM   1255  O   TYR   163      19.476   3.683  23.339  1.00  0.00           O
ATOM   1256  N   GLY   164      20.903   5.261  24.069  1.00  0.00           N
ATOM   1257  CA  GLY   164      22.069   4.482  23.770  1.00  0.00           C
ATOM   1258  C   GLY   164      22.045   3.224  24.577  1.00  0.00           C
ATOM   1259  O   GLY   164      22.488   2.176  24.111  1.00  0.00           O
ATOM   1260  N   LYS   165      21.576   3.305  25.835  1.00  0.00           N
ATOM   1261  CA  LYS   165      21.547   2.142  26.674  1.00  0.00           C
ATOM   1262  CB  LYS   165      21.146   2.463  28.121  1.00  0.00           C
ATOM   1263  CG  LYS   165      22.147   3.390  28.813  1.00  0.00           C
ATOM   1264  CD  LYS   165      23.576   2.846  28.825  1.00  0.00           C
ATOM   1265  CE  LYS   165      23.859   1.825  29.925  1.00  0.00           C
ATOM   1266  NZ  LYS   165      25.248   1.336  29.782  1.00  0.00           N
ATOM   1267  C   LYS   165      20.570   1.146  26.126  1.00  0.00           C
ATOM   1268  O   LYS   165      20.848  -0.051  26.094  1.00  0.00           O
ATOM   1269  N   THR   166      19.390   1.613  25.674  1.00  0.00           N
ATOM   1270  CA  THR   166      18.397   0.696  25.193  1.00  0.00           C
ATOM   1271  CB  THR   166      17.077   1.340  24.855  1.00  0.00           C
ATOM   1272  OG1 THR   166      16.087   0.337  24.682  1.00  0.00           O
ATOM   1273  CG2 THR   166      17.213   2.161  23.564  1.00  0.00           C
ATOM   1274  C   THR   166      18.914   0.008  23.968  1.00  0.00           C
ATOM   1275  O   THR   166      18.710  -1.192  23.796  1.00  0.00           O
ATOM   1276  N   VAL   167      19.610   0.744  23.081  1.00  0.00           N
ATOM   1277  CA  VAL   167      20.088   0.128  21.875  1.00  0.00           C
ATOM   1278  CB  VAL   167      20.767   1.080  20.923  1.00  0.00           C
ATOM   1279  CG1 VAL   167      22.140   1.488  21.481  1.00  0.00           C
ATOM   1280  CG2 VAL   167      20.827   0.416  19.535  1.00  0.00           C
ATOM   1281  C   VAL   167      21.063  -0.948  22.240  1.00  0.00           C
ATOM   1282  O   VAL   167      21.078  -2.014  21.625  1.00  0.00           O
ATOM   1283  N   ALA   168      21.903  -0.691  23.260  1.00  0.00           N
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ATOM   1284  CA  ALA   168      22.906  -1.631  23.675  1.00  0.00           C
ATOM   1285  CB  ALA   168      23.776  -1.103  24.828  1.00  0.00           C
ATOM   1286  C   ALA   168      22.232  -2.875  24.148  1.00  0.00           C
ATOM   1287  O   ALA   168      22.691  -3.982  23.869  1.00  0.00           O
ATOM   1288  N   GLU   169      21.108  -2.726  24.872  1.00  0.00           N
ATOM   1289  CA  GLU   169      20.424  -3.877  25.383  1.00  0.00           C
ATOM   1290  CB  GLU   169      19.141  -3.536  26.159  1.00  0.00           C
ATOM   1291  CG  GLU   169      19.390  -2.866  27.511  1.00  0.00           C
ATOM   1292  CD  GLU   169      18.048  -2.716  28.213  1.00  0.00           C
ATOM   1293  OE1 GLU   169      17.042  -2.418  27.514  1.00  0.00           O
ATOM   1294  OE2 GLU   169      18.012  -2.906  29.458  1.00  0.00           O
ATOM   1295  C   GLU   169      20.007  -4.707  24.216  1.00  0.00           C
ATOM   1296  O   GLU   169      20.043  -5.935  24.274  1.00  0.00           O
ATOM   1297  N   LYS   170      19.593  -4.043  23.124  1.00  0.00           N
ATOM   1298  CA  LYS   170      19.133  -4.728  21.953  1.00  0.00           C
ATOM   1299  CB  LYS   170      18.697  -3.747  20.849  1.00  0.00           C
ATOM   1300  CG  LYS   170      17.556  -2.820  21.280  1.00  0.00           C
ATOM   1301  CD  LYS   170      17.368  -1.607  20.365  1.00  0.00           C
ATOM   1302  CE  LYS   170      16.249  -0.667  20.820  1.00  0.00           C
ATOM   1303  NZ  LYS   170      16.165   0.495  19.910  1.00  0.00           N
ATOM   1304  C   LYS   170      20.256  -5.555  21.399  1.00  0.00           C
ATOM   1305  O   LYS   170      20.067  -6.716  21.044  1.00  0.00           O
ATOM   1306  N   ALA   171      21.468  -4.972  21.323  1.00  0.00           N
ATOM   1307  CA  ALA   171      22.604  -5.655  20.765  1.00  0.00           C
ATOM   1308  CB  ALA   171      23.869  -4.780  20.743  1.00  0.00           C
ATOM   1309  C   ALA   171      22.907  -6.853  21.606  1.00  0.00           C
ATOM   1310  O   ALA   171      23.235  -7.922  21.093  1.00  0.00           O
ATOM   1311  N   ALA   172      22.798  -6.693  22.936  1.00  0.00           N
ATOM   1312  CA  ALA   172      23.099  -7.750  23.855  1.00  0.00           C
ATOM   1313  CB  ALA   172      22.896  -7.314  25.316  1.00  0.00           C
ATOM   1314  C   ALA   172      22.163  -8.887  23.587  1.00  0.00           C
ATOM   1315  O   ALA   172      22.564 -10.049  23.598  1.00  0.00           O
ATOM   1316  N   TRP   173      20.882  -8.566  23.331  1.00  0.00           N
ATOM   1317  CA  TRP   173      19.870  -9.549  23.074  1.00  0.00           C
ATOM   1318  CB  TRP   173      18.506  -8.920  22.741  1.00  0.00           C
ATOM   1319  CG  TRP   173      17.460  -9.911  22.282  1.00  0.00           C
ATOM   1320  CD2 TRP   173      16.420 -10.459  23.109  1.00  0.00           C
ATOM   1321  CD1 TRP   173      17.275 -10.434  21.035  1.00  0.00           C
ATOM   1322  NE1 TRP   173      16.193 -11.281  21.036  1.00  0.00           N
ATOM   1323  CE2 TRP   173      15.654 -11.302  22.304  1.00  0.00           C
ATOM   1324  CE3 TRP   173      16.124 -10.269  24.429  1.00  0.00           C
ATOM   1325  CZ2 TRP   173      14.578 -11.973  22.809  1.00  0.00           C
ATOM   1326  CZ3 TRP   173      15.040 -10.950  24.936  1.00  0.00           C
ATOM   1327  CH2 TRP   173      14.283 -11.784  24.141  1.00  0.00           C
ATOM   1328  C   TRP   173      20.266 -10.317  21.856  1.00  0.00           C
ATOM   1329  O   TRP   173      20.185 -11.542  21.833  1.00  0.00           O
ATOM   1330  N   GLU   174      20.711  -9.599  20.809  1.00  0.00           N
ATOM   1331  CA  GLU   174      21.063 -10.211  19.561  1.00  0.00           C
ATOM   1332  CB  GLU   174      21.551  -9.192  18.520  1.00  0.00           C
ATOM   1333  CG  GLU   174      21.930  -9.831  17.182  1.00  0.00           C
ATOM   1334  CD  GLU   174      22.489  -8.739  16.282  1.00  0.00           C
ATOM   1335  OE1 GLU   174      22.383  -7.544  16.664  1.00  0.00           O
ATOM   1336  OE2 GLU   174      23.034  -9.088  15.200  1.00  0.00           O
ATOM   1337  C   GLU   174      22.188 -11.168  19.772  1.00  0.00           C
ATOM   1338  O   GLU   174      22.208 -12.246  19.182  1.00  0.00           O
ATOM   1339  N   ARG   175      23.162 -10.796  20.619  1.00  0.00           N
ATOM   1340  CA  ARG   175      24.315 -11.623  20.824  1.00  0.00           C
ATOM   1341  CB  ARG   175      25.257 -11.038  21.893  1.00  0.00           C
ATOM   1342  CG  ARG   175      25.749  -9.617  21.598  1.00  0.00           C
ATOM   1343  CD  ARG   175      27.251  -9.517  21.328  1.00  0.00           C
ATOM   1344  NE  ARG   175      27.467  -9.645  19.860  1.00  0.00           N
ATOM   1345  CZ  ARG   175      28.493  -8.961  19.273  1.00  0.00           C
ATOM   1346  NH1 ARG   175      29.295  -8.158  20.029  1.00  0.00           N
ATOM   1347  NH2 ARG   175      28.713  -9.074  17.930  1.00  0.00           N
ATOM   1348  C   ARG   175      23.849 -12.940  21.353  1.00  0.00           C
ATOM   1349  O   ARG   175      24.255 -13.998  20.875  1.00  0.00           O
ATOM   1350  N   ALA   176      22.966 -12.900  22.365  1.00  0.00           N
ATOM   1351  CA  ALA   176      22.484 -14.103  22.973  1.00  0.00           C
ATOM   1352  CB  ALA   176      21.566 -13.829  24.175  1.00  0.00           C
ATOM   1353  C   ALA   176      21.695 -14.889  21.978  1.00  0.00           C
ATOM   1354  O   ALA   176      21.825 -16.108  21.888  1.00  0.00           O
ATOM   1355  N   LYS   177      20.842 -14.213  21.197  1.00  0.00           N
ATOM   1356  CA  LYS   177      20.026 -14.944  20.280  1.00  0.00           C
ATOM   1357  CB  LYS   177      19.073 -14.017  19.503  1.00  0.00           C
ATOM   1358  CG  LYS   177      18.131 -14.741  18.540  1.00  0.00           C
ATOM   1359  CD  LYS   177      16.973 -13.863  18.057  1.00  0.00           C
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ATOM   1360  CE  LYS   177      17.424 -12.569  17.375  1.00  0.00           C
ATOM   1361  NZ  LYS   177      16.244 -11.818  16.890  1.00  0.00           N
ATOM   1362  C   LYS   177      20.904 -15.644  19.289  1.00  0.00           C
ATOM   1363  O   LYS   177      20.788 -16.854  19.095  1.00  0.00           O
ATOM   1364  N   ASP   178      21.804 -14.893  18.626  1.00  0.00           N
ATOM   1365  CA  ASP   178      22.633 -15.500  17.625  1.00  0.00           C
ATOM   1366  CB  ASP   178      23.430 -14.460  16.818  1.00  0.00           C
ATOM   1367  CG  ASP   178      22.456 -13.677  15.951  1.00  0.00           C
ATOM   1368  OD1 ASP   178      21.473 -14.295  15.460  1.00  0.00           O
ATOM   1369  OD2 ASP   178      22.679 -12.450  15.767  1.00  0.00           O
ATOM   1370  C   ASP   178      23.636 -16.439  18.224  1.00  0.00           C
ATOM   1371  O   ASP   178      23.630 -17.636  17.944  1.00  0.00           O
ATOM   1372  N   LYS   179      24.533 -15.894  19.070  1.00  0.00           N
ATOM   1373  CA  LYS   179      25.619 -16.642  19.637  1.00  0.00           C
ATOM   1374  CB  LYS   179      26.716 -15.747  20.232  1.00  0.00           C
ATOM   1375  CG  LYS   179      28.023 -16.495  20.492  1.00  0.00           C
ATOM   1376  CD  LYS   179      29.216 -15.564  20.711  1.00  0.00           C
ATOM   1377  CE  LYS   179      30.549 -16.301  20.839  1.00  0.00           C
ATOM   1378  NZ  LYS   179      30.937 -16.877  19.533  1.00  0.00           N
ATOM   1379  C   LYS   179      25.162 -17.577  20.707  1.00  0.00           C
ATOM   1380  O   LYS   179      25.659 -18.696  20.820  1.00  0.00           O
ATOM   1381  N   GLY   180      24.194 -17.149  21.533  1.00  0.00           N
ATOM   1382  CA  GLY   180      23.797 -17.975  22.636  1.00  0.00           C
ATOM   1383  C   GLY   180      24.702 -17.633  23.781  1.00  0.00           C
ATOM   1384  O   GLY   180      24.881 -18.418  24.710  1.00  0.00           O
ATOM   1385  N   LEU   181      25.293 -16.425  23.731  1.00  0.00           N
ATOM   1386  CA  LEU   181      26.223 -15.951  24.714  1.00  0.00           C
ATOM   1387  CB  LEU   181      26.853 -14.608  24.294  1.00  0.00           C
ATOM   1388  CG  LEU   181      28.015 -14.129  25.179  1.00  0.00           C
ATOM   1389  CD2 LEU   181      28.356 -12.653  24.909  1.00  0.00           C
ATOM   1390  CD1 LEU   181      29.232 -15.056  25.031  1.00  0.00           C
ATOM   1391  C   LEU   181      25.488 -15.750  26.003  1.00  0.00           C
ATOM   1392  O   LEU   181      24.292 -15.456  26.029  1.00  0.00           O
ATOM   1393  N   ASP   182      26.207 -15.936  27.124  1.00  0.00           N
ATOM   1394  CA  ASP   182      25.624 -15.796  28.420  1.00  0.00           C
ATOM   1395  CB  ASP   182      26.455 -16.510  29.492  1.00  0.00           C
ATOM   1396  CG  ASP   182      26.640 -17.956  29.053  1.00  0.00           C
ATOM   1397  OD1 ASP   182      26.004 -18.375  28.051  1.00  0.00           O
ATOM   1398  OD2 ASP   182      27.453 -18.658  29.707  1.00  0.00           O
ATOM   1399  C   ASP   182      25.699 -14.342  28.738  1.00  0.00           C
ATOM   1400  O   ASP   182      26.714 -13.866  29.244  1.00  0.00           O
ATOM   1401  N   LEU   183      24.631 -13.580  28.441  1.00  0.00           N
ATOM   1402  CA  LEU   183      24.757 -12.181  28.727  1.00  0.00           C
ATOM   1403  CB  LEU   183      24.681 -11.305  27.459  1.00  0.00           C
ATOM   1404  CG  LEU   183      25.084  -9.822  27.628  1.00  0.00           C
ATOM   1405  CD2 LEU   183      24.237  -9.085  28.679  1.00  0.00           C
ATOM   1406  CD1 LEU   183      25.046  -9.102  26.272  1.00  0.00           C
ATOM   1407  C   LEU   183      23.653 -11.801  29.659  1.00  0.00           C
ATOM   1408  O   LEU   183      22.502 -12.198  29.475  1.00  0.00           O
ATOM   1409  N   VAL   184      23.989 -11.026  30.710  1.00  0.00           N
ATOM   1410  CA  VAL   184      22.984 -10.605  31.637  1.00  0.00           C
ATOM   1411  CB  VAL   184      23.270 -10.989  33.059  1.00  0.00           C
ATOM   1412  CG1 VAL   184      23.282 -12.524  33.157  1.00  0.00           C
ATOM   1413  CG2 VAL   184      24.585 -10.322  33.498  1.00  0.00           C
ATOM   1414  C   VAL   184      22.910  -9.120  31.578  1.00  0.00           C
ATOM   1415  O   VAL   184      23.929  -8.441  31.448  1.00  0.00           O
ATOM   1416  N   VAL   185      21.678  -8.578  31.642  1.00  0.00           N
ATOM   1417  CA  VAL   185      21.538  -7.157  31.634  1.00  0.00           C
ATOM   1418  CB  VAL   185      20.634  -6.637  30.546  1.00  0.00           C
ATOM   1419  CG1 VAL   185      21.295  -6.938  29.190  1.00  0.00           C
ATOM   1420  CG2 VAL   185      19.236  -7.266  30.688  1.00  0.00           C
ATOM   1421  C   VAL   185      20.981  -6.764  32.961  1.00  0.00           C
ATOM   1422  O   VAL   185      19.882  -7.159  33.347  1.00  0.00           O
ATOM   1423  N   VAL   186      21.754  -5.965  33.711  1.00  0.00           N
ATOM   1424  CA  VAL   186      21.270  -5.514  34.973  1.00  0.00           C
ATOM   1425  CB  VAL   186      22.323  -5.469  36.043  1.00  0.00           C
ATOM   1426  CG1 VAL   186      22.795  -6.906  36.324  1.00  0.00           C
ATOM   1427  CG2 VAL   186      23.449  -4.530  35.581  1.00  0.00           C
ATOM   1428  C   VAL   186      20.824  -4.126  34.715  1.00  0.00           C
ATOM   1429  O   VAL   186      21.501  -3.386  34.006  1.00  0.00           O
ATOM   1430  N   ASN   187      19.642  -3.752  35.236  1.00  0.00           N
ATOM   1431  CA  ASN   187      19.186  -2.409  35.047  1.00  0.00           C
ATOM   1432  CB  ASN   187      17.699  -2.302  34.673  1.00  0.00           C
ATOM   1433  CG  ASN   187      17.521  -2.827  33.258  1.00  0.00           C
ATOM   1434  OD1 ASN   187      17.216  -4.001  33.057  1.00  0.00           O
ATOM   1435  ND2 ASN   187      17.714  -1.936  32.250  1.00  0.00           N
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ATOM   1436  C   ASN   187      19.332  -1.744  36.366  1.00  0.00           C
ATOM   1437  O   ASN   187      18.485  -1.886  37.247  1.00  0.00           O
ATOM   1438  N   PRO   188      20.405  -1.041  36.548  1.00  0.00           N
ATOM   1439  CA  PRO   188      20.528  -0.381  37.804  1.00  0.00           C
ATOM   1440  CD  PRO   188      21.695  -1.515  36.084  1.00  0.00           C
ATOM   1441  CB  PRO   188      22.017  -0.338  38.153  1.00  0.00           C
ATOM   1442  CG  PRO   188      22.724  -0.657  36.829  1.00  0.00           C
ATOM   1443  C   PRO   188      19.917   0.951  37.736  1.00  0.00           C
ATOM   1444  O   PRO   188      19.654   1.462  36.647  1.00  0.00           O
ATOM   1445  N   CYS   189      19.674   1.538  38.905  1.00  0.00           N
ATOM   1446  CA  CYS   189      19.240   2.876  38.822  1.00  0.00           C
ATOM   1447  CB  CYS   189      18.150   3.291  39.806  1.00  0.00           C
ATOM   1448  SG  CYS   189      17.421   4.837  39.200  1.00  0.00           S
ATOM   1449  C   CYS   189      20.492   3.609  39.131  1.00  0.00           C
ATOM   1450  O   CYS   189      21.573   3.150  38.768  1.00  0.00           O
ATOM   1451  N   VAL   190      20.419   4.769  39.790  1.00  0.00           N
ATOM   1452  CA  VAL   190      21.677   5.380  40.055  1.00  0.00           C
ATOM   1453  CB  VAL   190      21.675   6.874  39.916  1.00  0.00           C
ATOM   1454  CG1 VAL   190      21.618   7.214  38.418  1.00  0.00           C
ATOM   1455  CG2 VAL   190      20.446   7.417  40.647  1.00  0.00           C
ATOM   1456  C   VAL   190      22.166   4.947  41.395  1.00  0.00           C
ATOM   1457  O   VAL   190      21.407   4.765  42.347  1.00  0.00           O
ATOM   1458  N   VAL   191      23.487   4.724  41.474  1.00  0.00           N
ATOM   1459  CA  VAL   191      24.084   4.237  42.676  1.00  0.00           C
ATOM   1460  CB  VAL   191      25.218   3.294  42.405  1.00  0.00           C
ATOM   1461  CG1 VAL   191      26.280   4.033  41.577  1.00  0.00           C
ATOM   1462  CG2 VAL   191      25.737   2.766  43.749  1.00  0.00           C
ATOM   1463  C   VAL   191      24.600   5.396  43.467  1.00  0.00           C
ATOM   1464  O   VAL   191      25.071   6.384  42.903  1.00  0.00           O
ATOM   1465  N   LEU   192      24.492   5.299  44.812  1.00  0.00           N
ATOM   1466  CA  LEU   192      24.925   6.351  45.684  1.00  0.00           C
ATOM   1467  CB  LEU   192      23.793   7.016  46.491  1.00  0.00           C
ATOM   1468  CG  LEU   192      23.071   6.153  47.546  1.00  0.00           C
ATOM   1469  CD2 LEU   192      21.694   6.747  47.877  1.00  0.00           C
ATOM   1470  CD1 LEU   192      23.923   5.922  48.805  1.00  0.00           C
ATOM   1471  C   LEU   192      25.909   5.809  46.656  1.00  0.00           C
ATOM   1472  O   LEU   192      25.913   4.622  46.977  1.00  0.00           O
ATOM   1473  N   GLY   193      26.767   6.709  47.162  1.00  0.00           N
ATOM   1474  CA  GLY   193      27.777   6.354  48.104  1.00  0.00           C
ATOM   1475  C   GLY   193      28.890   7.293  47.812  1.00  0.00           C
ATOM   1476  O   GLY   193      28.707   8.265  47.084  1.00  0.00           O
ATOM   1477  N   PRO   194      30.052   7.037  48.319  1.00  0.00           N
ATOM   1478  CA  PRO   194      31.127   7.959  48.097  1.00  0.00           C
ATOM   1479  CD  PRO   194      30.209   6.303  49.560  1.00  0.00           C
ATOM   1480  CB  PRO   194      32.205   7.605  49.129  1.00  0.00           C
ATOM   1481  CG  PRO   194      31.730   6.281  49.763  1.00  0.00           C
ATOM   1482  C   PRO   194      31.613   8.030  46.672  1.00  0.00           C
ATOM   1483  O   PRO   194      31.602   6.990  46.019  1.00  0.00           O
ATOM   1484  N   VAL   195      31.992   9.260  46.203  1.00  0.00           N
ATOM   1485  CA  VAL   195      32.576   9.658  44.936  1.00  0.00           C
ATOM   1486  CB  VAL   195      32.460   8.679  43.801  1.00  0.00           C
ATOM   1487  CG1 VAL   195      33.406   7.489  44.039  1.00  0.00           C
ATOM   1488  CG2 VAL   195      30.979   8.309  43.644  1.00  0.00           C
ATOM   1489  C   VAL   195      31.956  10.936  44.471  1.00  0.00           C
ATOM   1490  O   VAL   195      30.818  11.258  44.810  1.00  0.00           O
ATOM   1491  N   LEU   196      32.721  11.713  43.677  1.00  0.00           N
ATOM   1492  CA  LEU   196      32.205  12.917  43.104  1.00  0.00           C
ATOM   1493  CB  LEU   196      31.868  14.004  44.136  1.00  0.00           C
ATOM   1494  CG  LEU   196      31.487  15.346  43.486  1.00  0.00           C
ATOM   1495  CD2 LEU   196      31.291  16.440  44.546  1.00  0.00           C
ATOM   1496  CD1 LEU   196      30.279  15.194  42.549  1.00  0.00           C
ATOM   1497  C   LEU   196      33.236  13.486  42.196  1.00  0.00           C
ATOM   1498  O   LEU   196      34.223  14.059  42.651  1.00  0.00           O
ATOM   1499  N   GLN   197      33.018  13.368  40.877  1.00  0.00           N
ATOM   1500  CA  GLN   197      33.905  13.992  39.947  1.00  0.00           C
ATOM   1501  CB  GLN   197      33.778  13.445  38.516  1.00  0.00           C
ATOM   1502  CG  GLN   197      34.377  12.044  38.357  1.00  0.00           C
ATOM   1503  CD  GLN   197      33.704  11.097  39.341  1.00  0.00           C
ATOM   1504  OE1 GLN   197      34.293  10.708  40.349  1.00  0.00           O
ATOM   1505  NE2 GLN   197      32.435  10.707  39.048  1.00  0.00           N
ATOM   1506  C   GLN   197      33.480  15.414  39.968  1.00  0.00           C
ATOM   1507  O   GLN   197      32.460  15.735  40.574  1.00  0.00           O
ATOM   1508  N   SER   198      34.258  16.315  39.346  1.00  0.00           N
ATOM   1509  CA  SER   198      33.875  17.694  39.408  1.00  0.00           C
ATOM   1510  CB  SER   198      34.823  18.637  38.648  1.00  0.00           C
ATOM   1511  OG  SER   198      34.365  19.977  38.763  1.00  0.00           O
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ATOM   1512  C   SER   198      32.520  17.821  38.798  1.00  0.00           C
ATOM   1513  O   SER   198      32.167  17.050  37.906  1.00  0.00           O
ATOM   1514  N   SER   199      31.726  18.784  39.314  1.00  0.00           N
ATOM   1515  CA  SER   199      30.404  19.094  38.836  1.00  0.00           C
ATOM   1516  CB  SER   199      30.394  19.963  37.564  1.00  0.00           C
ATOM   1517  OG  SER   199      29.057  20.227  37.170  1.00  0.00           O
ATOM   1518  C   SER   199      29.647  17.837  38.556  1.00  0.00           C
ATOM   1519  O   SER   199      29.455  17.484  37.393  1.00  0.00           O
ATOM   1520  N   ILE   200      29.218  17.100  39.603  1.00  0.00           N
ATOM   1521  CA  ILE   200      28.508  15.898  39.290  1.00  0.00           C
ATOM   1522  CB  ILE   200      28.109  15.050  40.461  1.00  0.00           C
ATOM   1523  CG2 ILE   200      27.083  15.823  41.306  1.00  0.00           C
ATOM   1524  CG1 ILE   200      27.606  13.692  39.933  1.00  0.00           C
ATOM   1525  CD1 ILE   200      27.484  12.603  40.994  1.00  0.00           C
ATOM   1526  C   ILE   200      27.280  16.306  38.566  1.00  0.00           C
ATOM   1527  O   ILE   200      26.552  17.202  38.982  1.00  0.00           O
ATOM   1528  N   ASN   201      27.052  15.668  37.411  1.00  0.00           N
ATOM   1529  CA  ASN   201      25.938  16.055  36.615  1.00  0.00           C
ATOM   1530  CB  ASN   201      25.882  15.288  35.284  1.00  0.00           C
ATOM   1531  CG  ASN   201      27.102  15.700  34.469  1.00  0.00           C
ATOM   1532  OD1 ASN   201      26.586  14.630  34.786  1.00  0.00           O
ATOM   1533  ND2 ASN   201      26.884  17.027  34.671  1.00  0.00           N
ATOM   1534  C   ASN   201      24.691  15.767  37.369  1.00  0.00           C
ATOM   1535  O   ASN   201      23.803  16.612  37.461  1.00  0.00           O
ATOM   1536  N   SER   202      24.587  14.567  37.960  1.00  0.00           N
ATOM   1537  CA  SER   202      23.347  14.332  38.617  1.00  0.00           C
ATOM   1538  CB  SER   202      22.222  13.905  37.665  1.00  0.00           C
ATOM   1539  OG  SER   202      21.957  14.942  36.733  1.00  0.00           O
ATOM   1540  C   SER   202      23.506  13.245  39.600  1.00  0.00           C
ATOM   1541  O   SER   202      24.615  12.853  39.953  1.00  0.00           O
ATOM   1542  N   SER   203      22.341  12.816  40.113  1.00  0.00           N
ATOM   1543  CA  SER   203      22.218  11.723  41.018  1.00  0.00           C
ATOM   1544  CB  SER   203      23.351  10.676  40.988  1.00  0.00           C
ATOM   1545  OG  SER   203      23.394  10.035  39.722  1.00  0.00           O
ATOM   1546  C   SER   203      22.084  12.219  42.405  1.00  0.00           C
ATOM   1547  O   SER   203      21.599  13.323  42.657  1.00  0.00           O
ATOM   1548  N   ILE   204      22.482  11.348  43.345  1.00  0.00           N
ATOM   1549  CA  ILE   204      22.436  11.607  44.746  1.00  0.00           C
ATOM   1550  CB  ILE   204      22.927  10.483  45.601  1.00  0.00           C
ATOM   1551  CG2 ILE   204      22.666  10.867  47.067  1.00  0.00           C
ATOM   1552  CG1 ILE   204      22.283   9.163  45.182  1.00  0.00           C
ATOM   1553  CD1 ILE   204      22.968   8.575  43.947  1.00  0.00           C
ATOM   1554  C   ILE   204      23.397  12.695  45.001  1.00  0.00           C
ATOM   1555  O   ILE   204      23.113  13.573  45.802  1.00  0.00           O
ATOM   1556  N   ILE   205      24.573  12.633  44.347  1.00  0.00           N
ATOM   1557  CA  ILE   205      25.590  13.624  44.532  1.00  0.00           C
ATOM   1558  CB  ILE   205      26.851  13.331  43.779  1.00  0.00           C
ATOM   1559  CG2 ILE   205      27.785  14.534  43.975  1.00  0.00           C
ATOM   1560  CG1 ILE   205      27.472  12.006  44.260  1.00  0.00           C
ATOM   1561  CD1 ILE   205      26.650  10.767  43.906  1.00  0.00           C
ATOM   1562  C   ILE   205      25.024  14.898  44.041  1.00  0.00           C
ATOM   1563  O   ILE   205      25.234  15.955  44.629  1.00  0.00           O
ATOM   1564  N   HIS   206      24.282  14.811  42.930  1.00  0.00           N
ATOM   1565  CA  HIS   206      23.618  15.958  42.405  1.00  0.00           C
ATOM   1566  ND1 HIS   206      22.060  17.787  40.132  1.00  0.00           N
ATOM   1567  CG  HIS   206      21.755  16.603  40.761  1.00  0.00           C
ATOM   1568  NE2 HIS   206      19.842  17.701  40.295  1.00  0.00           N
ATOM   1569  CD2 HIS   206      20.397  16.565  40.852  1.00  0.00           C
ATOM   1570  CE1 HIS   206      20.878  18.403  39.875  1.00  0.00           C
ATOM   1571  CB  HIS   206      22.743  15.578  41.211  1.00  0.00           C
ATOM   1572  C   HIS   206      22.706  16.442  43.470  1.00  0.00           C
ATOM   1573  O   HIS   206      22.694  17.622  43.797  1.00  0.00           O
ATOM   1574  N   ILE   207      21.932  15.534  44.079  1.00  0.00           N
ATOM   1575  CA  ILE   207      20.994  16.029  45.033  1.00  0.00           C
ATOM   1576  CB  ILE   207      20.136  14.956  45.606  1.00  0.00           C
ATOM   1577  CG2 ILE   207      19.104  15.646  46.518  1.00  0.00           C
ATOM   1578  CG1 ILE   207      19.482  14.167  44.467  1.00  0.00           C
ATOM   1579  CD1 ILE   207      19.035  12.784  44.909  1.00  0.00           C
ATOM   1580  C   ILE   207      21.727  16.671  46.170  1.00  0.00           C
ATOM   1581  O   ILE   207      21.386  17.764  46.608  1.00  0.00           O
ATOM   1582  N   LEU   208      22.778  16.002  46.658  1.00  0.00           N
ATOM   1583  CA  LEU   208      23.536  16.403  47.802  1.00  0.00           C
ATOM   1584  CB  LEU   208      24.554  15.301  48.147  1.00  0.00           C
ATOM   1585  CG  LEU   208      25.238  15.415  49.515  1.00  0.00           C
ATOM   1586  CD2 LEU   208      26.183  14.222  49.733  1.00  0.00           C
ATOM   1587  CD1 LEU   208      24.200  15.512  50.643  1.00  0.00           C
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ATOM   1588  C   LEU   208      24.226  17.720  47.552  1.00  0.00           C
ATOM   1589  O   LEU   208      24.220  18.594  48.415  1.00  0.00           O
ATOM   1590  N   LYS   209      24.838  17.900  46.363  1.00  0.00           N
ATOM   1591  CA  LYS   209      25.543  19.110  46.005  1.00  0.00           C
ATOM   1592  CB  LYS   209      26.221  18.992  44.629  1.00  0.00           C
ATOM   1593  CG  LYS   209      26.932  20.256  44.135  1.00  0.00           C
ATOM   1594  CD  LYS   209      28.247  20.598  44.833  1.00  0.00           C
ATOM   1595  CE  LYS   209      28.959  21.800  44.203  1.00  0.00           C
ATOM   1596  NZ  LYS   209      29.229  21.539  42.769  1.00  0.00           N
ATOM   1597  C   LYS   209      24.575  20.239  45.922  1.00  0.00           C
ATOM   1598  O   LYS   209      24.846  21.362  46.347  1.00  0.00           O
ATOM   1599  N   TYR   210      23.411  19.956  45.327  1.00  0.00           N
ATOM   1600  CA  TYR   210      22.391  20.935  45.172  1.00  0.00           C
ATOM   1601  CB  TYR   210      21.334  20.427  44.165  1.00  0.00           C
ATOM   1602  CG  TYR   210      21.976  20.508  42.796  1.00  0.00           C
ATOM   1603  CD1 TYR   210      23.211  19.962  42.515  1.00  0.00           C
ATOM   1604  CD2 TYR   210      21.330  21.107  41.742  1.00  0.00           C
ATOM   1605  CE1 TYR   210      23.780  20.028  41.264  1.00  0.00           C
ATOM   1606  CE2 TYR   210      21.878  21.193  40.483  1.00  0.00           C
ATOM   1607  CZ  TYR   210      23.115  20.653  40.240  1.00  0.00           C
ATOM   1608  OH  TYR   210      23.685  20.734  38.952  1.00  0.00           O
ATOM   1609  C   TYR   210      21.892  21.263  46.557  1.00  0.00           C
ATOM   1610  O   TYR   210      21.673  22.424  46.905  1.00  0.00           O
ATOM   1611  N   LEU   211      21.751  20.240  47.419  1.00  0.00           N
ATOM   1612  CA  LEU   211      21.385  20.494  48.783  1.00  0.00           C
ATOM   1613  CB  LEU   211      21.111  19.232  49.613  1.00  0.00           C
ATOM   1614  CG  LEU   211      19.642  18.771  49.525  1.00  0.00           C
ATOM   1615  CD2 LEU   211      19.196  18.469  48.088  1.00  0.00           C
ATOM   1616  CD1 LEU   211      18.733  19.813  50.195  1.00  0.00           C
ATOM   1617  C   LEU   211      22.471  21.304  49.412  1.00  0.00           C
ATOM   1618  O   LEU   211      22.211  22.126  50.287  1.00  0.00           O
ATOM   1619  N   THR   212      23.722  21.103  48.958  1.00  0.00           N
ATOM   1620  CA  THR   212      24.859  21.819  49.457  1.00  0.00           C
ATOM   1621  CB  THR   212      26.139  21.442  48.769  1.00  0.00           C
ATOM   1622  OG1 THR   212      26.385  20.053  48.916  1.00  0.00           O
ATOM   1623  CG2 THR   212      27.294  22.254  49.379  1.00  0.00           C
ATOM   1624  C   THR   212      24.612  23.264  49.172  1.00  0.00           C
ATOM   1625  O   THR   212      25.080  24.137  49.900  1.00  0.00           O
ATOM   1626  N   GLY   213      23.851  23.562  48.101  1.00  0.00           N
ATOM   1627  CA  GLY   213      23.597  24.934  47.777  1.00  0.00           C
ATOM   1628  C   GLY   213      24.139  25.213  46.419  1.00  0.00           C
ATOM   1629  O   GLY   213      23.980  26.312  45.890  1.00  0.00           O
ATOM   1630  N   SER   214      24.793  24.213  45.808  1.00  0.00           N
ATOM   1631  CA  SER   214      25.300  24.423  44.489  1.00  0.00           C
ATOM   1632  CB  SER   214      25.963  23.170  43.898  1.00  0.00           C
ATOM   1633  OG  SER   214      24.981  22.176  43.644  1.00  0.00           O
ATOM   1634  C   SER   214      24.126  24.740  43.618  1.00  0.00           C
ATOM   1635  O   SER   214      24.198  25.635  42.777  1.00  0.00           O
ATOM   1636  N   ALA   215      23.001  24.017  43.806  1.00  0.00           N
ATOM   1637  CA  ALA   215      21.851  24.259  42.981  1.00  0.00           C
ATOM   1638  CB  ALA   215      22.078  23.945  41.496  1.00  0.00           C
ATOM   1639  C   ALA   215      20.709  23.428  43.492  1.00  0.00           C
ATOM   1640  O   ALA   215      20.702  23.048  44.659  1.00  0.00           O
ATOM   1641  N   LYS   216      19.659  23.174  42.674  1.00  0.00           N
ATOM   1642  CA  LYS   216      18.618  22.344  43.217  1.00  0.00           C
ATOM   1643  CB  LYS   216      17.270  23.065  43.371  1.00  0.00           C
ATOM   1644  CG  LYS   216      16.489  22.598  44.604  1.00  0.00           C
ATOM   1645  CD  LYS   216      16.203  21.101  44.670  1.00  0.00           C
ATOM   1646  CE  LYS   216      15.941  20.604  46.090  1.00  0.00           C
ATOM   1647  NZ  LYS   216      17.169  20.780  46.899  1.00  0.00           N
ATOM   1648  C   LYS   216      18.445  21.172  42.288  1.00  0.00           C
ATOM   1649  O   LYS   216      18.675  21.280  41.085  1.00  0.00           O
ATOM   1650  N   THR   217      18.035  20.008  42.832  1.00  0.00           N
ATOM   1651  CA  THR   217      17.928  18.794  42.073  1.00  0.00           C
ATOM   1652  CB  THR   217      17.677  17.583  42.913  1.00  0.00           C
ATOM   1653  OG1 THR   217      16.373  17.635  43.473  1.00  0.00           O
ATOM   1654  CG2 THR   217      18.704  17.579  44.047  1.00  0.00           C
ATOM   1655  C   THR   217      16.737  18.889  41.198  1.00  0.00           C
ATOM   1656  O   THR   217      16.185  19.965  40.987  1.00  0.00           O
ATOM   1657  N   TYR   218      16.337  17.729  40.645  1.00  0.00           N
ATOM   1658  CA  TYR   218      15.173  17.682  39.822  1.00  0.00           C
ATOM   1659  CB  TYR   218      15.286  16.688  38.657  1.00  0.00           C
ATOM   1660  CG  TYR   218      16.495  16.928  37.814  1.00  0.00           C
ATOM   1661  CD1 TYR   218      17.733  16.526  38.261  1.00  0.00           C
ATOM   1662  CD2 TYR   218      16.399  17.506  36.566  1.00  0.00           C
ATOM   1663  CE1 TYR   218      18.859  16.722  37.494  1.00  0.00           C
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ATOM   1664  CE2 TYR   218      17.522  17.701  35.795  1.00  0.00           C
ATOM   1665  CZ  TYR   218      18.756  17.313  36.257  1.00  0.00           C
ATOM   1666  OH  TYR   218      19.906  17.515  35.463  1.00  0.00           O
ATOM   1667  C   TYR   218      14.145  17.064  40.711  1.00  0.00           C
ATOM   1668  O   TYR   218      14.132  15.850  40.906  1.00  0.00           O
ATOM   1669  N   ALA   219      13.264  17.888  41.298  1.00  0.00           N
ATOM   1670  CA  ALA   219      12.254  17.351  42.149  1.00  0.00           C
ATOM   1671  CB  ALA   219      11.350  18.431  42.761  1.00  0.00           C
ATOM   1672  C   ALA   219      11.396  16.510  41.286  1.00  0.00           C
ATOM   1673  O   ALA   219      11.037  15.391  41.643  1.00  0.00           O
ATOM   1674  N   ASN   220      11.055  17.059  40.110  1.00  0.00           N
ATOM   1675  CA  ASN   220      10.203  16.386  39.189  1.00  0.00           C
ATOM   1676  CB  ASN   220       9.701  17.288  38.048  1.00  0.00           C
ATOM   1677  CG  ASN   220      10.894  17.813  37.264  1.00  0.00           C
ATOM   1678  OD1 ASN   220      11.385  18.909  37.527  1.00  0.00           O
ATOM   1679  ND2 ASN   220      11.376  17.013  36.276  1.00  0.00           N
ATOM   1680  C   ASN   220      10.892  15.204  38.585  1.00  0.00           C
ATOM   1681  O   ASN   220      10.272  14.163  38.399  1.00  0.00           O
ATOM   1682  N   SER   221      12.194  15.309  38.271  1.00  0.00           N
ATOM   1683  CA  SER   221      12.793  14.203  37.582  1.00  0.00           C
ATOM   1684  CB  SER   221      14.228  14.445  37.083  1.00  0.00           C
ATOM   1685  OG  SER   221      14.719  13.291  36.418  1.00  0.00           O
ATOM   1686  C   SER   221      12.800  13.001  38.470  1.00  0.00           C
ATOM   1687  O   SER   221      12.584  13.089  39.679  1.00  0.00           O
ATOM   1688  N   VAL   222      13.016  11.824  37.849  1.00  0.00           N
ATOM   1689  CA  VAL   222      12.995  10.601  38.590  1.00  0.00           C
ATOM   1690  CB  VAL   222      12.196   9.524  37.913  1.00  0.00           C
ATOM   1691  CG1 VAL   222      12.246   8.256  38.780  1.00  0.00           C
ATOM   1692  CG2 VAL   222      10.790  10.050  37.608  1.00  0.00           C
ATOM   1693  C   VAL   222      14.388  10.063  38.618  1.00  0.00           C
ATOM   1694  O   VAL   222      14.998   9.838  37.576  1.00  0.00           O
ATOM   1695  N   GLN   223      14.931   9.834  39.829  1.00  0.00           N
ATOM   1696  CA  GLN   223      16.222   9.228  39.945  1.00  0.00           C
ATOM   1697  CB  GLN   223      17.346  10.227  40.260  1.00  0.00           C
ATOM   1698  CG  GLN   223      17.619  11.214  39.120  1.00  0.00           C
ATOM   1699  CD  GLN   223      18.294  10.445  37.994  1.00  0.00           C
ATOM   1700  OE1 GLN   223      19.404   9.936  38.146  1.00  0.00           O
ATOM   1701  NE2 GLN   223      17.601  10.352  36.827  1.00  0.00           N
ATOM   1702  C   GLN   223      16.114   8.312  41.109  1.00  0.00           C
ATOM   1703  O   GLN   223      15.578   8.713  42.134  1.00  0.00           O
ATOM   1704  N   ALA   224      16.609   7.067  40.998  1.00  0.00           N
ATOM   1705  CA  ALA   224      16.463   6.138  42.088  1.00  0.00           C
ATOM   1706  CB  ALA   224      15.644   4.920  41.682  1.00  0.00           C
ATOM   1707  C   ALA   224      17.827   5.705  42.510  1.00  0.00           C
ATOM   1708  O   ALA   224      18.705   5.500  41.675  1.00  0.00           O
ATOM   1709  N   TYR   225      18.055   5.540  43.827  1.00  0.00           N
ATOM   1710  CA  TYR   225      19.418   5.316  44.195  1.00  0.00           C
ATOM   1711  CB  TYR   225      19.913   6.450  45.103  1.00  0.00           C
ATOM   1712  CG  TYR   225      19.447   7.727  44.475  1.00  0.00           C
ATOM   1713  CD1 TYR   225      20.099   8.301  43.416  1.00  0.00           C
ATOM   1714  CD2 TYR   225      18.320   8.359  44.940  1.00  0.00           C
ATOM   1715  CE1 TYR   225      19.664   9.475  42.844  1.00  0.00           C
ATOM   1716  CE2 TYR   225      17.869   9.532  44.383  1.00  0.00           C
ATOM   1717  CZ  TYR   225      18.541  10.098  43.330  1.00  0.00           C
ATOM   1718  OH  TYR   225      18.077  11.302  42.757  1.00  0.00           O
ATOM   1719  C   TYR   225      19.585   4.021  44.932  1.00  0.00           C
ATOM   1720  O   TYR   225      18.736   3.590  45.712  1.00  0.00           O
ATOM   1721  N   VAL   226      20.728   3.360  44.678  1.00  0.00           N
ATOM   1722  CA  VAL   226      21.050   2.122  45.326  1.00  0.00           C
ATOM   1723  CB  VAL   226      21.222   0.995  44.362  1.00  0.00           C
ATOM   1724  CG1 VAL   226      19.896   0.819  43.615  1.00  0.00           C
ATOM   1725  CG2 VAL   226      22.413   1.304  43.439  1.00  0.00           C
ATOM   1726  C   VAL   226      22.375   2.340  45.971  1.00  0.00           C
ATOM   1727  O   VAL   226      23.221   3.042  45.422  1.00  0.00           O
ATOM   1728  N   HIS   227      22.588   1.748  47.161  1.00  0.00           N
ATOM   1729  CA  HIS   227      23.828   1.940  47.851  1.00  0.00           C
ATOM   1730  ND1 HIS   227      26.277   1.489  50.019  1.00  0.00           N
ATOM   1731  CG  HIS   227      24.948   1.845  50.115  1.00  0.00           C
ATOM   1732  NE2 HIS   227      26.139   3.000  51.647  1.00  0.00           N
ATOM   1733  CD2 HIS   227      24.883   2.767  51.115  1.00  0.00           C
ATOM   1734  CE1 HIS   227      26.943   2.210  50.956  1.00  0.00           C
ATOM   1735  CB  HIS   227      23.854   1.297  49.250  1.00  0.00           C
ATOM   1736  C   HIS   227      24.875   1.289  47.016  1.00  0.00           C
ATOM   1737  O   HIS   227      24.671   0.191  46.501  1.00  0.00           O
ATOM   1738  N   VAL   228      26.033   1.953  46.864  1.00  0.00           N
ATOM   1739  CA  VAL   228      27.063   1.432  46.013  1.00  0.00           C
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ATOM   1740  CB  VAL   228      28.268   2.318  45.914  1.00  0.00           C
ATOM   1741  CG1 VAL   228      28.944   2.405  47.294  1.00  0.00           C
ATOM   1742  CG2 VAL   228      29.177   1.760  44.803  1.00  0.00           C
ATOM   1743  C   VAL   228      27.517   0.113  46.535  1.00  0.00           C
ATOM   1744  O   VAL   228      27.820  -0.802  45.770  1.00  0.00           O
ATOM   1745  N   ARG   229      27.588  -0.018  47.867  1.00  0.00           N
ATOM   1746  CA  ARG   229      28.047  -1.254  48.417  1.00  0.00           C
ATOM   1747  CB  ARG   229      28.013  -1.276  49.956  1.00  0.00           C
ATOM   1748  CG  ARG   229      28.327  -2.657  50.536  1.00  0.00           C
ATOM   1749  CD  ARG   229      27.987  -2.812  52.022  1.00  0.00           C
ATOM   1750  NE  ARG   229      29.002  -2.059  52.811  1.00  0.00           N
ATOM   1751  CZ  ARG   229      29.395  -2.525  54.034  1.00  0.00           C
ATOM   1752  NH1 ARG   229      28.869  -3.685  54.525  1.00  0.00           N
ATOM   1753  NH2 ARG   229      30.320  -1.831  54.760  1.00  0.00           N
ATOM   1754  C   ARG   229      27.124  -2.341  47.976  1.00  0.00           C
ATOM   1755  O   ARG   229      27.559  -3.433  47.615  1.00  0.00           O
ATOM   1756  N   ASP   230      25.810  -2.069  48.010  1.00  0.00           N
ATOM   1757  CA  ASP   230      24.857  -3.089  47.698  1.00  0.00           C
ATOM   1758  CB  ASP   230      23.418  -2.672  48.024  1.00  0.00           C
ATOM   1759  CG  ASP   230      22.693  -3.961  48.356  1.00  0.00           C
ATOM   1760  OD1 ASP   230      22.790  -4.391  49.536  1.00  0.00           O
ATOM   1761  OD2 ASP   230      22.048  -4.541  47.447  1.00  0.00           O
ATOM   1762  C   ASP   230      24.947  -3.459  46.248  1.00  0.00           C
ATOM   1763  O   ASP   230      24.830  -4.630  45.889  1.00  0.00           O
ATOM   1764  N   VAL   231      25.155  -2.467  45.362  1.00  0.00           N
ATOM   1765  CA  VAL   231      25.191  -2.766  43.960  1.00  0.00           C
ATOM   1766  CB  VAL   231      25.282  -1.548  43.086  1.00  0.00           C
ATOM   1767  CG1 VAL   231      26.651  -0.882  43.290  1.00  0.00           C
ATOM   1768  CG2 VAL   231      25.008  -1.981  41.636  1.00  0.00           C
ATOM   1769  C   VAL   231      26.364  -3.653  43.653  1.00  0.00           C
ATOM   1770  O   VAL   231      26.255  -4.587  42.859  1.00  0.00           O
ATOM   1771  N   ALA   232      27.521  -3.383  44.287  1.00  0.00           N
ATOM   1772  CA  ALA   232      28.711  -4.139  44.013  1.00  0.00           C
ATOM   1773  CB  ALA   232      29.923  -3.664  44.835  1.00  0.00           C
ATOM   1774  C   ALA   232      28.465  -5.573  44.359  1.00  0.00           C
ATOM   1775  O   ALA   232      28.872  -6.478  43.632  1.00  0.00           O
ATOM   1776  N   GLU   233      27.776  -5.812  45.484  1.00  0.00           N
ATOM   1777  CA  GLU   233      27.506  -7.142  45.941  1.00  0.00           C
ATOM   1778  CB  GLU   233      26.649  -7.118  47.221  1.00  0.00           C
ATOM   1779  CG  GLU   233      26.596  -8.430  48.002  1.00  0.00           C
ATOM   1780  CD  GLU   233      27.653  -8.361  49.095  1.00  0.00           C
ATOM   1781  OE1 GLU   233      28.867  -8.356  48.751  1.00  0.00           O
ATOM   1782  OE2 GLU   233      27.258  -8.310  50.290  1.00  0.00           O
ATOM   1783  C   GLU   233      26.688  -7.838  44.893  1.00  0.00           C
ATOM   1784  O   GLU   233      26.929  -9.001  44.572  1.00  0.00           O
ATOM   1785  N   ALA   234      25.692  -7.134  44.326  1.00  0.00           N
ATOM   1786  CA  ALA   234      24.795  -7.710  43.360  1.00  0.00           C
ATOM   1787  CB  ALA   234      23.697  -6.733  42.908  1.00  0.00           C
ATOM   1788  C   ALA   234      25.548  -8.126  42.139  1.00  0.00           C
ATOM   1789  O   ALA   234      25.275  -9.173  41.556  1.00  0.00           O
ATOM   1790  N   HIS   235      26.518  -7.308  41.707  1.00  0.00           N
ATOM   1791  CA  HIS   235      27.233  -7.628  40.511  1.00  0.00           C
ATOM   1792  ND1 HIS   235      26.867  -4.867  38.860  1.00  0.00           N
ATOM   1793  CG  HIS   235      27.688  -5.193  39.915  1.00  0.00           C
ATOM   1794  NE2 HIS   235      27.133  -3.010  40.053  1.00  0.00           N
ATOM   1795  CD2 HIS   235      27.842  -4.048  40.634  1.00  0.00           C
ATOM   1796  CE1 HIS   235      26.565  -3.550  38.991  1.00  0.00           C
ATOM   1797  CB  HIS   235      28.271  -6.559  40.136  1.00  0.00           C
ATOM   1798  C   HIS   235      27.978  -8.907  40.710  1.00  0.00           C
ATOM   1799  O   HIS   235      28.005  -9.756  39.820  1.00  0.00           O
ATOM   1800  N   ILE   236      28.609  -9.088  41.886  1.00  0.00           N
ATOM   1801  CA  ILE   236      29.388 -10.275  42.049  1.00  0.00           C
ATOM   1802  CB  ILE   236      30.175 -10.322  43.330  1.00  0.00           C
ATOM   1803  CG2 ILE   236      29.218 -10.497  44.518  1.00  0.00           C
ATOM   1804  CG1 ILE   236      31.240 -11.427  43.243  1.00  0.00           C
ATOM   1805  CD1 ILE   236      32.282 -11.347  44.356  1.00  0.00           C
ATOM   1806  C   ILE   236      28.506 -11.483  41.977  1.00  0.00           C
ATOM   1807  O   ILE   236      28.855 -12.469  41.330  1.00  0.00           O
ATOM   1808  N   LEU   237      27.338 -11.458  42.647  1.00  0.00           N
ATOM   1809  CA  LEU   237      26.515 -12.630  42.598  1.00  0.00           C
ATOM   1810  CB  LEU   237      25.389 -12.683  43.640  1.00  0.00           C
ATOM   1811  CG  LEU   237      25.952 -12.939  45.052  1.00  0.00           C
ATOM   1812  CD2 LEU   237      27.110 -13.952  45.020  1.00  0.00           C
ATOM   1813  CD1 LEU   237      24.845 -13.346  46.032  1.00  0.00           C
ATOM   1814  C   LEU   237      25.968 -12.856  41.225  1.00  0.00           C
ATOM   1815  O   LEU   237      25.905 -13.996  40.769  1.00  0.00           O
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ATOM   1816  N   VAL   238      25.559 -11.791  40.513  1.00  0.00           N
ATOM   1817  CA  VAL   238      25.032 -11.997  39.193  1.00  0.00           C
ATOM   1818  CB  VAL   238      24.561 -10.726  38.535  1.00  0.00           C
ATOM   1819  CG1 VAL   238      25.765  -9.815  38.236  1.00  0.00           C
ATOM   1820  CG2 VAL   238      23.749 -11.110  37.287  1.00  0.00           C
ATOM   1821  C   VAL   238      26.124 -12.596  38.363  1.00  0.00           C
ATOM   1822  O   VAL   238      25.901 -13.475  37.538  1.00  0.00           O
ATOM   1823  N   TYR   239      27.365 -12.136  38.552  1.00  0.00           N
ATOM   1824  CA  TYR   239      28.429 -12.723  37.799  1.00  0.00           C
ATOM   1825  CB  TYR   239      29.794 -12.069  38.074  1.00  0.00           C
ATOM   1826  CG  TYR   239      30.798 -13.143  37.826  1.00  0.00           C
ATOM   1827  CD1 TYR   239      31.124 -13.553  36.555  1.00  0.00           C
ATOM   1828  CD2 TYR   239      31.416 -13.748  38.899  1.00  0.00           C
ATOM   1829  CE1 TYR   239      32.046 -14.556  36.364  1.00  0.00           C
ATOM   1830  CE2 TYR   239      32.339 -14.749  38.717  1.00  0.00           C
ATOM   1831  CZ  TYR   239      32.653 -15.154  37.443  1.00  0.00           C
ATOM   1832  OH  TYR   239      33.597 -16.183  37.240  1.00  0.00           O
ATOM   1833  C   TYR   239      28.583 -14.167  38.145  1.00  0.00           C
ATOM   1834  O   TYR   239      28.725 -15.008  37.260  1.00  0.00           O
ATOM   1835  N   GLU   240      28.585 -14.495  39.448  1.00  0.00           N
ATOM   1836  CA  GLU   240      28.831 -15.852  39.831  1.00  0.00           C
ATOM   1837  CB  GLU   240      29.029 -16.024  41.347  1.00  0.00           C
ATOM   1838  CG  GLU   240      30.311 -15.363  41.862  1.00  0.00           C
ATOM   1839  CD  GLU   240      30.412 -15.606  43.361  1.00  0.00           C
ATOM   1840  OE1 GLU   240      30.422 -16.799  43.767  1.00  0.00           O
ATOM   1841  OE2 GLU   240      30.490 -14.604  44.122  1.00  0.00           O
ATOM   1842  C   GLU   240      27.721 -16.770  39.418  1.00  0.00           C
ATOM   1843  O   GLU   240      27.983 -17.835  38.864  1.00  0.00           O
ATOM   1844  N   SER   241      26.449 -16.408  39.680  1.00  0.00           N
ATOM   1845  CA  SER   241      25.415 -17.362  39.381  1.00  0.00           C
ATOM   1846  CB  SER   241      24.077 -17.092  40.110  1.00  0.00           C
ATOM   1847  OG  SER   241      24.253 -17.181  41.516  1.00  0.00           O
ATOM   1848  C   SER   241      25.212 -17.540  37.893  1.00  0.00           C
ATOM   1849  O   SER   241      25.240 -18.677  37.431  1.00  0.00           O
ATOM   1850  N   PRO   242      25.000 -16.505  37.112  1.00  0.00           N
ATOM   1851  CA  PRO   242      24.844 -16.722  35.688  1.00  0.00           C
ATOM   1852  CD  PRO   242      24.012 -15.526  37.559  1.00  0.00           C
ATOM   1853  CB  PRO   242      24.093 -15.510  35.146  1.00  0.00           C
ATOM   1854  CG  PRO   242      23.212 -15.087  36.326  1.00  0.00           C
ATOM   1855  C   PRO   242      26.021 -17.099  34.830  1.00  0.00           C
ATOM   1856  O   PRO   242      25.804 -17.366  33.647  1.00  0.00           O
ATOM   1857  N   SER   243      27.263 -17.111  35.343  1.00  0.00           N
ATOM   1858  CA  SER   243      28.354 -17.395  34.455  1.00  0.00           C
ATOM   1859  CB  SER   243      29.731 -17.379  35.142  1.00  0.00           C
ATOM   1860  OG  SER   243      29.825 -18.456  36.061  1.00  0.00           O
ATOM   1861  C   SER   243      28.169 -18.747  33.839  1.00  0.00           C
ATOM   1862  O   SER   243      27.705 -19.693  34.475  1.00  0.00           O
ATOM   1863  N   ALA   244      28.544 -18.852  32.549  1.00  0.00           N
ATOM   1864  CA  ALA   244      28.477 -20.080  31.814  1.00  0.00           C
ATOM   1865  CB  ALA   244      29.278 -21.218  32.474  1.00  0.00           C
ATOM   1866  C   ALA   244      27.056 -20.523  31.670  1.00  0.00           C
ATOM   1867  O   ALA   244      26.797 -21.661  31.284  1.00  0.00           O
ATOM   1868  N   SER   245      26.087 -19.626  31.929  1.00  0.00           N
ATOM   1869  CA  SER   245      24.727 -20.040  31.755  1.00  0.00           C
ATOM   1870  CB  SER   245      23.822 -19.693  32.950  1.00  0.00           C
ATOM   1871  OG  SER   245      24.254 -20.380  34.115  1.00  0.00           O
ATOM   1872  C   SER   245      24.213 -19.287  30.576  1.00  0.00           C
ATOM   1873  O   SER   245      24.074 -18.066  30.618  1.00  0.00           O
ATOM   1874  N   GLY   246      23.923 -20.006  29.477  1.00  0.00           N
ATOM   1875  CA  GLY   246      23.455 -19.347  28.298  1.00  0.00           C
ATOM   1876  C   GLY   246      22.053 -18.887  28.521  1.00  0.00           C
ATOM   1877  O   GLY   246      21.195 -19.676  28.910  1.00  0.00           O
ATOM   1878  N   ARG   247      21.806 -17.586  28.256  1.00  0.00           N
ATOM   1879  CA  ARG   247      20.504 -16.985  28.355  1.00  0.00           C
ATOM   1880  CB  ARG   247      19.593 -17.544  29.466  1.00  0.00           C
ATOM   1881  CG  ARG   247      20.176 -17.452  30.878  1.00  0.00           C
ATOM   1882  CD  ARG   247      19.393 -18.283  31.896  1.00  0.00           C
ATOM   1883  NE  ARG   247      19.603 -19.714  31.538  1.00  0.00           N
ATOM   1884  CZ  ARG   247      18.714 -20.667  31.943  1.00  0.00           C
ATOM   1885  NH1 ARG   247      17.625 -20.318  32.688  1.00  0.00           N
ATOM   1886  NH2 ARG   247      18.908 -21.970  31.587  1.00  0.00           N
ATOM   1887  C   ARG   247      20.697 -15.533  28.629  1.00  0.00           C
ATOM   1888  O   ARG   247      21.810 -15.084  28.901  1.00  0.00           O
ATOM   1889  N   TYR   248      19.599 -14.756  28.544  1.00  0.00           N
ATOM   1890  CA  TYR   248      19.693 -13.367  28.866  1.00  0.00           C
ATOM   1891  CB  TYR   248      19.227 -12.424  27.732  1.00  0.00           C
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ATOM   1892  CG  TYR   248      17.831 -12.765  27.345  1.00  0.00           C
ATOM   1893  CD1 TYR   248      17.598 -13.809  26.482  1.00  0.00           C
ATOM   1894  CD2 TYR   248      16.760 -12.056  27.840  1.00  0.00           C
ATOM   1895  CE1 TYR   248      16.316 -14.144  26.115  1.00  0.00           C
ATOM   1896  CE2 TYR   248      15.477 -12.389  27.480  1.00  0.00           C
ATOM   1897  CZ  TYR   248      15.252 -13.435  26.618  1.00  0.00           C
ATOM   1898  OH  TYR   248      13.934 -13.775  26.251  1.00  0.00           O
ATOM   1899  C   TYR   248      18.867 -13.175  30.091  1.00  0.00           C
ATOM   1900  O   TYR   248      17.649 -13.336  30.083  1.00  0.00           O
ATOM   1901  N   LEU   249      19.531 -12.857  31.213  1.00  0.00           N
ATOM   1902  CA  LEU   249      18.781 -12.660  32.414  1.00  0.00           C
ATOM   1903  CB  LEU   249      19.372 -13.339  33.661  1.00  0.00           C
ATOM   1904  CG  LEU   249      18.543 -13.090  34.936  1.00  0.00           C
ATOM   1905  CD2 LEU   249      19.303 -13.553  36.188  1.00  0.00           C
ATOM   1906  CD1 LEU   249      17.134 -13.694  34.832  1.00  0.00           C
ATOM   1907  C   LEU   249      18.758 -11.198  32.670  1.00  0.00           C
ATOM   1908  O   LEU   249      19.792 -10.532  32.642  1.00  0.00           O
ATOM   1909  N   CYS   250      17.558 -10.647  32.909  1.00  0.00           N
ATOM   1910  CA  CYS   250      17.498  -9.239  33.139  1.00  0.00           C
ATOM   1911  CB  CYS   250      16.549  -8.519  32.169  1.00  0.00           C
ATOM   1912  SG  CYS   250      16.627  -6.720  32.359  1.00  0.00           S
ATOM   1913  C   CYS   250      16.988  -9.036  34.526  1.00  0.00           C
ATOM   1914  O   CYS   250      15.945  -9.570  34.898  1.00  0.00           O
ATOM   1915  N   ALA   251      17.724  -8.262  35.347  1.00  0.00           N
ATOM   1916  CA  ALA   251      17.245  -8.057  36.678  1.00  0.00           C
ATOM   1917  CB  ALA   251      18.022  -8.859  37.736  1.00  0.00           C
ATOM   1918  C   ALA   251      17.394  -6.614  37.011  1.00  0.00           C
ATOM   1919  O   ALA   251      18.397  -5.985  36.677  1.00  0.00           O
ATOM   1920  N   GLU   252      16.375  -6.045  37.679  1.00  0.00           N
ATOM   1921  CA  GLU   252      16.503  -4.681  38.067  1.00  0.00           C
ATOM   1922  CB  GLU   252      15.165  -4.033  38.462  1.00  0.00           C
ATOM   1923  CG  GLU   252      14.115  -4.108  37.353  1.00  0.00           C
ATOM   1924  CD  GLU   252      14.736  -3.573  36.072  1.00  0.00           C
ATOM   1925  OE1 GLU   252      15.376  -2.489  36.126  1.00  0.00           O
ATOM   1926  OE2 GLU   252      14.569  -4.241  35.017  1.00  0.00           O
ATOM   1927  C   GLU   252      17.362  -4.734  39.279  1.00  0.00           C
ATOM   1928  O   GLU   252      17.130  -5.552  40.163  1.00  0.00           O
ATOM   1929  N   SER   253      18.405  -3.893  39.354  1.00  0.00           N
ATOM   1930  CA  SER   253      19.186  -3.914  40.552  1.00  0.00           C
ATOM   1931  CB  SER   253      20.682  -4.183  40.317  1.00  0.00           C
ATOM   1932  OG  SER   253      20.875  -5.496  39.811  1.00  0.00           O
ATOM   1933  C   SER   253      19.069  -2.548  41.075  1.00  0.00           C
ATOM   1934  O   SER   253      19.807  -1.648  40.678  1.00  0.00           O
ATOM   1935  N   VAL   254      18.126  -2.351  42.000  1.00  0.00           N
ATOM   1936  CA  VAL   254      17.951  -0.999  42.369  1.00  0.00           C
ATOM   1937  CB  VAL   254      17.081  -0.220  41.418  1.00  0.00           C
ATOM   1938  CG1 VAL   254      17.667  -0.120  40.001  1.00  0.00           C
ATOM   1939  CG2 VAL   254      15.719  -0.917  41.443  1.00  0.00           C
ATOM   1940  C   VAL   254      17.120  -0.951  43.570  1.00  0.00           C
ATOM   1941  O   VAL   254      16.858  -1.922  44.279  1.00  0.00           O
ATOM   1942  N   LEU   255      16.744   0.302  43.769  1.00  0.00           N
ATOM   1943  CA  LEU   255      15.726   0.839  44.572  1.00  0.00           C
ATOM   1944  CB  LEU   255      16.312   1.688  45.704  1.00  0.00           C
ATOM   1945  CG  LEU   255      17.116   0.846  46.714  1.00  0.00           C
ATOM   1946  CD2 LEU   255      16.287  -0.340  47.238  1.00  0.00           C
ATOM   1947  CD1 LEU   255      17.693   1.716  47.842  1.00  0.00           C
ATOM   1948  C   LEU   255      15.221   1.766  43.495  1.00  0.00           C
ATOM   1949  O   LEU   255      15.934   2.717  43.231  1.00  0.00           O
ATOM   1950  N   HIS   256      14.085   1.464  42.798  1.00  0.00           N
ATOM   1951  CA  HIS   256      13.401   2.137  41.690  1.00  0.00           C
ATOM   1952  ND1 HIS   256      12.285  -0.944  39.752  1.00  0.00           N
ATOM   1953  CG  HIS   256      12.888   0.254  40.060  1.00  0.00           C
ATOM   1954  NE2 HIS   256      14.161  -0.849  38.560  1.00  0.00           N
ATOM   1955  CD2 HIS   256      14.028   0.299  39.318  1.00  0.00           C
ATOM   1956  CE1 HIS   256      13.090  -1.563  38.854  1.00  0.00           C
ATOM   1957  CB  HIS   256      12.327   1.259  41.022  1.00  0.00           C
ATOM   1958  C   HIS   256      12.770   3.551  41.796  1.00  0.00           C
ATOM   1959  O   HIS   256      13.084   4.355  40.923  1.00  0.00           O
ATOM   1960  N   ARG   257      11.869   3.957  42.751  1.00  0.00           N
ATOM   1961  CA  ARG   257      11.368   5.346  42.709  1.00  0.00           C
ATOM   1962  CB  ARG   257      10.252   5.472  41.652  1.00  0.00           C
ATOM   1963  CG  ARG   257       9.412   6.747  41.574  1.00  0.00           C
ATOM   1964  CD  ARG   257      10.063   7.931  40.868  1.00  0.00           C
ATOM   1965  NE  ARG   257       9.020   8.994  40.838  1.00  0.00           N
ATOM   1966  CZ  ARG   257       8.023   8.931  39.909  1.00  0.00           C
ATOM   1967  NH1 ARG   257       7.973   7.872  39.048  1.00  0.00           N
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ATOM   1968  NH2 ARG   257       7.070   9.908  39.859  1.00  0.00           N
ATOM   1969  C   ARG   257      10.813   5.882  44.036  1.00  0.00           C
ATOM   1970  O   ARG   257      10.681   5.172  45.027  1.00  0.00           O
ATOM   1971  N   GLY   258      10.533   7.219  44.094  1.00  0.00           N
ATOM   1972  CA  GLY   258       9.854   7.912  45.177  1.00  0.00           C
ATOM   1973  C   GLY   258      10.642   8.392  46.375  1.00  0.00           C
ATOM   1974  O   GLY   258      11.344   9.403  46.350  1.00  0.00           O
ATOM   1975  N   ASP   259      10.493   7.659  47.491  1.00  0.00           N
ATOM   1976  CA  ASP   259      10.848   8.073  48.821  1.00  0.00           C
ATOM   1977  CB  ASP   259      10.504   7.034  49.899  1.00  0.00           C
ATOM   1978  CG  ASP   259       8.989   7.057  50.064  1.00  0.00           C
ATOM   1979  OD1 ASP   259       8.340   7.951  49.458  1.00  0.00           O
ATOM   1980  OD2 ASP   259       8.464   6.185  50.806  1.00  0.00           O
ATOM   1981  C   ASP   259      12.270   8.504  49.003  1.00  0.00           C
ATOM   1982  O   ASP   259      12.571   9.130  50.017  1.00  0.00           O
ATOM   1983  N   VAL   260      13.196   8.179  48.086  1.00  0.00           N
ATOM   1984  CA  VAL   260      14.556   8.608  48.288  1.00  0.00           C
ATOM   1985  CB  VAL   260      15.465   8.296  47.155  1.00  0.00           C
ATOM   1986  CG1 VAL   260      16.707   9.188  47.249  1.00  0.00           C
ATOM   1987  CG2 VAL   260      15.780   6.792  47.161  1.00  0.00           C
ATOM   1988  C   VAL   260      14.619  10.077  48.458  1.00  0.00           C
ATOM   1989  O   VAL   260      15.446  10.571  49.226  1.00  0.00           O
ATOM   1990  N   VAL   261      13.772  10.821  47.732  1.00  0.00           N
ATOM   1991  CA  VAL   261      13.803  12.231  47.951  1.00  0.00           C
ATOM   1992  CB  VAL   261      12.750  13.035  47.257  1.00  0.00           C
ATOM   1993  CG1 VAL   261      11.361  12.385  47.414  1.00  0.00           C
ATOM   1994  CG2 VAL   261      12.824  14.434  47.880  1.00  0.00           C
ATOM   1995  C   VAL   261      13.494  12.459  49.372  1.00  0.00           C
ATOM   1996  O   VAL   261      14.160  13.260  50.013  1.00  0.00           O
ATOM   1997  N   ASP   262      12.500  11.741  49.908  1.00  0.00           N
ATOM   1998  CA  ASP   262      12.125  11.974  51.264  1.00  0.00           C
ATOM   1999  CB  ASP   262      11.002  11.035  51.737  1.00  0.00           C
ATOM   2000  CG  ASP   262      10.491  11.519  53.091  1.00  0.00           C
ATOM   2001  OD1 ASP   262      11.126  12.437  53.677  1.00  0.00           O
ATOM   2002  OD2 ASP   262       9.450  10.973  53.550  1.00  0.00           O
ATOM   2003  C   ASP   262      13.318  11.714  52.115  1.00  0.00           C
ATOM   2004  O   ASP   262      13.590  12.457  53.053  1.00  0.00           O
ATOM   2005  N   SER   263      14.076  10.653  51.806  1.00  0.00           N
ATOM   2006  CA  SER   263      15.190  10.340  52.650  1.00  0.00           C
ATOM   2007  CB  SER   263      15.905   9.051  52.214  1.00  0.00           C
ATOM   2008  OG  SER   263      15.014   7.948  52.290  1.00  0.00           O
ATOM   2009  C   SER   263      16.216  11.435  52.642  1.00  0.00           C
ATOM   2010  O   SER   263      16.572  11.965  53.695  1.00  0.00           O
ATOM   2011  N   LEU   264      16.746  11.800  51.457  1.00  0.00           N
ATOM   2012  CA  LEU   264      17.790  12.788  51.464  1.00  0.00           C
ATOM   2013  CB  LEU   264      18.492  12.977  50.110  1.00  0.00           C
ATOM   2014  CG  LEU   264      19.598  14.046  50.203  1.00  0.00           C
ATOM   2015  CD2 LEU   264      20.278  14.288  48.850  1.00  0.00           C
ATOM   2016  CD1 LEU   264      20.621  13.681  51.289  1.00  0.00           C
ATOM   2017  C   LEU   264      17.229  14.103  51.877  1.00  0.00           C
ATOM   2018  O   LEU   264      17.846  14.849  52.628  1.00  0.00           O
ATOM   2019  N   ALA   265      16.023  14.415  51.394  1.00  0.00           N
ATOM   2020  CA  ALA   265      15.398  15.663  51.689  1.00  0.00           C
ATOM   2021  CB  ALA   265      14.001  15.791  51.062  1.00  0.00           C
ATOM   2022  C   ALA   265      15.221  15.732  53.160  1.00  0.00           C
ATOM   2023  O   ALA   265      15.360  16.781  53.780  1.00  0.00           O
ATOM   2024  N   SER   266      14.871  14.610  53.786  1.00  0.00           N
ATOM   2025  CA  SER   266      14.727  14.744  55.192  1.00  0.00           C
ATOM   2026  CB  SER   266      14.170  13.479  55.877  1.00  0.00           C
ATOM   2027  OG  SER   266      15.083  12.398  55.758  1.00  0.00           O
ATOM   2028  C   SER   266      16.063  15.049  55.791  1.00  0.00           C
ATOM   2029  O   SER   266      16.236  16.066  56.461  1.00  0.00           O
ATOM   2030  N   MET   267      17.054  14.171  55.549  1.00  0.00           N
ATOM   2031  CA  MET   267      18.300  14.313  56.241  1.00  0.00           C
ATOM   2032  CB  MET   267      19.239  13.118  56.007  1.00  0.00           C
ATOM   2033  CG  MET   267      18.643  11.798  56.499  1.00  0.00           C
ATOM   2034  SD  MET   267      18.232  11.761  58.270  1.00  0.00           S
ATOM   2035  CE  MET   267      19.957  11.685  58.828  1.00  0.00           C
ATOM   2036  C   MET   267      19.044  15.557  55.890  1.00  0.00           C
ATOM   2037  O   MET   267      19.464  16.304  56.771  1.00  0.00           O
ATOM   2038  N   PHE   268      19.256  15.808  54.592  1.00  0.00           N
ATOM   2039  CA  PHE   268      20.060  16.927  54.216  1.00  0.00           C
ATOM   2040  CB  PHE   268      20.646  16.833  52.792  1.00  0.00           C
ATOM   2041  CG  PHE   268      21.768  17.813  52.747  1.00  0.00           C
ATOM   2042  CD1 PHE   268      21.538  19.151  52.523  1.00  0.00           C
ATOM   2043  CD2 PHE   268      23.057  17.391  52.968  1.00  0.00           C
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ATOM   2044  CE1 PHE   268      22.580  20.048  52.491  1.00  0.00           C
ATOM   2045  CE2 PHE   268      24.104  18.280  52.938  1.00  0.00           C
ATOM   2046  CZ  PHE   268      23.866  19.611  52.698  1.00  0.00           C
ATOM   2047  C   PHE   268      19.321  18.203  54.362  1.00  0.00           C
ATOM   2048  O   PHE   268      19.912  19.186  54.798  1.00  0.00           O
ATOM   2049  N   PRO   269      18.085  18.256  53.939  1.00  0.00           N
ATOM   2050  CA  PRO   269      17.390  19.491  54.127  1.00  0.00           C
ATOM   2051  CD  PRO   269      17.758  17.670  52.646  1.00  0.00           C
ATOM   2052  CB  PRO   269      16.179  19.416  53.216  1.00  0.00           C
ATOM   2053  CG  PRO   269      16.675  18.570  52.035  1.00  0.00           C
ATOM   2054  C   PRO   269      17.079  19.780  55.546  1.00  0.00           C
ATOM   2055  O   PRO   269      15.916  19.654  55.928  1.00  0.00           O
ATOM   2056  N   GLN   270      18.085  20.211  56.322  1.00  0.00           N
ATOM   2057  CA  GLN   270      17.856  20.603  57.669  1.00  0.00           C
ATOM   2058  CB  GLN   270      19.162  20.965  58.394  1.00  0.00           C
ATOM   2059  CG  GLN   270      18.981  21.422  59.842  1.00  0.00           C
ATOM   2060  CD  GLN   270      20.366  21.738  60.396  1.00  0.00           C
ATOM   2061  OE1 GLN   270      21.330  21.024  60.121  1.00  0.00           O
ATOM   2062  NE2 GLN   270      20.477  22.848  61.175  1.00  0.00           N
ATOM   2063  C   GLN   270      17.067  21.854  57.546  1.00  0.00           C
ATOM   2064  O   GLN   270      16.024  22.028  58.171  1.00  0.00           O
ATOM   2065  N   TYR   271      17.581  22.762  56.697  1.00  0.00           N
ATOM   2066  CA  TYR   271      16.896  23.979  56.404  1.00  0.00           C
ATOM   2067  CB  TYR   271      17.611  25.194  57.019  1.00  0.00           C
ATOM   2068  CG  TYR   271      16.866  26.443  56.705  1.00  0.00           C
ATOM   2069  CD1 TYR   271      15.690  26.733  57.357  1.00  0.00           C
ATOM   2070  CD2 TYR   271      17.357  27.336  55.784  1.00  0.00           C
ATOM   2071  CE1 TYR   271      15.001  27.890  57.082  1.00  0.00           C
ATOM   2072  CE2 TYR   271      16.673  28.496  55.506  1.00  0.00           C
ATOM   2073  CZ  TYR   271      15.493  28.775  56.152  1.00  0.00           C
ATOM   2074  OH  TYR   271      14.792  29.965  55.863  1.00  0.00           O
ATOM   2075  C   TYR   271      16.933  24.097  54.914  1.00  0.00           C
ATOM   2076  O   TYR   271      17.851  24.677  54.342  1.00  0.00           O
ATOM   2077  N   PRO   272      15.955  23.488  54.306  1.00  0.00           N
ATOM   2078  CA  PRO   272      15.807  23.440  52.873  1.00  0.00           C
ATOM   2079  CD  PRO   272      15.304  22.357  54.945  1.00  0.00           C
ATOM   2080  CB  PRO   272      14.995  22.189  52.563  1.00  0.00           C
ATOM   2081  CG  PRO   272      14.323  21.823  53.896  1.00  0.00           C
ATOM   2082  C   PRO   272      15.143  24.610  52.220  1.00  0.00           C
ATOM   2083  O   PRO   272      14.985  24.557  51.003  1.00  0.00           O
ATOM   2084  N   ILE   273      14.712  25.644  52.962  1.00  0.00           N
ATOM   2085  CA  ILE   273      13.889  26.636  52.330  1.00  0.00           C
ATOM   2086  CB  ILE   273      13.494  27.748  53.258  1.00  0.00           C
ATOM   2087  CG2 ILE   273      12.818  28.841  52.416  1.00  0.00           C
ATOM   2088  CG1 ILE   273      12.607  27.210  54.393  1.00  0.00           C
ATOM   2089  CD1 ILE   273      11.303  26.597  53.887  1.00  0.00           C
ATOM   2090  C   ILE   273      14.574  27.253  51.152  1.00  0.00           C
ATOM   2091  O   ILE   273      13.967  27.357  50.087  1.00  0.00           O
ATOM   2092  N   PRO   274      15.804  27.644  51.262  1.00  0.00           N
ATOM   2093  CA  PRO   274      16.480  28.263  50.159  1.00  0.00           C
ATOM   2094  CD  PRO   274      16.428  27.950  52.537  1.00  0.00           C
ATOM   2095  CB  PRO   274      17.729  28.924  50.748  1.00  0.00           C
ATOM   2096  CG  PRO   274      17.870  28.320  52.158  1.00  0.00           C
ATOM   2097  C   PRO   274      16.793  27.331  49.026  1.00  0.00           C
ATOM   2098  O   PRO   274      17.101  27.825  47.943  1.00  0.00           O
ATOM   2099  N   THR   275      16.753  26.000  49.230  1.00  0.00           N
ATOM   2100  CA  THR   275      17.201  25.140  48.170  1.00  0.00           C
ATOM   2101  CB  THR   275      17.312  23.700  48.576  1.00  0.00           C
ATOM   2102  OG1 THR   275      16.041  23.199  48.965  1.00  0.00           O
ATOM   2103  CG2 THR   275      18.302  23.599  49.748  1.00  0.00           C
ATOM   2104  C   THR   275      16.320  25.216  46.963  1.00  0.00           C
ATOM   2105  O   THR   275      15.296  24.544  46.869  1.00  0.00           O
ATOM   2106  N   LYS   276      16.723  26.032  45.973  1.00  0.00           N
ATOM   2107  CA  LYS   276      15.990  26.088  44.743  1.00  0.00           C
ATOM   2108  CB  LYS   276      14.775  27.039  44.734  1.00  0.00           C
ATOM   2109  CG  LYS   276      13.539  26.510  45.466  1.00  0.00           C
ATOM   2110  CD  LYS   276      13.562  26.665  46.989  1.00  0.00           C
ATOM   2111  CE  LYS   276      12.626  27.767  47.491  1.00  0.00           C
ATOM   2112  NZ  LYS   276      11.243  27.486  47.049  1.00  0.00           N
ATOM   2113  C   LYS   276      16.918  26.605  43.701  1.00  0.00           C
ATOM   2114  O   LYS   276      17.597  27.609  43.901  1.00  0.00           O
ATOM   2115  N   VAL   277      16.979  25.922  42.546  1.00  0.00           N
ATOM   2116  CA  VAL   277      17.806  26.406  41.488  1.00  0.00           C
ATOM   2117  CB  VAL   277      19.199  25.871  41.544  1.00  0.00           C
ATOM   2118  CG1 VAL   277      19.957  26.320  40.284  1.00  0.00           C
ATOM   2119  CG2 VAL   277      19.819  26.379  42.857  1.00  0.00           C
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ATOM   2120  C   VAL   277      17.172  25.991  40.207  1.00  0.00           C
ATOM   2121  O   VAL   277      16.463  24.987  40.147  1.00  0.00           O
ATOM   2122  N   LYS   278      17.393  26.783  39.141  1.00  0.00           N
ATOM   2123  CA  LYS   278      16.795  26.424  37.895  1.00  0.00           C
ATOM   2124  CB  LYS   278      16.381  27.600  36.997  1.00  0.00           C
ATOM   2125  CG  LYS   278      15.685  27.120  35.721  1.00  0.00           C
ATOM   2126  CD  LYS   278      14.904  28.209  34.985  1.00  0.00           C
ATOM   2127  CE  LYS   278      14.112  27.685  33.784  1.00  0.00           C
ATOM   2128  NZ  LYS   278      13.365  28.796  33.150  1.00  0.00           N
ATOM   2129  C   LYS   278      17.761  25.610  37.112  1.00  0.00           C
ATOM   2130  O   LYS   278      18.972  25.816  37.166  1.00  0.00           O
ATOM   2131  N   GLU   279      17.202  24.639  36.376  1.00  0.00           N
ATOM   2132  CA  GLU   279      17.883  23.743  35.497  1.00  0.00           C
ATOM   2133  CB  GLU   279      18.951  22.853  36.158  1.00  0.00           C
ATOM   2134  CG  GLU   279      20.295  23.551  36.370  1.00  0.00           C
ATOM   2135  CD  GLU   279      20.954  23.707  35.005  1.00  0.00           C
ATOM   2136  OE1 GLU   279      20.620  24.699  34.299  1.00  0.00           O
ATOM   2137  OE2 GLU   279      21.791  22.841  34.642  1.00  0.00           O
ATOM   2138  C   GLU   279      16.801  22.845  35.033  1.00  0.00           C
ATOM   2139  O   GLU   279      15.637  23.057  35.370  1.00  0.00           O
ATOM   2140  N   ASP   280      17.131  21.824  34.230  1.00  0.00           N
ATOM   2141  CA  ASP   280      16.056  20.950  33.900  1.00  0.00           C
ATOM   2142  CB  ASP   280      16.420  19.844  32.895  1.00  0.00           C
ATOM   2143  CG  ASP   280      16.663  20.498  31.539  1.00  0.00           C
ATOM   2144  OD1 ASP   280      16.960  21.721  31.517  1.00  0.00           O
ATOM   2145  OD2 ASP   280      16.550  19.781  30.508  1.00  0.00           O
ATOM   2146  C   ASP   280      15.711  20.317  35.202  1.00  0.00           C
ATOM   2147  O   ASP   280      16.551  20.241  36.098  1.00  0.00           O
ATOM   2148  N   GLY   281      14.453  19.884  35.372  1.00  0.00           N
ATOM   2149  CA  GLY   281      14.099  19.372  36.658  1.00  0.00           C
ATOM   2150  C   GLY   281      13.783  20.601  37.449  1.00  0.00           C
ATOM   2151  O   GLY   281      14.096  21.697  36.987  1.00  0.00           O
ATOM   2152  N   LYS   282      13.177  20.455  38.653  1.00  0.00           N
ATOM   2153  CA  LYS   282      12.778  21.600  39.431  1.00  0.00           C
ATOM   2154  CB  LYS   282      11.255  21.698  39.638  1.00  0.00           C
ATOM   2155  CG  LYS   282      10.464  21.855  38.337  1.00  0.00           C
ATOM   2156  CD  LYS   282      10.795  23.131  37.560  1.00  0.00           C
ATOM   2157  CE  LYS   282       9.849  24.296  37.859  1.00  0.00           C
ATOM   2158  NZ  LYS   282      10.250  25.487  37.079  1.00  0.00           N
ATOM   2159  C   LYS   282      13.396  21.514  40.793  1.00  0.00           C
ATOM   2160  O   LYS   282      13.723  20.450  41.306  1.00  0.00           O
ATOM   2161  N   PRO   283      13.583  22.668  41.359  1.00  0.00           N
ATOM   2162  CA  PRO   283      14.164  22.841  42.669  1.00  0.00           C
ATOM   2163  CD  PRO   283      13.703  23.863  40.543  1.00  0.00           C
ATOM   2164  CB  PRO   283      14.578  24.308  42.739  1.00  0.00           C
ATOM   2165  CG  PRO   283      13.865  24.993  41.562  1.00  0.00           C
ATOM   2166  C   PRO   283      13.285  22.483  43.826  1.00  0.00           C
ATOM   2167  O   PRO   283      13.771  22.507  44.955  1.00  0.00           O
ATOM   2168  N   ARG   284      12.000  22.176  43.596  1.00  0.00           N
ATOM   2169  CA  ARG   284      11.095  22.027  44.698  1.00  0.00           C
ATOM   2170  CB  ARG   284       9.669  21.651  44.259  1.00  0.00           C
ATOM   2171  CG  ARG   284       8.666  21.713  45.411  1.00  0.00           C
ATOM   2172  CD  ARG   284       7.368  20.938  45.173  1.00  0.00           C
ATOM   2173  NE  ARG   284       6.762  21.410  43.897  1.00  0.00           N
ATOM   2174  CZ  ARG   284       6.799  20.602  42.798  1.00  0.00           C
ATOM   2175  NH1 ARG   284       7.375  19.367  42.880  1.00  0.00           N
ATOM   2176  NH2 ARG   284       6.244  21.016  41.622  1.00  0.00           N
ATOM   2177  C   ARG   284      11.524  20.958  45.653  1.00  0.00           C
ATOM   2178  O   ARG   284      11.477  21.157  46.867  1.00  0.00           O
ATOM   2179  N   VAL   285      11.961  19.789  45.158  1.00  0.00           N
ATOM   2180  CA  VAL   285      12.133  18.747  46.120  1.00  0.00           C
ATOM   2181  CB  VAL   285      10.969  17.781  46.038  1.00  0.00           C
ATOM   2182  CG1 VAL   285      11.075  16.658  47.079  1.00  0.00           C
ATOM   2183  CG2 VAL   285       9.675  18.603  46.162  1.00  0.00           C
ATOM   2184  C   VAL   285      13.432  18.034  45.863  1.00  0.00           C
ATOM   2185  O   VAL   285      14.098  18.242  44.851  1.00  0.00           O
ATOM   2186  N   LYS   286      13.819  17.184  46.832  1.00  0.00           N
ATOM   2187  CA  LYS   286      15.006  16.386  46.901  1.00  0.00           C
ATOM   2188  CB  LYS   286      15.235  16.064  48.396  1.00  0.00           C
ATOM   2189  CG  LYS   286      15.847  17.240  49.164  1.00  0.00           C
ATOM   2190  CD  LYS   286      15.006  18.522  49.141  1.00  0.00           C
ATOM   2191  CE  LYS   286      13.577  18.349  49.660  1.00  0.00           C
ATOM   2192  NZ  LYS   286      12.866  19.648  49.629  1.00  0.00           N
ATOM   2193  C   LYS   286      14.903  15.171  45.936  1.00  0.00           C
ATOM   2194  O   LYS   286      14.454  15.418  44.821  1.00  0.00           O
ATOM   2195  N   PRO   287      15.295  13.907  46.215  1.00  0.00           N
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ATOM   2196  CA  PRO   287      15.260  12.781  45.250  1.00  0.00           C
ATOM   2197  CD  PRO   287      16.480  13.734  47.054  1.00  0.00           C
ATOM   2198  CB  PRO   287      16.313  11.773  45.699  1.00  0.00           C
ATOM   2199  CG  PRO   287      16.752  12.232  47.088  1.00  0.00           C
ATOM   2200  C   PRO   287      14.039  11.963  44.845  1.00  0.00           C
ATOM   2201  O   PRO   287      12.973  12.531  44.602  1.00  0.00           O
ATOM   2202  N   TRP   288      14.272  10.629  44.602  1.00  0.00           N
ATOM   2203  CA  TRP   288      13.311   9.556  44.336  1.00  0.00           C
ATOM   2204  CB  TRP   288      12.583   9.624  42.979  1.00  0.00           C
ATOM   2205  CG  TRP   288      11.397  10.564  43.066  1.00  0.00           C
ATOM   2206  CD2 TRP   288      10.710  11.181  41.964  1.00  0.00           C
ATOM   2207  CD1 TRP   288      10.757  10.987  44.195  1.00  0.00           C
ATOM   2208  NE1 TRP   288       9.723  11.828  43.872  1.00  0.00           N
ATOM   2209  CE2 TRP   288       9.678  11.953  42.503  1.00  0.00           C
ATOM   2210  CE3 TRP   288      10.920  11.119  40.620  1.00  0.00           C
ATOM   2211  CZ2 TRP   288       8.841  12.676  41.705  1.00  0.00           C
ATOM   2212  CZ3 TRP   288      10.058  11.838  39.823  1.00  0.00           C
ATOM   2213  CH2 TRP   288       9.038  12.601  40.347  1.00  0.00           C
ATOM   2214  C   TRP   288      13.922   8.175  44.624  1.00  0.00           C
ATOM   2215  O   TRP   288      15.131   7.994  44.500  1.00  0.00           O
ATOM   2216  N   LYS   289      13.078   7.157  44.987  1.00  0.00           N
ATOM   2217  CA  LYS   289      13.418   5.885  45.643  1.00  0.00           C
ATOM   2218  CB  LYS   289      12.587   5.678  46.925  1.00  0.00           C
ATOM   2219  CG  LYS   289      13.159   4.643  47.896  1.00  0.00           C
ATOM   2220  CD  LYS   289      12.547   4.709  49.295  1.00  0.00           C
ATOM   2221  CE  LYS   289      11.106   4.200  49.365  1.00  0.00           C
ATOM   2222  NZ  LYS   289      11.092   2.747  49.636  1.00  0.00           N
ATOM   2223  C   LYS   289      13.458   4.537  44.914  1.00  0.00           C
ATOM   2224  O   LYS   289      14.197   4.396  43.947  1.00  0.00           O
ATOM   2225  N   VAL   290      12.659   3.498  45.368  1.00  0.00           N
ATOM   2226  CA  VAL   290      12.795   2.046  45.126  1.00  0.00           C
ATOM   2227  CB  VAL   290      12.814   1.285  46.421  1.00  0.00           C
ATOM   2228  CG1 VAL   290      13.895   1.841  47.354  1.00  0.00           C
ATOM   2229  CG2 VAL   290      11.402   1.350  47.027  1.00  0.00           C
ATOM   2230  C   VAL   290      11.754   1.254  44.333  1.00  0.00           C
ATOM   2231  O   VAL   290      10.668   1.726  44.020  1.00  0.00           O
ATOM   2232  N   SER   291      12.160  -0.017  43.964  1.00  0.00           N
ATOM   2233  CA  SER   291      11.407  -1.120  43.364  1.00  0.00           C
ATOM   2234  CB  SER   291      10.491  -0.727  42.188  1.00  0.00           C
ATOM   2235  OG  SER   291       9.354  -0.016  42.655  1.00  0.00           O
ATOM   2236  C   SER   291      12.361  -2.193  42.847  1.00  0.00           C
ATOM   2237  O   SER   291      13.236  -1.899  42.038  1.00  0.00           O
ATOM   2238  N   ASN   292      12.232  -3.482  43.271  1.00  0.00           N
ATOM   2239  CA  ASN   292      13.121  -4.495  42.730  1.00  0.00           C
ATOM   2240  CB  ASN   292      14.548  -4.339  43.283  1.00  0.00           C
ATOM   2241  CG  ASN   292      15.535  -5.176  42.481  1.00  0.00           C
ATOM   2242  OD1 ASN   292      16.735  -4.928  42.586  1.00  0.00           O
ATOM   2243  ND2 ASN   292      15.052  -6.172  41.689  1.00  0.00           N
ATOM   2244  C   ASN   292      12.624  -5.862  43.144  1.00  0.00           C
ATOM   2245  O   ASN   292      13.139  -6.451  44.095  1.00  0.00           O
ATOM   2246  N   GLN   293      11.620  -6.410  42.431  1.00  0.00           N
ATOM   2247  CA  GLN   293      11.048  -7.690  42.764  1.00  0.00           C
ATOM   2248  CB  GLN   293       9.662  -7.918  42.137  1.00  0.00           C
ATOM   2249  CG  GLN   293       9.047  -9.265  42.528  1.00  0.00           C
ATOM   2250  CD  GLN   293       7.808  -9.479  41.670  1.00  0.00           C
ATOM   2251  OE1 GLN   293       6.862 -10.158  42.066  1.00  0.00           O
ATOM   2252  NE2 GLN   293       7.821  -8.893  40.443  1.00  0.00           N
ATOM   2253  C   GLN   293      11.861  -8.907  42.386  1.00  0.00           C
ATOM   2254  O   GLN   293      11.964  -9.839  43.182  1.00  0.00           O
ATOM   2255  N   LYS   294      12.456  -8.962  41.173  1.00  0.00           N
ATOM   2256  CA  LYS   294      12.970 -10.242  40.739  1.00  0.00           C
ATOM   2257  CB  LYS   294      12.912 -10.439  39.214  1.00  0.00           C
ATOM   2258  CG  LYS   294      13.924  -9.594  38.434  1.00  0.00           C
ATOM   2259  CD  LYS   294      14.113 -10.066  36.990  1.00  0.00           C
ATOM   2260  CE  LYS   294      14.888 -11.382  36.876  1.00  0.00           C
ATOM   2261  NZ  LYS   294      14.777 -11.930  35.505  1.00  0.00           N
ATOM   2262  C   LYS   294      14.389 -10.486  41.127  1.00  0.00           C
ATOM   2263  O   LYS   294      15.061 -11.323  40.526  1.00  0.00           O
ATOM   2264  N   LEU   295      14.879  -9.807  42.165  1.00  0.00           N
ATOM   2265  CA  LEU   295      16.206 -10.053  42.641  1.00  0.00           C
ATOM   2266  CB  LEU   295      16.629  -9.084  43.741  1.00  0.00           C
ATOM   2267  CG  LEU   295      16.911  -7.644  43.302  1.00  0.00           C
ATOM   2268  CD2 LEU   295      17.940  -7.584  42.159  1.00  0.00           C
ATOM   2269  CD1 LEU   295      17.326  -6.793  44.514  1.00  0.00           C
ATOM   2270  C   LEU   295      16.223 -11.412  43.265  1.00  0.00           C
ATOM   2271  O   LEU   295      17.267 -12.059  43.324  1.00  0.00           O
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ATOM   2272  N   LYS   296      15.050 -11.869  43.749  1.00  0.00           N
ATOM   2273  CA  LYS   296      14.912 -13.069  44.525  1.00  0.00           C
ATOM   2274  CB  LYS   296      13.444 -13.447  44.792  1.00  0.00           C
ATOM   2275  CG  LYS   296      12.727 -12.513  45.771  1.00  0.00           C
ATOM   2276  CD  LYS   296      13.296 -12.545  47.194  1.00  0.00           C
ATOM   2277  CE  LYS   296      14.146 -11.326  47.555  1.00  0.00           C
ATOM   2278  NZ  LYS   296      15.443 -11.383  46.849  1.00  0.00           N
ATOM   2279  C   LYS   296      15.550 -14.224  43.823  1.00  0.00           C
ATOM   2280  O   LYS   296      16.119 -15.088  44.487  1.00  0.00           O
ATOM   2281  N   ASP   297      15.478 -14.286  42.478  1.00  0.00           N
ATOM   2282  CA  ASP   297      16.080 -15.394  41.789  1.00  0.00           C
ATOM   2283  CB  ASP   297      16.027 -15.241  40.260  1.00  0.00           C
ATOM   2284  CG  ASP   297      14.584 -15.366  39.793  1.00  0.00           C
ATOM   2285  OD1 ASP   297      13.809 -16.112  40.450  1.00  0.00           O
ATOM   2286  OD2 ASP   297      14.241 -14.718  38.768  1.00  0.00           O
ATOM   2287  C   ASP   297      17.526 -15.402  42.165  1.00  0.00           C
ATOM   2288  O   ASP   297      18.092 -16.439  42.510  1.00  0.00           O
ATOM   2289  N   LEU   298      18.156 -14.217  42.123  1.00  0.00           N
ATOM   2290  CA  LEU   298      19.523 -14.079  42.517  1.00  0.00           C
ATOM   2291  CB  LEU   298      20.072 -12.664  42.257  1.00  0.00           C
ATOM   2292  CG  LEU   298      20.161 -12.285  40.765  1.00  0.00           C
ATOM   2293  CD2 LEU   298      18.784 -12.350  40.088  1.00  0.00           C
ATOM   2294  CD1 LEU   298      21.219 -13.127  40.036  1.00  0.00           C
ATOM   2295  C   LEU   298      19.593 -14.326  43.987  1.00  0.00           C
ATOM   2296  O   LEU   298      20.538 -14.938  44.487  1.00  0.00           O
ATOM   2297  N   GLY   299      18.572 -13.847  44.723  1.00  0.00           N
ATOM   2298  CA  GLY   299      18.552 -14.016  46.145  1.00  0.00           C
ATOM   2299  C   GLY   299      19.266 -12.855  46.756  1.00  0.00           C
ATOM   2300  O   GLY   299      19.584 -12.867  47.944  1.00  0.00           O
ATOM   2301  N   LEU   300      19.543 -11.813  45.951  1.00  0.00           N
ATOM   2302  CA  LEU   300      20.223 -10.664  46.473  1.00  0.00           C
ATOM   2303  CB  LEU   300      21.321 -10.115  45.546  1.00  0.00           C
ATOM   2304  CG  LEU   300      22.572 -11.003  45.491  1.00  0.00           C
ATOM   2305  CD2 LEU   300      22.234 -12.424  45.012  1.00  0.00           C
ATOM   2306  CD1 LEU   300      23.300 -10.978  46.843  1.00  0.00           C
ATOM   2307  C   LEU   300      19.224  -9.572  46.654  1.00  0.00           C
ATOM   2308  O   LEU   300      18.326  -9.400  45.839  1.00  0.00           O
ATOM   2309  N   GLU   301      19.335  -8.806  47.752  1.00  0.00           N
ATOM   2310  CA  GLU   301      18.423  -7.716  47.933  1.00  0.00           C
ATOM   2311  CB  GLU   301      17.334  -7.969  48.990  1.00  0.00           C
ATOM   2312  CG  GLU   301      16.355  -9.085  48.621  1.00  0.00           C
ATOM   2313  CD  GLU   301      15.337  -9.194  49.748  1.00  0.00           C
ATOM   2314  OE1 GLU   301      14.487  -8.272  49.866  1.00  0.00           O
ATOM   2315  OE2 GLU   301      15.396 -10.198  50.508  1.00  0.00           O
ATOM   2316  C   GLU   301      19.237  -6.571  48.423  1.00  0.00           C
ATOM   2317  O   GLU   301      20.274  -6.776  49.052  1.00  0.00           O
ATOM   2318  N   PHE   302      18.807  -5.325  48.134  1.00  0.00           N
ATOM   2319  CA  PHE   302      19.588  -4.235  48.631  1.00  0.00           C
ATOM   2320  CB  PHE   302      19.188  -2.871  48.033  1.00  0.00           C
ATOM   2321  CG  PHE   302      19.711  -2.830  46.637  1.00  0.00           C
ATOM   2322  CD1 PHE   302      18.990  -3.356  45.590  1.00  0.00           C
ATOM   2323  CD2 PHE   302      20.942  -2.273  46.376  1.00  0.00           C
ATOM   2324  CE1 PHE   302      19.486  -3.319  44.307  1.00  0.00           C
ATOM   2325  CE2 PHE   302      21.442  -2.233  45.095  1.00  0.00           C
ATOM   2326  CZ  PHE   302      20.713  -2.755  44.055  1.00  0.00           C
ATOM   2327  C   PHE   302      19.408  -4.203  50.110  1.00  0.00           C
ATOM   2328  O   PHE   302      18.295  -4.058  50.612  1.00  0.00           O
ATOM   2329  N   THR   303      20.516  -4.422  50.839  1.00  0.00           N
ATOM   2330  CA  THR   303      20.528  -4.387  52.270  1.00  0.00           C
ATOM   2331  CB  THR   303      21.610  -5.231  52.907  1.00  0.00           C
ATOM   2332  OG1 THR   303      22.912  -4.848  52.495  1.00  0.00           O
ATOM   2333  CG2 THR   303      21.350  -6.697  52.522  1.00  0.00           C
ATOM   2334  C   THR   303      20.556  -2.983  52.799  1.00  0.00           C
ATOM   2335  O   THR   303      19.955  -2.736  53.843  1.00  0.00           O
ATOM   2336  N   PRO   304      21.206  -2.033  52.163  1.00  0.00           N
ATOM   2337  CA  PRO   304      21.245  -0.734  52.767  1.00  0.00           C
ATOM   2338  CD  PRO   304      22.398  -2.283  51.367  1.00  0.00           C
ATOM   2339  CB  PRO   304      22.369   0.028  52.073  1.00  0.00           C
ATOM   2340  CG  PRO   304      23.320  -1.078  51.594  1.00  0.00           C
ATOM   2341  C   PRO   304      19.925  -0.065  52.674  1.00  0.00           C
ATOM   2342  O   PRO   304      19.254  -0.192  51.651  1.00  0.00           O
ATOM   2343  N   ALA   305      19.542   0.649  53.745  1.00  0.00           N
ATOM   2344  CA  ALA   305      18.303   1.350  53.752  1.00  0.00           C
ATOM   2345  CB  ALA   305      17.763   1.637  55.163  1.00  0.00           C
ATOM   2346  C   ALA   305      18.558   2.653  53.092  1.00  0.00           C
ATOM   2347  O   ALA   305      19.694   3.117  53.026  1.00  0.00           O
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ATOM   2348  N   LYS   306      17.490   3.279  52.579  1.00  0.00           N
ATOM   2349  CA  LYS   306      17.679   4.525  51.925  1.00  0.00           C
ATOM   2350  CB  LYS   306      16.356   5.127  51.427  1.00  0.00           C
ATOM   2351  CG  LYS   306      15.689   4.286  50.339  1.00  0.00           C
ATOM   2352  CD  LYS   306      15.258   2.899  50.824  1.00  0.00           C
ATOM   2353  CE  LYS   306      14.267   2.934  51.989  1.00  0.00           C
ATOM   2354  NZ  LYS   306      13.884   1.556  52.372  1.00  0.00           N
ATOM   2355  C   LYS   306      18.261   5.464  52.930  1.00  0.00           C
ATOM   2356  O   LYS   306      19.233   6.152  52.632  1.00  0.00           O
ATOM   2357  N   GLN   307      17.734   5.474  54.172  1.00  0.00           N
ATOM   2358  CA  GLN   307      18.186   6.430  55.146  1.00  0.00           C
ATOM   2359  CB  GLN   307      17.534   6.252  56.528  1.00  0.00           C
ATOM   2360  CG  GLN   307      16.029   6.524  56.532  1.00  0.00           C
ATOM   2361  CD  GLN   307      15.333   5.324  55.906  1.00  0.00           C
ATOM   2362  OE1 GLN   307      15.934   4.266  55.730  1.00  0.00           O
ATOM   2363  NE2 GLN   307      14.026   5.487  55.567  1.00  0.00           N
ATOM   2364  C   GLN   307      19.653   6.254  55.334  1.00  0.00           C
ATOM   2365  O   GLN   307      20.397   7.230  55.417  1.00  0.00           O
ATOM   2366  N   CYS   308      20.108   4.994  55.378  1.00  0.00           N
ATOM   2367  CA  CYS   308      21.500   4.746  55.573  1.00  0.00           C
ATOM   2368  CB  CYS   308      21.834   3.246  55.587  1.00  0.00           C
ATOM   2369  SG  CYS   308      23.601   2.931  55.858  1.00  0.00           S
ATOM   2370  C   CYS   308      22.246   5.366  54.436  1.00  0.00           C
ATOM   2371  O   CYS   308      23.247   6.045  54.640  1.00  0.00           O
ATOM   2372  N   LEU   309      21.763   5.169  53.196  1.00  0.00           N
ATOM   2373  CA  LEU   309      22.459   5.692  52.054  1.00  0.00           C
ATOM   2374  CB  LEU   309      21.769   5.342  50.724  1.00  0.00           C
ATOM   2375  CG  LEU   309      22.078   3.935  50.187  1.00  0.00           C
ATOM   2376  CD2 LEU   309      21.453   3.750  48.798  1.00  0.00           C
ATOM   2377  CD1 LEU   309      21.671   2.830  51.164  1.00  0.00           C
ATOM   2378  C   LEU   309      22.548   7.186  52.092  1.00  0.00           C
ATOM   2379  O   LEU   309      23.632   7.743  51.936  1.00  0.00           O
ATOM   2380  N   TYR   310      21.417   7.888  52.293  1.00  0.00           N
ATOM   2381  CA  TYR   310      21.472   9.321  52.234  1.00  0.00           C
ATOM   2382  CB  TYR   310      20.094   9.980  52.062  1.00  0.00           C
ATOM   2383  CG  TYR   310      19.686   9.285  50.817  1.00  0.00           C
ATOM   2384  CD1 TYR   310      20.187   9.649  49.588  1.00  0.00           C
ATOM   2385  CD2 TYR   310      18.842   8.211  50.903  1.00  0.00           C
ATOM   2386  CE1 TYR   310      19.818   8.950  48.461  1.00  0.00           C
ATOM   2387  CE2 TYR   310      18.468   7.507  49.792  1.00  0.00           C
ATOM   2388  CZ  TYR   310      18.965   7.877  48.573  1.00  0.00           C
ATOM   2389  OH  TYR   310      18.578   7.146  47.434  1.00  0.00           O
ATOM   2390  C   TYR   310      22.218   9.852  53.405  1.00  0.00           C
ATOM   2391  O   TYR   310      22.973  10.813  53.286  1.00  0.00           O
ATOM   2392  N   GLU   311      22.031   9.228  54.575  1.00  0.00           N
ATOM   2393  CA  GLU   311      22.685   9.687  55.760  1.00  0.00           C
ATOM   2394  CB  GLU   311      22.300   8.785  56.945  1.00  0.00           C
ATOM   2395  CG  GLU   311      22.726   9.275  58.326  1.00  0.00           C
ATOM   2396  CD  GLU   311      22.067   8.337  59.333  1.00  0.00           C
ATOM   2397  OE1 GLU   311      20.813   8.371  59.435  1.00  0.00           O
ATOM   2398  OE2 GLU   311      22.807   7.566  60.004  1.00  0.00           O
ATOM   2399  C   GLU   311      24.165   9.611  55.535  1.00  0.00           C
ATOM   2400  O   GLU   311      24.893  10.565  55.808  1.00  0.00           O
ATOM   2401  N   THR   312      24.643   8.475  54.992  1.00  0.00           N
ATOM   2402  CA  THR   312      26.045   8.277  54.763  1.00  0.00           C
ATOM   2403  CB  THR   312      26.365   6.898  54.250  1.00  0.00           C
ATOM   2404  OG1 THR   312      25.731   6.674  52.998  1.00  0.00           O
ATOM   2405  CG2 THR   312      25.900   5.860  55.289  1.00  0.00           C
ATOM   2406  C   THR   312      26.536   9.262  53.748  1.00  0.00           C
ATOM   2407  O   THR   312      27.609   9.840  53.910  1.00  0.00           O
ATOM   2408  N   VAL   313      25.770   9.474  52.661  1.00  0.00           N
ATOM   2409  CA  VAL   313      26.223  10.350  51.617  1.00  0.00           C
ATOM   2410  CB  VAL   313      25.355  10.329  50.390  1.00  0.00           C
ATOM   2411  CG1 VAL   313      23.964  10.882  50.733  1.00  0.00           C
ATOM   2412  CG2 VAL   313      26.071  11.127  49.290  1.00  0.00           C
ATOM   2413  C   VAL   313      26.305  11.766  52.101  1.00  0.00           C
ATOM   2414  O   VAL   313      27.278  12.464  51.820  1.00  0.00           O
ATOM   2415  N   ILE   314      25.289  12.229  52.854  1.00  0.00           N
ATOM   2416  CA  ILE   314      25.249  13.597  53.289  1.00  0.00           C
ATOM   2417  CB  ILE   314      24.044  13.897  54.129  1.00  0.00           C
ATOM   2418  CG2 ILE   314      24.215  15.309  54.712  1.00  0.00           C
ATOM   2419  CG1 ILE   314      22.750  13.704  53.324  1.00  0.00           C
ATOM   2420  CD1 ILE   314      21.495  13.699  54.194  1.00  0.00           C
ATOM   2421  C   ILE   314      26.434  13.869  54.156  1.00  0.00           C
ATOM   2422  O   ILE   314      27.125  14.872  53.984  1.00  0.00           O
ATOM   2423  N   SER   315      26.711  12.965  55.109  1.00  0.00           N
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ATOM   2424  CA  SER   315      27.791  13.190  56.021  1.00  0.00           C
ATOM   2425  CB  SER   315      27.945  12.059  57.052  1.00  0.00           C
ATOM   2426  OG  SER   315      29.029  12.339  57.925  1.00  0.00           O
ATOM   2427  C   SER   315      29.072  13.281  55.256  1.00  0.00           C
ATOM   2428  O   SER   315      29.916  14.128  55.547  1.00  0.00           O
ATOM   2429  N   LEU   316      29.252  12.415  54.240  1.00  0.00           N
ATOM   2430  CA  LEU   316      30.486  12.435  53.509  1.00  0.00           C
ATOM   2431  CB  LEU   316      30.572  11.350  52.423  1.00  0.00           C
ATOM   2432  CG  LEU   316      31.904  11.380  51.649  1.00  0.00           C
ATOM   2433  CD2 LEU   316      31.857  10.479  50.407  1.00  0.00           C
ATOM   2434  CD1 LEU   316      33.089  11.056  52.574  1.00  0.00           C
ATOM   2435  C   LEU   316      30.620  13.763  52.829  1.00  0.00           C
ATOM   2436  O   LEU   316      31.688  14.370  52.861  1.00  0.00           O
ATOM   2437  N   GLN   317      29.538  14.262  52.201  1.00  0.00           N
ATOM   2438  CA  GLN   317      29.659  15.487  51.457  1.00  0.00           C
ATOM   2439  CB  GLN   317      28.396  15.899  50.696  1.00  0.00           C
ATOM   2440  CG  GLN   317      28.651  17.070  49.743  1.00  0.00           C
ATOM   2441  CD  GLN   317      27.337  17.437  49.076  1.00  0.00           C
ATOM   2442  OE1 GLN   317      28.432  17.043  48.679  1.00  0.00           O
ATOM   2443  NE2 GLN   317      26.743  17.739  50.262  1.00  0.00           N
ATOM   2444  C   GLN   317      29.977  16.616  52.376  1.00  0.00           C
ATOM   2445  O   GLN   317      30.810  17.464  52.058  1.00  0.00           O
ATOM   2446  N   GLU   318      29.308  16.674  53.539  1.00  0.00           N
ATOM   2447  CA  GLU   318      29.596  17.768  54.412  1.00  0.00           C
ATOM   2448  CB  GLU   318      28.691  17.837  55.655  1.00  0.00           C
ATOM   2449  CG  GLU   318      28.863  16.669  56.625  1.00  0.00           C
ATOM   2450  CD  GLU   318      28.002  16.961  57.846  1.00  0.00           C
ATOM   2451  OE1 GLU   318      27.272  17.987  57.826  1.00  0.00           O
ATOM   2452  OE2 GLU   318      28.070  16.164  58.819  1.00  0.00           O
ATOM   2453  C   GLU   318      31.010  17.619  54.884  1.00  0.00           C
ATOM   2454  O   GLU   318      31.746  18.599  54.986  1.00  0.00           O
ATOM   2455  N   LYS   319      31.428  16.369  55.175  1.00  0.00           N
ATOM   2456  CA  LYS   319      32.743  16.117  55.694  1.00  0.00           C
ATOM   2457  CB  LYS   319      33.018  14.620  55.935  1.00  0.00           C
ATOM   2458  CG  LYS   319      32.282  14.002  57.126  1.00  0.00           C
ATOM   2459  CD  LYS   319      32.702  14.576  58.482  1.00  0.00           C
ATOM   2460  CE  LYS   319      31.618  15.408  59.168  1.00  0.00           C
ATOM   2461  NZ  LYS   319      30.644  14.511  59.830  1.00  0.00           N
ATOM   2462  C   LYS   319      33.773  16.574  54.713  1.00  0.00           C
ATOM   2463  O   LYS   319      34.682  17.322  55.071  1.00  0.00           O
ATOM   2464  N   GLY   320      33.661  16.160  53.437  1.00  0.00           N
ATOM   2465  CA  GLY   320      34.683  16.575  52.522  1.00  0.00           C
ATOM   2466  C   GLY   320      34.046  16.905  51.218  1.00  0.00           C
ATOM   2467  O   GLY   320      33.718  16.024  50.427  1.00  0.00           O
ATOM   2468  N   HIS   321      33.894  18.213  50.951  1.00  0.00           N
ATOM   2469  CA  HIS   321      33.315  18.634  49.714  1.00  0.00           C
ATOM   2470  ND1 HIS   321      30.772  20.694  48.723  1.00  0.00           N
ATOM   2471  CG  HIS   321      32.128  20.540  48.539  1.00  0.00           C
ATOM   2472  NE2 HIS   321      31.172  21.112  46.576  1.00  0.00           N
ATOM   2473  CD2 HIS   321      32.356  20.799  47.221  1.00  0.00           C
ATOM   2474  CE1 HIS   321      30.248  21.035  47.518  1.00  0.00           C
ATOM   2475  CB  HIS   321      33.079  20.153  49.635  1.00  0.00           C
ATOM   2476  C   HIS   321      34.280  18.243  48.639  1.00  0.00           C
ATOM   2477  O   HIS   321      33.876  17.861  47.542  1.00  0.00           O
ATOM   2478  N   ILE   322      35.592  18.335  48.946  1.00  0.00           N
ATOM   2479  CA  ILE   322      36.646  18.030  48.018  1.00  0.00           C
ATOM   2480  CB  ILE   322      38.013  18.291  48.577  1.00  0.00           C
ATOM   2481  CG2 ILE   322      38.108  19.790  48.907  1.00  0.00           C
ATOM   2482  CG1 ILE   322      38.295  17.377  49.779  1.00  0.00           C
ATOM   2483  CD1 ILE   322      39.760  17.389  50.211  1.00  0.00           C
ATOM   2484  C   ILE   322      36.583  16.582  47.642  1.00  0.00           C
ATOM   2485  O   ILE   322      36.746  16.232  46.476  1.00  0.00           O
ATOM   2486  N   SER   323      36.340  15.693  48.625  1.00  0.00           N
ATOM   2487  CA  SER   323      36.287  14.289  48.333  1.00  0.00           C
ATOM   2488  CB  SER   323      35.231  13.940  47.272  1.00  0.00           C
ATOM   2489  OG  SER   323      35.222  12.541  47.027  1.00  0.00           O
ATOM   2490  C   SER   323      37.626  13.896  47.821  1.00  0.00           C
ATOM   2491  O   SER   323      37.767  12.953  47.046  1.00  0.00           O
ATOM   2492  N   LYS   324      38.661  14.623  48.267  1.00  0.00           N
ATOM   2493  CA  LYS   324      39.986  14.302  47.851  1.00  0.00           C
ATOM   2494  CB  LYS   324      41.025  15.341  48.317  1.00  0.00           C
ATOM   2495  CG  LYS   324      42.454  15.091  47.818  1.00  0.00           C
ATOM   2496  CD  LYS   324      43.123  13.840  48.397  1.00  0.00           C
ATOM   2497  CE  LYS   324      44.534  13.591  47.860  1.00  0.00           C
ATOM   2498  NZ  LYS   324      44.467  13.217  46.429  1.00  0.00           N
ATOM   2499  C   LYS   324      40.316  12.958  48.489  1.00  0.00           C
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ATOM   2500  O   LYS   324      40.216  11.924  47.775  1.00  0.00           O
ATOM   2501  OXT LYS   324      40.672  12.951  49.697  1.00  0.00           O
END
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Pinus taeda Cinnamyl Alcohol Dehydrogenase

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REMARK Pinus taeda CAD molecular model
REMARK  CAD_ COMPLIES WITH FORMAT V. 2.0, 28-MAY-2002
ATOM      1  N   LEU     1      24.599   2.823 -11.066  1.00  0.00           N
ATOM      2  CA  LEU     1      23.173   2.941 -10.688  1.00  0.00           C
ATOM      3  CB  LEU     1      22.551   1.559 -10.375  1.00  0.00           C
ATOM      4  CG  LEU     1      23.367   0.607  -9.471  1.00  0.00           C
ATOM      5  CD2 LEU     1      23.678   1.238  -8.109  1.00  0.00           C
ATOM      6  CD1 LEU     1      24.619   0.063 -10.180  1.00  0.00           C
ATOM      7  C   LEU     1      22.955   3.889  -9.557  1.00  0.00           C
ATOM      8  O   LEU     1      23.561   4.958  -9.510  1.00  0.00           O
ATOM      9  N   GLU     2      22.078   3.516  -8.607  1.00  0.00           N
ATOM     10  CA  GLU     2      21.739   4.380  -7.515  1.00  0.00           C
ATOM     11  CB  GLU     2      20.672   3.770  -6.586  1.00  0.00           C
ATOM     12  CG  GLU     2      21.072   2.425  -5.972  1.00  0.00           C
ATOM     13  CD  GLU     2      21.933   2.685  -4.743  1.00  0.00           C
ATOM     14  OE1 GLU     2      21.972   3.855  -4.277  1.00  0.00           O
ATOM     15  OE2 GLU     2      22.562   1.711  -4.248  1.00  0.00           O
ATOM     16  C   GLU     2      22.969   4.635  -6.714  1.00  0.00           C
ATOM     17  O   GLU     2      23.172   5.733  -6.198  1.00  0.00           O
ATOM     18  N   SER     3      23.840   3.620  -6.608  1.00  0.00           N
ATOM     19  CA  SER     3      25.008   3.755  -5.802  1.00  0.00           C
ATOM     20  CB  SER     3      25.907   2.507  -5.801  1.00  0.00           C
ATOM     21  OG  SER     3      26.432   2.285  -7.102  1.00  0.00           O
ATOM     22  C   SER     3      25.824   4.905  -6.292  1.00  0.00           C
ATOM     23  O   SER     3      25.784   5.267  -7.465  1.00  0.00           O
ATOM     24  N   GLU     4      26.582   5.510  -5.356  1.00  0.00           N
ATOM     25  CA  GLU     4      27.482   6.595  -5.615  1.00  0.00           C
ATOM     26  CB  GLU     4      28.539   6.215  -6.677  1.00  0.00           C
ATOM     27  CG  GLU     4      29.637   7.254  -6.930  1.00  0.00           C
ATOM     28  CD  GLU     4      29.378   7.923  -8.275  1.00  0.00           C
ATOM     29  OE1 GLU     4      28.369   7.555  -8.934  1.00  0.00           O
ATOM     30  OE2 GLU     4      30.185   8.811  -8.660  1.00  0.00           O
ATOM     31  C   GLU     4      26.745   7.829  -6.038  1.00  0.00           C
ATOM     32  O   GLU     4      27.324   8.720  -6.654  1.00  0.00           O
ATOM     33  N   LYS     5      25.453   7.956  -5.690  1.00  0.00           N
ATOM     34  CA  LYS     5      24.796   9.184  -6.032  1.00  0.00           C
ATOM     35  CB  LYS     5      23.861   9.101  -7.250  1.00  0.00           C
ATOM     36  CG  LYS     5      24.576   8.819  -8.571  1.00  0.00           C
ATOM     37  CD  LYS     5      23.619   8.612  -9.747  1.00  0.00           C
ATOM     38  CE  LYS     5      22.578   7.516  -9.515  1.00  0.00           C
ATOM     39  NZ  LYS     5      21.527   7.997  -8.590  1.00  0.00           N
ATOM     40  C   LYS     5      23.940   9.565  -4.873  1.00  0.00           C
ATOM     41  O   LYS     5      23.553   8.717  -4.073  1.00  0.00           O
ATOM     42  N   THR     6      23.633  10.870  -4.742  1.00  0.00           N
ATOM     43  CA  THR     6      22.753  11.275  -3.691  1.00  0.00           C
ATOM     44  CB  THR     6      22.618  12.763  -3.551  1.00  0.00           C
ATOM     45  OG1 THR     6      23.886  13.348  -3.290  1.00  0.00           O
ATOM     46  CG2 THR     6      21.647  13.062  -2.396  1.00  0.00           C
ATOM     47  C   THR     6      21.426  10.729  -4.086  1.00  0.00           C
ATOM     48  O   THR     6      21.164  10.549  -5.274  1.00  0.00           O
ATOM     49  N   VAL     7      20.553  10.420  -3.109  1.00  0.00           N
ATOM     50  CA  VAL     7      19.298   9.853  -3.519  1.00  0.00           C
ATOM     51  CB  VAL     7      18.805   8.725  -2.660  1.00  0.00           C
ATOM     52  CG1 VAL     7      19.819   7.571  -2.719  1.00  0.00           C
ATOM     53  CG2 VAL     7      18.514   9.265  -1.250  1.00  0.00           C
ATOM     54  C   VAL     7      18.245  10.911  -3.458  1.00  0.00           C
ATOM     55  O   VAL     7      18.221  11.720  -2.531  1.00  0.00           O
ATOM     56  N   THR     8      17.377  10.920  -4.495  1.00  0.00           N
ATOM     57  CA  THR     8      16.288  11.842  -4.698  1.00  0.00           C
ATOM     58  CB  THR     8      15.665  11.695  -6.055  1.00  0.00           C
ATOM     59  OG1 THR     8      16.638  11.908  -7.067  1.00  0.00           O
ATOM     60  CG2 THR     8      14.529  12.724  -6.188  1.00  0.00           C
ATOM     61  C   THR     8      15.193  11.654  -3.692  1.00  0.00           C
ATOM     62  O   THR     8      14.698  12.643  -3.169  1.00  0.00           O
ATOM     63  N   GLY     9      14.787  10.386  -3.456  1.00  0.00           N
ATOM     64  CA  GLY     9      13.828   9.797  -2.541  1.00  0.00           C
ATOM     65  C   GLY     9      12.600  10.581  -2.174  1.00  0.00           C
ATOM     66  O   GLY     9      12.491  11.797  -2.315  1.00  0.00           O
ATOM     67  N   TYR    10      11.620   9.826  -1.632  1.00  0.00           N
ATOM     68  CA  TYR    10      10.378  10.348  -1.147  1.00  0.00           C
ATOM     69  CB  TYR    10       9.156   9.794  -1.892  1.00  0.00           C
ATOM     70  CG  TYR    10       9.211  10.283  -3.299  1.00  0.00           C
ATOM     71  CD1 TYR    10       9.987   9.638  -4.235  1.00  0.00           C
ATOM     72  CD2 TYR    10       8.483  11.386  -3.683  1.00  0.00           C
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ATOM     73  CE1 TYR    10      10.036  10.088  -5.533  1.00  0.00           C
ATOM     74  CE2 TYR    10       8.528  11.840  -4.980  1.00  0.00           C
ATOM     75  CZ  TYR    10       9.307  11.191  -5.908  1.00  0.00           C
ATOM     76  OH  TYR    10       9.356  11.654  -7.240  1.00  0.00           O
ATOM     77  C   TYR    10      10.280   9.913   0.281  1.00  0.00           C
ATOM     78  O   TYR    10      10.631   8.784   0.621  1.00  0.00           O
ATOM     79  N   ALA    11       9.812  10.815   1.163  1.00  0.00           N
ATOM     80  CA  ALA    11       9.735  10.492   2.553  1.00  0.00           C
ATOM     81  CB  ALA    11      10.804  11.195   3.407  1.00  0.00           C
ATOM     82  C   ALA    11       8.409  10.939   3.059  1.00  0.00           C
ATOM     83  O   ALA    11       7.763  11.813   2.482  1.00  0.00           O
ATOM     84  N   ALA    12       7.973  10.325   4.171  1.00  0.00           N
ATOM     85  CA  ALA    12       6.709  10.654   4.746  1.00  0.00           C
ATOM     86  CB  ALA    12       5.748   9.463   4.901  1.00  0.00           C
ATOM     87  C   ALA    12       6.976  11.150   6.111  1.00  0.00           C
ATOM     88  O   ALA    12       8.101  11.122   6.609  1.00  0.00           O
ATOM     89  N   ARG    13       5.926  11.687   6.738  1.00  0.00           N
ATOM     90  CA  ARG    13       6.104  12.254   8.027  1.00  0.00           C
ATOM     91  CB  ARG    13       6.568  11.251   9.108  1.00  0.00           C
ATOM     92  CG  ARG    13       6.646  11.896  10.496  1.00  0.00           C
ATOM     93  CD  ARG    13       6.409  10.967  11.686  1.00  0.00           C
ATOM     94  NE  ARG    13       6.099  11.870  12.831  1.00  0.00           N
ATOM     95  CZ  ARG    13       5.178  11.524  13.775  1.00  0.00           C
ATOM     96  NH1 ARG    13       4.643  10.268  13.784  1.00  0.00           N
ATOM     97  NH2 ARG    13       4.770  12.454  14.687  1.00  0.00           N
ATOM     98  C   ARG    13       7.101  13.347   7.865  1.00  0.00           C
ATOM     99  O   ARG    13       7.801  13.710   8.808  1.00  0.00           O
ATOM    100  N   ASP    14       7.216  13.894   6.636  1.00  0.00           N
ATOM    101  CA  ASP    14       8.026  15.057   6.564  1.00  0.00           C
ATOM    102  CB  ASP    14       8.169  15.640   5.148  1.00  0.00           C
ATOM    103  CG  ASP    14       9.038  14.696   4.329  1.00  0.00           C
ATOM    104  OD1 ASP    14       9.627  13.761   4.932  1.00  0.00           O
ATOM    105  OD2 ASP    14       9.121  14.898   3.088  1.00  0.00           O
ATOM    106  C   ASP    14       7.191  15.983   7.365  1.00  0.00           C
ATOM    107  O   ASP    14       6.113  16.384   6.927  1.00  0.00           O
ATOM    108  N   SER    15       7.637  16.306   8.588  1.00  0.00           N
ATOM    109  CA  SER    15       6.787  17.110   9.402  1.00  0.00           C
ATOM    110  CB  SER    15       6.712  16.640  10.865  1.00  0.00           C
ATOM    111  OG  SER    15       6.126  15.348  10.933  1.00  0.00           O
ATOM    112  C   SER    15       7.354  18.479   9.395  1.00  0.00           C
ATOM    113  O   SER    15       8.482  18.703   9.831  1.00  0.00           O
ATOM    114  N   SER    16       6.570  19.427   8.856  1.00  0.00           N
ATOM    115  CA  SER    16       6.988  20.792   8.802  1.00  0.00           C
ATOM    116  CB  SER    16       6.031  21.678   7.990  1.00  0.00           C
ATOM    117  OG  SER    16       6.501  23.019   7.975  1.00  0.00           O
ATOM    118  C   SER    16       7.013  21.319  10.196  1.00  0.00           C
ATOM    119  O   SER    16       7.936  22.033  10.584  1.00  0.00           O
ATOM    120  N   GLY    17       5.995  20.956  11.001  1.00  0.00           N
ATOM    121  CA  GLY    17       5.945  21.484  12.329  1.00  0.00           C
ATOM    122  C   GLY    17       5.175  20.540  13.192  1.00  0.00           C
ATOM    123  O   GLY    17       4.679  19.512  12.734  1.00  0.00           O
ATOM    124  N   HIS    18       5.060  20.894  14.486  1.00  0.00           N
ATOM    125  CA  HIS    18       4.379  20.086  15.453  1.00  0.00           C
ATOM    126  ND1 HIS    18       6.485  19.514  18.176  1.00  0.00           N
ATOM    127  CG  HIS    18       5.961  20.544  17.426  1.00  0.00           C
ATOM    128  NE2 HIS    18       8.092  21.039  17.985  1.00  0.00           N
ATOM    129  CD2 HIS    18       6.957  21.466  17.317  1.00  0.00           C
ATOM    130  CE1 HIS    18       7.760  19.862  18.484  1.00  0.00           C
ATOM    131  CB  HIS    18       4.555  20.577  16.904  1.00  0.00           C
ATOM    132  C   HIS    18       2.910  20.159  15.184  1.00  0.00           C
ATOM    133  O   HIS    18       2.414  21.130  14.614  1.00  0.00           O
ATOM    134  N   LEU    19       2.181  19.100  15.585  1.00  0.00           N
ATOM    135  CA  LEU    19       0.753  19.062  15.465  1.00  0.00           C
ATOM    136  CB  LEU    19       0.048  20.129  16.320  1.00  0.00           C
ATOM    137  CG  LEU    19       0.259  19.944  17.834  1.00  0.00           C
ATOM    138  CD2 LEU    19       1.745  20.064  18.209  1.00  0.00           C
ATOM    139  CD1 LEU    19      -0.382  18.640  18.333  1.00  0.00           C
ATOM    140  C   LEU    19       0.351  19.270  14.042  1.00  0.00           C
ATOM    141  O   LEU    19      -0.654  19.925  13.769  1.00  0.00           O
ATOM    142  N   SER    20       1.119  18.708  13.090  1.00  0.00           N
ATOM    143  CA  SER    20       0.760  18.857  11.711  1.00  0.00           C
ATOM    144  CB  SER    20       1.746  19.722  10.908  1.00  0.00           C
ATOM    145  OG  SER    20       1.747  21.052  11.405  1.00  0.00           O
ATOM    146  C   SER    20       0.774  17.492  11.102  1.00  0.00           C
ATOM    147  O   SER    20       1.381  16.562  11.630  1.00  0.00           O
ATOM    148  N   PRO    21       0.074  17.362  10.008  1.00  0.00           N
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ATOM    149  CA  PRO    21       0.035  16.100   9.322  1.00  0.00           C
ATOM    150  CD  PRO    21      -1.181  18.085   9.873  1.00  0.00           C
ATOM    151  CB  PRO    21      -1.190  16.145   8.414  1.00  0.00           C
ATOM    152  CG  PRO    21      -2.128  17.133   9.125  1.00  0.00           C
ATOM    153  C   PRO    21       1.306  15.862   8.576  1.00  0.00           C
ATOM    154  O   PRO    21       2.048  16.811   8.332  1.00  0.00           O
ATOM    155  N   TYR    22       1.557  14.591   8.209  1.00  0.00           N
ATOM    156  CA  TYR    22       2.741  14.171   7.523  1.00  0.00           C
ATOM    157  CB  TYR    22       2.950  12.652   7.620  1.00  0.00           C
ATOM    158  CG  TYR    22       2.824  12.395   9.075  1.00  0.00           C
ATOM    159  CD1 TYR    22       3.873  12.652   9.913  1.00  0.00           C
ATOM    160  CD2 TYR    22       1.643  11.949   9.616  1.00  0.00           C
ATOM    161  CE1 TYR    22       3.769  12.446  11.265  1.00  0.00           C
ATOM    162  CE2 TYR    22       1.528  11.738  10.968  1.00  0.00           C
ATOM    163  CZ  TYR    22       2.592  11.988  11.798  1.00  0.00           C
ATOM    164  OH  TYR    22       2.470  11.779  13.188  1.00  0.00           O
ATOM    165  C   TYR    22       2.574  14.509   6.081  1.00  0.00           C
ATOM    166  O   TYR    22       1.476  14.416   5.534  1.00  0.00           O
ATOM    167  N   THR    23       3.663  14.970   5.439  1.00  0.00           N
ATOM    168  CA  THR    23       3.593  15.269   4.040  1.00  0.00           C
ATOM    169  CB  THR    23       3.917  16.698   3.717  1.00  0.00           C
ATOM    170  OG1 THR    23       5.250  16.997   4.103  1.00  0.00           O
ATOM    171  CG2 THR    23       2.931  17.607   4.470  1.00  0.00           C
ATOM    172  C   THR    23       4.608  14.411   3.358  1.00  0.00           C
ATOM    173  O   THR    23       5.740  14.275   3.820  1.00  0.00           O
ATOM    174  N   TYR    24       4.218  13.803   2.224  1.00  0.00           N
ATOM    175  CA  TYR    24       5.102  12.946   1.490  1.00  0.00           C
ATOM    176  CB  TYR    24       4.278  11.983   0.613  1.00  0.00           C
ATOM    177  CG  TYR    24       5.098  10.866   0.073  1.00  0.00           C
ATOM    178  CD1 TYR    24       5.457   9.820   0.891  1.00  0.00           C
ATOM    179  CD2 TYR    24       5.471  10.841  -1.250  1.00  0.00           C
ATOM    180  CE1 TYR    24       6.198   8.770   0.404  1.00  0.00           C
ATOM    181  CE2 TYR    24       6.212   9.794  -1.743  1.00  0.00           C
ATOM    182  CZ  TYR    24       6.578   8.759  -0.915  1.00  0.00           C
ATOM    183  OH  TYR    24       7.339   7.684  -1.422  1.00  0.00           O
ATOM    184  C   TYR    24       5.892  13.872   0.607  1.00  0.00           C
ATOM    185  O   TYR    24       5.313  14.586  -0.208  1.00  0.00           O
ATOM    186  N   ASN    25       7.239  13.893   0.742  1.00  0.00           N
ATOM    187  CA  ASN    25       8.028  14.829  -0.026  1.00  0.00           C
ATOM    188  CB  ASN    25       8.369  16.119   0.738  1.00  0.00           C
ATOM    189  CG  ASN    25       7.085  16.919   0.910  1.00  0.00           C
ATOM    190  OD1 ASN    25       6.231  16.944   0.027  1.00  0.00           O
ATOM    191  ND2 ASN    25       6.944  17.596   2.082  1.00  0.00           N
ATOM    192  C   ASN    25       9.335  14.201  -0.419  1.00  0.00           C
ATOM    193  O   ASN    25       9.547  13.006  -0.235  1.00  0.00           O
ATOM    194  N   LEU    26      10.253  15.001  -1.008  1.00  0.00           N
ATOM    195  CA  LEU    26      11.513  14.465  -1.460  1.00  0.00           C
ATOM    196  CB  LEU    26      11.850  14.846  -2.913  1.00  0.00           C
ATOM    197  CG  LEU    26      10.854  14.282  -3.943  1.00  0.00           C
ATOM    198  CD2 LEU    26      11.367  14.472  -5.379  1.00  0.00           C
ATOM    199  CD1 LEU    26       9.446  14.862  -3.734  1.00  0.00           C
ATOM    200  C   LEU    26      12.636  14.977  -0.595  1.00  0.00           C
ATOM    201  O   LEU    26      12.591  16.104  -0.107  1.00  0.00           O
ATOM    202  N   ARG    27      13.674  14.133  -0.372  1.00  0.00           N
ATOM    203  CA  ARG    27      14.834  14.510   0.408  1.00  0.00           C
ATOM    204  CB  ARG    27      14.701  14.131   1.895  1.00  0.00           C
ATOM    205  CG  ARG    27      15.907  14.527   2.748  1.00  0.00           C
ATOM    206  CD  ARG    27      15.762  14.149   4.223  1.00  0.00           C
ATOM    207  NE  ARG    27      15.853  12.665   4.318  1.00  0.00           N
ATOM    208  CZ  ARG    27      17.073  12.062   4.431  1.00  0.00           C
ATOM    209  NH1 ARG    27      18.208  12.819   4.465  1.00  0.00           N
ATOM    210  NH2 ARG    27      17.158  10.702   4.515  1.00  0.00           N
ATOM    211  C   ARG    27      16.057  13.795  -0.141  1.00  0.00           C
ATOM    212  O   ARG    27      15.927  12.915  -0.985  1.00  0.00           O
ATOM    213  N   LYS    28      17.292  14.150   0.314  1.00  0.00           N
ATOM    214  CA  LYS    28      18.496  13.543  -0.234  1.00  0.00           C
ATOM    215  CB  LYS    28      19.394  14.545  -0.981  1.00  0.00           C
ATOM    216  CG  LYS    28      19.960  15.643  -0.078  1.00  0.00           C
ATOM    217  CD  LYS    28      18.884  16.504   0.589  1.00  0.00           C
ATOM    218  CE  LYS    28      19.450  17.602   1.491  1.00  0.00           C
ATOM    219  NZ  LYS    28      18.348  18.383   2.094  1.00  0.00           N
ATOM    220  C   LYS    28      19.345  12.924   0.862  1.00  0.00           C
ATOM    221  O   LYS    28      19.185  13.275   2.029  1.00  0.00           O
ATOM    222  N   LYS    29      20.280  11.984   0.515  1.00  0.00           N
ATOM    223  CA  LYS    29      21.096  11.315   1.527  1.00  0.00           C
ATOM    224  CB  LYS    29      20.661   9.867   1.813  1.00  0.00           C
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ATOM    225  CG  LYS    29      21.421   8.836   0.973  1.00  0.00           C
ATOM    226  CD  LYS    29      21.365   9.069  -0.537  1.00  0.00           C
ATOM    227  CE  LYS    29      22.339   8.185  -1.319  1.00  0.00           C
ATOM    228  NZ  LYS    29      23.733   8.570  -1.009  1.00  0.00           N
ATOM    229  C   LYS    29      22.577  11.198   1.107  1.00  0.00           C
ATOM    230  O   LYS    29      22.868  11.373  -0.075  1.00  0.00           O
ATOM    231  N   GLY    30      23.530  10.843   2.056  1.00  0.00           N
ATOM    232  CA  GLY    30      25.000  10.775   1.869  1.00  0.00           C
ATOM    233  C   GLY    30      25.721   9.550   2.544  1.00  0.00           C
ATOM    234  O   GLY    30      25.026   8.627   2.962  1.00  0.00           O
ATOM    235  N   PRO    31      27.104   9.523   2.605  1.00  0.00           N
ATOM    236  CA  PRO    31      28.055   8.448   3.071  1.00  0.00           C
ATOM    237  CD  PRO    31      27.747  10.351   1.595  1.00  0.00           C
ATOM    238  CB  PRO    31      29.266   8.556   2.143  1.00  0.00           C
ATOM    239  CG  PRO    31      29.239  10.002   1.634  1.00  0.00           C
ATOM    240  C   PRO    31      28.572   8.209   4.514  1.00  0.00           C
ATOM    241  O   PRO    31      28.116   8.864   5.447  1.00  0.00           O
ATOM    242  N   GLU    32      29.566   7.259   4.690  1.00  0.00           N
ATOM    243  CA  GLU    32      30.265   6.815   5.909  1.00  0.00           C
ATOM    244  CB  GLU    32      30.870   7.969   6.722  1.00  0.00           C
ATOM    245  CG  GLU    32      31.625   7.509   7.972  1.00  0.00           C
ATOM    246  CD  GLU    32      32.166   8.746   8.674  1.00  0.00           C
ATOM    247  OE1 GLU    32      31.870   9.874   8.196  1.00  0.00           O
ATOM    248  OE2 GLU    32      32.884   8.582   9.697  1.00  0.00           O
ATOM    249  C   GLU    32      29.271   6.136   6.745  1.00  0.00           C
ATOM    250  O   GLU    32      29.418   5.848   7.939  1.00  0.00           O
ATOM    251  N   ASP    33      28.212   5.803   6.039  1.00  0.00           N
ATOM    252  CA  ASP    33      27.132   5.206   6.686  1.00  0.00           C
ATOM    253  CB  ASP    33      25.949   6.175   6.798  1.00  0.00           C
ATOM    254  CG  ASP    33      26.289   7.260   7.811  1.00  0.00           C
ATOM    255  OD1 ASP    33      27.293   7.092   8.552  1.00  0.00           O
ATOM    256  OD2 ASP    33      25.540   8.272   7.859  1.00  0.00           O
ATOM    257  C   ASP    33      26.732   4.117   5.779  1.00  0.00           C
ATOM    258  O   ASP    33      27.480   3.705   4.892  1.00  0.00           O
ATOM    259  N   VAL    34      25.529   3.605   6.032  1.00  0.00           N
ATOM    260  CA  VAL    34      24.974   2.616   5.187  1.00  0.00           C
ATOM    261  CB  VAL    34      24.619   1.362   5.928  1.00  0.00           C
ATOM    262  CG1 VAL    34      23.838   0.431   4.990  1.00  0.00           C
ATOM    263  CG2 VAL    34      25.918   0.748   6.475  1.00  0.00           C
ATOM    264  C   VAL    34      23.713   3.229   4.695  1.00  0.00           C
ATOM    265  O   VAL    34      22.993   3.876   5.452  1.00  0.00           O
ATOM    266  N   ILE    35      23.429   3.069   3.395  1.00  0.00           N
ATOM    267  CA  ILE    35      22.216   3.605   2.875  1.00  0.00           C
ATOM    268  CB  ILE    35      22.417   4.365   1.596  1.00  0.00           C
ATOM    269  CG2 ILE    35      23.254   5.614   1.920  1.00  0.00           C
ATOM    270  CG1 ILE    35      23.045   3.469   0.519  1.00  0.00           C
ATOM    271  CD1 ILE    35      23.006   4.086  -0.879  1.00  0.00           C
ATOM    272  C   ILE    35      21.334   2.427   2.667  1.00  0.00           C
ATOM    273  O   ILE    35      21.721   1.444   2.037  1.00  0.00           O
ATOM    274  N   VAL    36      20.122   2.483   3.248  1.00  0.00           N
ATOM    275  CA  VAL    36      19.286   1.326   3.182  1.00  0.00           C
ATOM    276  CB  VAL    36      19.015   0.725   4.528  1.00  0.00           C
ATOM    277  CG1 VAL    36      20.345   0.236   5.125  1.00  0.00           C
ATOM    278  CG2 VAL    36      18.302   1.783   5.384  1.00  0.00           C
ATOM    279  C   VAL    36      17.969   1.672   2.579  1.00  0.00           C
ATOM    280  O   VAL    36      17.462   2.783   2.724  1.00  0.00           O
ATOM    281  N   LYS    37      17.395   0.700   1.848  1.00  0.00           N
ATOM    282  CA  LYS    37      16.081   0.871   1.310  1.00  0.00           C
ATOM    283  CB  LYS    37      15.851   0.127  -0.015  1.00  0.00           C
ATOM    284  CG  LYS    37      14.441   0.322  -0.576  1.00  0.00           C
ATOM    285  CD  LYS    37      14.270  -0.155  -2.018  1.00  0.00           C
ATOM    286  CE  LYS    37      12.854   0.056  -2.555  1.00  0.00           C
ATOM    287  NZ  LYS    37      12.767  -0.426  -3.949  1.00  0.00           N
ATOM    288  C   LYS    37      15.173   0.271   2.334  1.00  0.00           C
ATOM    289  O   LYS    37      15.376  -0.866   2.759  1.00  0.00           O
ATOM    290  N   VAL    38      14.136   1.018   2.760  1.00  0.00           N
ATOM    291  CA  VAL    38      13.340   0.498   3.834  1.00  0.00           C
ATOM    292  CB  VAL    38      12.813   1.557   4.760  1.00  0.00           C
ATOM    293  CG1 VAL    38      14.011   2.236   5.444  1.00  0.00           C
ATOM    294  CG2 VAL    38      11.922   2.527   3.968  1.00  0.00           C
ATOM    295  C   VAL    38      12.180  -0.276   3.296  1.00  0.00           C
ATOM    296  O   VAL    38      11.362   0.256   2.545  1.00  0.00           O
ATOM    297  N   ILE    39      12.134  -1.601   3.572  1.00  0.00           N
ATOM    298  CA  ILE    39      10.962  -2.304   3.146  1.00  0.00           C
ATOM    299  CB  ILE    39      11.125  -3.739   2.716  1.00  0.00           C
ATOM    300  CG2 ILE    39      12.135  -3.728   1.557  1.00  0.00           C
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ATOM    301  CG1 ILE    39      11.494  -4.722   3.822  1.00  0.00           C
ATOM    302  CD1 ILE    39      11.283  -6.148   3.308  1.00  0.00           C
ATOM    303  C   ILE    39       9.803  -2.145   4.095  1.00  0.00           C
ATOM    304  O   ILE    39       8.677  -1.948   3.647  1.00  0.00           O
ATOM    305  N   TYR    40      10.025  -2.240   5.430  1.00  0.00           N
ATOM    306  CA  TYR    40       8.906  -2.124   6.340  1.00  0.00           C
ATOM    307  CB  TYR    40       8.452  -3.472   6.930  1.00  0.00           C
ATOM    308  CG  TYR    40       7.848  -4.299   5.846  1.00  0.00           C
ATOM    309  CD1 TYR    40       6.523  -4.143   5.517  1.00  0.00           C
ATOM    310  CD2 TYR    40       8.599  -5.233   5.165  1.00  0.00           C
ATOM    311  CE1 TYR    40       5.961  -4.901   4.521  1.00  0.00           C
ATOM    312  CE2 TYR    40       8.039  -5.996   4.165  1.00  0.00           C
ATOM    313  CZ  TYR    40       6.713  -5.828   3.841  1.00  0.00           C
ATOM    314  OH  TYR    40       6.126  -6.602   2.817  1.00  0.00           O
ATOM    315  C   TYR    40       9.273  -1.260   7.518  1.00  0.00           C
ATOM    316  O   TYR    40      10.418  -1.261   7.964  1.00  0.00           O
ATOM    317  N   CYS    41       8.287  -0.504   8.062  1.00  0.00           N
ATOM    318  CA  CYS    41       8.508   0.366   9.192  1.00  0.00           C
ATOM    319  CB  CYS    41       8.769   1.824   8.774  1.00  0.00           C
ATOM    320  SG  CYS    41       8.780   2.975  10.181  1.00  0.00           S
ATOM    321  C   CYS    41       7.263   0.393  10.040  1.00  0.00           C
ATOM    322  O   CYS    41       6.160   0.573   9.524  1.00  0.00           O
ATOM    323  N   GLY    42       7.411   0.226  11.375  1.00  0.00           N
ATOM    324  CA  GLY    42       6.264   0.231  12.249  1.00  0.00           C
ATOM    325  C   GLY    42       5.994   1.616  12.757  1.00  0.00           C
ATOM    326  O   GLY    42       6.846   2.500  12.682  1.00  0.00           O
ATOM    327  N   ILE    43       4.786   1.821  13.332  1.00  0.00           N
ATOM    328  CA  ILE    43       4.407   3.107  13.852  1.00  0.00           C
ATOM    329  CB  ILE    43       3.028   3.524  13.428  1.00  0.00           C
ATOM    330  CG2 ILE    43       2.688   4.842  14.146  1.00  0.00           C
ATOM    331  CG1 ILE    43       2.947   3.621  11.896  1.00  0.00           C
ATOM    332  CD1 ILE    43       3.908   4.642  11.291  1.00  0.00           C
ATOM    333  C   ILE    43       4.394   2.996  15.344  1.00  0.00           C
ATOM    334  O   ILE    43       3.477   2.418  15.927  1.00  0.00           O
ATOM    335  N   CYS    44       5.415   3.585  15.995  1.00  0.00           N
ATOM    336  CA  CYS    44       5.568   3.523  17.421  1.00  0.00           C
ATOM    337  CB  CYS    44       7.044   3.411  17.845  1.00  0.00           C
ATOM    338  SG  CYS    44       7.279   3.337  19.645  1.00  0.00           S
ATOM    339  C   CYS    44       5.008   4.781  18.009  1.00  0.00           C
ATOM    340  O   CYS    44       4.985   5.828  17.367  1.00  0.00           O
ATOM    341  N   HIS    45       4.570   4.700  19.280  1.00  0.00           N
ATOM    342  CA  HIS    45       3.931   5.788  19.966  1.00  0.00           C
ATOM    343  ND1 HIS    45       1.349   6.643  21.927  1.00  0.00           N
ATOM    344  CG  HIS    45       2.709   6.486  22.078  1.00  0.00           C
ATOM    345  NE2 HIS    45       2.021   8.238  23.323  1.00  0.00           N
ATOM    346  CD2 HIS    45       3.103   7.469  22.933  1.00  0.00           C
ATOM    347  CE1 HIS    45       0.989   7.704  22.693  1.00  0.00           C
ATOM    348  CB  HIS    45       3.512   5.416  21.400  1.00  0.00           C
ATOM    349  C   HIS    45       4.886   6.935  20.049  1.00  0.00           C
ATOM    350  O   HIS    45       4.475   8.094  20.036  1.00  0.00           O
ATOM    351  N   SER    46       6.191   6.639  20.162  1.00  0.00           N
ATOM    352  CA  SER    46       7.180   7.672  20.284  1.00  0.00           C
ATOM    353  CB  SER    46       8.601   7.101  20.401  1.00  0.00           C
ATOM    354  OG  SER    46       9.538   8.157  20.527  1.00  0.00           O
ATOM    355  C   SER    46       7.136   8.556  19.075  1.00  0.00           C
ATOM    356  O   SER    46       7.341   9.764  19.163  1.00  0.00           O
ATOM    357  N   ASP    47       6.858   7.987  17.894  1.00  0.00           N
ATOM    358  CA  ASP    47       6.827   8.810  16.718  1.00  0.00           C
ATOM    359  CB  ASP    47       6.510   8.007  15.441  1.00  0.00           C
ATOM    360  CG  ASP    47       7.690   7.087  15.147  1.00  0.00           C
ATOM    361  OD1 ASP    47       8.851   7.571  15.206  1.00  0.00           O
ATOM    362  OD2 ASP    47       7.446   5.882  14.872  1.00  0.00           O
ATOM    363  C   ASP    47       5.732   9.814  16.900  1.00  0.00           C
ATOM    364  O   ASP    47       5.901  10.993  16.595  1.00  0.00           O
ATOM    365  N   LEU    48       4.582   9.365  17.439  1.00  0.00           N
ATOM    366  CA  LEU    48       3.440  10.219  17.608  1.00  0.00           C
ATOM    367  CB  LEU    48       2.185   9.488  18.114  1.00  0.00           C
ATOM    368  CG  LEU    48       1.587   8.506  17.092  1.00  0.00           C
ATOM    369  CD2 LEU    48       1.503   9.136  15.693  1.00  0.00           C
ATOM    370  CD1 LEU    48       0.236   7.963  17.581  1.00  0.00           C
ATOM    371  C   LEU    48       3.750  11.305  18.585  1.00  0.00           C
ATOM    372  O   LEU    48       3.265  12.428  18.442  1.00  0.00           O
ATOM    373  N   VAL    49       4.560  11.011  19.618  1.00  0.00           N
ATOM    374  CA  VAL    49       4.795  12.035  20.589  1.00  0.00           C
ATOM    375  CB  VAL    49       5.501  11.584  21.846  1.00  0.00           C
ATOM    376  CG1 VAL    49       4.582  10.577  22.558  1.00  0.00           C
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ATOM    377  CG2 VAL    49       6.889  11.024  21.531  1.00  0.00           C
ATOM    378  C   VAL    49       5.491  13.199  19.947  1.00  0.00           C
ATOM    379  O   VAL    49       5.299  14.334  20.378  1.00  0.00           O
ATOM    380  N   GLN    50       6.326  12.961  18.915  1.00  0.00           N
ATOM    381  CA  GLN    50       6.994  14.042  18.236  1.00  0.00           C
ATOM    382  CB  GLN    50       7.971  13.567  17.149  1.00  0.00           C
ATOM    383  CG  GLN    50       8.681  14.721  16.436  1.00  0.00           C
ATOM    384  CD  GLN    50       9.624  14.135  15.395  1.00  0.00           C
ATOM    385  OE1 GLN    50       9.735  12.919  15.251  1.00  0.00           O
ATOM    386  NE2 GLN    50      10.322  15.027  14.642  1.00  0.00           N
ATOM    387  C   GLN    50       5.978  14.926  17.563  1.00  0.00           C
ATOM    388  O   GLN    50       6.146  16.145  17.534  1.00  0.00           O
ATOM    389  N   MET    51       4.915  14.342  16.973  1.00  0.00           N
ATOM    390  CA  MET    51       3.904  15.137  16.320  1.00  0.00           C
ATOM    391  CB  MET    51       2.794  14.290  15.676  1.00  0.00           C
ATOM    392  CG  MET    51       1.725  15.131  14.973  1.00  0.00           C
ATOM    393  SD  MET    51       0.391  14.169  14.200  1.00  0.00           S
ATOM    394  CE  MET    51      -0.498  15.621  13.572  1.00  0.00           C
ATOM    395  C   MET    51       3.273  15.983  17.366  1.00  0.00           C
ATOM    396  O   MET    51       3.055  17.179  17.181  1.00  0.00           O
ATOM    397  N   ARG    52       2.984  15.374  18.524  1.00  0.00           N
ATOM    398  CA  ARG    52       2.464  16.154  19.596  1.00  0.00           C
ATOM    399  CB  ARG    52       1.854  15.319  20.733  1.00  0.00           C
ATOM    400  CG  ARG    52       1.299  16.166  21.878  1.00  0.00           C
ATOM    401  CD  ARG    52       0.695  15.339  23.013  1.00  0.00           C
ATOM    402  NE  ARG    52      -0.483  14.609  22.465  1.00  0.00           N
ATOM    403  CZ  ARG    52      -1.133  13.691  23.237  1.00  0.00           C
ATOM    404  NH1 ARG    52      -0.708  13.449  24.512  1.00  0.00           N
ATOM    405  NH2 ARG    52      -2.208  13.015  22.737  1.00  0.00           N
ATOM    406  C   ARG    52       3.687  16.816  20.114  1.00  0.00           C
ATOM    407  O   ARG    52       4.767  16.662  19.565  1.00  0.00           O
ATOM    408  N   ASN    53       3.605  17.654  21.133  1.00  0.00           N
ATOM    409  CA  ASN    53       4.886  18.148  21.525  1.00  0.00           C
ATOM    410  CB  ASN    53       4.872  19.643  21.887  1.00  0.00           C
ATOM    411  CG  ASN    53       3.968  19.823  23.098  1.00  0.00           C
ATOM    412  OD1 ASN    53       2.863  19.286  23.149  1.00  0.00           O
ATOM    413  ND2 ASN    53       4.453  20.595  24.108  1.00  0.00           N
ATOM    414  C   ASN    53       5.259  17.399  22.759  1.00  0.00           C
ATOM    415  O   ASN    53       6.046  17.877  23.574  1.00  0.00           O
ATOM    416  N   GLU    54       4.707  16.180  22.910  1.00  0.00           N
ATOM    417  CA  GLU    54       4.967  15.383  24.071  1.00  0.00           C
ATOM    418  CB  GLU    54       4.106  14.108  24.118  1.00  0.00           C
ATOM    419  CG  GLU    54       4.255  13.316  25.417  1.00  0.00           C
ATOM    420  CD  GLU    54       3.458  14.037  26.494  1.00  0.00           C
ATOM    421  OE1 GLU    54       3.536  15.294  26.545  1.00  0.00           O
ATOM    422  OE2 GLU    54       2.757  13.342  27.277  1.00  0.00           O
ATOM    423  C   GLU    54       6.395  14.953  24.057  1.00  0.00           C
ATOM    424  O   GLU    54       7.088  15.025  25.070  1.00  0.00           O
ATOM    425  N   MET    55       6.883  14.517  22.882  1.00  0.00           N
ATOM    426  CA  MET    55       8.224  14.031  22.815  1.00  0.00           C
ATOM    427  CB  MET    55       8.610  13.404  21.467  1.00  0.00           C
ATOM    428  CG  MET    55      10.028  12.827  21.454  1.00  0.00           C
ATOM    429  SD  MET    55      10.512  12.051  19.884  1.00  0.00           S
ATOM    430  CE  MET    55      12.175  11.584  20.444  1.00  0.00           C
ATOM    431  C   MET    55       9.092  15.196  22.982  1.00  0.00           C
ATOM    432  O   MET    55       8.728  16.279  22.517  1.00  0.00           O
ATOM    433  N   GLY    56      10.243  14.963  23.659  1.00  0.00           N
ATOM    434  CA  GLY    56      11.218  15.982  23.870  1.00  0.00           C
ATOM    435  C   GLY    56      11.414  16.509  22.508  1.00  0.00           C
ATOM    436  O   GLY    56      11.717  15.757  21.583  1.00  0.00           O
ATOM    437  N   MET    57      11.203  17.828  22.388  1.00  0.00           N
ATOM    438  CA  MET    57      11.137  18.496  21.133  1.00  0.00           C
ATOM    439  CB  MET    57      11.156  20.030  21.248  1.00  0.00           C
ATOM    440  CG  MET    57      12.490  20.587  21.751  1.00  0.00           C
ATOM    441  SD  MET    57      12.543  22.398  21.899  1.00  0.00           S
ATOM    442  CE  MET    57      14.258  22.455  22.492  1.00  0.00           C
ATOM    443  C   MET    57      12.288  18.084  20.297  1.00  0.00           C
ATOM    444  O   MET    57      13.369  17.780  20.792  1.00  0.00           O
ATOM    445  N   SER    58      12.025  17.995  18.988  1.00  0.00           N
ATOM    446  CA  SER    58      13.035  17.621  18.055  1.00  0.00           C
ATOM    447  CB  SER    58      12.701  16.343  17.266  1.00  0.00           C
ATOM    448  OG  SER    58      13.750  16.045  16.358  1.00  0.00           O
ATOM    449  C   SER    58      13.094  18.741  17.081  1.00  0.00           C
ATOM    450  O   SER    58      12.184  19.567  17.019  1.00  0.00           O
ATOM    451  N   HIS    59      14.196  18.821  16.316  1.00  0.00           N
ATOM    452  CA  HIS    59      14.309  19.878  15.362  1.00  0.00           C
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ATOM    453  ND1 HIS    59      17.426  19.509  16.554  1.00  0.00           N
ATOM    454  CG  HIS    59      16.764  20.400  15.739  1.00  0.00           C
ATOM    455  NE2 HIS    59      18.230  21.526  17.032  1.00  0.00           N
ATOM    456  CD2 HIS    59      17.267  21.627  16.044  1.00  0.00           C
ATOM    457  CE1 HIS    59      18.290  20.235  17.306  1.00  0.00           C
ATOM    458  CB  HIS    59      15.712  20.008  14.745  1.00  0.00           C
ATOM    459  C   HIS    59      13.355  19.584  14.253  1.00  0.00           C
ATOM    460  O   HIS    59      13.060  18.428  13.957  1.00  0.00           O
ATOM    461  N   TYR    60      12.825  20.650  13.625  1.00  0.00           N
ATOM    462  CA  TYR    60      11.921  20.504  12.521  1.00  0.00           C
ATOM    463  CB  TYR    60      10.524  21.104  12.763  1.00  0.00           C
ATOM    464  CG  TYR    60       9.816  20.240  13.749  1.00  0.00           C
ATOM    465  CD1 TYR    60      10.110  20.316  15.089  1.00  0.00           C
ATOM    466  CD2 TYR    60       8.849  19.357  13.327  1.00  0.00           C
ATOM    467  CE1 TYR    60       9.453  19.516  15.993  1.00  0.00           C
ATOM    468  CE2 TYR    60       8.188  18.554  14.225  1.00  0.00           C
ATOM    469  CZ  TYR    60       8.492  18.633  15.561  1.00  0.00           C
ATOM    470  OH  TYR    60       7.816  17.809  16.485  1.00  0.00           O
ATOM    471  C   TYR    60      12.527  21.253  11.383  1.00  0.00           C
ATOM    472  O   TYR    60      13.286  22.200  11.585  1.00  0.00           O
ATOM    473  N   PRO    61      12.236  20.839  10.182  1.00  0.00           N
ATOM    474  CA  PRO    61      11.378  19.710   9.952  1.00  0.00           C
ATOM    475  CD  PRO    61      12.217  21.769   9.066  1.00  0.00           C
ATOM    476  CB  PRO    61      10.840  19.861   8.527  1.00  0.00           C
ATOM    477  CG  PRO    61      11.748  20.920   7.878  1.00  0.00           C
ATOM    478  C   PRO    61      12.129  18.440  10.175  1.00  0.00           C
ATOM    479  O   PRO    61      13.358  18.472  10.168  1.00  0.00           O
ATOM    480  N   MET    62      11.419  17.314  10.386  1.00  0.00           N
ATOM    481  CA  MET    62      12.114  16.089  10.633  1.00  0.00           C
ATOM    482  CB  MET    62      12.270  15.769  12.129  1.00  0.00           C
ATOM    483  CG  MET    62      13.044  14.478  12.405  1.00  0.00           C
ATOM    484  SD  MET    62      13.247  14.085  14.168  1.00  0.00           S
ATOM    485  CE  MET    62      14.180  12.553  13.882  1.00  0.00           C
ATOM    486  C   MET    62      11.368  14.954  10.013  1.00  0.00           C
ATOM    487  O   MET    62      10.175  15.052   9.729  1.00  0.00           O
ATOM    488  N   VAL    63      12.090  13.848   9.748  1.00  0.00           N
ATOM    489  CA  VAL    63      11.479  12.647   9.265  1.00  0.00           C
ATOM    490  CB  VAL    63      12.115  12.112   8.008  1.00  0.00           C
ATOM    491  CG1 VAL    63      13.618  11.882   8.240  1.00  0.00           C
ATOM    492  CG2 VAL    63      11.347  10.850   7.581  1.00  0.00           C
ATOM    493  C   VAL    63      11.610  11.641  10.370  1.00  0.00           C
ATOM    494  O   VAL    63      12.688  11.157  10.709  1.00  0.00           O
ATOM    495  N   PRO    64      10.485  11.355  10.946  1.00  0.00           N
ATOM    496  CA  PRO    64      10.443  10.438  12.060  1.00  0.00           C
ATOM    497  CD  PRO    64       9.556  12.456  11.133  1.00  0.00           C
ATOM    498  CB  PRO    64       9.197  10.799  12.860  1.00  0.00           C
ATOM    499  CG  PRO    64       8.997  12.291  12.551  1.00  0.00           C
ATOM    500  C   PRO    64      10.495   9.007  11.631  1.00  0.00           C
ATOM    501  O   PRO    64      10.737   8.730  10.457  1.00  0.00           O
ATOM    502  N   GLY    65      10.305   8.075  12.584  1.00  0.00           N
ATOM    503  CA  GLY    65      10.296   6.677  12.265  1.00  0.00           C
ATOM    504  C   GLY    65      11.594   6.115  12.743  1.00  0.00           C
ATOM    505  O   GLY    65      12.654   6.705  12.535  1.00  0.00           O
ATOM    506  N   HIS    66      11.541   4.939  13.401  1.00  0.00           N
ATOM    507  CA  HIS    66      12.751   4.387  13.935  1.00  0.00           C
ATOM    508  ND1 HIS    66      10.810   5.720  16.279  1.00  0.00           N
ATOM    509  CG  HIS    66      11.819   4.783  16.252  1.00  0.00           C
ATOM    510  NE2 HIS    66      10.259   4.151  17.753  1.00  0.00           N
ATOM    511  CD2 HIS    66      11.467   3.832  17.159  1.00  0.00           C
ATOM    512  CE1 HIS    66       9.903   5.292  17.193  1.00  0.00           C
ATOM    513  CB  HIS    66      13.021   4.886  15.362  1.00  0.00           C
ATOM    514  C   HIS    66      12.658   2.894  14.012  1.00  0.00           C
ATOM    515  O   HIS    66      13.671   2.229  14.224  1.00  0.00           O
ATOM    516  N   GLU    67      11.447   2.325  13.852  1.00  0.00           N
ATOM    517  CA  GLU    67      11.275   0.900  13.951  1.00  0.00           C
ATOM    518  CB  GLU    67       9.983   0.555  14.718  1.00  0.00           C
ATOM    519  CG  GLU    67       9.745  -0.925  15.019  1.00  0.00           C
ATOM    520  CD  GLU    67       8.467  -0.991  15.836  1.00  0.00           C
ATOM    521  OE1 GLU    67       7.452  -0.418  15.360  1.00  0.00           O
ATOM    522  OE2 GLU    67       8.487  -1.592  16.943  1.00  0.00           O
ATOM    523  C   GLU    67      11.146   0.380  12.550  1.00  0.00           C
ATOM    524  O   GLU    67      10.091   0.533  11.935  1.00  0.00           O
ATOM    525  N   VAL    68      12.205  -0.270  12.006  1.00  0.00           N
ATOM    526  CA  VAL    68      12.098  -0.677  10.625  1.00  0.00           C
ATOM    527  CB  VAL    68      12.441   0.418   9.654  1.00  0.00           C
ATOM    528  CG1 VAL    68      11.507   1.615   9.856  1.00  0.00           C
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ATOM    529  CG2 VAL    68      13.930   0.758   9.829  1.00  0.00           C
ATOM    530  C   VAL    68      13.082  -1.756  10.274  1.00  0.00           C
ATOM    531  O   VAL    68      13.943  -2.147  11.055  1.00  0.00           O
ATOM    532  N   VAL    69      12.952  -2.283   9.040  1.00  0.00           N
ATOM    533  CA  VAL    69      13.891  -3.240   8.525  1.00  0.00           C
ATOM    534  CB  VAL    69      13.435  -4.661   8.624  1.00  0.00           C
ATOM    535  CG1 VAL    69      14.526  -5.543   7.998  1.00  0.00           C
ATOM    536  CG2 VAL    69      13.144  -4.986  10.098  1.00  0.00           C
ATOM    537  C   VAL    69      14.059  -2.929   7.071  1.00  0.00           C
ATOM    538  O   VAL    69      13.145  -2.402   6.436  1.00  0.00           O
ATOM    539  N   GLY    70      15.240  -3.241   6.495  1.00  0.00           N
ATOM    540  CA  GLY    70      15.435  -2.899   5.114  1.00  0.00           C
ATOM    541  C   GLY    70      16.591  -3.671   4.553  1.00  0.00           C
ATOM    542  O   GLY    70      17.148  -4.555   5.204  1.00  0.00           O
ATOM    543  N   ILE    71      16.966  -3.333   3.297  1.00  0.00           N
ATOM    544  CA  ILE    71      18.045  -3.971   2.591  1.00  0.00           C
ATOM    545  CB  ILE    71      17.632  -4.548   1.271  1.00  0.00           C
ATOM    546  CG2 ILE    71      18.898  -5.037   0.553  1.00  0.00           C
ATOM    547  CG1 ILE    71      16.599  -5.661   1.482  1.00  0.00           C
ATOM    548  CD1 ILE    71      17.159  -6.851   2.256  1.00  0.00           C
ATOM    549  C   ILE    71      19.062  -2.916   2.298  1.00  0.00           C
ATOM    550  O   ILE    71      18.711  -1.757   2.088  1.00  0.00           O
ATOM    551  N   VAL    72      20.358  -3.293   2.280  1.00  0.00           N
ATOM    552  CA  VAL    72      21.390  -2.309   2.103  1.00  0.00           C
ATOM    553  CB  VAL    72      22.709  -2.739   2.676  1.00  0.00           C
ATOM    554  CG1 VAL    72      23.748  -1.644   2.388  1.00  0.00           C
ATOM    555  CG2 VAL    72      22.518  -3.048   4.171  1.00  0.00           C
ATOM    556  C   VAL    72      21.594  -2.045   0.640  1.00  0.00           C
ATOM    557  O   VAL    72      21.971  -2.936  -0.120  1.00  0.00           O
ATOM    558  N   THR    73      21.283  -0.804   0.198  1.00  0.00           N
ATOM    559  CA  THR    73      21.498  -0.422  -1.170  1.00  0.00           C
ATOM    560  CB  THR    73      20.739   0.813  -1.567  1.00  0.00           C
ATOM    561  OG1 THR    73      21.145   1.919  -0.779  1.00  0.00           O
ATOM    562  CG2 THR    73      19.237   0.552  -1.369  1.00  0.00           C
ATOM    563  C   THR    73      22.961  -0.204  -1.447  1.00  0.00           C
ATOM    564  O   THR    73      23.497  -0.740  -2.415  1.00  0.00           O
ATOM    565  N   GLU    74      23.657   0.575  -0.588  1.00  0.00           N
ATOM    566  CA  GLU    74      25.049   0.867  -0.814  1.00  0.00           C
ATOM    567  CB  GLU    74      25.329   2.267  -1.367  1.00  0.00           C
ATOM    568  CG  GLU    74      24.780   2.624  -2.736  1.00  0.00           C
ATOM    569  CD  GLU    74      25.151   4.092  -2.895  1.00  0.00           C
ATOM    570  OE1 GLU    74      26.332   4.427  -2.612  1.00  0.00           O
ATOM    571  OE2 GLU    74      24.269   4.894  -3.301  1.00  0.00           O
ATOM    572  C   GLU    74      25.707   0.991   0.523  1.00  0.00           C
ATOM    573  O   GLU    74      25.046   1.264   1.523  1.00  0.00           O
ATOM    574  N   ILE    75      27.048   0.826   0.555  1.00  0.00           N
ATOM    575  CA  ILE    75      27.797   1.029   1.765  1.00  0.00           C
ATOM    576  CB  ILE    75      28.599  -0.156   2.227  1.00  0.00           C
ATOM    577  CG2 ILE    75      27.618  -1.303   2.522  1.00  0.00           C
ATOM    578  CG1 ILE    75      29.692  -0.518   1.209  1.00  0.00           C
ATOM    579  CD1 ILE    75      29.143  -0.937  -0.151  1.00  0.00           C
ATOM    580  C   ILE    75      28.757   2.140   1.470  1.00  0.00           C
ATOM    581  O   ILE    75      29.312   2.223   0.374  1.00  0.00           O
ATOM    582  N   GLY    76      28.960   3.042   2.448  1.00  0.00           N
ATOM    583  CA  GLY    76      29.798   4.186   2.242  1.00  0.00           C
ATOM    584  C   GLY    76      31.210   3.823   2.489  1.00  0.00           C
ATOM    585  O   GLY    76      31.533   2.673   2.769  1.00  0.00           O
ATOM    586  N   SER    77      32.095   4.829   2.393  1.00  0.00           N
ATOM    587  CA  SER    77      33.481   4.572   2.599  1.00  0.00           C
ATOM    588  CB  SER    77      34.378   5.799   2.354  1.00  0.00           C
ATOM    589  OG  SER    77      34.293   6.204   0.995  1.00  0.00           O
ATOM    590  C   SER    77      33.650   4.165   4.022  1.00  0.00           C
ATOM    591  O   SER    77      32.946   4.652   4.906  1.00  0.00           O
ATOM    592  N   GLU    78      34.616   3.253   4.248  1.00  0.00           N
ATOM    593  CA  GLU    78      34.992   2.743   5.535  1.00  0.00           C
ATOM    594  CB  GLU    78      35.406   3.864   6.505  1.00  0.00           C
ATOM    595  CG  GLU    78      36.675   4.609   6.080  1.00  0.00           C
ATOM    596  CD  GLU    78      36.809   5.849   6.953  1.00  0.00           C
ATOM    597  OE1 GLU    78      37.294   5.713   8.108  1.00  0.00           O
ATOM    598  OE2 GLU    78      36.418   6.949   6.477  1.00  0.00           O
ATOM    599  C   GLU    78      33.891   1.954   6.186  1.00  0.00           C
ATOM    600  O   GLU    78      33.837   1.891   7.412  1.00  0.00           O
ATOM    601  N   VAL    79      33.009   1.290   5.407  1.00  0.00           N
ATOM    602  CA  VAL    79      31.964   0.505   6.018  1.00  0.00           C
ATOM    603  CB  VAL    79      30.654   0.592   5.280  1.00  0.00           C
ATOM    604  CG1 VAL    79      29.683  -0.448   5.863  1.00  0.00           C
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ATOM    605  CG2 VAL    79      30.129   2.034   5.371  1.00  0.00           C
ATOM    606  C   VAL    79      32.364  -0.947   5.994  1.00  0.00           C
ATOM    607  O   VAL    79      32.387  -1.570   4.934  1.00  0.00           O
ATOM    608  N   LYS    80      32.769  -1.492   7.164  1.00  0.00           N
ATOM    609  CA  LYS    80      33.144  -2.877   7.342  1.00  0.00           C
ATOM    610  CB  LYS    80      34.057  -3.094   8.559  1.00  0.00           C
ATOM    611  CG  LYS    80      34.308  -4.578   8.841  1.00  0.00           C
ATOM    612  CD  LYS    80      35.440  -4.848   9.832  1.00  0.00           C
ATOM    613  CE  LYS    80      36.732  -5.328   9.170  1.00  0.00           C
ATOM    614  NZ  LYS    80      36.534  -6.682   8.603  1.00  0.00           N
ATOM    615  C   LYS    80      32.010  -3.868   7.508  1.00  0.00           C
ATOM    616  O   LYS    80      32.024  -4.939   6.902  1.00  0.00           O
ATOM    617  N   LYS    81      31.010  -3.534   8.353  1.00  0.00           N
ATOM    618  CA  LYS    81      29.994  -4.449   8.833  1.00  0.00           C
ATOM    619  CB  LYS    81      29.074  -3.831   9.903  1.00  0.00           C
ATOM    620  CG  LYS    81      29.651  -3.798  11.320  1.00  0.00           C
ATOM    621  CD  LYS    81      28.752  -3.050  12.310  1.00  0.00           C
ATOM    622  CE  LYS    81      29.046  -3.369  13.779  1.00  0.00           C
ATOM    623  NZ  LYS    81      30.311  -2.735  14.202  1.00  0.00           N
ATOM    624  C   LYS    81      29.062  -5.014   7.800  1.00  0.00           C
ATOM    625  O   LYS    81      28.767  -6.208   7.835  1.00  0.00           O
ATOM    626  N   PHE    82      28.541  -4.191   6.874  1.00  0.00           N
ATOM    627  CA  PHE    82      27.546  -4.698   5.963  1.00  0.00           C
ATOM    628  CB  PHE    82      26.247  -3.880   5.883  1.00  0.00           C
ATOM    629  CG  PHE    82      25.444  -3.941   7.126  1.00  0.00           C
ATOM    630  CD1 PHE    82      25.632  -3.028   8.139  1.00  0.00           C
ATOM    631  CD2 PHE    82      24.479  -4.903   7.258  1.00  0.00           C
ATOM    632  CE1 PHE    82      24.872  -3.082   9.283  1.00  0.00           C
ATOM    633  CE2 PHE    82      23.726  -4.949   8.398  1.00  0.00           C
ATOM    634  CZ  PHE    82      23.912  -4.049   9.416  1.00  0.00           C
ATOM    635  C   PHE    82      28.024  -4.567   4.556  1.00  0.00           C
ATOM    636  O   PHE    82      28.916  -3.774   4.256  1.00  0.00           O
ATOM    637  N   LYS    83      27.384  -5.356   3.662  1.00  0.00           N
ATOM    638  CA  LYS    83      27.607  -5.356   2.242  1.00  0.00           C
ATOM    639  CB  LYS    83      27.921  -6.741   1.655  1.00  0.00           C
ATOM    640  CG  LYS    83      29.110  -7.461   2.278  1.00  0.00           C
ATOM    641  CD  LYS    83      29.132  -8.951   1.930  1.00  0.00           C
ATOM    642  CE  LYS    83      29.918  -9.283   0.661  1.00  0.00           C
ATOM    643  NZ  LYS    83      31.282  -9.731   1.023  1.00  0.00           N
ATOM    644  C   LYS    83      26.280  -5.027   1.628  1.00  0.00           C
ATOM    645  O   LYS    83      25.245  -5.138   2.282  1.00  0.00           O
ATOM    646  N   VAL    84      26.266  -4.621   0.343  1.00  0.00           N
ATOM    647  CA  VAL    84      25.006  -4.310  -0.265  1.00  0.00           C
ATOM    648  CB  VAL    84      25.126  -3.645  -1.607  1.00  0.00           C
ATOM    649  CG1 VAL    84      25.831  -2.292  -1.418  1.00  0.00           C
ATOM    650  CG2 VAL    84      25.851  -4.601  -2.570  1.00  0.00           C
ATOM    651  C   VAL    84      24.261  -5.593  -0.454  1.00  0.00           C
ATOM    652  O   VAL    84      24.850  -6.632  -0.746  1.00  0.00           O
ATOM    653  N   GLY    85      22.926  -5.545  -0.265  1.00  0.00           N
ATOM    654  CA  GLY    85      22.094  -6.697  -0.453  1.00  0.00           C
ATOM    655  C   GLY    85      21.834  -7.352   0.867  1.00  0.00           C
ATOM    656  O   GLY    85      20.983  -8.235   0.964  1.00  0.00           O
ATOM    657  N   GLU    86      22.551  -6.931   1.925  1.00  0.00           N
ATOM    658  CA  GLU    86      22.373  -7.536   3.214  1.00  0.00           C
ATOM    659  CB  GLU    86      23.509  -7.199   4.197  1.00  0.00           C
ATOM    660  CG  GLU    86      24.881  -7.727   3.767  1.00  0.00           C
ATOM    661  CD  GLU    86      24.935  -9.225   4.036  1.00  0.00           C
ATOM    662  OE1 GLU    86      24.127  -9.709   4.871  1.00  0.00           O
ATOM    663  OE2 GLU    86      25.791  -9.904   3.408  1.00  0.00           O
ATOM    664  C   GLU    86      21.095  -7.028   3.814  1.00  0.00           C
ATOM    665  O   GLU    86      20.686  -5.895   3.568  1.00  0.00           O
ATOM    666  N   HIS    87      20.419  -7.881   4.613  1.00  0.00           N
ATOM    667  CA  HIS    87      19.218  -7.478   5.289  1.00  0.00           C
ATOM    668  ND1 HIS    87      18.261 -10.166   3.603  1.00  0.00           N
ATOM    669  CG  HIS    87      17.624  -9.283   4.447  1.00  0.00           C
ATOM    670  NE2 HIS    87      16.181  -9.951   2.844  1.00  0.00           N
ATOM    671  CD2 HIS    87      16.355  -9.164   3.969  1.00  0.00           C
ATOM    672  CE1 HIS    87      17.352 -10.535   2.664  1.00  0.00           C
ATOM    673  CB  HIS    87      18.272  -8.643   5.641  1.00  0.00           C
ATOM    674  C   HIS    87      19.675  -6.882   6.575  1.00  0.00           C
ATOM    675  O   HIS    87      20.549  -7.430   7.244  1.00  0.00           O
ATOM    676  N   VAL    88      19.107  -5.724   6.957  1.00  0.00           N
ATOM    677  CA  VAL    88      19.607  -5.112   8.145  1.00  0.00           C
ATOM    678  CB  VAL    88      20.612  -4.036   7.818  1.00  0.00           C
ATOM    679  CG1 VAL    88      19.999  -3.113   6.756  1.00  0.00           C
ATOM    680  CG2 VAL    88      21.008  -3.278   9.092  1.00  0.00           C
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ATOM    681  C   VAL    88      18.489  -4.493   8.906  1.00  0.00           C
ATOM    682  O   VAL    88      17.486  -4.054   8.341  1.00  0.00           O
ATOM    683  N   GLY    89      18.611  -4.511  10.248  1.00  0.00           N
ATOM    684  CA  GLY    89      17.688  -3.711  10.959  1.00  0.00           C
ATOM    685  C   GLY    89      18.186  -2.430  10.480  1.00  0.00           C
ATOM    686  O   GLY    89      19.292  -2.039  10.873  1.00  0.00           O
ATOM    687  N   VAL    90      17.324  -1.743   9.697  1.00  0.00           N
ATOM    688  CA  VAL    90      17.662  -0.556   8.979  1.00  0.00           C
ATOM    689  CB  VAL    90      16.480   0.198   8.451  1.00  0.00           C
ATOM    690  CG1 VAL    90      16.962   1.588   8.001  1.00  0.00           C
ATOM    691  CG2 VAL    90      15.850  -0.606   7.309  1.00  0.00           C
ATOM    692  C   VAL    90      18.276   0.310   9.975  1.00  0.00           C
ATOM    693  O   VAL    90      19.222   1.044   9.690  1.00  0.00           O
ATOM    694  N   GLY    91      17.767   0.239  11.205  1.00  0.00           N
ATOM    695  CA  GLY    91      18.521   1.082  12.035  1.00  0.00           C
ATOM    696  C   GLY    91      18.344   0.729  13.453  1.00  0.00           C
ATOM    697  O   GLY    91      17.367   0.101  13.860  1.00  0.00           O
ATOM    698  N   CYS    92      19.347   1.153  14.235  1.00  0.00           N
ATOM    699  CA  CYS    92      19.328   0.988  15.643  1.00  0.00           C
ATOM    700  CB  CYS    92      20.631   0.385  16.190  1.00  0.00           C
ATOM    701  SG  CYS    92      20.905  -1.315  15.609  1.00  0.00           S
ATOM    702  C   CYS    92      19.220   2.370  16.206  1.00  0.00           C
ATOM    703  O   CYS    92      20.105   3.200  16.012  1.00  0.00           O
ATOM    704  N   ILE    93      18.113   2.657  16.910  1.00  0.00           N
ATOM    705  CA  ILE    93      17.940   3.935  17.534  1.00  0.00           C
ATOM    706  CB  ILE    93      16.623   4.070  18.247  1.00  0.00           C
ATOM    707  CG2 ILE    93      16.482   2.884  19.215  1.00  0.00           C
ATOM    708  CG1 ILE    93      16.516   5.446  18.930  1.00  0.00           C
ATOM    709  CD1 ILE    93      16.536   6.637  17.977  1.00  0.00           C
ATOM    710  C   ILE    93      19.013   4.060  18.553  1.00  0.00           C
ATOM    711  O   ILE    93      19.561   5.143  18.756  1.00  0.00           O
ATOM    712  N   VAL    94      19.309   2.947  19.252  1.00  0.00           N
ATOM    713  CA  VAL    94      20.365   2.964  20.214  1.00  0.00           C
ATOM    714  CB  VAL    94      20.049   2.195  21.472  1.00  0.00           C
ATOM    715  CG1 VAL    94      18.867   2.890  22.162  1.00  0.00           C
ATOM    716  CG2 VAL    94      19.755   0.724  21.135  1.00  0.00           C
ATOM    717  C   VAL    94      21.549   2.345  19.541  1.00  0.00           C
ATOM    718  O   VAL    94      21.501   1.204  19.086  1.00  0.00           O
ATOM    719  N   GLY    95      22.655   3.105  19.447  1.00  0.00           N
ATOM    720  CA  GLY    95      23.812   2.628  18.750  1.00  0.00           C
ATOM    721  C   GLY    95      24.627   1.784  19.666  1.00  0.00           C
ATOM    722  O   GLY    95      24.371   1.716  20.867  1.00  0.00           O
ATOM    723  N   SER    96      25.621   1.078  19.089  1.00  0.00           N
ATOM    724  CA  SER    96      26.548   0.339  19.889  1.00  0.00           C
ATOM    725  CB  SER    96      26.258  -1.171  19.927  1.00  0.00           C
ATOM    726  OG  SER    96      25.002  -1.410  20.546  1.00  0.00           O
ATOM    727  C   SER    96      27.893   0.521  19.258  1.00  0.00           C
ATOM    728  O   SER    96      28.353  -0.319  18.488  1.00  0.00           O
ATOM    729  N   CYS    97      28.582   1.617  19.616  1.00  0.00           N
ATOM    730  CA  CYS    97      29.868   1.931  19.062  1.00  0.00           C
ATOM    731  CB  CYS    97      30.396   3.300  19.507  1.00  0.00           C
ATOM    732  SG  CYS    97      30.691   3.354  21.293  1.00  0.00           S
ATOM    733  C   CYS    97      30.836   0.887  19.516  1.00  0.00           C
ATOM    734  O   CYS    97      31.803   0.575  18.825  1.00  0.00           O
ATOM    735  N   ARG    98      30.586   0.318  20.709  1.00  0.00           N
ATOM    736  CA  ARG    98      31.444  -0.685  21.268  1.00  0.00           C
ATOM    737  CB  ARG    98      31.806  -1.791  20.260  1.00  0.00           C
ATOM    738  CG  ARG    98      30.588  -2.580  19.775  1.00  0.00           C
ATOM    739  CD  ARG    98      30.044  -3.573  20.804  1.00  0.00           C
ATOM    740  NE  ARG    98      31.046  -4.665  20.949  1.00  0.00           N
ATOM    741  CZ  ARG    98      30.969  -5.766  20.148  1.00  0.00           C
ATOM    742  NH1 ARG    98      29.978  -5.862  19.214  1.00  0.00           N
ATOM    743  NH2 ARG    98      31.882  -6.773  20.280  1.00  0.00           N
ATOM    744  C   ARG    98      32.712  -0.043  21.737  1.00  0.00           C
ATOM    745  O   ARG    98      33.676  -0.736  22.062  1.00  0.00           O
ATOM    746  N   SER    99      32.748   1.304  21.801  1.00  0.00           N
ATOM    747  CA  SER    99      33.915   1.949  22.333  1.00  0.00           C
ATOM    748  CB  SER    99      34.821   2.547  21.242  1.00  0.00           C
ATOM    749  OG  SER    99      34.125   3.555  20.524  1.00  0.00           O
ATOM    750  C   SER    99      33.461   3.082  23.203  1.00  0.00           C
ATOM    751  O   SER    99      33.831   4.236  22.996  1.00  0.00           O
ATOM    752  N   CYS   100      32.663   2.760  24.232  1.00  0.00           N
ATOM    753  CA  CYS   100      32.161   3.702  25.188  1.00  0.00           C
ATOM    754  CB  CYS   100      30.686   4.106  25.027  1.00  0.00           C
ATOM    755  SG  CYS   100      30.369   5.348  23.757  1.00  0.00           S
ATOM    756  C   CYS   100      32.148   2.962  26.470  1.00  0.00           C
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ATOM    757  O   CYS   100      32.138   1.733  26.486  1.00  0.00           O
ATOM    758  N   GLY   101      32.113   3.700  27.588  1.00  0.00           N
ATOM    759  CA  GLY   101      32.103   3.027  28.844  1.00  0.00           C
ATOM    760  C   GLY   101      30.874   2.183  28.899  1.00  0.00           C
ATOM    761  O   GLY   101      30.906   1.040  29.349  1.00  0.00           O
ATOM    762  N   ASN   102      29.747   2.740  28.432  1.00  0.00           N
ATOM    763  CA  ASN   102      28.490   2.064  28.519  1.00  0.00           C
ATOM    764  CB  ASN   102      27.364   2.956  27.977  1.00  0.00           C
ATOM    765  CG  ASN   102      27.427   4.248  28.784  1.00  0.00           C
ATOM    766  OD1 ASN   102      27.822   4.242  29.948  1.00  0.00           O
ATOM    767  ND2 ASN   102      27.051   5.391  28.150  1.00  0.00           N
ATOM    768  C   ASN   102      28.533   0.802  27.713  1.00  0.00           C
ATOM    769  O   ASN   102      28.177  -0.265  28.211  1.00  0.00           O
ATOM    770  N   CYS   103      28.986   0.875  26.447  1.00  0.00           N
ATOM    771  CA  CYS   103      28.954  -0.315  25.648  1.00  0.00           C
ATOM    772  CB  CYS   103      29.058  -0.085  24.127  1.00  0.00           C
ATOM    773  SG  CYS   103      30.406   0.997  23.613  1.00  0.00           S
ATOM    774  C   CYS   103      29.930  -1.342  26.134  1.00  0.00           C
ATOM    775  O   CYS   103      29.662  -2.537  26.025  1.00  0.00           O
ATOM    776  N   ASN   104      31.097  -0.939  26.670  1.00  0.00           N
ATOM    777  CA  ASN   104      31.990  -1.968  27.122  1.00  0.00           C
ATOM    778  CB  ASN   104      33.399  -1.488  27.523  1.00  0.00           C
ATOM    779  CG  ASN   104      33.326  -0.642  28.783  1.00  0.00           C
ATOM    780  OD1 ASN   104      33.323   0.583  28.707  1.00  0.00           O
ATOM    781  ND2 ASN   104      33.279  -1.304  29.970  1.00  0.00           N
ATOM    782  C   ASN   104      31.385  -2.666  28.304  1.00  0.00           C
ATOM    783  O   ASN   104      31.505  -3.883  28.436  1.00  0.00           O
ATOM    784  N   GLN   105      30.714  -1.911  29.199  1.00  0.00           N
ATOM    785  CA  GLN   105      30.170  -2.500  30.393  1.00  0.00           C
ATOM    786  CB  GLN   105      29.619  -1.472  31.397  1.00  0.00           C
ATOM    787  CG  GLN   105      29.132  -2.107  32.702  1.00  0.00           C
ATOM    788  CD  GLN   105      28.643  -0.993  33.614  1.00  0.00           C
ATOM    789  OE1 GLN   105      28.471  -1.195  34.815  1.00  0.00           O
ATOM    790  NE2 GLN   105      28.418   0.215  33.033  1.00  0.00           N
ATOM    791  C   GLN   105      29.064  -3.436  30.027  1.00  0.00           C
ATOM    792  O   GLN   105      28.239  -3.152  29.160  1.00  0.00           O
ATOM    793  N   SER   106      29.034  -4.603  30.700  1.00  0.00           N
ATOM    794  CA  SER   106      28.076  -5.629  30.408  1.00  0.00           C
ATOM    795  CB  SER   106      28.313  -6.910  31.226  1.00  0.00           C
ATOM    796  OG  SER   106      29.564  -7.487  30.879  1.00  0.00           O
ATOM    797  C   SER   106      26.685  -5.161  30.711  1.00  0.00           C
ATOM    798  O   SER   106      25.758  -5.442  29.955  1.00  0.00           O
ATOM    799  N   MET   107      26.496  -4.465  31.846  1.00  0.00           N
ATOM    800  CA  MET   107      25.189  -4.043  32.265  1.00  0.00           C
ATOM    801  CB  MET   107      25.167  -3.477  33.695  1.00  0.00           C
ATOM    802  CG  MET   107      25.793  -2.087  33.817  1.00  0.00           C
ATOM    803  SD  MET   107      25.683  -1.363  35.482  1.00  0.00           S
ATOM    804  CE  MET   107      26.177   0.304  34.959  1.00  0.00           C
ATOM    805  C   MET   107      24.605  -2.988  31.374  1.00  0.00           C
ATOM    806  O   MET   107      23.407  -3.012  31.099  1.00  0.00           O
ATOM    807  N   GLU   108      25.419  -2.021  30.908  1.00  0.00           N
ATOM    808  CA  GLU   108      24.858  -0.894  30.210  1.00  0.00           C
ATOM    809  CB  GLU   108      25.658   0.406  30.387  1.00  0.00           C
ATOM    810  CG  GLU   108      24.887   1.643  29.924  1.00  0.00           C
ATOM    811  CD  GLU   108      25.533   2.859  30.566  1.00  0.00           C
ATOM    812  OE1 GLU   108      26.457   2.666  31.400  1.00  0.00           O
ATOM    813  OE2 GLU   108      25.109   3.999  30.235  1.00  0.00           O
ATOM    814  C   GLU   108      24.663  -1.148  28.748  1.00  0.00           C
ATOM    815  O   GLU   108      25.156  -2.127  28.191  1.00  0.00           O
ATOM    816  N   GLN   109      23.868  -0.264  28.101  1.00  0.00           N
ATOM    817  CA  GLN   109      23.601  -0.373  26.698  1.00  0.00           C
ATOM    818  CB  GLN   109      22.235  -1.011  26.379  1.00  0.00           C
ATOM    819  CG  GLN   109      21.026  -0.153  26.776  1.00  0.00           C
ATOM    820  CD  GLN   109      20.647   0.782  25.625  1.00  0.00           C
ATOM    821  OE1 GLN   109      19.811   1.668  25.784  1.00  0.00           O
ATOM    822  NE2 GLN   109      21.265   0.592  24.430  1.00  0.00           N
ATOM    823  C   GLN   109      23.543   1.005  26.108  1.00  0.00           C
ATOM    824  O   GLN   109      23.802   1.191  24.922  1.00  0.00           O
ATOM    825  N   TYR   110      23.189   2.015  26.923  1.00  0.00           N
ATOM    826  CA  TYR   110      22.975   3.343  26.420  1.00  0.00           C
ATOM    827  CB  TYR   110      22.545   4.242  27.599  1.00  0.00           C
ATOM    828  CG  TYR   110      21.958   5.549  27.194  1.00  0.00           C
ATOM    829  CD1 TYR   110      20.651   5.607  26.771  1.00  0.00           C
ATOM    830  CD2 TYR   110      22.686   6.714  27.276  1.00  0.00           C
ATOM    831  CE1 TYR   110      20.083   6.806  26.414  1.00  0.00           C
ATOM    832  CE2 TYR   110      22.122   7.917  26.920  1.00  0.00           C
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ATOM    833  CZ  TYR   110      20.819   7.963  26.485  1.00  0.00           C
ATOM    834  OH  TYR   110      20.234   9.194  26.120  1.00  0.00           O
ATOM    835  C   TYR   110      24.301   3.819  25.905  1.00  0.00           C
ATOM    836  O   TYR   110      25.142   4.279  26.674  1.00  0.00           O
ATOM    837  N   CYS   111      24.495   3.779  24.567  1.00  0.00           N
ATOM    838  CA  CYS   111      25.756   4.169  23.996  1.00  0.00           C
ATOM    839  CB  CYS   111      25.954   3.699  22.543  1.00  0.00           C
ATOM    840  SG  CYS   111      27.554   4.217  21.856  1.00  0.00           S
ATOM    841  C   CYS   111      25.839   5.664  24.004  1.00  0.00           C
ATOM    842  O   CYS   111      24.826   6.361  24.018  1.00  0.00           O
ATOM    843  N   SER   112      27.081   6.189  24.006  1.00  0.00           N
ATOM    844  CA  SER   112      27.319   7.604  24.072  1.00  0.00           C
ATOM    845  CB  SER   112      28.807   7.956  24.211  1.00  0.00           C
ATOM    846  OG  SER   112      29.310   7.470  25.445  1.00  0.00           O
ATOM    847  C   SER   112      26.813   8.277  22.831  1.00  0.00           C
ATOM    848  O   SER   112      26.458   9.453  22.862  1.00  0.00           O
ATOM    849  N   LYS   113      26.785   7.552  21.700  1.00  0.00           N
ATOM    850  CA  LYS   113      26.349   8.096  20.442  1.00  0.00           C
ATOM    851  CB  LYS   113      26.724   7.242  19.222  1.00  0.00           C
ATOM    852  CG  LYS   113      28.202   7.420  18.860  1.00  0.00           C
ATOM    853  CD  LYS   113      28.671   6.602  17.657  1.00  0.00           C
ATOM    854  CE  LYS   113      30.076   6.972  17.175  1.00  0.00           C
ATOM    855  NZ  LYS   113      30.452   6.145  16.006  1.00  0.00           N
ATOM    856  C   LYS   113      24.875   8.375  20.448  1.00  0.00           C
ATOM    857  O   LYS   113      24.378   9.102  19.589  1.00  0.00           O
ATOM    858  N   ARG   114      24.137   7.777  21.400  1.00  0.00           N
ATOM    859  CA  ARG   114      22.706   7.890  21.490  1.00  0.00           C
ATOM    860  CB  ARG   114      22.160   7.419  22.851  1.00  0.00           C
ATOM    861  CG  ARG   114      22.733   8.192  24.045  1.00  0.00           C
ATOM    862  CD  ARG   114      22.197   9.620  24.192  1.00  0.00           C
ATOM    863  NE  ARG   114      22.842  10.232  25.387  1.00  0.00           N
ATOM    864  CZ  ARG   114      24.034  10.888  25.262  1.00  0.00           C
ATOM    865  NH1 ARG   114      24.630  10.993  24.040  1.00  0.00           N
ATOM    866  NH2 ARG   114      24.623  11.444  26.360  1.00  0.00           N
ATOM    867  C   ARG   114      22.216   9.298  21.267  1.00  0.00           C
ATOM    868  O   ARG   114      22.856  10.288  21.614  1.00  0.00           O
ATOM    869  N   ILE   115      21.039   9.341  20.611  1.00  0.00           N
ATOM    870  CA  ILE   115      20.173  10.379  20.112  1.00  0.00           C
ATOM    871  CB  ILE   115      19.181   9.805  19.135  1.00  0.00           C
ATOM    872  CG2 ILE   115      18.254  10.918  18.614  1.00  0.00           C
ATOM    873  CG1 ILE   115      19.935   9.097  17.996  1.00  0.00           C
ATOM    874  CD1 ILE   115      20.848  10.029  17.199  1.00  0.00           C
ATOM    875  C   ILE   115      19.412  11.167  21.148  1.00  0.00           C
ATOM    876  O   ILE   115      18.996  12.284  20.860  1.00  0.00           O
ATOM    877  N   TRP   116      19.176  10.637  22.361  1.00  0.00           N
ATOM    878  CA  TRP   116      18.193  11.170  23.278  1.00  0.00           C
ATOM    879  CB  TRP   116      18.273  10.559  24.686  1.00  0.00           C
ATOM    880  CG  TRP   116      17.579   9.226  24.826  1.00  0.00           C
ATOM    881  CD2 TRP   116      18.100   7.973  24.360  1.00  0.00           C
ATOM    882  CD1 TRP   116      16.362   8.958  25.380  1.00  0.00           C
ATOM    883  NE1 TRP   116      16.095   7.614  25.300  1.00  0.00           N
ATOM    884  CE2 TRP   116      17.155   6.995  24.672  1.00  0.00           C
ATOM    885  CE3 TRP   116      19.264   7.665  23.717  1.00  0.00           C
ATOM    886  CZ2 TRP   116      17.362   5.686  24.350  1.00  0.00           C
ATOM    887  CZ3 TRP   116      19.472   6.342  23.400  1.00  0.00           C
ATOM    888  CH2 TRP   116      18.540   5.374  23.712  1.00  0.00           C
ATOM    889  C   TRP   116      18.184  12.664  23.449  1.00  0.00           C
ATOM    890  O   TRP   116      17.114  13.213  23.709  1.00  0.00           O
ATOM    891  N   THR   117      19.323  13.372  23.368  1.00  0.00           N
ATOM    892  CA  THR   117      19.280  14.799  23.572  1.00  0.00           C
ATOM    893  CB  THR   117      20.658  15.375  23.691  1.00  0.00           C
ATOM    894  OG1 THR   117      20.587  16.727  24.111  1.00  0.00           O
ATOM    895  CG2 THR   117      21.360  15.278  22.326  1.00  0.00           C
ATOM    896  C   THR   117      18.571  15.529  22.450  1.00  0.00           C
ATOM    897  O   THR   117      18.834  16.710  22.222  1.00  0.00           O
ATOM    898  N   TYR   118      17.625  14.869  21.749  1.00  0.00           N
ATOM    899  CA  TYR   118      16.806  15.445  20.712  1.00  0.00           C
ATOM    900  CB  TYR   118      15.659  16.335  21.239  1.00  0.00           C
ATOM    901  CG  TYR   118      16.204  17.451  22.066  1.00  0.00           C
ATOM    902  CD1 TYR   118      16.627  18.625  21.486  1.00  0.00           C
ATOM    903  CD2 TYR   118      16.289  17.320  23.433  1.00  0.00           C
ATOM    904  CE1 TYR   118      17.127  19.649  22.255  1.00  0.00           C
ATOM    905  CE2 TYR   118      16.788  18.340  24.208  1.00  0.00           C
ATOM    906  CZ  TYR   118      17.208  19.507  23.619  1.00  0.00           C
ATOM    907  OH  TYR   118      17.721  20.556  24.411  1.00  0.00           O
ATOM    908  C   TYR   118      17.605  16.177  19.685  1.00  0.00           C
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ATOM    909  O   TYR   118      17.189  17.227  19.196  1.00  0.00           O
ATOM    910  N   ASN   119      18.765  15.624  19.295  1.00  0.00           N
ATOM    911  CA  ASN   119      19.499  16.229  18.232  1.00  0.00           C
ATOM    912  CB  ASN   119      21.025  16.129  18.390  1.00  0.00           C
ATOM    913  CG  ASN   119      21.438  17.022  19.550  1.00  0.00           C
ATOM    914  OD1 ASN   119      20.684  17.896  19.977  1.00  0.00           O
ATOM    915  ND2 ASN   119      22.675  16.807  20.072  1.00  0.00           N
ATOM    916  C   ASN   119      19.114  15.409  17.050  1.00  0.00           C
ATOM    917  O   ASN   119      19.124  14.184  17.110  1.00  0.00           O
ATOM    918  N   ASP   120      18.708  16.049  15.947  1.00  0.00           N
ATOM    919  CA  ASP   120      18.343  15.253  14.817  1.00  0.00           C
ATOM    920  CB  ASP   120      17.160  15.831  14.020  1.00  0.00           C
ATOM    921  CG  ASP   120      16.830  14.878  12.878  1.00  0.00           C
ATOM    922  OD1 ASP   120      17.529  13.838  12.748  1.00  0.00           O
ATOM    923  OD2 ASP   120      15.869  15.177  12.120  1.00  0.00           O
ATOM    924  C   ASP   120      19.531  15.289  13.936  1.00  0.00           C
ATOM    925  O   ASP   120      19.609  16.105  13.020  1.00  0.00           O
ATOM    926  N   VAL   121      20.494  14.391  14.205  1.00  0.00           N
ATOM    927  CA  VAL   121      21.717  14.483  13.490  1.00  0.00           C
ATOM    928  CB  VAL   121      22.599  15.484  14.157  1.00  0.00           C
ATOM    929  CG1 VAL   121      23.016  14.938  15.530  1.00  0.00           C
ATOM    930  CG2 VAL   121      23.750  15.817  13.228  1.00  0.00           C
ATOM    931  C   VAL   121      22.394  13.145  13.516  1.00  0.00           C
ATOM    932  O   VAL   121      22.003  12.239  14.249  1.00  0.00           O
ATOM    933  N   ASN   122      23.438  13.009  12.680  1.00  0.00           N
ATOM    934  CA  ASN   122      24.241  11.838  12.524  1.00  0.00           C
ATOM    935  CB  ASN   122      24.528  11.559  11.036  1.00  0.00           C
ATOM    936  CG  ASN   122      25.297  10.263  10.863  1.00  0.00           C
ATOM    937  OD1 ASN   122      24.724   9.175  10.889  1.00  0.00           O
ATOM    938  ND2 ASN   122      26.633  10.386  10.642  1.00  0.00           N
ATOM    939  C   ASN   122      25.521  12.177  13.209  1.00  0.00           C
ATOM    940  O   ASN   122      25.681  13.282  13.726  1.00  0.00           O
ATOM    941  N   HIS   123      26.472  11.231  13.246  1.00  0.00           N
ATOM    942  CA  HIS   123      27.700  11.501  13.923  1.00  0.00           C
ATOM    943  ND1 HIS   123      28.591   7.804  14.050  1.00  0.00           N
ATOM    944  CG  HIS   123      28.138   9.060  14.380  1.00  0.00           C
ATOM    945  NE2 HIS   123      26.947   7.520  15.520  1.00  0.00           N
ATOM    946  CD2 HIS   123      27.134   8.869  15.281  1.00  0.00           C
ATOM    947  CE1 HIS   123      27.844   6.920  14.759  1.00  0.00           C
ATOM    948  CB  HIS   123      28.690  10.331  13.807  1.00  0.00           C
ATOM    949  C   HIS   123      28.321  12.697  13.263  1.00  0.00           C
ATOM    950  O   HIS   123      28.812  13.599  13.940  1.00  0.00           O
ATOM    951  N   ASP   124      28.289  12.743  11.916  1.00  0.00           N
ATOM    952  CA  ASP   124      28.908  13.803  11.168  1.00  0.00           C
ATOM    953  CB  ASP   124      29.043  13.549   9.647  1.00  0.00           C
ATOM    954  CG  ASP   124      27.694  13.522   8.944  1.00  0.00           C
ATOM    955  OD1 ASP   124      26.831  12.688   9.323  1.00  0.00           O
ATOM    956  OD2 ASP   124      27.522  14.329   7.992  1.00  0.00           O
ATOM    957  C   ASP   124      28.213  15.111  11.391  1.00  0.00           C
ATOM    958  O   ASP   124      28.826  16.164  11.229  1.00  0.00           O
ATOM    959  N   GLY   125      26.921  15.114  11.771  1.00  0.00           N
ATOM    960  CA  GLY   125      26.317  16.405  11.949  1.00  0.00           C
ATOM    961  C   GLY   125      25.302  16.660  10.871  1.00  0.00           C
ATOM    962  O   GLY   125      24.819  17.782  10.725  1.00  0.00           O
ATOM    963  N   THR   126      24.942  15.623  10.087  1.00  0.00           N
ATOM    964  CA  THR   126      23.943  15.774   9.059  1.00  0.00           C
ATOM    965  CB  THR   126      24.413  15.328   7.707  1.00  0.00           C
ATOM    966  OG1 THR   126      24.778  13.956   7.744  1.00  0.00           O
ATOM    967  CG2 THR   126      25.620  16.189   7.298  1.00  0.00           C
ATOM    968  C   THR   126      22.770  14.911   9.449  1.00  0.00           C
ATOM    969  O   THR   126      22.831  14.248  10.476  1.00  0.00           O
ATOM    970  N   PRO   127      21.685  14.897   8.712  1.00  0.00           N
ATOM    971  CA  PRO   127      20.527  14.117   9.117  1.00  0.00           C
ATOM    972  CD  PRO   127      21.301  16.063   7.938  1.00  0.00           C
ATOM    973  CB  PRO   127      19.326  14.736   8.397  1.00  0.00           C
ATOM    974  CG  PRO   127      19.938  15.679   7.343  1.00  0.00           C
ATOM    975  C   PRO   127      20.630  12.615   8.939  1.00  0.00           C
ATOM    976  O   PRO   127      21.332  12.211   8.015  1.00  0.00           O
ATOM    977  N   THR   128      19.926  11.791   9.788  1.00  0.00           N
ATOM    978  CA  THR   128      19.986  10.326   9.788  1.00  0.00           C
ATOM    979  CB  THR   128      21.079   9.803  10.677  1.00  0.00           C
ATOM    980  OG1 THR   128      21.306   8.421  10.447  1.00  0.00           O
ATOM    981  CG2 THR   128      20.671  10.042  12.141  1.00  0.00           C
ATOM    982  C   THR   128      18.656   9.673  10.244  1.00  0.00           C
ATOM    983  O   THR   128      17.608  10.270   9.999  1.00  0.00           O
ATOM    984  N   GLN   129      18.682   8.428  10.877  1.00  0.00           N
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ATOM    985  CA  GLN   129      17.589   7.566  11.351  1.00  0.00           C
ATOM    986  CB  GLN   129      17.209   7.807  12.820  1.00  0.00           C
ATOM    987  CG  GLN   129      16.240   6.764  13.369  1.00  0.00           C
ATOM    988  CD  GLN   129      15.952   7.119  14.816  1.00  0.00           C
ATOM    989  OE1 GLN   129      15.334   6.339  15.535  1.00  0.00           O
ATOM    990  NE2 GLN   129      16.412   8.321  15.257  1.00  0.00           N
ATOM    991  C   GLN   129      16.415   7.859  10.480  1.00  0.00           C
ATOM    992  O   GLN   129      16.569   8.067   9.286  1.00  0.00           O
ATOM    993  N   GLY   130      15.184   7.876  10.999  1.00  0.00           N
ATOM    994  CA  GLY   130      14.189   8.303  10.057  1.00  0.00           C
ATOM    995  C   GLY   130      13.848   7.235   9.060  1.00  0.00           C
ATOM    996  O   GLY   130      14.323   7.223   7.925  1.00  0.00           O
ATOM    997  N   GLY   131      13.036   6.274   9.528  1.00  0.00           N
ATOM    998  CA  GLY   131      12.477   5.153   8.819  1.00  0.00           C
ATOM    999  C   GLY   131      11.374   5.545   7.873  1.00  0.00           C
ATOM   1000  O   GLY   131      11.020   4.774   6.982  1.00  0.00           O
ATOM   1001  N   PHE   132      10.742   6.712   8.089  1.00  0.00           N
ATOM   1002  CA  PHE   132       9.595   7.152   7.336  1.00  0.00           C
ATOM   1003  CB  PHE   132       8.831   8.380   7.872  1.00  0.00           C
ATOM   1004  CG  PHE   132       7.955   7.922   8.992  1.00  0.00           C
ATOM   1005  CD1 PHE   132       7.064   6.889   8.807  1.00  0.00           C
ATOM   1006  CD2 PHE   132       7.965   8.558  10.208  1.00  0.00           C
ATOM   1007  CE1 PHE   132       6.246   6.470   9.832  1.00  0.00           C
ATOM   1008  CE2 PHE   132       7.151   8.147  11.237  1.00  0.00           C
ATOM   1009  CZ  PHE   132       6.290   7.094  11.054  1.00  0.00           C
ATOM   1010  C   PHE   132       9.921   7.397   5.895  1.00  0.00           C
ATOM   1011  O   PHE   132       9.042   7.803   5.139  1.00  0.00           O
ATOM   1012  N   ALA   133      11.202   7.309   5.494  1.00  0.00           N
ATOM   1013  CA  ALA   133      11.543   7.557   4.118  1.00  0.00           C
ATOM   1014  CB  ALA   133      12.729   8.521   3.954  1.00  0.00           C
ATOM   1015  C   ALA   133      11.909   6.278   3.414  1.00  0.00           C
ATOM   1016  O   ALA   133      12.180   5.253   4.037  1.00  0.00           O
ATOM   1017  N   SER   134      11.883   6.313   2.062  1.00  0.00           N
ATOM   1018  CA  SER   134      12.186   5.174   1.239  1.00  0.00           C
ATOM   1019  CB  SER   134      11.992   5.457  -0.260  1.00  0.00           C
ATOM   1020  OG  SER   134      12.911   6.450  -0.692  1.00  0.00           O
ATOM   1021  C   SER   134      13.618   4.788   1.437  1.00  0.00           C
ATOM   1022  O   SER   134      13.937   3.603   1.507  1.00  0.00           O
ATOM   1023  N   SER   135      14.526   5.780   1.525  1.00  0.00           N
ATOM   1024  CA  SER   135      15.911   5.468   1.723  1.00  0.00           C
ATOM   1025  CB  SER   135      16.824   5.957   0.585  1.00  0.00           C
ATOM   1026  OG  SER   135      16.511   5.279  -0.623  1.00  0.00           O
ATOM   1027  C   SER   135      16.347   6.178   2.962  1.00  0.00           C
ATOM   1028  O   SER   135      15.834   7.245   3.292  1.00  0.00           O
ATOM   1029  N   MET   136      17.309   5.578   3.687  1.00  0.00           N
ATOM   1030  CA  MET   136      17.773   6.123   4.928  1.00  0.00           C
ATOM   1031  CB  MET   136      17.129   5.378   6.116  1.00  0.00           C
ATOM   1032  CG  MET   136      17.082   6.066   7.484  1.00  0.00           C
ATOM   1033  SD  MET   136      18.670   6.448   8.279  1.00  0.00           S
ATOM   1034  CE  MET   136      18.748   8.173   7.676  1.00  0.00           C
ATOM   1035  C   MET   136      19.241   5.826   4.975  1.00  0.00           C
ATOM   1036  O   MET   136      19.706   4.858   4.376  1.00  0.00           O
ATOM   1037  N   VAL   137      20.006   6.682   5.676  1.00  0.00           N
ATOM   1038  CA  VAL   137      21.418   6.544   5.859  1.00  0.00           C
ATOM   1039  CB  VAL   137      22.158   7.735   5.327  1.00  0.00           C
ATOM   1040  CG1 VAL   137      23.660   7.552   5.565  1.00  0.00           C
ATOM   1041  CG2 VAL   137      21.776   7.926   3.852  1.00  0.00           C
ATOM   1042  C   VAL   137      21.682   6.494   7.335  1.00  0.00           C
ATOM   1043  O   VAL   137      21.342   7.416   8.071  1.00  0.00           O
ATOM   1044  N   VAL   138      22.331   5.417   7.806  1.00  0.00           N
ATOM   1045  CA  VAL   138      22.555   5.226   9.210  1.00  0.00           C
ATOM   1046  CB  VAL   138      21.990   3.913   9.646  1.00  0.00           C
ATOM   1047  CG1 VAL   138      22.440   3.650  11.072  1.00  0.00           C
ATOM   1048  CG2 VAL   138      20.475   3.907   9.455  1.00  0.00           C
ATOM   1049  C   VAL   138      24.020   5.068   9.425  1.00  0.00           C
ATOM   1050  O   VAL   138      24.715   4.522   8.574  1.00  0.00           O
ATOM   1051  N   ASP   139      24.521   5.508  10.596  1.00  0.00           N
ATOM   1052  CA  ASP   139      25.908   5.318  10.891  1.00  0.00           C
ATOM   1053  CB  ASP   139      26.350   5.911  12.240  1.00  0.00           C
ATOM   1054  CG  ASP   139      26.478   7.415  12.099  1.00  0.00           C
ATOM   1055  OD1 ASP   139      27.211   7.849  11.172  1.00  0.00           O
ATOM   1056  OD2 ASP   139      25.854   8.146  12.913  1.00  0.00           O
ATOM   1057  C   ASP   139      26.091   3.852  11.006  1.00  0.00           C
ATOM   1058  O   ASP   139      25.149   3.112  11.282  1.00  0.00           O
ATOM   1059  N   GLN   140      27.337   3.403  10.806  1.00  0.00           N
ATOM   1060  CA  GLN   140      27.635   2.005  10.875  1.00  0.00           C
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ATOM   1061  CB  GLN   140      29.134   1.705  10.736  1.00  0.00           C
ATOM   1062  CG  GLN   140      29.732   2.047   9.375  1.00  0.00           C
ATOM   1063  CD  GLN   140      31.221   1.746   9.462  1.00  0.00           C
ATOM   1064  OE1 GLN   140      31.753   0.922   8.722  1.00  0.00           O
ATOM   1065  NE2 GLN   140      31.919   2.430  10.409  1.00  0.00           N
ATOM   1066  C   GLN   140      27.259   1.548  12.246  1.00  0.00           C
ATOM   1067  O   GLN   140      26.807   0.420  12.436  1.00  0.00           O
ATOM   1068  N   MET   141      27.438   2.430  13.245  1.00  0.00           N
ATOM   1069  CA  MET   141      27.181   2.080  14.612  1.00  0.00           C
ATOM   1070  CB  MET   141      27.478   3.186  15.635  1.00  0.00           C
ATOM   1071  CG  MET   141      27.169   2.708  17.058  1.00  0.00           C
ATOM   1072  SD  MET   141      27.247   3.977  18.355  1.00  0.00           S
ATOM   1073  CE  MET   141      25.754   4.850  17.799  1.00  0.00           C
ATOM   1074  C   MET   141      25.738   1.747  14.786  1.00  0.00           C
ATOM   1075  O   MET   141      25.401   0.994  15.702  1.00  0.00           O
ATOM   1076  N   PHE   142      24.824   2.350  13.994  1.00  0.00           N
ATOM   1077  CA  PHE   142      23.500   1.917  14.300  1.00  0.00           C
ATOM   1078  CB  PHE   142      22.593   3.017  14.894  1.00  0.00           C
ATOM   1079  CG  PHE   142      22.210   4.121  13.972  1.00  0.00           C
ATOM   1080  CD1 PHE   142      23.126   5.064  13.569  1.00  0.00           C
ATOM   1081  CD2 PHE   142      20.913   4.210  13.519  1.00  0.00           C
ATOM   1082  CE1 PHE   142      22.751   6.080  12.722  1.00  0.00           C
ATOM   1083  CE2 PHE   142      20.532   5.225  12.672  1.00  0.00           C
ATOM   1084  CZ  PHE   142      21.455   6.162  12.272  1.00  0.00           C
ATOM   1085  C   PHE   142      22.857   1.138  13.194  1.00  0.00           C
ATOM   1086  O   PHE   142      21.759   1.450  12.735  1.00  0.00           O
ATOM   1087  N   VAL   143      23.521   0.036  12.788  1.00  0.00           N
ATOM   1088  CA  VAL   143      22.983  -0.888  11.834  1.00  0.00           C
ATOM   1089  CB  VAL   143      23.454  -0.679  10.423  1.00  0.00           C
ATOM   1090  CG1 VAL   143      22.678   0.489   9.804  1.00  0.00           C
ATOM   1091  CG2 VAL   143      24.962  -0.392  10.468  1.00  0.00           C
ATOM   1092  C   VAL   143      23.341  -2.271  12.261  1.00  0.00           C
ATOM   1093  O   VAL   143      24.481  -2.556  12.625  1.00  0.00           O
ATOM   1094  N   VAL   144      22.353  -3.183  12.228  1.00  0.00           N
ATOM   1095  CA  VAL   144      22.643  -4.527  12.623  1.00  0.00           C
ATOM   1096  CB  VAL   144      21.845  -4.995  13.803  1.00  0.00           C
ATOM   1097  CG1 VAL   144      22.159  -6.480  14.042  1.00  0.00           C
ATOM   1098  CG2 VAL   144      22.159  -4.086  15.003  1.00  0.00           C
ATOM   1099  C   VAL   144      22.286  -5.411  11.479  1.00  0.00           C
ATOM   1100  O   VAL   144      21.199  -5.298  10.917  1.00  0.00           O
ATOM   1101  N   ARG   145      23.208  -6.323  11.111  1.00  0.00           N
ATOM   1102  CA  ARG   145      22.971  -7.242  10.038  1.00  0.00           C
ATOM   1103  CB  ARG   145      24.264  -7.830   9.446  1.00  0.00           C
ATOM   1104  CG  ARG   145      24.034  -8.936   8.414  1.00  0.00           C
ATOM   1105  CD  ARG   145      25.320  -9.676   8.036  1.00  0.00           C
ATOM   1106  NE  ARG   145      24.928 -10.894   7.273  1.00  0.00           N
ATOM   1107  CZ  ARG   145      25.864 -11.843   6.979  1.00  0.00           C
ATOM   1108  NH1 ARG   145      27.165 -11.651   7.348  1.00  0.00           N
ATOM   1109  NH2 ARG   145      25.502 -12.983   6.322  1.00  0.00           N
ATOM   1110  C   ARG   145      22.146  -8.352  10.569  1.00  0.00           C
ATOM   1111  O   ARG   145      22.393  -8.845  11.665  1.00  0.00           O
ATOM   1112  N   ILE   146      21.133  -8.775   9.794  1.00  0.00           N
ATOM   1113  CA  ILE   146      20.266  -9.821  10.243  1.00  0.00           C
ATOM   1114  CB  ILE   146      18.864  -9.358  10.520  1.00  0.00           C
ATOM   1115  CG2 ILE   146      18.927  -8.313  11.648  1.00  0.00           C
ATOM   1116  CG1 ILE   146      18.196  -8.845   9.234  1.00  0.00           C
ATOM   1117  CD1 ILE   146      16.689  -8.634   9.379  1.00  0.00           C
ATOM   1118  C   ILE   146      20.202 -10.868   9.171  1.00  0.00           C
ATOM   1119  O   ILE   146      20.685 -10.675   8.057  1.00  0.00           O
ATOM   1120  N   PRO   147      19.636 -11.998   9.499  1.00  0.00           N
ATOM   1121  CA  PRO   147      19.567 -13.073   8.543  1.00  0.00           C
ATOM   1122  CD  PRO   147      19.706 -12.493  10.865  1.00  0.00           C
ATOM   1123  CB  PRO   147      19.170 -14.314   9.335  1.00  0.00           C
ATOM   1124  CG  PRO   147      19.722 -14.027  10.745  1.00  0.00           C
ATOM   1125  C   PRO   147      18.693 -12.769   7.364  1.00  0.00           C
ATOM   1126  O   PRO   147      17.674 -12.098   7.516  1.00  0.00           O
ATOM   1127  N   GLU   148      19.084 -13.283   6.182  1.00  0.00           N
ATOM   1128  CA  GLU   148      18.431 -13.042   4.924  1.00  0.00           C
ATOM   1129  CB  GLU   148      19.126 -13.768   3.760  1.00  0.00           C
ATOM   1130  CG  GLU   148      20.540 -13.270   3.460  1.00  0.00           C
ATOM   1131  CD  GLU   148      21.079 -14.101   2.302  1.00  0.00           C
ATOM   1132  OE1 GLU   148      20.994 -15.355   2.388  1.00  0.00           O
ATOM   1133  OE2 GLU   148      21.574 -13.493   1.316  1.00  0.00           O
ATOM   1134  C   GLU   148      17.035 -13.574   4.965  1.00  0.00           C
ATOM   1135  O   GLU   148      16.120 -12.995   4.382  1.00  0.00           O
ATOM   1136  N   ASN   149      16.847 -14.709   5.651  1.00  0.00           N
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ATOM   1137  CA  ASN   149      15.594 -15.403   5.696  1.00  0.00           C
ATOM   1138  CB  ASN   149      15.686 -16.744   6.443  1.00  0.00           C
ATOM   1139  CG  ASN   149      14.326 -17.422   6.351  1.00  0.00           C
ATOM   1140  OD1 ASN   149      13.976 -18.010   5.329  1.00  0.00           O
ATOM   1141  ND2 ASN   149      13.535 -17.342   7.455  1.00  0.00           N
ATOM   1142  C   ASN   149      14.521 -14.599   6.370  1.00  0.00           C
ATOM   1143  O   ASN   149      13.343 -14.789   6.076  1.00  0.00           O
ATOM   1144  N   LEU   150      14.872 -13.704   7.310  1.00  0.00           N
ATOM   1145  CA  LEU   150      13.849 -13.063   8.097  1.00  0.00           C
ATOM   1146  CB  LEU   150      14.401 -12.217   9.258  1.00  0.00           C
ATOM   1147  CG  LEU   150      15.028 -13.062  10.382  1.00  0.00           C
ATOM   1148  CD2 LEU   150      15.375 -12.197  11.603  1.00  0.00           C
ATOM   1149  CD1 LEU   150      16.222 -13.876   9.868  1.00  0.00           C
ATOM   1150  C   LEU   150      12.910 -12.205   7.301  1.00  0.00           C
ATOM   1151  O   LEU   150      13.297 -11.464   6.399  1.00  0.00           O
ATOM   1152  N   PRO   151      11.642 -12.352   7.629  1.00  0.00           N
ATOM   1153  CA  PRO   151      10.611 -11.545   7.028  1.00  0.00           C
ATOM   1154  CD  PRO   151      11.131 -13.637   8.080  1.00  0.00           C
ATOM   1155  CB  PRO   151       9.285 -12.224   7.362  1.00  0.00           C
ATOM   1156  CG  PRO   151       9.675 -13.697   7.585  1.00  0.00           C
ATOM   1157  C   PRO   151      10.718 -10.157   7.572  1.00  0.00           C
ATOM   1158  O   PRO   151      10.542  -9.974   8.775  1.00  0.00           O
ATOM   1159  N   LEU   152      10.936  -9.158   6.703  1.00  0.00           N
ATOM   1160  CA  LEU   152      11.142  -7.819   7.164  1.00  0.00           C
ATOM   1161  CB  LEU   152      11.740  -6.885   6.108  1.00  0.00           C
ATOM   1162  CG  LEU   152      13.080  -7.414   5.548  1.00  0.00           C
ATOM   1163  CD2 LEU   152      13.933  -8.084   6.637  1.00  0.00           C
ATOM   1164  CD1 LEU   152      13.837  -6.331   4.763  1.00  0.00           C
ATOM   1165  C   LEU   152       9.888  -7.232   7.732  1.00  0.00           C
ATOM   1166  O   LEU   152       9.944  -6.357   8.594  1.00  0.00           O
ATOM   1167  N   GLU   153       8.716  -7.661   7.241  1.00  0.00           N
ATOM   1168  CA  GLU   153       7.505  -7.084   7.748  1.00  0.00           C
ATOM   1169  CB  GLU   153       6.235  -7.583   7.029  1.00  0.00           C
ATOM   1170  CG  GLU   153       5.999  -9.094   7.103  1.00  0.00           C
ATOM   1171  CD  GLU   153       6.800  -9.763   5.995  1.00  0.00           C
ATOM   1172  OE1 GLU   153       7.595  -9.054   5.323  1.00  0.00           O
ATOM   1173  OE2 GLU   153       6.625 -10.996   5.804  1.00  0.00           O
ATOM   1174  C   GLU   153       7.369  -7.393   9.212  1.00  0.00           C
ATOM   1175  O   GLU   153       6.897  -6.556   9.976  1.00  0.00           O
ATOM   1176  N   GLN   154       7.702  -8.631   9.634  1.00  0.00           N
ATOM   1177  CA  GLN   154       7.604  -9.042  11.016  1.00  0.00           C
ATOM   1178  CB  GLN   154       7.599 -10.574  11.161  1.00  0.00           C
ATOM   1179  CG  GLN   154       6.398 -11.248  10.494  1.00  0.00           C
ATOM   1180  CD  GLN   154       6.522 -12.750  10.707  1.00  0.00           C
ATOM   1181  OE1 GLN   154       7.623 -13.298  10.735  1.00  0.00           O
ATOM   1182  NE2 GLN   154       5.360 -13.437  10.870  1.00  0.00           N
ATOM   1183  C   GLN   154       8.727  -8.539  11.882  1.00  0.00           C
ATOM   1184  O   GLN   154       8.520  -8.065  12.997  1.00  0.00           O
ATOM   1185  N   ALA   155       9.961  -8.651  11.370  1.00  0.00           N
ATOM   1186  CA  ALA   155      11.203  -8.388  12.052  1.00  0.00           C
ATOM   1187  CB  ALA   155      12.429  -8.756  11.199  1.00  0.00           C
ATOM   1188  C   ALA   155      11.350  -6.948  12.436  1.00  0.00           C
ATOM   1189  O   ALA   155      12.097  -6.615  13.352  1.00  0.00           O
ATOM   1190  N   ALA   156      10.699  -6.036  11.705  1.00  0.00           N
ATOM   1191  CA  ALA   156      10.869  -4.629  11.941  1.00  0.00           C
ATOM   1192  CB  ALA   156       9.963  -3.768  11.044  1.00  0.00           C
ATOM   1193  C   ALA   156      10.532  -4.300  13.367  1.00  0.00           C
ATOM   1194  O   ALA   156      11.156  -3.408  13.937  1.00  0.00           O
ATOM   1195  N   PRO   157       9.570  -4.946  13.969  1.00  0.00           N
ATOM   1196  CA  PRO   157       9.259  -4.641  15.339  1.00  0.00           C
ATOM   1197  CD  PRO   157       8.357  -5.269  13.232  1.00  0.00           C
ATOM   1198  CB  PRO   157       7.971  -5.402  15.637  1.00  0.00           C
ATOM   1199  CG  PRO   157       7.236  -5.359  14.284  1.00  0.00           C
ATOM   1200  C   PRO   157      10.385  -4.860  16.294  1.00  0.00           C
ATOM   1201  O   PRO   157      10.352  -4.305  17.389  1.00  0.00           O
ATOM   1202  N   LEU   158      11.388  -5.655  15.908  1.00  0.00           N
ATOM   1203  CA  LEU   158      12.540  -5.918  16.724  1.00  0.00           C
ATOM   1204  CB  LEU   158      13.477  -6.990  16.142  1.00  0.00           C
ATOM   1205  CG  LEU   158      12.871  -8.406  16.157  1.00  0.00           C
ATOM   1206  CD2 LEU   158      13.930  -9.474  15.848  1.00  0.00           C
ATOM   1207  CD1 LEU   158      11.634  -8.512  15.256  1.00  0.00           C
ATOM   1208  C   LEU   158      13.329  -4.650  16.886  1.00  0.00           C
ATOM   1209  O   LEU   158      14.153  -4.523  17.788  1.00  0.00           O
ATOM   1210  N   LEU   159      13.161  -3.699  15.957  1.00  0.00           N
ATOM   1211  CA  LEU   159      13.870  -2.452  15.992  1.00  0.00           C
ATOM   1212  CB  LEU   159      13.833  -1.664  14.683  1.00  0.00           C
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ATOM   1213  CG  LEU   159      14.733  -2.349  13.647  1.00  0.00           C
ATOM   1214  CD2 LEU   159      14.202  -3.744  13.282  1.00  0.00           C
ATOM   1215  CD1 LEU   159      16.199  -2.372  14.105  1.00  0.00           C
ATOM   1216  C   LEU   159      13.435  -1.587  17.125  1.00  0.00           C
ATOM   1217  O   LEU   159      14.131  -0.622  17.445  1.00  0.00           O
ATOM   1218  N   CYS   160      12.238  -1.827  17.704  1.00  0.00           N
ATOM   1219  CA  CYS   160      11.844  -0.977  18.790  1.00  0.00           C
ATOM   1220  CB  CYS   160      11.132   0.302  18.326  1.00  0.00           C
ATOM   1221  SG  CYS   160      10.648   1.358  19.725  1.00  0.00           S
ATOM   1222  C   CYS   160      10.895  -1.676  19.721  1.00  0.00           C
ATOM   1223  O   CYS   160      11.288  -2.169  20.778  1.00  0.00           O
ATOM   1224  N   ALA   161       9.606  -1.726  19.336  1.00  0.00           N
ATOM   1225  CA  ALA   161       8.557  -2.127  20.230  1.00  0.00           C
ATOM   1226  CB  ALA   161       7.185  -2.155  19.546  1.00  0.00           C
ATOM   1227  C   ALA   161       8.746  -3.476  20.834  1.00  0.00           C
ATOM   1228  O   ALA   161       8.660  -3.592  22.051  1.00  0.00           O
ATOM   1229  N   GLY   162       9.010  -4.529  20.047  1.00  0.00           N
ATOM   1230  CA  GLY   162       9.091  -5.834  20.650  1.00  0.00           C
ATOM   1231  C   GLY   162      10.272  -5.981  21.541  1.00  0.00           C
ATOM   1232  O   GLY   162      10.163  -6.484  22.659  1.00  0.00           O
ATOM   1233  N   VAL   163      11.445  -5.549  21.062  1.00  0.00           N
ATOM   1234  CA  VAL   163      12.625  -5.752  21.830  1.00  0.00           C
ATOM   1235  CB  VAL   163      13.848  -5.272  21.128  1.00  0.00           C
ATOM   1236  CG1 VAL   163      14.131  -6.212  19.943  1.00  0.00           C
ATOM   1237  CG2 VAL   163      13.573  -3.825  20.701  1.00  0.00           C
ATOM   1238  C   VAL   163      12.487  -5.010  23.107  1.00  0.00           C
ATOM   1239  O   VAL   163      12.886  -5.509  24.158  1.00  0.00           O
ATOM   1240  N   THR   164      11.974  -3.768  23.049  1.00  0.00           N
ATOM   1241  CA  THR   164      11.890  -2.997  24.247  1.00  0.00           C
ATOM   1242  CB  THR   164      11.387  -1.598  24.034  1.00  0.00           C
ATOM   1243  OG1 THR   164      10.117  -1.614  23.404  1.00  0.00           O
ATOM   1244  CG2 THR   164      12.392  -0.835  23.164  1.00  0.00           C
ATOM   1245  C   THR   164      10.993  -3.674  25.208  1.00  0.00           C
ATOM   1246  O   THR   164      11.359  -3.881  26.346  1.00  0.00           O
ATOM   1247  N   VAL   165       9.780  -4.073  24.850  1.00  0.00           N
ATOM   1248  CA  VAL   165       9.095  -4.694  25.936  1.00  0.00           C
ATOM   1249  CB  VAL   165       7.683  -4.718  25.783  1.00  0.00           C
ATOM   1250  CG1 VAL   165       7.241  -3.444  26.525  1.00  0.00           C
ATOM   1251  CG2 VAL   165       7.543  -4.725  24.257  1.00  0.00           C
ATOM   1252  C   VAL   165       9.628  -5.998  26.321  1.00  0.00           C
ATOM   1253  O   VAL   165       9.752  -6.237  27.507  1.00  0.00           O
ATOM   1254  N   PHE   166      10.011  -6.842  25.366  1.00  0.00           N
ATOM   1255  CA  PHE   166      10.469  -8.165  25.657  1.00  0.00           C
ATOM   1256  CB  PHE   166      11.029  -8.773  24.354  1.00  0.00           C
ATOM   1257  CG  PHE   166      11.408 -10.208  24.464  1.00  0.00           C
ATOM   1258  CD1 PHE   166      12.566 -10.606  25.092  1.00  0.00           C
ATOM   1259  CD2 PHE   166      10.606 -11.165  23.885  1.00  0.00           C
ATOM   1260  CE1 PHE   166      12.903 -11.939  25.165  1.00  0.00           C
ATOM   1261  CE2 PHE   166      10.938 -12.498  23.952  1.00  0.00           C
ATOM   1262  CZ  PHE   166      12.087 -12.887  24.597  1.00  0.00           C
ATOM   1263  C   PHE   166      11.597  -8.070  26.642  1.00  0.00           C
ATOM   1264  O   PHE   166      11.565  -8.739  27.674  1.00  0.00           O
ATOM   1265  N   SER   167      12.626  -7.233  26.382  1.00  0.00           N
ATOM   1266  CA  SER   167      13.707  -7.259  27.324  1.00  0.00           C
ATOM   1267  CB  SER   167      15.055  -6.752  26.866  1.00  0.00           C
ATOM   1268  OG  SER   167      15.997  -6.850  27.924  1.00  0.00           O
ATOM   1269  C   SER   167      13.384  -6.598  28.623  1.00  0.00           C
ATOM   1270  O   SER   167      13.963  -7.044  29.602  1.00  0.00           O
ATOM   1271  N   PRO   168      12.600  -5.554  28.750  1.00  0.00           N
ATOM   1272  CA  PRO   168      12.303  -5.215  30.088  1.00  0.00           C
ATOM   1273  CD  PRO   168      13.200  -4.326  28.321  1.00  0.00           C
ATOM   1274  CB  PRO   168      11.603  -3.867  30.079  1.00  0.00           C
ATOM   1275  CG  PRO   168      12.310  -3.195  28.897  1.00  0.00           C
ATOM   1276  C   PRO   168      11.789  -6.253  30.999  1.00  0.00           C
ATOM   1277  O   PRO   168      12.135  -6.162  32.173  1.00  0.00           O
ATOM   1278  N   MET   169      10.964  -7.215  30.575  1.00  0.00           N
ATOM   1279  CA  MET   169      10.798  -8.179  31.624  1.00  0.00           C
ATOM   1280  CB  MET   169       9.489  -8.972  31.732  1.00  0.00           C
ATOM   1281  CG  MET   169       8.334  -8.028  32.077  1.00  0.00           C
ATOM   1282  SD  MET   169       6.687  -8.778  32.047  1.00  0.00           S
ATOM   1283  CE  MET   169       7.054  -9.809  33.492  1.00  0.00           C
ATOM   1284  C   MET   169      11.962  -9.122  31.717  1.00  0.00           C
ATOM   1285  O   MET   169      12.356  -9.516  32.811  1.00  0.00           O
ATOM   1286  N   LYS   170      12.522  -9.529  30.560  1.00  0.00           N
ATOM   1287  CA  LYS   170      13.536 -10.547  30.468  1.00  0.00           C
ATOM   1288  CB  LYS   170      13.794 -10.946  29.001  1.00  0.00           C
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ATOM   1289  CG  LYS   170      14.858 -12.028  28.813  1.00  0.00           C
ATOM   1290  CD  LYS   170      14.847 -12.670  27.423  1.00  0.00           C
ATOM   1291  CE  LYS   170      15.906 -13.757  27.241  1.00  0.00           C
ATOM   1292  NZ  LYS   170      15.517 -14.969  27.997  1.00  0.00           N
ATOM   1293  C   LYS   170      14.851 -10.143  31.044  1.00  0.00           C
ATOM   1294  O   LYS   170      15.448 -10.888  31.824  1.00  0.00           O
ATOM   1295  N   HIS   171      15.348  -8.948  30.679  1.00  0.00           N
ATOM   1296  CA  HIS   171      16.665  -8.571  31.087  1.00  0.00           C
ATOM   1297  ND1 HIS   171      19.244  -6.428  30.929  1.00  0.00           N
ATOM   1298  CG  HIS   171      18.914  -7.642  30.376  1.00  0.00           C
ATOM   1299  NE2 HIS   171      21.121  -7.616  30.846  1.00  0.00           N
ATOM   1300  CD2 HIS   171      20.072  -8.359  30.332  1.00  0.00           C
ATOM   1301  CE1 HIS   171      20.574  -6.463  31.190  1.00  0.00           C
ATOM   1302  CB  HIS   171      17.528  -8.019  29.938  1.00  0.00           C
ATOM   1303  C   HIS   171      16.605  -7.506  32.131  1.00  0.00           C
ATOM   1304  O   HIS   171      17.253  -7.625  33.169  1.00  0.00           O
ATOM   1305  N   PHE   172      15.870  -6.407  31.881  1.00  0.00           N
ATOM   1306  CA  PHE   172      15.932  -5.361  32.862  1.00  0.00           C
ATOM   1307  CB  PHE   172      15.298  -4.057  32.350  1.00  0.00           C
ATOM   1308  CG  PHE   172      15.960  -2.954  33.097  1.00  0.00           C
ATOM   1309  CD1 PHE   172      17.257  -2.610  32.790  1.00  0.00           C
ATOM   1310  CD2 PHE   172      15.300  -2.251  34.071  1.00  0.00           C
ATOM   1311  CE1 PHE   172      17.900  -1.598  33.460  1.00  0.00           C
ATOM   1312  CE2 PHE   172      15.938  -1.238  34.746  1.00  0.00           C
ATOM   1313  CZ  PHE   172      17.239  -0.912  34.446  1.00  0.00           C
ATOM   1314  C   PHE   172      15.280  -5.785  34.162  1.00  0.00           C
ATOM   1315  O   PHE   172      15.904  -5.738  35.222  1.00  0.00           O
ATOM   1316  N   ALA   173      13.999  -6.212  34.107  1.00  0.00           N
ATOM   1317  CA  ALA   173      13.210  -6.646  35.242  1.00  0.00           C
ATOM   1318  CB  ALA   173      11.720  -6.810  34.901  1.00  0.00           C
ATOM   1319  C   ALA   173      13.685  -7.969  35.765  1.00  0.00           C
ATOM   1320  O   ALA   173      13.651  -8.221  36.970  1.00  0.00           O
ATOM   1321  N   MET   174      14.138  -8.859  34.859  1.00  0.00           N
ATOM   1322  CA  MET   174      14.531 -10.190  35.235  1.00  0.00           C
ATOM   1323  CB  MET   174      15.804 -10.213  36.097  1.00  0.00           C
ATOM   1324  CG  MET   174      17.040  -9.695  35.363  1.00  0.00           C
ATOM   1325  SD  MET   174      17.592 -10.758  33.998  1.00  0.00           S
ATOM   1326  CE  MET   174      18.179 -12.073  35.102  1.00  0.00           C
ATOM   1327  C   MET   174      13.436 -10.849  36.020  1.00  0.00           C
ATOM   1328  O   MET   174      13.662 -11.364  37.115  1.00  0.00           O
ATOM   1329  N   THR   175      12.209 -10.871  35.459  1.00  0.00           N
ATOM   1330  CA  THR   175      11.095 -11.478  36.136  1.00  0.00           C
ATOM   1331  CB  THR   175       9.813 -11.396  35.365  1.00  0.00           C
ATOM   1332  OG1 THR   175       9.933 -12.074  34.124  1.00  0.00           O
ATOM   1333  CG2 THR   175       9.503  -9.909  35.131  1.00  0.00           C
ATOM   1334  C   THR   175      11.417 -12.912  36.413  1.00  0.00           C
ATOM   1335  O   THR   175      12.125 -13.568  35.652  1.00  0.00           O
ATOM   1336  N   GLU   176      10.912 -13.434  37.548  1.00  0.00           N
ATOM   1337  CA  GLU   176      11.228 -14.777  37.939  1.00  0.00           C
ATOM   1338  CB  GLU   176      11.690 -14.897  39.401  1.00  0.00           C
ATOM   1339  CG  GLU   176      12.119 -16.315  39.785  1.00  0.00           C
ATOM   1340  CD  GLU   176      12.565 -16.301  41.240  1.00  0.00           C
ATOM   1341  OE1 GLU   176      11.790 -15.797  42.096  1.00  0.00           O
ATOM   1342  OE2 GLU   176      13.693 -16.791  41.513  1.00  0.00           O
ATOM   1343  C   GLU   176      10.012 -15.626  37.776  1.00  0.00           C
ATOM   1344  O   GLU   176       8.883 -15.141  37.725  1.00  0.00           O
ATOM   1345  N   PRO   177      10.239 -16.905  37.667  1.00  0.00           N
ATOM   1346  CA  PRO   177       9.133 -17.797  37.483  1.00  0.00           C
ATOM   1347  CD  PRO   177      11.446 -17.398  37.024  1.00  0.00           C
ATOM   1348  CB  PRO   177       9.736 -19.130  37.051  1.00  0.00           C
ATOM   1349  CG  PRO   177      11.038 -18.715  36.341  1.00  0.00           C
ATOM   1350  C   PRO   177       8.261 -17.871  38.693  1.00  0.00           C
ATOM   1351  O   PRO   177       8.780 -17.914  39.807  1.00  0.00           O
ATOM   1352  N   GLY   178       6.930 -17.897  38.483  1.00  0.00           N
ATOM   1353  CA  GLY   178       5.987 -18.033  39.554  1.00  0.00           C
ATOM   1354  C   GLY   178       5.593 -16.686  40.085  1.00  0.00           C
ATOM   1355  O   GLY   178       4.726 -16.593  40.953  1.00  0.00           O
ATOM   1356  N   LYS   179       6.204 -15.600  39.579  1.00  0.00           N
ATOM   1357  CA  LYS   179       5.898 -14.299  40.099  1.00  0.00           C
ATOM   1358  CB  LYS   179       7.064 -13.304  39.976  1.00  0.00           C
ATOM   1359  CG  LYS   179       8.160 -13.640  40.991  1.00  0.00           C
ATOM   1360  CD  LYS   179       9.513 -12.970  40.758  1.00  0.00           C
ATOM   1361  CE  LYS   179      10.540 -13.367  41.823  1.00  0.00           C
ATOM   1362  NZ  LYS   179      11.882 -12.858  41.470  1.00  0.00           N
ATOM   1363  C   LYS   179       4.667 -13.751  39.449  1.00  0.00           C
ATOM   1364  O   LYS   179       4.148 -14.317  38.488  1.00  0.00           O
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ATOM   1365  N   LYS   180       4.138 -12.648  40.020  1.00  0.00           N
ATOM   1366  CA  LYS   180       2.957 -12.011  39.513  1.00  0.00           C
ATOM   1367  CB  LYS   180       1.931 -11.708  40.627  1.00  0.00           C
ATOM   1368  CG  LYS   180       0.616 -11.048  40.184  1.00  0.00           C
ATOM   1369  CD  LYS   180       0.739  -9.626  39.630  1.00  0.00           C
ATOM   1370  CE  LYS   180      -0.600  -9.019  39.205  1.00  0.00           C
ATOM   1371  NZ  LYS   180      -1.436  -8.749  40.397  1.00  0.00           N
ATOM   1372  C   LYS   180       3.384 -10.703  38.930  1.00  0.00           C
ATOM   1373  O   LYS   180       4.007  -9.884  39.606  1.00  0.00           O
ATOM   1374  N   CYS   181       3.042 -10.464  37.649  1.00  0.00           N
ATOM   1375  CA  CYS   181       3.441  -9.233  37.036  1.00  0.00           C
ATOM   1376  CB  CYS   181       4.348  -9.438  35.816  1.00  0.00           C
ATOM   1377  SG  CYS   181       5.924 -10.195  36.314  1.00  0.00           S
ATOM   1378  C   CYS   181       2.220  -8.475  36.623  1.00  0.00           C
ATOM   1379  O   CYS   181       1.160  -9.051  36.383  1.00  0.00           O
ATOM   1380  N   GLY   182       2.346  -7.134  36.559  1.00  0.00           N
ATOM   1381  CA  GLY   182       1.250  -6.311  36.148  1.00  0.00           C
ATOM   1382  C   GLY   182       1.797  -5.354  35.139  1.00  0.00           C
ATOM   1383  O   GLY   182       2.800  -4.685  35.387  1.00  0.00           O
ATOM   1384  N   ILE   183       1.130  -5.251  33.972  1.00  0.00           N
ATOM   1385  CA  ILE   183       1.622  -4.390  32.935  1.00  0.00           C
ATOM   1386  CB  ILE   183       1.761  -5.067  31.597  1.00  0.00           C
ATOM   1387  CG2 ILE   183       2.799  -6.190  31.739  1.00  0.00           C
ATOM   1388  CG1 ILE   183       0.393  -5.546  31.082  1.00  0.00           C
ATOM   1389  CD1 ILE   183       0.377  -5.874  29.592  1.00  0.00           C
ATOM   1390  C   ILE   183       0.665  -3.255  32.755  1.00  0.00           C
ATOM   1391  O   ILE   183      -0.536  -3.448  32.574  1.00  0.00           O
ATOM   1392  N   LEU   184       1.188  -2.015  32.814  1.00  0.00           N
ATOM   1393  CA  LEU   184       0.342  -0.873  32.625  1.00  0.00           C
ATOM   1394  CB  LEU   184       0.683   0.308  33.546  1.00  0.00           C
ATOM   1395  CG  LEU   184      -0.235   1.528  33.343  1.00  0.00           C
ATOM   1396  CD2 LEU   184       0.305   2.761  34.083  1.00  0.00           C
ATOM   1397  CD1 LEU   184      -1.686   1.200  33.704  1.00  0.00           C
ATOM   1398  C   LEU   184       0.524  -0.408  31.219  1.00  0.00           C
ATOM   1399  O   LEU   184       1.561   0.156  30.873  1.00  0.00           O
ATOM   1400  N   GLY   185      -0.509  -0.617  30.379  1.00  0.00           N
ATOM   1401  CA  GLY   185      -0.454  -0.208  29.006  1.00  0.00           C
ATOM   1402  C   GLY   185      -0.426  -1.435  28.143  1.00  0.00           C
ATOM   1403  O   GLY   185       0.543  -2.188  28.111  1.00  0.00           O
ATOM   1404  N   LEU   186      -1.551  -1.650  27.444  1.00  0.00           N
ATOM   1405  CA  LEU   186      -1.893  -2.708  26.535  1.00  0.00           C
ATOM   1406  CB  LEU   186      -3.390  -3.045  26.521  1.00  0.00           C
ATOM   1407  CG  LEU   186      -3.882  -3.566  27.882  1.00  0.00           C
ATOM   1408  CD2 LEU   186      -2.884  -4.565  28.494  1.00  0.00           C
ATOM   1409  CD1 LEU   186      -5.312  -4.123  27.795  1.00  0.00           C
ATOM   1410  C   LEU   186      -1.406  -2.519  25.127  1.00  0.00           C
ATOM   1411  O   LEU   186      -1.841  -3.266  24.252  1.00  0.00           O
ATOM   1412  N   GLY   187      -0.647  -1.445  24.828  1.00  0.00           N
ATOM   1413  CA  GLY   187      -0.241  -1.165  23.473  1.00  0.00           C
ATOM   1414  C   GLY   187       0.764  -2.175  22.981  1.00  0.00           C
ATOM   1415  O   GLY   187       0.934  -3.244  23.563  1.00  0.00           O
ATOM   1416  N   GLY   188       1.432  -1.860  21.845  1.00  0.00           N
ATOM   1417  CA  GLY   188       2.356  -2.766  21.208  1.00  0.00           C
ATOM   1418  C   GLY   188       3.498  -3.085  22.109  1.00  0.00           C
ATOM   1419  O   GLY   188       3.965  -4.223  22.169  1.00  0.00           O
ATOM   1420  N   VAL   189       4.010  -2.061  22.797  1.00  0.00           N
ATOM   1421  CA  VAL   189       5.101  -2.254  23.694  1.00  0.00           C
ATOM   1422  CB  VAL   189       5.527  -0.879  24.166  1.00  0.00           C
ATOM   1423  CG1 VAL   189       6.703  -0.935  25.141  1.00  0.00           C
ATOM   1424  CG2 VAL   189       5.811  -0.034  22.917  1.00  0.00           C
ATOM   1425  C   VAL   189       4.561  -3.108  24.814  1.00  0.00           C
ATOM   1426  O   VAL   189       5.081  -4.172  25.111  1.00  0.00           O
ATOM   1427  N   GLY   190       3.417  -2.746  25.413  1.00  0.00           N
ATOM   1428  CA  GLY   190       2.960  -3.492  26.557  1.00  0.00           C
ATOM   1429  C   GLY   190       2.743  -4.946  26.235  1.00  0.00           C
ATOM   1430  O   GLY   190       3.082  -5.815  27.038  1.00  0.00           O
ATOM   1431  N   HIS   191       2.204  -5.265  25.046  1.00  0.00           N
ATOM   1432  CA  HIS   191       1.951  -6.645  24.750  1.00  0.00           C
ATOM   1433  ND1 HIS   191       2.419  -8.293  21.774  1.00  0.00           N
ATOM   1434  CG  HIS   191       1.929  -7.073  22.186  1.00  0.00           C
ATOM   1435  NE2 HIS   191       2.922  -6.836  20.173  1.00  0.00           N
ATOM   1436  CD2 HIS   191       2.250  -6.193  21.197  1.00  0.00           C
ATOM   1437  CE1 HIS   191       3.001  -8.094  20.565  1.00  0.00           C
ATOM   1438  CB  HIS   191       1.147  -6.883  23.453  1.00  0.00           C
ATOM   1439  C   HIS   191       3.240  -7.399  24.683  1.00  0.00           C
ATOM   1440  O   HIS   191       3.297  -8.572  25.048  1.00  0.00           O
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ATOM   1441  N   MET   192       4.316  -6.771  24.180  1.00  0.00           N
ATOM   1442  CA  MET   192       5.532  -7.519  24.123  1.00  0.00           C
ATOM   1443  CB  MET   192       6.478  -7.135  22.981  1.00  0.00           C
ATOM   1444  CG  MET   192       5.764  -7.616  21.710  1.00  0.00           C
ATOM   1445  SD  MET   192       6.524  -7.378  20.082  1.00  0.00           S
ATOM   1446  CE  MET   192       6.113  -5.614  19.960  1.00  0.00           C
ATOM   1447  C   MET   192       6.104  -7.755  25.484  1.00  0.00           C
ATOM   1448  O   MET   192       6.759  -8.770  25.716  1.00  0.00           O
ATOM   1449  N   GLY   193       5.853  -6.837  26.436  1.00  0.00           N
ATOM   1450  CA  GLY   193       6.276  -7.061  27.786  1.00  0.00           C
ATOM   1451  C   GLY   193       5.593  -8.306  28.289  1.00  0.00           C
ATOM   1452  O   GLY   193       6.202  -9.162  28.931  1.00  0.00           O
ATOM   1453  N   VAL   194       4.293  -8.458  27.981  1.00  0.00           N
ATOM   1454  CA  VAL   194       3.542  -9.593  28.442  1.00  0.00           C
ATOM   1455  CB  VAL   194       2.138  -9.619  27.914  1.00  0.00           C
ATOM   1456  CG1 VAL   194       1.447 -10.901  28.409  1.00  0.00           C
ATOM   1457  CG2 VAL   194       1.432  -8.322  28.334  1.00  0.00           C
ATOM   1458  C   VAL   194       4.211 -10.821  27.925  1.00  0.00           C
ATOM   1459  O   VAL   194       4.338 -11.821  28.629  1.00  0.00           O
ATOM   1460  N   LYS   195       4.670 -10.770  26.667  1.00  0.00           N
ATOM   1461  CA  LYS   195       5.290 -11.907  26.066  1.00  0.00           C
ATOM   1462  CB  LYS   195       5.707 -11.647  24.610  1.00  0.00           C
ATOM   1463  CG  LYS   195       6.119 -12.921  23.875  1.00  0.00           C
ATOM   1464  CD  LYS   195       4.965 -13.908  23.691  1.00  0.00           C
ATOM   1465  CE  LYS   195       3.947 -13.487  22.629  1.00  0.00           C
ATOM   1466  NZ  LYS   195       4.388 -13.939  21.291  1.00  0.00           N
ATOM   1467  C   LYS   195       6.518 -12.252  26.850  1.00  0.00           C
ATOM   1468  O   LYS   195       6.824 -13.425  27.060  1.00  0.00           O
ATOM   1469  N   ILE   196       7.256 -11.231  27.320  1.00  0.00           N
ATOM   1470  CA  ILE   196       8.488 -11.471  28.014  1.00  0.00           C
ATOM   1471  CB  ILE   196       8.979 -10.325  28.765  1.00  0.00           C
ATOM   1472  CG2 ILE   196      10.401 -10.717  29.160  1.00  0.00           C
ATOM   1473  CG1 ILE   196       8.853  -9.007  28.045  1.00  0.00           C
ATOM   1474  CD1 ILE   196       8.659  -7.992  29.152  1.00  0.00           C
ATOM   1475  C   ILE   196       8.174 -12.232  29.253  1.00  0.00           C
ATOM   1476  O   ILE   196       8.857 -13.185  29.624  1.00  0.00           O
ATOM   1477  N   ALA   197       7.138 -11.742  29.956  1.00  0.00           N
ATOM   1478  CA  ALA   197       6.754 -12.241  31.242  1.00  0.00           C
ATOM   1479  CB  ALA   197       5.468 -11.578  31.757  1.00  0.00           C
ATOM   1480  C   ALA   197       6.429 -13.682  31.080  1.00  0.00           C
ATOM   1481  O   ALA   197       6.776 -14.503  31.927  1.00  0.00           O
ATOM   1482  N   LYS   198       5.743 -14.016  29.975  1.00  0.00           N
ATOM   1483  CA  LYS   198       5.343 -15.368  29.736  1.00  0.00           C
ATOM   1484  CB  LYS   198       4.499 -15.515  28.458  1.00  0.00           C
ATOM   1485  CG  LYS   198       3.767 -16.854  28.344  1.00  0.00           C
ATOM   1486  CD  LYS   198       4.687 -18.072  28.271  1.00  0.00           C
ATOM   1487  CE  LYS   198       5.342 -18.262  26.902  1.00  0.00           C
ATOM   1488  NZ  LYS   198       6.211 -19.460  26.919  1.00  0.00           N
ATOM   1489  C   LYS   198       6.569 -16.215  29.582  1.00  0.00           C
ATOM   1490  O   LYS   198       6.620 -17.340  30.076  1.00  0.00           O
ATOM   1491  N   ALA   199       7.598 -15.691  28.889  1.00  0.00           N
ATOM   1492  CA  ALA   199       8.804 -16.440  28.665  1.00  0.00           C
ATOM   1493  CB  ALA   199       9.827 -15.680  27.800  1.00  0.00           C
ATOM   1494  C   ALA   199       9.452 -16.730  29.981  1.00  0.00           C
ATOM   1495  O   ALA   199       9.968 -17.823  30.206  1.00  0.00           O
ATOM   1496  N   PHE   200       9.435 -15.743  30.892  1.00  0.00           N
ATOM   1497  CA  PHE   200      10.043 -15.886  32.183  1.00  0.00           C
ATOM   1498  CB  PHE   200      10.277 -14.566  32.925  1.00  0.00           C
ATOM   1499  CG  PHE   200      11.577 -14.169  32.329  1.00  0.00           C
ATOM   1500  CD1 PHE   200      11.641 -13.752  31.023  1.00  0.00           C
ATOM   1501  CD2 PHE   200      12.733 -14.247  33.072  1.00  0.00           C
ATOM   1502  CE1 PHE   200      12.848 -13.405  30.473  1.00  0.00           C
ATOM   1503  CE2 PHE   200      13.945 -13.899  32.528  1.00  0.00           C
ATOM   1504  CZ  PHE   200      13.997 -13.476  31.225  1.00  0.00           C
ATOM   1505  C   PHE   200       9.328 -16.894  33.013  1.00  0.00           C
ATOM   1506  O   PHE   200       9.934 -17.498  33.896  1.00  0.00           O
ATOM   1507  N   GLY   201       8.022 -17.105  32.773  1.00  0.00           N
ATOM   1508  CA  GLY   201       7.362 -18.122  33.536  1.00  0.00           C
ATOM   1509  C   GLY   201       6.575 -17.508  34.640  1.00  0.00           C
ATOM   1510  O   GLY   201       6.274 -18.175  35.629  1.00  0.00           O
ATOM   1511  N   LEU   202       6.204 -16.220  34.514  1.00  0.00           N
ATOM   1512  CA  LEU   202       5.441 -15.689  35.600  1.00  0.00           C
ATOM   1513  CB  LEU   202       5.176 -14.168  35.574  1.00  0.00           C
ATOM   1514  CG  LEU   202       4.339 -13.609  34.409  1.00  0.00           C
ATOM   1515  CD2 LEU   202       4.377 -12.076  34.443  1.00  0.00           C
ATOM   1516  CD1 LEU   202       2.895 -14.138  34.402  1.00  0.00           C
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ATOM   1517  C   LEU   202       4.149 -16.437  35.681  1.00  0.00           C
ATOM   1518  O   LEU   202       3.602 -16.877  34.670  1.00  0.00           O
ATOM   1519  N   HIS   203       3.656 -16.634  36.918  1.00  0.00           N
ATOM   1520  CA  HIS   203       2.430 -17.338  37.158  1.00  0.00           C
ATOM   1521  ND1 HIS   203       0.837 -19.760  38.860  1.00  0.00           N
ATOM   1522  CG  HIS   203       0.920 -18.386  38.901  1.00  0.00           C
ATOM   1523  NE2 HIS   203      -1.200 -19.015  39.348  1.00  0.00           N
ATOM   1524  CD2 HIS   203      -0.333 -17.947  39.200  1.00  0.00           C
ATOM   1525  CE1 HIS   203      -0.453 -20.083  39.134  1.00  0.00           C
ATOM   1526  CB  HIS   203       2.181 -17.611  38.650  1.00  0.00           C
ATOM   1527  C   HIS   203       1.271 -16.540  36.653  1.00  0.00           C
ATOM   1528  O   HIS   203       0.374 -17.085  36.010  1.00  0.00           O
ATOM   1529  N   VAL   204       1.239 -15.223  36.944  1.00  0.00           N
ATOM   1530  CA  VAL   204       0.117 -14.463  36.481  1.00  0.00           C
ATOM   1531  CB  VAL   204      -0.907 -14.204  37.547  1.00  0.00           C
ATOM   1532  CG1 VAL   204      -0.234 -13.435  38.690  1.00  0.00           C
ATOM   1533  CG2 VAL   204      -2.099 -13.466  36.915  1.00  0.00           C
ATOM   1534  C   VAL   204       0.586 -13.148  35.942  1.00  0.00           C
ATOM   1535  O   VAL   204       1.528 -12.546  36.456  1.00  0.00           O
ATOM   1536  N   THR   205      -0.063 -12.690  34.851  1.00  0.00           N
ATOM   1537  CA  THR   205       0.217 -11.413  34.253  1.00  0.00           C
ATOM   1538  CB  THR   205       0.640 -11.433  32.804  1.00  0.00           C
ATOM   1539  OG1 THR   205      -0.290 -12.176  32.032  1.00  0.00           O
ATOM   1540  CG2 THR   205       2.062 -11.966  32.624  1.00  0.00           C
ATOM   1541  C   THR   205      -1.077 -10.678  34.217  1.00  0.00           C
ATOM   1542  O   THR   205      -2.043 -11.139  33.611  1.00  0.00           O
ATOM   1543  N   VAL   206      -1.128  -9.497  34.853  1.00  0.00           N
ATOM   1544  CA  VAL   206      -2.343  -8.748  34.808  1.00  0.00           C
ATOM   1545  CB  VAL   206      -2.755  -8.192  36.141  1.00  0.00           C
ATOM   1546  CG1 VAL   206      -4.004  -7.317  35.941  1.00  0.00           C
ATOM   1547  CG2 VAL   206      -2.961  -9.363  37.117  1.00  0.00           C
ATOM   1548  C   VAL   206      -2.101  -7.589  33.899  1.00  0.00           C
ATOM   1549  O   VAL   206      -1.134  -6.848  34.060  1.00  0.00           O
ATOM   1550  N   ILE   207      -3.001  -7.400  32.918  1.00  0.00           N
ATOM   1551  CA  ILE   207      -2.846  -6.340  31.965  1.00  0.00           C
ATOM   1552  CB  ILE   207      -3.219  -6.743  30.571  1.00  0.00           C
ATOM   1553  CG2 ILE   207      -2.249  -7.844  30.115  1.00  0.00           C
ATOM   1554  CG1 ILE   207      -4.702  -7.148  30.527  1.00  0.00           C
ATOM   1555  CD1 ILE   207      -5.263  -7.295  29.116  1.00  0.00           C
ATOM   1556  C   ILE   207      -3.774  -5.244  32.366  1.00  0.00           C
ATOM   1557  O   ILE   207      -4.921  -5.494  32.733  1.00  0.00           O
ATOM   1558  N   SER   208      -3.283  -3.988  32.342  1.00  0.00           N
ATOM   1559  CA  SER   208      -4.140  -2.909  32.732  1.00  0.00           C
ATOM   1560  CB  SER   208      -3.665  -2.178  33.999  1.00  0.00           C
ATOM   1561  OG  SER   208      -2.424  -1.532  33.754  1.00  0.00           O
ATOM   1562  C   SER   208      -4.186  -1.895  31.637  1.00  0.00           C
ATOM   1563  O   SER   208      -3.154  -1.477  31.116  1.00  0.00           O
ATOM   1564  N   SER   209      -5.411  -1.473  31.262  1.00  0.00           N
ATOM   1565  CA  SER   209      -5.560  -0.459  30.262  1.00  0.00           C
ATOM   1566  CB  SER   209      -5.494  -0.977  28.815  1.00  0.00           C
ATOM   1567  OG  SER   209      -6.631  -1.777  28.528  1.00  0.00           O
ATOM   1568  C   SER   209      -6.901   0.170  30.445  1.00  0.00           C
ATOM   1569  O   SER   209      -7.820  -0.436  30.993  1.00  0.00           O
ATOM   1570  N   SER   210      -7.033   1.432  30.005  1.00  0.00           N
ATOM   1571  CA  SER   210      -8.277   2.136  30.101  1.00  0.00           C
ATOM   1572  CB  SER   210      -8.140   3.631  29.767  1.00  0.00           C
ATOM   1573  OG  SER   210      -9.402   4.273  29.880  1.00  0.00           O
ATOM   1574  C   SER   210      -9.237   1.550  29.111  1.00  0.00           C
ATOM   1575  O   SER   210     -10.439   1.490  29.372  1.00  0.00           O
ATOM   1576  N   ASP   211      -8.739   1.102  27.936  1.00  0.00           N
ATOM   1577  CA  ASP   211      -9.685   0.615  26.978  1.00  0.00           C
ATOM   1578  CB  ASP   211      -9.457   1.068  25.525  1.00  0.00           C
ATOM   1579  CG  ASP   211      -8.209   0.401  24.992  1.00  0.00           C
ATOM   1580  OD1 ASP   211      -7.100   0.712  25.498  1.00  0.00           O
ATOM   1581  OD2 ASP   211      -8.357  -0.441  24.067  1.00  0.00           O
ATOM   1582  C   ASP   211      -9.715  -0.878  27.004  1.00  0.00           C
ATOM   1583  O   ASP   211      -8.703  -1.557  26.842  1.00  0.00           O
ATOM   1584  N   LYS   212     -10.928  -1.414  27.206  1.00  0.00           N
ATOM   1585  CA  LYS   212     -11.206  -2.815  27.309  1.00  0.00           C
ATOM   1586  CB  LYS   212     -12.634  -3.109  27.798  1.00  0.00           C
ATOM   1587  CG  LYS   212     -12.803  -2.761  29.280  1.00  0.00           C
ATOM   1588  CD  LYS   212     -14.250  -2.753  29.776  1.00  0.00           C
ATOM   1589  CE  LYS   212     -14.369  -2.427  31.267  1.00  0.00           C
ATOM   1590  NZ  LYS   212     -15.789  -2.429  31.683  1.00  0.00           N
ATOM   1591  C   LYS   212     -10.969  -3.498  25.996  1.00  0.00           C
ATOM   1592  O   LYS   212     -10.804  -4.714  25.947  1.00  0.00           O
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ATOM   1593  N   LYS   213     -10.973  -2.746  24.884  1.00  0.00           N
ATOM   1594  CA  LYS   213     -10.829  -3.349  23.587  1.00  0.00           C
ATOM   1595  CB  LYS   213     -10.808  -2.318  22.446  1.00  0.00           C
ATOM   1596  CG  LYS   213     -12.134  -1.584  22.246  1.00  0.00           C
ATOM   1597  CD  LYS   213     -12.490  -0.641  23.395  1.00  0.00           C
ATOM   1598  CE  LYS   213     -13.818   0.087  23.186  1.00  0.00           C
ATOM   1599  NZ  LYS   213     -14.084   0.982  24.332  1.00  0.00           N
ATOM   1600  C   LYS   213      -9.534  -4.108  23.508  1.00  0.00           C
ATOM   1601  O   LYS   213      -9.451  -5.131  22.832  1.00  0.00           O
ATOM   1602  N   LYS   214      -8.480  -3.613  24.178  1.00  0.00           N
ATOM   1603  CA  LYS   214      -7.163  -4.192  24.148  1.00  0.00           C
ATOM   1604  CB  LYS   214      -6.115  -3.333  24.866  1.00  0.00           C
ATOM   1605  CG  LYS   214      -5.809  -2.009  24.171  1.00  0.00           C
ATOM   1606  CD  LYS   214      -4.991  -1.066  25.056  1.00  0.00           C
ATOM   1607  CE  LYS   214      -4.524   0.207  24.362  1.00  0.00           C
ATOM   1608  NZ  LYS   214      -3.693   1.023  25.276  1.00  0.00           N
ATOM   1609  C   LYS   214      -7.113  -5.550  24.795  1.00  0.00           C
ATOM   1610  O   LYS   214      -6.226  -6.350  24.500  1.00  0.00           O
ATOM   1611  N   GLU   215      -8.046  -5.838  25.716  1.00  0.00           N
ATOM   1612  CA  GLU   215      -8.009  -7.017  26.542  1.00  0.00           C
ATOM   1613  CB  GLU   215      -9.323  -7.214  27.310  1.00  0.00           C
ATOM   1614  CG  GLU   215      -9.761  -6.006  28.126  1.00  0.00           C
ATOM   1615  CD  GLU   215     -11.125  -6.322  28.729  1.00  0.00           C
ATOM   1616  OE1 GLU   215     -11.509  -7.522  28.731  1.00  0.00           O
ATOM   1617  OE2 GLU   215     -11.802  -5.367  29.195  1.00  0.00           O
ATOM   1618  C   GLU   215      -7.894  -8.277  25.738  1.00  0.00           C
ATOM   1619  O   GLU   215      -7.099  -9.153  26.077  1.00  0.00           O
ATOM   1620  N   GLU   216      -8.676  -8.416  24.653  1.00  0.00           N
ATOM   1621  CA  GLU   216      -8.721  -9.680  23.971  1.00  0.00           C
ATOM   1622  CB  GLU   216      -9.623  -9.652  22.723  1.00  0.00           C
ATOM   1623  CG  GLU   216     -11.109  -9.479  23.041  1.00  0.00           C
ATOM   1624  CD  GLU   216     -11.649 -10.817  23.526  1.00  0.00           C
ATOM   1625  OE1 GLU   216     -11.056 -11.864  23.152  1.00  0.00           O
ATOM   1626  OE2 GLU   216     -12.664 -10.811  24.271  1.00  0.00           O
ATOM   1627  C   GLU   216      -7.359 -10.080  23.505  1.00  0.00           C
ATOM   1628  O   GLU   216      -6.927 -11.209  23.733  1.00  0.00           O
ATOM   1629  N   ALA   217      -6.641  -9.168  22.832  1.00  0.00           N
ATOM   1630  CA  ALA   217      -5.355  -9.519  22.309  1.00  0.00           C
ATOM   1631  CB  ALA   217      -4.768  -8.458  21.368  1.00  0.00           C
ATOM   1632  C   ALA   217      -4.384  -9.778  23.416  1.00  0.00           C
ATOM   1633  O   ALA   217      -3.554 -10.680  23.318  1.00  0.00           O
ATOM   1634  N   MET   218      -4.463  -9.002  24.512  1.00  0.00           N
ATOM   1635  CA  MET   218      -3.507  -9.159  25.570  1.00  0.00           C
ATOM   1636  CB  MET   218      -3.761  -8.206  26.750  1.00  0.00           C
ATOM   1637  CG  MET   218      -3.520  -6.727  26.421  1.00  0.00           C
ATOM   1638  SD  MET   218      -1.783  -6.282  26.129  1.00  0.00           S
ATOM   1639  CE  MET   218      -1.674  -7.095  24.507  1.00  0.00           C
ATOM   1640  C   MET   218      -3.600 -10.566  26.069  1.00  0.00           C
ATOM   1641  O   MET   218      -2.585 -11.206  26.337  1.00  0.00           O
ATOM   1642  N   GLU   219      -4.829 -11.098  26.183  1.00  0.00           N
ATOM   1643  CA  GLU   219      -5.035 -12.431  26.672  1.00  0.00           C
ATOM   1644  CB  GLU   219      -6.528 -12.787  26.774  1.00  0.00           C
ATOM   1645  CG  GLU   219      -6.785 -14.135  27.448  1.00  0.00           C
ATOM   1646  CD  GLU   219      -8.288 -14.367  27.492  1.00  0.00           C
ATOM   1647  OE1 GLU   219      -9.042 -13.514  26.953  1.00  0.00           O
ATOM   1648  OE2 GLU   219      -8.702 -15.406  28.072  1.00  0.00           O
ATOM   1649  C   GLU   219      -4.392 -13.415  25.738  1.00  0.00           C
ATOM   1650  O   GLU   219      -3.829 -14.416  26.176  1.00  0.00           O
ATOM   1651  N   VAL   220      -4.463 -13.163  24.417  1.00  0.00           N
ATOM   1652  CA  VAL   220      -3.914 -14.075  23.449  1.00  0.00           C
ATOM   1653  CB  VAL   220      -4.139 -13.624  22.037  1.00  0.00           C
ATOM   1654  CG1 VAL   220      -3.429 -14.607  21.090  1.00  0.00           C
ATOM   1655  CG2 VAL   220      -5.654 -13.516  21.798  1.00  0.00           C
ATOM   1656  C   VAL   220      -2.433 -14.187  23.657  1.00  0.00           C
ATOM   1657  O   VAL   220      -1.865 -15.274  23.567  1.00  0.00           O
ATOM   1658  N   LEU   221      -1.777 -13.043  23.923  1.00  0.00           N
ATOM   1659  CA  LEU   221      -0.360 -12.929  24.138  1.00  0.00           C
ATOM   1660  CB  LEU   221       0.157 -11.477  24.140  1.00  0.00           C
ATOM   1661  CG  LEU   221       0.232 -10.850  22.734  1.00  0.00           C
ATOM   1662  CD2 LEU   221      -1.137 -10.839  22.040  1.00  0.00           C
ATOM   1663  CD1 LEU   221       1.314 -11.537  21.885  1.00  0.00           C
ATOM   1664  C   LEU   221       0.071 -13.575  25.426  1.00  0.00           C
ATOM   1665  O   LEU   221       1.231 -13.972  25.531  1.00  0.00           O
ATOM   1666  N   GLY   222      -0.814 -13.700  26.446  1.00  0.00           N
ATOM   1667  CA  GLY   222      -0.330 -14.293  27.667  1.00  0.00           C
ATOM   1668  C   GLY   222      -0.909 -13.676  28.916  1.00  0.00           C
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ATOM   1669  O   GLY   222      -0.665 -14.189  30.007  1.00  0.00           O
ATOM   1670  N   ALA   223      -1.681 -12.574  28.830  1.00  0.00           N
ATOM   1671  CA  ALA   223      -2.230 -12.018  30.041  1.00  0.00           C
ATOM   1672  CB  ALA   223      -2.974 -10.690  29.819  1.00  0.00           C
ATOM   1673  C   ALA   223      -3.212 -12.986  30.641  1.00  0.00           C
ATOM   1674  O   ALA   223      -4.066 -13.536  29.949  1.00  0.00           O
ATOM   1675  N   ASP   224      -3.081 -13.232  31.963  1.00  0.00           N
ATOM   1676  CA  ASP   224      -3.961 -14.096  32.705  1.00  0.00           C
ATOM   1677  CB  ASP   224      -3.401 -14.440  34.098  1.00  0.00           C
ATOM   1678  CG  ASP   224      -4.271 -15.515  34.738  1.00  0.00           C
ATOM   1679  OD1 ASP   224      -5.502 -15.287  34.884  1.00  0.00           O
ATOM   1680  OD2 ASP   224      -3.706 -16.580  35.104  1.00  0.00           O
ATOM   1681  C   ASP   224      -5.275 -13.409  32.899  1.00  0.00           C
ATOM   1682  O   ASP   224      -6.332 -14.035  32.832  1.00  0.00           O
ATOM   1683  N   ALA   225      -5.231 -12.092  33.178  1.00  0.00           N
ATOM   1684  CA  ALA   225      -6.431 -11.349  33.412  1.00  0.00           C
ATOM   1685  CB  ALA   225      -6.891 -11.368  34.880  1.00  0.00           C
ATOM   1686  C   ALA   225      -6.151  -9.926  33.052  1.00  0.00           C
ATOM   1687  O   ALA   225      -4.999  -9.506  32.957  1.00  0.00           O
ATOM   1688  N   TYR   226      -7.231  -9.155  32.827  1.00  0.00           N
ATOM   1689  CA  TYR   226      -7.168  -7.780  32.427  1.00  0.00           C
ATOM   1690  CB  TYR   226      -7.718  -7.608  31.002  1.00  0.00           C
ATOM   1691  CG  TYR   226      -8.090  -6.194  30.714  1.00  0.00           C
ATOM   1692  CD1 TYR   226      -9.359  -5.746  31.020  1.00  0.00           C
ATOM   1693  CD2 TYR   226      -7.196  -5.321  30.142  1.00  0.00           C
ATOM   1694  CE1 TYR   226      -9.737  -4.455  30.752  1.00  0.00           C
ATOM   1695  CE2 TYR   226      -7.571  -4.026  29.872  1.00  0.00           C
ATOM   1696  CZ  TYR   226      -8.841  -3.595  30.173  1.00  0.00           C
ATOM   1697  OH  TYR   226      -9.236  -2.272  29.894  1.00  0.00           O
ATOM   1698  C   TYR   226      -8.072  -7.004  33.331  1.00  0.00           C
ATOM   1699  O   TYR   226      -9.094  -7.519  33.777  1.00  0.00           O
ATOM   1700  N   LEU   227      -7.711  -5.737  33.612  1.00  0.00           N
ATOM   1701  CA  LEU   227      -8.562  -4.919  34.431  1.00  0.00           C
ATOM   1702  CB  LEU   227      -8.175  -4.940  35.920  1.00  0.00           C
ATOM   1703  CG  LEU   227      -9.082  -4.063  36.800  1.00  0.00           C
ATOM   1704  CD2 LEU   227      -8.492  -3.883  38.209  1.00  0.00           C
ATOM   1705  CD1 LEU   227     -10.522  -4.606  36.819  1.00  0.00           C
ATOM   1706  C   LEU   227      -8.438  -3.504  33.970  1.00  0.00           C
ATOM   1707  O   LEU   227      -7.466  -3.128  33.311  1.00  0.00           O
ATOM   1708  N   VAL   228      -9.445  -2.666  34.307  1.00  0.00           N
ATOM   1709  CA  VAL   228      -9.398  -1.281  33.958  1.00  0.00           C
ATOM   1710  CB  VAL   228     -10.646  -0.769  33.299  1.00  0.00           C
ATOM   1711  CG1 VAL   228     -10.445   0.724  32.994  1.00  0.00           C
ATOM   1712  CG2 VAL   228     -10.936  -1.631  32.059  1.00  0.00           C
ATOM   1713  C   VAL   228      -9.238  -0.539  35.255  1.00  0.00           C
ATOM   1714  O   VAL   228      -9.686  -1.000  36.304  1.00  0.00           O
ATOM   1715  N   SER   229      -8.587   0.635  35.211  1.00  0.00           N
ATOM   1716  CA  SER   229      -8.255   1.382  36.394  1.00  0.00           C
ATOM   1717  CB  SER   229      -7.505   2.685  36.077  1.00  0.00           C
ATOM   1718  OG  SER   229      -6.256   2.393  35.468  1.00  0.00           O
ATOM   1719  C   SER   229      -9.477   1.749  37.159  1.00  0.00           C
ATOM   1720  O   SER   229      -9.458   1.789  38.388  1.00  0.00           O
ATOM   1721  N   LYS   230     -10.584   2.030  36.461  1.00  0.00           N
ATOM   1722  CA  LYS   230     -11.742   2.462  37.176  1.00  0.00           C
ATOM   1723  CB  LYS   230     -12.922   2.883  36.280  1.00  0.00           C
ATOM   1724  CG  LYS   230     -13.683   1.727  35.632  1.00  0.00           C
ATOM   1725  CD  LYS   230     -12.840   0.871  34.692  1.00  0.00           C
ATOM   1726  CE  LYS   230     -13.625  -0.266  34.036  1.00  0.00           C
ATOM   1727  NZ  LYS   230     -14.652   0.288  33.125  1.00  0.00           N
ATOM   1728  C   LYS   230     -12.219   1.363  38.070  1.00  0.00           C
ATOM   1729  O   LYS   230     -12.777   1.619  39.134  1.00  0.00           O
ATOM   1730  N   ASP   231     -12.011   0.100  37.659  1.00  0.00           N
ATOM   1731  CA  ASP   231     -12.585  -1.012  38.360  1.00  0.00           C
ATOM   1732  CB  ASP   231     -12.218  -2.359  37.713  1.00  0.00           C
ATOM   1733  CG  ASP   231     -12.931  -2.446  36.368  1.00  0.00           C
ATOM   1734  OD1 ASP   231     -14.032  -1.847  36.240  1.00  0.00           O
ATOM   1735  OD2 ASP   231     -12.382  -3.111  35.450  1.00  0.00           O
ATOM   1736  C   ASP   231     -12.199  -1.096  39.818  1.00  0.00           C
ATOM   1737  O   ASP   231     -13.087  -1.182  40.664  1.00  0.00           O
ATOM   1738  N   THR   232     -10.899  -1.070  40.194  1.00  0.00           N
ATOM   1739  CA  THR   232     -10.668  -1.282  41.604  1.00  0.00           C
ATOM   1740  CB  THR   232     -10.364  -2.711  41.948  1.00  0.00           C
ATOM   1741  OG1 THR   232     -10.360  -2.885  43.357  1.00  0.00           O
ATOM   1742  CG2 THR   232      -8.991  -3.078  41.361  1.00  0.00           C
ATOM   1743  C   THR   232      -9.524  -0.465  42.123  1.00  0.00           C
ATOM   1744  O   THR   232      -8.639  -0.040  41.383  1.00  0.00           O
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ATOM   1745  N   GLU   233      -9.562  -0.213  43.449  1.00  0.00           N
ATOM   1746  CA  GLU   233      -8.594   0.566  44.170  1.00  0.00           C
ATOM   1747  CB  GLU   233      -9.077   0.955  45.579  1.00  0.00           C
ATOM   1748  CG  GLU   233      -9.348  -0.241  46.494  1.00  0.00           C
ATOM   1749  CD  GLU   233     -10.707  -0.827  46.135  1.00  0.00           C
ATOM   1750  OE1 GLU   233     -11.420  -0.209  45.300  1.00  0.00           O
ATOM   1751  OE2 GLU   233     -11.052  -1.901  46.695  1.00  0.00           O
ATOM   1752  C   GLU   233      -7.262  -0.119  44.347  1.00  0.00           C
ATOM   1753  O   GLU   233      -6.225   0.504  44.125  1.00  0.00           O
ATOM   1754  N   LYS   234      -7.230  -1.410  44.749  1.00  0.00           N
ATOM   1755  CA  LYS   234      -5.943  -1.975  45.083  1.00  0.00           C
ATOM   1756  CB  LYS   234      -5.720  -2.132  46.597  1.00  0.00           C
ATOM   1757  CG  LYS   234      -5.639  -0.802  47.349  1.00  0.00           C
ATOM   1758  CD  LYS   234      -5.725  -0.954  48.869  1.00  0.00           C
ATOM   1759  CE  LYS   234      -5.637   0.374  49.624  1.00  0.00           C
ATOM   1760  NZ  LYS   234      -6.895   1.133  49.461  1.00  0.00           N
ATOM   1761  C   LYS   234      -5.765  -3.337  44.484  1.00  0.00           C
ATOM   1762  O   LYS   234      -6.589  -3.795  43.693  1.00  0.00           O
ATOM   1763  N   MET   235      -4.633  -4.002  44.843  1.00  0.00           N
ATOM   1764  CA  MET   235      -4.333  -5.310  44.339  1.00  0.00           C
ATOM   1765  CB  MET   235      -2.834  -5.532  44.075  1.00  0.00           C
ATOM   1766  CG  MET   235      -2.521  -6.901  43.466  1.00  0.00           C
ATOM   1767  SD  MET   235      -0.765  -7.168  43.080  1.00  0.00           S
ATOM   1768  CE  MET   235      -0.228  -7.191  44.814  1.00  0.00           C
ATOM   1769  C   MET   235      -4.774  -6.356  45.309  1.00  0.00           C
ATOM   1770  O   MET   235      -3.956  -7.010  45.955  1.00  0.00           O
ATOM   1771  N   MET   236      -6.101  -6.537  45.418  1.00  0.00           N
ATOM   1772  CA  MET   236      -6.680  -7.569  46.227  1.00  0.00           C
ATOM   1773  CB  MET   236      -8.203  -7.417  46.387  1.00  0.00           C
ATOM   1774  CG  MET   236      -8.616  -6.171  47.173  1.00  0.00           C
ATOM   1775  SD  MET   236     -10.411  -5.966  47.372  1.00  0.00           S
ATOM   1776  CE  MET   236     -10.293  -4.421  48.320  1.00  0.00           C
ATOM   1777  C   MET   236      -6.428  -8.879  45.551  1.00  0.00           C
ATOM   1778  O   MET   236      -6.226  -9.901  46.204  1.00  0.00           O
ATOM   1779  N   GLU   237      -6.429  -8.868  44.200  1.00  0.00           N
ATOM   1780  CA  GLU   237      -6.340 -10.078  43.433  1.00  0.00           C
ATOM   1781  CB  GLU   237      -6.276  -9.816  41.919  1.00  0.00           C
ATOM   1782  CG  GLU   237      -7.570  -9.233  41.347  1.00  0.00           C
ATOM   1783  CD  GLU   237      -7.370  -9.024  39.853  1.00  0.00           C
ATOM   1784  OE1 GLU   237      -6.260  -9.351  39.353  1.00  0.00           O
ATOM   1785  OE2 GLU   237      -8.325  -8.538  39.190  1.00  0.00           O
ATOM   1786  C   GLU   237      -5.103 -10.813  43.812  1.00  0.00           C
ATOM   1787  O   GLU   237      -5.151 -12.011  44.084  1.00  0.00           O
ATOM   1788  N   ALA   238      -3.952 -10.127  43.850  1.00  0.00           N
ATOM   1789  CA  ALA   238      -2.803 -10.828  44.326  1.00  0.00           C
ATOM   1790  CB  ALA   238      -1.500 -10.463  43.594  1.00  0.00           C
ATOM   1791  C   ALA   238      -2.694 -10.315  45.707  1.00  0.00           C
ATOM   1792  O   ALA   238      -2.531  -9.112  45.877  1.00  0.00           O
ATOM   1793  N   ALA   239      -2.789 -11.190  46.725  1.00  0.00           N
ATOM   1794  CA  ALA   239      -2.821 -10.657  48.052  1.00  0.00           C
ATOM   1795  CB  ALA   239      -3.107 -11.716  49.129  1.00  0.00           C
ATOM   1796  C   ALA   239      -1.498 -10.047  48.355  1.00  0.00           C
ATOM   1797  O   ALA   239      -0.547 -10.735  48.720  1.00  0.00           O
ATOM   1798  N   GLU   240      -1.439  -8.709  48.218  1.00  0.00           N
ATOM   1799  CA  GLU   240      -0.282  -7.926  48.508  1.00  0.00           C
ATOM   1800  CB  GLU   240      -0.084  -7.729  50.028  1.00  0.00           C
ATOM   1801  CG  GLU   240       1.016  -6.740  50.435  1.00  0.00           C
ATOM   1802  CD  GLU   240       2.196  -7.518  51.007  1.00  0.00           C
ATOM   1803  OE1 GLU   240       2.049  -8.755  51.195  1.00  0.00           O
ATOM   1804  OE2 GLU   240       3.256  -6.887  51.262  1.00  0.00           O
ATOM   1805  C   GLU   240       0.920  -8.572  47.894  1.00  0.00           C
ATOM   1806  O   GLU   240       1.972  -8.642  48.524  1.00  0.00           O
ATOM   1807  N   SER   241       0.827  -9.072  46.644  1.00  0.00           N
ATOM   1808  CA  SER   241       2.036  -9.655  46.142  1.00  0.00           C
ATOM   1809  CB  SER   241       2.093 -11.180  46.345  1.00  0.00           C
ATOM   1810  OG  SER   241       1.025 -11.811  45.656  1.00  0.00           O
ATOM   1811  C   SER   241       2.211  -9.391  44.679  1.00  0.00           C
ATOM   1812  O   SER   241       2.127 -10.313  43.869  1.00  0.00           O
ATOM   1813  N   LEU   242       2.514  -8.140  44.278  1.00  0.00           N
ATOM   1814  CA  LEU   242       2.825  -8.018  42.886  1.00  0.00           C
ATOM   1815  CB  LEU   242       2.173  -6.851  42.106  1.00  0.00           C
ATOM   1816  CG  LEU   242       2.957  -5.531  41.928  1.00  0.00           C
ATOM   1817  CD2 LEU   242       2.003  -4.466  41.390  1.00  0.00           C
ATOM   1818  CD1 LEU   242       4.178  -5.638  40.992  1.00  0.00           C
ATOM   1819  C   LEU   242       4.304  -7.878  42.860  1.00  0.00           C
ATOM   1820  O   LEU   242       4.856  -6.904  43.367  1.00  0.00           O
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ATOM   1821  N   ASP   243       4.981  -8.889  42.297  1.00  0.00           N
ATOM   1822  CA  ASP   243       6.410  -8.905  42.252  1.00  0.00           C
ATOM   1823  CB  ASP   243       6.958 -10.266  41.797  1.00  0.00           C
ATOM   1824  CG  ASP   243       6.652 -11.268  42.901  1.00  0.00           C
ATOM   1825  OD1 ASP   243       6.989 -10.974  44.079  1.00  0.00           O
ATOM   1826  OD2 ASP   243       6.060 -12.333  42.583  1.00  0.00           O
ATOM   1827  C   ASP   243       6.932  -7.866  41.311  1.00  0.00           C
ATOM   1828  O   ASP   243       7.898  -7.175  41.627  1.00  0.00           O
ATOM   1829  N   TYR   244       6.320  -7.733  40.118  1.00  0.00           N
ATOM   1830  CA  TYR   244       6.869  -6.805  39.175  1.00  0.00           C
ATOM   1831  CB  TYR   244       7.620  -7.488  38.020  1.00  0.00           C
ATOM   1832  CG  TYR   244       8.757  -8.271  38.579  1.00  0.00           C
ATOM   1833  CD1 TYR   244       9.932  -7.650  38.925  1.00  0.00           C
ATOM   1834  CD2 TYR   244       8.651  -9.632  38.747  1.00  0.00           C
ATOM   1835  CE1 TYR   244      10.982  -8.374  39.436  1.00  0.00           C
ATOM   1836  CE2 TYR   244       9.698 -10.363  39.258  1.00  0.00           C
ATOM   1837  CZ  TYR   244      10.867  -9.731  39.604  1.00  0.00           C
ATOM   1838  OH  TYR   244      11.948 -10.468  40.128  1.00  0.00           O
ATOM   1839  C   TYR   244       5.766  -6.040  38.531  1.00  0.00           C
ATOM   1840  O   TYR   244       4.680  -6.557  38.277  1.00  0.00           O
ATOM   1841  N   ILE   245       6.034  -4.759  38.250  1.00  0.00           N
ATOM   1842  CA  ILE   245       5.114  -3.976  37.499  1.00  0.00           C
ATOM   1843  CB  ILE   245       4.156  -3.154  38.319  1.00  0.00           C
ATOM   1844  CG2 ILE   245       2.943  -4.044  38.630  1.00  0.00           C
ATOM   1845  CG1 ILE   245       4.835  -2.569  39.561  1.00  0.00           C
ATOM   1846  CD1 ILE   245       6.053  -1.729  39.258  1.00  0.00           C
ATOM   1847  C   ILE   245       5.888  -3.237  36.469  1.00  0.00           C
ATOM   1848  O   ILE   245       7.073  -2.967  36.656  1.00  0.00           O
ATOM   1849  N   MET   246       5.231  -2.915  35.330  1.00  0.00           N
ATOM   1850  CA  MET   246       5.885  -2.220  34.256  1.00  0.00           C
ATOM   1851  CB  MET   246       6.145  -3.120  33.039  1.00  0.00           C
ATOM   1852  CG  MET   246       6.964  -4.365  33.379  1.00  0.00           C
ATOM   1853  SD  MET   246       8.647  -4.033  33.973  1.00  0.00           S
ATOM   1854  CE  MET   246       9.023  -5.780  34.286  1.00  0.00           C
ATOM   1855  C   MET   246       4.988  -1.115  33.781  1.00  0.00           C
ATOM   1856  O   MET   246       3.797  -1.326  33.555  1.00  0.00           O
ATOM   1857  N   ASP   247       5.520   0.114  33.608  1.00  0.00           N
ATOM   1858  CA  ASP   247       4.625   1.091  33.062  1.00  0.00           C
ATOM   1859  CB  ASP   247       4.514   2.464  33.750  1.00  0.00           C
ATOM   1860  CG  ASP   247       5.818   3.197  33.591  1.00  0.00           C
ATOM   1861  OD1 ASP   247       6.861   2.502  33.661  1.00  0.00           O
ATOM   1862  OD2 ASP   247       5.802   4.440  33.388  1.00  0.00           O
ATOM   1863  C   ASP   247       5.045   1.310  31.655  1.00  0.00           C
ATOM   1864  O   ASP   247       6.200   1.631  31.369  1.00  0.00           O
ATOM   1865  N   THR   248       4.109   1.069  30.724  1.00  0.00           N
ATOM   1866  CA  THR   248       4.427   1.260  29.347  1.00  0.00           C
ATOM   1867  CB  THR   248       4.440  -0.025  28.573  1.00  0.00           C
ATOM   1868  OG1 THR   248       3.159  -0.637  28.610  1.00  0.00           O
ATOM   1869  CG2 THR   248       5.491  -0.960  29.196  1.00  0.00           C
ATOM   1870  C   THR   248       3.380   2.146  28.732  1.00  0.00           C
ATOM   1871  O   THR   248       2.767   1.759  27.738  1.00  0.00           O
ATOM   1872  N   ILE   249       3.113   3.343  29.313  1.00  0.00           N
ATOM   1873  CA  ILE   249       2.158   4.205  28.661  1.00  0.00           C
ATOM   1874  CB  ILE   249       0.779   4.065  29.260  1.00  0.00           C
ATOM   1875  CG2 ILE   249      -0.241   4.764  28.338  1.00  0.00           C
ATOM   1876  CG1 ILE   249       0.408   2.586  29.426  1.00  0.00           C
ATOM   1877  CD1 ILE   249      -0.802   2.394  30.342  1.00  0.00           C
ATOM   1878  C   ILE   249       2.569   5.635  28.913  1.00  0.00           C
ATOM   1879  O   ILE   249       1.715   6.492  29.072  1.00  0.00           O
ATOM   1880  N   PRO   250       3.782   5.979  28.674  1.00  0.00           N
ATOM   1881  CA  PRO   250       4.395   7.183  29.227  1.00  0.00           C
ATOM   1882  CD  PRO   250       4.248   5.675  27.333  1.00  0.00           C
ATOM   1883  CB  PRO   250       5.242   7.731  28.094  1.00  0.00           C
ATOM   1884  CG  PRO   250       5.461   6.564  27.118  1.00  0.00           C
ATOM   1885  C   PRO   250       3.585   8.319  29.813  1.00  0.00           C
ATOM   1886  O   PRO   250       3.308   9.291  29.116  1.00  0.00           O
ATOM   1887  N   VAL   251       3.279   8.251  31.127  1.00  0.00           N
ATOM   1888  CA  VAL   251       2.611   9.340  31.787  1.00  0.00           C
ATOM   1889  CB  VAL   251       1.116   9.221  31.829  1.00  0.00           C
ATOM   1890  CG1 VAL   251       0.559  10.457  32.559  1.00  0.00           C
ATOM   1891  CG2 VAL   251       0.591   9.057  30.391  1.00  0.00           C
ATOM   1892  C   VAL   251       3.115   9.337  33.191  1.00  0.00           C
ATOM   1893  O   VAL   251       3.254   8.280  33.799  1.00  0.00           O
ATOM   1894  N   ALA   252       3.404  10.529  33.755  1.00  0.00           N
ATOM   1895  CA  ALA   252       3.993  10.598  35.062  1.00  0.00           C
ATOM   1896  CB  ALA   252       4.283  12.042  35.507  1.00  0.00           C
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ATOM   1897  C   ALA   252       3.069  10.000  36.064  1.00  0.00           C
ATOM   1898  O   ALA   252       3.487   9.212  36.913  1.00  0.00           O
ATOM   1899  N   HIS   253       1.772  10.338  35.988  1.00  0.00           N
ATOM   1900  CA  HIS   253       0.914   9.794  36.987  1.00  0.00           C
ATOM   1901  ND1 HIS   253      -2.151   9.891  35.161  1.00  0.00           N
ATOM   1902  CG  HIS   253      -1.174  10.685  35.721  1.00  0.00           C
ATOM   1903  NE2 HIS   253      -1.822  11.580  33.753  1.00  0.00           N
ATOM   1904  CD2 HIS   253      -0.986  11.712  34.847  1.00  0.00           C
ATOM   1905  CE1 HIS   253      -2.502  10.472  33.986  1.00  0.00           C
ATOM   1906  CB  HIS   253      -0.510  10.403  37.036  1.00  0.00           C
ATOM   1907  C   HIS   253       0.896   8.305  36.870  1.00  0.00           C
ATOM   1908  O   HIS   253       0.989   7.654  37.899  1.00  0.00           O
ATOM   1909  N   PRO   254       0.837   7.676  35.735  1.00  0.00           N
ATOM   1910  CA  PRO   254       0.814   6.243  35.742  1.00  0.00           C
ATOM   1911  CD  PRO   254       0.194   8.214  34.553  1.00  0.00           C
ATOM   1912  CB  PRO   254       0.486   5.815  34.314  1.00  0.00           C
ATOM   1913  CG  PRO   254      -0.332   6.999  33.771  1.00  0.00           C
ATOM   1914  C   PRO   254       2.081   5.680  36.265  1.00  0.00           C
ATOM   1915  O   PRO   254       2.041   4.554  36.736  1.00  0.00           O
ATOM   1916  N   LEU   255       3.218   6.396  36.197  1.00  0.00           N
ATOM   1917  CA  LEU   255       4.391   5.786  36.741  1.00  0.00           C
ATOM   1918  CB  LEU   255       5.702   6.592  36.605  1.00  0.00           C
ATOM   1919  CG  LEU   255       6.450   6.462  35.261  1.00  0.00           C
ATOM   1920  CD2 LEU   255       7.886   6.996  35.386  1.00  0.00           C
ATOM   1921  CD1 LEU   255       5.693   7.090  34.090  1.00  0.00           C
ATOM   1922  C   LEU   255       4.175   5.587  38.204  1.00  0.00           C
ATOM   1923  O   LEU   255       4.558   4.552  38.744  1.00  0.00           O
ATOM   1924  N   GLU   256       3.574   6.586  38.886  1.00  0.00           N
ATOM   1925  CA  GLU   256       3.423   6.524  40.315  1.00  0.00           C
ATOM   1926  CB  GLU   256       2.965   7.860  40.930  1.00  0.00           C
ATOM   1927  CG  GLU   256       2.802   7.808  42.450  1.00  0.00           C
ATOM   1928  CD  GLU   256       2.343   9.180  42.922  1.00  0.00           C
ATOM   1929  OE1 GLU   256       2.218  10.090  42.059  1.00  0.00           O
ATOM   1930  OE2 GLU   256       2.112   9.338  44.150  1.00  0.00           O
ATOM   1931  C   GLU   256       2.496   5.419  40.782  1.00  0.00           C
ATOM   1932  O   GLU   256       2.941   4.611  41.594  1.00  0.00           O
ATOM   1933  N   PRO   257       1.262   5.276  40.348  1.00  0.00           N
ATOM   1934  CA  PRO   257       0.520   4.161  40.872  1.00  0.00           C
ATOM   1935  CD  PRO   257       0.381   6.434  40.317  1.00  0.00           C
ATOM   1936  CB  PRO   257      -0.938   4.406  40.507  1.00  0.00           C
ATOM   1937  CG  PRO   257      -1.043   5.933  40.619  1.00  0.00           C
ATOM   1938  C   PRO   257       1.052   2.838  40.498  1.00  0.00           C
ATOM   1939  O   PRO   257       0.792   1.843  41.168  1.00  0.00           O
ATOM   1940  N   TYR   258       1.781   2.813  39.399  1.00  0.00           N
ATOM   1941  CA  TYR   258       2.415   1.660  38.911  1.00  0.00           C
ATOM   1942  CB  TYR   258       2.730   2.069  37.494  1.00  0.00           C
ATOM   1943  CG  TYR   258       3.909   1.423  37.095  1.00  0.00           C
ATOM   1944  CD1 TYR   258       3.876   0.079  37.169  1.00  0.00           C
ATOM   1945  CD2 TYR   258       4.945   2.195  36.642  1.00  0.00           C
ATOM   1946  CE1 TYR   258       5.009  -0.508  36.794  1.00  0.00           C
ATOM   1947  CE2 TYR   258       6.088   1.582  36.255  1.00  0.00           C
ATOM   1948  CZ  TYR   258       6.064   0.223  36.359  1.00  0.00           C
ATOM   1949  OH  TYR   258       7.171  -0.499  36.009  1.00  0.00           O
ATOM   1950  C   TYR   258       3.506   1.279  39.885  1.00  0.00           C
ATOM   1951  O   TYR   258       3.723   0.097  40.156  1.00  0.00           O
ATOM   1952  N   LEU   259       4.219   2.269  40.459  1.00  0.00           N
ATOM   1953  CA  LEU   259       5.189   2.016  41.495  1.00  0.00           C
ATOM   1954  CB  LEU   259       5.953   3.289  41.897  1.00  0.00           C
ATOM   1955  CG  LEU   259       7.004   3.069  43.000  1.00  0.00           C
ATOM   1956  CD2 LEU   259       7.524   4.414  43.536  1.00  0.00           C
ATOM   1957  CD1 LEU   259       8.127   2.135  42.535  1.00  0.00           C
ATOM   1958  C   LEU   259       4.490   1.513  42.713  1.00  0.00           C
ATOM   1959  O   LEU   259       4.905   0.527  43.320  1.00  0.00           O
ATOM   1960  N   ALA   260       3.383   2.184  43.072  1.00  0.00           N
ATOM   1961  CA  ALA   260       2.625   1.910  44.260  1.00  0.00           C
ATOM   1962  CB  ALA   260       1.445   2.878  44.447  1.00  0.00           C
ATOM   1963  C   ALA   260       2.063   0.527  44.208  1.00  0.00           C
ATOM   1964  O   ALA   260       1.952  -0.142  45.234  1.00  0.00           O
ATOM   1965  N   LEU   261       1.678   0.067  43.008  1.00  0.00           N
ATOM   1966  CA  LEU   261       1.047  -1.212  42.875  1.00  0.00           C
ATOM   1967  CB  LEU   261       0.602  -1.500  41.428  1.00  0.00           C
ATOM   1968  CG  LEU   261      -0.347  -2.707  41.294  1.00  0.00           C
ATOM   1969  CD2 LEU   261      -0.545  -3.099  39.821  1.00  0.00           C
ATOM   1970  CD1 LEU   261      -1.674  -2.458  42.028  1.00  0.00           C
ATOM   1971  C   LEU   261       2.019  -2.258  43.331  1.00  0.00           C
ATOM   1972  O   LEU   261       1.634  -3.305  43.843  1.00  0.00           O
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ATOM   1973  N   LEU   262       3.318  -2.010  43.102  1.00  0.00           N
ATOM   1974  CA  LEU   262       4.400  -2.848  43.534  1.00  0.00           C
ATOM   1975  CB  LEU   262       5.638  -2.462  42.709  1.00  0.00           C
ATOM   1976  CG  LEU   262       6.870  -3.308  42.971  1.00  0.00           C
ATOM   1977  CD2 LEU   262       6.498  -4.786  42.773  1.00  0.00           C
ATOM   1978  CD1 LEU   262       7.502  -2.951  44.325  1.00  0.00           C
ATOM   1979  C   LEU   262       4.581  -2.489  45.005  1.00  0.00           C
ATOM   1980  O   LEU   262       4.134  -1.422  45.409  1.00  0.00           O
ATOM   1981  N   LYS   263       5.191  -3.342  45.873  1.00  0.00           N
ATOM   1982  CA  LYS   263       5.288  -3.009  47.281  1.00  0.00           C
ATOM   1983  CB  LYS   263       4.531  -4.000  48.186  1.00  0.00           C
ATOM   1984  CG  LYS   263       4.243  -3.462  49.592  1.00  0.00           C
ATOM   1985  CD  LYS   263       3.220  -4.289  50.373  1.00  0.00           C
ATOM   1986  CE  LYS   263       2.935  -3.744  51.775  1.00  0.00           C
ATOM   1987  NZ  LYS   263       1.938  -4.597  52.459  1.00  0.00           N
ATOM   1988  C   LYS   263       6.729  -2.968  47.728  1.00  0.00           C
ATOM   1989  O   LYS   263       7.606  -2.469  47.025  1.00  0.00           O
ATOM   1990  N   THR   264       6.990  -3.449  48.965  1.00  0.00           N
ATOM   1991  CA  THR   264       8.289  -3.408  49.579  1.00  0.00           C
ATOM   1992  CB  THR   264       8.280  -3.953  50.976  1.00  0.00           C
ATOM   1993  OG1 THR   264       7.919  -5.326  50.965  1.00  0.00           O
ATOM   1994  CG2 THR   264       7.271  -3.147  51.812  1.00  0.00           C
ATOM   1995  C   THR   264       9.286  -4.212  48.800  1.00  0.00           C
ATOM   1996  O   THR   264      10.373  -3.720  48.505  1.00  0.00           O
ATOM   1997  N   ASN   265       8.968  -5.474  48.445  1.00  0.00           N
ATOM   1998  CA  ASN   265       9.961  -6.229  47.734  1.00  0.00           C
ATOM   1999  CB  ASN   265      10.229  -7.608  48.369  1.00  0.00           C
ATOM   2000  CG  ASN   265       8.926  -8.397  48.420  1.00  0.00           C
ATOM   2001  OD1 ASN   265       7.897  -7.894  48.868  1.00  0.00           O
ATOM   2002  ND2 ASN   265       8.968  -9.668  47.939  1.00  0.00           N
ATOM   2003  C   ASN   265       9.509  -6.427  46.328  1.00  0.00           C
ATOM   2004  O   ASN   265       9.346  -7.549  45.850  1.00  0.00           O
ATOM   2005  N   GLY   266       9.351  -5.327  45.585  1.00  0.00           N
ATOM   2006  CA  GLY   266       8.910  -5.530  44.249  1.00  0.00           C
ATOM   2007  C   GLY   266       9.701  -4.639  43.359  1.00  0.00           C
ATOM   2008  O   GLY   266      10.436  -3.769  43.823  1.00  0.00           O
ATOM   2009  N   LYS   267       9.547  -4.835  42.038  1.00  0.00           N
ATOM   2010  CA  LYS   267      10.287  -4.040  41.107  1.00  0.00           C
ATOM   2011  CB  LYS   267      11.245  -4.863  40.229  1.00  0.00           C
ATOM   2012  CG  LYS   267      12.076  -4.012  39.267  1.00  0.00           C
ATOM   2013  CD  LYS   267      13.101  -3.121  39.972  1.00  0.00           C
ATOM   2014  CE  LYS   267      14.259  -3.901  40.599  1.00  0.00           C
ATOM   2015  NZ  LYS   267      13.758  -4.749  41.704  1.00  0.00           N
ATOM   2016  C   LYS   267       9.323  -3.351  40.188  1.00  0.00           C
ATOM   2017  O   LYS   267       8.291  -3.901  39.805  1.00  0.00           O
ATOM   2018  N   LEU   268       9.671  -2.102  39.832  1.00  0.00           N
ATOM   2019  CA  LEU   268       8.923  -1.188  39.015  1.00  0.00           C
ATOM   2020  CB  LEU   268       8.748   0.098  39.856  1.00  0.00           C
ATOM   2021  CG  LEU   268       8.080   1.362  39.275  1.00  0.00           C
ATOM   2022  CD2 LEU   268       6.589   1.148  39.094  1.00  0.00           C
ATOM   2023  CD1 LEU   268       8.795   1.951  38.047  1.00  0.00           C
ATOM   2024  C   LEU   268       9.818  -0.793  37.879  1.00  0.00           C
ATOM   2025  O   LEU   268      10.735  -0.007  38.096  1.00  0.00           O
ATOM   2026  N   VAL   269       9.571  -1.271  36.641  1.00  0.00           N
ATOM   2027  CA  VAL   269      10.391  -0.844  35.531  1.00  0.00           C
ATOM   2028  CB  VAL   269      10.830  -1.978  34.650  1.00  0.00           C
ATOM   2029  CG1 VAL   269      11.669  -1.406  33.496  1.00  0.00           C
ATOM   2030  CG2 VAL   269      11.579  -3.006  35.515  1.00  0.00           C
ATOM   2031  C   VAL   269       9.669   0.155  34.650  1.00  0.00           C
ATOM   2032  O   VAL   269       8.647  -0.135  34.027  1.00  0.00           O
ATOM   2033  N   MET   270      10.227   1.377  34.524  1.00  0.00           N
ATOM   2034  CA  MET   270       9.578   2.387  33.730  1.00  0.00           C
ATOM   2035  CB  MET   270       9.875   3.821  34.209  1.00  0.00           C
ATOM   2036  CG  MET   270      11.355   4.208  34.136  1.00  0.00           C
ATOM   2037  SD  MET   270      11.725   5.898  34.695  1.00  0.00           S
ATOM   2038  CE  MET   270      11.086   6.709  33.202  1.00  0.00           C
ATOM   2039  C   MET   270       9.992   2.278  32.291  1.00  0.00           C
ATOM   2040  O   MET   270      11.122   2.600  31.925  1.00  0.00           O
ATOM   2041  N   LEU   271       9.091   1.717  31.451  1.00  0.00           N
ATOM   2042  CA  LEU   271       9.300   1.602  30.031  1.00  0.00           C
ATOM   2043  CB  LEU   271       8.500   0.450  29.400  1.00  0.00           C
ATOM   2044  CG  LEU   271       8.918  -0.939  29.915  1.00  0.00           C
ATOM   2045  CD2 LEU   271       8.301  -2.061  29.065  1.00  0.00           C
ATOM   2046  CD1 LEU   271       8.620  -1.093  31.416  1.00  0.00           C
ATOM   2047  C   LEU   271       8.928   2.854  29.288  1.00  0.00           C
ATOM   2048  O   LEU   271       9.631   3.273  28.370  1.00  0.00           O
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ATOM   2049  N   GLY  272       7.786   3.474  29.664  1.00  0.00           N
ATOM   2050  CA  GLY  272       7.255   4.590  28.928  1.00  0.00           C
ATOM   2051  C   GLY  272       8.182   5.761  29.052  1.00  0.00           C
ATOM   2052  O   GLY  272       8.873   5.915  30.055  1.00  0.00           O
ATOM   2053  N   VAL  273       8.198   6.632  28.018  1.00  0.00           N
ATOM   2054  CA  VAL  273       9.058   7.781  27.999  1.00  0.00           C
ATOM   2055  CB  VAL  273       9.598   8.088  26.630  1.00  0.00           C
ATOM   2056  CG1 VAL  273      10.422   9.385  26.700  1.00  0.00           C
ATOM   2057  CG2 VAL  273      10.390   6.869  26.128  1.00  0.00           C
ATOM   2058  C   VAL  273       8.283   8.982  28.438  1.00  0.00           C
ATOM   2059  O   VAL  273       7.398   9.464  27.736  1.00  0.00           O
ATOM   2060  N   VAL  274       8.654   9.533  29.606  1.00  0.00           N
ATOM   2061  CA  VAL  274       7.989  10.654  30.202  1.00  0.00           C
ATOM   2062  CB  VAL  274       8.644  11.092  31.484  1.00  0.00           C
ATOM   2063  CG1 VAL  274       7.931  12.341  32.028  1.00  0.00           C
ATOM   2064  CG2 VAL  274       8.642   9.900  32.456  1.00  0.00           C
ATOM   2065  C   VAL  274       8.005  11.806  29.248  1.00  0.00           C
ATOM   2066  O   VAL  274       8.873  11.950  28.387  1.00  0.00           O
ATOM   2067  N   PRO  275       7.014  12.635  29.413  1.00  0.00           N
ATOM   2068  CA  PRO  275       6.857  13.778  28.562  1.00  0.00           C
ATOM   2069  CD  PRO  275       5.740  12.171  29.942  1.00  0.00           C
ATOM   2070  CB  PRO  275       5.473  14.341  28.883  1.00  0.00           C
ATOM   2071  CG  PRO  275       4.679  13.105  29.341  1.00  0.00           C
ATOM   2072  C   PRO  275       7.973  14.743  28.758  1.00  0.00           C
ATOM   2073  O   PRO  275       8.726  14.597  29.721  1.00  0.00           O
ATOM   2074  N   GLU  276       8.077  15.730  27.842  1.00  0.00           N
ATOM   2075  CA  GLU  276       9.102  16.738  27.832  1.00  0.00           C
ATOM   2076  CB  GLU  276       8.768  17.922  26.906  1.00  0.00           C
ATOM   2077  CG  GLU  276       8.800  17.561  25.421  1.00  0.00           C
ATOM   2078  CD  GLU  276       8.455  18.814  24.629  1.00  0.00           C
ATOM   2079  OE1 GLU  276       8.215  19.871  25.272  1.00  0.00           O
ATOM   2080  OE2 GLU  276       8.427  18.733  23.372  1.00  0.00           O
ATOM   2081  C   GLU  276       9.217  17.236  29.225  1.00  0.00           C
ATOM   2082  O   GLU  276       8.236  17.189  29.960  1.00  0.00           O
ATOM   2083  N   PRO  277      10.380  17.728  29.578  1.00  0.00           N
ATOM   2084  CA  PRO  277      10.738  17.962  30.953  1.00  0.00           C
ATOM   2085  CD  PRO  277      11.113  18.610  28.682  1.00  0.00           C
ATOM   2086  CB  PRO  277      11.947  18.896  30.930  1.00  0.00           C
ATOM   2087  CG  PRO  277      11.802  19.637  29.592  1.00  0.00           C
ATOM   2088  C   PRO  277       9.679  18.430  31.895  1.00  0.00           C
ATOM   2089  O   PRO  277       9.326  19.608  31.916  1.00  0.00           O
ATOM   2090  N   LEU  278       9.201  17.463  32.698  1.00  0.00           N
ATOM   2091  CA  LEU  278       8.293  17.612  33.791  1.00  0.00           C
ATOM   2092  CB  LEU  278       6.860  17.093  33.554  1.00  0.00           C
ATOM   2093  CG  LEU  278       5.913  18.099  32.866  1.00  0.00           C
ATOM   2094  CD2 LEU  278       4.474  17.560  32.833  1.00  0.00           C
ATOM   2095  CD1 LEU  278       6.409  18.536  31.483  1.00  0.00           C
ATOM   2096  C   LEU  278       8.909  16.793  34.868  1.00  0.00           C
ATOM   2097  O   LEU  278       9.594  15.811  34.586  1.00  0.00           O
ATOM   2098  N   HIS  279       8.712  17.183  36.137  1.00  0.00           N
ATOM   2099  CA  HIS  279       9.368  16.435  37.166  1.00  0.00           C
ATOM   2100  ND1 HIS  279       8.505  17.790  40.120  1.00  0.00           N
ATOM   2101  CG  HIS  279       9.170  18.193  38.983  1.00  0.00           C
ATOM   2102  NE2 HIS  279       7.916  19.903  39.755  1.00  0.00           N
ATOM   2103  CD2 HIS  279       8.799  19.486  38.775  1.00  0.00           C
ATOM   2104  CE1 HIS  279       7.770  18.851  40.540  1.00  0.00           C
ATOM   2105  CB  HIS  279      10.097  17.314  38.197  1.00  0.00           C
ATOM   2106  C   HIS  279       8.354  15.638  37.911  1.00  0.00           C
ATOM   2107  O   HIS  279       7.244  16.095  38.173  1.00  0.00           O
ATOM   2108  N   PHE  280       8.727  14.392  38.248  1.00  0.00           N
ATOM   2109  CA  PHE  280       7.881  13.548  39.031  1.00  0.00           C
ATOM   2110  CB  PHE  280       7.268  12.381  38.242  1.00  0.00           C
ATOM   2111  CG  PHE  280       6.421  11.599  39.186  1.00  0.00           C
ATOM   2112  CD1 PHE  280       5.128  11.988  39.451  1.00  0.00           C
ATOM   2113  CD2 PHE  280       6.920  10.477  39.806  1.00  0.00           C
ATOM   2114  CE1 PHE  280       4.346  11.269  40.323  1.00  0.00           C
ATOM   2115  CE2 PHE  280       6.142   9.754  40.679  1.00  0.00           C
ATOM   2116  CZ  PHE  280       4.850  10.151  40.939  1.00  0.00           C
ATOM   2117  C   PHE  280       8.761  12.954  40.079  1.00  0.00           C
ATOM   2118  O   PHE  280       9.927  12.662  39.822  1.00  0.00           O
ATOM   2119  N   VAL  281       8.238  12.786  41.307  1.00  0.00           N
ATOM   2120  CA  VAL  281       9.077  12.187  42.297  1.00  0.00           C
ATOM   2121  CB  VAL  281       9.961  13.167  43.008  1.00  0.00           C
ATOM   2122  CG1 VAL  281       9.074  14.160  43.777  1.00  0.00           C
ATOM   2123  CG2 VAL  281      10.938  12.385  43.905  1.00  0.00           C
ATOM   2124  C   VAL  281       8.208  11.551  43.334  1.00  0.00           C
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ATOM   2125  O   VAL   281       7.107  12.024  43.611  1.00  0.00           O
ATOM   2126  N   THR   282       8.682  10.424  43.898  1.00  0.00           N
ATOM   2127  CA  THR   282       8.010   9.788  44.995  1.00  0.00           C
ATOM   2128  CB  THR   282       6.929   8.830  44.552  1.00  0.00           C
ATOM   2129  OG1 THR   282       6.305   8.242  45.682  1.00  0.00           O
ATOM   2130  CG2 THR   282       7.494   7.769  43.592  1.00  0.00           C
ATOM   2131  C   THR   282       9.055   9.071  45.808  1.00  0.00           C
ATOM   2132  O   THR   282       9.327   7.889  45.612  1.00  0.00           O
ATOM   2133  N   PRO   283       9.696   9.770  46.707  1.00  0.00           N
ATOM   2134  CA  PRO   283      10.714   9.149  47.514  1.00  0.00           C
ATOM   2135  CD  PRO   283       9.944  11.186  46.516  1.00  0.00           C
ATOM   2136  CB  PRO   283      11.589  10.289  48.046  1.00  0.00           C
ATOM   2137  CG  PRO   283      10.802  11.575  47.730  1.00  0.00           C
ATOM   2138  C   PRO   283      10.249   8.206  48.583  1.00  0.00           C
ATOM   2139  O   PRO   283      10.967   7.254  48.880  1.00  0.00           O
ATOM   2140  N   LEU   284       9.075   8.456  49.190  1.00  0.00           N
ATOM   2141  CA  LEU   284       8.622   7.665  50.300  1.00  0.00           C
ATOM   2142  CB  LEU   284       7.351   8.237  50.951  1.00  0.00           C
ATOM   2143  CG  LEU   284       6.845   7.404  52.144  1.00  0.00           C
ATOM   2144  CD2 LEU   284       5.445   7.862  52.588  1.00  0.00           C
ATOM   2145  CD1 LEU   284       7.863   7.401  53.296  1.00  0.00           C
ATOM   2146  C   LEU   284       8.307   6.270  49.874  1.00  0.00           C
ATOM   2147  O   LEU   284       8.644   5.306  50.559  1.00  0.00           O
ATOM   2148  N   LEU   285       7.643   6.126  48.715  1.00  0.00           N
ATOM   2149  CA  LEU   285       7.165   4.847  48.288  1.00  0.00           C
ATOM   2150  CB  LEU   285       6.381   4.922  46.966  1.00  0.00           C
ATOM   2151  CG  LEU   285       5.078   5.737  47.075  1.00  0.00           C
ATOM   2152  CD2 LEU   285       4.199   5.225  48.228  1.00  0.00           C
ATOM   2153  CD1 LEU   285       4.331   5.778  45.733  1.00  0.00           C
ATOM   2154  C   LEU   285       8.291   3.893  48.074  1.00  0.00           C
ATOM   2155  O   LEU   285       8.198   2.737  48.481  1.00  0.00           O
ATOM   2156  N   ILE   286       9.396   4.333  47.446  1.00  0.00           N
ATOM   2157  CA  ILE   286      10.376   3.343  47.118  1.00  0.00           C
ATOM   2158  CB  ILE   286      11.052   3.643  45.804  1.00  0.00           C
ATOM   2159  CG2 ILE   286      10.028   3.370  44.692  1.00  0.00           C
ATOM   2160  CG1 ILE   286      11.637   5.074  45.759  1.00  0.00           C
ATOM   2161  CD1 ILE   286      12.846   5.351  46.652  1.00  0.00           C
ATOM   2162  C   ILE   286      11.402   3.154  48.177  1.00  0.00           C
ATOM   2163  O   ILE   286      12.574   2.930  47.879  1.00  0.00           O
ATOM   2164  N   LEU   287      11.001   3.166  49.456  1.00  0.00           N
ATOM   2165  CA  LEU   287      12.031   2.851  50.389  1.00  0.00           C
ATOM   2166  CB  LEU   287      11.578   2.995  51.851  1.00  0.00           C
ATOM   2167  CG  LEU   287      12.681   2.663  52.873  1.00  0.00           C
ATOM   2168  CD2 LEU   287      12.112   2.576  54.300  1.00  0.00           C
ATOM   2169  CD1 LEU   287      13.860   3.637  52.761  1.00  0.00           C
ATOM   2170  C   LEU   287      12.371   1.412  50.157  1.00  0.00           C
ATOM   2171  O   LEU   287      13.523   1.059  49.913  1.00  0.00           O
ATOM   2172  N   GLY   288      11.336   0.551  50.227  1.00  0.00           N
ATOM   2173  CA  GLY   288      11.462  -0.871  50.060  1.00  0.00           C
ATOM   2174  C   GLY   288      11.678  -1.311  48.642  1.00  0.00           C
ATOM   2175  O   GLY   288      12.533  -2.153  48.375  1.00  0.00           O
ATOM   2176  N   ARG   289      10.892  -0.774  47.684  1.00  0.00           N
ATOM   2177  CA  ARG   289      10.950  -1.326  46.357  1.00  0.00           C
ATOM   2178  CB  ARG   289       9.640  -1.239  45.550  1.00  0.00           C
ATOM   2179  CG  ARG   289       9.184   0.184  45.241  1.00  0.00           C
ATOM   2180  CD  ARG   289       8.762   0.959  46.483  1.00  0.00           C
ATOM   2181  NE  ARG   289       7.543   0.311  47.045  1.00  0.00           N
ATOM   2182  CZ  ARG   289       6.305   0.773  46.702  1.00  0.00           C
ATOM   2183  NH1 ARG   289       6.183   1.817  45.831  1.00  0.00           N
ATOM   2184  NH2 ARG   289       5.191   0.198  47.239  1.00  0.00           N
ATOM   2185  C   ARG   289      12.015  -0.678  45.548  1.00  0.00           C
ATOM   2186  O   ARG   289      12.549   0.372  45.903  1.00  0.00           O
ATOM   2187  N   ARG   290      12.361  -1.339  44.424  1.00  0.00           N
ATOM   2188  CA  ARG   290      13.369  -0.828  43.550  1.00  0.00           C
ATOM   2189  CB  ARG   290      14.392  -1.890  43.109  1.00  0.00           C
ATOM   2190  CG  ARG   290      15.480  -1.346  42.181  1.00  0.00           C
ATOM   2191  CD  ARG   290      16.511  -2.399  41.769  1.00  0.00           C
ATOM   2192  NE  ARG   290      17.238  -2.815  43.002  1.00  0.00           N
ATOM   2193  CZ  ARG   290      18.214  -3.767  42.936  1.00  0.00           C
ATOM   2194  NH1 ARG   290      18.533  -4.337  41.738  1.00  0.00           N
ATOM   2195  NH2 ARG   290      18.870  -4.149  44.072  1.00  0.00           N
ATOM   2196  C   ARG   290      12.685  -0.317  42.325  1.00  0.00           C
ATOM   2197  O   ARG   290      11.795  -0.965  41.775  1.00  0.00           O
ATOM   2198  N   SER   291      13.088   0.889  41.881  1.00  0.00           N
ATOM   2199  CA  SER   291      12.524   1.465  40.703  1.00  0.00           C
ATOM   2200  CB  SER   291      11.982   2.889  40.905  1.00  0.00           C
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ATOM   2201  OG  SER   291      11.441   3.382  39.687  1.00  0.00           O
ATOM   2202  C   SER   291      13.640   1.555  39.719  1.00  0.00           C
ATOM   2203  O   SER   291      14.746   1.982  40.051  1.00  0.00           O
ATOM   2204  N   ILE   292      13.376   1.122  38.474  1.00  0.00           N
ATOM   2205  CA  ILE   292      14.407   1.115  37.483  1.00  0.00           C
ATOM   2206  CB  ILE   292      15.013  -0.250  37.359  1.00  0.00           C
ATOM   2207  CG2 ILE   292      15.752  -0.563  38.673  1.00  0.00           C
ATOM   2208  CG1 ILE   292      13.927  -1.277  36.998  1.00  0.00           C
ATOM   2209  CD1 ILE   292      14.449  -2.706  36.853  1.00  0.00           C
ATOM   2210  C   ILE   292      13.818   1.546  36.176  1.00  0.00           C
ATOM   2211  O   ILE   292      12.624   1.380  35.933  1.00  0.00           O
ATOM   2212  N   ALA   293      14.656   2.131  35.300  1.00  0.00           N
ATOM   2213  CA  ALA   293      14.198   2.615  34.028  1.00  0.00           C
ATOM   2214  CB  ALA   293      14.620   4.064  33.731  1.00  0.00           C
ATOM   2215  C   ALA   293      14.802   1.756  32.972  1.00  0.00           C
ATOM   2216  O   ALA   293      15.778   1.050  33.217  1.00  0.00           O
ATOM   2217  N   GLY   294      14.218   1.761  31.758  1.00  0.00           N
ATOM   2218  CA  GLY   294      14.787   0.889  30.774  1.00  0.00           C
ATOM   2219  C   GLY   294      14.753   1.530  29.432  1.00  0.00           C
ATOM   2220  O   GLY   294      13.749   2.093  29.004  1.00  0.00           O
ATOM   2221  N   SER   295      15.883   1.430  28.713  1.00  0.00           N
ATOM   2222  CA  SER   295      15.914   1.931  27.384  1.00  0.00           C
ATOM   2223  CB  SER   295      17.035   2.959  27.163  1.00  0.00           C
ATOM   2224  OG  SER   295      18.258   2.453  27.673  1.00  0.00           O
ATOM   2225  C   SER   295      16.119   0.755  26.495  1.00  0.00           C
ATOM   2226  O   SER   295      17.043  -0.037  26.684  1.00  0.00           O
ATOM   2227  N   PHE   296      15.217   0.633  25.504  1.00  0.00           N
ATOM   2228  CA  PHE   296      15.285  -0.372  24.500  1.00  0.00           C
ATOM   2229  CB  PHE   296      16.350  -0.008  23.444  1.00  0.00           C
ATOM   2230  CG  PHE   296      16.270  -0.902  22.256  1.00  0.00           C
ATOM   2231  CD1 PHE   296      15.338  -0.671  21.270  1.00  0.00           C
ATOM   2232  CD2 PHE   296      17.146  -1.952  22.115  1.00  0.00           C
ATOM   2233  CE1 PHE   296      15.274  -1.484  20.164  1.00  0.00           C
ATOM   2234  CE2 PHE   296      17.085  -2.769  21.012  1.00  0.00           C
ATOM   2235  CZ  PHE   296      16.144  -2.541  20.038  1.00  0.00           C
ATOM   2236  C   PHE   296      15.598  -1.709  25.081  1.00  0.00           C
ATOM   2237  O   PHE   296      16.689  -2.212  24.833  1.00  0.00           O
ATOM   2238  N   ILE   297      14.698  -2.381  25.849  1.00  0.00           N
ATOM   2239  CA  ILE   297      15.138  -3.721  26.181  1.00  0.00           C
ATOM   2240  CB  ILE   297      15.443  -4.646  24.915  1.00  0.00           C
ATOM   2241  CG2 ILE   297      15.196  -4.060  23.507  1.00  0.00           C
ATOM   2242  CG1 ILE   297      16.785  -5.397  24.932  1.00  0.00           C
ATOM   2243  CD1 ILE   297      16.881  -6.504  23.883  1.00  0.00           C
ATOM   2244  C   ILE   297      16.245  -3.517  27.173  1.00  0.00           C
ATOM   2245  O   ILE   297      16.197  -2.513  27.843  1.00  0.00           O
ATOM   2246  N   GLY   298      17.117  -4.462  27.528  1.00  0.00           N
ATOM   2247  CA  GLY   298      18.298  -4.090  28.259  1.00  0.00           C
ATOM   2248  C   GLY   298      19.116  -3.450  27.228  1.00  0.00           C
ATOM   2249  O   GLY   298      19.900  -2.549  27.495  1.00  0.00           O
ATOM   2250  N   SER   299      18.981  -4.011  26.017  1.00  0.00           N
ATOM   2251  CA  SER   299      19.510  -3.439  24.828  1.00  0.00           C
ATOM   2252  CB  SER   299      19.658  -1.914  24.828  1.00  0.00           C
ATOM   2253  OG  SER   299      19.851  -1.488  23.486  1.00  0.00           O
ATOM   2254  C   SER   299      20.783  -4.029  24.339  1.00  0.00           C
ATOM   2255  O   SER   299      20.885  -5.221  24.180  1.00  0.00           O
ATOM   2256  N   MET   300      21.800  -3.220  24.025  1.00  0.00           N
ATOM   2257  CA  MET   300      22.973  -3.730  23.359  1.00  0.00           C
ATOM   2258  CB  MET   300      23.673  -4.895  24.081  1.00  0.00           C
ATOM   2259  CG  MET   300      24.426  -4.456  25.339  1.00  0.00           C
ATOM   2260  SD  MET   300      25.274  -5.795  26.228  1.00  0.00           S
ATOM   2261  CE  MET   300      26.157  -4.674  27.351  1.00  0.00           C
ATOM   2262  C   MET   300      22.472  -4.190  22.030  1.00  0.00           C
ATOM   2263  O   MET   300      22.412  -5.379  21.719  1.00  0.00           O
ATOM   2264  N   GLU   301      22.122  -3.197  21.195  1.00  0.00           N
ATOM   2265  CA  GLU   301      21.430  -3.428  19.964  1.00  0.00           C
ATOM   2266  CB  GLU   301      20.872  -2.148  19.322  1.00  0.00           C
ATOM   2267  CG  GLU   301      19.820  -2.458  18.253  1.00  0.00           C
ATOM   2268  CD  GLU   301      18.974  -1.215  18.023  1.00  0.00           C
ATOM   2269  OE1 GLU   301      19.347  -0.139  18.561  1.00  0.00           O
ATOM   2270  OE2 GLU   301      17.944  -1.322  17.306  1.00  0.00           O
ATOM   2271  C   GLU   301      22.189  -4.192  18.930  1.00  0.00           C
ATOM   2272  O   GLU   301      21.615  -5.073  18.293  1.00  0.00           O
ATOM   2273  N   GLU   302      23.482  -3.899  18.712  1.00  0.00           N
ATOM   2274  CA  GLU   302      24.143  -4.590  17.641  1.00  0.00           C
ATOM   2275  CB  GLU   302      25.605  -4.147  17.458  1.00  0.00           C
ATOM   2276  CG  GLU   302      25.747  -2.717  16.935  1.00  0.00           C
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ATOM   2277  CD  GLU   302      27.230  -2.411  16.801  1.00  0.00           C
ATOM   2278  OE1 GLU   302      28.049  -3.278  17.207  1.00  0.00           O
ATOM   2279  OE2 GLU   302      27.564  -1.310  16.286  1.00  0.00           O
ATOM   2280  C   GLU   302      24.146  -6.060  17.920  1.00  0.00           C
ATOM   2281  O   GLU   302      23.854  -6.861  17.035  1.00  0.00           O
ATOM   2282  N   THR   303      24.490  -6.455  19.158  1.00  0.00           N
ATOM   2283  CA  THR   303      24.575  -7.849  19.494  1.00  0.00           C
ATOM   2284  CB  THR   303      25.247  -8.075  20.817  1.00  0.00           C
ATOM   2285  OG1 THR   303      26.554  -7.522  20.802  1.00  0.00           O
ATOM   2286  CG2 THR   303      25.318  -9.588  21.081  1.00  0.00           C
ATOM   2287  C   THR   303      23.231  -8.524  19.570  1.00  0.00           C
ATOM   2288  O   THR   303      23.041  -9.607  19.020  1.00  0.00           O
ATOM   2289  N   GLN   304      22.266  -7.898  20.271  1.00  0.00           N
ATOM   2290  CA  GLN   304      20.987  -8.480  20.594  1.00  0.00           C
ATOM   2291  CB  GLN   304      20.223  -7.668  21.653  1.00  0.00           C
ATOM   2292  CG  GLN   304      20.893  -7.708  23.026  1.00  0.00           C
ATOM   2293  CD  GLN   304      20.775  -9.128  23.562  1.00  0.00           C
ATOM   2294  OE1 GLN   304      20.181  -9.997  22.926  1.00  0.00           O
ATOM   2295  NE2 GLN   304      21.356  -9.371  24.767  1.00  0.00           N
ATOM   2296  C   GLN   304      20.061  -8.678  19.428  1.00  0.00           C
ATOM   2297  O   GLN   304      19.300  -9.643  19.395  1.00  0.00           O
ATOM   2298  N   GLU   305      20.098  -7.779  18.438  1.00  0.00           N
ATOM   2299  CA  GLU   305      19.141  -7.721  17.367  1.00  0.00           C
ATOM   2300  CB  GLU   305      19.409  -6.556  16.398  1.00  0.00           C
ATOM   2301  CG  GLU   305      18.337  -6.415  15.317  1.00  0.00           C
ATOM   2302  CD  GLU   305      18.708  -5.236  14.429  1.00  0.00           C
ATOM   2303  OE1 GLU   305      18.983  -4.141  14.987  1.00  0.00           O
ATOM   2304  OE2 GLU   305      18.713  -5.412  13.181  1.00  0.00           O
ATOM   2305  C   GLU   305      19.032  -8.980  16.529  1.00  0.00           C
ATOM   2306  O   GLU   305      18.002  -9.169  15.893  1.00  0.00           O
ATOM   2307  N   THR   306      20.049  -9.865  16.477  1.00  0.00           N
ATOM   2308  CA  THR   306      20.137 -10.972  15.536  1.00  0.00           C
ATOM   2309  CB  THR   306      21.481 -11.654  15.639  1.00  0.00           C
ATOM   2310  OG1 THR   306      22.497 -10.662  15.633  1.00  0.00           O
ATOM   2311  CG2 THR   306      21.721 -12.540  14.398  1.00  0.00           C
ATOM   2312  C   THR   306      18.984 -12.022  15.584  1.00  0.00           C
ATOM   2313  O   THR   306      17.812 -11.669  15.577  1.00  0.00           O
ATOM   2314  N   LEU   307      19.317 -13.348  15.576  1.00  0.00           N
ATOM   2315  CA  LEU   307      18.639 -14.621  15.308  1.00  0.00           C
ATOM   2316  CB  LEU   307      19.651 -15.778  15.212  1.00  0.00           C
ATOM   2317  CG  LEU   307      20.496 -15.984  16.486  1.00  0.00           C
ATOM   2318  CD2 LEU   307      21.671 -16.940  16.222  1.00  0.00           C
ATOM   2319  CD1 LEU   307      19.634 -16.423  17.680  1.00  0.00           C
ATOM   2320  C   LEU   307      17.472 -15.168  16.117  1.00  0.00           C
ATOM   2321  O   LEU   307      16.731 -15.977  15.563  1.00  0.00           O
ATOM   2322  N   ASP   308      17.250 -14.832  17.399  1.00  0.00           N
ATOM   2323  CA  ASP   308      16.306 -15.562  18.231  1.00  0.00           C
ATOM   2324  CB  ASP   308      16.112 -14.864  19.592  1.00  0.00           C
ATOM   2325  CG  ASP   308      15.312 -15.757  20.529  1.00  0.00           C
ATOM   2326  OD1 ASP   308      14.131 -16.056  20.209  1.00  0.00           O
ATOM   2327  OD2 ASP   308      15.876 -16.154  21.582  1.00  0.00           O
ATOM   2328  C   ASP   308      14.940 -15.762  17.607  1.00  0.00           C
ATOM   2329  O   ASP   308      14.330 -16.816  17.791  1.00  0.00           O
ATOM   2330  N   PHE   309      14.410 -14.781  16.860  1.00  0.00           N
ATOM   2331  CA  PHE   309      13.095 -14.891  16.278  1.00  0.00           C
ATOM   2332  CB  PHE   309      12.733 -13.620  15.483  1.00  0.00           C
ATOM   2333  CG  PHE   309      11.419 -13.786  14.794  1.00  0.00           C
ATOM   2334  CD1 PHE   309      11.346 -14.385  13.557  1.00  0.00           C
ATOM   2335  CD2 PHE   309      10.258 -13.326  15.371  1.00  0.00           C
ATOM   2336  CE1 PHE   309      10.139 -14.535  12.914  1.00  0.00           C
ATOM   2337  CE2 PHE   309       9.049 -13.473  14.733  1.00  0.00           C
ATOM   2338  CZ  PHE   309       8.985 -14.079  13.502  1.00  0.00           C
ATOM   2339  C   PHE   309      13.015 -16.051  15.328  1.00  0.00           C
ATOM   2340  O   PHE   309      12.063 -16.829  15.379  1.00  0.00           O
ATOM   2341  N   CYS   310      14.014 -16.202  14.438  1.00  0.00           N
ATOM   2342  CA  CYS   310      13.970 -17.223  13.427  1.00  0.00           C
ATOM   2343  CB  CYS   310      15.126 -17.145  12.410  1.00  0.00           C
ATOM   2344  SG  CYS   310      16.762 -17.478  13.124  1.00  0.00           S
ATOM   2345  C   CYS   310      13.986 -18.568  14.065  1.00  0.00           C
ATOM   2346  O   CYS   310      13.415 -19.519  13.532  1.00  0.00           O
ATOM   2347  N   ALA   311      14.640 -18.683  15.232  1.00  0.00           N
ATOM   2348  CA  ALA   311      14.712 -19.950  15.891  1.00  0.00           C
ATOM   2349  CB  ALA   311      15.424 -19.876  17.252  1.00  0.00           C
ATOM   2350  C   ALA   311      13.306 -20.370  16.132  1.00  0.00           C
ATOM   2351  O   ALA   311      12.984 -21.550  16.028  1.00  0.00           O
ATOM   2352  N   GLU   312      12.453 -19.388  16.468  1.00  0.00           N
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ATOM   2353  CA  GLU   312      11.056 -19.531  16.753  1.00  0.00           C
ATOM   2354  CB  GLU   312      10.533 -20.949  17.064  1.00  0.00           C
ATOM   2355  CG  GLU   312      10.267 -21.793  15.813  1.00  0.00           C
ATOM   2356  CD  GLU   312       9.105 -21.157  15.062  1.00  0.00           C
ATOM   2357  OE1 GLU   312       8.243 -20.525  15.730  1.00  0.00           O
ATOM   2358  OE2 GLU   312       9.064 -21.293  13.810  1.00  0.00           O
ATOM   2359  C   GLU   312      10.904 -18.725  17.974  1.00  0.00           C
ATOM   2360  O   GLU   312      11.024 -17.502  17.950  1.00  0.00           O
ATOM   2361  N   LYS   313      10.624 -19.411  19.084  1.00  0.00           N
ATOM   2362  CA  LYS   313      10.561 -18.718  20.323  1.00  0.00           C
ATOM   2363  CB  LYS   313      11.764 -17.792  20.572  1.00  0.00           C
ATOM   2364  CG  LYS   313      13.087 -18.563  20.587  1.00  0.00           C
ATOM   2365  CD  LYS   313      13.137 -19.689  21.621  1.00  0.00           C
ATOM   2366  CE  LYS   313      14.387 -20.565  21.510  1.00  0.00           C
ATOM   2367  NZ  LYS   313      14.302 -21.418  20.304  1.00  0.00           N
ATOM   2368  C   LYS   313       9.276 -17.960  20.385  1.00  0.00           C
ATOM   2369  O   LYS   313       8.317 -18.429  20.993  1.00  0.00           O
ATOM   2370  N   LYS   314       9.205 -16.757  19.781  1.00  0.00           N
ATOM   2371  CA  LYS   314       7.967 -16.043  19.911  1.00  0.00           C
ATOM   2372  CB  LYS   314       8.069 -14.773  20.781  1.00  0.00           C
ATOM   2373  CG  LYS   314       9.084 -13.737  20.295  1.00  0.00           C
ATOM   2374  CD  LYS   314       8.691 -13.033  18.996  1.00  0.00           C
ATOM   2375  CE  LYS   314       9.645 -11.900  18.614  1.00  0.00           C
ATOM   2376  NZ  LYS   314      10.994 -12.441  18.333  1.00  0.00           N
ATOM   2377  C   LYS   314       7.425 -15.663  18.570  1.00  0.00           C
ATOM   2378  O   LYS   314       8.129 -15.720  17.561  1.00  0.00           O
ATOM   2379  N   VAL   315       6.122 -15.289  18.542  1.00  0.00           N
ATOM   2380  CA  VAL   315       5.474 -14.917  17.316  1.00  0.00           C
ATOM   2381  CB  VAL   315       4.230 -15.712  17.031  1.00  0.00           C
ATOM   2382  CG1 VAL   315       4.632 -17.187  16.868  1.00  0.00           C
ATOM   2383  CG2 VAL   315       3.199 -15.473  18.147  1.00  0.00           C
ATOM   2384  C   VAL   315       5.101 -13.463  17.360  1.00  0.00           C
ATOM   2385  O   VAL   315       4.387 -13.005  18.251  1.00  0.00           O
ATOM   2386  N   SER   316       5.613 -12.696  16.379  1.00  0.00           N
ATOM   2387  CA  SER   316       5.393 -11.282  16.251  1.00  0.00           C
ATOM   2388  CB  SER   316       6.480 -10.588  15.412  1.00  0.00           C
ATOM   2389  OG  SER   316       7.740 -10.696  16.059  1.00  0.00           O
ATOM   2390  C   SER   316       4.071 -10.986  15.602  1.00  0.00           C
ATOM   2391  O   SER   316       3.630  -9.838  15.585  1.00  0.00           O
ATOM   2392  N   SER   317       3.390 -12.008  15.061  1.00  0.00           N
ATOM   2393  CA  SER   317       2.212 -11.794  14.264  1.00  0.00           C
ATOM   2394  CB  SER   317       1.554 -13.109  13.813  1.00  0.00           C
ATOM   2395  OG  SER   317       2.425 -13.825  12.949  1.00  0.00           O
ATOM   2396  C   SER   317       1.162 -11.006  14.994  1.00  0.00           C
ATOM   2397  O   SER   317       0.384 -10.294  14.361  1.00  0.00           O
ATOM   2398  N   MET   318       1.089 -11.085  16.335  1.00  0.00           N
ATOM   2399  CA  MET   318       0.004 -10.390  16.979  1.00  0.00           C
ATOM   2400  CB  MET   318      -0.278 -10.957  18.378  1.00  0.00           C
ATOM   2401  CG  MET   318      -0.560 -12.460  18.396  1.00  0.00           C
ATOM   2402  SD  MET   318      -0.567 -13.185  20.063  1.00  0.00           S
ATOM   2403  CE  MET   318      -0.428 -14.901  19.485  1.00  0.00           C
ATOM   2404  C   MET   318       0.370  -8.938  17.203  1.00  0.00           C
ATOM   2405  O   MET   318       0.430  -8.512  18.351  1.00  0.00           O
ATOM   2406  N   ILE   319       0.540  -8.137  16.121  1.00  0.00           N
ATOM   2407  CA  ILE   319       0.912  -6.728  16.105  1.00  0.00           C
ATOM   2408  CB  ILE   319       2.333  -6.498  15.656  1.00  0.00           C
ATOM   2409  CG2 ILE   319       3.275  -7.147  16.679  1.00  0.00           C
ATOM   2410  CG1 ILE   319       2.564  -7.001  14.225  1.00  0.00           C
ATOM   2411  CD1 ILE   319       3.890  -6.512  13.645  1.00  0.00           C
ATOM   2412  C   ILE   319      -0.054  -5.895  15.161  1.00  0.00           C
ATOM   2413  O   ILE   319      -0.909  -5.255  15.757  1.00  0.00           O
ATOM   2414  N   GLU   320       0.073  -5.760  13.761  1.00  0.00           N
ATOM   2415  CA  GLU   320      -0.874  -5.130  12.760  1.00  0.00           C
ATOM   2416  CB  GLU   320      -1.964  -4.207  13.348  1.00  0.00           C
ATOM   2417  CG  GLU   320      -3.055  -5.000  14.066  1.00  0.00           C
ATOM   2418  CD  GLU   320      -3.421  -6.184  13.171  1.00  0.00           C
ATOM   2419  OE1 GLU   320      -3.562  -5.978  11.936  1.00  0.00           O
ATOM   2420  OE2 GLU   320      -3.537  -7.316  13.712  1.00  0.00           O
ATOM   2421  C   GLU   320      -0.201  -4.422  11.547  1.00  0.00           C
ATOM   2422  O   GLU   320       0.922  -3.948  11.679  1.00  0.00           O
ATOM   2423  N   VAL   321      -0.844  -4.306  10.318  1.00  0.00           N
ATOM   2424  CA  VAL   321      -0.139  -3.701   9.165  1.00  0.00           C
ATOM   2425  CB  VAL   321       0.761  -4.679   8.453  1.00  0.00           C
ATOM   2426  CG1 VAL   321       1.816  -5.218   9.435  1.00  0.00           C
ATOM   2427  CG2 VAL   321      -0.107  -5.769   7.793  1.00  0.00           C
ATOM   2428  C   VAL   321      -0.999  -3.095   8.036  1.00  0.00           C
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ATOM   2429  O   VAL   321      -2.184  -3.401   7.906  1.00  0.00           O
ATOM   2430  N   VAL   322      -0.370  -2.212   7.174  1.00  0.00           N
ATOM   2431  CA  VAL   322      -0.883  -1.614   5.930  1.00  0.00           C
ATOM   2432  CB  VAL   322      -1.994  -0.603   6.008  1.00  0.00           C
ATOM   2433  CG1 VAL   322      -3.273  -1.291   6.515  1.00  0.00           C
ATOM   2434  CG2 VAL   322      -1.502   0.633   6.773  1.00  0.00           C
ATOM   2435  C   VAL   322       0.235  -0.945   5.138  1.00  0.00           C
ATOM   2436  O   VAL   322       1.404  -1.004   5.511  1.00  0.00           O
ATOM   2437  N   GLY   323      -0.112  -0.305   3.985  1.00  0.00           N
ATOM   2438  CA  GLY   323       0.832   0.309   3.064  1.00  0.00           C
ATOM   2439  C   GLY   323       1.339   1.647   3.551  1.00  0.00           C
ATOM   2440  O   GLY   323       0.679   2.349   4.313  1.00  0.00           O
ATOM   2441  N   LEU   324       2.534   2.041   3.044  1.00  0.00           N
ATOM   2442  CA  LEU   324       3.290   3.227   3.389  1.00  0.00           C
ATOM   2443  CB  LEU   324       4.672   3.229   2.692  1.00  0.00           C
ATOM   2444  CG  LEU   324       5.679   4.328   3.115  1.00  0.00           C
ATOM   2445  CD2 LEU   324       5.167   5.756   2.863  1.00  0.00           C
ATOM   2446  CD1 LEU   324       7.035   4.103   2.429  1.00  0.00           C
ATOM   2447  C   LEU   324       2.538   4.463   3.012  1.00  0.00           C
ATOM   2448  O   LEU   324       2.575   5.467   3.723  1.00  0.00           O
ATOM   2449  N   ASP   325       1.838   4.426   1.872  1.00  0.00           N
ATOM   2450  CA  ASP   325       1.159   5.592   1.402  1.00  0.00           C
ATOM   2451  CB  ASP   325       0.392   5.315   0.099  1.00  0.00           C
ATOM   2452  CG  ASP   325      -0.059   6.635  -0.501  1.00  0.00           C
ATOM   2453  OD1 ASP   325       0.094   7.687   0.176  1.00  0.00           O
ATOM   2454  OD2 ASP   325      -0.566   6.609  -1.655  1.00  0.00           O
ATOM   2455  C   ASP   325       0.169   6.012   2.443  1.00  0.00           C
ATOM   2456  O   ASP   325      -0.022   7.206   2.666  1.00  0.00           O
ATOM   2457  N   TYR   326      -0.485   5.047   3.122  1.00  0.00           N
ATOM   2458  CA  TYR   326      -1.474   5.455   4.079  1.00  0.00           C
ATOM   2459  CB  TYR   326      -2.654   4.471   4.176  1.00  0.00           C
ATOM   2460  CG  TYR   326      -3.401   4.495   2.885  1.00  0.00           C
ATOM   2461  CD1 TYR   326      -4.352   5.462   2.649  1.00  0.00           C
ATOM   2462  CD2 TYR   326      -3.158   3.551   1.914  1.00  0.00           C
ATOM   2463  CE1 TYR   326      -5.047   5.489   1.463  1.00  0.00           C
ATOM   2464  CE2 TYR   326      -3.850   3.573   0.724  1.00  0.00           C
ATOM   2465  CZ  TYR   326      -4.796   4.544   0.498  1.00  0.00           C
ATOM   2466  OH  TYR   326      -5.507   4.569  -0.721  1.00  0.00           O
ATOM   2467  C   TYR   326      -0.853   5.511   5.440  1.00  0.00           C
ATOM   2468  O   TYR   326      -1.302   4.849   6.375  1.00  0.00           O
ATOM   2469  N   ILE   327       0.177   6.358   5.589  1.00  0.00           N
ATOM   2470  CA  ILE   327       0.858   6.566   6.833  1.00  0.00           C
ATOM   2471  CB  ILE   327       2.064   7.450   6.671  1.00  0.00           C
ATOM   2472  CG2 ILE   327       1.612   8.766   6.017  1.00  0.00           C
ATOM   2473  CG1 ILE   327       2.797   7.634   8.010  1.00  0.00           C
ATOM   2474  CD1 ILE   327       4.145   8.344   7.878  1.00  0.00           C
ATOM   2475  C   ILE   327      -0.076   7.237   7.793  1.00  0.00           C
ATOM   2476  O   ILE   327      -0.119   6.902   8.976  1.00  0.00           O
ATOM   2477  N   ASN   328      -0.847   8.225   7.302  1.00  0.00           N
ATOM   2478  CA  ASN   328      -1.716   8.976   8.160  1.00  0.00           C
ATOM   2479  CB  ASN   328      -2.436  10.129   7.439  1.00  0.00           C
ATOM   2480  CG  ASN   328      -1.420  11.239   7.193  1.00  0.00           C
ATOM   2481  OD1 ASN   328      -0.469  11.413   7.952  1.00  0.00           O
ATOM   2482  ND2 ASN   328      -1.628  12.020   6.100  1.00  0.00           N
ATOM   2483  C   ASN   328      -2.751   8.073   8.750  1.00  0.00           C
ATOM   2484  O   ASN   328      -3.101   8.211   9.921  1.00  0.00           O
ATOM   2485  N   THR   329      -3.272   7.120   7.958  1.00  0.00           N
ATOM   2486  CA  THR   329      -4.298   6.251   8.459  1.00  0.00           C
ATOM   2487  CB  THR   329      -4.799   5.280   7.431  1.00  0.00           C
ATOM   2488  OG1 THR   329      -3.755   4.404   7.034  1.00  0.00           O
ATOM   2489  CG2 THR   329      -5.323   6.067   6.218  1.00  0.00           C
ATOM   2490  C   THR   329      -3.732   5.452   9.588  1.00  0.00           C
ATOM   2491  O   THR   329      -4.398   5.223  10.597  1.00  0.00           O
ATOM   2492  N   ALA   330      -2.473   5.005   9.448  1.00  0.00           N
ATOM   2493  CA  ALA   330      -1.888   4.182  10.463  1.00  0.00           C
ATOM   2494  CB  ALA   330      -0.449   3.755  10.128  1.00  0.00           C
ATOM   2495  C   ALA   330      -1.840   4.942  11.748  1.00  0.00           C
ATOM   2496  O   ALA   330      -2.167   4.404  12.805  1.00  0.00           O
ATOM   2497  N   MET   331      -1.415   6.217  11.698  1.00  0.00           N
ATOM   2498  CA  MET   331      -1.318   6.973  12.908  1.00  0.00           C
ATOM   2499  CB  MET   331      -0.419   8.208  12.768  1.00  0.00           C
ATOM   2500  CG  MET   331       1.036   7.730  12.706  1.00  0.00           C
ATOM   2501  SD  MET   331       2.301   8.991  12.411  1.00  0.00           S
ATOM   2502  CE  MET   331       2.171   8.886  10.604  1.00  0.00           C
ATOM   2503  C   MET   331      -2.669   7.285  13.465  1.00  0.00           C
ATOM   2504  O   MET   331      -2.859   7.274  14.680  1.00  0.00           O
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ATOM   2505  N   LYS   332      -3.658   7.559  12.599  1.00  0.00           N
ATOM   2506  CA  LYS   332      -4.957   7.882  13.110  1.00  0.00           C
ATOM   2507  CB  LYS   332      -5.944   8.310  12.009  1.00  0.00           C
ATOM   2508  CG  LYS   332      -7.280   8.815  12.554  1.00  0.00           C
ATOM   2509  CD  LYS   332      -8.060   9.677  11.557  1.00  0.00           C
ATOM   2510  CE  LYS   332      -7.891   9.248  10.098  1.00  0.00           C
ATOM   2511  NZ  LYS   332      -8.751   8.085   9.797  1.00  0.00           N
ATOM   2512  C   LYS   332      -5.498   6.691  13.837  1.00  0.00           C
ATOM   2513  O   LYS   332      -6.120   6.828  14.890  1.00  0.00           O
ATOM   2514  N   ARG   333      -5.257   5.481  13.298  1.00  0.00           N
ATOM   2515  CA  ARG   333      -5.743   4.275  13.907  1.00  0.00           C
ATOM   2516  CB  ARG   333      -5.422   3.007  13.094  1.00  0.00           C
ATOM   2517  CG  ARG   333      -6.162   2.927  11.758  1.00  0.00           C
ATOM   2518  CD  ARG   333      -7.502   2.188  11.830  1.00  0.00           C
ATOM   2519  NE  ARG   333      -8.539   3.163  12.271  1.00  0.00           N
ATOM   2520  CZ  ARG   333      -9.850   2.924  11.975  1.00  0.00           C
ATOM   2521  NH1 ARG   333     -10.194   1.815  11.258  1.00  0.00           N
ATOM   2522  NH2 ARG   333     -10.814   3.787  12.409  1.00  0.00           N
ATOM   2523  C   ARG   333      -5.106   4.126  15.254  1.00  0.00           C
ATOM   2524  O   ARG   333      -5.736   3.650  16.196  1.00  0.00           O
ATOM   2525  N   LEU   334      -3.823   4.505  15.384  1.00  0.00           N
ATOM   2526  CA  LEU   334      -3.168   4.348  16.651  1.00  0.00           C
ATOM   2527  CB  LEU   334      -1.669   4.691  16.585  1.00  0.00           C
ATOM   2528  CG  LEU   334      -0.935   4.508  17.926  1.00  0.00           C
ATOM   2529  CD2 LEU   334       0.506   5.040  17.850  1.00  0.00           C
ATOM   2530  CD1 LEU   334      -0.991   3.046  18.392  1.00  0.00           C
ATOM   2531  C   LEU   334      -3.816   5.240  17.668  1.00  0.00           C
ATOM   2532  O   LEU   334      -4.105   4.814  18.785  1.00  0.00           O
ATOM   2533  N   GLU   335      -4.079   6.507  17.295  1.00  0.00           N
ATOM   2534  CA  GLU   335      -4.650   7.469  18.197  1.00  0.00           C
ATOM   2535  CB  GLU   335      -4.791   8.858  17.558  1.00  0.00           C
ATOM   2536  CG  GLU   335      -5.390   9.907  18.497  1.00  0.00           C
ATOM   2537  CD  GLU   335      -5.523  11.204  17.712  1.00  0.00           C
ATOM   2538  OE1 GLU   335      -5.205  11.189  16.493  1.00  0.00           O
ATOM   2539  OE2 GLU   335      -5.947  12.225  18.317  1.00  0.00           O
ATOM   2540  C   GLU   335      -6.024   7.030  18.588  1.00  0.00           C
ATOM   2541  O   GLU   335      -6.445   7.203  19.730  1.00  0.00           O
ATOM   2542  N   LYS   336      -6.759   6.451  17.624  1.00  0.00           N
ATOM   2543  CA  LYS   336      -8.123   6.033  17.782  1.00  0.00           C
ATOM   2544  CB  LYS   336      -8.770   5.567  16.470  1.00  0.00           C
ATOM   2545  CG  LYS   336      -8.997   6.726  15.499  1.00  0.00           C
ATOM   2546  CD  LYS   336      -9.462   6.301  14.108  1.00  0.00           C
ATOM   2547  CE  LYS   336      -9.823   7.491  13.220  1.00  0.00           C
ATOM   2548  NZ  LYS   336     -10.345   7.018  11.922  1.00  0.00           N
ATOM   2549  C   LYS   336      -8.228   4.934  18.789  1.00  0.00           C
ATOM   2550  O   LYS   336      -9.301   4.730  19.356  1.00  0.00           O
ATOM   2551  N   ASN   337      -7.123   4.195  19.022  1.00  0.00           N
ATOM   2552  CA  ASN   337      -7.104   3.066  19.909  1.00  0.00           C
ATOM   2553  CB  ASN   337      -7.891   3.327  21.218  1.00  0.00           C
ATOM   2554  CG  ASN   337      -7.599   2.287  22.295  1.00  0.00           C
ATOM   2555  OD1 ASN   337      -7.758   1.080  22.122  1.00  0.00           O
ATOM   2556  ND2 ASN   337      -7.168   2.786  23.485  1.00  0.00           N
ATOM   2557  C   ASN   337      -7.741   1.961  19.137  1.00  0.00           C
ATOM   2558  O   ASN   337      -7.909   0.842  19.615  1.00  0.00           O
ATOM   2559  N   ASP   338      -8.056   2.243  17.861  1.00  0.00           N
ATOM   2560  CA  ASP   338      -8.612   1.230  17.021  1.00  0.00           C
ATOM   2561  CB  ASP   338      -8.975   1.739  15.616  1.00  0.00           C
ATOM   2562  CG  ASP   338      -9.720   0.622  14.905  1.00  0.00           C
ATOM   2563  OD1 ASP   338      -9.877  -0.470  15.515  1.00  0.00           O
ATOM   2564  OD2 ASP   338     -10.148   0.850  13.744  1.00  0.00           O
ATOM   2565  C   ASP   338      -7.552   0.206  16.863  1.00  0.00           C
ATOM   2566  O   ASP   338      -7.807  -0.993  16.946  1.00  0.00           O
ATOM   2567  N   VAL   339      -6.313   0.670  16.626  1.00  0.00           N
ATOM   2568  CA  VAL   339      -5.240  -0.257  16.563  1.00  0.00           C
ATOM   2569  CB  VAL   339      -4.371  -0.117  15.341  1.00  0.00           C
ATOM   2570  CG1 VAL   339      -5.211  -0.543  14.130  1.00  0.00           C
ATOM   2571  CG2 VAL   339      -3.850   1.325  15.204  1.00  0.00           C
ATOM   2572  C   VAL   339      -4.462  -0.008  17.793  1.00  0.00           C
ATOM   2573  O   VAL   339      -3.467   0.715  17.831  1.00  0.00           O
ATOM   2574  N   ARG   340      -4.853  -0.629  18.909  1.00  0.00           N
ATOM   2575  CA  ARG   340      -3.923  -0.363  19.951  1.00  0.00           C
ATOM   2576  CB  ARG   340      -4.535  -0.197  21.337  1.00  0.00           C
ATOM   2577  CG  ARG   340      -4.553   1.291  21.651  1.00  0.00           C
ATOM   2578  CD  ARG   340      -3.123   1.738  21.949  1.00  0.00           C
ATOM   2579  NE  ARG   340      -3.126   3.195  22.207  1.00  0.00           N
ATOM   2580  CZ  ARG   340      -2.050   3.693  22.872  1.00  0.00           C
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ATOM   2581  NH1 ARG   340      -1.110   2.814  23.326  1.00  0.00           N
ATOM   2582  NH2 ARG   340      -1.908   5.036  23.065  1.00  0.00           N
ATOM   2583  C   ARG   340      -2.902  -1.433  19.897  1.00  0.00           C
ATOM   2584  O   ARG   340      -2.607  -2.123  20.872  1.00  0.00           O
ATOM   2585  N   TYR   341      -2.318  -1.526  18.689  1.00  0.00           N
ATOM   2586  CA  TYR   341      -1.361  -2.482  18.306  1.00  0.00           C
ATOM   2587  CB  TYR   341      -1.995  -3.756  17.749  1.00  0.00           C
ATOM   2588  CG  TYR   341      -2.479  -4.404  18.996  1.00  0.00           C
ATOM   2589  CD1 TYR   341      -1.577  -5.101  19.767  1.00  0.00           C
ATOM   2590  CD2 TYR   341      -3.783  -4.275  19.425  1.00  0.00           C
ATOM   2591  CE1 TYR   341      -1.971  -5.701  20.940  1.00  0.00           C
ATOM   2592  CE2 TYR   341      -4.183  -4.871  20.601  1.00  0.00           C
ATOM   2593  CZ  TYR   341      -3.278  -5.581  21.357  1.00  0.00           C
ATOM   2594  OH  TYR   341      -3.702  -6.183  22.559  1.00  0.00           O
ATOM   2595  C   TYR   341      -0.443  -1.814  17.369  1.00  0.00           C
ATOM   2596  O   TYR   341      -0.403  -0.585  17.320  1.00  0.00           O
ATOM   2597  N   ARG   342       0.377  -2.581  16.639  1.00  0.00           N
ATOM   2598  CA  ARG   342       1.254  -1.821  15.820  1.00  0.00           C
ATOM   2599  CB  ARG   342       2.739  -2.128  15.997  1.00  0.00           C
ATOM   2600  CG  ARG   342       3.593  -1.105  15.266  1.00  0.00           C
ATOM   2601  CD  ARG   342       4.835  -0.770  16.063  1.00  0.00           C
ATOM   2602  NE  ARG   342       4.345  -0.226  17.357  1.00  0.00           N
ATOM   2603  CZ  ARG   342       5.227   0.237  18.284  1.00  0.00           C
ATOM   2604  NH1 ARG   342       6.565   0.182  18.037  1.00  0.00           N
ATOM   2605  NH2 ARG   342       4.757   0.786  19.442  1.00  0.00           N
ATOM   2606  C   ARG   342       0.882  -1.988  14.407  1.00  0.00           C
ATOM   2607  O   ARG   342       0.427  -3.049  13.988  1.00  0.00           O
ATOM   2608  N   PHE   343       1.062  -0.901  13.644  1.00  0.00           N
ATOM   2609  CA  PHE   343       0.705  -0.900  12.269  1.00  0.00           C
ATOM   2610  CB  PHE   343      -0.054   0.382  11.917  1.00  0.00           C
ATOM   2611  CG  PHE   343      -1.255  -0.108  11.222  1.00  0.00           C
ATOM   2612  CD1 PHE   343      -2.365  -0.472  11.952  1.00  0.00           C
ATOM   2613  CD2 PHE   343      -1.264  -0.236   9.860  1.00  0.00           C
ATOM   2614  CE1 PHE   343      -3.494  -0.939  11.325  1.00  0.00           C
ATOM   2615  CE2 PHE   343      -2.393  -0.704   9.242  1.00  0.00           C
ATOM   2616  CZ  PHE   343      -3.511  -1.052   9.958  1.00  0.00           C
ATOM   2617  C   PHE   343       2.005  -0.916  11.537  1.00  0.00           C
ATOM   2618  O   PHE   343       2.895  -0.117  11.825  1.00  0.00           O
ATOM   2619  N   VAL   344       2.173  -1.862  10.597  1.00  0.00           N
ATOM   2620  CA  VAL   344       3.407  -1.880   9.873  1.00  0.00           C
ATOM   2621  CB  VAL   344       4.008  -3.246   9.700  1.00  0.00           C
ATOM   2622  CG1 VAL   344       5.257  -3.127   8.810  1.00  0.00           C
ATOM   2623  CG2 VAL   344       4.301  -3.832  11.093  1.00  0.00           C
ATOM   2624  C   VAL   344       3.135  -1.320   8.522  1.00  0.00           C
ATOM   2625  O   VAL   344       2.137  -1.654   7.883  1.00  0.00           O
ATOM   2626  N   VAL   345       4.025  -0.419   8.064  1.00  0.00           N
ATOM   2627  CA  VAL   345       3.836   0.182   6.779  1.00  0.00           C
ATOM   2628  CB  VAL   345       4.053   1.668   6.769  1.00  0.00           C
ATOM   2629  CG1 VAL   345       2.968   2.325   7.639  1.00  0.00           C
ATOM   2630  CG2 VAL   345       5.486   1.960   7.243  1.00  0.00           C
ATOM   2631  C   VAL   345       4.833  -0.428   5.852  1.00  0.00           C
ATOM   2632  O   VAL   345       6.025  -0.498   6.149  1.00  0.00           O
ATOM   2633  N   ASP   346       4.348  -0.904   4.690  1.00  0.00           N
ATOM   2634  CA  ASP   346       5.184  -1.528   3.706  1.00  0.00           C
ATOM   2635  CB  ASP   346       4.487  -2.702   2.990  1.00  0.00           C
ATOM   2636  CG  ASP   346       5.479  -3.382   2.053  1.00  0.00           C
ATOM   2637  OD1 ASP   346       6.703  -3.130   2.207  1.00  0.00           O
ATOM   2638  OD2 ASP   346       5.029  -4.169   1.178  1.00  0.00           O
ATOM   2639  C   ASP   346       5.478  -0.499   2.663  1.00  0.00           C
ATOM   2640  O   ASP   346       4.631   0.334   2.347  1.00  0.00           O
ATOM   2641  N   VAL   347       6.702  -0.519   2.103  1.00  0.00           N
ATOM   2642  CA  VAL   347       7.011   0.438   1.086  1.00  0.00           C
ATOM   2643  CB  VAL   347       8.474   0.766   0.971  1.00  0.00           C
ATOM   2644  CG1 VAL   347       8.919   1.480   2.258  1.00  0.00           C
ATOM   2645  CG2 VAL   347       9.255  -0.529   0.690  1.00  0.00           C
ATOM   2646  C   VAL   347       6.563  -0.131  -0.216  1.00  0.00           C
ATOM   2647  O   VAL   347       6.939  -1.239  -0.595  1.00  0.00           O
ATOM   2648  N   ALA   348       5.712   0.624  -0.933  1.00  0.00           N
ATOM   2649  CA  ALA   348       5.228   0.154  -2.193  1.00  0.00           C
ATOM   2650  CB  ALA   348       3.943   0.857  -2.660  1.00  0.00           C
ATOM   2651  C   ALA   348       6.281   0.405  -3.218  1.00  0.00           C
ATOM   2652  O   ALA   348       7.026   1.382  -3.143  1.00  0.00           O
ATOM   2653  N   ALA   349       6.365  -0.498  -4.211  1.00  0.00           N
ATOM   2654  CA  ALA   349       7.305  -0.339  -5.277  1.00  0.00           C
ATOM   2655  CB  ALA   349       7.866  -1.668  -5.812  1.00  0.00           C
ATOM   2656  C   ALA   349       6.558   0.305  -6.392  1.00  0.00           C
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ATOM   2657  O   ALA   349       5.334   0.205  -6.467  1.00  0.00           O
ATOM   2658  N   SER   350       7.277   1.010  -7.285  1.00  0.00           N
ATOM   2659  CA  SER   350       6.595   1.630  -8.377  1.00  0.00           C
ATOM   2660  CB  SER   350       7.457   2.638  -9.155  1.00  0.00           C
ATOM   2661  OG  SER   350       6.708   3.202 -10.222  1.00  0.00           O
ATOM   2662  C   SER   350       6.204   0.538  -9.317  1.00  0.00           C
ATOM   2663  O   SER   350       6.842  -0.513  -9.361  1.00  0.00           O
ATOM   2664  N   LYS   351       5.119   0.757 -10.082  1.00  0.00           N
ATOM   2665  CA  LYS   351       4.686  -0.247 -11.004  1.00  0.00           C
ATOM   2666  CB  LYS   351       3.220  -0.094 -11.443  1.00  0.00           C
ATOM   2667  CG  LYS   351       2.223  -0.323 -10.307  1.00  0.00           C
ATOM   2668  CD  LYS   351       2.303  -1.723  -9.691  1.00  0.00           C
ATOM   2669  CE  LYS   351       1.736  -2.821 -10.594  1.00  0.00           C
ATOM   2670  NZ  LYS   351       1.853  -4.136  -9.926  1.00  0.00           N
ATOM   2671  C   LYS   351       5.542  -0.135 -12.218  1.00  0.00           C
ATOM   2672  O   LYS   351       6.016   0.950 -12.553  1.00  0.00           O
ATOM   2673  N   LEU   352       5.758  -1.276 -12.901  1.00  0.00           N
ATOM   2674  CA  LEU   352       6.572  -1.320 -14.079  1.00  0.00           C
ATOM   2675  CB  LEU   352       5.919  -0.646 -15.299  1.00  0.00           C
ATOM   2676  C   LEU   352       7.890  -0.614 -13.791  1.00  0.00           C
ATOM   2677  O   LEU   352       8.210   0.363 -14.520  1.00  0.00           O
ATOM   2678  OXT LEU   352       8.595  -1.042 -12.837  1.00  0.00           O
ATOM   2679  CG  LEU   352       4.636  -1.349 -15.781  1.00  0.00           C
ATOM   2680  CD2 LEU   352       3.542  -1.320 -14.702  1.00  0.00           C
ATOM   2681  CD1 LEU   352       4.936  -2.766 -16.294  1.00  0.00           C
END
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Appendix 2. EST-derived consensus sequences of the *Pinus taeda* 4CL, CCR and CAD subfamilies

4-Coumarate:Coenzyme A ligase (4CL)

tBLASTn report

4CL gi|13068764	gb|BG275445.1|BG275445	NXSI_141_H05_F NXSI (Nsf...	318	1e-87	495	99
4CL gi|9993266	gb|BE662594.1|BE662594	ST88/ST88D05 Pine TriplEx..	299	6e-82	480	95
4CL gi|6696172	gb|AW289536.1|AW289536	NXNV002B02F Nsf Xylem Nor..	290	3e-79	460	97
4CL gi|10798130	gb|BF049733.1|BF049733	NXCI_106_E02_F NXCI (Nsf...	287	3e-78	456	95
4CL gi|6696097	gb|AW289461.1|AW289461	NXNV001C01F Nsf Xylem Nor..	285	9e-78	462	94
4CL gi|11606879	gb|BF518234.1|BF518234	NXSI_036_F06_F NXSI (Nsf...	285	1e-77	512	84
4CL gi|9982694	gb|BE656758.1|BE656758	NXCI_056_E08_F NXCI (Nsf ..	271	1e-73	444	93
4CL gi|11054109	gb|BF169470.1|BF169470	NXCI_123_A06_F NXCI (Nsf...	268	1e-72	512	80
4CL gi|13536798	gb|BG526919.1|BG526919	NXPV_057_D07_F NXPV (Nsf...	267	2e-72	550	83
4CL gi|8179651	gb|AW985299.1|AW985299	NXNV_135_E09_F Nsf Xylem ..	267	2e-72	467	86
4CL gi|10191872	gb|BE761948.1|BE761948	NXCI_075_B08_F NXCI (Nsf...	259	9e-70	394	98
4CL gi|11126612	gb|BF220480.1|BF220480	NXCI_147_A06_F NXCI (Nsf...	256	4e-69	419	94
4CL gi|9458063	gb|BE452059.1|BE452059	NXCI_007_H11_F NXCI (Nsf ..	254	2e-68	410	93
4CL gi|8179270	gb|AW984914.1|AW984914	NXNV_100_H07_F Nsf Xylem ..	248	1e-66	413	91
4CL gi|14515963	gb|BI077306.1|BI077306	NXPV_095_D09_F NXPV (Nsf...	248	2e-66	482	80
4CL gi|11068595	gb|BF186422.1|BF186422	NXCI_137_B11_F NXCI (Nsf...	240	3e-64	368	96
4CL gi|8666540	gb|BE187356.1|BE187356	NXNV_162_H09_F Nsf Xylem ..	236	5e-63	384	92
4CL gi|12482910	gb|BG040325.1|BG040325	NXSI_107_A08_F NXSI (Nsf...	234	3e-62	528	88
4CL gi|11068509	gb|BF186336.1|BF186336	NXCI_136_E11_F NXCI (Nsf...	231	2e-61	377	95
4CL gi|3365962	gb|AA556948.1|AA556948	790 Loblolly pine C Pinus..	213	3e-61	669	86
4CL gi|3365945	gb|AA556931.1|AA556931	773 Loblolly pine C Pinus..	221	9e-61	633	88
4CL gi|13068750	gb|BG275438.1|BG275438	NXSI_141_H06_F NXSI (Nsf...	227	4e-60	400	89
4CL gi|5044108	gb|AI725289.1|AI725289	1155 PtIFG2 Pinus taeda c..	223	5e-59	651	72
4CL gi|11054171	gb|BF169555.1|BF169555	NXCI_124_B09_F NXCI (Nsf...	214	2e-56	346	93
4CL gi|11054054	gb|BF169416.1|BF169416	NXCI_120_G08_F NXCI (Nsf...	213	7e-56	348	95
4CL gi|6696815	gb|AW290167.1|AW290167	NXNV015G05F Nsf Xylem Nor..	209	8e-55	553	81
4CL gi|5423605	gb|AI812407.1|AI812407	10A6 Pine Lambda Zap Xyle..	206	9e-54	610	80
4CL gi|9689875	gb|BE496477.1|BE496477	NXCI_018_E12_F NXCI (Nsf ..	200	5e-52	319	93
4CL gi|7838491	gb|AW784067.1|AW784067	NXNV_117_C12_F Nsf Xylem ..	196	9e-51	501	82
4CL gi|9956845	gb|BE644238.1|BE644238	NXCI_051_G09_F NXCI (Nsf ..	195	1e-50	323	91
4CL gi|9488824	gb|BE458121.1|BE458121	NXCI_010_A08_F NXCI (Nsf ..	194	2e-50	486	83
4CL gi|11068356	gb|BF186183.1|BF186183	NXCI_131_C04_F NXCI (Nsf...	191	3e-49	293	95
4CL gi|13068766	gb|BG275446.1|BG275446	NXSI_141_G12_F NXSI (Nsf...	189	6e-49	480	84
4CL gi|9956449	gb|BE643842.1|BE643842	NXCI_047_H11_F NXCI (Nsf ..	180	5e-46	450	86
4CL gi|11126758	gb|BF220710.1|BF220710	NXCI_149_F08_F NXCI (Nsf...	171	3e-43	437	87
4CL gi|10682045	gb|BE997195.1|BE997195	NXCI_107_E10_F NXCI (Nsf...	164	2e-41	272	93
4CL gi|12125405	gb|BF777505.1|BF777505	NXSI_069_D03_F NXSI (Nsf...	162	8e-41	427	88
4CL gi|13127087	gb|BG317657.1|BG317657	NXPV_004_C07_F NXPV (Nsf...	161	2e-40	552	77
4CL gi|15553845	gb|BI643841.1|BI643841	NXPV_123_F05_F NXPV (Nsf...	161	2e-40	518	77
4CL gi|12125443	gb|BF777543.1|BF777543	NXSI_069_G07_F NXSI (Nsf...	156	8e-39	387	90
4CL gi|10710819	gb|BF010545.1|BF010545	NXCI_085_G04_F NXCI (Nsf...	152	9e-38	395	84
4CL gi|7031487	gb|AW461270.1|AW461270	NXNV060G01F Nsf Xylem Nor..	147	3e-36	362	100
4CL gi|7676542	gb|AW754726.1|AW754726	PC07B01 Pine TriplEx poll..	141	2e-34	308	74
4CL gi|14189367	gb|BG832725.1|BG832725	NXPV_079_A01_F NXPV (Nsf...	139	1e-33	214	95
4CL gi|9689658	gb|BE496260.1|BE496260	NXCI_012_H08_F NXCI (Nsf ..	137	4e-33	345	94
4CL gi|9982990	gb|BE657098.1|BE657098	NXCI_042_F05_F NXCI (Nsf ..	136	6e-33	209	95
4CL gi|9457484	gb|BE451781.1|BE451781	NXCI_002_B08_F NXCI (Nsf ..	130	6e-31	322	89
4CL gi|2778557	gb|AA740006.1|AA740006	771 PtIFG2 Pinus taeda cD..	129	1e-30	553	64
4CL gi|9457401	gb|BE451741.1|BE451741	NXCI_001_E12_F NXCI (Nsf ..	128	2e-30	323	92
4CL gi|9833314	gb|BE582366.1|BE582366	NXCI_032_E08_F NXCI (Nsf ..	127	4e-30	328	95
4CL gi|9833310	gb|BE582362.1|BE582362	NXCI_032_E04_F NXCI (Nsf ..	127	4e-30	325	95
4CL gi|10710850	gb|BF010576.1|BF010576	NXCI_086_C09_F NXCI (Nsf...	126	7e-30	234	80
4CL gi|10192052	gb|BE762128.1|BE762128	NXCI_081_G08_F NXCI (Nsf...	123	6e-29	325	89
4CL gi|3365751	gb|AA556736.1|AA556736	973 Loblolly pine NA Pinu..	121	3e-28	520	82
4CL gi|9833002	gb|BE582138.1|BE582138	NXCI_029_G07_F NXCI (Nsf ..	120	4e-28	340	95
4CL gi|11126608	gb|BF220476.1|BF220476	NXCI_146_H09_F NXCI (Nsf...	115	2e-26	329	88
4CL gi|13128019	gb|BG318589.1|BG318589	NXPV_015_E11_F NXPV (Nsf...	108	1e-24	286	69
4CL gi|8517081	gb|BE123767.1|BE123767	NXNV_156_A10_F Nsf Xylem ..	108	1e-24	203	88
4CL gi|8179552	gb|AW985215.1|AW985215	NXNV_132_E10_F Nsf Xylem ..	105	1e-23	377	43
4CL gi|10681747	gb|BE996982.1|BE996982	NXCI_093_G03_F NXCI (Nsf...	105	2e-23	299	92
4CL gi|11127107	gb|BF220975.1|BF220975	NXCI_153_D01_F NXCI (Nsf...	100	4e-22	293	90
4CL gi|7274639	gb|AW587610.1|AW587610	ST60E04 Pine TriplEx shoo..	99	2e-21	445	41
4CL gi|13127363	gb|BG317933.1|BG317933	NXPV_007_E06_F NXPV (Nsf...	92	1e-19	375	80
4CL gi|6697351	gb|AW290715.1|AW290715	NXNV046A10F Nsf Xylem Nor..	91	4e-19	380	79
4CL gi|2778293	gb|AA739742.1|AA739742	507 PtIFG2 Pinus taeda cD..	76	1e-14	351	92
4CL gi|5423581	gb|AI812383.1|AI812383	1G2 Pine Lambda Zap Xylem..	74	5e-14	584	32
4CL gi|11605885	gb|BF517821.1|BF517821	NXSI_027_F01_F NXSI (Nsf...	72	2e-13	346	100
4CL gi|11068483	gb|BF186310.1|BF186310	NXCI_135_H07_F NXCI (Nsf...	69	2e-12	242	88

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4CL gi|11054182 |gb|BF169566.1|BF169566  NXCI_124_D02_F NXCI (Nsf...    68   3e-12 227  90
4CL gi|10192119 |gb|BE762195.1|BE762195  NXCI_083_C08_F NXCI (Nsf...    68   4e-12 230  88
4CL gi|11068399 |gb|BF186226.1|BF186226  NXCI_134_F03_F NXCI (Nsf...    66   1e-11 236  87
4CL gi|15144802 |gb|BI397738.1|BI397738  NXPV_104_G03_F NXPV (Nsf...    64   7e-11 441  36
4CL gi|5424240  |gb|AI812889.1|AI812889  22B5 Pine Lambda Zap Xyle..    49   2e-06 566  25
4CL gi|7690469  |gb|AW758552.1|AW758552  NXNV_085_D05_F Nsf Xylem ..    47   7e-06 285  30
4CL gi|7690500  |gb|AW758582.1|AW758582  NXNV_075_B12_F Nsf Xylem ..    46   2e-05 309  52
4CL gi|13127035 |gb|BG317605.1|BG317605  NXPV_003_F08_F NXPV (Nsf...    45   3e-05 545  32
4CL gi|5424292  |gb|AI812941.1|AI812941  22G1 Pine Lambda Zap Xyle..    42   3e-04 515  29
4CL gi|13536766 |gb|BG526887.1|BG526887  NXPV_057_A05_F NXPV (Nsf...    40   0.001 441  33
4CL gi|7579940  |gb|AW697581.1|AW697581  ST59C08 Pine TriplEx shoo..    39   0.002 454  25
4CL gi|13128512 |gb|BG319082.1|BG319082  NXPV_023_E04_F NXPV (Nsf...    37   0.007 352  37
4CL gi|11778484 |gb|BF610134.1|BF610134  NXSI_055_B04_F NXSI (Nsf...    36   0.016 327  25
4CL gi|13128768 |gb|BG319338.1|BG319338  NXPV_026_G09_F NXPV (Nsf...    31   0.500 357  41
4CL gi|7580743  |gb|AW698157.1|AW698157  NXNV_073_H03_F Nsf Xylem ..    28   4.200 297  40
4CL gi|17243751 |gb|BM158264.1|BM158264  NXLV_031_F05_F NXLV (Nsf...    27   5.600 475  40
4CL gi|8666243  |gb|BE187023.1|BE187023  NXNV_154_C08_F Nsf Xylem ..    27   7.200 310  35
4CL gi|7644696  |gb|AW736832.1|AW736832  NXNV_083_E02_F Nsf Xylem ..    27   7.200 403  35
4CL gi|6696767  |gb|AW290131.1|AW290131  NXNV012E02F Nsf Xylem Nor..    27   9.500 522  21
4CL gi|6696248  |gb|AW289612.1|AW289612  NXNV003D02F Nsf Xylem Nor..    27   9.500 492  21
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>4CL subfamily 1 Pinus_taeda
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GCGTTCGTGGTGAAGTCGTCGGAAATCAGCGAGCAGGAAATCAAGGAGTTCGTGGCAAAG
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 V  P  P  I  V  L  D  I  T  K  S  P  I  V  S  Q  Y  D  V  S
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 S  V  R  I  I  M  S  G  A  A  P  L  G  K  E  L  E  D  A  L
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 P  S  G  K  I  L  R  K  D  L  R  S  R  L  A  A  K  -
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Cinnamoyl Coenzyme A reductase (CCR)

tBLASTn report

CCR gi|7676637	gb|AW754917.1|AW754917	PC08D01 Pine TriplEx poll..	171	1e-43	434	59
CCR gi|6555678	gb|AW226382.1|AW226382	ST81F10 Pine TriplEx shoo..	160	3e-40	369	72
CCR gi|8173485	gb|AW981912.1|AW981912	PC20C06 Pine TriplEx poll..	127	2e-30	516	72
CCR gi|5929199	gb|AW056441.1|AW056441	ST51H10 Pine TriplEx shoo..	125	7e-30	462	43
CCR gi|11778385	gb|BF610086.1|BF610086	NXSI_054_E12_F NXSI (Nsf...	124	2e-29	490	41
CCR gi|13128715	gb|BG319285.1|BG319285	NXPV_026_B01_F NXPV (Nsf...	122	6e-29	490	41
CCR gi|7676593	gb|AW754777.1|AW754777	PC07G05 Pine TriplEx poll..	108	9e-25	490	39
CCR gi|18613783	gb|BM492852.1|BM492852	NXRV_033_A06_F NXRV (Nsf...	107	3e-24	509	46
CCR gi|7676293	gb|AW754573.1|AW754573	PC03H02 Pine TriplEx poll..	105	1e-23	490	61
CCR gi|6020091	gb|AW065019.1|AW065019	ST38F06 Pine TriplEx shoo..	105	1e-23	449	61
CCR gi|5929503	gb|AW056808.1|AW056808	ST56D11 Pine TriplEx shoo..	104	2e-23	370	53
CCR gi|7676840	gb|AW755120.1|AW755120	PC11B10 Pine TriplEx poll..	104	2e-23	458	37
CCR gi|11605374	gb|BF517479.1|BF517479	NXSI_022_E03_F NXSI (Nsf...	101	2e-22	515	43
CCR gi|6555506	gb|AW226210.1|AW226210	ST79F04 Pine TriplEx shoo..	101	2e-22	396	42
CCR gi|7676424	gb|AW754704.1|AW754704	PC05D10 Pine TriplEx poll..	99	9e-22	545	43
CCR gi|12481880	gb|BG039295.1|BG039295	NXSI_097_E03_F NXSI (Nsf...	99	9e-22	365	57
CCR gi|5903436	gb|AW042907.1|AW042907	ST26H07 Pine TriplEx shoo..	92	2e-20	563	48
CCR gi|7031450	gb|AW461233.1|AW461233	NXNV052F10F Nsf Xylem Nor..	90	4e-19	280	47
CCR gi|6973304	gb|AW437998.1|AW437998	ST83C11 Pine TriplEx shoo..	84	3e-17	306	48
CCR gi|6019765	gb|AW064693.1|AW064693	ST34F04 Pine TriplEx shoo..	80	3e-16	590	62
CCR gi|8173059	gb|AW981496.1|AW981496	PC13A10 Pine TriplEx poll..	77	3e-15	630	91
CCR gi|10192100	gb|BE762176.1|BE762176	NXCI_083_A03_F NXCI (Nsf...	77	5e-15	251	57
CCR gi|9993111	gb|BE662440.1|BE662440	ST85/ST85C11 Pine TriplEx..	68	2e-12	309	58
CCR gi|6555061	gb|AW225765.1|AW225765	ST71E09 Pine TriplEx shoo..	68	2e-12	432	32
CCR gi|7676652	gb|AW754932.1|AW754932	PC08E08 Pine TriplEx poll..	68	2e-12	393	96
CCR gi|3365551	gb|AA556536.1|AA556536	391 Loblolly pine C Pinus..	61	2e-10	728	28
CCR gi|11606774	gb|BF518182.1|BF518182	NXSI_036_B01_F NXSI (Nsf...	60	5e-10	503	36
CCR gi|14515850	gb|BI077193.1|BI077193	NXPV_094_B05_F NXPV (Nsf...	56	7e-09	517	34
CCR gi|8173633	gb|AW982065.1|AW982065	PC23D07 Pine TriplEx poll..	56	9e-09	514	33
CCR gi|13128654	gb|BG319224.1|BG319224	NXPV_019_C11_F NXPV (Nsf...	50	5e-07	328	36
CCR gi|7676370	gb|AW754650.1|AW754650	PC04G01 Pine TriplEx poll..	47	4e-06	305	29
CCR gi|11127580	gb|BF221448.1|BF221448	NXCI_165_H04_F NXCI (Nsf...	47	5e-06	317	80
CCR gi|8789596	gb|BE209344.1|BE209344	NXNV_166_F05_F Nsf Xylem ..	46	9e-06	203	86
CCR gi|10798149	gb|BF049752.1|BF049752	NXCI_106_G05_F NXCI (Nsf...	44	3e-05	455	60
CCR gi|9993149	gb|BE662478.1|BE662478	ST86/ST86D05 Pine TriplEx..	42	1e-04	367	29
CCR gi|11127180	gb|BF221048.1|BF221048	NXCI_162_F04_F NXCI (Nsf...	37	0.004	415	24
CCR gi|13069174	gb|BG275650.1|BG275650	NXSI_144_D03_F NXSI (Nsf...	34	0.036	643	32
CCR gi|5424089	gb|AI812993.1|AI812993	2E11 Pine Lambda Zap Xyle..	34	0.036	543	27
CCR gi|11126974	gb|BF220842.1|BF220842	NXCI_154_E08_F NXCI (Nsf...	33	0.061	391	26
CCR gi|12482629	gb|BG040044.1|BG040044	NXSI_105_H04_F NXSI (Nsf...	32	0.100	502	27

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CCR gi|6555177  |gb|AW225881.1|AW225881  ST72G11 Pine TriplEx shoo..    32   0.140 458  35
CCR gi|7676874  |gb|AW755154.1|AW755154  PC11F03 Pine TriplEx poll..    30   0.520 376  37
CCR gi|8050099  |gb|AW888016.1|AW888016  NXNV_105_H05_F Nsf Xylem ..    29   0.890 415  27
CCR gi|13068984 |gb|BG275555.1|BG275555  NXSI_143_B10_F NXSI (Nsf...    29   1.200 625  26
CCR gi|6697128  |gb|AW290492.1|AW290492  NXNV027E06F Nsf Xylem Nor..    29   1.200 546  32
CCR gi|8789470  |gb|BE209218.1|BE209218  NXNV_147_E01_F Nsf Xylem ..    29   1.200 580  26
CCR gi|12483353 |gb|BG040768.1|BG040768  NXSI_114_H01_F NXSI (Nsf...    29   1.200 533  26
CCR gi|5649878  |gb|AI920246.1|AI920246  1776 Pine Lambda Zap Xyle..    29   1.200 625  26
CCR gi|12483505 |gb|BG040920.1|BG040920  NXSI_116_F10_F NXSI (Nsf...    29   1.200 546  32
CCR gi|12125518 |gb|BF777618.1|BF777618  NXSI_070_F01_F NXSI (Nsf...    29   1.200 442  26
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>CCR subfamily 1 Pinus_taeda
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 H  I  S  K

>CCR subfamily 2 Pinus_taeda
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Cinnamyl alcohol dehydrogenase (CAD)

tBLASTn report

CAD gi|11779142 |gb|BF610463.1|BF610463	NXSI_058_G06_F NXSI (Nsf...	335	6e-93	536	97
CAD gi|12482543 |gb|BG039862.1|BG039862	NXSI_104_H07_F NXSI (Nsf...	332	7e-92	558	89
CAD gi|14668812 |gb|BI202840.1|BI202840	NXPV_091_C09_F NXPV (Nsf...	306	4e-84	537	92
CAD gi|10798224 |gb|BF049827.1|BF049827	NXCI_111_D08_F NXCI (Nsf...	296	4e-81	454	99
CAD gi|12482616 |gb|BG040031.1|BG040031	NXSI_105_G03_F NXSI (Nsf...	276	3e-75	532	83
CAD gi|13068352 |gb|BG275227.1|BG275227	NXSI_138_C04_F NXSI (Nsf...	276	3e-75	488	93
CAD gi|12483465 |gb|BG040880.1|BG040880	NXSI_116_C06_F NXSI (Nsf...	276	3e-75	547	95
CAD gi|8517057 |gb|BE123743.1|BE123743	NXNV_153_E12_F Nsf Xylem...	275	8e-75	525	83
CAD gi|9833253 |gb|BE582305.1|BE582305	NXCI_031_G09_F NXCI (Nsf...	257	2e-69	459	92
CAD gi|12126129 |gb|BF778313.1|BF778313	NXSI_080_G04_F NXSI (Nsf...	256	3e-69	428	95
CAD gi|11604149 |gb|BF516866.1|BF516866	NXSI_004_E02_F NXSI (Nsf...	226	5e-60	398	92
CAD gi|18433745 |gb|BM428051.1|BM428051	NXRV_008_B03_F NXRV (Nsf...	223	5e-59	401	92
CAD gi|13128430 |gb|BG319000.1|BG319000	NXPV_022_D09_F NXPV (Nsf...	195	1e-50	361	92
CAD gi|5043829 |gb|AI724977.1|AI724977	876 PtIFG2 Pinus taeda cD..	194	2e-50	673	54
CAD gi|8666516 |gb|BE187332.1|BE187332	NXNV_162_F07_F Nsf Xylem ..	193	3e-50	304	92
CAD gi|14515615 |gb|BI076958.1|BI076958	NXPV_085_C05_F NXPV (Nsf...	187	3e-48	491	56
CAD gi|8666475 |gb|BE187291.1|BE187291	NXNV_162_B03_F Nsf Xylem...	184	2e-47	490	100
CAD gi|13127551 |gb|BG318121.1|BG318121	NXPV_010_F11_F NXPV (Nsf...	183	4e-47	491	54
CAD gi|17243629 |gb|BM158200.1|BM158200	NXLV_030_G08_F NXLV (Nsf...	176	6e-45	301	94
CAD gi|12482332 |gb|BG039747.1|BG039747	NXSI_103_D11_F NXSI (Nsf...	175	8e-45	544	48
CAD gi|9956384 |gb|BE643777.1|BE643777	NXCI_047_B02_F NXCI (Nsf ..	173	3e-44	320	94
CAD gi|13126952 |gb|BG317522.1|BG317522	NXPV_002_G08_F NXPV (Nsf...	172	9e-44	439	60
CAD gi|7690507 |gb|AW758589.1|AW758589	NXNV_075_C04_F Nsf Xylem ..	170	3e-43	260	93
CAD gi|10711175 |gb|BF010901.1|BF010901	NXCI_094_D10_F NXCI (Nsf...	166	4e-42	294	93
CAD gi|7580767 |gb|AW698181.1|AW698181	NXNV_074_C12_F Nsf Xylem ..	166	7e-42	341	78
CAD gi|3365598 |gb|AA556583.1|AA556583	438 Loblolly pine C Pinus..	163	3e-41	555	73

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CAD gi|18613961 |gb|BM493030.1|BM493030  NXRV_037_A01_F NXRV (Nsf...   157   3e-39 280  89
CAD gi|9956800  |gb|BE644193.1|BE644193  NXCI_049_G06_F NXCI (Nsf ..   155   9e-39 261  93
CAD gi|17244595 |gb|BM158723.1|BM158723  NXLV_039_D03_F NXLV (Nsf...   145   9e-37 284  57
CAD gi|9884400  |gb|BE607164.1|BE607164  NXCI_037_F11_F NXCI (Nsf...   147   2e-36 272  94
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CAD gi|5044186  |gb|AI725214.1|AI725214  1233 PtIFG2 Pinus taeda ...   143   3e-35 602  47
CAD gi|11068530 |gb|BF186357.1|BF186357  NXCI_136_H08_F NXCI (Nsf...   143   5e-35 404  55
CAD gi|9832987  |gb|BE582123.1|BE582123  NXCI_029_D01_F NXCI (Nsf ..   142   1e-34 270  93
CAD gi|11054340 |gb|BF169721.1|BF169721  NXCI_128_B05_F NXCI (Nsf...   139   7e-34 257  89
CAD gi|18613453 |gb|BM492522.1|BM492522  NXRV_026_E09_F NXRV (Nsf...   124   2e-29 408  53
CAD gi|5858893  |gb|AW010115.1|AW010115  ST02B03 Pine TriplEx shoo..   124   3e-29 470  64
CAD gi|11606165 |gb|BF517781.1|BF517781  NXSI_031_B08_F NXSI (Nsf...   122   1e-28 266  75
CAD gi|7676753  |gb|AW755033.1|AW755033  PC09H04 Pine TriplEx poll..   118   2e-27 383  59
CAD gi|5929284  |gb|AW056589.1|AW056589  ST53A05 Pine TriplEx shoo..   109   6e-25 453  45
CAD gi|7580578  |gb|AW697980.1|AW697980  NXNV_079_A08_F Nsf Xylem ..   108   1e-24 408  40
CAD gi|9956508  |gb|BE643901.1|BE643901  NXCI_048_G10_F NXCI (Nsf ..   105   1e-23 385  53
CAD gi|5423701  |gb|AI812486.1|AI812486  11G1 Pine Lambda Zap Xyle..   102   9e-23 453  40
CAD gi|2778629  |gb|AA740078.1|AA740078  843 PtIFG2 Pinus taeda cD..    95   2e-20 657  45
CAD gi|12481790 |gb|BG039205.1|BG039205  NXSI_096_B09_F NXSI (Nsf...    95   2e-20 289  55
CAD gi|18613821 |gb|BM492890.1|BM492890  NXRV_033_E05_F NXRV (Nsf...    94   4e-20 272  53
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CAD gi|8517100  |gb|BE123786.1|BE123786  NXNV_156_D04_F Nsf Xylem ..    82   1e-16 245  52
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CAD gi|10819555 |gb|BF060645.1|BF060645  NXCI_118_H04_F NXCI (Nsf...    67   3e-12 205  55
CAD gi|12483392 |gb|BG040807.1|BG040807  NXSI_115_D01_F NXSI (Nsf...    59   1e-09 541  30
CAD gi|5424039  |gb|AI812824.1|AI812824  19F8 Pine Lambda Zap Xyle..    57   3e-09 500  30
CAD gi|6696630  |gb|AW289994.1|AW289994  NXNV009F07F Nsf Xylem Nor..    57   3e-09 537  30
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CAD gi|13127446 |gb|BG318016.1|BG318016  NXPV_008_E09_F NXPV (Nsf...    51   2e-07 581  31
CAD gi|13127516 |gb|BG318086.1|BG318086  NXPV_010_C12_F NXPV (Nsf...    51   2e-07 553  31
CAD gi|12482565 |gb|BG039884.1|BG039884  NXSI_105_C02_F NXSI (Nsf...    50   5e-07 491  31
CAD gi|10710853 |gb|BF010579.1|BF010579  NXCI_086_D01_F NXCI (Nsf...    49   2e-06 201  40
CAD gi|5424461  |gb|AI813246.1|AI813246  3G4 Pine Lambda Zap Xylem..    48   3e-06 665  27
CAD gi|5423623  |gb|AI812425.1|AI812425  10D5 Pine Lambda Zap Xyle..    47   6e-06 715  29
CAD gi|12125104 |gb|BF777204.1|BF777204  NXSI_066_D12_F NXSI (Nsf...    47   6e-06 553  29
CAD gi|3365675  |gb|AA556660.1|AA556660  515 Loblolly pine CA Pinu..    45   2e-05 594  31
CAD gi|11777683 |gb|BF609735.1|BF609735  NXSI_048_G09_F NXSI (Nsf...    45   2e-05 319  34
CAD gi|5649825  |gb|AI920193.1|AI920193  1723 Pine Lambda Zap Xyle..    44   3e-05 617  27
CAD gi|5929417  |gb|AW056722.1|AW056722  ST55A03 Pine TriplEx shoo..    44   3e-05 550  27
CAD gi|5903174  |gb|AW042597.1|AW042597  ST23G07 Pine TriplEx shoo..    44   3e-05 594  27
CAD gi|6020137  |gb|AW065065.1|AW065065  ST39B11 Pine TriplEx shoo..    43   6e-05 601  27
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CAD gi|17243651 |gb|BM158212.1|BM158212  NXLV_030_H08_F NXLV (Nsf...    43   8e-05 200  36
CAD gi|12483340 |gb|BG040755.1|BG040755  NXSI_114_F12_F NXSI (Nsf...    42   1e-04 536  27
CAD gi|7274700  |gb|AW587673.1|AW587673  ST63C09 Pine TriplEx shoo..    42   2e-04 427  37
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CAD gi|11607035 |gb|BF518352.1|BF518352  NXSI_038_D06_F NXSI (Nsf...    41   3e-04 274  37
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CAD gi|10711072 |gb|BF010798.1|BF010798  NXCI_068_H03_F NXCI (Nsf...    40   5e-04 402  27
CAD gi|10681852 |gb|BE996907.1|BE996907  NXCI_097_D12_F NXCI (Nsf...    39   0.001 319  31
CAD gi|11127168 |gb|BF221036.1|BF221036  NXCI_162_D10_F NXCI (Nsf...    39   0.001 460  32
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CAD gi|5929457  |gb|AW056762.1|AW056762  ST55E09 Pine TriplEx shoo..    39   0.002 516  22
CAD gi|13126996 |gb|BG317566.1|BG317566  NXPV_003_C09_F NXPV (Nsf...    37   0.005 443  32
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CAD gi|10711024 |gb|BF010750.1|BF010750  NXCI_068_A11_F NXCI (Nsf...    35   0.023 405  30
CAD gi|13433329 |gb|BG485762.1|BG485762  NXPV_038_E06_F NXPV (Nsf...    35   0.023 435  33
CAD gi|12483260 |gb|BG040675.1|BG040675  NXSI_113_G12_F NXSI (Nsf...    34   0.039 539  28
CAD gi|11127376 |gb|BF221244.1|BF221244  NXCI_156_D10_F NXCI (Nsf...    33   0.051 377  30
CAD gi|12126036 |gb|BF778136.1|BF778136  NXSI_077_E12_F NXSI (Nsf...    33   0.051 393  31
CAD gi|11606740 |gb|BF518165.1|BF518165  NXSI_035_H05_F NXSI (Nsf...    33   0.087 223  31
CAD gi|7644760  |gb|AW736896.1|AW736896  NXNV_081_B11_F Nsf Xylem ..    32   0.110 293  27
CAD gi|6696150  |gb|AW289514.1|AW289514  NXNV001D05F Nsf Xylem Nor..    32   0.150 332  29
CAD gi|11606624 |gb|BF518107.1|BF518107  NXSI_035_A11_F NXSI (Nsf...    32   0.190 320  29
CAD gi|12481779 |gb|BG039194.1|BG039194  NXSI_096_A09_F NXSI (Nsf...    32   0.190 246  36
CAD gi|12483547 |gb|BG040962.1|BG040962  NXSI_117_B05_F NXSI (Nsf...    31   0.330 258  50
CAD gi|12125290 |gb|BF777390.1|BF777390  NXSI_071_A08_F NXSI (Nsf...    30   0.740 250  33
CAD gi|3366060  |gb|AA557046.1|AA557046  888 Loblolly pine N Pinus..    27   3.700 557  45
CAD gi|11605883 |gb|BF517820.1|BF517820  NXSI_027_E12_F NXSI (Nsf...    27   4.800 493  22
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>CAD subfamily 1 Pinus_taeda
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