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(54) Title: METHODS AND COMPOSITIONS FOR DETERMINING ENZYMATIC ACTIVITY

(57) Abstract: The present invention comprises crystalline polyketide synthases, isolated non-native polyketide synthases having the structural coordinates of said crystalline polyketide synthases, and nucleic acids encoding such non-native polyketide synthases. Also disclosed are methods of predicting the activity and/or substrate specificity of putative polyketide synthase, methods of identifying potential polyketide synthase substrates, and methods of identifying potential polyketide synthase inhibitors.

METHODS AND COMPOSITIONS FOR DETERMINING ENZYMATIC ACTIVITY

FIELD OF THE INVENTION

The present invention relates to methods for designing mutant polyketide synthases, and to predicting the activity and/or substrate specificity of putative native and mutant polyketide synthases. The present invention further relates to methods for identifying polyketide synthase substrates and/or inhibitors.

BACKGROUND

Advances in molecular biology have allowed the development of biological agents useful in modulating protein or nucleic acid activity or expression, respectively. Many of these advances are based on identifying the primary sequence of the molecule to be modulated. For example, determining the nucleic acid sequence of DNA or RNA allows the development of antisense or ribozyme molecules. Similarly, identifying the primary sequence allows for the identification of sequences that may be useful in creating monoclonal antibodies. However, often the primary sequence of a protein is insufficient to develop therapeutic or diagnostic molecules due to the secondary, tertiary or quartenary structure of the protein from which the primary sequence is obtained. The process of designing potent and specific inhibitors or activators has improved with the arrival of techniques for determining the three-dimensional structure of an enzyme or polypeptide to be modulated.

The phenylpropanoid synthetic pathway in plants produces a class of compounds know as anthocyanins, which are used for a variety of applications. Anthocyanins are involved in pigmentation and protection against UV photodamage, synthesis of anti-microbial phytoalexins, and are flavonoid inducers of *Rhizobium* modulation genes l-4. As medicinal natural products, the phenylpropanoids exhibit cancer chemopreventive activity, as well as anti-mitotic, estrogenic, anti-malarial, anti-oxidant, and antiasthmatic activities. The benefits of consuming red wine, which contains significant amounts of 3,4',5-trihydroxystilbene (resveratrol) and other phenylpropanoids, highlight the dietary importance of these compounds. Chalcone

synthase (CHS), a polyketide synthase, plays an essential role in the biosynthesis of plant phenylpropanoids.

An improvement in the understanding of the structure/function of these enzymes would allow for the exploitation of the synthetic capabilities of known enzymes for production of useful new chemical compounds, or allow for the creation of novel non-native enzymes having new synthetic capabilities. A need exists, therefore, for a detailed understanding of the molecular basis of the chemical reactions involved in polyketide synthesis. The present invention addresses this and related needs.

SUMMARY OF THE INVENTION

In accordance with the present invention there are presented crystalline polyketide synthases and the three-dimensional coordinates derived therefrom. Three-dimensional coordinates have been obtained for an active form of chalcone synthase and several inactive mutants thereof, both with and without substrate or substrate analog. Similar results have been obtained for the polyketide synthases stilbene synthase and pyrone synthase.

One aspect of the present invention that is made possible by results described herein is that the three-dimensional properties of polyketide synthase proteins are determined, in particular the three-dimensional properties of the active site. The invention features specific coordinates of at least fourteen α carbon atoms defined for the active site in three-dimensional space. R-groups attached to said α-carbons are defined such that mutants can be made by changing at least one R-group found in the synthase active site. Such mutants may have unique and useful properties. Thus, in another embodiment of the invention, there are provided isolated non-native (*e.g.*, mutant) synthase(s) having at least fourteen active site α-carbons having the structural coordinates disclosed herein and one or more R-groups other than those found in native chalcone synthase(s).

The three-dimensional coordinates disclosed herein can be employed in a variety of methods. The polyketide synthase used in the crystallization studies

disclosed herein is a chalcone synthase derived from *Medicago sataiva* (alfalfa). A large number of proteins have been isolated and sequenced which have primary amino acid sequence similar to that of chalcone synthase, but for which substrate specificity and/or product is unknown. Thus, in another embodiment of the present invention, there are provided methods for predicting the activity and/or substrate specificity of a putative polyketide synthase. There are further provided methods for identifying potential substrates for a polyketide synthase, as well as inhibitors thereof.

Other aspects, embodiments, advantages, and features of the present invention will become apparent from the following specification.

BRIEF DESCRIPTION OF FIGURES

Figure 1A presents the chemical structures of chalcone, naringenin, resveratrol, and cerulenin. **Figure 1B** presents final SIGMAA-weighted 2Fo-Fc electron density map of the CHS-resveratrol complex in the vicinity of the resveratrol binding site. The map is contoured at 1σ.

Figure 2A shows a ribbon representation of the CHS homodimer. The approximate alpha carbon positions of Met 137 from each of the monomers are labeled accordingly. Naringenin completely fills the coumaroyl-binding and cyclization pockets while the CoA binding tunnels are highlighted by black arrows. Produced with MOLSCRIPT and rendered with POV-Ray. **Figure 2B** presents a stereoview of the monomer's alpha carbon backbone. The orientation of the left-hand monomer is exactly the same as in **Figure 2A**. Every twenty residues are numbered starting with residue 3 and include the C-terminal residue, 389.

Figure 3 shows a comparison of chalcone synthase and 3-ketoacyl-CoA thiolase. Ribbon view of the CHS monomer is oriented perpendicular to the dimer interface. The active site cysteine (Cys 164) and the location of bound CoA are rendered as ball and stick models. In addition, strands β1d and β2d of the cyclization pocket are noted. The reaction catalyzed by CHS is illustrated with the coumaroyl- and malonyl-derived portions of chalcone, respectively. The thiolase monomer is depicted in the same orientation as CHS with the Active site cysteine (Cys 125)

modeled and the reaction of thiolase as indicated. Figure prepared with MOLSCRIPT and rendered with POV-Ray.

Figure 4 collectively shows structures of CHS-Acyl-CoA complexes. The ribbon diagram in panel **Figure 4A** (on the top left) is the same as **Figure 2A**. The CoA binding region depicted in stereo is bounded by a black box in the upper ribbon diagram. Close-up stereoviews of the $C_{164}S$ mutant CoA binding region for the malonyl-and hexanoyl-CoA complexes are depicted in **Figures 4B** and **4C**, respectively. This mutant retains decarboxylation activity and an acetyl-CoA complex is observed crystallographically for the malonyl-CoA complex. In each complex, placement of the Met 137 loop originating from the dyad-related molecule spatially defines one wall of the cyclization pocket. Hydrogen bonds are depicted as spheres. Figure prepared with MOLSCRIPT and rendered with POV-Ray.

Figure 5A shows the CHS-naringenin complex viewed down the CoA-binding tunnel. The ribbon diagram at the top left has been rotated 90 degrees around the y-axis from the orientation shown in **Figure 2A**. This view approximates the global orientation of the CHS dimer used for the close-up view of the natingenin binding site depicted in stereo. Again, the black box highlights the region of CHS shown in stereo close-up. Hydrogen bonds are depicted as dashed cylinders. **Figure 5B** illustrates a comparison of the CHS apoenzyme, CHS-naringenin, and CHS-resveratrol structures. Protein backbone atoms for the three refined structures (apoenzyme, naringenin, and resveratrol) were superimposed by least squares fit in O. The position of bound naringenin and resveratrol are shown. For reference, a modeled low energy conformation of chalcone is indicated by dashed cylinders. Strands β1d and β2d for each complex are also depicted (see **Figure 3**). β2d does not change in all the complexes examined, but β1d moves in the CHS-resveratrol complex. **Figure 5C** presents representative sequence alignment of the β1d -β2d region is given with positions 255, 266, and 268 highlighted. The first three sequences follow a CHS-like cyclization pathway, while the last three use the STS-cyclization pathway. Figure prepared with MOLSCRIPT and rendered with POV-Ray.

Figure 6 presents the proposed reaction mechanism for chalcone synthesis. The three boxed regions labeled 1, 2, and 3 depict the addition of acetate units derived from malonyl-CoA during the elongation of polyketide intermediates. Box I is depicted in expanded fashion to illustrate the mechanistic details governing the decarboxylation, enolization, and condensation phase of ketide elongation. Smaller black arrows depict the flow of electrons. Each acetate unit of the malonyl-CoA thioesters is coded to emphasize the portions of chalcone derived from each of three elongation reactions using malonyl-CoA. Cyclization and aromatization of the enzyme bound tetraketide leads to formation of chalcone. Hydrogen bonds are shown as dashed lines. Coenzyme A is symbolized as a circle.

Figure 7 collectively presents three-dimensional models of the elongation and cyclization reaction in CHS and STS. Views are shown in stereo. **Figure 7A** illustrates the elongation of the triketide covalently attached to Cys 164 by the acetyl-CoA carbanion produces the tetraketide CoA thioester reaction intermediate that subsequently reattaches to Cys 164. **Figure 7B** illustrates the folding of the tetraketide intermediate in CHS positions the oxygen of Cl near the hydrogen of C6 facilitating internal proton transfer and expulsion of chalcone upon cyclization. **Figure 7C** illustrates alternate folding of the tetraketide intermediate and positioning of the oxygen of C7 near the hydrogen of C2 in STS allows formation of resveratrol using an internal proton transfer followed by hydrolysis and decarboxylation. Rendered and dashed lines illustrate potential hydrogen bonding interactions. Figure prepared with MOLSCREPIT and rendered with POV-Ray.

Figure 8 presents a comparison of the active site volumes of CHS and GCHS2. The active site volumes available for binding ketide intermediates were calculated with VOID00 for the CHS-COA complex and for a homology model of GCHS2 with CoA. The cavities are shown as a wire mesh. The homology model of GCHS2 was generated using MODELER and the volume calculated and displayed as for CHS. The numbering scheme is for alfalfa CHS homodimer. Figure prepared with MOLSCRIPT and rendered with POV-Ray.

Figure 9 shows an example of a computer system in block diagram form.

DETAILED DESCRIPTION OF THE INVENTION

The phenylpropanoid synthetic pathway in plants produces a class of compounds know as anthocyanins, which are used for a variety of applications. Anthocyanins are involved in pigmentation and protection against UV photodamage, synthesis of anti-microbial phytoalexins, and are flavonoid inducers of *Rhizobium* modulation genes l-4. As medicinal natural products, the phenylpropanoids exhibit cancer chemopreventive activity, as well as anti-mitotic, estrogenic, anti-malarial, anti-oxidant, and antiasthmatic activities. The benefits of consuming red wine, which contains significant amounts of 3,4',5-trihydroxystilbene (resveratrol) and other phenylpropanoids, highlight the dietary importance of these compounds.

Polyketides are a large class of compounds and include a broad range of antibiotics, immunosuppressants and anticancer agents which together account for sales of over $5 billion per year. Polyketides are molecules which are an extremely rich source of bioactivities, including antibiotics (*e.g.*, tetracyclines and erythromycin), anti-cancer agents (*e.g.*, daunomycin), immunosuppressants (*e.g.*, FK506 and rapamycin), and veterinary products (*e.g.*, monensin) and the like. Many polyketides (produced by polyketide synthases) are valuable as therapeutic agents. Polyketide synthases are multifunctional enzymes that catalyze the biosynthesis of a huge variety of carbon chains differing in length and patterns of functionality and cyclization.

Chalcone synthase (CHS), a polyketide synthase, plays an essential role in the biosynthesis of plant phenylpropanoids. CHS supplies 4,2',4',6'-tetrahydroxychalcone (chalcone) to downstream enzymes that synthesize a diverse set of flavonoid phytoalexins and anthocyanin pigments. Synthesis of chalcone by CHS involves the sequential condensation of one p-coumaroyl- and three malonyl-Coenzyme-A (CoA) molecules (Kreuzaler and Hahlbrock, Eur. J. Biochem. 56:205-213, 1975). After initial capture of the p-coumaroyl moiety, each subsequent condensation step begins

with decarboxylation of malonyl-CoA at the CHS active site; the resulting acetyl-CoA carbanion then serves as the nucleophile for chain elongation.

Ultimately, these reactions generate a tetraketide intermediate that cyclizes by a Claisen condensation into a hydroxylated aromatic ring system. This mechanism mirrors those of the fatty acid and polyketide synthases but with significant differences. CHS uses CoA-thioesters for shuttling substrates and intermediate polyketides instead of the acyl carrier proteins used by the fatty acid synthases. Also, unlike these enzymes, which function as either multichain or multimodular enzyme complexes catalyzing distinct reactions at different active sites, CHS functions as a unimodular polyketide synthase and carries out a series of decarboxylation, condensation, cyclization, and aromatization reactions at a single active site.

A number of plant polyketide synthases related to CHS by sequence identity, including stilbene synthase (STS), bibenzyl synthase (BBS), and acridone synthase (ACS), share a common chemical mechanism, but differ from CHS in their substrate specificity and/or in the stereochemistry of the polyketide cyclization reaction. For example, STS condenses one coumaroyl- and three malonyl-CoA molecules, like CHS, but synthesizes resveratrol (resveratrol) through a structurally distinct cyclization intermediate.

While the cloning of nearly 150 CHS-related genes, and characterization of some of these proteins, provides insight into their biological function, it remains unclear how these enzymes perform multiple decarboxylation and condensation reactions and how they dictate the stereochemistry of the final polyketide cyclization reaction. Furthermore, despite significant advances in the biosynthetic manipulation of structurally complex and biologically important natural products, there remains a lack of structural information on polyketide synthases from any source.

As used herein, "naturally occurring amino acid" and "naturally occurring R-group" includes L-isomers of the twenty amino acids naturally occurring in proteins. Naturally occurring amino acids are glycine, alanine, valine, leucine, isoleucine, serine, methionine, threonine, phenylalanine, tyrosine, tryptophan, cysteine, proline,

histidine, aspartic acid, asparagine, glutamic acid, glutamine, arginine, and lysine. Unless specially indicated, all amino acids referred to in this application are in the L-form.

"Unnatural amino acid" and "unnatural R-group" includes amino acids that are not naturally found in proteins. Examples of unnatural amino acids included herein are racemic mixtures of selenocysteine and selenomethionine. In addition, unnatural amino acids include the D or L forms of, for example, nor-leucine, para-nitrophenylalanine, homophenylalanine, para-fluorophenylalanine, 3-amino-2-benzylpropionic acid, homoarginines, D-phenylalanine, and the like.

"R-group" refers to the substituent attached to the α-carbon of an amino acid residue. An R-group is an important determinant of the overall chemical character of an amino acid. There are twenty natural R-groups found in proteins, which make up the twenty naturally occurring amino acids.

"α-carbon" refers to the chiral carbon atom found in an amino acid residue. Typically, four substituents will be covalently bound to said α-carbon including an amine group, a carboxylic acid group, a hydrogen atom, and an R-group.

"Positively charged amino acid" and "positively charged R-group" includes any naturally occurring or unnatural amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged, naturally occurring amino acids include arginine, lysine, histidine, and the like.

"Negatively charged amino acid" and "negatively charged R-group" includes any naturally occurring or unnatural amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged, naturally occurring amino acids include aspartic acid, glutamic acid, and the like.

"Hydrophobic amino acid" and "hydrophobic R-group" includes any naturally occurring or unnatural amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of naturally occurring hydrophobic amino acids are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan, methionine, and the like.

"Hydrophilic amino acid" and "hydrophilic R-group" includes any naturally occurring or unnatural amino acid having a charged polar side chain that is relatively soluble in water. Examples of naturally occurring hydrophilic amino acids include serine, threonine, tyrosine, asparagine, glutamine, cysteine, and the like.

"Mutant" or "mutated synthase" refers to a polyketide synthase polypeptide, having the three-dimensional coordinates as set forth in Protein Data Bank (PDB) Accession No. 1BI5 (the content of which is incorporated herein by reference in its entirety), and having R-groups on each α-carbon other than the prescribed arrangements of R-groups associated with each α-carbon of a known isolated polyketide synthase (Accession No. 1BI5). Examples of mutant or mutated synthase polypeptides include those having Protein Data Base Accession No. 1D6F, 1K6I, and 1D6H (the content of which are incorporated herein by reference in their entirety). Access to the foregoing information in the Protein Data Bank can be found at www.rcsb.org.

The R-groups of known isolated polyketide synthases can be readily determined by consulting sequence databases well known in the art, such as, for example, Genbank. Additional R-groups found inside and/or outside of the active site may or may not be the same. R-groups may be a natural R-group, unnatural R-group, hydrophobic R-group, hydrophilic R-group, positively charged R-group, negatively charged R-group, and the like. The term "mutant" only refers to the configuration of R-groups within the active site; therefore, mutations outside of the residues found in the active site are not considered to be mutants in light of the present invention.

"Nonmutated synthase" includes a synthase wherein no R-group(s) are changed relative to the active site of CHS (see, for example, PDB Accession No. 1BI5). A nonmutated synthase according to the present invention may or may not have amino acid residues outside of the active site that are the same as those taught for native CHS. In addition, a nonmutated synthase is a synthase having an active site comprising α-carbons having the coordinates as given in Table 1 and having the arrangements of R-groups associated with α-carbons as given in Table 1.

TABLE 1

Structural Cartesian coordinates of α-carbons found in the active site of a polyketide synthase of the present invention.

Active Site –Carbon Number	X Position	Y Position	Z Position	Amino Acid
1	25.378	49.320	57.979	Thr 132
2	26.089	45.704	56.981	Ser 133
3	35.423	42.296	66.622	Met 137*
4	25.212	49.977	62.196	Gln 161
5	22.745	44.120	51.193	Thr 194
6	19.022	42.892	54.600	Thr 197
7	13.850	48.144	50.791	Gly 211
8	22.118	48.048	46.357	Gly 216
9	13.001	54.666	59.688	Ile 254
10	16.434	48.819	61.334	Gly 256
11	18.715	43.328	59.526	Leu 263
12	13.943	47.516	57.567	Phe 265
13	9.252	52.715	57.456	Leu 267
14	23.141	53.552	52.148	Ser 338

* Met 137 from the second monomer

"Non-native" or "non-native synthase" refers to synthase proteins that are not found in nature, whether isolated or not. A non-native synthase may, for example, be a mutated synthase (see, for example, PDB Accession No. 1D6F, 1D6I and 1D6H).

"Native" or "native synthase" refers to synthase proteins that are produced in nature, *e.g.*, are not mutants (see, for example, PDB Accession No. 1BI5).

"Isolated" refers to a protein or nucleic acid that has been identified and separated from its natural environment. Contaminant components of its natural environment may include enzymes, hormones, and other proteinaceous or non-proteinaceous solutes. In one embodiment, the isolated molecule, in the case of a protein, will be purified to a degree sufficient to obtain at least 15 residues of

N-terminal or internal amino acid sequence or to homogeneity by SDS-PAGE under reducing or non-reducing conditions using Coomassie blue or silver stain. In the case of a nucleic acid the isolated molecule will preferably be purified to a degree sufficient to obtain a nucleic acid sequence using standard sequencing methods.

"Degenerate variations thereof" refers to changing a gene sequence using the degenerate nature of the genetic code to encode proteins having the same amino acid sequence yet having a different gene sequence. For example, polyketide synthases of the present invention are based on amino acid sequences. Degenerate gene variations thereof can be made encoding the same protein due to the plasticity of the genetic code, as described herein.

"Expression" refers to transcription of a gene or nucleic acid sequence, stable accumulation of nucleic acid, and the translation of that nucleic acid to a polypeptide sequence. Expression of genes also involves transcription of the gene to make RNA, processing of RNA into mRNA in eukaryotic systems, and translation of mRNA into proteins. It is not necessary for the genes to integrate into the genome of a cell in order to achieve expression. This definition in no way limits expression to a particular system or to being confined to cells or a particular cell type and is meant to include cellular, transient, *in vitro, in vivo*, and viral expression systems in both prokaryotic, eukaryotic cells, and the like.

"Foreign" or "heterologous" genes refers to a gene encoding a protein whose exact amino acid sequence is not normally found in the host cell.

"Promoter" and "promoter regulatory element", and the like, refers to a nucleotide sequence element within a nucleic acid fragment or gene that controls the expression of that gene. These can also include expression control sequences. Promoter regulatory elements, and the like, from a variety of sources can be used efficiently to promote gene expression. Promoter regulatory elements are meant to include constitutive, tissue-specific, developmental-specific, inducible, subgenomic promoters, and the like. Promoter regulatory elements may also include certain enhancer elements or silencing elements that improve or regulate transcriptional

efficiency. Promoter regulatory elements are recognized by RNA polymerases, promote the binding thereof, and facilitate RNA transcription.

A polypeptide is a chain of amino acids, regardless of length or post-translational modification (*e.g.*, glycosylation or phosphorylation). A polypeptide or protein refers to a polymer in which the monomers are amino acid residues, which are joined together through amide bonds. When the amino acids are alpha-amino acids, either the L-optical isomer or the D-optical isomer can be used, the L-isomers being typical. A synthase polypeptide of the invention is intended to encompass an amino acid sequence as set forth in SEQ ID NO:1 (see, Table 2) or SEQ ID NO:1 having one or more of the following mutations: C164A, H303Q, and N336A, mutants, variants and conservative substitutions thereof comprising L- or D- amino acids and include modified sequences such as glycoproteins.

TABLE 2 (SEQ ID NO:1)

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MVSVSEIRKA QRAEGPATIL AIGTANPANC VEQSTYPDFY FKITNSEHKT ELKEKFQRMC
DKSMIKRRYM YLTEEILKEN PNVCEYMAPS LDARQDMVVV EVPRLGKEAA VKAIKEWGQP
KSKITHLIVC TTSGVDMPGA DYQLTKLLGL RPYVKRYMMY QQGXFAGGTV LRLAKDLAEN
NKGARVLVVC SEVTAVTFRG PSDTHLDSLV GQALFGDGAA ALIVGSDPVP EIEKPIFEMV
WTAQTIAPDS EGAIDGHLRE AGLTFHLLKD VPGIVSKNIT KALVEAFEPL GISDYNSIFW
IAHPGGPAIL DQVEQKLALK PEKMNATREV LSEYGNMSSA CVLFILDEMR KKSTQNGLKT
TGEGLEWGVL FGFGPGLTIE TVVLRSVAI
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Accordingly, the polypeptides of the invention are intended to cover naturally occurring proteins, as well as those which are recombinantly or synthetically synthesized. Polypeptide or protein fragments are also encompassed by the invention. Fragments can have the same or substantially the same amino acid sequence as the naturally occurring protein. A polypeptide or peptide having substantially the same sequence means that an amino acid sequence is largely, but not entirely, the same, but retains a functional activity of the sequence to which it is related. In general polypeptides of the invention include peptides, or full-length protein, that contains substitutions, deletions, or insertions into the protein backbone, that would still have an

approximately 70%-90% homology to the original protein over the corresponding portion. A yet greater degree of departure from homology is allowed if like-amino acids, *i.e.* conservative amino acid substitutions, do not count as a change in the sequence.

A polypeptide may be substantially related but for a conservative variation, such polypeptides being encompassed by the invention. A conservative variation denotes the replacement of an amino acid residue by another, biologically similar residue. Examples of conservative variations include the substitution of one hydrophobic residue such as isoleucine, valine, leucine or methionine for another, or the substitution of one polar residue for another, such as the substitution of arginine for lysine, glutamic for aspartic acids, or glutamine for asparagine, and the like. Other illustrative examples of conservative substitutions include the changes of: alanine to serine; arginine to lysine; asparagine to glutamine or histidine; aspartate to glutamate; cysteine to serine; glutamine to asparagine; glutamate to aspartate; glycine to proline; histidine to asparagine or glutamine; isoleucine to leucine or valine; leucine to valine or isoleucine; lysine to arginine, glutamine, or glutamate; methionine to leucine or isoleucine; phenylalanine to tyrosine, leucine or methionine; serine to threonine; threonine to serine; tryptophan to tyrosine; tyrosine to tryptophan or phenylalanine; valine to isoleucine or leucine, and the like. The term "conservative variation" also includes the use of a substituted amino acid in place of an unsubstituted parent amino acid provided that antibodies raised to the substituted polypeptide also immunoreact with the unsubstituted polypeptide.

Modifications and substitutions are not limited to replacement of amino acids. For a variety of purposes, such as increased stability, solubility, or configuration concerns, one skilled in the art will recognize the need to introduce, (by deletion, replacement, or addition) other modifications. Examples of such other modifications include incorporation of rare amino acids, dextra-amino acids, glycosylation sites, cytosine for specific disulfide bridge formation. The modified peptides can be chemically synthesized, or the isolated gene can be site-directed mutagenized, or a

synthetic gene can be synthesized and expressed in bacteria, yeast, baculovirus, tissue culture and so on.

Chalcone synthase polypeptides of the invention include synthase polypeptides from plants, prokaryotes, eukaryotes, including, for example, invertebrates, mammals and humans and include sequences as set forth in SEQ ID NO:1, as well as sequences that have at least 70% homology to the sequence of SEQ ID NO:1, fragments, variants, or conservative substitutions of any of the foregoing sequences.

The term "variant" refers to polypeptides modified at one or more amino acid residues yet still retain the biological activity of a synthase polypeptide. Variants can be produced by any number of means known in the art, including, for example, methods such as, for example, error-prone PCR, shuffling, oligonucleotide-directed mutagenesis, assembly PCR, sexual PCR mutagenesis, and the like, as well as any combination thereof.

By "substantially identical" is meant a polypeptide or nucleic acid exhibiting at least 50%, preferably 85%, more preferably 90%, and most preferably 95% homology to a reference amino acid or nucleic acid sequence.

Homology or identity is often measured using sequence analysis software (*e.g.*, Sequence Analysis Software Package of the Genetics Computer Group, University of Wisconsin Biotechnology Center, 1710 University Avenue, Madison, WI 53705). Such software matches similar sequences by assigning degrees of homology to various deletions, substitutions and other modifications. The terms "homology" and "identity" in the context of two or more nucleic acids or polypeptide sequences, refer to two or more sequences or subsequences that are the same or have a specified percentage of amino acid residues or nucleotides that are the same when compared and aligned for maximum correspondence over a comparison window or designated region as measured using any number of sequence comparison algorithms or by manual alignment and visual inspection.

For sequence comparison, typically one sequence acts as a reference sequence, to which test sequences are compared. When using a sequence comparison algorithm, test and reference sequences are entered into a computer, subsequence coordinates are designated, if necessary, and sequence algorithm program parameters are designated. Default program parameters can be used, or alternative parameters can be designated. The sequence comparison algorithm then calculates the percent sequence identities for the test sequences relative to the reference sequence, based on the program parameters.

A "comparison window", as used herein, includes reference to a segment of any one of the number of contiguous positions selected from the group consisting of from 20 to 600, usually about 50 to about 200, more usually about 100 to about 150 in which a sequence may be compared to a reference sequence of the same number of contiguous positions after the two sequences are optimally aligned. Methods of alignment of sequence for comparison are well-known in the art. Optimal alignment of sequences for comparison can be conducted, *e.g.*, by the local homology algorithm of Smith & Waterman, Adv. Appl. Math. 2:482, 1981, by the homology alignment algorithm of Needleman & Wunsch, J. Mol. Biol 48:443, 1970, by the search for similarity method of Person & Lipman, Proc. Nat'l. Acad. Sci. USA 85:2444, 1988, by computerized implementations of these algorithms (GAP, BESTFIT, FASTA, and TFASTA in the Wisconsin Genetics Software Package, Genetics Computer Group, 575 Science Dr., Madison, WI), or by manual alignment and visual inspection. Other algorithms for determining homology or identity include, for example, in addition to a BLAST program (Basic Local Alignment Search Tool at the National Center for Biological Information), ALIGN, AMAS (Analysis of Multiply Aligned Sequences), AMPS (Protein Multiple Sequence Alignment), ASSET (Aligned Segment Statistical Evaluation Tool), BANDS, BESTSCOR, BIOSCAN (Biological Sequence Comparative Analysis Node), BLIMPS (BLocks IMProved Searcher), FASTA, Intervals & Points, BMB, CLUSTAL V, CLUSTAL W, CONSENSUS, LCONSENSUS, WCONSENSUS, Smith-Waterman algorithm, DARWIN, Las Vegas algorithm, FNAT (Forced Nucleotide Alignment Tool), Framealign, Framesearch, DYNAMIC, FILTER, FSAP (Fristensky Sequence Analysis Package), GAP (Global

Alignment Program), GENAL, GIBBS, GenQuest, ISSC (Sensitive Sequence Comparison), LALIGN (Local Sequence Alignment), LCP (Local Content Program), MACAW (Multiple Alignment Construction & Analysis Workbench), MAP (Multiple Alignment Program), MBLKP, MBLKN, PIMA (Pattern-Induced Multi-sequence Alignment), SAGA (Sequence Alignment by Genetic Algorithm) and WHAT-IF. Such alignment programs can also be used to screen genome databases to identify polynucleotide sequences having substantially identical sequences. A number of genome databases are available, for example, a substantial portion of the human genome is available as part of the Human Genome Sequencing Project (J. Roach, http://weber.u.Washington.edu/~roach/human_ genome_ progress 2.html) (Gibbs, 1995). At least twenty-one other genomes have already been sequenced, including, for example, *M. genitalium* (Fraser *et al.*, 1995), M. jannaschii (Bult *et al.*, 1996), *H. influenzae* (Fleischmann *et al.*, 1995), *E. coli* (Blattner *et al.*, 1997), and yeast (*S. cerevisiae*) (Mewes *et al.*, 1997), and *D. melanogaster* (Adams *et al.*, 2000). Significant progress has also been made in sequencing the genomes of model organism, such as mouse, *C. elegans*, and *Arabadopsis sp.* Several databases containing genomic information annotated with some functional information are maintained by different organization, and are accessible via the internet, for example, http://wwwtigr.org/tdb; http://www.genetics.wisc.edu; http://genome-www.stanford.edu/~ball; http://hiv-web.lanl.gov; http://www.ncbi.nlm.nih.gov; http://www.ebi.ac.uk; http://Pasteur.fr/other/biology; and http:// www.genome.wi.mit.edu.

One example of a useful algorithm is BLAST and BLAST 2.0 algorithms, which are described in Altschul *et al.*, Nuc. Acids Res. 25:3389-3402, 1977, and Altschul *et al.*, J. Mol. Biol. 215:403-410, 1990, respectively. Software for performing BLAST analyses is publicly available through the National Center for Biotechnology Information (http://www.ncbi.nlm.nih. gov). This algorithm involves first identifying high scoring sequence pairs (HSPs) by identifying short words of length W in the query sequence, which either match or satisfy some positive-valued threshold score T when aligned with a word of the same length in a database sequence. T is referred to as the neighborhood word score threshold (Altschul *et al.*, *supra*). These initial neighborhood

word hits act as seeds for initiating searches to find longer HSPs containing them. The word hits are extended in both directions along each sequence for as far as the cumulative alignment score can be increased. Cumulative scores are calculated using, for nucleotide sequences, the parameters M (reward score for a pair of matching residues; always >0). For amino acid sequences, a scoring matrix is used to calculate the cumulative score. Extension of the word hits in each direction are halted when: the cumulative alignment score falls off by the quantity X from its maximum achieved value; the cumulative score goes to zero or below, due to the accumulation of one or more negative-scoring residue alignments; or the end of either sequence is reached. The BLAST algorithm parameters W, T, and X determine the sensitivity and speed of the alignment. The BLASTN program (for nucleotide sequences) uses as defaults a wordlength (W) of 11, an expectation (E) of 10, M=5, N=-4 and a comparison of both strands. For amino acid sequences, the BLASTP program uses as defaults a wordlength of 3, and expectations (E) of 10, and the BLOSUM62 scoring matrix (see Henikoff & Henikoff, Proc. Natl. Acad. Sci. USA 89:10915, 1989) alignments (B) of 50, expectation (E) of 10, M=5, N= -4, and a comparison of both strands.

The BLAST algorithm also performs a statistical analysis of the similarity between two sequences (see, *e.g.*, Karlin & Altschul, Proc. Natl. Acad. Sci. USA 90:5873, 1993). One measure of similarity provided by BLAST algorithm is the smallest sum probability (P(N)), which provides an indication of the probability by which a match between two nucleotide or amino acid sequences would occur by chance. For example, a nucleic acid is considered similar to a references sequence if the smallest sum probability in a comparison of the test nucleic acid to the reference nucleic acid is less than about 0.2, more preferably less than about 0.01, and most preferably less than about 0.001.

In one embodiment, protein and nucleic acid sequence homologies are evaluated using the Basic Local Alignment Search Tool ("BLAST") In particular, five specific BLAST programs are used to perform the following task:

(1) BLASTP and BLAST3 compare an amino acid query sequence against a protein sequence database;

(2) BLASTN compares a nucleotide query sequence against a nucleotide sequence database;

(3) BLASTX compares the six-frame conceptual translation products of a query nucleotide sequence (both strands) against a protein sequence database;

(4) TBLASTN compares a query protein sequence against a nucleotide sequence database translated in all six reading frames (both strands); and

(5) TBLASTX compares the six-frame translations of a nucleotide query sequence against the six-frame translations of a nucleotide sequence database.

The BLAST programs identify homologous sequences by identifying similar segments, which are referred to herein as "high-scoring segment pairs," between a query amino or nucleic acid sequence and a test sequence which is preferably obtained from a protein or nucleic acid sequence database. High-scoring segment pairs are preferably identified (*i.e.*, aligned) by means of a scoring matrix, many of which are known in the art. Preferably, the scoring matrix used is the BLOSUM62 matrix (Gonnet *et al.*, Science 256:1443-1445, 1992; Henikoff and Henikoff, Proteins 17:49-61, 1993). Less preferably, the PAM or PAM250 matrices may also be used (see, *e.g.*, Schwartz and Dayhoff, eds., 1978, *Matrices for Detecting Distance Relationships: Atlas of Protein Sequence and Structure*, Washington: National Biomedical Research Foundation). BLAST programs are accessible through the U.S. National Library of Medicine, *e.g.*, at www.ncbi.nlm.nih.gov.

The parameters used with the above algorithms may be adapted depending on the sequence length and degree of homology studied. In some embodiments, the

parameters may be the default parameters used by the algorithms in the absence of instructions from the user.

By a "substantially pure polypeptide" is meant a synthase polypeptide (e.g., a chalcone synthase) which has been separated from components which naturally accompany it. Typically, the polypeptide is substantially pure when it is at least 60%, by weight, free from the proteins and naturally-occurring organic molecules with which it is naturally associated. Preferably, the preparation is at least 75%, more preferably at least 90%, and most preferably at least 99%, by weight, synthase polypeptide. A substantially pure synthase polypeptide may be obtained, for example, by extraction from a natural source; by expression of a recombinant nucleic acid encoding an synthase polypeptide; or by chemically synthesizing the protein. Purity can be measured by any appropriate method (*e.g.*, column chromatography, polyacrylamide gel electrophoresis, or by HPLC analysis).

One aspect of the invention resides in obtaining crystals of the synthase polypeptide chalcone synthase of sufficient quality to determine the three dimensional (tertiary) structure of the protein by X-ray diffraction methods. The knowledge obtained concerning the three-dimensional structure of chalcone synthase can be used in the determination of the three dimensional structure of other synthase polypeptides in the polyketide synthesis pathway. The structural coordinates of chalcone synthase can be used to develop new polyketide synthesis enzymes or synthase inhibitors using various computer models. Based on the structural coordinates of the chalcone synthase polypeptide (*e.g.*, the three dimensional protein structure), as described herein, novel polyketide synthases can be engineered. In addition, small molecules which mimic or are capable of interacting with a functional domain of a synthase molecule, can be designed and synthesized to modulate chalcone synthase, pyrone synthase, and other polyketide synthase biological functions as well as the biological functions of other polyketide synthases. Accordingly, in one embodiment, the invention provides a method of "rational" enzyme or drug design. Another approach

to "rational" enzyme or drug design is based on a lead compound that is discovered using high throughput screens; the lead compound is further modified based on a crystal structure of the binding regions of the molecule in question. Accordingly, another aspect of the invention is to provide related protein sequences or material which is a starting material in the rational design of new synthases or drugs which lead to the synthesis of new polyketides or modify the polyketide synthesis pathway.

"Active Site" refers to a site in a synthase defined by amino acid residues that interact with substrate and facilitate a biosynthetic reaction that allows one or more products to be produced. An active site is comprised of α-carbon atoms that are indirectly linked via peptide bonds and have the structural coordinates disclosed in Table 1 ± 2.3 angstroms. Other active site amino acids for chalcone synthase include C164, H303, and N336. The position in three-dimensional space of an α-carbon at the active site of a synthase and of R-groups associated therewith can be determined using techniques such as three-dimensional modeling, X-ray crystallography, and/or techniques associated therewith.

"Altered substrate specificity" includes a change in the ability of a mutant synthase to produce a polyketide product as compared to a non-mutated synthase. Altered substrate specificity may include the ability of a synthase to exhibit different enzymatic parameters relative to a non-mutated synthase (K_m, V_{max}. etc), use different substrates, and/or produce products that are different from those of known non-native synthases.

"Structure coordinates" refers to Cartesian coordinates (x, y, and z positions) derived from mathematical equations involving Fourier synthesis as determined from patterns obtained via diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a polyketide synthase molecule in crystal form. Diffraction data are used to calculate electron density maps of repeating protein units in the crystal (unit cell). Electron density maps are used to establish the positions of individual atoms within a crystal's unit cell. The term "crystal structure coordinates" refers to mathematical coordinates derived from mathematical equations related to the

patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a synthase polypeptide (*e.g.*, a chalcone synthase protein molecule) in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal. The crystal structure coordinates of a synthase can be obtained from a chalcone synthase protein crystal having space group $P3_221$ (a = b = 97.54 Å, c = 65.52 with a single monomer per asymmetric unit). The coordinates of the cynthase polypeptide can also be obtained by means of computational analysis.

The term "selenomethionine substitution" refers to the method of producing a chemically modified form of the crystal of a synthase (e.g., a chalcone synthase). The synthase protein is expressed by bacteria in media that is depleted in methionine and supplement with selenomethionine. Selenium is thereby incorporated into the crystal in place of methionine sulfurs. The location(s) of selenium are determined by X-ray diffraction analysis of the crystal. This information is used to generate the phase information used to construct a three-dimensional structure of the protein.

"Heavy atom derivatization" refers to a method of producing a chemically modified form of a synthase crystal. In practice, a crystal is soaked in a solution containing heavy atom salts or organometallic compounds, *e.g.*, lead chloride, gold thiomalate, thimerosal, uranyl acetate, and the like, which can diffuse through the crystal and bind to the protein's surface. Locations of the bound heavy atoms can be determined by X-ray diffraction analysis of the soaked crystal. This information is then used to construct phase information which can then be used to construct three-dimensional structures of the enzyme as described in Blundel, T. L., and Johnson, N. L., Protein Crystallography, Academic Press (1976), which is incorporated herein by reference.

"Unit cell" refers to a basic parallelepiped shaped block. Regular assembly of such blocks may construct the entire volume of a crystal. Each unit cell comprises a complete representation of the unit pattern, the repetition of which builds up the

crystal.

"Mutagenesis" refers to the changing of one R-group for another as defined herein. This can be most easily performed by changing the coding sequence of the nucleic acid encoding the amino acid residue. In the context of the present invention, mutagenesis does not change the carbon coordinates beyond the limits defined herein.

"Space Group" refers to the arrangement of symmetry elements within a crystal.

"Molecular replacement" refers to generating a preliminary model of a polyketide synthase whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal (Lattman, E., 1985, in Methods in Enzymology, 11 5.55-77; Rossmann, MG., ed., "The Molecular Replacement Method" 1972, Int, Sci. Rev. Ser., No. 13, Gordon & Breach, New York). Using structure coordinates of the polyketide synthase provided in Figure 1 molecular replacement may be used to determine the structural coordinates of a crystalline mutant, homologue, or a different crystal form of polyketide synthase.

A "synthase" or a "polyketide synthase" includes any one of a family of enzymes that catalyze the formation of polyketide compounds. Polyketide synthases are generally homodimers, with each monomer being enzymatically acitve.

"Substrate" refers to the Coenzyme-A (CoA) thioesters that are acted on by the polyketide synthases and mutants thereof disclosed herein, such as malonyl-CoA, coumaroyl-CoA, hexamoyl-CoA, and the like.

The present invention relates to crystallized polyketide synthases and mutants thereof from which the position of specific α-carbon atoms and R-groups associated therewith comprising the active site can be determined in three-dimensional space.

The invention also relates to structural coordinates of said polyketide synthases, use of said structural coordinates to develop structural information related to polyketide synthase homologues, mutants, and the like, and to crystal forms of such synthases. Furthermore, the invention, as disclosed herein, provides a method whereby said α-carbon structural coordinates specifically determined for atoms comprising the active site of said synthase, as shown in Table 1 and including C164, H303, and N336, can be used to develop synthases wherein R-groups associated with active site α-carbon atoms are different from the R-groups found in native CHS, *e.g.*, are mutant synthases. In addition, the present invention provides for production of mutant polyketide synthases based on the structural information provided herein and for use of said mutant synthases to make a variety of polyketide compounds using a variety of substrates.

The present invention further provides, for the first time, crystals of several polyketide synthases, as exemplified by chalcone synthase (CHS; PDB Accession No. 1B15), stilbene synthase (STS), and pyrone synthase (PS); see Table 3 for coordinates of PS ("molecule" denoted in the table refers to the particular monomer of the PS dimer). Also provided are coordinates for crystals which are grown in the presence and absence of substrate and substrate analogues, thus allowing definition of the structural or atomic coordinates associated therewith. Said structural coordinates allow determination of the carbon atoms comprising the active site, R-groups associated therewith, and the interaction of said α-carbons and said R-groups with each other. For example, Table 4 identifies various substrates and substrate analogues that were grown with chalcone synthase as well as their PDB accession numbers, all of which are incorporated herein by reference in their entirety.

TABLE 3

Atom	Atom Type	Res.	#	X	Y	Z	OCC	B	Molec
1	N	GLY	20	32.834	42.457	65.617	1.00	27.09	A
2	CA	GLY	20	33.866	41.428	65.356	1.00	23.93	A
3	C	GLY	20	33.175	40.130	64.906	1.00	21.83	A
4	O	GLY	20	31.967	40.073	64.809	1.00	20.10	A
5	N	LEU	21	34.001	39.120	64.701	1.00	19.92	A
6	CA	LEU	21	33.519	37.812	64.301	1.00	21.97	A

7	CB	LEU	21	34.698	36.928	63.924	1.00	20.90	A
8	CG	LEU	21	35.592	37.425	62.769	1.00	25.38	A
9	CD2	LEU	21	34.861	37.362	61.428	1.00	26.08	A
10	CD1	LEU	21	36.862	36.561	62.728	1.00	24.02	A
11	C	LEU	21	32.710	37.113	65.406	1.00	22.68	A
12	O	LEU	21	33.076	37.172	66.591	1.00	21.48	A
13	N	ALA	22	31.662	36.430	64.988	1.00	19.98	A
14	CA	ALA	22	30.941	35.520	65.863	1.00	19.22	A
15	CB	ALA	22	29.897	34.702	65.083	1.00	16.98	A
16	C	ALA	22	31.951	34.602	66.522	1.00	18.97	A
17	O	ALA	22	32.771	33.961	65.852	1.00	19.26	A
18	N	THR	23	31.887	34.515	67.854	1.00	17.74	A
19	CA	THR	23	32.840	33.659	68.577	1.00	15.74	A
20	CB	THR	23	33.699	34.563	69.497	1.00	17.10	A
21	OG1	THR	23	34.155	35.652	68.678	1.00	16.29	A
22	CG2	THR	23	34.824	33.809	70.184	1.00	18.53	A
23	C	THR	23	32.138	32.654	69.465	1.00	16.14	A
24	O	THR	23	31.100	32.951	70.060	1.00	15.79	A
25	N	ILE	24	32.680	31.455	69.500	1.00	15.97	A
26	CA	ILE	24	32.183	30.385	70.313	1.00	18.48	A
27	CB	ILE	24	32.620	29.024	69.816	1.00	17.83	A
28	CG2	ILE	24	32.097	27.975	70.825	1.00	18.50	A
29	CG1	ILE	24	32.052	28.700	68.408	1.00	18.53	A
30	CD1	ILE	24	32.633	27.424	67.841	1.00	16.89	A
31	C	ILE	24	32.790	30.650	71.729	1.00	20.41	A
32	O	ILE	24	34.005	30.764	71.810	1.00	19.04	A
33	N	LEU	25	31.928	30.814	72.709	1.00	20.83	A
34	CA	LEU	25	32.236	31.175	74.068	1.00	20.33	A
35	CB	LEU	25	31.368	32.388	74.458	1.00	19.36	A
36	CG	LEU	25	31.475	33.620	73.571	1.00	19.02	A
37	CD2	LEU	25	32.876	34.236	73.516	1.00	19.47	A
38	CD1	LEU	25	30.514	34.693	74.104	1.00	17.79	A
39	C	LEU	25	32.009	30.093	75.092	1.00	19.34	A
40	O	LEU	25	32.480	30.255	76.215	1.00	17.65	A
41	N	ALA	26	31.231	29.051	74.796	1.00	17.56	A
42	CA	ALA	26	31.065	27.958	75.712	1.00	18.21	A
43	CB	ALA	26	30.071	28.315	76.844	1.00	16.77	A
44	C	ALA	26	30.487	26.777	74.961	1.00	20.23	A
45	O	ALA	26	29.882	26.972	73.895	1.00	18.85	A
46	N	ILE	27	30.855	25.588	75.429	1.00	18.15	A
47	CA	ILE	27	30.356	24.366	74.843	1.00	19.79	A
48	CB	ILE	27	31.390	23.696	73.930	1.00	18.91	A
49	CG2	ILE	27	30.719	22.521	73.240	1.00	17.49	A
50	CG1	ILE	27	31.984	24.650	72.859	1.00	17.58	A
51	CD1	ILE	27	33.157	24.057	72.094	1.00	17.89	A
52	C	ILE	27	29.968	23.380	75.929	1.00	19.93	A
53	O	ILE	27	30.842	23.024	76.725	1.00	20.00	A
54	N	GLY	28	28.798	22.788	75.853	1.00	19.91	A
55	CA	GLY	28	28.297	21.759	76.759	1.00	18.80	A
56	C	GLY	28	27.802	20.540	75.993	1.00	20.61	A
57	O	GLY	28	27.170	20.667	74.905	1.00	19.24	A
58	N	THR	29	28.111	19.333	76.457	1.00	16.87	A

59	CA	THR	29	27.545	18.133	75.816	1.00	19.02	A
60	CB	THR	29	28.603	17.320	75.080	1.00	20.16	A
61	OG1	THR	29	29.629	16.843	75.950	1.00	21.21	A
62	CG2	THR	29	29.373	18.154	74.032	1.00	20.41	A
63	C	THR	29	26.787	17.267	76.813	1.00	20.90	A
64	O	THR	29	27.106	17.274	78.025	1.00	22.12	A
65	N	ALA	30	25.942	16.358	76.393	1.00	17.49	A
66	CA	ALA	30	25.211	15.395	77.185	1.00	17.35	A
67	CB	ALA	30	23.866	15.947	77.664	1.00	14.17	A
68	C	ALA	30	24.876	14.187	76.310	1.00	18.08	A
69	O	ALA	30	24.631	14.306	75.082	1.00	17.60	A
70	N	THR	31	24.696	13.046	76.908	1.00	19.58	A
71	CA	THR	31	24.246	11.823	76.246	1.00	19.85	A
72	CB	THR	31	25.412	10.856	76.014	1.00	21.41	A
73	OG1	THR	31	26.049	10.534	77.282	1.00	26.09	A
74	CG2	THR	31	26.542	11.344	75.122	1.00	19.56	A
75	C	THR	31	23.225	11.139	77.136	1.00	22.26	A
76	O	THR	31	23.198	11.407	78.329	1.00	20.45	A
77	N	PRO	32	22.355	10.302	76.602	1.00	21.50	A
78	CA	PRO	32	21.537	9.421	77.401	1.00	21.71	A
79	CD	PRO	32	22.201	10.080	75.137	1.00	21.81	A
80	CB	PRO	32	20.893	8.493	76.344	1.00	19.90	A
81	CG	PRO	32	20.880	9.325	75.091	1.00	21.81	A
82	C	PRO	32	22.424	8.561	78.299	1.00	22.41	A
83	O	PRO	32	23.584	8.337	77.979	1.00	22.75	A
84	N	PRO	33	21.905	8.074	79.421	1.00	24.52	A
85	CA	PRO	33	22.653	7.254	80.353	1.00	26.49	A
86	CD	PRO	33	20.524	8.372	79.888	1.00	24.57	A
87	CB	PRO	33	21.713	7.159	81.571	1.00	26.31	A
88	CG	PRO	33	20.346	7.355	81.014	1.00	27.68	A
89	C	PRO	33	23.045	5.870	79.845	1.00	27.55	A
90	O	PRO	33	24.179	5.435	80.070	1.00	28.73	A
91	N	ASN	34	22.175	5.154	79.163	1.00	29.66	A
92	CA	ASN	34	22.410	3.783	78.649	1.00	32.41	A
93	CB	ASN	34	21.101	3.280	78.056	1.00	36.26	A
94	CG	ASN	34	20.948	2.142	77.083	1.00	38.95	A
95	OD1	ASN	34	21.662	1.127	77.183	1.00	39.62	A
96	ND2	ASN	34	19.989	2.192	76.138	1.00	35.37	A
97	C	ASN	34	23.523	3.807	77.609	1.00	32.31	A
98	O	ASN	34	23.469	4.526	76.610	1.00	29.54	A
99	N	CYS	35	24.576	3.052	77.829	1.00	30.93	A
100	CA	CYS	35	25.723	2.919	76.965	1.00	31.69	A
101	CB	CYS	35	26.917	3.153	77.906	1.00	35.11	A
102	SG	CYS	35	28.474	3.296	77.056	1.00	37.85	A
103	C	CYS	35	25.768	1.499	76.438	1.00	31.58	A
104	O	CYS	35	25.523	0.623	77.272	1.00	31.97	A
105	N	VAL	36	26.041	1.225	75.182	1.00	30.94	A
106	CA	VAL	36	26.161	-0.144	74.669	1.00	31.93	A
107	CB	VAL	36	25.047	-0.605	73.706	1.00	32.84	A
108	CG1	VAL	36	25.372	-1.969	73.087	1.00	33.47	A
109	CG2	VAL	36	23.689	-0.721	74.407	1.00	33.32	A
110	C	VAL	36	27.500	-0.299	73.944	1.00	31.29	A

111	O	VAL	36	27.768	0.506	73.036	1.00	30.05	A
112	N	ALA	37	28.310	-1.286	74.343	1.00	30.79	A
113	CA	ALA	37	29.594	-1.466	73.680	1.00	29.79	A
114	CB	ALA	37	30.543	-2.436	74.385	1.00	29.23	A
115	C	ALA	37	29.342	-1.982	72.250	1.00	28.16	A
116	O	ALA	37	28.620	-2.955	72.083	1.00	26.46	A
117	N	GLN	38	30.143	-1.521	71.312	1.00	28.15	A
118	CA	GLN	38	30.007	-1.958	69.912	1.00	27.67	A
119	CB	GLN	38	30.846	-1.049	69.021	1.00	28.50	A
120	CG	GLN	38	30.657	-1.221	67.506	1.00	26.41	A
121	CD	GLN	38	29.350	-0.581	67.053	1.00	27.26	A
122	OE1	GLN	38	28.360	-0.689	67.767	1.00	26.46	A
123	NE2	GLN	38	29.296	0.067	65.877	1.00	25.63	A
124	C	GLN	38	30.382	-3.409	69.734	1.00	29.10	A
125	O	GLN	38	29.688	-4.212	69.107	1.00	27.00	A
126	N	ALA	39	31.355	-3.895	70.531	1.00	31.28	A
127	CA	ALA	39	31.738	-5.301	70.547	1.00	31.16	A
128	CB	ALA	39	32.950	-5.519	71.448	1.00	32.49	A
129	C	ALA	39	30.592	-6.189	71.009	1.00	32.31	A
130	O	ALA	39	30.519	-7.353	70.605	1.00	34.94	A
131	N	ASP	40	29.574	-5.650	71.681	1.00	31.27	A
132	CA	ASP	40	28.403	-6.433	72.036	1.00	32.18	A
133	CB	ASP	40	28.042	-6.187	73.503	1.00	33.60	A
134	CG	ASP	40	29.167	-6.530	74.462	1.00	35.07	A
135	OD1	ASP	40	29.914	-7.480	74.174	1.00	35.48	A
136	OD2	ASP	40	29.312	-5.832	75.481	1.00	36.82	A
137	C	ASP	40	27.156	-6.106	71.203	1.00	30.15	A
138	O	ASP	40	26.137	-6.760	71.362	1.00	27.91	A
139	N	TYR	41	27.225	-5.055	70.383	1.00	29.82	A
140	CA	TYR	41	26.045	-4.632	69.634	1.00	27.44	A
141	CB	TYR	41	26.336	-3.302	68.891	1.00	28.10	A
142	CG	TYR	41	24.958	-2.680	68.620	1.00	28.23	A
143	CD1	TYR	41	24.354	-1.940	69.628	1.00	28.38	A
144	CD2	TYR	41	24.306	-2.853	67.404	1.00	26.85	A
145	CE1	TYR	41	23.104	-1.367	69.427	1.00	30.06	A
146	CE2	TYR	41	23.066	-2.289	67.183	1.00	27.54	A
147	CZ	TYR	41	22.468	-1.558	68.190	1.00	30.20	A
148	OH	TYR	41	21.230	-0.987	68.015	1.00	31.22	A
149	C	TYR	41	25.416	-5.639	68.706	1.00	26.97	A
150	O	TYR	41	24.185	-5.796	68.753	1.00	24.64	A
151	N	ALA	42	26.191	-6.432	67.949	1.00	27.02	A
152	CA	ALA	42	25.599	-7.424	67.061	1.00	27.20	A
153	CB	ALA	42	26.651	-8.140	66.232	1.00	26.68	A
154	C	ALA	42	24.723	-8.413	67.805	1.00	28.00	A
155	O	ALA	42	23.616	-8.774	67.405	1.00	26.11	A
156	N	ASP	43	25.240	-8.969	68.907	1.00	30.84	A
157	CA	ASP	43	24.475	-9.891	69.734	1.00	31.33	A
158	CB	ASP	43	25.385	-10.470	70.825	1.00	34.03	A
159	CG	ASP	43	26.273	-11.584	70.276	1.00	36.27	A
160	OD1	ASP	43	27.305	-11.885	70.905	1.00	37.42	A
161	OD2	ASP	43	25.960	-12.163	69.214	1.00	37.57	A
162	C	ASP	43	23.237	-9.246	70.351	1.00	30.78	A

163	O	ASP	43	22.130	-9.796	70.356	1.00	31.39	A
164	N	TYR	44	23.350	-8.026	70.836	1.00	28.82	A
165	CA	TYR	44	22.211	-7.302	71.395	1.00	30.46	A
166	CB	TYR	44	22.687	-5.932	71.934	1.00	31.63	A
167	CG	TYR	44	21.497	-5.043	72.238	1.00	34.09	A
168	CD1	TYR	44	20.706	-5.350	73.352	1.00	34.43	A
169	CD2	TYR	44	21.139	-3.967	71.435	1.00	33.42	A
170	CE1	TYR	44	19.606	-4.577	73.661	1.00	35.43	A
171	CE2	TYR	44	20.031	-3.205	71.749	1.00	35.16	A
172	CZ	TYR	44	19.266	-3.514	72.859	1.00	35.11	A
173	OH	TYR	44	18.149	-2.773	73.173	1.00	36.24	A
174	C	TYR	44	21.124	-7.090	70.351	1.00	28.76	A
175	O	TYR	44	19.933	-7.443	70.461	1.00	29.56	A
176	N	TYR	45	21.556	-6.598	69.182	1.00	28.20	A
177	CA	TYR	45	20.616	-6.219	68.115	1.00	25.74	A
178	CB	TYR	45	21.435	-5.417	67.073	1.00	26.31	A
179	CG	TYR	45	20.733	-5.127	65.770	1.00	25.68	A
180	CD1	TYR	45	19.830	-4.066	65.699	1.00	25.75	A
181	CD2	TYR	45	20.938	-5.887	64.626	1.00	26.97	A
182	CE1	TYR	45	19.165	-3.757	64.534	1.00	26.81	A
183	CE2	TYR	45	20.273	-5.584	63.439	1.00	27.53	A
184	CZ	TYR	45	19.389	-4.531	63.406	1.00	26.52	A
185	OH	TYR	45	18.722	-4.205	62.248	1.00	25.82	A
186	C	TYR	45	19.800	-7.359	67.578	1.00	25.23	A
187	O	TYR	45	18.547	-7.365	67.499	1.00	25.18	A
188	N	PHE	46	20.460	-8.466	67.240	1.00	25.33	A
189	CA	PHE	46	19.805	-9.655	66.710	1.00	26.13	A
190	CB	PHE	46	20.872	-10.562	66.065	1.00	25.99	A
191	CG	PHE	46	21.118	-10.169	64.623	1.00	24.71	A
192	CD1	PHE	46	21.993	-9.158	64.295	1.00	24.42	A
193	CD2	PHE	46	20.408	-10.779	63.609	1.00	25.49	A
194	CE1	PHE	46	22.221	-8.832	62.952	1.00	24.01	A
195	CE2	PHE	46	20.609	-10.411	62.272	1.00	26.54	A
196	CZ	PHE	46	21.473	-9.380	61.941	1.00	22.32	A
197	C	PHE	46	18.980	-10.383	67.767	1.00	28.00	A
198	O	PHE	46	17.944	-10.985	67.459	1.00	29.01	A
199	N	ARG	47	19.297	-10.167	69.014	1.00	27.89	A
200	CA	ARG	47	18.537	-10.764	70.120	1.00	29.09	A
201	CB	ARG	47	19.399	-10.735	71.377	1.00	31.22	A
202	CG	ARG	47	18.961	-11.670	72.511	1.00	32.64	A
203	CD	ARG	47	19.652	-11.266	73.821	1.00	34.71	A
204	NE	ARG	47	18.780	-10.430	74.611	1.00	36.52	A
205	CZ	ARG	47	19.000	-9.232	75.181	1.00	36.76	A
206	NH1	ARG	47	20.169	-8.598	75.167	1.00	36.52	A
207	NH2	ARG	47	18.003	-8.579	75.805	1.00	38.61	A
208	C	ARG	47	17.230	-9.970	70.323	1.00	29.38	A
209	O	ARG	47	16.130	-10.531	70.338	1.00	27.87	A
210	N	VAL	48	17.371	-8.614	70.501	1.00	31.39	A
211	CA	VAL	48	16.155	-7.803	70.723	1.00	31.67	A
212	CB	VAL	48	16.483	-6.382	71.230	1.00	32.60	A
213	CG1	VAL	48	17.272	-6.551	72.529	1.00	34.07	A
214	CG2	VAL	48	17.262	-5.532	70.225	1.00	31.26	A

215	C	VAL	48	15.235	-7.692	69.524	1.00	31.64	A
216	O	VAL	48	14.027	-7.461	69.678	1.00	31.80	A
217	N	THR	49	15.773	-7.869	68.326	1.00	30.64	A
218	CA	THR	49	14.909	-7.845	67.137	1.00	31.47	A
219	CB	THR	49	15.625	-7.226	65.928	1.00	29.40	A
220	OG1	THR	49	16.731	-8.068	65.630	1.00	28.79	A
221	CG2	THR	49	16.076	-5.809	66.244	1.00	29.44	A
222	C	THR	49	14.501	-9.264	66.767	1.00	32.37	A
223	O	THR	49	13.890	-9.440	65.735	1.00	31.92	A
224	N	LYS	50	14.803	-10.271	67.599	1.00	35.30	A
225	CA	LYS	50	14.352	-11.635	67.379	1.00	36.93	A
226	CB	LYS	50	12.830	-11.671	67.617	1.00	39.91	A
227	CG	LYS	50	12.448	-11.295	69.053	1.00	43.14	A
228	CD	LYS	50	10.925	-11.120	69.148	1.00	46.09	A
229	CE	LYS	50	10.531	-10.612	70.521	1.00	48.94	A
230	NZ	LYS	50	9.159	-11.061	70.920	1.00	51.49	A
231	C	LYS	50	14.703	-12.190	65.998	1.00	36.27	A
232	O	LYS	50	13.882	-12.803	65.304	1.00	35.23	A
233	N	SER	51	15.952	-11.983	65.588	1.00	34.72	A
234	CA	SER	51	16.357	-12.292	64.227	1.00	36.62	A
235	CB	SER	51	16.761	-11.007	63.490	1.00	35.04	A
236	OG	SER	51	15.632	-10.153	63.401	1.00	35.75	A
237	C	SER	51	17.530	-13.264	64.196	1.00	37.21	A
238	O	SER	51	18.250	-13.326	63.202	1.00	35.82	A
239	N	GLU	52	17.644	-14.064	65.250	1.00	37.90	A
240	CA	GLU	52	18.726	-15.024	65.378	1.00	41.24	A
241	CB	GLU	52	18.664	-15.821	66.687	1.00	41.73	A
242	CG	GLU	52	18.714	-14.913	67.912	1.00	43.24	A
243	CD	GLU	52	20.093	-14.326	68.139	1.00	43.08	A
244	OE1	GLU	52	20.922	-14.295	67.206	1.00	43.85	A
245	OE2	GLU	52	20.335	-13.886	69.276	1.00	42.33	A
246	C	GLU	52	18.852	-16.016	64.237	1.00	41.56	A
247	O	GLU	52	19.962	-16.418	63.923	1.00	41.47	A
248	N	HIS	53	17.765	-16.368	63.591	1.00	43.15	A
249	CA	HIS	53	17.757	-17.277	62.462	1.00	46.02	A
250	ND1	HIS	53	15.020	-15.790	63.161	1.00	57.14	A
251	CG	HIS	53	15.414	-16.524	62.053	1.00	55.58	A
252	CB	HIS	53	16.321	-17.714	62.158	1.00	50.66	A
253	NE2	HIS	53	14.105	-14.866	61.430	1.00	57.55	A
254	CD2	HIS	53	14.842	-15.934	60.966	1.00	57.42	A
255	CE1	HIS	53	14.232	-14.810	62.745	1.00	58.02	A
256	C	HIS	53	18.409	-16.654	61.237	1.00	44.57	A
257	O	HIS	53	18.924	-17.441	60.437	1.00	44.24	A
258	N	MET	54	18.572	-15.331	61.178	1.00	41.09	A
259	CA	MET	54	19.348	-14.712	60.113	1.00	40.86	A
260	CB	MET	54	18.865	-13.279	59.877	1.00	39.34	A
261	CG	MET	54	17.345	-13.172	59.756	1.00	38.82	A
262	SD	MET	54	16.834	-11.433	59.565	1.00	38.46	A
263	CE	MET	54	15.087	-11.625	59.282	1.00	39.63	A
264	C	MET	54	20.843	-14.743	60.444	1.00	38.70	A
265	O	MET	54	21.471	-13.709	60.604	1.00	36.96	A
266	N	VAL	55	21.423	-15.930	60.471	1.00	37.47	A

267	CA	VAL	55	22.806	-16.179	60.826	1.00	38.20	A
268	CB	VAL	55	23.074	-17.704	60.781	1.00	37.95	A
269	CG1	VAL	55	24.539	-18.029	60.988	1.00	37.15	A
270	CG2	VAL	55	22.200	-18.366	61.852	1.00	38.75	A
271	C	VAL	55	23.808	-15.423	59.964	1.00	37.34	A
272	O	VAL	55	24.678	-14.746	60.485	1.00	35.85	A
273	N	ASP	56	23.671	-15.506	58.651	1.00	37.85	A
274	CA	ASP	56	24.592	-14.871	57.712	1.00	40.33	A
275	CB	ASP	56	24.342	-15.403	56.297	1.00	44.16	A
276	CG	ASP	56	24.760	-16.863	56.131	1.00	48.56	A
277	OD1	ASP	56	25.297	-17.563	57.035	1.00	49.83	A
278	OD2	ASP	56	24.494	-17.330	54.992	1.00	50.70	A
279	C	ASP	56	24.537	-13.352	57.759	1.00	38.30	A
280	O	ASP	56	25.568	-12.680	57.818	1.00	38.20	A
281	N	LEU	57	23.340	-12.789	57.909	1.00	35.70	A
282	CA	LEU	57	23.179	-11.369	58.144	1.00	34.76	A
283	CB	LEU	57	21.700	-10.988	58.141	1.00	36.41	A
284	CG	LEU	57	21.328	-9.731	57.367	1.00	38.75	A
285	CD2	LEU	57	19.810	-9.657	57.233	1.00	39.19	A
286	CD1	LEU	57	21.984	-9.704	55.983	1.00	38.62	A
287	C	LEU	57	23.777	-10.975	59.492	1.00	31.73	A
288	O	LEU	57	24.409	-9.936	59.642	1.00	30.50	A
289	N	LYS	58	23.517	-11.816	60.504	1.00	30.83	A
290	CA	LYS	58	24.186	-11.616	61.791	1.00	29.23	A
291	CB	LYS	58	23.802	-12.695	62.816	1.00	29.15	A
292	CG	LYS	58	24.327	-12.284	64.198	1.00	29.77	A
293	CD	LYS	58	23.767	-13.189	65.296	1.00	28.95	A
294	CE	LYS	58	24.413	-12.778	66.620	1.00	29.21	A
295	NZ	LYS	58	23.929	-13.667	67.738	1.00	30.34	A
296	C	LYS	58	25.691	-11.592	61.599	1.00	28.39	A
297	O	LYS	58	26.412	-10.672	62.017	1.00	26.22	A
298	N	GLU	59	26.223	-12.590	60.873	1.00	28.92	A
299	CA	GLU	59	27.676	-12.592	60.652	1.00	30.78	A
300	CB	GLU	59	28.071	-13.810	59.789	1.00	36.02	A
301	CG	GLU	59	28.228	-15.069	60.615	1.00	41.00	A
302	CD	GLU	59	29.133	-14.949	61.820	1.00	43.84	A
303	OE1	GLU	59	30.081	-14.148	61.926	1.00	46.35	A
304	OE2	GLU	59	28.890	-15.739	62.770	1.00	47.23	A
305	C	GLU	59	28.131	-11.334	59.950	1.00	28.91	A
306	O	GLU	59	29.200	-10.804	60.211	1.00	26.29	A
307	N	LYS	60	27.365	-10.903	58.932	1.00	27.65	A
308	CA	LYS	60	27.756	-9.676	58.235	1.00	28.35	A
309	CB	LYS	60	26.908	-9.608	56.978	1.00	31.60	A
310	CG	LYS	60	26.369	-8.247	56.605	1.00	34.59	A
311	CD	LYS	60	27.107	-7.755	55.389	1.00	36.17	A
312	CE	LYS	60	26.120	-7.195	54.355	1.00	34.07	A
313	NZ	LYS	60	26.854	-7.291	53.037	1.00	30.49	A
314	C	LYS	60	27.622	-8.441	59.120	1.00	27.63	A
315	O	LYS	60	28.495	-7.592	59.158	1.00	25.96	A
316	N	PHE	61	26.605	-8.378	59.980	1.00	27.76	A
317	CA	PHE	61	26.533	-7.279	60.954	1.00	27.20	A
318	CB	PHE	61	25.175	-7.344	61.691	1.00	26.83	A

319	CG	PHE	61	24.870	-6.020	62.361	1.00	25.57	A
320	CD1	PHE	61	24.793	-4.848	61.636	1.00	23.19	A
321	CD2	PHE	61	24.705	-5.974	63.742	1.00	25.42	A
322	CE1	PHE	61	24.589	-3.642	62.279	1.00	22.77	A
323	CE2	PHE	61	24.431	-4.765	64.394	1.00	24.47	A
324	CZ	PHE	61	24.410	-3.600	63.658	1.00	23.21	A
325	C	PHE	61	27.706	-7.291	61.918	1.00	27.60	A
326	O	PHE	61	28.204	-6.228	62.306	1.00	25.06	A
327	N	LYS	62	28.248	-8.470	62.281	1.00	28.63	A
328	CA	LYS	62	29.440	-8.434	63.161	1.00	30.01	A
329	CB	LYS	62	29.817	-9.798	63.712	1.00	33.50	A
330	CG	LYS	62	28.933	-10.363	64.817	1.00	36.21	A
331	CD	LYS	62	29.313	-11.795	65.201	1.00	39.57	A
332	CE	LYS	62	28.868	-12.139	66.632	1.00	42.71	A
333	NZ	LYS	62	28.743	-13.618	66.867	1.00	43.80	A
334	C	LYS	62	30.633	-7.820	62.432	1.00	27.66	A
335	O	LYS	62	31.408	-7.040	62.961	1.00	25.63	A
336	N	ARG	63	30.812	-8.129	61.160	1.00	28.40	A
337	CA	ARG	63	31.886	-7.532	60.345	1.00	26.83	A
338	CB	ARG	63	31.923	-8.166	58.949	1.00	28.80	A
339	CG	ARG	63	32.205	-9.670	58.860	1.00	31.04	A
340	CD	ARG	63	32.605	-10.075	57.429	1.00	31.67	A
341	NE	ARG	63	31.458	-10.007	56.496	1.00	31.18	A
342	CZ	ARG	63	30.568	-10.993	56.412	1.00	33.98	A
343	NH1	ARG	63	30.675	-12.080	57.183	1.00	33.69	A
344	NH2	ARG	63	29.552	-10.945	55.537	1.00	35.02	A
345	C	ARG	63	31.725	-6.028	60.234	1.00	26.47	A
346	O	ARG	63	32.707	-5.281	60.285	1.00	27.57	A
347	N	ILE	64	30.517	-5.531	59.967	1.00	26.34	A
348	CA	ILE	64	30.285	-4.079	59.832	1.00	25.94	A
349	CB	ILE	64	28.797	-3.821	59.461	1.00	25.49	A
350	CG2	ILE	64	28.386	-2.381	59.606	1.00	25.16	A
351	CG1	ILE	64	28.502	-4.295	58.011	1.00	24.16	A
352	CD1	ILE	64	27.030	-4.611	57.772	1.00	20.75	A
353	C	ILE	64	30.604	-3.364	61.149	1.00	26.57	A
354	O	ILE	64	31.299	-2.343	61.183	1.00	25.13	A
355	N	CYS	65	30.119	-3.920	62.268	1.00	25.79	A
356	CA	CYS	65	30.373	-3.275	63.569	1.00	29.16	A
357	CB	CYS	65	29.703	-4.001	64.744	1.00	27.03	A
358	SG	CYS	65	27.900	-3.813	64.788	1.00	27.03	A
359	C	CYS	65	31.870	-3.230	63.861	1.00	29.65	A
360	O	CYS	65	32.384	-2.241	64.393	1.00	27.74	A
361	N	GLU	66	32.557	-4.333	63.495	1.00	32.64	A
362	CA	GLU	66	34.017	-4.324	63.693	1.00	34.70	A
363	CB	GLU	66	34.616	-5.684	63.344	1.00	38.03	A
364	CG	GLU	66	36.078	-5.831	63.720	1.00	42.01	A
365	CD	GLU	66	37.051	-5.375	62.644	1.00	45.51	A
366	OE1	GLU	66	36.749	-5.306	61.421	1.00	45.11	A
367	OE2	GLU	66	38.211	-5.061	63.034	1.00	47.20	A
368	C	GLU	66	34.645	-3.235	62.842	1.00	33.45	A
369	O	GLU	66	35.633	-2.642	63.271	1.00	34.26	A
370	N	LYS	67	34.187	-2.990	61.610	1.00	31.58	A

371	CA	LYS	67	34.775	-1.966	60.759	1.00	30.20	A
372	CB	LYS	67	34.159	-2.078	59.335	1.00	30.36	A
373	CG	LYS	67	34.698	-3.350	58.673	1.00	31.77	A
374	CD	LYS	67	36.139	-3.095	58.230	1.00	30.35	A
375	CE	LYS	67	36.519	-4.248	57.282	1.00	32.61	A
376	NZ	LYS	67	37.969	-4.223	56.965	1.00	31.38	A
377	C	LYS	67	34.530	-0.539	61.207	1.00	28.50	A
378	O	LYS	67	35.301	0.330	60.826	1.00	26.35	A
379	N	THR	68	33.485	-0.253	61.990	1.00	28.16	A
380	CA	THR	68	33.117	1.117	62.321	1.00	26.38	A
381	CB	THR	68	31.755	1.142	63.079	1.00	28.00	A
382	OG1	THR	68	31.822	0.406	64.297	1.00	25.98	A
383	CG2	THR	68	30.640	0.516	62.232	1.00	26.36	A
384	C	THR	68	34.127	1.962	63.067	1.00	26.03	A
385	O	THR	68	34.035	3.198	63.074	1.00	23.26	A
386	N	ALA	69	35.020	1.367	63.862	1.00	25.08	A
387	CA	ALA	69	35.959	2.110	64.689	1.00	26.12	A
388	CB	ALA	69	36.881	3.014	63.885	1.00	24.83	A
389	C	ALA	69	35.146	2.920	65.730	1.00	25.89	A
390	O	ALA	69	35.516	4.026	66.108	1.00	25.89	A
391	N	ILE	70	34.088	2.282	66.214	1.00	25.60	A
392	CA	ILE	70	33.264	2.842	67.291	1.00	25.62	A
393	CB	ILE	70	31.757	2.933	66.959	1.00	24.18	A
394	CG2	ILE	70	30.904	3.310	68.168	1.00	21.69	A
395	CG1	ILE	70	31.559	3.928	65.795	1.00	22.58	A
396	CD1	ILE	70	30.160	3.904	65.163	1.00	20.62	A
397	C	ILE	70	33.454	1.913	68.493	1.00	25.45	A
398	O	ILE	70	33.249	0.715	68.340	1.00	23.85	A
399	N	LYS	71	33.762	2.463	69.667	1.00	26.85	A
400	CA	LYS	71	33.835	1.597	70.865	1.00	28.48	A
401	CB	LYS	71	34.913	2.162	71.797	1.00	31.60	A
402	CG	LYS	71	35.196	1.430	73.078	1.00	34.19	A
403	CD	LYS	71	36.308	2.012	73.935	1.00	36.61	A
404	CE	LYS	71	37.382	2.812	73.249	1.00	38.89	A
405	NZ	LYS	71	38.738	2.685	73.870	1.00	42.37	A
406	C	LYS	71	32.506	1.455	71.584	1.00	27.13	A
407	O	LYS	71	32.183	0.367	72.087	1.00	27.37	A
408	N	LYS	72	31.724	2.520	71.728	1.00	25.23	A
409	CA	LYS	72	30.442	2.474	72.414	1.00	25.15	A
410	CB	LYS	72	30.572	2.715	73.924	1.00	26.70	A
411	CG	LYS	72	31.332	3.981	74.244	1.00	28.08	A
412	CD	LYS	72	31.600	4.138	75.752	1.00	31.06	A
413	CE	LYS	72	32.583	5.268	75.965	1.00	34.19	A
414	NZ	LYS	72	32.080	6.648	75.842	1.00	30.79	A
415	C	LYS	72	29.588	3.650	71.915	1.00	24.42	A
416	O	LYS	72	30.117	4.578	71.299	1.00	20.97	A
417	N	ARG	73	28.302	3.536	72.187	1.00	22.40	A
418	CA	ARG	73	27.331	4.559	71.833	1.00	23.39	A
419	CB	ARG	73	26.539	4.093	70.579	1.00	22.84	A
420	CG	ARG	73	27.403	4.138	69.304	1.00	23.07	A
421	CD	ARG	73	26.641	3.582	68.115	1.00	24.33	A
422	NE	ARG	73	26.448	2.175	67.974	1.00	21.31	A

423	CZ	ARG	73	25.538	1.589	67.211	1.00	22.61	A
424	NH1	ARG	73	25.470	0.280	67.165	1.00	21.98	A
425	NH2	ARG	73	24.660	2.250	66.446	1.00	23.67	A
426	C	ARG	73	26.362	4.735	73.009	1.00	21.07	A
427	O	ARG	73	25.989	3.699	73.545	1.00	20.95	A
428	N	TYR	74	25.869	5.907	73.273	1.00	20.99	A
429	CA	TYR	74	24.812	6.072	74.270	1.00	20.56	A
430	CB	TYR	74	25.038	7.416	74.957	1.00	21.25	A
431	CG	TYR	74	26.352	7.376	75.718	1.00	23.79	A
432	CD1	TYR	74	27.511	7.806	75.099	1.00	25.16	A
433	CD2	TYR	74	26.369	6.913	77.030	1.00	23.96	A
434	CE1	TYR	74	28.712	7.779	75.806	1.00	27.20	A
435	CE2	TYR	74	27.563	6.900	77.752	1.00	24.67	A
436	CZ	TYR	74	28.701	7.327	77.131	1.00	26.17	A
437	OH	TYR	74	29.894	7.334	77.795	1.00	28.39	A
438	C	TYR	74	23.464	6.090	73.583	1.00	20.11	A
439	O	TYR	74	23.401	6.600	72.434	1.00	22.54	A
440	N	LEU	75	22.467	5.355	74.035	1.00	20.26	A
441	CA	LEU	75	21.201	5.266	73.291	1.00	22.57	A
442	CB	LEU	75	21.119	3.864	72.671	1.00	22.46	A
443	CG	LEU	75	22.251	3.500	71.686	1.00	22.93	A
444	CD2	LEU	75	21.988	4.281	70.390	1.00	22.07	A
445	CD1	LEU	75	22.304	1.995	71.423	1.00	22.36	A
446	C	LEU	75	20.032	5.489	74.242	1.00	24.64	A
447	O	LEU	75	19.972	4.805	75.265	1.00	23.88	A
448	N	ALA	76	19.129	6.383	73.895	1.00	22.83	A
449	CA	ALA	76	17.935	6.662	74.660	1.00	24.54	A
450	CB	ALA	76	17.287	7.977	74.206	1.00	22.44	A
451	C	ALA	76	16.935	5.535	74.428	1.00	24.70	A
452	O	ALA	76	16.159	5.190	75.303	1.00	25.26	A
453	N	LEU	77	17.018	4.839	73.284	1.00	23.09	A
454	CA	LEU	77	16.187	3.672	73.024	1.00	22.26	A
455	CB	LEU	77	16.375	3.085	71.623	1.00	23.19	A
456	CG	LEU	77	15.196	2.566	70.826	1.00	25.81	A
457	CD2	LEU	77	13.985	2.125	71.624	1.00	24.97	A
458	CD1	LEU	77	15.597	1.526	69.775	1.00	26.58	A
459	C	LEU	77	16.565	2.512	73.969	1.00	22.32	A
460	O	LEU	77	17.692	2.038	73.916	1.00	21.09	A
461	N	THR	78	15.602	1.990	74.719	1.00	23.09	A
462	CA	THR	78	15.918	0.875	75.627	1.00	23.42	A
463	CB	THR	78	15.463	1.118	77.082	1.00	23.04	A
464	OG1	THR	78	14.015	1.098	77.049	1.00	21.65	A
465	CG2	THR	78	15.990	2.406	77.693	1.00	22.61	A
466	C	THR	78	15.313	-0.421	75.135	1.00	23.97	A
467	O	THR	78	14.357	-0.475	74.363	1.00	21.55	A
468	N	GLU	79	15.805	-1.535	75.697	1.00	25.13	A
469	CA	GLU	79	15.223	-2.840	75.440	1.00	25.90	A
470	CB	GLU	79	16.075	-3.912	76.147	1.00	29.42	A
471	CG	GLU	79	15.500	-5.306	75.879	1.00	32.50	A
472	CD	GLU	79	16.417	-6.432	76.330	1.00	33.94	A
473	OE1	GLU	79	17.572	-6.275	76.719	1.00	33.93	A
474	OE2	GLU	79	15.928	-7.572	76.300	1.00	34.93	A

475	C	GLU	79	13.786	-2.939	75.909	1.00	26.56	A
476	O	GLU	79	12.933	-3.542	75.219	1.00	26.00	A
477	N	ASP	80	13.469	-2.306	77.047	1.00	25.28	A
478	CA	ASP	80	12.130	-2.360	77.604	1.00	26.58	A
479	CB	ASP	80	11.991	-1.707	78.992	1.00	29.59	A
480	CG	ASP	80	12.565	-2.545	80.145	1.00	34.54	A
481	OD1	ASP	80	13.268	-3.561	80.003	1.00	36.70	A
482	OD2	ASP	80	12.324	-2.141	81.293	1.00	35.94	A
483	C	ASP	80	11.185	-1.624	76.630	1.00	23.74	A
484	O	ASP	80	10.052	-1.982	76.364	1.00	20.67	A
485	N	TYR	81	11.655	-0.470	76.146	1.00	21.73	A
486	CA	TYR	81	10.830	0.280	75.179	1.00	21.01	A
487	CB	TYR	81	11.538	1.572	74.807	1.00	22.38	A
488	CG	TYR	81	10.553	2.569	74.238	1.00	20.79	A
489	CD1	TYR	81	9.658	3.258	75.038	1.00	22.40	A
490	CD2	TYR	81	10.539	2.777	72.863	1.00	21.60	A
491	CE1	TYR	81	8.774	4.180	74.482	1.00	22.22	A
492	CE2	TYR	81	9.653	3.680	72.284	1.00	21.70	A
493	CZ	TYR	81	8.780	4.368	73.083	1.00	21.39	A
494	OH	TYR	81	7.857	5.281	72.616	1.00	16.70	A
495	C	TYR	81	10.538	-0.518	73.927	1.00	21.01	A
496	O	TYR	81	9.414	-0.513	73.417	1.00	23.40	A
497	N	LEU	82	11.502	-1.279	73.447	1.00	22.80	A
498	CA	LEU	82	11.360	-2.117	72.269	1.00	25.21	A
499	CB	LEU	82	12.729	-2.691	71.876	1.00	25.32	A
500	CG	LEU	82	13.677	-1.731	71.130	1.00	25.98	A
501	CD2	LEU	82	13.000	-1.237	69.843	1.00	24.58	A
502	CD1	LEU	82	14.986	-2.446	70.884	1.00	26.48	A
503	C	LEU	82	10.427	-3.297	72.489	1.00	26.98	A
504	O	LEU	82	9.554	-3.654	71.680	1.00	26.48	A
505	N	GLN	83	10.470	-3.811	73.739	1.00	27.34	A
506	CA	GLN	83	9.551	-4.924	74.047	1.00	27.90	A
507	CB	GLN	83	10.054	-5.610	75.334	1.00	34.21	A
508	CG	GLN	83	11.214	-6.537	75.052	1.00	43.19	A
509	CD	GLN	83	11.745	-7.361	76.215	1.00	48.60	A
510	OE1	GLN	83	11.137	-7.539	77.284	1.00	52.11	A
511	NE2	GLN	83	12.957	-7.920	76.033	1.00	48.78	A
512	C	GLN	83	8.140	-4.386	74.173	1.00	23.34	A
513	O	GLN	83	7.165	-5.046	73.827	1.00	23.48	A
514	N	GLU	84	7.989	-3.150	74.641	1.00	21.80	A
515	CA	GLU	84	6.664	-2.532	74.774	1.00	24.16	A
516	CB	GLU	84	6.714	-1.345	75.751	1.00	27.24	A
517	CG	GLU	84	7.145	-1.787	77.172	1.00	35.14	A
518	CD	GLU	84	7.088	-0.745	78.267	1.00	38.58	A
519	OE1	GLU	84	6.536	0.370	78.077	1.00	42.49	A
520	OE2	GLU	84	7.598	-0.973	79.396	1.00	39.80	A
521	C	GLU	84	6.119	-2.062	73.410	1.00	24.58	A
522	O	GLU	84	4,910	-1.871	73.194	1.00	22.41	A
523	N	ASN	85	7.041	-1.795	72.475	1.00	20.65	A
524	CA	ASN	85	6.620	-1.284	71.143	1.00	22.51	A
525	CB	ASN	85	7.195	0.155	71.062	1.00	20.97	A
526	CG	ASN	85	6.600	1.055	72.157	1.00	23.78	A

527	OD1	ASN	85	7.224	1.315	73.225	1.00	24.08	A
528	ND2	ASN	85	5.402	1.527	71.973	1.00	22.00	A
529	C	ASN	85	7.201	-2.159	70.073	1.00	22.06	A
530	O	ASN	85	8.196	-1.765	69.417	1.00	22.54	A
531	N	PRO	86	6.768	-3.408	69.944	1.00	22.24	A
532	CA	PRO	86	7.455	-4.412	69.147	1.00	22.73	A
533	CD	PRO	86	5.579	-4.002	70.612	1.00	23.00	A
534	CB	PRO	86	6.642	-5.700	69.362	1.00	21.97	A
535	CG	PRO	86	5.268	-5.173	69.702	1.00	22.61	A
536	C	PRO	86	7.574	-4.119	67.655	1.00	21.69	A
537	O	PRO	86	8.435	-4.678	66.960	1.00	21.61	A
538	N	THR	87	6.700	-3.276	67.148	1.00	21.21	A
539	CA	THR	87	6.722	-2.936	65.704	1.00	22.08	A
540	CB	THR	87	5.501	-2.171	65.242	1.00	22.22	A
541	OG1	THR	87	5.367	-0.934	65.949	1.00	20.60	A
542	CG2	THR	87	4.223	-3.026	65.356	1.00	24.78	A
543	C	THR	87	7.946	-2.127	65.342	1.00	22.35	A
544	O	THR	87	8.374	-2.191	64.187	1.00	22.21	A
545	N	MET	88	8.672	-1.544	66.313	1.00	21.23	A
546	CA	MET	88	9.949	-0.933	66.036	1.00	24.04	A
547	CB	MET	88	10.510	-0.178	67.257	1.00	22.23	A
548	CG	MET	88	9.720	1.118	67.459	1.00	22.19	A
549	SD	MET	88	10.285	2.038	68.920	1.00	22.06	A
550	CE	MET	88	11.960	2.446	68.441	1.00	20.27	A
551	C	MET	88	10.972	-1.939	65.533	1.00	25.74	A
552	O	MET	88	11.933	-1.517	64.887	1.00	25.43	A
553	N	CYS	89	10.841	-3.217	65.850	1.00	28.09	A
554	CA	CYS	89	11.782	-4.230	65.434	1.00	31.78	A
555	CB	CYS	89	11.943	-5.303	66.544	1.00	31.86	A
556	SG	CYS	89	12.464	-4.554	68.102	1.00	33.92	A
557	C	CYS	89	11.381	-4.988	64.175	1.00	32.89	A
558	O	CYS	89	12.193	-5.791	63.718	1.00	33.74	A
559	N	GLU	90	10.199	-4.765	63.654	1.00	35.14	A
560	CA	GLU	90	9.642	-5.420	62.477	1.00	35.99	A
561	CB	GLU	90	8.163	-5.761	62.680	1.00	39.05	A
562	CG	GLU	90	7.781	-6.609	63.870	1.00	43.25	A
563	CD	GLU	90	6.323	-6.617	64.296	1.00	45.32	A
564	OE1	GLU	90	5.381	-6.341	63.517	1.00	45.87	A
565	OE2	GLU	90	6.084	-6.930	65.499	1.00	46.74	A
566	C	GLU	90	9.827	-4.495	61.266	1.00	35.00	A
567	O	GLU	90	9.299	-3.382	61.198	1.00	30.90	A
568	N	PHE	91	10.664	-4.939	60.336	1.00	35.74	A
569	CA	PHE	91	11.073	-4.068	59.227	1.00	37.10	A
570	CB	PHE	91	12.146	-4.707	58.353	1.00	37.29	A
571	CG	PHE	91	12.830	-3.748	57.416	1.00	37.01	A
572	CD1	PHE	91	13.960	-3.053	57.790	1.00	37.87	A
573	CD2	PHE	91	12.304	-3.526	56.152	1.00	37.36	A
574	CE1	PHE	91	14.568	-2.151	56.927	1.00	38.21	A
575	CE2	PHE	91	12.896	-2.622	55.278	1.00	37.76	A
576	CZ	PHE	91	14.012	-1.925	55.677	1.00	38.01	A
577	C	PHE	91	9.837	-3.535	58.508	1.00	37.33	A
578	O	PHE	91	8.908	-4.199	58.081	1.00	37.45	A

579	N	MET	92	9.721	-2.218	58.577	1.00	37.74	A
580	CA	MET	92	8.643	-1.430	58.010	1.00	39.99	A
581	CB	MET	92	8.708	-1.524	56.475	1.00	42.01	A
582	CG	MET	92	10.005	-0.872	55.965	1.00	44.68	A
583	SD	MET	92	10.124	0.894	56.343	1.00	48.32	A
584	CE	MET	92	11.755	0.952	57.098	1.00	47.67	A
585	C	MET	92	7.246	-1.634	58.579	1.00	38.29	A
586	O	MET	92	6.265	-1.145	57.986	1.00	37.09	A
587	N	ALA	93	7.088	-2.278	59.744	1.00	33.03	A
588	CA	ALA	93	5.776	-2.292	60.378	1.00	30.77	A
589	CB	ALA	93	5.784	-3.241	61.579	1.00	30.88	A
590	C	ALA	93	5.566	-0.833	60.801	1.00	26.21	A
591	O	ALA	93	6.519	-0.061	60.984	1.00	26.39	A
592	N	PRO	94	4.339	-0.414	60.993	1.00	25.45	A
593	CA	PRO	94	4.001	0.911	61.454	1.00	24.71	A
594	CD	PRO	94	3.138	-1.282	60.866	1.00	27.05	A
595	CB	PRO	94	2.498	0.937	61.426	1.00	24.24	A
596	CG	PRO	94	2.063	-0.488	61.540	1.00	27.58	A
597	C	PRO	94	4.586	1.134	62.853	1.00	23.01	A
598	O	PRO	94	4.182	0.405	63.771	1.00	22.00	A
599	N	SER	95	5.380	2.177	63.030	1.00	21.95	A
600	CA	SER	95	6.074	2.390	64.307	1.00	19.65	A
601	CB	SER	95	7.371	1.567	64.279	1.00	17.85	A
602	OG	SER	95	8.170	1.976	63.168	1.00	19.02	A
603	C	SER	95	6.433	3.842	64.540	1.00	21.19	A
604	O	SER	95	6.984	4.232	65.590	1.00	20.42	A
605	N	LEU	96	6.014	4.734	63.620	1.00	19.13	A
606	CA	LEU	96	6.309	6.159	63.800	1.00	18.01	A
607	CB	LEU	96	5.732	6.987	62.625	1.00	15.73	A
608	CG	LEU	96	6.021	8.495	62.787	1.00	18.09	A
609	CD2	LEU	96	5.344	9.254	61.649	1.00	19.36	A
610	CD1	LEU	96	7.517	8.788	62.715	1.00	17.55	A
611	C	LEU	96	5.786	6.727	65.121	1.00	17.50	A
612	O	LEU	96	6.447	7.588	65.720	1.00	16.57	A
613	N	ASN	97	4.572	6.396	65.508	1.00	17.74	A
614	CA	ASN	97	3.962	6.946	66.729	1.00	17.67	A
615	CB	ASN	97	2.536	6.418	66.878	1.00	18.54	A
616	CG	ASN	97	1.559	6.945	65.844	1.00	20.15	A
617	OD1	ASN	97	0.373	6.530	65.830	1.00	22.49	A
618	ND2	ASN	97	1.996	7.888	65.040	1.00	14.75	A
619	C	ASN	97	4.789	6.539	67.971	1.00	17.57	A
620	O	ASN	97	5.114	7.411	68.765	1.00	17.20	A
621	N	ALA	98	5.239	5.299	68.063	1.00	17.89	A
622	CA	ALA	98	6.116	4.874	69.156	1.00	19.90	A
623	CB	ALA	98	6.459	3.382	69.117	1.00	18.51	A
624	C	ALA	98	7.418	5.641	69.147	1.00	18.57	A
625	O	ALA	98	8.035	6.005	70.196	1.00	18.22	A
626	N	ARG	99	8.000	5.788	67.939	1.00	15.38	A
627	CA	ARG	99	9.198	6.584	67.808	1.00	15.91	A
628	CB	ARG	99	9.736	6.561	66.322	1.00	17.77	A
629	CG	ARG	99	9.922	5.102	65.894	1.00	18.85	A
630	CD	ARG	99	10.377	5.051	64.441	1.00	17.09	A

631	NE	ARG	99	10.364	3.734	63.832	1.00	17.08	A
632	CZ	ARG	99	11.483	3.005	63.837	1.00	19.23	A
633	NH1	ARG	99	12.582	3.470	64.438	1.00	15.98	A
634	NH2	ARG	99	11.439	1.825	63.211	1.00	21.09	A
635	C	ARG	99	9.010	8.007	68.270	1.00	14.62	A
636	O	ARG	99	9.813	8.566	69.052	1.00	16.83	A
637	N	GLN	100	8.013	8.687	67.759	1.00	14.76	A
638	CA	GLN	100	7.755	10.093	68.096	1.00	15.89	A
639	CB	GLN	100	6.471	10.518	67.386	1.00	16.39	A
640	CG	GLN	100	6.589	10.774	65.861	1.00	16.04	A
641	CD	GLN	100	7.193	12.136	65.634	1.00	14.40	A
642	OE1	GLN	100	6.499	12.946	65.003	1.00	21.02	A
643	NE2	GLN	100	8.372	12.458	66.071	1.00	14.10	A
644	C	GLN	100	7.475	10.202	69.622	1.00	15.87	A
645	O	GLN	100	7.777	11.189	70.280	1.00	17.94	A
646	N	ASP	101	6.725	9.238	70.173	1.00	16.61	A
647	CA	ASP	101	6.404	9.336	71.629	1.00	19.76	A
648	CB	ASP	101	5.522	8.146	72.016	1.00	20.02	A
649	CG	ASP	101	4.103	8.330	71.534	1.00	19.83	A
650	OD1	ASP	101	3.727	9.441	71.188	1.00	17.95	A
651	OD2	ASP	101	3.359	7.357	71.523	1.00	24.70	A
652	C	ASP	101	7.715	9.313	72.423	1.00	20.87	A
653	O	ASP	101	7.824	10.021	73.446	1.00	27.99	A
654	N	LEU	102	8.774	8.667	71.954	1.00	19.31	A
655	CA	LEU	102	10.082	8.718	72.603	1.00	16.53	A
656	CB	LEU	102	10.931	7.530	72.208	1.00	18.29	A
657	CG	LEU	102	12.276	7.281	72.888	1.00	19.63	A
658	CD2	LEU	102	13.256	8.393	72.584	1.00	25.96	A
659	CD1	LEU	102	13.019	6.034	72.414	1.00	20.49	A
660	C	LEU	102	10.752	10.043	72.329	1.00	19.62	A
661	O	LEU	102	11.269	10.746	73.227	1.00	17.52	A
662	N	VAL	103	10.980	10.374	71.032	1.00	18.18	A
663	CA	VAL	103	11.888	11.468	70.699	1.00	15.75	A
664	CB	VAL	103	12.449	11.309	69.236	1.00	18.04	A
665	CG1	VAL	103	13.122	9.941	69.142	1.00	14.19	A
666	CG2	VAL	103	11.350	11.445	68.181	1.00	13.15	A
667	C	VAL	103	11.299	12.833	70.858	1.00	13.49	A
668	O	VAL	103	12.044	13.813	71.001	1.00	13.92	A
669	N	VAL	104	9.981	13.018	70.850	1.00	14.88	A
670	CA	VAL	104	9.346	14.321	71.017	1.00	14.37	A
671	CB	VAL	104	7.856	14.282	70.698	1.00	18.72	A
672	CG1	VAL	104	7.102	15.492	71.202	1.00	17.65	A
673	CG2	VAL	104	7.622	14.322	69.122	1.00	16.40	A
674	C	VAL	104	9.589	14.926	72.420	1.00	17.96	A
675	O	VAL	104	9.844	16.140	72.563	1.00	16.58	A
676	N	THR	105	9.657	14.018	73.414	1.00	14.93	A
677	CA	THR	105	10.082	14.554	74.730	1.00	18.23	A
678	CB	THR	105	9.356	13.736	75.842	1.00	18.83	A
679	OG1	THR	105	9.653	12.375	75.611	1.00	20.03	A
680	CG2	THR	105	7.843	13.834	75.729	1.00	19.34	A
681	C	THR	105	11.581	14.428	74.919	1.00	17.76	A
682	O	THR	105	12.297	15.321	75.390	1.00	16.74	A

683	N	GLY	106	12.156	13.355	74.408	1.00	18.35	A
684	CA	GLY	106	13.588	13.075	74.646	1.00	20.22	A
685	C	GLY	106	14.573	14.040	74.076	1.00	17.61	A
686	O	GLY	106	15.617	14.427	74.619	1.00	18.07	A
687	N	VAL	107	14.283	14.500	72.828	1.00	18.39	A
688	CA	VAL	107	15.253	15.382	72.150	1.00	14.98	A
689	CB	VAL	107	14.794	15.578	70.688	1.00	15.76	A
690	CG1	VAL	107	15.372	16.793	70.033	1.00	12.18	A
691	CG2	VAL	107	15.172	14.301	69.879	1.00	14.81	A
692	C	VAL	107	15.409	16.665	72.929	1.00	14.08	A
693	O	VAL	107	16.524	17.141	73.159	1.00	14.20	A
694	N	PRO	108	14.341	17.395	73.241	1.00	14.43	A
695	CA	PRO	108	14.438	18.640	73.962	1.00	16.42	A
696	CD	PRO	108	12.948	17.026	72.949	1.00	16.38	A
697	CB	PRO	108	13.039	19.206	73.945	1.00	17.29	A
698	CG	PRO	108	12.103	18.080	73.638	1.00	17.10	A
699	C	PRO	108	15.030	18.462	75.375	1.00	17.39	A
700	O	PRO	108	15.717	19.340	75.899	1.00	16.11	A
701	N	MET	109	14.681	17.377	76.050	1.00	18.23	A
702	CA	MET	109	15.216	17.142	77.417	1.00	19.54	A
703	CB	MET	109	14.579	15.892	78.030	1.00	18.80	A
704	CG	MET	109	15.141	15.705	79.453	1.00	24.55	A
705	SD	MET	109	14.681	17.096	80.548	1.00	30.03	A
706	CE	MET	109	12.892	17.062	80.237	1.00	23.66	A
707	C	MET	109	16.726	16.932	77.368	1.00	19.02	A
708	O	MET	109	17.498	17.514	78.126	1.00	17.91	A
709	N	LEU	110	17.197	16.076	76.453	1.00	18.49	A
710	CA	LEU	110	18.611	15.843	76.232	1.00	18.20	A
711	CB	LEU	110	18.821	14.757	75.163	1.00	18.64	A
712	CG	LEU	110	20.275	14.405	74.813	1.00	19.58	A
713	CD2	LEU	110	20.325	13.371	73.673	1.00	18.33	A
714	CD1	LEU	110	20.970	13.816	76.051	1.00	18.07	A
715	C	LEU	110	19.337	17.100	75.806	1.00	18.48	A
716	O	LEU	110	20.433	17.435	76.297	1.00	20.76	A
717	N	GLY	111	18.711	17.945	74.981	1.00	16.22	A
718	CA	GLY	111	19.304	19.235	74.604	1.00	14.18	A
719	C	GLY	111	19.371	20.178	75.812	1.00	16.43	A
720	O	GLY	111	20.299	20.948	76.061	1.00	15.13	A
721	N	LYS	112	18.371	20.116	76.685	1.00	15.61	A
722	CA	LYS	112	18.401	20.945	77.898	1.00	16.57	A
723	CB	LYS	112	17.103	20.710	78.684	1.00	18.18	A
724	CG	LYS	112	16.987	21.680	79.892	1.00	20.77	A
725	CD	LYS	112	16.318	20.904	81.048	1.00	22.71	A
726	CE	LYS	112	17.323	19.962	81.667	1.00	27.09	A
727	NZ	LYS	112	16.687	19.337	82.890	1.00	32.10	A
728	C	LYS	112	19.597	20.512	78.747	1.00	14.36	A
729	O	LYS	112	20.258	21.371	79.299	1.00	16.03	A
730	N	GLU	113	19.915	19.227	78.831	1.00	17.89	A
731	CA	GLU	113	21.055	18.838	79.690	1.00	19.13	A
732	CB	GLU	113	21.089	17.313	79.820	1.00	22.35	A
733	CG	GLU	113	19.889	16.849	80.643	1.00	27.59	A
734	CD	GLU	113	19.575	15.381	80.477	1.00	30.72	A

735	OE1	GLU	113	20.383	14.636	79.816	1.00	34.90	A
736	OE2	GLU	113	18.516	14.896	81.021	1.00	33.21	A
737	C	GLU	113	22.372	19.390	79.154	1.00	20.94	A
738	O	GLU	113	23.264	19.789	79.915	1.00	15.83	A
739	N	ALA	114	22.498	19.420	77.852	1.00	17.27	A
740	CA	ALA	114	23.708	19.962	77.235	1.00	16.41	A
741	CB	ALA	114	23.731	19.648	75.742	1.00	13.77	A
742	C	ALA	114	23.749	21.485	77.439	1.00	14.62	A
743	O	ALA	114	24.791	22.066	77.757	1.00	13.91	A
744	N	ALA	115	22.598	22.115	77.260	1.00	13.33	A
745	CA	ALA	115	22.480	23.585	77.361	1.00	13.34	A
746	CB	ALA	115	21.060	24.038	77.044	1.00	13.34	A
747	C	ALA	115	22.825	24.103	78.766	1.00	16.12	A
748	O	ALA	115	23.455	25.153	78.930	1.00	14.73	A
749	N	VAL	116	22.393	23.380	79.782	1.00	16.09	A
750	CA	VAL	116	22.668	23.795	81.168	1.00	17.57	A
751	CB	VAL	116	22.046	22.819	82.168	1.00	16.56	A
752	CG1	VAL	116	22.547	23.031	83.602	1.00	16.83	A
753	CG2	VAL	116	20.521	22.936	82.249	1.00	14.36	A
754	C	VAL	116	24.182	23.858	81.387	1.00	16.32	A
755	O	VAL	116	24.702	24.791	82.013	1.00	17.09	A
756	N	LYS	117	24.861	22.859	80.850	1.00	18.67	A
757	CA	LYS	117	26.324	22.751	80.965	1.00	19.95	A
758	CB	LYS	117	26.822	21.443	80.365	1.00	20.22	A
759	CG	LYS	117	26.532	20.235	81.251	1.00	23.41	A
760	CD	LYS	117	27.018	18.925	80.638	1.00	25.60	A
761	CE	LYS	117	26.247	17.704	81.136	1.00	27.45	A
762	NZ	LYS	117	26.879	16.439	80.735	1.00	27.56	A
763	C	LYS	117	27.024	23.902	80.231	1.00	19.45	A
764	O	LYS	117	27.988	24.489	80.726	1.00	17.34	A
765	N	ALA	118	26.549	24.220	79.039	1.00	17.17	A
766	CA	ALA	118	27.157	25.309	78.250	1.00	15.71	A
767	CB	ALA	118	26.501	25.415	76.875	1.00	17.47	A
768	C	ALA	118	26.985	26.651	78.976	1.00	15.84	A
769	O	ALA	118	27.908	27.466	79.068	1.00	16.06	A
770	N	ILE	119	25.792	26.861	79.486	1.00	18.12	A
771	CA	ILE	119	25.446	28.109	80.181	1.00	18.00	A
772	CB	ILE	119	23.937	28.145	80.409	1.00	19.24	A
773	CG2	ILE	119	23.498	29.252	81.368	1.00	18.79	A
774	CG1	ILE	119	23.163	28.373	79.109	1.00	18.13	A
775	CD1	ILE	119	21.670	28.086	79.241	1.00	16.38	A
776	C	ILE	119	26.190	28.215	81.517	1.00	18.79	A
777	O	ILE	119	26.612	29.301	81.913	1.00	20.34	A
778	N	ASP	120	26.457	27.099	82.123	0.50	19.78	A
779	CA	ASP	120	27.191	27.069	83.392	0.50	21.23	A
780	CB	ASP	120	27.043	25.701	84.032	0.50	21.61	A
781	CG	ASP	120	25.743	25.622	84.821	0.50	23.09	A
782	OD1	ASP	120	25.277	24.484	85.185	0.50	25.77	A
783	OD2	ASP	120	25.114	26.712	85.115	0.50	24.50	A
784	C	ASP	120	28.652	27.452	83.140	0.50	21.63	A
785	O	ASP	120	29.263	28.203	83.913	0.50	20.32	A
778	N	2ASP	120	26.430	27.095	82.148	0.50	18.97	A

779	CA	2ASP	120	27.176	27.073	83.414	0.50	19.78	A
780	CB	2ASP	120	27.105	25.691	84.055	0.50	18.04	A
781	CG	2ASP	120	27.823	25.634	85.402	0.50	18.53	A
782	OD	12ASP	120	27.378	26.311	86.405	0.50	18.96	A
783	OD	22ASP	120	28.811	24.912	85.525	0.50	14.37	A
784	C	2ASP	120	28.633	27.483	83.139	0.50	20.73	A
785	O	2ASP	120	29.225	28.289	83.868	0.50	19.80	A
794	N	GLU	121	29.255	26.892	82.096	1.00	20.48	A
795	CA	GLU	121	30.577	27.296	81.668	1.00	19.07	A
796	CB	GLU	121	31.089	26.472	80.454	1.00	20.06	A
797	CG	GLU	121	32.459	27.012	79.979	1.00	21.09	A
798	CD	GLU	121	32.816	26.412	78.600	1.00	22.32	A
799	OE1	GLU	121	32.182	25.479	78.093	1.00	21.05	A
800	OE2	GLU	121	33.843	26.890	78.072	1.00	22.00	A
801	C	GLU	121	30.625	28.776	81.369	1.00	20.81	A
802	O	GLU	121	31.521	29.554	81.776	1.00	20.90	A
803	N	TRP	122	29.653	29.236	80.583	1.00	18.77	A
804	CA	TRP	122	29.584	30.620	80.181	1.00	18.63	A
805	CB	TRP	122	28.334	30.801	79.294	1.00	16.48	A
806	CG	TRP	122	28.155	32.174	78.726	1.00	16.28	A
807	CD2	TRP	122	26.923	32.873	78.518	1.00	15.79	A
808	CD1	TRP	122	29.116	32.990	78.194	1.00	16.70	A
809	NE1	TRP	122	28.583	34.161	77.731	1.00	16.88	A
810	CE2	TRP	122	27.211	34.093	77.901	1.00	15.08	A
811	CE3	TRP	122	25.577	32.560	78.829	1.00	17.00	A
812	CZ2	TRP	122	26.262	35.047	77.609	1.00	13.22	A
813	CZ3	TRP	122	24.614	33.522	78.531	1.00	13.93	A
814	CH2	TRP	122	24.969	34.717	77.916	1.00	13.27	A
815	C	TRP	122	29.538	31.499	81.441	1.00	21.18	A
816	O	TRP	122	30.143	32.595	81.471	1.00	21.65	A
817	N	GLY	123	28.546	31.276	82.290	1.00	21.20	A
818	CA	GLY	123	28.464	31.926	83.601	1.00	20.30	A
819	C	GLY	123	27.636	33.178	83.633	1.00	22.55	A
820	O	GLY	123	27.223	33.591	84.711	1.00	23.03	A
821	N	LEU	124	27.214	33.734	82.476	1.00	19.56	A
822	CA	LEU	124	26.387	34.911	82.452	1.00	18.14	A
823	CB	LEU	124	26.671	35.733	81.199	1.00	23.08	A
824	CG	LEU	124	27.898	36.660	81.262	1.00	24.54	A
825	CD2	LEU	124	27.913	37.634	80.089	1.00	23.57	A
826	CD1	LEU	124	29.206	35.864	81.321	1.00	24.28	A
827	C	LEU	124	24.926	34.504	82.604	1.00	18.48	A
828	O	LEU	124	24.566	33.340	82.410	1.00	18.76	A
829	N	PRO	125	24.055	35.423	82.938	1.00	19.11	A
830	CA	PRO	125	22.654	35.144	83.097	1.00	20.89	A
831	CD	PRO	125	24.389	36.861	83.156	1.00	19.83	A
832	CB	PRO	125	22.040	36.459	83.557	1.00	21.21	A
833	CG	PRO	125	23.163	37.368	83.904	1.00	23.77	A
834	C	PRO	125	22.003	34.619	81.809	1.00	21.34	A
835	O	PRO	125	22.193	35.136	80.694	1.00	21.43	A
836	N	LYS	126	21.174	33.600	81.942	1.00	19.50	A
837	CA	LYS	126	20.433	32.982	80.835	1.00	21.62	A
838	CB	LYS	126	19.846	31.624	81.228	1.00	20.60	A

839	CG	LYS	126	18.716	31.656	82.265	1.00	24.65	A
840	CD	LYS	126	18.268	30.231	82.580	1.00	24.08	A
841	CE	LYS	126	17.293	30.086	83.743	1.00	27.19	A
842	NZ	LYS	126	16.268	31.128	83.772	1.00	28.11	A
843	C	LYS	126	19.451	33.949	80.210	1.00	20.79	A
844	O	LYS	126	19.057	33.887	79.024	1.00	19.00	A
845	N	SER	127	19.054	35.006	80.960	1.00	18.95	A
846	CA	SER	127	18.198	36.061	80.448	1.00	19.28	A
847	CB	SER	127	17.769	37.070	81.561	1.00	18.43	A
848	OG	SER	127	18.972	37.718	81.982	1.00	20.37	A
849	C	SER	127	18.880	36.875	79.350	1.00	19.12	A
850	O	SER	127	18.226	37.612	78.598	1.00	19.26	A
851	N	LYS	128	20.207	36.775	79.241	1.00	18.44	A
852	CA	LYS	128	20.934	37.466	78.202	1.00	19.59	A
853	CB	LYS	128	22.371	37.809	78.645	1.00	22.71	A
854	CG	LYS	128	22.360	38.988	79.650	1.00	28.47	A
855	CD	LYS	128	23.798	39.358	80.030	1.00	33.65	A
856	CE	LYS	128	23.837	40.734	80.699	1.00	37.84	A
857	NZ	LYS	128	25.066	40.919	81.542	1.00	40.83	A
858	C	LYS	128	20.970	36.648	76.886	1.00	17.61	A
859	O	LYS	128	21.654	37.100	75.975	1.00	17.90	A
860	N	ILE	129	20.492	35.446	76.817	1.00	16.00	A
861	CA	ILE	129	20.418	34.665	75.559	1.00	15.86	A
862	CB	ILE	129	20.184	33.196	75.852	1.00	14.94	A
863	CG2	ILE	129	19.853	32.386	74.563	1.00	13.22	A
864	CG1	ILE	129	21.464	32.641	76.525	1.00	15.39	A
865	CD1	ILE	129	21.251	31.266	77.182	1.00	12.48	A
866	C	ILE	129	19.323	35.309	74.719	1.00	16.47	A
867	O	ILE	129	18.190	35.359	75.206	1.00	15.12	A
868	N	THR	130	19.660	35.830	73.526	1.00	14.40	A
869	CA	THR	130	18.674	36.537	72.722	1.00	15.90	A
870	CB	THR	130	19.356	37.780	72.073	1.00	16.78	A
871	OG1	THR	130	20.588	37.405	71.457	1.00	14.61	A
872	CG2	THR	130	19.600	38.797	73.226	1.00	20.14	A
873	C	THR	130	18.116	35.718	71.552	1.00	14.97	A
874	O	THR	130	17.072	36.074	71.030	1.00	13.58	A
875	N	HIS	131	18.817	34.672	71.133	1.00	14.54	A
876	CA	HIS	131	18.460	33.849	69.997	1.00	14.88	A
877	ND1	HIS	131	19.656	36.778	68.871	1.00	14.87	A
878	CG	HIS	131	19.134	35.633	68.252	1.00	14.61	A
879	CB	HIS	131	19.347	34.251	68.754	1.00	11.60	A
880	NE2	HIS	131	18.565	37.480	67.118	1.00	12.92	A
881	CD2	HIS	131	18.458	36.092	67.140	1.00	10.98	A
882	CE1	HIS	131	19.361	37.852	68.159	1.00	15.43	A
883	C	HIS	131	18.769	32.417	70.382	1.00	15.66	A
884	O	HIS	131	19.744	32.127	71.106	1.00	14.95	A
885	N	LEU	132	17.935	31.487	69.947	1.00	11.48	A
886	CA	LEU	132	18.046	30.095	70.167	1.00	13.97	A
887	CB	LEU	132	16.883	29.525	71.004	1.00	11.50	A
888	CG	LEU	132	16.800	28.010	71.055	1.00	13.95	A
889	CD2	LEU	132	15.496	27.637	71.783	1.00	12.94	A
890	CD1	LEU	132	17.976	27.318	71.746	1.00	13.85	A

891	C	LEU	132	17.915	29.322	68.823	1.00	14.21	A
892	O	LEU	132	16.909	29.490	68.133	1.00	12.57	A
893	N	ILE	133	18.927	28.543	68.531	1.00	16.16	A
894	CA	ILE	133	18.880	27.710	67.311	1.00	14.73	A
895	CB	ILE	133	20.145	27.803	66.434	1.00	14.29	A
896	CG2	ILE	133	20.083	26.754	65.321	1.00	13.55	A
897	CG1	ILE	133	20.306	29.227	65.887	1.00	12.77	A
898	CD1	ILE	133	21.732	29.488	65.391	1.00	13.14	A
899	C	ILE	133	18.758	26.263	67.829	1.00	14.02	A
900	O	ILE	133	19.669	25.807	68.529	1.00	15.60	A
901	N	PHE	134	17.637	25.617	67.546	1.00	12.75	A
902	CA	PHE	134	17.508	24.222	67.961	1.00	14.31	A
903	CB	PHE	134	16.173	23.968	68.718	1.00	13.08	A
904	CG	PHE	134	16.243	22.661	69.465	1.00	14.84	A
905	CD1	PHE	134	16.267	22.700	70.896	1.00	13.62	A
906	CD2	PHE	134	16.177	21.453	68.831	1.00	13.56	A
907	CE1	PHE	134	16.304	21.485	71.584	1.00	12.53	A
908	CE2	PHE	134	16.288	20.257	69.520	1.00	15.13	A
909	CZ	PHE	134	16.360	20.278	70.926	1.00	14.68	A
910	C	PHE	134	17.524	23.349	66.693	1.00	15.71	A
911	O	PHE	134	16.787	23.619	65.706	1.00	16.42	A
912	N	CYS	135	18.358	22.353	66.708	1.00	15.75	A
913	CA	CYS	135	18.522	21.499	65.502	1.00	16.73	A
914	CB	CYS	135	19.884	21.859	64.834	1.00	15.26	A
915	SG	CYS	135	20.328	20.732	63.445	1.00	15.19	A
916	C	CYS	135	18.465	20.056	65.836	1.00	15.01	A
917	O	CYS	135	19.009	19.629	66.880	1.00	13.86	A
918	N	THR	136	17.663	19.285	65.092	1.00	13.11	A
919	CA	THR	136	17.623	17.854	65.246	1.00	12.65	A
920	CB	THR	136	16.572	17.458	66.335	1.00	11.65	A
921	OG1	THR	136	16.660	16.068	66.616	1.00	10.20	A
922	CG2	THR	136	15.131	17.740	65.909	1.00	9.93	A
923	C	THR	136	17.249	17.186	63.922	1.00	14.69	A
924	O	THR	136	16.870	17.854	62.950	1.00	16.07	A
925	N	THR	137	17.383	15.874	63.928	1.00	12.78	A
926	CA	THR	137	17.043	15.032	62.777	1.00	15.31	A
927	CB	THR	137	18.310	14.389	62.186	1.00	15.76	A
928	OG1	THR	137	19.338	15.362	62.046	1.00	14.12	A
929	CG2	THR	137	18.077	13.777	60.800	1.00	17.92	A
930	C	THR	137	16.079	13.931	63.231	1.00	16.12	A
931	O	THR	137	15.720	13.030	62.467	1.00	15.44	A
932	N	ALA	138	15.649	14.027	64.484	1.00	14.51	A
933	CA	ALA	138	14.776	12.996	65.074	1.00	15.90	A
934	CB	ALA	138	15.496	12.320	66.243	1.00	16.72	A
935	C	ALA	138	13.447	13.566	65.597	1.00	16.75	A
936	O	ALA	138	13.405	14.229	66.644	1.00	16.22	A
937	N	GLY	139	12.400	13.265	64.836	1.00	15.47	A
938	CA	GLY	139	11.003	13.646	65.154	1.00	16.54	A
939	C	GLY	139	10.724	15.135	64.881	1.00	13.58	A
940	O	GLY	139	11.632	15.933	64.641	1.00	16.14	A
941	N	VAL	140	9.439	15.447	64.906	1.00	12.00	A
942	CA	VAL	140	8.917	16.821	64.769	1.00	14.02	A

943	CB	VAL	140	8.583	17.186	63.313	1.00	14.96	A
944	CG1	VAL	140	9.745	16.964	62.348	1.00	14.96	A
945	CG2	VAL	140	7.402	16.393	62.754	1.00	15.30	A
946	C	VAL	140	7.642	16.903	65.587	1.00	11.68	A
947	O	VAL	140	7.008	15.887	65.877	1.00	15.88	A
948	N	ASP	141	7.288	18.095	65.956	1.00	12.22	A
949	CA	ASP	141	6.082	18.329	66.748	1.00	14.96	A
950	CB	ASP	141	6.343	17.905	68.200	1.00	15.56	A
951	CG	ASP	141	5.068	17.708	69.024	1.00	18.13	A
952	OD1	ASP	141	4.036	17.140	68.502	1.00	19.29	A
953	OD2	ASP	141	5.026	18.111	70.249	1.00	18.44	A
954	C	ASP	141	5.777	19.796	66.672	1.00	15.17	A
955	O	ASP	141	6.630	20.646	66.329	1.00	16.33	A
956	N	MET	142	4.573	20.198	67.043	1.00	12.47	A
957	CA	MET	142	4.163	21.576	67.107	1.00	12.35	A
958	CB	MET	142	3.274	22.034	65.937	1.00	12.65	A
959	CG	MET	142	3.849	21.519	64.560	1.00	13.17	A
960	SD	MET	142	2.778	22.129	63.249	1.00	17.73	A
961	CE	MET	142	3.238	23.820	63.168	1.00	12.70	A
962	C	MET	142	3.430	21.833	68.425	1.00	14.69	A
963	O	MET	142	2.530	21.028	68.630	1.00	11.86	A
964	N	PRO	143	3.862	22.750	69.210	1.00	15.28	A
965	CA	PRO	143	5.051	23.558	69.203	1.00	13.24	A
966	CD	PRO	143	3.201	23.007	70.527	1.00	16.57	A
967	CB	PRO	143	5.128	24.447	70.428	1.00	16.21	A
968	CG	PRO	143	3.868	24.173	71.156	1.00	17.09	A
969	C	PRO	143	6.270	22.671	69.122	1.00	11.50	A
970	O	PRO	143	6.231	21.479	69.430	1.00	11.80	A
971	N	GLY	144	7.360	23.233	68.554	1.00	12.53	A
972	CA	GLY	144	8.509	22.371	68.317	1.00	14.94	A
973	C	GLY	144	9.454	22.196	69.510	1.00	15.09	A
974	O	GLY	144	9.214	22.737	70.580	1.00	15.08	A
975	N	ALA	145	10.535	21.443	69.291	1.00	13.80	A
976	CA	ALA	145	11.507	21.238	70.340	1.00	14.14	A
977	CB	ALA	145	12.609	20.293	69.930	1.00	12.47	A
978	C	ALA	145	12.124	22.560	70.844	1.00	15.66	A
979	O	ALA	145	12.599	22.643	71.986	1.00	16.32	A
980	N	ASP	146	12.118	23.600	70.015	1.00	13.22	A
981	CA	ASP	146	12.685	24.908	70.430	1.00	15.87	A
982	CB	ASP	146	12.738	25.912	69.268	1.00	14.01	A
983	CG	ASP	146	11.381	26.189	68.621	1.00	15.41	A
984	OD1	ASP	146	10.555	25.222	68.427	1.00	13.88	A
985	OD2	ASP	146	11.069	27.386	68.257	1.00	14.80	A
986	C	ASP	146	11.848	25.508	71.565	1.00	16.26	A
987	O	ASP	146	12.383	26.053	72.542	1.00	13.83	A
988	N	TYR	147	10.545	25.393	71.410	1.00	15.62	A
989	CA	TYR	147	9.603	25.906	72.404	1.00	17.56	A
990	CB	TYR	147	8.168	25.788	71.901	1.00	19.53	A
991	CG	TYR	147	7.155	25.905	73.035	1.00	21.75	A
992	CD1	TYR	147	6.720	27.164	73.453	1.00	22.18	A
993	CD2	TYR	147	6.675	24.750	73.659	1.00	21.43	A
994	CE1	TYR	147	5.808	27.271	74.503	1.00	24.05	A

995	CE2	TYR	147	5.764	24.859	74.715	1.00	22.89	A
996	CZ	TYR	147	5.332	26.121	75.137	1.00	25.54	A
997	OH	TYR	147	4.451	26.235	76.165	1.00	26.85	A
998	C	TYR	147	9.747	25.121	73.716	1.00	15.68	A
999	O	TYR	147	9.762	25.699	74.810	1.00	17.55	A
1000	N	GLN	148	9.854	23.800	73.597	1.00	14.99	A
1001	CA	GLN	148	10.007	22.931	74.782	1.00	17.49	A
1002	CB	GLN	148	10.130	21.449	74.400	1.00	16.80	A
1003	CG	GLN	148	8.907	20.883	73.674	1.00	19.62	A
1004	CD	GLN	148	7.584	21.077	74.426	1.00	22.64	A
1005	OE1	GLN	148	7.583	21.469	75.592	1.00	17.96	A
1006	NE2	GLN	148	6.440	20.831	73.808	1.00	18.78	A
1007	C	GLN	148	11.278	23.313	75.549	1.00	18.28	A
1008	O	GLN	148	11.298	23.343	76.787	1.00	16.95	A
1009	N	LEU	149	12.325	23.605	74.786	1.00	16.52	A
1010	CA	LEU	149	13.630	23.968	75.363	1.00	16.17	A
1011	CB	LEU	149	14.715	24.128	74.302	1.00	17.15	A
1012	CG	LEU	149	16.068	24.444	74.947	1.00	18.85	A
1013	CD2	LEU	149	17.171	24.749	73.939	1.00	20.01	A
1014	CD1	LEU	149	16.590	23.296	75.816	1.00	17.08	A
1015	C	LEU	149	13.560	25.293	76.138	1.00	16.77	A
1016	O	LEU	149	14.180	25.447	77.198	1.00	13.50	A
1017	N	VAL	150	12.816	26.246	75.606	1.00	14.16	A
1018	CA	VAL	150	12.653	27.557	76.263	1.00	18.01	A
1019	CB	VAL	150	11.792	28.485	75.406	1.00	18.11	A
1020	CG1	VAL	150	11.328	29.731	76.168	1.00	17.86	A
1021	CG2	VAL	150	12.526	28.994	74.163	1.00	15.15	A
1022	C	VAL	150	11.982	27.372	77.636	1.00	19.70	A
1023	O	VAL	150	12.395	27.973	78.635	1.00	19.11	A
1024	N	LYS	151	10.961	26.534	77.638	1.00	17.83	A
1025	CA	LYS	151	10.164	26.208	78.842	1.00	21.77	A
1026	CB	LYS	151	9.010	25.297	78.420	1.00	24.68	A
1027	CG	LYS	151	8.072	24.921	79.561	1.00	30.91	A
1028	CD	LYS	151	6.971	23.958	79.115	1.00	34.30	A
1029	CE	LYS	151	5.718	24.044	79.983	1.00	37.33	A
1030	NZ	LYS	151	4.774	22.947	79.728	1.00	38.19	A
1031	C	LYS	151	11.031	25.487	79.880	1.00	21.42	A
1032	O	LYS	151	11.128	25.883	81.027	1.00	19.15	A
1033	N	LEU	152	11.742	24.446	79.471	1.00	17.46	A
1034	CA	LEU	152	12.633	23.653	80.236	1.00	21.09	A
1035	CB	LEU	152	13.200	22.522	79.373	1.00	22.56	A
1036	CG	LEU	152	12.813	21.079	79.538	1.00	27.28	A
1037	CD2	LEU	152	12.742	20.286	78.238	1.00	25.41	A
1038	CD1	LEU	152	11.558	20.840	80.389	1.00	29.19	A
1039	C	LEU	152	13.763	24.480	80.833	1.00	23.13	A
1040	O	LEU	152	14.106	24.209	81.996	1.00	20.16	A
1041	N	LEU	153	14.358	25.403	80.070	1.00	18.40	A
1042	CA	LEU	153	15.503	26.119	80.574	1.00	20.40	A
1043	CB	LEU	153	16.382	26.485	79.359	1.00	20.57	A
1044	CG	LEU	153	17.877	26.358	79.291	1.00	24.59	A
1045	CD2	LEU	153	18.308	26.399	77.813	1.00	22.59	A
1046	CD1	LEU	153	18.411	25.111	80.019	1.00	23.12	A

1047	C	LEU	153	15.101	27.398	81.283	1.00	19.64	A
1048	O	LEU	153	15.945	27.971	81.967	1.00	17.34	A
1049	N	GLY	154	13.914	27.915	81.043	1.00	17.94	A
1050	CA	GLY	154	13.496	29.218	81.518	1.00	19.41	A
1051	C	GLY	154	14.175	30.350	80.739	1.00	20.74	A
1052	O	GLY	154	14.546	31.389	81.322	1.00	19.81	A
1053	N	LEU	155	14.299	30.195	79.399	1.00	18.06	A
1054	CA	LEU	155	14.766	31.359	78.612	1.00	15.78	A
1055	CB	LEU	155	15.148	30.916	77.196	1.00	14.66	A
1056	CG	LEU	155	16.221	29.829	77.137	1.00	16.04	A
1057	CD2	LEU	155	17.522	30.344	77.738	1.00	13.61	A
1058	CD1	LEU	155	16.555	29.414	75.701	1.00	17.31	A
1059	C	LEU	155	13.675	32.397	78.493	1.00	16.11	A
1060	O	LEU	155	12.512	32.103	78.776	1.00	15.33	A
1061	N	SER	156	14.004	33.608	78.057	1.00	14.91	A
1062	CA	SER	156	13.052	34.662	77.854	1.00	15.86	A
1063	CB	SER	156	13.735	35.930	77.301	1.00	16.39	A
1064	OG	SER	156	12.766	36.841	76.777	1.00	19.30	A
1065	C	SER	156	11.985	34.196	76.887	1.00	19.09	A
1066	O	SER	156	12.285	33.526	75.906	1.00	17.54	A
1067	N	PRO	157	10.716	34.489	77.156	1.00	20.48	A
1068	CA	PRO	157	9.620	34.161	76.291	1.00	18.95	A
1069	CD	PRO	157	10.268	35.254	78.374	1.00	20.56	A
1070	CB	PRO	157	8.354	34.731	76.945	1.00	19.94	A
1071	CG	PRO	157	8.761	35.066	78.359	1.00	24.08	A
1072	C	PRO	157	9.825	34.836	74.935	1.00	16.61	A
1073	O	PRO	157	9.197	34.433	73.935	1.00	16.75	A
1074	N	SER	158	10.577	35.929	74.902	1.00	15.33	A
1075	CA	SER	158	10.845	36.681	73.714	1.00	16.28	A
1076	CB	SER	158	10.896	38.175	74.113	1.00	14.87	A
1077	OG	SER	158	9.537	38.540	74.283	1.00	16.79	A
1078	C	SER	158	12.142	36.283	73.006	1.00	17.03	A
1079	O	SER	158	12.630	37.122	72.222	1.00	16.14	A
1080	N	VAL	159	12.735	35.168	73.382	1.00	16.44	A
1081	CA	VAL	159	13.966	34.735	72.740	1.00	17.16	A
1082	CB	VAL	159	14.577	33.517	73.432	1.00	15.62	A
1083	CG1	VAL	159	13.754	32.261	73.262	1.00	16.89	A
1084	CG2	VAL	159	15.983	33.232	72.875	1.00	17.19	A
1085	C	VAL	159	13.586	34.422	71.247	1.00	18.63	A
1086	O	VAL	159	12.501	33.899	70.964	1.00	15.76	A
1087	N	LYS	160	14.497	34.792	70.343	1.00	17.02	A
1088	CA	LYS	160	14.195	34.594	68.899	1.00	16.47	A
1089	CB	LYS	160	14.946	35.648	68.051	1.00	17.21	A
1090	CG	LYS	160	14.129	36.945	67.956	1.00	18.56	A
1091	CD	LYS	160	14.968	38.011	67.176	1.00	19.23	A
1092	CE	LYS	160	14.133	39.270	66.945	1.00	22.12	A
1093	NZ	LYS	160	14.866	40.323	66.149	1.00	18.24	A
1094	C	LYS	160	14.629	33.212	68.520	1.00	15.67	A
1095	O	LYS	160	15.775	32.823	68.712	1.00	13.89	A
1096	N	ARG	161	13.722	32.382	68.017	1.00	16.27	A
1097	CA	ARG	161	13.994	31.006	67.744	1.00	15.63	A
1098	CB	ARG	161	12.920	30.092	68.418	1.00	14.77	A

1099	CG	ARG	161	12.859	30.457	69.955	1.00	13.42	A
1100	CD	ARG	161	11.629	29.691	70.465	1.00	15.07	A
1101	NE	ARG	161	10.485	30.516	70.367	1.00	16.22	A
1102	CZ	ARG	161	9.230	30.233	70.015	1.00	15.96	A
1103	NH1	ARG	161	8.942	29.048	69.548	1.00	15.82	A
1104	NH2	ARG	161	8.378	31.242	70.124	1.00	13.11	A
1105	C	ARG	161	14.081	30.571	66.279	1.00	15.67	A
1106	O	ARG	161	13.536	31.211	65.414	1.00	16.22	A
1107	N	TYR	162	14.886	29.535	66.068	1.00	13.46	A
1108	CA	TYR	162	15.183	29.022	64.699	1.00	14.97	A
1109	CB	TYR	162	16.603	29.451	64.219	1.00	12.61	A
1110	CG	TYR	162	16.719	30.966	64.212	1.00	15.38	A
1111	CD1	TYR	162	16.990	31.658	65.423	1.00	13.80	A
1112	CD2	TYR	162	16.410	31.745	63.117	1.00	13.23	A
1113	CE1	TYR	162	16.851	33.033	65.496	1.00	13.36	A
1114	CE2	TYR	162	16.385	33.119	63.142	1.00	14.86	A
1115	CZ	TYR	162	16.591	33.775	64.371	1.00	14.39	A
1116	OH	TYR	162	16.511	35.148	64.453	1.00	11.49	A
1117	C	TYR	162	15.086	27.512	64.810	1.00	12.99	A
1118	O	TYR	162	15.963	26.894	65.399	1.00	16.13	A
1119	N	MET	163	13.928	26.973	64.441	1.00	13.54	A
1120	CA	MET	163	13.702	25.539	64.663	1.00	11.42	A
1121	CB	MET	163	12.225	25.362	65.030	1.00	12.72	A
1122	CG	MET	163	11.753	23.939	65.240	1.00	13.77	A
1123	SD	MET	163	12.554	23.120	66.666	1.00	14.60	A
1124	CE	MET	163	13.550	21.883	65.892	1.00	14.05	A
1125	C	MET	163	14.051	24.763	63.396	1.00	15.21	A
1126	O	MET	163	13.257	24.841	62.437	1.00	9.57	A
1127	N	LEU	164	15.169	24.076	63.480	1.00	12.99	A
1128	CA	LEU	164	15.733	23.268	62.412	1.00	15.09	A
1129	CB	LEU	164	17.233	23.559	62.323	1.00	13.13	A
1130	CG	LEU	164	17.587	25.043	62.253	1.00	16.94	A
1131	CD2	LEU	164	16.854	25.783	61.134	1.00	17.73	A
1132	CD1	LEU	164	19.081	25.277	62.002	1.00	19.46	A
1133	C	LEU	164	15.472	21.773	62.629	1.00	15.31	A
1134	O	LEU	164	16.150	21.115	63.428	1.00	16.41	A
1135	N	TYR	165	14.489	21.302	61.875	1.00	13.24	A
1136	CA	TYR	165	14.031	19.901	61.897	1.00	12.58	A
1137	CB	TYR	165	12.494	19.860	61.889	1.00	13.09	A
1138	CG	TYR	165	11.838	19.868	63.280	1.00	13.99	A
1139	CD1	TYR	165	12.277	18.989	64.279	1.00	15.08	A
1140	CD2	TYR	165	10.781	20.751	63.548	1.00	13.57	A
1141	CE1	TYR	165	11.658	18.992	65.539	1.00	15.28	A
1142	CE2	TYR	165	10.162	20.752	64.804	1.00	14.15	A
1143	CZ	TYR	165	10.599	19.872	65.799	1.00	15.62	A
1144	OH	TYR	165	9.995	19.872	67.019	1.00	15.74	A
1145	C	TYR	165	14.508	19.150	60.634	1.00	13.25	A
1146	O	TYR	165	14.711	19.763	59.572	1.00	12.61	A
1147	N	GLN	166	14.658	17.838	60.813	1.00	13.51	A
1148	CA	GLN	166	15.057	16.877	59.749	1.00	16.56	A
1149	CB	GLN	166	13.934	16.754	58.711	1.00	16.59	A
1150	CG	GLN	166	13.819	15.349	58.130	1.00	14.49	A

1151	CD	GLN	166	13.619	14.297	59.214	1.00	18.48	A
1152	OE1	GLN	166	14.376	13.332	59.281	1.00	23.45	A
1153	NE2	GLN	166	12.635	14.435	60.083	1.00	11.19	A
1154	C	GLN	166	16.305	17.349	59.003	1.00	18.25	A
1155	O	GLN	166	16.386	17.232	57.772	1.00	16.01	A
1156	N	GLN	167	17.258	17.839	59.778	1.00	14.94	A
1157	CA	GLN	167	18.472	18.490	59.238	1.00	15.04	A
1158	CB	GLN	167	19.053	19.437	60.279	1.00	14.35	A
1159	CG	GLN	167	18.094	20.593	60.611	1.00	11.77	A
1160	CD	GLN	167	17.858	21.565	59.441	1.00	15.34	A
1161	OE1	GLN	167	18.805	22.183	58.950	1.00	13.72	A
1162	NE2	GLN	167	16.637	21.751	58.967	1.00	14.07	A
1163	C	GLN	167	19.556	17.508	58.748	1.00	16.24	A
1164	O	GLN	167	20.109	17.669	57.658	1.00	18.12	A
1165	N	GLY	168	19.908	16.510	59.531	1.00	14.08	A
1166	CA	GLY	168	20.893	15.502	59.065	1.00	13.80	A
1167	C	GLY	168	22.334	15.870	59.376	1.00	15.39	A
1168	O	GLY	168	22.695	16.824	60.095	1.00	15.87	A
1169	N	CYS	169	23.253	15.041	58.924	1.00	16.61	A
1170	CA	CYS	169	24.682	15.033	59.298	1.00	16.82	A
1171	CB	CYS	169	25.392	13.842	58.674	1.00	17.31	A
1172	SG	CYS	169	25.104	12.267	59.615	1.00	21.12	A
1173	C	CYS	169	25.514	16.259	58.887	1.00	17.71	A
1174	O	CYS	169	26.670	16.404	59.292	1.00	17.95	A
1177	N	ALA	170	25.000	17.157	58.089	1.00	15.93	A
1178	CA	ALA	170	25.814	18.331	57.718	1.00	16.42	A
1179	CB	ALA	170	25.609	18.686	56.245	1.00	16.83	A
1180	C	ALA	170	25.422	19.552	58.565	1.00	15.01	A
1181	O	ALA	170	26.081	20.595	58.520	1.00	12.25	A
1182	N	ALA	171	24.404	19.320	59.459	1.00	13.18	A
1183	CA	ALA	171	23.796	20.439	60.092	1.00	15.70	A
1184	CB	ALA	171	22.323	20.192	60.450	1.00	14.62	A
1185	C	ALA	171	24.522	20.972	61.337	1.00	13.32	A
1186	O	ALA	171	24.239	22.106	61.766	1.00	16.93	A
1187	N	GLY	172	25.605	20.304	61.727	1.00	14.02	A
1188	CA	GLY	172	26.464	20.929	62.776	1.00	14.32	A
1189	C	GLY	172	27.204	22.091	62.113	1.00	16.85	A
1190	O	GLY	172	27.435	23.150	62.690	1.00	15.28	A
1191	N	GLY	173	27.475	21.983	60.779	1.00	15.85	A
1192	CA	GLY	173	28.015	23.142	60.031	1.00	14.31	A
1193	C	GLY	173	26.917	24.195	59.844	1.00	13.19	A
1194	O	GLY	173	27.078	25.405	60.058	1.00	14.41	A
1195	N	THR	174	25.696	23.736	59.546	1.00	14.08	A
1196	CA	THR	174	24.559	24.669	59.387	1.00	14.30	A
1197	CB	THR	174	23.256	23.908	59.150	1.00	14.77	A
1198	OG1	THR	174	23.371	22.999	58.044	1.00	16.92	A
1199	CG2	THR	174	21.994	24.718	58.884	1.00	13.40	A
1200	C	THR	174	24.387	25.619	60.573	1.00	12.21	A
1201	O	THR	174	24.172	26.823	60.469	1.00	11.17	A
1202	N	VAL	175	24.253	25.072	61.798	1.00	12.71	A
1203	CA	VAL	175	23.972	25.900	62.985	1.00	11.72	A
1204	CB	VAL	175	23.782	25.045	64.260	1.00	9.02	A

1205	CG1	VAL	175	22.608	24.053	64.123	1.00	8.41	A
1206	CG2	VAL	175	24.965	24.150	64.598	1.00	9.19	A
1207	C	VAL	175	25.053	26.949	63.145	1.00	12.00	A
1208	O	VAL	175	24.783	28.079	63.531	1.00	14.66	A
1209	N	LEU	176	26.321	26.603	62.868	1.00	10.98	A
1210	CA	LEU	176	27.388	27.587	63.021	1.00	14.02	A
1211	CB	LEU	176	28.774	26.955	62.842	1.00	14.19	A
1212	CG	LEU	176	29.087	25.850	63.873	1.00	17.06	A
1213	CD2	LEU	176	29.215	26.495	65.278	1.00	18.24	A
1214	CD1	LEU	176	30.354	25.076	63.597	1.00	15.24	A
1215	C	LEU	176	27.214	28.669	61.980	1.00	14.29	A
1216	O	LEU	176	27.468	29.825	62.221	1.00	14.46	A
1217	N	ARG	177	26.849	28.243	60.752	1.00	13.39	A
1218	CA	ARG	177	26.635	29.238	59.649	1.00	13.19	A
1219	CB	ARG	177	26.339	28.381	58.383	1.00	10.10	A
1220	CG	ARG	177	25.772	29.254	57.250	1.00	12.26	A
1221	CD	ARG	177	25.868	28.471	55.943	1.00	12.34	A
1222	NE	ARG	177	25.193	27.181	55.925	1.00	11.28	A
1223	CZ	ARG	177	23.867	27.101	55.696	1.00	10.47	A
1224	NH1	ARG	177	23.120	28.157	55.494	1.00	14.49	A
1225	NH2	ARG	177	23.223	25.969	55.624	1.00	12.71	A
1226	C	ARG	177	25.557	30.211	59.969	1.00	11.64	A
1227	O	ARG	177	25.600	31.430	59.752	1.00	12.90	A
1228	N	LEU	178	24.429	29.643	60.505	1.00	13.45	A
1229	CA	LEU	178	23.350	30.539	60.953	1.00	12.99	A
1230	CB	LEU	178	22.125	29.678	61.304	1.00	14.12	A
1231	CG	LEU	178	20.929	30.356	61.974	1.00	15.67	A
1232	CD2	LEU	178	19.757	29.384	62.173	1.00	15.35	A
1233	CD1	LEU	178	20.337	31.455	61.031	1.00	16.46	A
1234	C	LEU	178	23.703	31.380	62.177	1.00	14.59	A
1235	O	LEU	178	23.447	32.558	62.244	1.00	10.66	A
1236	N	ALA	179	24.311	30.780	63.228	1.00	15.25	A
1237	CA	ALA	179	24.626	31.617	64.424	1.00	15.23	A
1238	CB	ALA	179	25.331	30.699	65.446	1.00	14.84	A
1239	C	ALA	179	25.567	32.747	64.126	1.00	14.68	A
1240	O	ALA	179	25.504	33.869	64.599	1.00	11.42	A
1241	N	LYS	180	26.496	32.500	63.150	1.00	16.39	A
1242	CA	LYS	180	27.444	33.589	62.797	1.00	16.05	A
1243	CB	LYS	180	28.389	33.004	61.699	1.00	17.99	A
1244	CG	LYS	180	29.171	34.095	60.937	1.00	18.86	A
1245	CD	LYS	180	30.424	33.429	60.340	1.00	20.68	A
1246	CE	LYS	180	31.167	34.451	59.505	1.00	21.58	A
1247	NZ	LYS	180	32.094	35.357	60.253	1.00	18.53	A
1248	C	LYS	180	26.758	34.834	62.307	1.00	16.60	A
1249	O	LYS	180	27.022	35.991	62.690	1.00	15.08	A
1250	N	ASP	181	25.747	34.703	61.412	1.00	12.78	A
1251	CA	ASP	181	25.033	35.864	60.910	1.00	13.37	A
1252	CB	ASP	181	24.129	35.506	59.687	1.00	14.96	A
1253	CG	ASP	181	24.955	35.406	58.367	1.00	18.01	A
1254	OD1	ASP	181	25.922	36.128	58.171	1.00	17.53	A
1255	OD2	ASP	181	24.596	34.523	57.518	1.00	16.78	A
1256	C	ASP	181	24.159	36.504	61.998	1.00	14.64	A

1257	O	ASP	181	24.037	37.711	62.116	1.00	14.14	A
1258	N	LEU	182	23.464	35.676	62.791	1.00	13.09	A
1259	CA	LEU	182	22.647	36.267	63.882	1.00	14.86	A
1260	CB	LEU	182	21.940	35.130	64.632	1.00	14.93	A
1261	CG	LEU	182	21.095	34.159	63.851	1.00	13.65	A
1262	CD2	LEU	182	19.988	34.928	63.166	1.00	13.56	A
1263	CD1	LEU	182	20.487	33.085	64.754	1.00	14.92	A
1264	C	LEU	182	23.510	36.991	64.913	1.00	13.35	A
1265	O	LEU	182	23.267	38.149	65.233	1.00	16.44	A
1266	N	ALA	183	24.642	36.381	65.294	1.00	14.86	A
1267	CA	ALA	183	25.462	37.136	66.296	1.00	17.00	A
1268	CB	ALA	183	26.553	36.188	66.788	1.00	17.27	A
1269	C	ALA	183	26.025	38.414	65.744	1.00	17.58	A
1270	O	ALA	183	26.111	39.473	66.378	1.00	16.18	A
1271	N	GLU	184	26.560	38.361	64.491	1.00	16.77	A
1272	CA	GLU	184	27.232	39.496	63.886	1.00	17.91	A
1273	CB	GLU	184	28.123	39.113	62.670	1.00	17.73	A
1274	CG	GLU	184	29.387	38.347	63.096	1.00	16.98	A
1275	CD	GLU	184	30.040	37.632	61.910	1.00	16.92	A
1276	OE1	GLU	184	29.602	37.871	60.746	1.00	16.69	A
1277	OE2	GLU	184	30.968	36.851	62.189	1.00	16.83	A
1278	C	GLU	184	26.295	40.607	63.446	1.00	18.12	A
1279	O	GLU	184	26.702	41.773	63.532	1.00	17.46	A
1280	N	ASN	185	25.035	40.318	63.153	1.00	16.96	A
1281	CA	ASN	185	24.107	41.367	62.780	1.00	17.76	A
1282	CB	ASN	185	23.063	40.888	61.747	1.00	16.68	A
1283	CG	ASN	185	22.468	42.081	61.003	1.00	17.01	A
1284	OD1	ASN	185	23.233	42.919	60.513	1.00	15.96	A
1285	ND2	ASN	185	21.149	42.265	60.951	1.00	15.43	A
1286	C	ASN	185	23.328	41.964	63.955	1.00	18.03	A
1287	O	ASN	185	22.731	43.013	63.716	1.00	18.68	A
1288	N	ASN	186	23.371	41.368	65.135	1.00	17.08	A
1289	CA	ASN	186	22.608	41.863	66.288	1.00	18.13	A
1290	CB	ASN	186	21.572	40.807	66.699	1.00	16.10	A
1291	CG	ASN	186	20.523	40.578	65.611	1.00	18.64	A
1292	OD1	ASN	186	19.547	41.299	65.579	1.00	19.86	A
1293	ND2	ASN	186	20.682	39.594	64.747	1.00	14.98	A
1294	C	ASN	186	23.499	42.226	67.487	1.00	18.41	A
1295	O	ASN	186	24.114	41.367	68.114	1.00	17.04	A
1296	N	LYS	187	23.815	43.507	67.599	1.00	20.13	A
1297	CA	LYS	187	24.735	43.999	68.612	1.00	25.18	A
1298	CB	LYS	187	24.825	45.515	68.465	1.00	29.17	A
1299	CG	LYS	187	25.281	46.242	69.710	1.00	36.89	A
1300	CD	LYS	187	26.705	46.759	69.568	1.00	40.48	A
1301	CE	LYS	187	26.622	48.236	69.176	1.00	42.38	A
1302	NZ	LYS	187	27.043	49.080	70.346	1.00	44.71	A
1303	C	LYS	187	24.293	43.578	70.027	1.00	21.89	A
1304	O	LYS	187	23.147	43.753	70.387	1.00	21.34	A
1305	N	GLY	188	25.201	42.940	70.743	1.00	22.90	A
1306	CA	GLY	188	24.942	42.452	72.108	1.00	22.17	A
1307	C	GLY	188	24.279	41.090	72.129	1.00	23.50	A
1308	O	GLY	188	24.146	40.430	73.170	1.00	20.50	A

1309	N	SER	189	23.977	40.511	70.908	1.00	17.92	A
1310	CA	SER	189	23.208	39.275	70.958	1.00	16.34	A
1311	CB	SER	189	22.596	38.969	69.534	1.00	17.81	A
1312	OG	SER	189	23.703	38.733	68.684	1.00	17.96	A
1313	C	SER	189	24.062	38.132	71.413	1.00	16.41	A
1314	O	SER	189	25.284	38.081	71.236	1.00	14.81	A
1315	N	ARG	190	23.377	37.146	72.057	1.00	13.48	A
1316	CA	ARG	190	24.074	35.932	72.446	1.00	15.78	A
1317	CB	ARG	190	24.387	35.898	73.980	1.00	15.30	A
1318	CG	ARG	190	25.474	36.948	74.311	1.00	13.88	A
1319	CD	ARG	190	26.866	36.358	74.045	1.00	14.87	A
1320	NE	ARG	190	27.965	37.244	74.479	1.00	15.65	A
1321	CZ	ARG	190	28.310	38.313	73.779	1.00	19.62	A
1322	NH1	ARG	190	27.701	38.627	72.589	1.00	19.54	A
1323	NH2	ARG	190	29.389	39.040	74.102	1.00	17.37	A
1324	C	ARG	190	23.168	34.787	72.015	1.00	15.73	A
1325	O	ARG	190	22.016	34.631	72.455	1.00	14.59	A
1326	N	VAL	191	23.774	33.904	71.215	1.00	17.00	A
1327	CA	VAL	191	23.000	32.845	70.579	1.00	16.41	A
1328	CB	VAL	191	23.477	32.589	69.110	1.00	16.72	A
1329	CG1	VAL	191	22.585	31.538	68.437	1.00	17.65	A
1330	CG2	VAL	191	23.506	33.925	68.368	1.00	15.63	A
1331	C	VAL	191	23.314	31.535	71.285	1.00	14.89	A
1332	O	VAL	191	24.477	31.161	71.305	1.00	16.89	A
1333	N	LEU	192	22.278	30.833	71.640	1.00	13.18	A
1334	CA	LEU	192	22.388	29.495	72.157	1.00	14.87	A
1335	CB	LEU	192	21.339	29.259	73.258	1.00	15.46	A
1336	CG	LEU	192	21.225	27.836	73.770	1.00	14.61	A
1337	CD2	LEU	192	20.226	27.716	74.951	1.00	13.51	A
1338	CD1	LEU	192	22.565	27.288	74.246	1.00	15.01	A
1339	C	LEU	192	22.035	28.561	70.981	1.00	14.56	A
1340	O	LEU	192	20.963	28.662	70.425	1.00	15.45	A
1341	N	ILE	193	22.942	27.654	70.681	1.00	14.79	A
1342	CA	ILE	193	22.789	26.668	69.667	1.00	14.89	A
1343	CB	ILE	193	24.110	26.468	68.853	1.00	16.51	A
1344	CG2	ILE	193	24.031	25.107	68.138	1.00	16.50	A
1345	CG1	ILE	193	24.419	27.631	67.941	1.00	17.44	A
1346	CD1	ILE	193	25.800	27.406	67.296	1.00	15.17	A
1347	C	ILE	193	22.575	25.355	70.404	1.00	14.33	A
1348	O	ILE	193	23.389	25.066	71.298	1.00	16.41	A
1349	N	VAL	194	21.534	24.615	70.077	1.00	12.33	A
1350	CA	VAL	194	21.446	23.263	70.571	1.00	13.58	A
1351	CB	VAL	194	20.284	23.160	71.617	1.00	14.48	A
1352	CG1	VAL	194	20.089	21.727	72.073	1.00	13.80	A
1353	CG2	VAL	194	20.576	24.108	72.783	1.00	14.46	A
1354	C	VAL	194	21.168	22.237	69.459	1.00	15.13	A
1355	O	VAL	194	20.115	22.302	68.808	1.00	14.72	A
1356	N	CYS	195	22.058	21.275	69.288	1.00	14.44	A
1357	CA	CYS	195	21.840	20.129	68.445	1.00	16.01	A
1358	CB	CYS	195	23.012	19.805	67.449	1.00	14.49	A
1359	SG	CYS	195	23.288	21.237	66.355	1.00	14.90	A
1360	C	CYS	195	21.621	18.905	69.326	1.00	15.76	A

1361	O	CYS	195	22.498	18.457	70.095	1.00	17.80	A
1362	N	SER	196	20.512	18.230	69.122	1.00	15.08	A
1363	CA	SER	196	20.194	17.064	69.931	1.00	15.38	A
1364	CB	SER	196	19.267	17.612	71.050	1.00	14.75	A
1365	OG	SER	196	18.738	16.521	71.723	1.00	15.86	A
1366	C	SER	196	19.588	15.963	69.093	1.00	14.38	A
1367	O	SER	196	18.577	16.134	68.396	1.00	12.93	A
1368	N	GLU	197	20.252	14.821	69.090	1.00	14.38	A
1369	CA	GLU	197	19.909	13.695	68.263	1.00	15.07	A
1370	CB	GLU	197	21.097	13.510	67.286	1.00	13.16	A
1371	CG	GLU	197	21.425	14.751	66.442	1.00	13.62	A
1372	CD	GLU	197	20.440	14.885	65.267	1.00	15.07	A
1373	OE1	GLU	197	19.321	14.316	65.326	1.00	13.89	A
1374	OE2	GLU	197	20.778	15.640	64.309	1.00	14.15	A
1375	C	GLU	197	19.705	12.424	69.072	1.00	16.83	A
1376	O	GLU	197	20.486	11.959	69.907	1.00	14.52	A
1377	N	ILE	198	18.557	11.810	68.811	1.00	17.45	A
1378	CA	ILE	198	18.225	10.502	69.365	1.00	19.36	A
1379	CB	ILE	198	16.999	10.591	70.293	1.00	18.13	A
1380	CG2	ILE	198	16.549	9.194	70.648	1.00	16.69	A
1381	CG1	ILE	198	17.415	11.418	71.536	1.00	19.63	A
1382	CD1	ILE	198	16.404	11.432	72.627	1.00	20.82	A
1383	C	ILE	198	17.917	9.599	68.162	1.00	18.68	A
1384	O	ILE	198	16.932	9.889	67.485	1.00	19.71	A
1385	N	THR	199	18.669	8.546	68.000	1.00	20.32	A
1386	CA	THR	199	18.566	7.649	66.867	1.00	20.53	A
1387	CB	THR	199	19.908	6.914	66.663	1.00	21.13	A
1388	OG1	THR	199	20.133	6.001	67.771	1.00	22.12	A
1389	CG2	THR	199	21.040	7.914	66.532	1.00	19.49	A
1390	C	THR	199	17.489	6.604	66.896	1.00	21.10	A
1391	O	THR	199	17.331	5.862	65.920	1.00	21.48	A
1392	N	ALA	200	16.593	6.623	67.874	1.00	20.86	A
1393	CA	ALA	200	15.422	5.794	67.919	1.00	20.57	A
1394	CB	ALA	200	14.586	6.016	69.159	1.00	17.68	A
1395	C	ALA	200	14.528	5.992	66.662	1.00	20.56	A
1396	O	ALA	200	13.901	5.003	66.291	1.00	17.87	A
1389	N	ILE	201	14.547	7.157	66.115	0.50	18.88	A
1390	CA	ILE	201	13.719	7.458	64.936	0.50	17.99	A
1391	CB	ILE	201	13.789	8.952	64.592	0.50	16.30	A
1392	CG2	ILE	201	15.132	9.358	63.985	0.50	16.91	A
1393	CG1	ILE	201	12.719	9.394	63.580	0.50	14.60	A
1394	CD1	ILE	201	11.286	9.202	64.089	0.50	11.06	A
1395	C	ILE	201	14.173	6.625	63.720	0.50	17.10	A
1396	O	ILE	201	13.389	6.383	62.788	0.50	18.59	A
1389	N	2ILE	201	14.461	7.125	66.061	0.50	21.70	A
1390	CA	2ILE	201	13.570	7.231	64.885	0.50	22.76	A
1391	CB	2ILE	201	13.310	8.649	64.373	0.50	25.16	A
1392	CG	22ILE	201	12.019	9.250	64.939	0.50	26.21	A
1393	CG	12ILE	201	14.427	9.629	64.673	0.50	25.65	A
1394	CD	12ILE	201	15.720	9.309	63.921	0.50	24.86	A
1395	C	2ILE	201	14.119	6.461	63.693	0.50	20.27	A
1396	O	2ILE	201	13.383	6.161	62.745	0.50	21.36	A

1413	N	LEU	202	15.425	6.166	63.668	1.00	18.05	A
1414	CA	LEU	202	15.958	5.380	62.578	1.00	18.89	A
1415	CB	LEU	202	17.156	6.013	61.864	1.00	18.54	A
1416	CG	LEU	202	18.292	6.576	62.683	1.00	21.58	A
1417	CD2	LEU	202	19.114	7.548	61.835	1.00	23.11	A
1418	CD1	LEU	202	19.180	5.447	63.207	1.00	23.74	A
1419	C	LEU	202	16.372	3.959	62.913	1.00	19.82	A
1420	O	LEU	202	16.979	3.290	62.059	1.00	17.73	A
1421	N	PHE	203	16.030	3.486	64.099	1.00	17.98	A
1422	CA	PHE	203	16.279	2.073	64.420	1.00	18.62	A
1423	CB	PHE	203	15.884	1.869	65.914	1.00	20.06	A
1424	CG	PHE	203	16.111	0.444	66.338	1.00	19.04	A
1425	CD1	PHE	203	15.077	-0.457	66.334	1.00	19.36	A
1426	CD2	PHE	203	17.365	0.075	66.797	1.00	21.11	A
1427	CE1	PHE	203	15.269	-1.767	66.759	1.00	22.06	A
1428	CE2	PHE	203	17.564	-1.245	67.228	1.00	20.23	A
1429	CZ	PHE	203	16.526	-2.143	67.219	1.00	21.46	A
1430	C	PHE	203	15.403	1.154	63.588	1.00	19.66	A
1431	O	PHE	203	14.192	1.422	63.431	1.00	21.19	A
1432	N	HIS	204	15.926	0.051	63.083	1.00	18.97	A
1433	CA	HIS	204	15.164	-0.889	62.266	1.00	22.20	A
1434	ND1	HIS	204	13.226	0.964	60.442	1.00	19.42	A
1435	CG	HIS	204	14.587	0.752	60.363	1.00	19.49	A
1436	CB	HIS	204	15.203	-0.575	60.729	1.00	19.31	A
1437	NE2	HIS	204	14.099	2.829	59.844	1.00	21.11	A
1438	CD2	HIS	204	15.140	1.937	59.994	1.00	19.11	A
1439	CE1	HIS	204	12.945	2.213	60.115	1.00	20.21	A
1440	C	HIS	204	15.725	-2.304	62.461	1.00	21.64	A
1441	O	HIS	204	16.945	-2.480	62.553	1.00	21.58	A
1442	N	GLY	205	14.849	-3.303	62.435	1.00	21.09	A
1443	CA	GLY	205	15.291	-4.707	62.453	1.00	23.18	A
1444	C	GLY	205	15.947	-5.065	61.114	1.00	24.77	A
1445	O	GLY	205	16.032	-4.267	60.168	1.00	25.98	A
1446	N	PRO	206	16.644	-6.190	61.054	1.00	25.87	A
1447	CA	PRO	206	17.458	-6.545	59.904	1.00	27.34	A
1448	CD	PRO	206	16.742	-7.204	62.137	1.00	26.44	A
1449	CB	PRO	206	18.398	-7.619	60.444	1.00	27.19	A
1450	CG	PRO	206	17.584	-8.280	61.507	1.00	26.88	A
1451	C	PRO	206	16.617	-7.054	58.768	1.00	29.39	A
1452	O	PRO	206	15.548	-7.658	58.967	1.00	30.52	A
1453	N	ASN	207	17.039	-6.756	57.545	1.00	31.69	A
1454	CA	ASN	207	16.328	-7.260	56.358	1.00	32.51	A
1455	CB	ASN	207	15.114	-6.402	56.029	1.00	33.65	A
1456	CG	ASN	207	14.435	-6.828	54.729	1.00	35.71	A
1457	OD1	ASN	207	14.943	-6.533	53.648	1.00	35.08	A
1458	ND2	ASN	207	13.310	-7.515	54.771	1.00	34.18	A
1459	C	ASN	207	17.302	-7.345	55.168	1.00	33.19	A
1460	O	ASN	207	17.979	-6.366	54.821	1.00	29.39	A
1461	N	GLU	208	17.310	-8.541	54.610	1.00	35.87	A
1462	CA	GLU	208	18.174	-8.962	53.489	1.00	39.04	A
1463	CB	GLU	208	17.633	-10.223	52.845	1.00	45.25	A
1464	CG	GLU	208	18.171	-11.507	53.439	1.00	51.38	A

1465	CD	GLU	208	17.231	-12.656	53.137	1.00	55.49	A
1466	OE1	GLU	208	16.975	-12.963	51.911	1.00	55.90	A
1467	OE2	GLU	208	16.679	-13.292	54.105	1.00	59.14	A
1468	C	GLU	208	18.217	-7.998	52.308	1.00	36.43	A
1469	O	GLU	208	19.268	-7.797	51.687	1.00	35.95	A
1470	N	ASN	209	17.074	-7.441	51.993	1.00	34.14	A
1471	CA	ASN	209	16.938	-6.577	50.818	1.00	34.13	A
1472	CB	ASN	209	15.522	-6.698	50.279	1.00	37.32	A
1473	CG	ASN	209	15.163	-8.157	50.012	1.00	39.65	A
1474	OD1	ASN	209	15.910	-8.850	49.320	1.00	40.89	A
1475	ND2	ASN	209	14.070	-8.676	50.533	1.00	39.96	A
1476	C	ASN	209	17.276	-5.115	51.130	1.00	32.88	A
1477	O	ASN	209	17.180	-4.237	50.270	1.00	32.04	A
1478	N	HIS	210	17.679	-4.841	52.354	1.00	31.55	A
1479	CA	HIS	210	18.060	-3.464	52.732	1.00	30.75	A
1480	ND1	HIS	210	14.723	-3.581	52.479	1.00	34.00	A
1481	CG	HIS	210	15.677	-2.583	52.636	1.00	34.22	A
1482	CB	HIS	210	16.921	-2.790	53.503	1.00	32.00	A
1483	NE2	HIS	210	14.076	-1.906	51.315	1.00	34.55	A
1484	CD2	HIS	210	15.246	-1.527	51.891	1.00	34.19	A
1485	CE1	HIS	210	13.779	-3.129	51.675	1.00	33.70	A
1486	C	HIS	210	19.335	-3.500	53.572	1.00	29.56	A
1487	O	HIS	210	19.313	-3.274	54.785	1.00	27.00	A
1488	N	LEU	211	20.435	-3.774	52.892	1.00	27.70	A
1489	CA	LEU	211	21.737	-3.913	53.553	1.00	28.08	A
1490	CB	LEU	211	22.744	-4.590	52.630	1.00	27.02	A
1491	CG	LEU	211	22.351	-6.031	52.294	1.00	29.47	A
1492	CD2	LEU	211	22.327	-6.959	53.513	1.00	30.67	A
1493	CD1	LEU	211	23.297	-6.685	51.286	1.00	29.25	A
1494	C	LEU	211	22.293	-2.583	54.019	1.00	26.99	A
1495	O	LEU	211	23.056	-2.576	54.983	1.00	24.96	A
1496	N	ASP	212	21.908	-1.479	53.384	1.00	27.06	A
1497	CA	ASP	212	22.377	-0.158	53.810	1.00	26.42	A
1498	CB	ASP	212	22.061	0.892	52.762	1.00	26.67	A
1499	CG	ASP	212	20.705	0.831	52.114	1.00	26.42	A
1500	OD1	ASP	212	19.920	-0.127	52.306	1.00	26.01	A
1501	OD2	ASP	212	20.376	1.811	51.396	1.00	26.03	A
1502	C	ASP	212	21.683	0.226	55.132	1.00	25.93	A
1503	O	ASP	212	22.225	0.860	56.034	1.00	23.85	A
1504	N	SER	213	20.410	-0.169	55.210	1.00	25.35	A
1505	CA	SER	213	19.657	0.004	56.454	1.00	28.05	A
1506	CB	SER	213	18.169	-0.310	56.239	1.00	29.07	A
1507	OG	SER	213	17.504	-0.103	57.466	1.00	34.43	A
1508	C	SER	213	20.269	-0.842	57.571	1.00	27.93	A
1509	O	SER	213	20.327	-0.407	58.727	1.00	27.08	A
1510	N	LEU	214	20.842	-2.005	57.258	1.00	26.89	A
1511	CA	LEU	214	21.562	-2.810	58.245	1.00	26.87	A
1512	CB	LEU	214	21.833	-4.241	57.732	1.00	25.91	A
1513	CG	LEU	214	22.581	-5.164	58.693	1.00	27.85	A
1514	CD2	LEU	214	23.032	-6.438	57.972	1.00	26.84	A
1515	CD1	LEU	214	21.682	-5.519	59.887	1.00	24.51	A
1516	C	LEU	214	22.857	-2.137	58.664	1.00	25.66	A

1517	O	LEU	214	23.122	-1.961	59.870	1.00	23.41	A
1518	N	VAL	215	23.617	-1.571	57.715	1.00	24.14	A
1519	CA	VAL	215	24.837	-0.863	58.008	1.00	24.72	A
1520	CB	VAL	215	25.566	-0.287	56.771	1.00	25.01	A
1521	CG1	VAL	215	26.611	0.742	57.174	1.00	21.78	A
1522	CG2	VAL	215	26.240	-1.392	55.945	1.00	26.32	A
1523	C	VAL	215	24.533	0.295	58.950	1.00	24.78	A
1524	O	VAL	215	25.259	0.482	59.939	1.00	25.77	A
1525	N	ALA	216	23.443	1.009	58.663	1.00	22.29	A
1526	CA	ALA	216	23.021	2.120	59.478	1.00	22.75	A
1527	CB	ALA	216	21.743	2.766	58.928	1.00	22.71	A
1528	C	ALA	216	22.722	1.774	60.943	1.00	23.23	A
1529	O	ALA	216	22.973	2.640	61.770	1.00	20.20	A
1530	N	GLN	217	22.412	0.526	61.287	1.00	24.45	A
1531	CA	GLN	217	22.177	0.159	62.695	1.00	24.33	A
1532	CB	GLN	217	21.419	-1.166	62.722	1.00	23.47	A
1533	CG	GLN	217	20.120	-1.190	61.895	1.00	24.28	A
1534	CD	GLN	217	19.244	0.031	62.195	1.00	24.61	A
1535	OE1	GLN	217	18.890	0.212	63.378	1.00	22.76	A
1536	NE2	GLN	217	18.951	0.862	61.205	1.00	19.95	A
1537	C	GLN	217	23.472	0.162	63.501	1.00	25.07	A
1538	O	GLN	217	23.441	0.169	64.758	1.00	26.55	A
1539	N	ALA	218	24.616	0.201	62.826	1.00	22.34	A
1540	CA	ALA	218	25.916	0.220	63.470	1.00	23.77	A
1541	CB	ALA	218	26.896	-0.742	62.787	1.00	22.04	A
1542	C	ALA	218	26.550	1.591	63.530	1.00	22.94	A
1543	O	ALA	218	27.586	1.694	64.221	1.00	23.52	A
1544	N	LEU	219	26.005	2.632	62.876	1.00	20.23	A
1545	CA	LEU	219	26.816	3.853	62.773	1.00	20.51	A
1546	CB	LEU	219	26.501	4.568	61.419	1.00	21.57	A
1547	CG	LEU	219	26.846	3.797	60.116	1.00	23.93	A
1548	CD2	LEU	219	28.345	3.552	60.007	1.00	23.19	A
1549	CD1	LEU	219	26.443	4.588	58.861	1.00	22.16	A
1550	C	LEU	219	26.567	4.911	63.838	1.00	20.63	A
1551	O	LEU	219	27.411	5.786	64.020	1.00	22.27	A
1552	N	PHE	220	25.307	5.047	64.276	1.00	18.63	A
1553	CA	PHE	220	24.840	6.263	64.910	1.00	18.81	A
1554	CB	PHE	220	23.429	6.607	64.343	1.00	19.71	A
1555	CG	PHE	220	23.451	6.886	62.842	1.00	19.21	A
1556	CD1	PHE	220	22.923	5.928	61.969	1.00	18.79	A
1557	CD2	PHE	220	24.015	8.040	62.364	1.00	18.11	A
1558	CE1	PHE	220	22.944	6.174	60.588	1.00	19.76	A
1559	CE2	PHE	220	24.023	8.299	60.982	1.00	22.11	A
1560	CZ	PHE	220	23.516	7.348	60.110	1.00	20.52	A
1561	C	PHE	220	24.662	6.123	66.429	1.00	17.23	A
1562	O	PHE	220	24.062	5.140	66.839	1.00	14.86	A
1563	N	GLY	221	24.914	7.207	67.127	1.00	19.72	A
1564	CA	GLY	221	24.738	7.156	68.607	1.00	22.07	A
1565	C	GLY	221	23.953	8.443	68.933	1.00	23.22	A
1566	O	GLY	221	23.705	9.294	68.031	1.00	20.48	A
1567	N	ASP	222	23.608	8.517	70.219	1.00	21.18	A
1568	CA	ASP	222	22.810	9.647	70.715	1.00	18.61	A

1569	CB	ASP	222	21.625	9.171	71.574	1.00	17.56	A
1570	CG	ASP	222	20.686	8.258	70.871	1.00	19.05	A
1571	OD1	ASP	222	20.865	7.974	69.631	1.00	19.17	A
1572	OD2	ASP	222	19.735	7.705	71.479	1.00	20.12	A
1573	C	ASP	222	23.581	10.656	71.492	1.00	16.80	A
1574	O	ASP	222	24.528	10.296	72.204	1.00	18.14	A
1575	N	GLY	223	23.198	11.939	71.329	1.00	16.62	A
1576	CA	GLY	223	23.863	13.007	72.027	1.00	16.89	A
1577	C	GLY	223	23.341	14.403	71.684	1.00	18.35	A
1578	O	GLY	223	22.634	14.608	70.699	1.00	19.09	A
1579	N	ALA	224	23.716	15.348	72.540	1.00	16.74	A
1580	CA	ALA	224	23.382	16.765	72.339	1.00	15.69	A
1581	CB	ALA	224	22.184	17.191	73.187	1.00	15.29	A
1582	C	ALA	224	24.574	17.641	72.719	1.00	16.88	A
1583	O	ALA	224	25.284	17.362	73.696	1.00	16.03	A
1584	N	ALA	225	24.748	18.662	71.915	1.00	17.12	A
1585	CA	ALA	225	25.781	19.675	72.125	1.00	17.04	A
1586	CB	ALA	225	26.822	19.628	71.005	1.00	17.62	A
1587	C	ALA	225	25.107	21.039	72.133	1.00	16.59	A
1588	O	ALA	225	24.143	21.276	71.394	1.00	16.15	A
1589	N	ALA	226	25.619	21.901	72.974	1.00	14.82	A
1590	CA	ALA	226	25.105	23.266	73.101	1.00	14.36	A
1591	CB	ALA	226	24.302	23.405	74.395	1.00	15.96	A
1592	C	ALA	226	26.277	24.237	73.106	1.00	15.68	A
1593	O	ALA	226	27.324	23.977	73.709	1.00	16.67	A
1594	N	LEU	227	26.079	25.338	72.426	1.00	14.94	A
1595	CA	LEU	227	27.102	26.376	72.311	1.00	15.69	A
1596	CB	LEU	227	27.635	26.458	70.871	1.00	15.95	A
1597	CG	LEU	227	28.772	25.490	70.547	1.00	18.96	A
1598	CD2	LEU	227	29.427	25.789	69.191	1.00	19.61	A
1599	CD1	LEU	227	28.306	24.038	70.472	1.00	21.33	A
1600	C	LEU	227	26.510	27.745	72.569	1.00	14.11	A
1601	O	LEU	227	25.330	27.989	72.297	1.00	15.41	A
1602	N	ILE	228	27.345	28.596	73.096	1.00	14.17	A
1603	CA	ILE	228	27.012	30.006	73.236	1.00	14.85	A
1604	CB	ILE	228	27.267	30.526	74.651	1.00	18.48	A
1605	CG2	ILE	228	26.980	32.030	74.778	1.00	19.00	A
1606	CG1	ILE	228	26.412	29.838	75.718	1.00	19.80	A
1607	CD1	ILE	228	24.934	30.231	75.668	1.00	16.73	A
1608	C	ILE	228	27.912	30.731	72.252	1.00	15.99	A
1609	O	ILE	228	29.141	30.575	72.293	1.00	14.79	A
1610	N	VAL	229	27.286	31.478	71.376	1.00	15.18	A
1611	CA	VAL	229	28.003	32.237	70.344	1.00	15.14	A
1612	CB	VAL	229	27.635	31.739	68.949	1.00	16.86	A
1613	CG1	VAL	229	28.226	32.615	67.839	1.00	14.92	A
1614	CG2	VAL	229	28.124	30.320	68.673	1.00	14.91	A
1615	C	VAL	229	27.623	33.703	70.402	1.00	15.54	A
1616	O	VAL	229	26.450	34.056	70.565	1.00	16.90	A
1617	N	GLY	230	28.626	34.534	70.256	1.00	15.38	A
1618	CA	GLY	230	28.415	35.976	70.275	1.00	15.59	A
1619	C	GLY	230	29.611	36.714	69.662	1.00	14.62	A
1620	O	GLY	230	30.710	36.182	69.655	1.00	15.54	A

1621	N	SER	231	29.365	37.939	69.206	1.00	15.66	A
1622	CA	SER	231	30.393	38.816	68.696	1.00	18.35	A
1623	CB	SER	231	29.874	39.655	67.476	1.00	19.73	A
1624	OG	SER	231	29.673	38.784	66.362	1.00	20.99	A
1625	C	SER	231	30.744	39.837	69.801	1.00	17.97	A
1626	O	SER	231	29.907	40.112	70.654	1.00	18.04	A
1627	N	GLY	232	31.911	40.446	69.789	1.00	17.80	A
1628	CA	GLY	232	32.231	41.445	70.839	1.00	19.53	A
1629	C	GLY	232	32.215	40.831	72.236	1.00	19.73	A
1630	O	GLY	232	31.435	41.187	73.120	1.00	22.75	A
1631	N	PRO	233	33.015	39.819	72.495	1.00	20.79	A
1632	CA	PRO	233	33.130	39.161	73.784	1.00	22.44	A
1633	CD	PRO	233	34.020	39.273	71.545	1.00	21.24	A
1634	CB	PRO	233	34.172	38.049	73.590	1.00	21.15	A
1635	CG	PRO	233	34.400	37.954	72.120	1.00	21.44	A
1636	C	PRO	233	33.604	40.149	74.864	1.00	22.27	A
1637	O	PRO	233	34.330	41.141	74.640	1.00	19.50	A
1638	N	HIS	234	32.901	40.097	76.002	1.00	22.16	A
1639	CA	HIS	234	33.339	40.937	77.165	1.00	23.15	A
1640	ND1	HIS	234	29.958	41.328	76.884	1.00	35.17	A
1641	CG	HIS	234	31.078	41.977	77.390	1.00	30.81	A
1642	CB	HIS	234	32.182	41.269	78.102	1.00	27.51	A
1643	NE2	HIS	234	29.741	43.370	76.323	1.00	35.82	A
1644	CD2	HIS	234	30.941	43.265	77.019	1.00	35.34	A
1645	CE1	HIS	234	29.175	42.190	76.256	1.00	34.13	A
1646	C	HIS	234	34.418	40.103	77.832	1.00	20.60	A
1647	O	HIS	234	34.116	39.200	78.630	1.00	19.16	A
1648	N	LEU	235	35.651	40.448	77.520	1.00	16.35	A
1649	CA	LEU	235	36.796	39.635	77.925	1.00	18.16	A
1650	CB	LEU	235	38.083	40.119	77.236	1.00	18.81	A
1651	CG	LEU	235	38.000	40.095	75.692	1.00	21.47	A
1652	CD2	LEU	235	37.807	38.679	75.168	1.00	21.10	A
1653	CD1	LEU	235	39.310	40.642	75.081	1.00	21.54	A
1654	C	LEU	235	37.066	39.504	79.428	1.00	17.07	A
1655	O	LEU	235	37.672	38.503	79.830	1.00	17.50	A
1656	N	ALA	236	36.583	40.438	80.209	1.00	19.10	A
1657	CA	ALA	236	36.751	40.302	81.675	1.00	21.23	A
1658	CB	ALA	236	36.162	41.556	82.316	1.00	20.52	A
1659	C	ALA	236	36.064	39.026	82.109	1.00	20.15	A
1660	O	ALA	236	36.467	38.329	83.046	1.00	20.26	A
1661	N	VAL	237	34.912	38.674	81.517	1.00	19.13	A
1662	CA	VAL	237	34.101	37.552	82.009	1.00	17.70	A
1663	CB	VAL	237	32.801	38.109	82.621	1.00	16.79	A
1664	CG1	VAL	237	33.087	39.149	83.738	1.00	17.70	A
1665	CG2	VAL	237	31.887	38.838	81.616	1.00	18.15	A
1666	C	VAL	237	33.776	36.489	80.979	1.00	20.33	A
1667	O	VAL	237	33.406	35.369	81.379	1.00	20.85	A
1668	N	GLU	238	33.953	36.754	79.675	1.00	20.13	A
1669	CA	GLU	238	33.642	35.691	78.681	1.00	20.82	A
1670	CB	GLU	238	32.698	36.229	77.592	1.00	21.43	A
1671	CG	GLU	238	31.368	36.751	78.026	1.00	20.52	A
1672	CD	GLU	238	30.490	37.238	76.859	1.00	22.45	A

1673	OE1	GLU	238	30.889	38.201	76.181	1.00	20.38	A
1674	OE2	GLU	238	29.398	36.671	76.665	1.00	21.83	A
1675	C	GLU	238	34.926	35.177	78.082	1.00	19.34	A
1676	O	GLU	238	35.877	35.955	77.983	1.00	21.58	A
1677	N	ARG	239	35.009	33.910	77.733	1.00	21.12	A
1678	CA	ARG	239	36.216	33.263	77.257	1.00	22.23	A
1679	CB	ARG	239	36.524	32.072	78.207	1.00	25.73	A
1680	CG	ARG	239	37.759	31.259	77.923	1.00	30.57	A
1681	CD	ARG	239	38.148	30.209	78.941	1.00	35.65	A
1682	NE	ARG	239	37.243	29.095	79.152	1.00	39.77	A
1683	CZ	ARG	239	37.280	27.784	79.297	1.00	42.53	A
1684	NH1	ARG	239	38.385	27.022	79.243	1.00	42.40	A
1685	NH2	ARG	239	36.137	27.097	79.519	1.00	42.16	A
1686	C	ARG	239	36.026	32.719	75.832	1.00	19.54	A
1687	O	ARG	239	35.664	31.556	75.686	1.00	18.01	A
1688	N	PRO	240	36.545	33.430	74.842	1.00	20.95	A
1689	CA	PRO	240	36.590	32.962	73.452	1.00	18.08	A
1690	CD	PRO	240	36.999	34.836	74.914	1.00	21.55	A
1691	CB	PRO	240	37.390	34.047	72.724	1.00	21.14	A
1692	CG	PRO	240	36.962	35.309	73.449	1.00	21.46	A
1693	C	PRO	240	37.277	31.643	73.337	1.00	19.07	A
1694	O	PRO	240	38.297	31.353	73.986	1.00	19.18	A
1695	N	ILE	241	36.721	30.753	72.523	1.00	18.31	A
1696	CA	ILE	241	37.291	29.428	72.275	1.00	19.83	A
1697	CB	ILE	241	36.234	28.333	72.548	1.00	19.49	A
1698	CG2	ILE	241	36.878	26.957	72.345	1.00	19.51	A
1699	CG1	ILE	241	35.632	28.482	73.949	1.00	20.96	A
1700	CD1	ILE	241	34.579	27.465	74.392	1.00	19.62	A
1701	C	ILE	241	37.791	29.336	70.829	1.00	21.55	A
1702	O	ILE	241	38.882	28.859	70.512	1.00	19.61	A
1703	N	PHE	242	36.934	29.754	69.894	1.00	20.18	A
1704	CA	PHE	242	37.174	29.805	68.462	1.00	21.43	A
1705	CB	PHE	242	36.689	28.534	67.733	1.00	18.71	A
1706	CG	PHE	242	37.494	27.318	68.067	1.00	20.98	A
1707	CD1	PHE	242	38.802	27.211	67.612	1.00	21.85	A
1708	CD2	PHE	242	36.968	26.314	68.866	1.00	19.93	A
1709	CE1	PHE	242	39.558	26.106	67.927	1.00	22.01	A
1710	CE2	PHE	242	37.725	25.213	69.185	1.00	20.01	A
1711	CZ	PHE	242	39.028	25.096	68.707	1.00	23.41	A
1712	C	PHE	242	36.346	30.925	67.827	1.00	21.27	A
1713	O	PHE	242	35.205	31.172	68.262	1.00	21.03	A
1714	N	GLU	243	36.884	31.605	66.819	1.00	21.66	A
1715	CA	GLU	243	36.073	32.593	66.108	1.00	21.05	A
1716	CB	GLU	243	36.812	33.838	65.740	1.00	23.06	A
1717	CG	GLU	243	37.306	34.658	66.935	1.00	26.19	A
1718	CD	GLU	243	38.280	35.712	66.421	1.00	28.12	A
1719	OE1	GLU	243	39.310	35.317	65.866	1.00	28.85	A
1720	OE2	GLU	243	37.934	36.889	66.576	1.00	29.67	A
1721	C	GLU	243	35.556	31.867	64.822	1.00	20.93	A
1722	O	GLU	243	36.297	31.031	64.298	1.00	19.28	A
1723	N	ILE	244	34.369	32.235	64.370	1.00	20.74	A
1724	CA	ILE	244	33.792	31.627	63.147	1.00	18.87	A

1725	CB	ILE	244	32.303	31.303	63.242	1.00	19.41	A
1726	CG2	ILE	244	31.879	30.417	62.045	1.00	17.16	A
1727	CG1	ILE	244	31.924	30.529	64.535	1.00	19.59	A
1728	CD1	ILE	244	30.399	30.611	64.826	1.00	19.07	A
1729	C	ILE	244	34.152	32.547	61.977	1.00	16.35	A
1730	O	ILE	244	33.588	33.605	61.829	1.00	16.20	A
1731	N	VAL	245	35.191	32.157	61.222	1.00	17.78	A
1732	CA	VAL	245	35.720	33.000	60.151	1.00	18.85	A
1733	CB	VAL	245	37.140	32.519	59.749	1.00	19.07	A
1734	CG1	VAL	245	37.680	33.512	58.717	1.00	19.26	A
1735	CG2	VAL	245	38.073	32.496	60.995	1.00	20.02	A
1736	C	VAL	245	34.866	33.034	58.877	1.00	16.35	A
1737	O	VAL	245	34.518	34.094	58.380	1.00	17.59	A
1738	N	SER	246	34.580	31.860	58.307	1.00	15.50	A
1739	CA	SER	246	33.761	31.847	57.092	1.00	15.90	A
1740	CB	SER	246	34.758	32.000	55.872	1.00	17.77	A
1741	OG	SER	246	35.465	30.750	55.794	1.00	18.94	A
1742	C	SER	246	33.005	30.556	57.051	1.00	16.37	A
1743	O	SER	246	33.348	29.541	57.697	1.00	14.51	A
1744	N	THR	247	31.898	30.536	56.278	1.00	15.35	A
1745	CA	THR	247	31.083	29.353	56.113	1.00	16.46	A
1746	CB	THR	247	29.760	29.445	56.919	1.00	16.78	A
1747	OG1	THR	247	29.052	30.622	56.477	1.00	17.47	A
1748	CG2	THR	247	30.077	29.665	58.403	1.00	16.52	A
1749	C	THR	247	30.694	29.237	54.622	1.00	18.21	A
1750	O	THR	247	30.504	30.205	53.889	1.00	16.99	A
1735	N	ASP	248	30.618	28.005	54.197	0.50	18.71	A
1736	CA	ASP	248	30.218	27.675	52.827	0.50	19.09	A
1737	CB	ASP	248	31.440	27.391	51.944	0.50	19.78	A
1738	CG	ASP	248	32.410	28.566	51.812	0.50	20.71	A
1739	OD1	ASP	248	31.968	29.747	51.547	0.50	21.41	A
1740	OD2	ASP	248	33.677	28.369	51.963	0.50	23.49	A
1741	C	ASP	248	29.379	26.409	52.848	0.50	19.03	A
1742	O	ASP	248	29.599	25.514	53.671	0.50	18.88	A
1735	N	2ASP	248	30.604	28.004	54.204	0.50	18.31	A
1736	CA	2ASP	248	30.193	27.679	52.839	0.50	18.44	A
1737	CB	2ASP	248	31.407	27.434	51.937	0.50	18.29	A
1738	CG	2ASP	248	31.017	26.889	50.555	0.50	18.92	A
1739	OD	12ASP	248	30.690	27.704	49.608	0.50	18.93	A
1740	OD	22ASP	248	31.012	25.617	50.335	0.50	19.50	A
1741	C	2ASP	248	29.358	26.413	52.864	0.50	18.56	A
1742	O	2ASP	248	29.566	25.532	53.705	0.50	18.48	A
1767	N	GLN	249	28.356	26.417	51.935	1.00	18.12	A
1768	CA	GLN	249	27.549	25.224	51.800	1.00	15.48	A
1769	CB	GLN	249	26.099	25.564	52.196	1.00	14.70	A
1770	CG	GLN	249	25.215	24.313	52.232	1.00	17.53	A
1771	CD	GLN	249	23.779	24.633	52.622	1.00	18.03	A
1772	OE1	GLN	249	23.386	25.788	52.526	1.00	20.85	A
1773	NE2	GLN	249	22.986	23.664	53.058	1.00	16.17	A
1774	C	GLN	249	27.516	24.887	50.297	1.00	17.28	A
1775	O	GLN	249	27.276	25.811	49.490	1.00	16.93	A
1752	N	THR	250	27.724	23.697	49.878	0.50	18.63	A

1753	CA	THR	250	27.626	23.389	48.445	0.50	19.72	A
1754	CB	THR	250	28.923	23.758	47.706	0.50	20.75	A
1755	OG1	THR	250	28.976	23.090	46.452	0.50	20.74	A
1756	CG2	THR	250	30.197	23.409	48.469	0.50	19.75	A
1757	C	THR	250	27.254	21.928	48.211	0.50	19.36	A
1758	O	THR	250	27.694	21.020	48.928	0.50	20.20	A
1752	N	2THR	250	27.757	23.701	49.893	0.50	17.80	A
1753	CA	2THR	250	27.697	23.337	48.471	0.50	18.17	A
1754	CB	2THR	250	29.094	23.333	47.827	0.50	17.92	A
1755	OG	12THR	250	29.903	22.324	48.410	0.50	19.85	A
1756	CG	22THR	250	29.837	24.663	47.974	0.50	13.72	A
1757	C	2THR	250	27.085	21.959	48.296	0.50	18.46	A
1758	O	2THR	250	27.144	21.111	49.195	0.50	19.35	A
1790	N	ILE	251	26.420	21.812	47.160	1.00	18.11	A
1791	CA	ILE	251	25.899	20.518	46.744	1.00	18.91	A
1792	CB	ILE	251	24.566	20.777	46.018	1.00	21.43	A
1793	CG2	ILE	251	24.079	19.563	45.255	1.00	21.91	A
1794	CG1	ILE	251	23.458	21.230	47.008	1.00	19.84	A
1795	CD1	ILE	251	22.343	21.902	46.184	1.00	21.62	A
1796	C	ILE	251	26.917	19.804	45.865	1.00	20.29	A
1797	O	ILE	251	27.373	20.421	44.904	1.00	18.39	A
1798	N	LEU	252	27.242	18.561	46.132	1.00	19.21	A
1799	CA	LEU	252	28.247	17.856	45.333	1.00	21.24	A
1800	CB	LEU	252	28.874	16.732	46.167	1.00	20.16	A
1801	CG	LEU	252	29.544	17.115	47.496	1.00	22.74	A
1802	CD2	LEU	252	30.589	18.196	47.306	1.00	20.38	A
1803	CD1	LEU	252	30.144	15.834	48.104	1.00	21.35	A
1804	C	LEU	252	27.540	17.343	44.067	1.00	21.53	A
1805	O	LEU	252	26.496	16.711	44.166	1.00	20.81	A
1806	N	PRO	253	28.125	17.540	42.891	1.00	23.96	A
1807	CA	PRO	253	27.503	17.137	41.637	1.00	24.00	A
1808	CD	PRO	253	29.384	18.295	42.669	1.00	24.04	A
1809	CB	PRO	253	28.477	17.645	40.537	1.00	27.26	A
1810	CG	PRO	253	29.758	17.845	41.256	1.00	26.43	A
1811	C	PRO	253	27.321	15.652	41.520	1.00	21.79	A
1812	O	PRO	253	28.160	14.836	41.927	1.00	23.62	A
1813	N	ASP	254	26.184	15.233	40.995	1.00	20.90	A
1814	CA	ASP	254	25.847	13.868	40.696	1.00	22.65	A
1815	CB	ASP	254	26.866	13.340	39.636	1.00	24.22	A
1816	CG	ASP	254	26.758	14.178	38.352	1.00	23.48	A
1817	OD1	ASP	254	25.656	14.260	37.820	1.00	23.35	A
1818	OD2	ASP	254	27.702	14.827	37.926	1.00	24.65	A
1819	C	ASP	254	25.915	12.933	41.901	1.00	23.89	A
1820	O	ASP	254	26.435	11.817	41.786	1.00	20.61	A
1821	N	THR	255	25.475	13.405	43.084	1.00	23.24	A
1822	CA	THR	255	25.539	12.504	44.271	1.00	22.38	A
1823	CB	THR	255	26.529	13.102	45.269	1.00	22.65	A
1824	OG1	THR	255	26.047	14.426	45.616	1.00	21.38	A
1825	CG2	THR	255	27.937	13.179	44.660	1.00	21.77	A
1826	C	THR	255	24.185	12.406	44.964	1.00	25.76	A
1827	O	THR	255	24.060	11.927	46.099	1.00	24.90	A
1828	N	GLU	256	23.128	12.826	44.279	1.00	26.04	A

1829	CA	GLU	256	21.798	12.886	44.836	1.00	30.86	A
1830	CB	GLU	256	20.747	13.428	43.862	1.00	32.70	A
1831	CG	GLU	256	19.388	13.594	44.527	1.00	36.12	A
1832	CD	GLU	256	18.316	14.007	43.540	1.00	38.83	A
1833	OE1	GLU	256	17.152	13.468	43.598	1.00	40.66	A
1834	OE2	GLU	256	18.588	14.893	42.648	1.00	38.96	A
1835	C	GLU	256	21.320	11.539	45.377	1.00	31.91	A
1836	O	GLU	256	20.679	11.464	46.430	1.00	31.93	A
1837	N	LYS	257	21.633	10.469	44.689	1.00	31.65	A
1838	CA	LYS	257	21.152	9.147	45.116	1.00	35.38	A
1839	CB	LYS	257	21.043	8.222	43.910	1.00	39.99	A
1840	CG	LYS	257	19.783	8.517	43.089	1.00	45.71	A
1841	CD	LYS	257	19.467	7.440	42.058	1.00	51.11	A
1842	CE	LYS	257	18.956	8.012	40.735	1.00	53.47	A
1843	NZ	LYS	257	18.536	6.968	39.790	1.00	56.09	A
1844	C	LYS	257	22.049	8.525	46.211	1.00	32.87	A
1845	O	LYS	257	21.790	7.419	46.698	1.00	34.25	A
1846	N	ALA	258	23.082	9.246	46.612	1.00	29.70	A
1847	CA	ALA	258	24.024	8.771	47.656	1.00	30.43	A
1848	CB	ALA	258	25.138	9.793	47.873	1.00	28.35	A
1849	C	ALA	258	23.323	8.565	49.021	1.00	27.90	A
1850	O	ALA	258	23.576	7.571	49.723	1.00	24.05	A
1851	N	MET	259	22.464	9.523	49.368	1.00	25.76	A
1852	CA	MET	259	21.726	9.522	50.658	1.00	25.87	A
1853	C	MET	259	20.309	10.047	50.545	1.00	21.93	A
1854	O	MET	259	20.083	11.221	50.262	1.00	23.58	A
1855	CB	MET	259	22.297	10.527	51.653	1.00	27.22	A
1856	CG	MET	259	23.705	10.233	52.098	1.00	28.27	A
1857	SD	MET	259	24.372	11.515	53.127	1.00	27.33	A
1858	CE	MET	259	26.025	11.066	53.579	1.00	25.33	A
1859	N	LYS	260	19.358	9.201	50.793	1.00	20.47	A
1860	CA	LYS	260	17.965	9.639	50.800	1.00	21.83	A
1861	CB	LYS	260	17.256	9.175	49.537	1.00	23.80	A
1862	CG	LYS	260	17.673	9.960	48.296	1.00	29.10	A
1863	CD	LYS	260	16.888	9.531	47.064	1.00	31.39	A
1864	CE	LYS	260	17.270	10.303	45.807	1.00	35.56	A
1865	NZ	LYS	260	16.189	10.333	44.812	1.00	38.58	A
1866	C	LYS	260	17.292	9.033	52.028	1.00	19.21	A
1867	O	LYS	260	17.425	7.840	52.275	1.00	22.29	A
1868	N	LEU	261	16.617	9.836	52.822	1.00	18.40	A
1869	CA	LEU	261	15.950	9.346	54.038	1.00	17.05	A
1870	CB	LEU	261	16.720	9.682	55.307	1.00	17.21	A
1871	CG	LEU	261	18.166	9.207	55.474	1.00	17.40	A
1872	CD2	LEU	261	18.529	9.086	56.953	1.00	16.95	A
1873	CD1	LEU	261	19.166	10.165	54.847	1.00	14.73	A
1874	C	LEU	261	14.536	9.894	54.066	1.00	16.09	A
1875	O	LEU	261	14.295	11.071	53.924	1.00	14.50	A
1876	N	HIS	262	13.548	9.015	54.169	1.00	18.30	A
1877	CA	HIS	262	12.152	9.422	54.155	1.00	17.72	A
1878	ND1	HIS	262	12.566	9.673	51.142	1.00	20.05	A
1879	CG	HIS	262	12.138	8.533	51.792	1.00	18.58	A
1880	CB	HIS	262	11.354	8.626	53.085	1.00	16.72	A

1881	NE2	HIS	262	13.145	7.985	49.930	1.00	19.75	A
1882	CD2	HIS	262	12.555	7.478	51.069	1.00	18.88	A
1883	CE1	HIS	262	13.214	9.296	50.004	1.00	21.26	A
1884	C	HIS	262	11.489	9.117	55.512	1.00	18.43	A
1885	O	HIS	262	11.784	8.058	56.049	1.00	18.61	A
1886	N	LEU	263	10.662	10.047	55.954	1.00	17.01	A
1887	CA	LEU	263	9.960	9.835	57.216	1.00	17.04	A
1888	CB	LEU	263	9.816	11.174	57.973	1.00	16.64	A
1889	CG	LEU	263	9.255	10.958	59.426	1.00	18.78	A
1890	CD2	LEU	263	9.028	12.298	60.090	1.00	17.69	A
1891	CD1	LEU	263	10.301	10.149	60.221	1.00	19.19	A
1892	C	LEU	263	8.608	9.231	56.922	1.00	16.73	A
1893	O	LEU	263	7.741	9.921	56.377	1.00	17.57	A
1894	N	ARG	264	8.469	7.931	57.163	1.00	16.36	A
1895	CA	ARG	264	7.290	7.216	56.840	1.00	17.70	A
1896	CB	ARG	264	7.666	6.046	55.898	1.00	20.34	A
1897	CG	ARG	264	8.681	6.392	54.814	1.00	22.37	A
1898	CD	ARG	264	7.994	7.130	53.685	1.00	20.91	A
1899	NE	ARG	264	7.169	6.277	52.808	1.00	20.51	A
1900	CZ	ARG	264	6.362	6.843	51.895	1.00	21.14	A
1901	NH1	ARG	264	6.375	8.164	51.651	1.00	20.32	A
1902	NH2	ARG	264	5.603	6.053	51.159	1.00	20.22	A
1903	C	ARG	264	6.594	6.569	58.039	1.00	20.22	A
1904	O	ARG	264	7.133	6.659	59.146	1.00	18.39	A
1905	N	GLU	265	5.471	5.899	57.772	1.00	17.87	A
1906	CA	GLU	265	4.790	5.177	58.862	1.00	18.98	A
1907	CB	GLU	265	3.556	4.407	58.303	1.00	16.37	A
1908	CG	GLU	265	2.643	5.476	57.656	1.00	20.82	A
1909	CD	GLU	265	1.563	4.861	56.766	1.00	20.66	A
1910	OE1	GLU	265	1.377	3.645	56.795	1.00	23.15	A
1911	OE2	GLU	265	0.921	5.616	56.020	1.00	22.61	A
1912	C	GLU	265	5.686	4.230	59.613	1.00	18.25	A
1913	O	GLU	265	5.444	3.929	60.795	1.00	18.46	A
1914	N	GLY	266	6.722	3.688	58.977	1.00	17.26	A
1915	CA	GLY	266	7.650	2.792	59.615	1.00	18.12	A
1916	C	GLY	266	8.861	3.481	60.227	1.00	17.40	A
1917	O	GLY	266	9.778	2.748	60.603	1.00	18.01	A
1918	N	GLY	267	8.923	4.798	60.337	1.00	19.74	A
1919	CA	GLY	267	10.100	5.458	60.917	1.00	20.63	A
1920	C	GLY	267	10.931	6.092	59.768	1.00	23.03	A
1921	O	GLY	267	10.497	6.138	58.616	1.00	20.28	A
1922	N	LEU	268	12.159	6.507	60.072	1.00	21.36	A
1923	CA	LEU	268	13.016	7.215	59.122	1.00	21.05	A
1924	CB	LEU	268	13.981	8.145	59.834	1.00	19.19	A
1925	CG	LEU	268	14.897	9.032	58.962	1.00	17.54	A
1926	CD2	LEU	268	15.779	9.886	59.886	1.00	17.15	A
1927	CD1	LEU	268	14.092	9.876	57.984	1.00	15.58	A
1928	C	LEU	268	13.778	6.178	58.285	1.00	21.30	A
1929	O	LEU	268	14.628	5.448	58.813	1.00	23.77	A
1930	N	THR	269	13.451	6.101	57.003	1.00	20.14	A
1931	CA	THR	269	14.056	5.101	56.137	1.00	22.90	A
1932	CB	THR	269	13.254	4.873	54.836	1.00	22.70	A

1933	OG1	THR	269	13.291	6.065	54.053	1.00	21.45	A
1934	CG2	THR	269	11.798	4.570	55.199	1.00	23.44	A
1935	C	THR	269	15.479	5.461	55.734	1.00	24.41	A
1936	O	THR	269	15.836	6.604	55.954	1.00	26.06	A
1937	N	PHE	270	16.186	4.525	55.142	1.00	25.77	A
1938	CA	PHE	270	17.545	4.694	54.678	1.00	30.89	A
1939	CB	PHE	270	18.501	3.800	55.499	1.00	33.60	A
1940	CG	PHE	270	19.068	4.507	56.692	1.00	35.25	A
1941	CD1	PHE	270	18.543	4.341	57.962	1.00	38.30	A
1942	CD2	PHE	270	20.116	5.377	56.499	1.00	36.35	A
1943	CE1	PHE	270	19.093	5.083	59.039	1.00	38.64	A
1944	CE2	PHE	270	20.654	6.118	57.517	1.00	37.80	A
1945	CZ	PHE	270	20.149	5.938	58.791	1.00	38.59	A
1946	C	PHE	270	17.781	4.204	53.238	1.00	31.79	A
1947	O	PHE	270	17.292	3.178	52.744	1.00	33.03	A
1948	N	GLN	271	18.437	5.045	52.478	1.00	29.75	A
1949	CA	GLN	271	19.027	4.697	51.203	1.00	30.30	A
1950	CB	GLN	271	18.181	5.184	50.041	1.00	32.83	A
1951	CG	GLN	271	18.831	5.074	48.669	1.00	37.28	A
1952	CD	GLN	271	17.923	5.507	47.534	1.00	40.09	A
1953	OE1	GLN	271	16.699	5.314	47.556	1.00	42.51	A
1954	NE2	GLN	271	18.436	6.098	46.459	1.00	40.55	A
1955	C	GLN	271	20.424	5.351	51.253	1.00	28.39	A
1956	O	GLN	271	20.552	6.564	51.138	1.00	27.71	A
1957	N	LEU	272	21.442	4.552	51.472	1.00	26.34	A
1958	CA	LEU	272	22.799	5.037	51.618	1.00	28.19	A
1959	CB	LEU	272	23.205	4.847	53.103	1.00	33.12	A
1960	CG	LEU	272	24.627	5.314	53.406	1.00	36.66	A
1961	CD2	LEU	272	25.100	4.817	54.771	1.00	38.65	A
1962	CD1	LEU	272	24.712	6.845	53.320	1.00	37.49	A
1963	C	LEU	272	23.744	4.251	50.704	1.00	27.33	A
1964	O	LEU	272	23.845	3.036	50.830	1.00	25.84	A
1965	N	HIS	273	24.286	4.916	49.706	1.00	27.33	A
1966	CA	HIS	273	25.070	4.272	48.676	1.00	29.58	A
1967	ND1	HIS	273	24.991	3.934	45.256	1.00	40.32	A
1968	CG	HIS	273	25.820	4.402	46.267	1.00	37.43	A
1969	CB	HIS	273	25.274	5.178	47.455	1.00	32.70	A
1970	NE2	HIS	273	26.990	3.337	44.776	1.00	40.36	A
1971	CD2	HIS	273	27.079	4.017	45.948	1.00	37.90	A
1972	CE1	HIS	273	25.742	3.297	44.378	1.00	39.49	A
1973	C	HIS	273	26.452	3.926	49.230	1.00	27.34	A
1974	O	HIS	273	27.034	4.676	50.023	1.00	24.81	A
1975	N	ARG	274	26.940	2.800	48.779	1.00	27.13	A
1976	CA	ARG	274	28.222	2.245	49.217	1.00	29.59	A
1977	CB	ARG	274	28.436	0.897	48.543	1.00	32.73	A
1978	CG	ARG	274	29.796	0.285	48.852	1.00	36.33	A
1979	CD	ARG	274	29.676	-1.035	49.605	1.00	38.66	A
1980	NE	ARG	274	30.959	-1.586	50.043	1.00	38.59	A
1981	CZ	ARG	274	31.496	-2.756	49.633	1.00	39.92	A
1982	NH1	ARG	274	30.899	-3.560	48.742	1.00	39.98	A
1983	NH2	ARG	274	32.670	-3.218	50.095	1.00	39.32	A
1984	C	ARG	274	29.427	3.145	48.864	1.00	27.69	A

1985	O	ARG	274	30.477	3.097	49.514	1.00	27.09	A
1986	N	ASP	275	29.301	3.971	47.837	1.00	24.66	A
1987	CA	ASP	275	30.438	4.816	47.405	1.00	26.48	A
1988	CB	ASP	275	30.422	5.042	45.901	1.00	30.30	A
1989	CG	ASP	275	30.708	3.772	45.112	1.00	35.19	A
1990	OD1	ASP	275	30.244	3.654	43.918	1.00	36.99	A
1991	OD2	ASP	275	31.402	2.826	45.645	1.00	37.66	A
1992	C	ASP	275	30.424	6.199	48.051	1.00	22.09	A
1993	O	ASP	275	31.151	7.111	47.643	1.00	19.23	A
1994	N	VAL	276	29.611	6.369	49.060	1.00	20.27	A
1995	CA	VAL	276	29.544	7.666	49.723	1.00	18.96	A
1996	CB	VAL	276	28.626	7.596	50.945	1.00	19.63	A
1997	CG1	VAL	276	28.923	8.677	51.989	1.00	19.71	A
1998	CG2	VAL	276	27.148	7.782	50.573	1.00	17.53	A
1999	C	VAL	276	30.971	8.126	50.086	1.00	18.02	A
2000	O	VAL	276	31.380	9.252	49.782	1.00	17.63	A
2001	N	PRO	277	31.831	7.331	50.754	1.00	18.36	A
2002	CA	PRO	277	33.169	7.800	51.096	1.00	20.79	A
2003	CD	PRO	277	31.512	5.973	51.202	1.00	19.97	A
2004	CB	PRO	277	33.785	6.649	51.849	1.00	19.99	A
2005	CG	PRO	277	32.739	5.555	51.962	1.00	19.83	A
2006	C	PRO	277	33.974	8.293	49.891	1.00	23.03	A
2007	O	PRO	277	34.726	9.302	50.018	1.00	21.62	A
2008	N	LEU	278	33.872	7.665	48.735	1.00	21.57	A
2009	CA	LEU	278	34.644	8.143	47.555	1.00	24.35	A
2010	CB	LEU	278	34.625	7.099	46.431	1.00	26.62	A
2011	CG	LEU	278	35.651	5.976	46.594	1.00	29.87	A
2012	CD2	LEU	278	37.099	6.467	46.565	1.00	27.31	A
2013	CD1	LEU	278	35.542	4.920	45.486	1.00	31.37	A
2014	C	LEU	278	34.025	9.394	46.975	1.00	23.03	A
2015	O	LEU	278	34.757	10.207	46.395	1.00	24.13	A
2016	N	MET	279	32.699	9.537	47.109	1.00	20.09	A
2017	CA	MET	279	32.098	10.793	46.607	1.00	20.81	A
2018	CB	MET	279	30.585	10.759	46.763	1.00	21.80	A
2019	CG	MET	279	29.956	9.554	46.087	1.00	21.49	A
2020	SD	MET	279	28.158	9.596	46.311	1.00	22.74	A
2021	CE	MET	279	27.814	7.886	45.932	1.00	22.20	A
2022	C	MET	279	32.620	11.950	47.432	1.00	21.26	A
2023	O	MET	279	32.843	13.056	46.902	1.00	21.41	A
2024	N	VAL	280	32.755	11.735	48.762	1.00	21.29	A
2025	CA	VAL	280	33.337	12.833	49.548	1.00	22.70	A
2026	CB	VAL	280	33.288	12.488	51.071	1.00	23.91	A
2027	CG1	VAL	280	34.082	13.494	51.898	1.00	22.39	A
2028	CG2	VAL	280	31.841	12.468	51.575	1.00	22.09	A
2029	C	VAL	280	34.770	13.083	49.071	1.00	24.53	A
2030	O	VAL	280	35.252	14.214	48.931	1.00	23.97	A
2031	N	ALA	281	35.564	12.025	48.891	1.00	25.87	A
2032	CA	ALA	281	36.967	12.124	48.489	1.00	27.38	A
2033	CB	ALA	281	37.578	10.723	48.367	1.00	27.95	A
2034	C	ALA	281	37.174	12.837	47.160	1.00	28.59	A
2035	O	ALA	281	38.056	13.701	47.016	1.00	29.65	A
2036	N	LYS	282	36.300	12.572	46.189	1.00	26.22	A

2037	CA	LYS	282	36.368	13.223	44.907	1.00	25.90	A
2038	CB	LYS	282	35.300	12.698	43.925	1.00	27.70	A
2039	CG	LYS	282	35.153	13.575	42.651	1.00	30.25	A
2040	CD	LYS	282	33.857	13.278	41.920	1.00	29.84	A
2041	CE	LYS	282	33.593	14.185	40.715	1.00	32.26	A
2042	NZ	LYS	282	32.243	13.849	40.139	1.00	30.29	A
2043	C	LYS	282	36.254	14.726	45.103	1.00	25.93	A
2044	O	LYS	282	36.845	15.456	44.303	1.00	23.37	A
2045	N	ASN	283	35.502	15.227	46.092	1.00	25.52	A
2046	CA	ASN	283	35.211	16.644	46.193	1.00	25.46	A
2047	CB	ASN	283	33.668	16.812	46.435	1.00	25.21	A
2048	CG	ASN	283	32.881	16.340	45.229	1.00	26.49	A
2049	OD1	ASN	283	32.704	17.126	44.310	1.00	25.47	A
2050	ND2	ASN	283	32.380	15.100	45.189	1.00	27.38	A
2051	C	ASN	283	35.863	17.400	47.333	1.00	24.11	A
2052	O	ASN	283	35.665	18.622	47.353	1.00	24.47	A
2053	N	ILE	284	36.517	16.739	48.251	1.00	25.53	A
2054	CA	ILE	284	36.995	17.393	49.477	1.00	26.10	A
2055	CB	ILE	284	37.328	16.279	50.494	1.00	26.34	A
2056	CG2	ILE	284	38.653	15.582	50.160	1.00	26.45	A
2057	CG1	ILE	284	37.371	16.753	51.938	1.00	26.40	A
2058	CD1	ILE	284	36.089	17.363	52.446	1.00	26.64	A
2059	C	ILE	284	38.133	18.365	49.270	1.00	28.21	A
2060	O	ILE	284	38.064	19.553	49.667	1.00	26.93	A
2061	N	GLU	285	39.048	18.054	48.349	1.00	28.53	A
2062	CA	GLU	285	40.191	18.985	48.139	1.00	30.46	A
2063	CB	GLU	285	41.241	18.332	47.222	1.00	33.52	A
2064	CG	GLU	285	42.182	19.313	46.561	1.00	39.10	A
2065	CD	GLU	285	43.388	19.749	47.365	1.00	42.79	A
2066	OE1	GLU	285	43.645	19.212	48.464	1.00	42.80	A
2067	OE2	GLU	285	44.117	20.670	46.879	1.00	44.61	A
2068	C	GLU	285	39.716	20.340	47.698	1.00	26.56	A
2069	O	GLU	285	40.175	21.419	48.100	1.00	25.80	A
2070	N	ASN	286	38.666	20.341	46.873	1.00	27.41	A
2071	CA	ASN	286	38.041	21.556	46.370	1.00	29.50	A
2072	CB	ASN	286	36.931	21.113	45.424	1.00	35.35	A
2073	CG	ASN	286	36.487	22.141	44.428	1.00	40.87	A
2074	OD1	ASN	286	36.837	22.003	43.230	1.00	45.15	A
2075	ND2	ASN	286	35.717	23.121	44.856	1.00	42.56	A
2076	C	ASN	286	37.392	22.389	47.486	1.00	26.71	A
2077	O	ASN	286	37.308	23.617	47.475	1.00	22.59	A
2078	N	ALA	287	36.790	21.654	48.434	1.00	24.05	A
2079	CA	ALA	287	36.132	22.320	49.573	1.00	23.78	A
2080	CB	ALA	287	35.286	21.334	50.345	1.00	22.36	A
2081	C	ALA	287	37.225	22.964	50.432	1.00	22.30	A
2082	O	ALA	287	37.135	24.138	50.758	1.00	24.71	A
2083	N	ALA	288	38.280	22.228	50.704	1.00	23.39	A
2084	CA	ALA	288	39.407	22.804	51.436	1.00	25.71	A
2085	CB	ALA	288	40.468	21.729	51.625	1.00	24.55	A
2086	C	ALA	288	40.000	24.044	50.791	1.00	25.87	A
2087	O	ALA	288	40.250	25.078	51.440	1.00	24.50	A
2088	N	GLU	289	40.198	23.985	49.463	1.00	27.07	A

2089	CA	GLU	289	40.813	25.091	48.741	1.00	28.27	A
2090	CB	GLU	289	41.130	24.674	47.271	1.00	30.88	A
2091	CG	GLU	289	42.340	23.762	47.245	1.00	35.87	A
2092	CD	GLU	289	42.625	23.071	45.921	1.00	40.56	A
2093	OE1	GLU	289	43.791	22.653	45.702	1.00	41.51	A
2094	OE2	GLU	289	41.708	22.906	45.088	1.00	41.76	A
2095	C	GLU	289	39.981	26.346	48.695	1.00	26.52	A
2096	O	GLU	289	40.511	27.452	48.830	1.00	25.15	A
2097	N	LYS	290	38.676	26.199	48.535	1.00	23.69	A
2098	CA	LYS	290	37.769	27.340	48.480	1.00	27.51	A
2099	CB	LYS	290	36.399	26.882	48.005	1.00	29.38	A
2100	CG	LYS	290	35.240	27.853	48.135	1.00	35.53	A
2101	CD	LYS	290	33.949	27.292	47.545	1.00	38.73	A
2102	CE	LYS	290	32.844	28.342	47.436	1.00	40.40	A
2103	NZ	LYS	290	31.560	27.684	47.011	1.00	41.39	A
2104	C	LYS	290	37.714	28.054	49.844	1.00	26.14	A
2105	O	LYS	290	37.657	29.278	49.879	1.00	24.24	A
2106	N	ALA	291	37.891	27.296	50.919	1.00	24.46	A
2107	CA	ALA	291	37.895	27.866	52.249	1.00	27.44	A
2108	CB	ALA	291	37.595	26.760	53.264	1.00	26.18	A
2109	C	ALA	291	39.262	28.465	52.626	1.00	27.57	A
2110	O	ALA	291	39.365	29.545	53.217	1.00	27.36	A
2111	N	LEU	292	40.304	27.720	52.266	1.00	26.84	A
2112	CA	LEU	292	41.624	28.202	52.710	1.00	28.86	A
2113	CB	LEU	292	42.422	26.986	53.134	1.00	26.99	A
2114	CG	LEU	292	41.871	26.217	54.337	1.00	28.38	A
2115	CD2	LEU	292	42.008	27.044	55.607	1.00	27.89	A
2116	CD1	LEU	292	42.631	24.899	54.444	1.00	26.16	A
2117	C	LEU	292	42.459	29.033	51.744	1.00	30.46	A
2118	O	LEU	292	43.188	29.940	52.207	1.00	30.17	A
2119	N	SER	293	42.120	29.018	50.451	1.00	31.81	A
2120	CA	SER	293	42.870	29.851	49.495	1.00	32.75	A
2121	CB	SER	293	42.477	29.604	48.025	1.00	32.73	A
2122	OG	SER	293	43.153	28.418	47.645	1.00	34.17	A
2123	C	SER	293	42.776	31.324	49.779	1.00	33.36	A
2124	O	SER	293	43.801	31.999	49.867	1.00	34.00	A
2125	N	PRO	294	41.603	31.876	50.029	1.00	34.41	A
2126	CA	PRO	294	41.480	33.287	50.381	1.00	35.42	A
2127	CD	PRO	294	40.295	31.190	50.023	1.00	34.17	A
2128	CB	PRO	294	39.981	33.501	50.548	1.00	34.86	A
2129	CG	PRO	294	39.306	32.337	49.921	1.00	34.65	A
2130	C	PRO	294	42.254	33.690	51.638	1.00	36.84	A
2131	O	PRO	294	42.481	34.881	51.909	1.00	36.47	A
2132	N	LEU	295	42.650	32.745	52.486	1.00	36.49	A
2133	CA	LEU	295	43.429	32.991	53.683	1.00	37.02	A
2134	CB	LEU	295	42.980	32.003	54.763	1.00	37.27	A
2135	CG	LEU	295	41.820	32.354	55.702	1.00	38.92	A
2136	CD2	LEU	295	41.008	31.102	56.046	1.00	38.57	A
2137	CD1	LEU	295	40.896	33.423	55.171	1.00	38.29	A
2138	C	LEU	295	44.925	32.827	53.416	1.00	36.97	A
2139	O	LEU	295	45.766	32.870	54.320	1.00	36.24	A
2140	N	GLY	296	45.308	32.560	52.176	1.00	36.33	A

2141	CA	GLY	296	46.679	32.361	51.749	1.00	36.08	A
2142	C	GLY	296	47.255	31.058	52.254	1.00	37.21	A
2143	O	GLY	296	48.472	30.915	52.457	1.00	37.99	A
2144	N	ILE	297	46.402	30.060	52.501	1.00	36.81	A
2145	CA	ILE	297	46.904	28.802	53.050	1.00	37.30	A
2146	CB	ILE	297	46.311	28.486	54.420	1.00	38.48	A
2147	CG2	ILE	297	45.103	29.359	54.728	1.00	40.59	A
2148	CG1	ILE	297	45.928	27.017	54.562	1.00	38.31	A
2149	CD1	ILE	297	46.901	26.269	55.416	1.00	40.48	A
2150	C	ILE	297	46.727	27.683	52.035	1.00	37.13	A
2151	O	ILE	297	45.686	27.505	51.409	1.00	37.08	A
2152	N	THR	298	47.803	26.927	51.890	1.00	36.87	A
2153	CA	THR	298	47.896	25.847	50.940	1.00	38.72	A
2154	CB	THR	298	48.874	26.221	49.786	1.00	39.90	A
2155	OG1	THR	298	50.117	26.627	50.374	1.00	39.12	A
2156	CG2	THR	298	48.278	27.325	48.927	1.00	39.83	A
2157	C	THR	298	48.369	24.568	51.589	1.00	39.07	A
2158	O	THR	298	48.122	23.494	51.045	1.00	42.28	A
2159	N	ASP	299	49.004	24.662	52.740	1.00	39.02	A
2160	CA	ASP	299	49.496	23.468	53.436	1.00	38.76	A
2161	CB	ASP	299	50.764	23.831	54.194	1.00	38.63	A
2162	CG	ASP	299	51.295	22.758	55.103	1.00	39.09	A
2163	OD1	ASP	299	50.863	21.591	55.031	1.00	37.72	A
2164	OD2	ASP	299	52.141	23.059	55.976	1.00	41.89	A
2165	C	ASP	299	48.408	22.909	54.362	1.00	38.43	A
2166	O	ASP	299	48.184	23.476	55.430	1.00	38.49	A
2167	N	TRP	300	47.826	21.767	54.023	1.00	37.66	A
2168	CA	TRP	300	46.745	21.149	54.790	1.00	37.33	A
2169	CB	TRP	300	46.076	20.035	54.030	1.00	35.24	A
2170	CG	TRP	300	45.615	20.311	52.635	1.00	33.53	A
2171	CD2	TRP	300	45.171	21.538	52.062	1.00	33.67	A
2172	CD1	TRP	300	45.493	19.374	51.649	1.00	33.49	A
2173	NE1	TRP	300	45.028	19.958	50.493	1.00	33.28	A
2174	CE2	TRP	300	44.800	21.288	50.730	1.00	34.25	A
2175	CE3	TRP	300	45.057	22.846	52.553	1.00	35.18	A
2176	CZ2	TRP	300	44.346	22.285	49.865	1.00	33.41	A
2177	CZ3	TRP	300	44.620	23.849	51.709	1.00	34.28	A
2178	CH2	TRP	300	44.241	23.551	50.385	1.00	34.92	A
2179	C	TRP	300	47.202	20.714	56.182	1.00	37.49	A
2180	O	TRP	300	46.418	20.813	57.163	1.00	36.40	A
2181	N	ASN	301	48.477	20.306	56.332	1.00	34.48	A
2182	CA	ASN	301	48.922	19.946	57.672	1.00	35.00	A
2183	CB	ASN	301	50.144	19.029	57.661	1.00	37.31	A
2184	CG	ASN	301	49.728	17.606	57.329	1.00	38.68	A
2185	OD1	ASN	301	48.920	16.951	57.987	1.00	37.57	A
2186	ND2	ASN	301	50.350	17.099	56.273	1.00	40.93	A
2187	C	ASN	301	49.175	21.173	58.550	1.00	32.26	A
2188	O	ASN	301	49.400	20.997	59.751	1.00	31.10	A
2189	N	SER	302	49.106	22.389	58.010	1.00	31.87	A
2190	CA	SER	302	49.245	23.552	58.893	1.00	32.12	A
2191	CB	SER	302	49.849	24.731	58.135	1.00	29.88	A
2192	OG	SER	302	48.880	25.107	57.168	1.00	32.74	A

2193	C	SER	302	47.906	23.992	59.499	1.00	30.90	A
2194	O	SER	302	47.842	25.052	60.118	1.00	31.20	A
2195	N	VAL	303	46.822	23.230	59.362	1.00	30.13	A
2196	CA	VAL	303	45.553	23.653	59.934	1.00	28.77	A
2197	CB	VAL	303	44.522	24.168	58.925	1.00	31.98	A
2198	CG1	VAL	303	45.062	25.161	57.904	1.00	32.26	A
2199	CG2	VAL	303	43.857	23.026	58.191	1.00	31.24	A
2200	C	VAL	303	44.978	22.498	60.741	1.00	26.82	A
2201	O	VAL	303	45.415	21.362	60.526	1.00	27.14	A
2202	N	PHE	304	44.090	22.798	61.685	1.00	24.01	A
2203	CA	PHE	304	43.475	21.704	62.438	1.00	23.42	A
2204	CB	PHE	304	43.325	22.054	63.911	1.00	23.36	A
2205	CG	PHE	304	42.463	23.232	64.237	1.00	22.32	A
2206	CD1	PHE	304	42.945	24.512	64.179	1.00	20.79	A
2207	CD2	PHE	304	41.127	23.039	64.629	1.00	24.15	A
2208	CE1	PHE	304	42.161	25.609	64.468	1.00	19.60	A
2209	CE2	PHE	304	40.346	24.133	64.947	1.00	21.08	A
2210	CZ	PHE	304	40.842	25.414	64.847	1.00	20.44	A
2211	C	PHE	304	42.147	21.355	61.776	1.00	24.89	A
2212	O	PHE	304	41.627	22.140	60.992	1.00	25.71	A
2213	N	TRP	305	41.666	20.119	61.929	1.00	25.44	A
2214	CA	TRP	305	40.584	19.613	61.118	1.00	25.60	A
2215	CB	TRP	305	41.051	18.536	60.093	1.00	25.55	A
2216	CG	TRP	305	41.959	19.100	59.049	1.00	26.83	A
2217	CD2	TRP	305	41.615	19.672	57.775	1.00	28.73	A
2218	CD1	TRP	305	43.318	19.207	59.176	1.00	27.96	A
2219	NE1	TRP	305	43.822	19.826	58.065	1.00	28.93	A
2220	CE2	TRP	305	42.806	20.120	57.187	1.00	29.39	A
2221	CE3	TRP	305	40.405	19.893	57.104	1.00	27.51	A
2222	CZ2	TRP	305	42.852	20.773	55.956	1.00	30.39	A
2223	CZ3	TRP	305	40.462	20.535	55.866	1.00	29.88	A
2224	CH2	TRP	305	41.657	20.981	55.292	1.00	30.23	A
2225	C	TRP	305	39.556	18.924	61.998	1.00	24.39	A
2226	O	TRP	305	39.918	18.180	62.892	1.00	25.90	A
2227	N	MET	306	38.308	19.223	61.746	1.00	22.65	A
2228	CA	MET	306	37.198	18.610	62.475	1.00	22.14	A
2229	CB	MET	306	36.522	19.736	63.268	1.00	22.15	A
2230	CG	MET	306	37.433	20.356	64.335	1.00	23.61	A
2231	SD	MET	306	37.057	22.087	64.614	1.00	24.09	A
2232	CE	MET	306	37.738	22.767	63.079	1.00	25.77	A
2233	C	MET	306	36.287	18.000	61.412	1.00	20.50	A
2234	O	MET	306	35.608	18.766	60.735	1.00	21.18	A
2235	N	VAL	307	36.296	16.682	61.268	1.00	19.97	A
2236	CA	VAL	307	35.652	16.070	60.113	1.00	20.97	A
2237	CB	VAL	307	36.711	15.240	59.325	1.00	22.15	A
2238	CG1	VAL	307	36.059	14.606	58.100	1.00	21.56	A
2239	CG2	VAL	307	37.843	16.138	58.808	1.00	19.03	A
2240	C	VAL	307	34.481	15.226	60.556	1.00	18.76	A
2241	O	VAL	307	34.671	14.319	61.368	1.00	18.36	A
2242	N	HIS	308	33.288	15.563	60.066	1.00	17.69	A
2243	CA	HIS	308	32.137	14.752	60.516	1.00	19.07	A
2244	ND1	HIS	308	29.082	14.287	61.340	1.00	19.45	A

2245	CG	HIS	308	29.736	14.291	60.117	1.00	18.52	A
2246	CB	HIS	308	30.860	15.253	59.823	1.00	17.91	A
2247	NE2	HIS	308	28.252	12.647	60.143	1.00	17.30	A
2248	CD2	HIS	308	29.273	13.240	59.426	1.00	18.98	A
2249	CE1	HIS	308	28.161	13.317	61.296	1.00	20.93	A
2250	C	HIS	308	32.401	13.295	60.187	1.00	22.00	A
2251	O	HIS	308	32.541	12.856	59.015	1.00	21.78	A
2252	N	PRO	309	32.393	12.441	61.212	1.00	20.32	A
2253	CA	PRO	309	32.739	11.051	61.029	1.00	20.18	A
2254	CD	PRO	309	32.301	12.831	62.657	1.00	20.49	A
2255	CB	PRO	309	33.298	10.657	62.401	1.00	20.80	A
2256	CG	PRO	309	32.498	11.496	63.364	1.00	20.59	A
2257	C	PRO	309	31.508	10.289	60.609	1.00	21.81	A
2258	O	PRO	309	30.997	9.378	61.269	1.00	19.24	A
2259	N	GLY	310	31.103	10.445	59.323	1.00	23.24	A
2260	CA	GLY	310	29.864	9.839	58.832	1.00	20.51	A
2261	C	GLY	310	30.019	8.326	58.903	1.00	20.61	A
2262	O	GLY	310	29.087	7.565	59.191	1.00	20.56	A
2263	N	GLY	311	31.239	7.863	58.784	1.00	22.70	A
2264	CA	GLY	311	31.640	6.482	59.010	1.00	22.41	A
2265	C	GLY	311	33.177	6.532	59.055	1.00	26.15	A
2266	O	GLY	311	33.732	7.545	58.622	1.00	23.11	A
2267	N	ARG	312	33.801	5.449	59.542	1.00	25.15	A
2268	CA	ARG	312	35.267	5.453	59.517	1.00	28.00	A
2269	CB	ARG	312	35.781	4.146	60.150	1.00	28.47	A
2270	CG	ARG	312	37.279	4.127	60.410	1.00	29.38	A
2271	CD	ARG	312	37.969	2.814	60.029	1.00	29.48	A
2272	NE	ARG	312	38.075	2.653	58.576	1.00	29.65	A
2273	CZ	ARG	312	37.412	1.794	57.833	1.00	29.04	A
2274	NH1	ARG	312	36.549	0.931	58.375	1.00	29.66	A
2275	NH2	ARG	312	37.562	1.804	56.502	1.00	29.86	A
2276	C	ARG	312	35.838	5.655	58.110	1.00	28.09	A
2277	O	ARG	312	36.840	6.360	57.932	1.00	26.45	A
2278	N	ALA	313	35.194	5.140	57.044	1.00	27.48	A
2279	CA	ALA	313	35.761	5.264	55.709	1.00	28.44	A
2280	CB	ALA	313	35.090	4.311	54.721	1.00	25.75	A
2281	C	ALA	313	35.789	6.710	55.238	1.00	27.78	A
2282	O	ALA	313	36.738	7.113	54.545	1.00	28.88	A
2283	N	ILE	314	34.847	7.571	55.640	1.00	25.33	A
2284	CA	ILE	314	34.863	8.967	55.278	1.00	24.23	A
2285	CB	ILE	314	33.593	9.715	55.711	1.00	24.88	A
2286	CG2	ILE	314	33.746	11.217	55.572	1.00	22.43	A
2287	CG1	ILE	314	32.389	9.150	54.926	1.00	25.63	A
2288	CD1	ILE	314	31.038	9.696	55.366	1.00	26.50	A
2289	C	ILE	314	36.096	9.645	55.864	1.00	25.33	A
2290	O	ILE	314	36.752	10.462	55.193	1.00	24.16	A
2291	N	LEU	315	36.403	9.283	57.131	1.00	23.77	A
2292	CA	LEU	315	37.587	9.932	57.718	1.00	24.34	A
2293	CB	LEU	315	37.682	9.524	59.191	1.00	24.34	A
2294	CG	LEU	315	36.536	10.054	60.091	1.00	25.06	A
2295	CD2	LEU	315	36.454	11.569	60.006	1.00	22.52	A
2296	CD1	LEU	315	36.748	9.592	61.524	1.00	24.58	A

2297	C	LEU	315	38.801	9.473	56.901	1.00	23.99	A
2298	O	LEU	315	39.630	10.293	56.546	1.00	20.41	A
2299	N	ASP	316	38.963	8.169	56.724	1.00	25.26	A
2300	CA	ASP	316	40.110	7.646	55.941	1.00	27.56	A
2301	CB	ASP	316	39.995	6.111	55.767	1.00	26.73	A
2302	CG	ASP	316	40.093	5.400	57.101	1.00	25.66	A
2303	OD1	ASP	316	40.437	6.079	58.096	1.00	26.87	A
2304	OD2	ASP	316	39.785	4.201	57.261	1.00	25.95	A
2305	C	ASP	316	40.253	8.299	54.580	1.00	29.51	A
2306	O	ASP	316	41.380	8.689	54.209	1.00	28.40	A
2307	N	GLN	317	39.156	8.489	53.828	1.00	28.98	A
2308	CA	GLN	317	39.264	9.121	52.514	1.00	29.43	A
2309	CB	GLN	317	37.937	9.114	51.714	1.00	29.81	A
2310	CG	GLN	317	37.628	7.668	51.398	1.00	32.45	A
2311	CD	GLN	317	38.330	7.080	50.206	1.00	34.76	A
2312	OE1	GLN	317	38.009	5.889	50.034	1.00	38.92	A
2313	NE2	GLN	317	39.119	7.750	49.373	1.00	31.51	A
2314	C	GLN	317	39.679	10.565	52.579	1.00	28.51	A
2315	O	GLN	317	40.430	11.043	51.730	1.00	26.77	A
2316	N	VAL	318	39.127	11.279	53.564	1.00	27.55	A
2317	CA	VAL	318	39.453	12.700	53.695	1.00	26.01	A
2318	CB	VAL	318	38.562	13.398	54.731	1.00	26.17	A
2319	CG1	VAL	318	39.100	14.786	55.062	1.00	24.19	A
2320	CG2	VAL	318	37.127	13.456	54.194	1.00	27.01	A
2321	C	VAL	318	40.931	12.801	54.056	1.00	27.36	A
2322	O	VAL	318	41.718	13.524	53.435	1.00	27.34	A
2323	N	GLU	319	41.346	11.967	55.006	1.00	26.26	A
2324	CA	GLU	319	42.771	11.972	55.396	1.00	29.48	A
2325	CB	GLU	319	42.954	10.913	56.476	1.00	28.76	A
2326	CG	GLU	319	44.416	10.778	56.949	1.00	32.30	A
2327	CD	GLU	319	44.448	9.601	57.916	1.00	33.55	A
2328	OE1	GLU	319	44.618	8.445	57.486	1.00	34.82	A
2329	OE2	GLU	319	44.106	9.866	59.086	1.00	34.46	A
2330	C	GLU	319	43.714	11.668	54.210	1.00	31.27	A
2331	O	GLU	319	44.646	12.423	53.936	1.00	29.97	A
2332	N	ARG	320	43.391	10.658	53.421	1.00	31.97	A
2333	CA	ARG	320	44.195	10.228	52.281	1.00	33.54	A
2334	CB	ARG	320	43.670	8.895	51.721	1.00	37.94	A
2335	CG	ARG	320	44.016	8.642	50.246	1.00	45.02	A
2336	CD	ARG	320	43.689	7.210	49.851	1.00	49.77	A
2337	NE	ARG	320	42.634	7.130	48.855	1.00	54.74	A
2338	CZ	ARG	320	42.006	6.021	48.473	1.00	57.64	A
2339	NH1	ARG	320	42.255	4.813	48.976	1.00	58.10	A
2340	NH2	ARG	320	41.067	6.113	47.529	1.00	59.70	A
2341	C	ARG	320	44.214	11.277	51.180	1.00	31.57	A
2342	O	ARG	320	45.260	11.735	50.748	1.00	26.69	A
2343	N	LYS	321	43.041	11.746	50.781	1.00	30.54	A
2344	CA	LYS	321	42.931	12.731	49.718	1.00	31.32	A
2345	CB	LYS	321	41.453	12.882	49.303	1.00	29.88	A
2346	CG	LYS	321	41.257	13.275	47.879	1.00	32.75	A
2347	CD	LYS	321	41.347	12.186	46.811	1.00	31.59	A
2348	CE	LYS	321	41.170	12.810	45.427	1.00	30.86	A

2349	NZ	LYS	321	40.794	11.823	44.359	1.00	28.78	A
2350	C	LYS	321	43.601	14.039	50.087	1.00	32.09	A
2351	O	LYS	321	44.231	14.651	49.185	1.00	30.42	A
2352	N	LEU	322	43.548	14.487	51.336	1.00	28.45	A
2353	CA	LEU	322	44.237	15.726	51.708	1.00	31.61	A
2354	CB	LEU	322	43.526	16.418	52.905	1.00	31.98	A
2355	CG	LEU	322	42.063	16.787	52.652	1.00	32.26	A
2356	CD2	LEU	322	41.968	17.752	51.468	1.00	31.43	A
2357	CD1	LEU	322	41.400	17.356	53.890	1.00	30.97	A
2358	C	LEU	322	45.687	15.492	52.143	1.00	32.01	A
2359	O	LEU	322	46.375	16.423	52.562	1.00	32.31	A
2360	N	ASN	323	46.106	14.241	52.199	1.00	33.80	A
2361	CA	ASN	323	47.422	13.770	52.591	1.00	33.98	A
2362	CB	ASN	323	48.475	14.261	51.561	1.00	35.66	A
2363	CG	ASN	323	49.791	13.511	51.684	1.00	38.31	A
2364	OD1	ASN	323	49.908	12.416	52.265	1.00	38.69	A
2365	ND2	ASN	323	50.842	14.144	51.159	1.00	40.45	A
2366	C	ASN	323	47.771	14.239	53.999	1.00	34.07	A
2367	O	ASN	323	48.867	14.696	54.276	1.00	29.61	A
2368	N	LEU	324	46.797	14.196	54.919	1.00	32.49	A
2369	CA	LEU	324	47.006	14.645	56.276	1.00	31.44	A
2370	CB	LEU	324	45.659	14.630	57.024	1.00	30.01	A
2371	CG	LEU	324	44.538	15.505	56.458	1.00	29.87	A
2372	CD2	LEU	324	45.051	16.888	56.068	1.00	29.03	A
2373	CD1	LEU	324	43.382	15.665	57.456	1.00	28.63	A
2374	C	LEU	324	48.003	13.734	56.980	1.00	32.17	A
2375	O	LEU	324	47.906	12.515	56.758	1.00	31.89	A
2376	N	LYS	325	48.830	14.261	57.884	1.00	32.78	A
2377	CA	LYS	325	49.671	13.326	58.647	1.00	36.55	A
2378	CB	LYS	325	50.820	13.917	59.442	1.00	38.31	A
2379	CG	LYS	325	50.604	15.247	60.115	1.00	40.84	A
2380	CD	LYS	325	51.767	16.183	59.765	1.00	43.98	A
2381	CE	LYS	325	51.719	17.381	60.709	1.00	45.41	A
2382	NZ	LYS	325	52.075	16.951	62.089	1.00	46.52	A
2383	C	LYS	325	48.795	12.493	59.587	1.00	36.64	A
2384	O	LYS	325	47.635	12.774	59.821	1.00	35.10	A
2385	N	ALA	326	49.375	11.426	60.088	1.00	37.18	A
2386	CA	ALA	326	48.791	10.409	60.914	1.00	40.51	A
2387	C	ALA	326	47.837	10.816	62.029	1.00	39.91	A
2388	O	ALA	326	46.852	10.108	62.288	1.00	41.58	A
2389	CB	ALA	326	49.955	9.618	61.562	1.00	41.19	A
2390	N	ASP	327	48.110	11.891	62.740	1.00	39.91	A
2391	CA	ASP	327	47.194	12.211	63.844	1.00	39.02	A
2392	CB	ASP	327	48.055	12.451	65.095	1.00	43.42	A
2393	CG	ASP	327	49.181	13.445	64.877	1.00	46.52	A
2394	OD1	ASP	327	50.142	13.411	65.694	1.00	50.17	A
2395	OD2	ASP	327	49.190	14.258	63.933	1.00	47.69	A
2396	C	ASP	327	46.335	13.405	63.535	1.00	35.51	A
2397	O	ASP	327	45.697	13.856	64.489	1.00	35.04	A
2398	N	LYS	328	46.284	13.931	62.295	1.00	31.04	A
2399	CA	LYS	328	45.477	15.122	62.094	1.00	29.47	A
2400	CB	LYS	328	45.546	15.701	60.680	1.00	29.91	A

2401	CG	LYS	328	46.875	16.254	60.230	1.00	31.30	A
2402	CD	LYS	328	47.479	17.280	61.208	1.00	30.94	A
2403	CE	LYS	328	46.703	18.557	61.104	1.00	30.10	A
2404	NZ	LYS	328	47.380	19.763	61.595	1.00	28.00	A
2405	C	LYS	328	44.002	14.872	62.475	1.00	26.96	A
2406	O	LYS	328	43.378	15.790	63.011	1.00	26.83	A
2407	N	LEU	329	43.456	13.707	62.207	1.00	24.37	A
2408	CA	LEU	329	42.034	13.458	62.500	1.00	24.60	A
2409	CB	LEU	329	41.499	12.602	61.342	1.00	23.58	A
2410	CG	LEU	329	41.496	13.306	59.962	1.00	23.22	A
2411	CD2	LEU	329	41.130	14.772	60.091	1.00	24.27	A
2412	CD1	LEU	329	40.574	12.571	58.994	1.00	21.79	A
2413	C	LEU	329	41.773	12.827	63.849	1.00	23.51	A
2414	O	LEU	329	40.705	12.252	64.112	1.00	23.49	A
2415	N	ARG	330	42.712	12.929	64.785	1.00	23.97	A
2416	CA	ARG	330	42.611	12.245	66.074	1.00	24.74	A
2417	CB	ARG	330	43.819	12.671	66.957	1.00	26.92	A
2418	CG	ARG	330	43.810	11.773	68.211	1.00	31.36	A
2419	CD	ARG	330	44.166	12.556	69.457	1.00	34.14	A
2420	NE	ARG	330	43.514	13.854	69.571	1.00	35.61	A
2421	CZ	ARG	330	42.415	14.135	70.285	1.00	35.45	A
2422	NH1	ARG	330	41.721	13.283	71.017	1.00	32.02	A
2423	NH2	ARG	330	41.988	15.386	70.304	1.00	35.69	A
2424	C	ARG	330	41.330	12.541	66.858	1.00	21.83	A
2425	O	ARG	330	40.580	11.694	67.327	1.00	22.99	A
2426	N	ALA	331	41.054	13.810	67.005	1.00	22.43	A
2427	CA	ALA	331	39.861	14.311	67.695	1.00	25.05	A
2428	CB	ALA	331	39.918	15.826	67.723	1.00	22.22	A
2429	C	ALA	331	38.584	13.791	67.027	1.00	23.68	A
2430	O	ALA	331	37.659	13.410	67.765	1.00	23.98	A
2431	N	SER	332	38.559	13.754	65.671	1.00	22.34	A
2432	CA	SER	332	37.361	13.275	64.986	1.00	21.43	A
2433	CB	SER	332	37.334	13.597	63.469	1.00	21.01	A
2434	OG	SER	332	37.614	14.946	63.212	1.00	22.05	A
2435	C	SER	332	37.186	11.789	65.222	1.00	22.98	A
2436	O	SER	332	36.098	11.271	65.497	1.00	21.41	A
2437	N	ARG	333	38.323	11.058	65.137	1.00	21.37	A
2438	CA	ARG	333	38.268	9.620	65.365	1.00	22.97	A
2439	CB	ARG	333	39.604	8.913	65.055	1.00	23.23	A
2440	CG	ARG	333	39.931	8.909	63.568	1.00	24.76	A
2441	CD	ARG	333	41.272	8.258	63.259	1.00	24.33	A
2442	NE	ARG	333	41.692	8.483	61.878	1.00	28.03	A
2443	CZ	ARG	333	41.188	7.825	60.832	1.00	25.05	A
2444	NH1	ARG	333	40.249	6.885	61.001	1.00	25.05	A
2445	NH2	ARG	333	41.568	8.043	59.568	1.00	26.62	A
2446	C	ARG	333	37.935	9.305	66.813	1.00	21.56	A
2447	O	ARG	333	37.314	8.273	67.116	1.00	19.77	A
2448	N	HIS	334	38.363	10.199	67.673	1.00	23.45	A
2449	CA	HIS	334	38.137	10.049	69.102	1.00	24.49	A
2450	ND1	HIS	334	39.373	10.257	72.270	1.00	32.33	A
2451	CG	HIS	334	38.572	10.993	71.400	1.00	29.22	A
2452	CB	HIS	334	38.881	11.104	69.907	1.00	26.66	A

2453	NE2	HIS	334	37.772	11.085	73.427	1.00	31.50	A
2454	CD2	HIS	334	37.567	11.508	72.152	1.00	30.73	A
2455	CE1	HIS	334	38.849	10.342	73.481	1.00	31.69	A
2456	C	HIS	334	36.641	10.147	69.435	1.00	22.86	A
2457	O	HIS	334	36.090	9.344	70.186	1.00	19.91	A
2458	N	VAL	335	35.895	11.125	68.906	1.00	22.31	A
2459	CA	VAL	335	34.474	11.147	69.315	1.00	21.53	A
2460	CB	VAL	335	33.777	12.523	69.238	1.00	24.33	A
2461	CG1	VAL	335	34.734	13.707	69.272	1.00	21.74	A
2462	CG2	VAL	335	32.872	12.708	68.024	1.00	23.21	A
2463	C	VAL	335	33.683	10.054	68.578	1.00	21.01	A
2464	O	VAL	335	32.677	9.556	69.084	1.00	20.79	A
2465	N	LEU	336	34.141	9.648	67.405	1.00	20.22	A
2466	CA	LEU	336	33.480	8.538	66.675	1.00	19.73	A
2467	CB	LEU	336	34.195	8.272	65.345	1.00	18.76	A
2468	CG	LEU	336	33.700	7.015	64.627	1.00	20.45	A
2469	CD2	LEU	336	34.552	6.652	63.407	1.00	21.80	A
2470	CD1	LEU	336	32.268	7.149	64.106	1.00	19.22	A
2471	C	LEU	336	33.557	7.265	67.510	1.00	19.35	A
2472	O	LEU	336	32.595	6.487	67.586	1.00	19.60	A
2473	N	SER	337	34.715	7.112	68.111	1.00	21.45	A
2474	CA	SER	337	35.045	5.950	68.934	1.00	22.61	A
2475	CB	SER	337	36.524	5.992	69.325	1.00	24.30	A
2476	OG	SER	337	36.847	4.864	70.124	1.00	24.53	A
2477	C	SER	337	34.223	5.914	70.225	1.00	21.12	A
2478	O	SER	337	33.638	4.885	70.583	1.00	21.62	A
2479	N	GLU	338	34.185	7.040	70.897	1.00	23.28	A
2480	CA	GLU	338	33.539	7.135	72.211	1.00	24.08	A
2481	CB	GLU	338	34.158	8.283	73.009	1.00	25.54	A
2482	CG	GLU	338	35.646	8.063	73.308	1.00	28.48	A
2483	CD	GLU	338	35.896	6.904	74.277	1.00	31.99	A
2484	OE1	GLU	338	34.960	6.520	75.077	1.00	32.49	A
2485	OE2	GLU	338	37.042	6.311	74.295	1.00	35.71	A
2486	C	GLU	338	32.016	7.368	72.142	1.00	24.98	A
2487	O	GLU	338	31.289	7.101	73.109	1.00	22.51	A
2488	N	TYR	339	31.510	7.851	71.012	1.00	22.37	A
2489	CA	TYR	339	30.068	8.187	70.920	1.00	21.48	A
2490	CB	TYR	339	29.868	9.700	70.855	1.00	22.32	A
2491	CG	TYR	339	30.391	10.422	72.084	1.00	22.93	A
2492	CD1	TYR	339	31.653	11.018	72.053	1.00	23.01	A
2493	CD2	TYR	339	29.604	10.485	73.235	1.00	22.61	A
2494	CE1	TYR	339	32.139	11.673	73.187	1.00	24.15	A
2495	CE2	TYR	339	30.091	11.137	74.370	1.00	25.87	A
2496	CZ	TYR	339	31.359	11.729	74.347	1.00	24.94	A
2497	OH	TYR	339	31.830	12.360	75.453	1.00	25.61	A
2498	C	TYR	339	29.354	7.673	69.667	1.00	21.23	A
2499	O	TYR	339	28.117	7.599	69.632	1.00	21.39	A
2500	N	GLY	340	30.114	7.335	68.654	1.00	20.88	A
2501	CA	GLY	340	29.532	6.927	67.362	1.00	18.86	A
2502	C	GLY	340	29.198	8.210	66.595	1.00	18.29	A
2503	O	GLY	340	29.529	9.317	67.031	1.00	16.14	A
2504	N	ASN	341	28.557	8.071	65.457	1.00	18.02	A

2505	CA	ASN	341	28.178	9.237	64.631	1.00	16.44	A
2506	CB	ASN	341	27.851	8.744	63.203	1.00	16.49	A
2507	CG	ASN	341	27.258	9.802	62.246	1.00	19.40	A
2508	OD1	ASN	341	26.919	10.909	62.657	1.00	16.32	A
2509	ND2	ASN	341	27.112	9.512	60.958	1.00	17.00	A
2510	C	ASN	341	26.946	9.900	65.254	1.00	15.55	A
2511	O	ASN	341	25.865	9.327	65.169	1.00	17.14	A
2512	N	LEU	342	27.075	11.088	65.794	1.00	15.07	A
2513	CA	LEU	342	26.022	11.805	66.477	1.00	16.85	A
2514	CB	LEU	342	26.592	12.599	67.636	1.00	16.75	A
2515	CG	LEU	342	27.392	11.768	68.685	1.00	18.49	A
2516	CD2	LEU	342	26.407	11.099	69.637	1.00	16.92	A
2517	CD1	LEU	342	28.336	12.687	69.441	1.00	17.96	A
2518	C	LEU	342	25.251	12.791	65.588	1.00	16.54	A
2519	O	LEU	342	24.662	13.772	66.027	1.00	13.14	A
2520	N	ILE	343	25.253	12.490	64.282	1.00	16.77	A
2521	CA	ILE	343	24.483	13.293	63.336	1.00	16.34	A
2522	CB	ILE	343	22.976	12.937	63.360	1.00	18.49	A
2523	CG2	ILE	343	22.340	13.465	62.050	1.00	19.03	A
2524	CG1	ILE	343	22.726	11.440	63.507	1.00	18.92	A
2525	CD1	ILE	343	21.287	10.952	63.369	1.00	18.26	A
2526	C	ILE	343	24.758	14.742	63.478	1.00	13.00	A
2527	O	ILE	343	25.974	15.082	63.555	1.00	14.01	A
2528	N	SER	344	23.791	15.673	63.583	1.00	13.53	A
2529	CA	SER	344	24.153	17.063	63.587	1.00	14.89	A
2530	CB	SER	344	22.943	18.003	63.525	1.00	15.82	A
2531	OG	SER	344	22.078	17.781	64.661	1.00	14.68	A
2532	C	SER	344	24.999	17.567	64.748	1.00	16.89	A
2533	O	SER	344	25.569	18.661	64.663	1.00	13.77	A
2534	N	ALA	345	24.957	16.858	65.866	1.00	18.14	A
2535	CA	ALA	345	25.788	17.298	66.982	1.00	19.06	A
2536	CB	ALA	345	25.213	16.583	68.249	1.00	17.68	A
2537	C	ALA	345	27.233	16.820	66.881	1.00	16.99	A
2538	O	ALA	345	28.076	17.324	67.643	1.00	16.29	A
2539	N	CYS	346	27.530	15.852	66.029	1.00	15.85	A
2540	CA	CYS	346	28.821	15.219	65.984	1.00	17.48	A
2541	CB	CYS	346	28.847	14.025	65.003	1.00	16.24	A
2542	SG	CYS	346	30.177	12.841	65.409	1.00	18.64	A
2543	C	CYS	346	30.039	16.118	65.840	1.00	18.21	A
2544	O	CYS	346	30.962	16.058	66.714	1.00	16.36	A
2545	N	VAL	347	29.990	17.100	64.942	1.00	17.34	A
2546	CA	VAL	347	31.124	18.004	64.761	1.00	16.15	A
2547	CB	VAL	347	31.090	18.801	63.461	1.00	18.24	A
2548	CG1	VAL	347	31.320	17.867	62.227	1.00	16.79	A
2549	CG2	VAL	347	29.802	19.570	63.224	1.00	15.47	A
2550	C	VAL	347	31.275	18.953	65.952	1.00	17.90	A
2551	O	VAL	347	32.346	19.518	66.204	1.00	17.22	A
2552	N	LEU	348	30.182	19.204	66.681	1.00	15.91	A
2553	CA	LEU	348	30.253	20.114	67.818	1.00	17.68	A
2554	CB	LEU	348	28.876	20.665	68.165	1.00	15.93	A
2555	CG	LEU	348	28.097	21.309	67.004	1.00	17.02	A
2556	CD2	LEU	348	28.818	22.548	66.483	1.00	11.37	A

2557	CD1	LEU	348	26.677	21.632	67.473	1.00	14.02	A
2558	C	LEU	348	30.922	19.412	69.020	1.00	17.18	A
2559	O	LEU	348	31.665	20.089	69.723	1.00	18.34	A
2560	N	PHE	349	30.772	18.110	69.128	1.00	17.77	A
2561	CA	PHE	349	31.489	17.315	70.110	1.00	20.37	A
2562	CB	PHE	349	31.015	15.893	70.220	1.00	18.65	A
2563	CG	PHE	349	29.812	15.572	71.076	1.00	17.81	A
2564	CD1	PHE	349	29.953	14.617	72.071	1.00	17.47	A
2565	CD2	PHE	349	28.573	16.149	70.840	1.00	16.73	A
2566	CE1	PHE	349	28.867	14.245	72.866	1.00	18.81	A
2567	CE2	PHE	349	27.469	15.824	71.627	1.00	15.30	A
2568	CZ	PHE	349	27.627	14.882	72.611	1.00	18.64	A
2569	C	PHE	349	32.981	17.269	69.715	1.00	22.63	A
2570	O	PHE	349	33.861	17.384	70.582	1.00	22.63	A
2571	N	ILE	350	33.242	17.259	68.400	1.00	20.47	A
2572	CA	ILE	350	34.634	17.300	67.944	1.00	20.13	A
2573	CB	ILE	350	34.781	16.955	66.449	1.00	19.92	A
2574	CG2	ILE	350	36.212	17.189	65.981	1.00	21.91	A
2575	CG1	ILE	350	34.380	15.492	66.269	1.00	22.03	A
2576	CD1	ILE	350	34.185	14.955	64.863	1.00	23.33	A
2577	C	ILE	350	35.241	18.642	68.284	1.00	18.34	A
2578	O	ILE	350	36.392	18.731	68.748	1.00	20.71	A
2579	N	ILE	351	34.563	19.759	68.097	1.00	15.23	A
2580	CA	ILE	351	35.113	21.067	68.451	1.00	15.59	A
2581	CB	ILE	351	34.097	22.179	68.172	1.00	16.23	A
2582	CG2	ILE	351	34.523	23.540	68.748	1.00	14.52	A
2583	CG1	ILE	351	33.911	22.394	66.616	1.00	16.07	A
2584	CD1	ILE	351	32.700	23.304	66.417	1.00	15.18	A
2585	C	ILE	351	35.478	21.063	69.958	1.00	19.03	A
2586	O	ILE	351	36.524	21.547	70.378	1.00	17.54	A
2587	N	ASP	352	34.642	20.452	70.794	1.00	18.69	A
2588	CA	ASP	352	34.905	20.482	72.268	1.00	19.86	A
2589	CB	ASP	352	33.659	19.938	72.959	1.00	17.51	A
2590	CG	ASP	352	33.525	20.315	74.445	1.00	17.73	A
2591	OD1	ASP	352	34.064	21.359	74.764	1.00	20.03	A
2592	OD2	ASP	352	32.878	19.514	75.136	1.00	17.82	A
2593	C	ASP	352	36.104	19.593	72.585	1.00	22.16	A
2594	O	ASP	352	36.945	19.946	73.433	1.00	22.49	A
2595	N	GLU	353	36.201	18.459	71.890	1.00	20.10	A
2596	CA	GLU	353	37.297	17.530	72.035	1.00	22.22	A
2597	CB	GLU	353	37.123	16.241	71.218	1.00	23.12	A
2598	CG	GLU	353	38.322	15.323	71.138	1.00	23.80	A
2599	CD	GLU	353	38.731	14.792	72.519	1.00	25.95	A
2600	OE1	GLU	353	37.898	14.679	73.443	1.00	24.69	A
2601	OE2	GLU	353	39.914	14.463	72.701	1.00	25.95	A
2602	C	GLU	353	38.598	18.227	71.651	1.00	23.07	A
2603	O	GLU	353	39.573	18.148	72.444	1.00	24.34	A
2604	N	VAL	354	38.657	18.959	70.560	1.00	21.51	A
2605	CA	VAL	354	39.856	19.673	70.127	1.00	20.65	A
2606	CB	VAL	354	39.648	20.396	68.779	1.00	20.92	A
2607	CG1	VAL	354	40.714	21.402	68.410	1.00	18.47	A
2608	CG2	VAL	354	39.581	19.346	67.669	1.00	23.03	A

2609	C	VAL	354	40.340	20.686	71.169	1.00	22.28	A
2610	O	VAL	354	41.538	20.670	71.535	1.00	19.37	A
2611	N	ARG	355	39.451	21.570	71.612	1.00	20.07	A
2612	CA	ARG	355	39.862	22.582	72.574	1.00	24.19	A
2613	CB	ARG	355	38.877	23.731	72.704	1.00	24.81	A
2614	CG	ARG	355	37.463	23.391	73.154	1.00	23.80	A
2615	CD	ARG	355	37.299	23.779	74.644	1.00	22.79	A
2616	NE	ARG	355	36.008	23.331	75.162	1.00	19.75	A
2617	CZ	ARG	355	35.280	24.057	76.030	1.00	21.29	A
2618	NH1	ARG	355	34.110	23.545	76.472	1.00	19.74	A
2619	NH2	ARG	355	35.690	25.217	76.527	1.00	17.69	A
2620	C	ARG	355	40.188	21.966	73.940	1.00	24.08	A
2621	O	ARG	355	41.151	22.428	74.534	1.00	25.32	A
2622	N	LYS	356	39.526	20.953	74.421	1.00	25.09	A
2623	CA	LYS	356	39.799	20.338	75.708	1.00	27.74	A
2624	CB	LYS	356	38.648	19.409	76.094	1.00	27.24	A
2625	CG	LYS	356	37.390	20.203	76.475	1.00	25.79	A
2626	CD	LYS	356	36.454	19.214	77.179	1.00	29.05	A
2627	CE	LYS	356	35.190	19.974	77.619	1.00	32.78	A
2628	NZ	LYS	356	34.318	19.032	78.386	1.00	36.70	A
2629	C	LYS	356	41.121	19.569	75.655	1.00	30.43	A
2630	O	LYS	356	41.947	19.680	76.565	1.00	27.52	A
2631	N	ARG	357	41.361	18.817	74.564	1.00	31.05	A
2632	CA	ARG	357	42.621	18.093	74.421	1.00	32.46	A
2633	CB	ARG	357	42.658	17.059	73.321	1.00	36.01	A
2634	CG	ARG	357	43.890	16.170	73.277	1.00	39.76	A
2635	CD	ARG	357	44.016	15.262	74.483	1.00	43.81	A
2636	NE	ARG	357	43.568	13.887	74.253	1.00	47.60	A
2637	CZ	ARG	357	44.317	13.006	73.567	1.00	50.39	A
2638	NH1	ARG	357	45.498	13.408	73.091	1.00	50.63	A
2639	NH2	ARG	357	43.900	11.761	73.354	1.00	52.74	A
2640	C	ARG	357	43.768	19.101	74.263	1.00	31.49	A
2641	O	ARG	357	44.814	18.907	74.929	1.00	29.47	A
2642	N	SER	358	43.528	20.233	73.605	1.00	27.94	A
2643	CA	SER	358	44.568	21.220	73.356	1.00	27.83	A
2644	CB	SER	358	44.117	22.313	72.371	1.00	26.50	A
2645	OG	SER	358	43.865	21.734	71.075	1.00	25.38	A
2646	C	SER	358	45.012	21.905	74.649	1.00	31.76	A
2647	O	SER	358	46.189	22.262	74.821	1.00	30.11	A
2648	N	MET	359	44.041	22.135	75.526	1.00	33.43	A
2649	CA	MET	359	44.364	22.748	76.811	1.00	36.99	A
2650	CB	MET	359	43.176	23.519	77.375	1.00	40.55	A
2651	CG	MET	359	42.966	24.791	76.524	1.00	45.08	A
2652	SD	MET	359	41.623	25.802	77.145	1.00	52.35	A
2653	CE	MET	359	40.359	24.601	77.538	1.00	48.97	A
2654	C	MET	359	44.954	21.716	77.750	1.00	35.16	A
2655	O	MET	359	45.929	22.078	78.412	1.00	35.83	A
2656	N	ALA	360	44.537	20.467	77.757	1.00	33.81	A
2657	CA	ALA	360	45.113	19.439	78.600	1.00	34.48	A
2658	CB	ALA	360	44.333	18.138	78.562	1.00	32.76	A
2659	C	ALA	360	46.574	19.153	78.219	1.00	36.33	A
2660	O	ALA	360	47.415	18.788	79.060	1.00	36.62	A

2661	N	GLU	361	46.928	19.300	76.949	1.00	35.22	A
2662	CA	GLU	361	48.292	19.058	76.489	1.00	35.33	A
2663	CB	GLU	361	48.299	18.568	75.036	1.00	34.20	A
2664	CG	GLU	361	47.649	17.207	74.839	1.00	36.67	A
2665	CD	GLU	361	47.522	16.832	73.369	1.00	36.07	A
2666	OE1	GLU	361	47.550	17.741	72.512	1.00	36.35	A
2667	OE2	GLU	361	47.428	15.624	73.088	1.00	37.56	A
2668	C	GLU	361	49.150	20.315	76.612	1.00	34.08	A
2669	O	GLU	361	50.302	20.258	76.180	1.00	32.86	A
2670	N	GLY	362	48.604	21.464	76.988	1.00	32.03	A
2671	CA	GLY	362	49.379	22.684	77.031	1.00	32.94	A
2672	C	GLY	362	49.730	23.307	75.688	1.00	33.44	A
2673	O	GLY	362	50.705	24.087	75.585	1.00	33.68	A
2674	N	LYS	363	48.944	23.049	74.654	1.00	30.95	A
2675	CA	LYS	363	49.193	23.643	73.341	1.00	32.10	A
2676	CB	LYS	363	48.229	23.096	72.281	1.00	34.04	A
2677	CG	LYS	363	48.245	21.589	72.100	1.00	36.23	A
2678	CD	LYS	363	49.675	21.121	71.840	1.00	40.53	A
2679	CE	LYS	363	49.688	19.986	70.821	1.00	42.21	A
2680	NZ	LYS	363	51.049	19.831	70.240	1.00	43.78	A
2681	C	LYS	363	49.095	25.150	73.474	1.00	29.77	A
2682	O	LYS	363	48.453	25.687	74.384	1.00	29.55	A
2683	N	SER	364	49.667	25.870	72.534	1.00	28.95	A
2684	CA	SER	364	49.649	27.325	72.569	1.00	28.77	A
2685	CB	SER	364	50.729	27.912	71.645	1.00	29.69	A
2686	OG	SER	364	50.550	27.443	70.314	1.00	30.42	A
2687	C	SER	364	48.325	27.920	72.116	1.00	26.66	A
2688	O	SER	364	48.166	29.123	72.216	1.00	23.83	A
2689	N	THR	365	47.454	27.155	71.452	1.00	26.85	A
2690	CA	THR	365	46.173	27.691	70.993	1.00	25.37	A
2691	CB	THR	365	46.096	28.110	69.509	1.00	26.90	A
2692	OG1	THR	365	45.908	26.904	68.742	1.00	22.84	A
2693	CG2	THR	365	47.305	28.882	68.987	1.00	26.67	A
2694	C	THR	365	45.075	26.655	71.253	1.00	24.62	A
2695	O	THR	365	45.373	25.479	71.461	1.00	25.62	A
2696	N	THR	366	43.801	27.030	71.180	1.00	23.49	A
2697	CA	THR	366	42.722	26.047	71.360	1.00	24.17	A
2698	CB	THR	366	41.362	26.761	71.570	1.00	22.41	A
2699	OG1	THR	366	41.195	27.696	70.499	1.00	20.38	A
2700	CG2	THR	366	41.325	27.528	72.880	1.00	23.95	A
2701	C	THR	366	42.551	25.109	70.164	1.00	23.10	A
2702	O	THR	366	41.855	24.097	70.270	1.00	21.41	A
2703	N	GLY	367	43.239	25.382	69.057	1.00	22.88	A
2704	CA	GLY	367	43.148	24.484	67.903	1.00	22.96	A
2705	C	GLY	367	44.462	23.746	67.678	1.00	23.68	A
2706	O	GLY	367	45.163	23.892	66.672	1.00	22.45	A
2707	N	GLU	368	44.834	22.922	68.642	1.00	22.76	A
2708	CA	GLU	368	45.999	22.046	68.632	1.00	25.26	A
2709	CB	GLU	368	45.767	20.982	67.542	1.00	24.97	A
2710	CG	GLU	368	44.482	20.181	67.744	1.00	26.24	A
2711	CD	GLU	368	44.200	19.090	66.749	1.00	26.19	A
2712	OE1	GLU	368	44.799	19.074	65.643	1.00	26.16	A

2713	OE2	GLU	368	43.352	18.215	67.011	1.00	26.44	A
2714	C	GLU	368	47.336	22.762	68.438	1.00	25.87	A
2715	O	GLU	368	48.273	22.206	67.826	1.00	25.65	A
2716	N	GLY	369	47.399	24.010	68.859	1.00	25.80	A
2717	CA	GLY	369	48.594	24.836	68.723	1.00	28.34	A
2718	C	GLY	369	48.656	25.551	67.394	1.00	29.47	A
2719	O	GLY	369	49.620	26.270	67.121	1.00	30.88	A
2720	N	LEU	370	47.682	25.345	66.514	1.00	28.55	A
2721	CA	LEU	370	47.632	25.953	65.206	1.00	28.68	A
2722	CB	LEU	370	47.219	24.933	64.126	1.00	25.24	A
2723	CG	LEU	370	48.087	23.679	64.134	1.00	27.19	A
2724	CD2	LEU	370	49.529	24.028	63.719	1.00	29.09	A
2725	CD1	LEU	370	47.540	22.629	63.195	1.00	26.28	A
2726	C	LEU	370	46.665	27.127	65.176	1.00	29.14	A
2727	O	LEU	370	45.843	27.293	66.083	1.00	27.98	A
2697	N	ASP	371	46.750	27.902	64.150	0.50	29.30	A
2698	CA	ASP	371	45.960	29.126	64.033	0.50	31.31	A
2699	CB	ASP	371	46.715	30.157	63.207	0.50	32.70	A
2700	CG	ASP	371	45.933	31.454	63.035	0.50	34.21	A
2701	OD1	ASP	371	45.675	32.198	64.055	0.50	35.27	A
2702	OD2	ASP	371	45.528	31.795	61.862	0.50	35.82	A
2703	C	ASP	371	44.570	28.897	63.404	0.50	30.67	A
2704	O	ASP	371	43.543	29.244	63.998	0.50	27.92	A
2697	N	2ASP	371	46.705	27.911	64.141	0.50	28.99	A
2698	CA	2ASP	371	45.915	29.152	64.058	0.50	30.87	A
2699	CB	2ASP	371	46.688	30.233	63.325	0.50	31.47	A
2700	CG	2ASP	371	47.790	30.848	64.182	0.50	32.85	A
2701	OD	12ASP	371	48.045	30.362	65.347	0.50	33.88	A
2702	OD	22ASP	371	48.466	31.846	63.731	0.50	31.60	A
2703	C	2ASP	371	44.563	29.022	63.333	0.50	30.36	A
2704	O	2ASP	371	43.571	29.636	63.734	0.50	28.09	A
2744	N	CYS	372	44.499	28.323	62.182	1.00	31.05	A
2745	CA	CYS	372	43.222	28.150	61.491	1.00	30.84	A
2746	CB	CYS	372	43.281	28.726	60.043	1.00	34.75	A
2747	SG	CYS	372	43.230	30.538	60.118	1.00	46.77	A
2748	C	CYS	372	42.771	26.726	61.387	1.00	27.81	A
2749	O	CYS	372	43.602	25.821	61.490	1.00	27.51	A
2750	N	GLY	373	41.450	26.476	61.320	1.00	25.16	A
2751	CA	GLY	373	40.983	25.098	61.238	1.00	22.49	A
2752	C	GLY	373	39.745	25.033	60.343	1.00	22.07	A
2753	O	GLY	373	39.087	26.034	60.091	1.00	20.72	A
2754	N	VAL	374	39.481	23.816	59.886	1.00	22.47	A
2755	CA	VAL	374	38.398	23.580	58.973	1.00	22.27	A
2756	CB	VAL	374	38.881	23.065	57.564	1.00	23.26	A
2757	CG1	VAL	374	37.691	22.725	56.672	1.00	22.41	A
2758	CG2	VAL	374	39.791	24.099	56.930	1.00	20.89	A
2759	C	VAL	374	37.529	22.467	59.506	1.00	19.69	A
2760	O	VAL	374	38.008	21.392	59.810	1.00	21.40	A
2761	N	LEU	375	36.263	22.800	59.562	1.00	18.61	A
2762	CA	LEU	375	35.227	21.858	59.985	1.00	20.84	A
2763	CB	LEU	375	34.399	22.581	61.033	1.00	19.48	A
2764	CG	LEU	375	32.960	22.370	61.454	1.00	24.36	A

2765	CD2	LEU	375	32.919	21.718	62.834	1.00	22.14	A
2766	CD1	LEU	375	31.916	21.827	60.498	1.00	21.76	A
2767	C	LEU	375	34.377	21.505	58.762	1.00	17.93	A
2768	O	LEU	375	34.032	22.409	57.997	1.00	17.39	A
2769	N	PHE	376	34.069	20.233	58.631	1.00	19.38	A
2770	CA	PHE	376	33.245	19.746	57.542	1.00	20.03	A
2771	CB	PHE	376	34.008	18.709	56.672	1.00	20.69	A
2772	CG	PHE	376	35.113	19.254	55.790	1.00	20.74	A
2773	CD1	PHE	376	36.372	18.688	55.794	1.00	20.92	A
2774	CD2	PHE	376	34.850	20.293	54.922	1.00	21.20	A
2775	CE1	PHE	376	37.362	19.182	54.955	1.00	21.74	A
2776	CE2	PHE	376	35.843	20.804	54.074	1.00	21.65	A
2777	CZ	PHE	376	37.105	20.254	54.097	1.00	21.09	A
2778	C	PHE	376	32.073	18.946	58.116	1.00	18.85	A
2779	O	PHE	376	32.268	18.040	58.913	1.00	20.24	A
2780	N	GLY	377	30.907	19.186	57.573	1.00	17.84	A
2781	CA	GLY	377	29.708	18.411	57.740	1.00	17.39	A
2782	C	GLY	377	29.323	17.792	56.379	1.00	17.57	A
2783	O	GLY	377	29.396	18.495	55.368	1.00	17.23	A
2784	N	PHE	378	28.794	16.596	56.360	1.00	17.66	A
2785	CA	PHE	378	28.372	15.939	55.104	1.00	19.03	A
2786	CB	PHE	378	29.288	14.720	54.791	1.00	17.54	A
2787	CG	PHE	378	30.774	15.021	54.880	1.00	18.27	A
2788	CD1	PHE	378	31.344	15.928	53.999	1.00	19.70	A
2789	CD2	PHE	378	31.589	14.415	55.812	1.00	19.70	A
2790	CE1	PHE	378	32.702	16.237	54.051	1.00	19.69	A
2791	CE2	PHE	378	32.959	14.670	55.856	1.00	18.59	A
2792	CZ	PHE	378	33.499	15.599	54.985	1.00	19.25	A
2793	C	PHE	378	26.956	15.424	55.248	1.00	21.11	A
2794	O	PHE	378	26.691	14.692	56.206	1.00	19.64	A
2795	N	GLY	379	26.024	15.749	54.358	1.00	18.60	A
2796	CA	GLY	379	24.655	15.284	54.458	1.00	18.83	A
2797	C	GLY	379	23.975	15.169	53.088	1.00	19.23	A
2798	O	GLY	379	24.676	15.268	52.089	1.00	16.57	A
2799	N	PRO	380	22.687	14.846	53.111	1.00	19.92	A
2800	CA	PRO	380	21.945	14.539	51.903	1.00	18.57	A
2801	CD	PRO	380	21.881	14.551	54.326	1.00	17.09	A
2802	CB	PRO	380	20.519	14.257	52.418	1.00	19.08	A
2803	CG	PRO	380	20.764	13.671	53.814	1.00	20.08	A
2804	C	PRO	380	22.017	15.713	50.940	1.00	17.30	A
2805	O	PRO	380	22.112	16.861	51.324	1.00	16.43	A
2806	N	GLY	381	22.008	15.392	49.637	1.00	18.61	A
2807	CA	GLY	381	22.098	16.455	48.592	1.00	16.07	A
2808	C	GLY	381	23.079	15.812	47.579	1.00	19.93	A
2809	O	GLY	381	22.724	15.621	46.442	1.00	17.52	A
2810	N	MET	382	24.286	15.299	47.676	1.00	18.83	A
2811	CA	MET	382	25.114	15.363	48.821	1.00	21.67	A
2812	CB	MET	382	26.411	14.578	48.884	1.00	23.56	A
2813	CG	MET	382	26.037	13.128	49.240	1.00	29.90	A
2814	SD	MET	382	27.518	12.143	49.463	1.00	35.81	A
2815	CE	MET	382	28.502	13.200	50.530	1.00	31.30	A
2816	C	MET	382	25.391	16.852	49.094	1.00	20.54	A

2817	O	MET	382	25.740	17.563	48.151	1.00	19.09	A
2818	N	THR	383	25.422	17.229	50.361	1.00	16.12	A
2819	CA	THR	383	25.811	18.613	50.712	1.00	18.02	A
2820	CB	THR	383	24.769	19.341	51.545	1.00	19.74	A
2821	OG1	THR	383	23.538	19.502	50.835	1.00	19.72	A
2822	CG2	THR	383	25.173	20.731	52.001	1.00	19.59	A
2823	C	THR	383	27.086	18.606	51.564	1.00	19.79	A
2824	O	THR	383	27.168	17.778	52.534	1.00	17.85	A
2825	N	VAL	384	27.977	19.564	51.364	1.00	18.96	A
2826	CA	VAL	384	29.141	19.665	52.260	1.00	19.75	A
2827	CB	VAL	384	30.529	19.605	51.599	1.00	22.71	A
2828	CG1	VAL	384	31.692	19.729	52.581	1.00	22.63	A
2829	CG2	VAL	384	30.661	18.336	50.801	1.00	24.06	A
2830	C	VAL	384	29.020	21.048	52.896	1.00	18.08	A
2831	O	VAL	384	28.778	22.056	52.209	1.00	17.98	A
2832	N	GLU	385	29.123	21.079	54.223	1.00	14.18	A
2833	CA	GLU	385	29.202	22.419	54.848	1.00	13.89	A
2834	CB	GLU	385	28.299	22.479	56.077	1.00	15.16	A
2835	CG	GLU	385	26.828	22.363	55.676	1.00	16.58	A
2836	CD	GLU	385	26.015	23.584	55.983	1.00	15.38	A
2837	OE1	GLU	385	26.525	24.650	56.402	1.00	18.10	A
2838	OE2	GLU	385	24.794	23.421	55.817	1.00	17.03	A
2839	C	GLU	385	30.674	22.620	55.247	1.00	14.43	A
2840	O	GLU	385	31.204	21.689	55.853	1.00	17.77	A
2841	N	THR	386	31.314	23.707	54.914	1.00	15.61	A
2842	CA	THR	386	32.715	23.927	55.296	1.00	16.74	A
2843	CB	THR	386	33.586	24.168	53.992	1.00	17.73	A
2844	OG1	THR	386	33.355	22.983	53.252	1.00	16.29	A
2845	CG2	THR	386	35.063	24.191	54.418	1.00	18.77	A
2846	C	THR	386	32.855	25.164	56.150	1.00	17.03	A
2847	O	THR	386	32.420	26.231	55.696	1.00	17.70	A
2848	N	VAL	387	33.308	25.006	57.417	1.00	16.84	A
2849	CA	VAL	387	33.355	26.208	58.276	1.00	17.13	A
2850	CB	VAL	387	32.508	25.999	59.558	1.00	17.99	A
2851	CG1	VAL	387	32.637	27.193	60.514	1.00	15.01	A
2852	CG2	VAL	387	31.034	25.779	59.133	1.00	17.10	A
2853	C	VAL	387	34.809	26.463	58.678	1.00	16.46	A
2854	O	VAL	387	35.443	25.504	59.132	1.00	17.67	A
2855	N	VAL	388	35.297	27.687	58.527	1.00	16.92	A
2856	CA	VAL	388	36.665	27.944	58.972	1.00	19.66	A
2857	CB	VAL	388	37.421	28.938	58.054	1.00	19.90	A
2858	CG1	VAL	388	38.737	29.427	58.644	1.00	21.93	A
2859	CG2	VAL	388	37.676	28.243	56.695	1.00	20.21	A
2860	C	VAL	388	36.588	28.537	60.402	1.00	19.79	A
2861	O	VAL	388	35.822	29.461	60.655	1.00	17.73	A
2862	N	LEU	389	37.399	27.914	61.275	1.00	20.60	A
2863	CA	LEU	389	37.505	28.438	62.639	1.00	22.00	A
2864	CB	LEU	389	37.299	27.352	63.703	1.00	19.81	A
2865	CG	LEU	389	35.932	26.671	63.609	1.00	19.87	A
2866	CD2	LEU	389	34.804	27.686	63.712	1.00	15.50	A
2867	CD1	LEU	389	35.782	25.592	64.677	1.00	21.26	A
2868	C	LEU	389	38.914	29.027	62.848	1.00	22.61	A

2869	O	LEU	389	39.864	28.586	62.198	1.00	20.80	A
2870	N	ARG	390	38.985	30.137	63.579	1.00	21.65	A
2871	CA	ARG	390	40.274	30.670	64.007	1.00	23.48	A
2872	CB	ARG	390	40.412	32.176	63.883	1.00	24.20	A
2873	CG	ARG	390	41.852	32.677	64.157	1.00	26.37	A
2874	CD	ARG	390	41.913	34.112	63.640	1.00	33.41	A
2875	NE	ARG	390	41.855	34.138	62.177	1.00	36.49	A
2876	CZ	ARG	390	41.265	34.873	61.257	1.00	39.62	A
2877	NH1	ARG	390	41.529	34.522	59.979	1.00	40.06	A
2878	NH2	ARG	390	40.440	35.914	61.389	1.00	37.97	A
2879	C	ARG	390	40.420	30.284	65.499	1.00	23.63	A
2880	O	ARG	390	39.512	30.603	66.269	1.00	21.29	A
2881	N	SER	391	41.536	29.674	65.881	1.00	24.10	A
2882	CA	SER	391	41.746	29.309	67.293	1.00	24.53	A
2883	CB	SER	391	42.907	28.303	67.371	1.00	25.80	A
2884	OG	SER	391	44.106	29.024	67.101	1.00	25.49	A
2885	C	SER	391	42.092	30.535	68.131	1.00	24.44	A
2886	O	SER	391	42.241	31.627	67.583	1.00	22.85	A
2887	N	VAL	392	42.135	30.383	69.462	1.00	25.39	A
2888	CA	VAL	392	42.446	31.497	70.350	1.00	27.60	A
2889	CB	VAL	392	41.215	31.668	71.270	1.00	29.90	A
2890	CG1	VAL	392	41.584	32.214	72.641	1.00	31.86	A
2891	CG2	VAL	392	40.138	32.520	70.627	1.00	29.27	A
2892	C	VAL	392	43.719	31.104	71.129	1.00	28.19	A
2893	O	VAL	392	43.979	29.932	71.429	1.00	23.40	A
2894	N	ARG	393	44.605	32.061	71.379	1.00	34.51	A
2895	CA	ARG	393	45.871	31.761	72.064	1.00	41.77	A
2896	CB	ARG	393	46.813	32.969	72.070	1.00	46.60	A
2897	CG	ARG	393	47.466	33.185	70.719	1.00	53.03	A
2898	CD	ARG	393	48.179	34.530	70.632	1.00	58.41	A
2899	NE	ARG	393	48.674	34.709	69.265	1.00	63.01	A
2900	CZ	ARG	393	49.502	35.647	68.825	1.00	65.65	A
2901	NH1	ARG	393	49.991	36.596	69.618	1.00	66.46	A
2902	NH2	ARG	393	49.820	35.628	67.530	1.00	66.47	A
2903	C	ARG	393	45.641	31.358	73.525	1.00	44.97	A
2904	O	ARG	393	44.855	32.011	74.195	1.00	41.97	A
2905	N	VAL	394	46.289	30.263	73.934	1.00	48.90	A
2906	CA	VAL	394	46.116	29.830	75.336	1.00	55.03	A
2907	CB	VAL	394	46.234	28.285	75.569	1.00	54.72	A
2908	CG1	VAL	394	45.934	28.121	77.130	1.00	54.65	A
2909	CG2	VAL	394	45.001	27.594	74.873	1.00	53.65	A
2910	C	VAL	394	47.334	30.484	76.041	1.00	59.46	A
2911	O	VAL	394	48.501	30.187	75.818	1.00	60.03	A
2912	N	THR	395	46.953	31.493	76.808	1.00	64.60	A
2913	CA	THR	395	47.832	32.357	77.563	1.00	68.25	A
2914	CB	THR	395	49.039	31.639	78.196	1.00	69.16	A
2915	OG1	THR	395	48.622	30.751	79.246	1.00	68.72	A
2916	CG2	THR	395	50.000	32.654	78.802	1.00	69.44	A
2917	C	THR	395	48.231	33.576	76.731	1.00	68.88	A
2918	OT	THR	395	48.680	33.459	75.570	1.00	71.94	A
2919	OXT	THR	395	48.680	33.459	75.570	1.00	71.94	A
2920	C8	AAC	396	29.088	-0.939	53.568	1.00	30.42	A

2921	N9	AAC	396	28.436	-2.108	53.270	1.00	32.14	A
2922	C4	AAC	396	27.290	-1.711	52.572	1.00	31.69	A
2923	C5	AAC	396	27.345	-0.331	52.498	1.00	30.04	A
2924	N7	AAC	396	28.425	0.168	53.194	1.00	30.04	A
2925	N3	AAC	396	26.249	-2.559	52.247	1.00	31.41	A
2926	C2	AAC	396	25.326	-1.874	51.601	1.00	30.53	A
2927	N1	AAC	396	25.230	-0.512	51.586	1.00	29.51	A
2928	C6	AAC	396	26.161	0.334	52.104	1.00	29.32	A
2929	N6	AAC	396	26.039	1.687	52.072	1.00	27.37	A
2930	C1'	AAC	396	28.970	-3.654	53.307	1.00	32.51	A
2931	C2'	AAC	396	30.145	-4.137	52.566	1.00	34.01	A
2932	O2'	AAC	396	29.559	-4.403	51.369	1.00	34.33	A
2933	C3'	AAC	396	30.770	-5.048	53.614	1.00	33.21	A
2934	O3'	AAC	396	30.180	-6.436	53.741	1.00	35.60	A
2935	C4'	AAC	396	30.447	-4.539	55.074	1.00	32.68	A
2936	O4'	AAC	396	29.243	-3.659	54.745	1.00	31.75	A
2937	C5'	AAC	396	31.558	-3.523	55.492	1.00	33.23	A
2938	O5'	AAC	396	32.462	-3.135	54.341	1.00	34.84	A
2939	P1	AAC	396	33.757	-3.149	54.009	1.00	35.11	A
2940	O11	AAC	396	33.972	-2.682	52.617	1.00	36.07	A
2941	O12	AAC	396	34.138	-4.565	54.285	1.00	34.22	A
2942	O6	AAC	396	34.317	-2.148	55.094	1.00	33.48	A
2943	P2	AAC	396	34.629	-0.608	55.274	1.00	31.67	A
2944	O21	AAC	396	34.091	0.157	54.141	1.00	29.47	A
2945	O22	AAC	396	36.088	-0.404	55.453	1.00	31.91	A
2946	O7	AAC	396	34.078	-0.103	56.587	1.00	33.38	A
2947	CPB	AAC	396	32.613	-0.372	56.779	1.00	31.59	A
2948	CPA	AAC	396	31.930	1.012	57.138	1.00	32.98	A
2949	CP7	AAC	396	32.377	2.047	56.089	1.00	32.64	A
2950	CP9	AAC	396	32.449	1.368	58.564	1.00	32.37	A
2951	CP8	AAC	396	30.388	0.907	57.120	1.00	31.38	A
2952	OP3	AAC	396	31.895	1.652	54.775	1.00	34.88	A
2953	CP6	AAC	396	31.780	3.481	56.251	1.00	32.61	A
2954	OP2	AAC	396	32.472	4.317	56.895	1.00	30.58	A
2955	NP2	AAC	396	30.924	3.796	55.273	1.00	31.11	A
2956	CP5	AAC	396	30.358	5.220	55.331	1.00	32.05	A
2957	CP4	AAC	396	29.035	5.178	56.067	1.00	32.87	A
2958	CP3	AAC	396	28.213	6.418	55.771	1.00	32.93	A
2959	OP1	AAC	396	27.905	6.418	54.570	1.00	32.85	A
2960	NP1	AAC	396	27.858	7.297	56.675	1.00	29.26	A
2961	CP2	AAC	396	27.034	8.515	56.304	1.00	28.60	A
2962	CP1	AAC	396	25.597	8.467	56.855	1.00	30.84	A
2963	S	AAC	396	24.755	9.968	56.383	1.00	33.02	A
2964	P3	AAC	396	30.702	-7.962	53.720	1.00	35.35	A
2965	O31	AAC	396	31.571	-8.202	54.889	1.00	34.33	A
2966	O32	AAC	396	31.470	-8.265	52.484	1.00	35.06	A
2967	O33	AAC	396	29.270	-8.684	53.804	1.00	36.14	A
2968	C51	AAC	396	23.138	9.614	56.893	1.00	35.73	A
2969	C52	AAC	396	22.130	10.649	56.436	1.00	37.65	A
2970	O51	AAC	396	22.832	8.462	57.127	1.00	37.20	A
2971	C53	AAC	396	21.523	11.431	57.594	1.00	38.75	A
2972	C54	AAC	396	20.940	10.674	58.762	1.00	37.79	A

2973	O52	AAC	396	21.600	12.643	57.568	1.00	38.80	A
2974	N	GLY	20	22.008	49.110	54.402	1.00	30.13	B
2975	CA	GLY	20	20.729	49.727	54.903	1.00	23.69	B
2976	C	GLY	20	19.882	48.505	55.299	1.00	20.92	B
2977	O	GLY	20	20.366	47.374	55.403	1.00	20.99	B
2978	N	LEU	21	18.625	48.779	55.519	1.00	17.75	B
2979	CA	LEU	21	17.682	47.768	55.953	1.00	20.77	B
2980	CB	LEU	21	16.341	48.472	56.276	1.00	18.00	B
2981	CG	LEU	21	16.409	49.431	57.481	1.00	21.40	B
2982	CD2	LEU	21	16.626	48.688	58.810	1.00	22.33	B
2983	CD1	LEU	21	15.145	50.253	57.628	1.00	19.17	B
2984	C	LEU	21	17.474	46.714	54.869	1.00	22.13	B
2985	O	LEU	21	17.475	47.035	53.636	1.00	19.43	B
2986	N	ALA	22	17.267	45.485	55.356	1.00	19.59	B
2987	CA	ALA	22	16.823	44.426	54.424	1.00	20.74	B
2988	CB	ALA	22	16.533	43.123	55.166	1.00	18.92	B
2989	C	ALA	22	15.560	44.925	53.725	1.00	19.75	B
2990	O	ALA	22	14.654	45.395	54.407	1.00	17.56	B
2991	N	THR	23	15.480	44.835	52.391	1.00	18.28	B
2992	CA	THR	23	14.275	45.344	51.708	1.00	17.46	B
2993	CB	THR	23	14.750	46.493	50.788	1.00	20.38	B
2994	OG1	THR	23	15.430	47.452	51.592	1.00	16.94	B
2995	CG2	THR	23	13.662	47.179	49.971	1.00	19.14	B
2996	C	THR	23	13.654	44.271	50.813	1.00	18.33	B
2997	O	THR	23	14.392	43.481	50.195	1.00	18.10	B
2998	N	ILE	24	12.338	44.231	50.809	1.00	15.97	B
2999	CA	ILE	24	11.616	43.299	49.966	1.00	16.44	B
3000	CB	ILE	24	10.167	43.151	50.443	1.00	16.72	B
3001	CG2	ILE	24	9.347	42.355	49.421	1.00	16.82	B
3002	CG1	ILE	24	10.141	42.392	51.809	1.00	17.90	B
3003	CD1	ILE	24	8.737	42.488	52.399	1.00	14.92	B
3004	C	ILE	24	11.634	43.907	48.544	1.00	15.66	B
3005	O	ILE	24	11.206	45.046	48.453	1.00	16.75	B
3006	N	LEU	25	12.196	43.200	47.566	1.00	17.77	B
3007	CA	LEU	25	12.300	43.723	46.203	1.00	18.64	B
3008	CB	LEU	25	13.748	43.484	45.728	1.00	17.20	B
3009	CG	LEU	25	14.865	44.002	46.651	1.00	17.92	B
3010	CD2	LEU	25	14.838	45.532	46.690	1.00	17.51	B
3011	CD1	LEU	25	16.263	43.583	46.185	1.00	20.19	B
3012	C	LEU	25	11.376	43.094	45.186	1.00	19.91	B
3013	O	LEU	25	11.280	43.565	44.022	1.00	20.36	B
3014	N	ALA	26	10.742	41.976	45.526	1.00	18.68	B
3015	CA	ALA	26	9.828	41.315	44.601	1.00	18.32	B
3016	CB	ALA	26	10.581	40.597	43.452	1.00	15.20	B
3017	C	ALA	26	9.007	40.302	45.374	1.00	18.51	B
3018	O	ALA	26	9.484	39.724	46.363	1.00	18.01	B
3019	N	ILE	27	7.758	40.130	44.969	1.00	15.99	B
3020	CA	ILE	27	6.897	39.116	45.522	1.00	18.77	B
3021	CB	ILE	27	5.792	39.725	46.452	1.00	17.13	B
3022	CG2	ILE	27	4.978	38.593	47.077	1.00	18.32	B
3023	CG1	ILE	27	6.452	40.581	47.537	1.00	20.55	B
3024	CD1	ILE	27	5.551	41.593	48.206	1.00	21.37	B

3025	C	ILE	27	6.199	38.314	44.451	1.00	16.71	B
3026	O	ILE	27	5.447	38.959	43.663	1.00	19.13	B
3027	N	GLY	28	6.238	36.988	44.527	1.00	17.02	B
3028	CA	GLY	28	5.416	36.216	43.587	1.00	18.19	B
3029	C	GLY	28	4.584	35.165	44.304	1.00	21.13	B
3030	O	GLY	28	5.026	34.712	45.367	1.00	19.81	B
3031	N	THR	29	3.373	34.841	43.855	1.00	16.70	B
3032	CA	THR	29	2.547	33.832	44.503	1.00	19.55	B
3033	CB	THR	29	1.326	34.437	45.216	1.00	19.77	B
3034	OG1	THR	29	0.531	35.210	44.302	1.00	19.35	B
3035	CG2	THR	29	1.778	35.415	46.306	1.00	16.94	B
3036	C	THR	29	2.025	32.802	43.504	1.00	20.47	B
3037	O	THR	29	1.910	33.080	42.300	1.00	18.54	B
3038	N	ALA	30	1.632	31.632	43.978	1.00	18.73	B
3039	CA	ALA	30	1.112	30.563	43.133	1.00	19.51	B
3040	CB	ALA	30	2.219	29.593	42.702	1.00	16.21	B
3041	C	ALA	30	0.154	29.747	44.000	1.00	21.06	B
3042	O	ALA	30	0.300	29.656	45.242	1.00	17.27	B
3043	N	THR	31	-0.779	29.058	43.380	1.00	18.81	B
3044	CA	THR	31	-1.678	28.138	44.037	1.00	20.19	B
3045	CB	THR	31	-3.071	28.716	44.280	1.00	21.90	B
3046	OG1	THR	31	-3.684	29.108	43.030	1.00	24.53	B
3047	CG2	THR	31	-3.097	30.004	45.138	1.00	20.79	B
3048	C	THR	31	-1.860	26.921	43.132	1.00	21.99	B
3049	O	THR	31	-1.635	27.056	41.944	1.00	20.19	B
3050	N	PRO	32	-2.230	25.791	43.694	1.00	20.90	B
3051	CA	PRO	32	-2.705	24.671	42.935	1.00	20.90	B
3052	CD	PRO	32	-2.474	25.621	45.182	1.00	19.82	B
3053	CB	PRO	32	-3.136	23.641	43.982	1.00	20.86	B
3054	CG	PRO	32	-2.397	24.104	45.236	1.00	19.96	B
3055	C	PRO	32	-3.900	25.112	42.079	1.00	20.14	B
3056	O	PRO	32	-4.609	26.075	42.354	1.00	18.10	B
3057	N	PRO	33	-4.067	24.465	40.936	1.00	21.96	B
3058	CA	PRO	33	-5.117	24.826	39.982	1.00	25.39	B
3059	CD	PRO	33	-3.227	23.355	40.446	1.00	22.41	B
3060	CB	PRO	33	-4.754	23.994	38.740	1.00	24.65	B
3061	CG	PRO	33	-4.085	22.781	39.334	1.00	26.31	B
3062	C	PRO	33	-6.536	24.549	40.458	1.00	25.18	B
3063	O	PRO	33	-7.360	25.395	40.193	1.00	28.12	B
3064	N	ASN	34	-6.852	23.480	41.129	1.00	27.34	B
3065	CA	ASN	34	-8.170	23.081	41.645	1.00	30.08	B
3066	CB	ASN	34	-8.087	21.643	42.171	1.00	33.39	B
3067	CG	ASN	34	-9.127	21.074	43.106	1.00	37.83	B
3068	OD1	ASN	34	-10.314	21.422	43.003	1.00	39.25	B
3069	ND2	ASN	34	-8.801	20.176	44.064	1.00	35.81	B
3070	C	ASN	34	-8.642	24.013	42.766	1.00	30.65	B
3071	O	ASN	34	-7.999	24.199	43.797	1.00	26.27	B
3072	N	CYS	35	-9.758	24.681	42.536	1.00	28.97	B
3073	CA	CYS	35	-10.386	25.618	43.431	1.00	30.72	B
3074	CB	CYS	35	-10.683	26.843	42.553	1.00	32.78	B
3075	SG	CYS	35	-11.330	28.291	43.356	1.00	34.81	B
3076	C	CYS	35	-11.733	25.077	43.899	1.00	30.56	B

3077	O	CYS	35	-12.564	24.726	43.026	1.00	28.14	B
3078	N	VAL	36	-12.010	25.115	45.195	1.00	27.43	B
3079	CA	VAL	36	-13.350	24.723	45.675	1.00	29.87	B
3080	CB	VAL	36	-13.365	23.513	46.620	1.00	29.99	B
3081	CG1	VAL	36	-14.794	23.072	46.955	1.00	32.05	B
3082	CG2	VAL	36	-12.676	22.281	46.041	1.00	29.23	B
3083	C	VAL	36	-13.999	25.907	46.381	1.00	31.35	B
3084	O	VAL	36	-13.382	26.519	47.293	1.00	30.21	B
3085	N	ALA	37	-15.257	26.231	46.004	1.00	28.89	B
3086	CA	ALA	37	-15.946	27.341	46.634	1.00	28.81	B
3087	CB	ALA	37	-17.171	27.768	45.838	1.00	30.11	B
3088	C	ALA	37	-16.333	26.966	48.066	1.00	28.01	B
3089	O	ALA	37	-16.783	25.827	48.269	1.00	27.02	B
3090	N	GLN	38	-16.248	27.912	49.003	1.00	28.89	B
3091	CA	GLN	38	-16.540	27.550	50.409	1.00	28.43	B
3092	CB	GLN	38	-16.187	28.665	51.390	1.00	28.73	B
3093	CG	GLN	38	-16.180	28.249	52.872	1.00	27.51	B
3094	CD	GLN	38	-15.036	27.352	53.262	1.00	25.61	B
3095	OE1	GLN	38	-14.701	26.373	52.601	1.00	24.71	B
3096	NE2	GLN	38	-14.350	27.608	54.384	1.00	23.66	B
3097	C	GLN	38	-18.013	27.191	50.566	1.00	29.33	B
3098	O	GLN	38	-18.363	26.188	51.189	1.00	28.34	B
3099	N	ALA	39	-18.862	27.896	49.808	1.00	30.07	B
3100	CA	ALA	39	-20.295	27.570	49.781	1.00	32.70	B
3101	CB	ALA	39	-21.051	28.568	48.896	1.00	33.57	B
3102	C	ALA	39	-20.549	26.146	49.335	1.00	30.85	B
3103	O	ALA	39	-21.575	25.584	49.736	1.00	33.70	B
3104	N	ASP	40	-19.654	25.458	48.632	1.00	30.62	B
3105	CA	ASP	40	-19.846	24.065	48.267	1.00	29.06	B
3106	CB	ASP	40	-19.346	23.872	46.817	1.00	32.72	B
3107	CG	ASP	40	-20.099	24.688	45.790	1.00	35.29	B
3108	OD1	ASP	40	-21.243	25.084	46.048	1.00	34.36	B
3109	OD2	ASP	40	-19.515	24.952	44.704	1.00	38.39	B
3110	C	ASP	40	-19.066	23.072	49.111	1.00	27.10	B
3111	O	ASP	40	-19.184	21.847	48.934	1.00	25.64	B
3112	N	TYR	41	-18.180	23.572	49.983	1.00	26.33	B
3113	CA	TYR	41	-17.195	22.686	50.602	1.00	25.45	B
3114	CB	TYR	41	-16.073	23.513	51.318	1.00	25.80	B
3115	CG	TYR	41	-14.950	22.533	51.647	1.00	26.69	B
3116	CD1	TYR	41	-14.085	22.167	50.613	1.00	26.77	B
3117	CD2	TYR	41	-14.762	21.968	52.905	1.00	26.47	B
3118	CE1	TYR	41	-13.046	21.271	50.818	1.00	28.14	B
3119	CE2	TYR	41	-13.722	21.066	53.108	1.00	27.32	B
3120	CZ	TYR	41	-12.866	20.718	52.081	1.00	29.44	B
3121	OH	TYR	41	-11.814	19.812	52.248	1.00	28.72	B
3122	C	TYR	41	-17.755	21.608	51.498	1.00	23.95	B
3123	O	TYR	41	-17.316	20.448	51.464	1.00	24.60	B
3124	N	ALA	42	-18.755	21.934	52.316	1.00	25.56	B
3125	CA	ALA	42	-19.353	20.914	53.201	1.00	25.76	B
3126	CB	ALA	42	-20.399	21.581	54.090	1.00	23.78	B
3127	C	ALA	42	-19.950	19.750	52.450	1.00	25.97	B
3128	O	ALA	42	-19.747	18.556	52.753	1.00	25.39	B

3129	N	ASP	43	-20.672	20.055	51.369	1.00	28.67	B
3130	CA	ASP	43	-21.195	18.932	50.555	1.00	30.08	B
3131	CB	ASP	43	-22.081	19.541	49.448	1.00	33.25	B
3132	CG	ASP	43	-23.443	19.995	49.962	1.00	34.98	B
3133	OD1	ASP	43	-23.930	19.541	51.007	1.00	33.60	B
3134	OD2	ASP	43	-24.052	20.858	49.282	1.00	37.96	B
3135	C	ASP	43	-20.077	18.126	49.912	1.00	28.64	B
3136	O	ASP	43	-20.097	16.901	49.768	1.00	27.36	B
3137	N	TYR	44	-19.069	18.830	49.357	1.00	28.91	B
3138	CA	TYR	44	-17.962	18.107	48.738	1.00	29.90	B
3139	CB	TYR	44	-16.920	19.101	48.198	1.00	32.45	B
3140	CG	TYR	44	-15.594	18.433	47.876	1.00	36.36	B
3141	CD1	TYR	44	-15.510	17.544	46.812	1.00	38.54	B
3142	CD2	TYR	44	-14.450	18.690	48.616	1.00	37.35	B
3143	CE1	TYR	44	-14.303	16.943	46.499	1.00	40.28	B
3144	CE2	TYR	44	-13.243	18.088	48.318	1.00	38.41	B
3145	CZ	TYR	44	-13.180	17.217	47.251	1.00	40.38	B
3146	OH	TYR	44	-12.000	16.594	46.922	1.00	41.35	B
3147	C	TYR	44	-17.309	17.225	49.814	1.00	29.19	B
3148	O	TYR	44	-17.130	16.030	49.643	1.00	28.55	B
3149	N	TYR	45	-17.041	17.861	50.971	1.00	27.03	B
3150	CA	TYR	45	-16.320	17.107	52.017	1.00	28.04	B
3151	CB	TYR	45	-15.961	18.141	53.101	1.00	25.24	B
3152	CG	TYR	45	-15.311	17.594	54.340	1.00	25.61	B
3153	CD1	TYR	45	-13.997	17.145	54.389	1.00	22.93	B
3154	CD2	TYR	45	-16.070	17.545	55.522	1.00	26.50	B
3155	CE1	TYR	45	-13.450	16.662	55.568	1.00	24.89	B
3156	CE2	TYR	45	-15.537	17.056	56.687	1.00	25.61	B
3157	CZ	TYR	45	-14.229	16.633	56.720	1.00	25.35	B
3158	OH	TYR	45	-13.730	16.155	57.908	1.00	23.72	B
3159	C	TYR	45	-17.099	15.943	52.584	1.00	27.22	B
3160	O	TYR	45	-16.593	14.809	52.694	1.00	30.23	B
3161	N	PHE	46	-18.371	16.127	52.930	1.00	27.26	B
3162	CA	PHE	46	-19.157	14.990	53.453	1.00	28.58	B
3163	CB	PHE	46	-20.503	15.493	53.995	1.00	27.85	B
3164	CG	PHE	46	-20.284	15.803	55.472	1.00	28.38	B
3165	CD1	PHE	46	-19.704	16.990	55.864	1.00	26.34	B
3166	CD2	PHE	46	-20.516	14.804	56.398	1.00	28.14	B
3167	CE1	PHE	46	-19.442	17.225	57.225	1.00	28.56	B
3168	CE2	PHE	46	-20.251	15.026	57.754	1.00	28.29	B
3169	CZ	PHE	46	-19.667	16.226	58.153	1.00	27.36	B
3170	C	PHE	46	-19.290	13.874	52.422	1.00	29.55	B
3171	O	PHE	46	-19.223	12.708	52.785	1.00	29.91	B
3172	N	ARG	47	-19.341	14.236	51.138	1.00	29.92	B
3173	CA	ARG	47	-19.427	13.212	50.087	1.00	29.82	B
3174	CB	ARG	47	-19.768	13.867	48.727	1.00	28.68	B
3175	CG	ARG	47	-19.805	12.878	47.555	1.00	31.40	B
3176	CD	ARG	47	-20.229	13.545	46.253	1.00	28.95	B
3177	NE	ARG	47	-19.376	14.627	45.753	1.00	27.46	B
3178	CZ	ARG	47	-18.239	14.330	45.107	1.00	26.32	B
3179	NH1	ARG	47	-17.870	13.079	44.917	1.00	26.37	B
3180	NH2	ARG	47	-17.457	15.269	44.656	1.00	27.46	B

3181	C	ARG	47	-18.103	12.488	49.936	1.00	27.74	B
3182	O	ARG	47	-18.094	11.272	50.065	1.00	26.68	B
3183	N	VAL	48	-16.999	13.213	49.690	1.00	27.28	B
3184	CA	VAL	48	-15.751	12.483	49.452	1.00	28.74	B
3185	CB	VAL	48	-14.552	13.314	48.955	1.00	31.08	B
3186	CG1	VAL	48	-14.846	13.784	47.514	1.00	33.19	B
3187	CG2	VAL	48	-14.201	14.486	49.857	1.00	29.64	B
3188	C	VAL	48	-15.314	11.665	50.651	1.00	28.98	B
3189	O	VAL	48	-14.649	10.649	50.437	1.00	27.72	B
3190	N	THR	49	-15.681	12.057	51.888	1.00	27.61	B
3191	CA	THR	49	-15.250	11.197	52.992	1.00	29.14	B
3192	CB	THR	49	-14.989	12.056	54.245	1.00	28.59	B
3193	OG1	THR	49	-16.199	12.664	54.686	1.00	26.82	B
3194	CG2	THR	49	-13.963	13.139	53.910	1.00	27.89	B
3195	C	THR	49	-16.256	10.105	53.263	1.00	32.25	B
3196	O	THR	49	-16.096	9.393	54.257	1.00	31.58	B
3197	N	LYS	50	-17.316	9.954	52.453	1.00	33.83	B
3198	CA	LYS	50	-18.345	8.930	52.695	1.00	34.87	B
3199	CB	LYS	50	-17.738	7.539	52.490	1.00	38.11	B
3200	CG	LYS	50	-17.129	7.347	51.099	1.00	40.70	B
3201	CD	LYS	50	-16.452	5.998	51.021	1.00	43.30	B
3202	CE	LYS	50	-15.934	5.688	49.621	1.00	45.65	B
3203	NZ	LYS	50	-15.174	4.391	49.724	1.00	47.82	B
3204	C	LYS	50	-18.992	9.033	54.076	1.00	34.08	B
3205	O	LYS	50	-19.219	8.064	54.802	1.00	32.77	B
3206	N	SER	51	-19.385	10.260	54.426	1.00	34.52	B
3207	CA	SER	51	-19.846	10.562	55.778	1.00	35.62	B
3208	CB	SER	51	-18.856	11.573	56.414	1.00	34.18	B
3209	OG	SER	51	-17.677	10.861	56.762	1.00	34.96	B
3210	C	SER	51	-21.228	11.171	55.798	1.00	35.96	B
3211	O	SER	51	-21.654	11.789	56.778	1.00	35.28	B
3212	N	GLU	52	-21.971	10.990	54.709	1.00	38.89	B
3213	CA	GLU	52	-23.324	11.491	54.550	1.00	40.11	B
3214	CB	GLU	52	-23.888	11.133	53.179	1.00	42.33	B
3215	CG	GLU	52	-23.062	11.610	51.985	1.00	44.09	B
3216	CD	GLU	52	-23.205	13.088	51.724	1.00	44.87	B
3217	OE1	GLU	52	-23.541	13.849	52.668	1.00	46.28	B
3218	OE2	GLU	52	-22.968	13.566	50.594	1.00	45.42	B
3219	C	GLU	52	-24.241	11.004	55.662	1.00	40.31	B
3220	O	GLU	52	-25.200	11.724	55.960	1.00	40.09	B
3221	N	HIS	53	-23.973	9.890	56.338	1.00	40.63	B
3222	CA	HIS	53	-24.778	9.462	57.468	1.00	43.33	B
3223	ND1	HIS	53	-22.007	7.845	57.264	1.00	48.85	B
3224	CG	HIS	53	-23.034	7.812	58.209	1.00	48.87	B
3225	CB	HIS	53	-24.475	8.000	57.818	1.00	45.61	B
3226	NE2	HIS	53	-21.114	7.488	59.199	1.00	49.66	B
3227	CD2	HIS	53	-22.472	7.597	59.426	1.00	48.98	B
3228	CE1	HIS	53	-20.866	7.646	57.906	1.00	49.30	B
3229	C	HIS	53	-24.600	10.323	58.714	1.00	42.97	B
3230	O	HIS	53	-25.449	10.299	59.615	1.00	40.95	B
3231	N	MET	54	-23.592	11.193	58.787	1.00	42.06	B
3232	CA	MET	54	-23.458	12.143	59.895	1.00	40.37	B

3233	CB	MET	54	-21.976	12.374	60.166	1.00	39.25	B
3234	CG	MET	54	-21.129	11.124	60.065	1.00	39.07	B
3235	SD	MET	54	-19.432	11.463	60.564	1.00	39.03	B
3236	CE	MET	54	-18.719	9.834	60.604	1.00	35.38	B
3237	C	MET	54	-24.133	13.462	59.580	1.00	40.50	B
3238	O	MET	54	-23.466	14.491	59.412	1.00	39.96	B
3239	N	VAL	55	-25.469	13.469	59.515	1.00	40.70	B
3240	CA	VAL	55	-26.225	14.645	59.127	1.00	41.24	B
3241	CB	VAL	55	-27.725	14.281	58.965	1.00	42.54	B
3242	CG1	VAL	55	-28.247	13.754	60.298	1.00	43.06	B
3243	CG2	VAL	55	-28.566	15.460	58.510	1.00	41.18	B
3244	C	VAL	55	-26.083	15.834	60.050	1.00	41.69	B
3245	O	VAL	55	-26.072	16.971	59.552	1.00	41.62	B
3246	N	ASP	56	-26.044	15.625	61.365	1.00	41.89	B
3247	CA	ASP	56	-25.971	16.772	62.276	1.00	42.82	B
3248	CB	ASP	56	-26.318	16.428	63.725	1.00	43.88	B
3249	CG	ASP	56	-27.747	15.911	63.870	1.00	47.81	B
3250	OD1	ASP	56	-27.958	14.828	64.467	1.00	48.73	B
3251	OD2	ASP	56	-28.711	16.529	63.373	1.00	48.34	B
3252	C	ASP	56	-24.580	17.408	62.166	1.00	39.80	B
3253	O	ASP	56	-24.486	18.615	62.022	1.00	39.83	B
3254	N	LEU	57	-23.543	16.580	62.126	1.00	38.46	B
3255	CA	LEU	57	-22.168	17.052	61.960	1.00	36.70	B
3256	CB	LEU	57	-21.208	15.880	62.088	1.00	37.93	B
3257	CG	LEU	57	-19.852	16.167	62.727	1.00	39.44	B
3258	CD2	LEU	57	-18.891	15.025	62.463	1.00	39.45	B
3259	CD1	LEU	57	-20.011	16.406	64.231	1.00	39.49	B
3260	C	LEU	57	-21.963	17.783	60.639	1.00	33.97	B
3261	O	LEU	57	-21.405	18.892	60.616	1.00	31.33	B
3262	N	LYS	58	-22.726	17.365	59.613	1.00	33.24	B
3263	CA	LYS	58	-22.690	18.074	58.335	1.00	31.91	B
3264	CB	LYS	58	-23.447	17.288	57.253	1.00	35.05	B
3265	CG	LYS	58	-23.342	17.963	55.885	1.00	35.27	B
3266	CD	LYS	58	-23.785	17.004	54.788	1.00	36.99	B
3267	CE	LYS	58	-24.081	17.788	53.522	1.00	38.02	B
3268	NZ	LYS	58	-24.138	16.923	52.309	1.00	38.14	B
3269	C	LYS	58	-23.278	19.454	58.476	1.00	31.37	B
3270	O	LYS	58	-22.764	20.468	57.989	1.00	29.09	B
3271	N	GLU	59	-24.409	19.515	59.214	1.00	31.49	B
3272	CA	GLU	59	-25.049	20.784	59.484	1.00	31.48	B
3273	CB	GLU	59	-26.360	20.582	60.291	1.00	35.68	B
3274	CG	GLU	59	-27.406	19.802	59.503	1.00	38.94	B
3275	CD	GLU	59	-28.727	19.621	60.251	1.00	42.98	B
3276	OE1	GLU	59	-29.707	19.210	59.577	1.00	42.91	B
3277	OE2	GLU	59	-28.801	19.894	61.476	1.00	42.63	B
3278	C	GLU	59	-24.105	21.696	60.260	1.00	30.72	B
3279	O	GLU	59	-23.912	22.872	59.932	1.00	32.00	B
3280	N	LYS	60	-23.491	21.165	61.306	1.00	30.16	B
3281	CA	LYS	60	-22.491	21.947	62.046	1.00	30.01	B
3282	CB	LYS	60	-21.904	21.105	63.180	1.00	29.34	B
3283	CG	LYS	60	-20.962	21.874	64.113	1.00	32.39	B
3284	CD	LYS	60	-20.162	20.902	64.990	1.00	32.26	B

3285	CE	LYS	60	-19.334	21.694	66.003	1.00	32.30	B
3286	NZ	LYS	60	-20.240	22.234	67.082	1.00	33.44	B
3287	C	LYS	60	-21.401	22.411	61.071	1.00	28.68	B
3288	O	LYS	60	-21.051	23.593	61.041	1.00	28.77	B
3289	N	PHE	61	-20.857	21.511	60.248	1.00	28.77	B
3290	CA	PHE	61	-19.768	21.971	59.340	1.00	27.65	B
3291	CB	PHE	61	-19.149	20.737	58.667	1.00	28.31	B
3292	CG	PHE	61	-17.881	21.034	57.904	1.00	26.08	B
3293	CD1	PHE	61	-16.802	21.661	58.507	1.00	25.71	B
3294	CD2	PHE	61	-17.803	20.688	56.559	1.00	26.70	B
3295	CE1	PHE	61	-15.652	21.924	57.767	1.00	26.72	B
3296	CE2	PHE	61	-16.640	20.942	55.817	1.00	26.65	B
3297	CZ	PHE	61	-15.557	21.547	56.438	1.00	26.34	B
3298	C	PHE	61	-20.246	23.020	58.376	1.00	28.42	B
3299	O	PHE	61	-19.525	23.965	58.031	1.00	29.26	B
3300	N	LYS	62	-21.524	22.978	57.941	1.00	30.24	B
3301	CA	LYS	62	-22.085	24.038	57.103	1.00	30.16	B
3302	CB	LYS	62	-23.503	23.658	56.642	1.00	33.40	B
3303	CG	LYS	62	-23.487	22.673	55.470	1.00	37.25	B
3304	CD	LYS	62	-24.767	22.671	54.634	1.00	40.54	B
3305	CE	LYS	62	-24.615	21.717	53.443	1.00	42.98	B
3306	NZ	LYS	62	-25.897	21.037	53.065	1.00	44.54	B
3307	C	LYS	62	-22.072	25.367	57.817	1.00	29.01	B
3308	O	LYS	62	-21.648	26.436	57.326	1.00	27.79	B
3309	N	ARG	63	-22.452	25.314	59.097	1.00	28.86	B
3310	CA	ARG	63	-22.337	26.528	59.927	1.00	27.90	B
3311	CB	ARG	63	-22.897	26.276	61.337	1.00	29.43	B
3312	CG	ARG	63	-24.422	26.185	61.444	1.00	31.90	B
3313	CD	ARG	63	-24.926	26.273	62.879	1.00	30.70	B
3314	NE	ARG	63	-24.460	25.182	63.711	1.00	32.36	B
3315	CZ	ARG	63	-24.895	23.936	63.817	1.00	33.89	B
3316	NH1	ARG	63	-25.922	23.479	63.102	1.00	34.24	B
3317	NH2	ARG	63	-24.339	23.077	64.678	1.00	32.87	B
3318	C	ARG	63	-20.884	26.992	60.005	1.00	27.06	B
3319	O	ARG	63	-20.596	28.194	59.911	1.00	26.93	B
3320	N	ILE	64	-19.951	26.093	60.300	1.00	26.97	B
3321	CA	ILE	64	-18.535	26.513	60.439	1.00	26.26	B
3322	CB	ILE	64	-17.663	25.318	60.850	1.00	26.23	B
3323	CG2	ILE	64	-16.163	25.617	60.649	1.00	26.15	B
3324	CG1	ILE	64	-17.861	24.910	62.322	1.00	23.46	B
3325	CD1	ILE	64	-17.695	23.413	62.551	1.00	24.95	B
3326	C	ILE	64	-18.036	27.210	59.168	1.00	26.51	B
3327	O	ILE	64	-17.593	28.372	59.180	1.00	24.26	B
3328	N	CYS	65	-18.293	26.615	57.993	1.00	27.01	B
3329	CA	CYS	65	-17.876	27.214	56.701	1.00	27.04	B
3330	CB	CYS	65	-18.262	26.250	55.579	1.00	25.72	B
3331	SG	CYS	65	-17.351	24.706	55.530	1.00	25.28	B
3332	C	CYS	65	-18.406	28.602	56.422	1.00	29.22	B
3333	O	CYS	65	-17.714	29.576	56.015	1.00	29.00	B
3334	N	GLU	66	-19.687	28.816	56.728	1.00	31.33	B
3335	CA	GLU	66	-20.340	30.110	56.626	1.00	33.56	B
3336	CB	GLU	66	-21.838	29.998	56.951	1.00	38.70	B

3337	CG	GLU	66	-22.626	31.310	56.818	1.00	44.46	B
3338	CD	GLU	66	-22.492	32.285	58.008	1.00	48.62	B
3339	OE1	GLU	66	-22.430	31.859	59.224	1.00	50.47	B
3340	OE2	GLU	66	-22.447	33.556	57.778	1.00	51.14	B
3341	C	GLU	66	-19.693	31.168	57.526	1.00	31.74	B
3342	O	GLU	66	-19.672	32.358	57.200	1.00	32.67	B
3343	N	LYS	67	-19.155	30.746	58.648	1.00	31.14	B
3344	CA	LYS	67	-18.549	31.692	59.602	1.00	28.65	B
3345	CB	LYS	67	-18.497	31.085	61.002	1.00	29.43	B
3346	CG	LYS	67	-19.869	30.994	61.664	1.00	29.62	B
3347	CD	LYS	67	-20.304	32.306	62.313	1.00	30.86	B
3348	CE	LYS	67	-21.584	32.167	63.134	1.00	30.74	B
3349	NZ	LYS	67	-22.186	33.465	63.467	1.00	32.87	B
3350	C	LYS	67	-17.101	32.068	59.231	1.00	27.59	B
3351	O	LYS	67	-16.571	33.089	59.681	1.00	25.43	B
3352	N	THR	68	-16.463	31.256	58.407	1.00	26.27	B
3353	CA	THR	68	-15.030	31.461	58.081	1.00	24.43	B
3354	CB	THR	68	-14.459	30.287	57.286	1.00	26.33	B
3355	OG1	THR	68	-15.189	30.094	56.086	1.00	27.29	B
3356	CG2	THR	68	-14.489	28.974	58.066	1.00	25.30	B
3357	C	THR	68	-14.739	32.730	57.259	1.00	23.11	B
3358	O	THR	68	-13.604	33.223	57.234	1.00	21.42	B
3359	N	ALA	69	-15.738	33.258	56.590	1.00	20.18	B
3360	CA	ALA	69	-15.548	34.442	55.727	1.00	18.52	B
3361	CB	ALA	69	-15.085	35.649	56.546	1.00	19.83	B
3362	C	ALA	69	-14.500	34.146	54.642	1.00	18.65	B
3363	O	ALA	69	-13.726	35.027	54.240	1.00	20.80	B
3364	N	ILE	70	-14.509	32.897	54.212	1.00	18.29	B
3365	CA	ILE	70	-13.647	32.403	53.123	1.00	21.02	B
3366	CB	ILE	70	-12.964	31.092	53.536	1.00	18.84	B
3367	CG2	ILE	70	-12.215	30.419	52.383	1.00	20.42	B
3368	CG1	ILE	70	-11.932	31.266	54.651	1.00	15.48	B
3369	CD1	ILE	70	-11.397	29.933	55.184	1.00	11.80	B
3370	C	ILE	70	-14.539	32.136	51.911	1.00	22.83	B
3371	O	ILE	70	-15.544	31.424	52.006	1.00	22.84	B
3372	N	LYS	71	-14.185	32.709	50.776	1.00	25.05	B
3373	CA	LYS	71	-15.000	32.535	49.558	1.00	28.31	B
3374	CB	LYS	71	-14.842	33.714	48.602	1.00	31.87	B
3375	CG	LYS	71	-15.875	33.684	47.469	1.00	36.10	B
3376	CD	LYS	71	-16.151	35.062	46.870	1.00	39.24	B
3377	CE	LYS	71	-15.029	35.543	45.950	1.00	41.09	B
3378	NZ	LYS	71	-15.126	36.972	45.626	1.00	43.39	B
3379	C	LYS	71	-14.614	31.257	48.805	1.00	27.83	B
3380	O	LYS	71	-15.477	30.508	48.329	1.00	29.51	B
3381	N	LYS	72	-13.321	31.026	48.703	1.00	27.04	B
3382	CA	LYS	72	-12.797	29.846	47.997	1.00	25.00	B
3383	CB	LYS	72	-12.757	30.116	46.492	1.00	25.89	B
3384	CG	LYS	72	-11.981	31.385	46.138	1.00	27.61	B
3385	CD	LYS	72	-12.203	31.838	44.695	1.00	28.83	B
3386	CE	LYS	72	-10.904	32.213	43.980	1.00	31.01	B
3387	NZ	LYS	72	-10.114	33.213	44.712	1.00	27.64	B
3388	C	LYS	72	-11.383	29.522	48.473	1.00	22.26	B

3389	O	LYS	72	-10.731	30.351	49.122	1.00	20.01	B
3390	N	ARG	73	-10.968	28.315	48.123	1.00	21.60	B
3391	CA	ARG	73	-9.637	27.786	48.463	1.00	22.36	B
3392	CB	ARG	73	-9.707	26.935	49.737	1.00	22.83	B
3393	CG	ARG	73	-9.954	27.764	50.996	1.00	22.90	B
3394	CD	ARG	73	-10.971	27.134	51.947	1.00	24.84	B
3395	NE	ARG	73	-10.648	25.750	52.247	1.00	21.88	B
3396	CZ	ARG	73	-11.387	24.791	52.828	1.00	24.18	B
3397	NH1	ARG	73	-12.644	24.923	53.218	1.00	23.73	B
3398	NH2	ARG	73	-10.817	23.640	53.204	1.00	21.04	B
3399	C	ARG	73	-9.117	26.879	47.346	1.00	23.89	B
3400	O	ARG	73	-9.870	26.102	46.748	1.00	22.54	B
3401	N	TYR	74	-7.830	27.005	47.084	1.00	21.64	B
3402	CA	TYR	74	-7.151	26.146	46.106	1.00	20.49	B
3403	CB	TYR	74	-6.076	26.933	45.369	1.00	20.77	B
3404	CG	TYR	74	-6.654	28.117	44.605	1.00	23.34	B
3405	CD1	TYR	74	-6.728	29.367	45.222	1.00	22.80	B
3406	CD2	TYR	74	-7.113	27.946	43.295	1.00	22.88	B
3407	CE1	TYR	74	-7.254	30.455	44.526	1.00	23.26	B
3408	CE2	TYR	74	-7.637	29.036	42.597	1.00	24.52	B
3409	CZ	TYR	74	-7.706	30.290	43.212	1.00	23.93	B
3410	OH	TYR	74	-8.212	31.351	42.531	1.00	28.25	B
3411	C	TYR	74	-6.548	24.980	46.876	1.00	19.76	B
3412	O	TYR	74	-5.942	25.162	47.940	1.00	19.96	B
3413	N	LEU	75	-6.730	23.797	46.339	1.00	17.38	B
3414	CA	LEU	75	-6.272	22.579	47.011	1.00	21.26	B
3415	CB	LEU	75	-7.476	21.856	47.611	1.00	20.25	B
3416	CG	LEU	75	-8.226	22.703	48.637	1.00	22.33	B
3417	CD2	LEU	75	-7.463	22.831	49.956	1.00	23.14	B
3418	CD1	LEU	75	-9.599	22.132	48.991	1.00	22.43	B
3419	C	LEU	75	-5.587	21.627	46.043	1.00	21.70	B
3420	O	LEU	75	-6.103	21.328	44.962	1.00	23.22	B
3421	N	ALA	76	-4.429	21.157	46.464	1.00	22.49	B
3422	CA	ALA	76	-3.651	20.202	45.670	1.00	21.99	B
3423	CB	ALA	76	-2.206	20.162	46.154	1.00	21.36	B
3424	C	ALA	76	-4.281	18.802	45.783	1.00	23.24	B
3425	O	ALA	76	-4.180	17.985	44.864	1.00	22.78	B
3426	N	LEU	77	-4.914	18.554	46.929	1.00	20.26	B
3427	CA	LEU	77	-5.626	17.275	47.211	1.00	21.63	B
3428	CB	LEU	77	-6.206	17.309	48.634	1.00	21.08	B
3429	CG	LEU	77	-6.036	16.032	49.475	1.00	24.27	B
3430	CD2	LEU	77	-6.094	14.731	48.678	1.00	22.09	B
3431	CD1	LEU	77	-7.115	15.900	50.566	1.00	21.69	B
3432	C	LEU	77	-6.836	17.157	46.285	1.00	19.11	B
3433	O	LEU	77	-7.734	18.003	46.317	1.00	18.26	B
3434	N	THR	78	-6.864	16.120	45.480	1.00	21.33	B
3435	CA	THR	78	-7.988	15.904	44.551	1.00	21.80	B
3436	CB	THR	78	-7.474	15.584	43.151	1.00	20.95	B
3437	OG1	THR	78	-6.745	14.365	43.168	1.00	20.65	B
3438	CG2	THR	78	-6.546	16.664	42.592	1.00	20.30	B
3439	C	THR	78	-8.826	14.713	45.004	1.00	21.99	B
3440	O	THR	78	-8.404	13.919	45.855	1.00	17.00	B

3441	N	GLU	79	-9.997	14.621	44.412	1.00	22.12	B
3442	CA	GLU	79	-10.936	13.534	44.694	1.00	22.76	B
3443	CB	GLU	79	-12.213	13.714	43.881	1.00	24.76	B
3444	CG	GLU	79	-13.136	14.782	44.455	1.00	31.51	B
3445	CD	GLU	79	-14.507	14.796	43.788	1.00	30.88	B
3446	OE1	GLU	79	-15.170	13.698	43.658	1.00	30.99	B
3447	OE2	GLU	79	-14.999	15.906	43.357	1.00	36.51	B
3448	C	GLU	79	-10.315	12.197	44.303	1.00	21.27	B
3449	O	GLU	79	-10.510	11.178	44.977	1.00	21.71	B
3450	N	ASP	80	-9.576	12.243	43.213	1.00	20.55	B
3451	CA	ASP	80	-8.928	11.052	42.659	1.00	21.74	B
3452	CB	ASP	80	-8.315	11.365	41.300	1.00	26.25	B
3453	CG	ASP	80	-9.287	11.078	40.154	1.00	30.13	B
3454	OD1	ASP	80	-10.537	10.879	40.408	1.00	31.09	B
3455	OD2	ASP	80	-8.861	11.036	38.939	1.00	31.25	B
3456	C	ASP	80	-7.849	10.525	43.607	1.00	20.12	B
3457	O	ASP	80	-7.704	9.314	43.808	1.00	20.55	B
3458	N	TYR	81	-7.084	11.423	44.198	1.00	19.89	B
3459	CA	TYR	81	-6.031	10.988	45.123	1.00	18.16	B
3460	CB	TYR	81	-5.151	12.153	45.578	1.00	18.76	B
3461	CG	TYR	81	-3.806	11.662	46.131	1.00	17.78	B
3462	CD1	TYR	81	-2.817	11.184	45.258	1.00	17.92	B
3463	CD2	TYR	81	-3.565	11.678	47.511	1.00	20.47	B
3464	CE1	TYR	81	-1.597	10.717	45.766	1.00	20.28	B
3465	CE2	TYR	81	-2.347	11.208	48.018	1.00	17.69	B
3466	CZ	TYR	81	-1.363	10.726	47.146	1.00	19.66	B
3467	OH	TYR	81	-0.182	10.265	47.640	1.00	17.94	B
3468	C	TYR	81	-6.663	10.316	46.349	1.00	16.11	B
3469	O	TYR	81	-6.168	9.296	46.846	1.00	19.25	B
3470	N	LEU	82	-7.761	10.898	46.809	1.00	18.19	B
3471	CA	LEU	82	-8.492	10.389	47.987	1.00	21.62	B
3472	CB	LEU	82	-9.627	11.340	48.368	1.00	21.73	B
3473	CG	LEU	82	-9.140	12.596	49.100	1.00	23.08	B
3474	CD2	LEU	82	-8.426	12.291	50.419	1.00	20.64	B
3475	CD1	LEU	82	-10.277	13.555	49.459	1.00	22.06	B
3476	C	LEU	82	-9.086	9.002	47.699	1.00	24.53	B
3477	O	LEU	82	-9.129	8.125	48.571	1.00	23.60	B
3478	N	GLN	83	-9.542	8.823	46.473	1.00	24.67	B
3479	CA	GLN	83	-10.128	7.545	46.045	1.00	25.38	B
3480	CB	GLN	83	-10.772	7.691	44.664	1.00	30.84	B
3481	CG	GLN	83	-11.992	8.615	44.677	1.00	36.26	B
3482	CD	GLN	83	-12.652	8.778	43.305	1.00	41.57	B
3483	OE1	GLN	83	-12.031	8.495	42.282	1.00	42.90	B
3484	NE2	GLN	83	-13.892	9.228	43.219	1.00	40.48	B
3485	C	GLN	83	-9.036	6.473	45.993	1.00	22.06	B
3486	O	GLN	83	-9.267	5.303	46.314	1.00	19.52	B
3487	N	GLU	84	-7.856	6.909	45.591	1.00	22.33	B
3488	CA	GLU	84	-6.691	6.020	45.457	1.00	24.13	B
3489	CB	GLU	84	-5.659	6.654	44.508	1.00	29.31	B
3490	CG	GLU	84	-6.195	6.801	43.076	1.00	32.81	B
3491	CD	GLU	84	-5.261	7.533	42.093	1.00	36.95	B
3492	OE1	GLU	84	-4.152	8.052	42.493	1.00	39.75	B

3493	OE2	GLU	84	-5.591	7.629	40.844	1.00	37.73	B
3494	C	GLU	84	-6.045	5.757	46.832	1.00	23.11	B
3495	O	GLU	84	-5.334	4.766	47.030	1.00	22.74	B
3496	N	ASN	85	-6.305	6.653	47.764	1.00	20.46	B
3497	CA	ASN	85	-5.740	6.574	49.127	1.00	22.14	B
3498	CB	ASN	85	-4.637	7.635	49.246	1.00	22.52	B
3499	CG	ASN	85	-3.539	7.471	48.183	1.00	24.04	B
3500	OD1	ASN	85	-2.645	6.642	48.353	1.00	26.52	B
3501	ND2	ASN	85	-3.552	8.211	47.087	1.00	20.49	B
3502	C	ASN	85	-6.871	6.812	50.134	1.00	19.09	B
3503	O	ASN	85	-6.929	7.869	50.779	1.00	22.00	B
3504	N	PRO	86	-7.777	5.823	50.317	1.00	20.37	B
3505	CA	PRO	86	-9.004	5.986	51.119	1.00	22.52	B
3506	CD	PRO	86	-7.621	4.488	49.726	1.00	22.90	B
3507	CB	PRO	86	-9.684	4.645	51.046	1.00	22.61	B
3508	CG	PRO	86	-8.809	3.721	50.223	1.00	23.46	B
3509	C	PRO	86	-8.753	6.261	52.570	1.00	24.83	B
3510	O	PRO	86	-9.589	6.949	53.233	1.00	27.06	B
3511	N	THR	87	-7.676	5.711	53.003	1.00	24.46	B
3512	CA	THR	87	-7.224	5.756	54.379	1.00	26.64	B
3513	CB	THR	87	-5.949	4.918	54.348	1.00	28.38	B
3514	OG1	THR	87	-6.082	3.795	55.204	1.00	29.91	B
3515	CG2	THR	87	-4.696	5.683	54.699	1.00	20.93	B
3516	C	THR	87	-7.125	7.240	54.852	1.00	25.88	B
3517	O	THR	87	-7.262	7.564	56.044	1.00	25.42	B
3518	N	MET	88	-6.920	8.147	53.905	1.00	25.14	B
3519	CA	MET	88	-6.837	9.592	54.201	1.00	24.00	B
3520	CB	MET	88	-6.437	10.384	52.951	1.00	23.65	B
3521	CG	MET	88	-4.962	10.208	52.585	1.00	21.30	B
3522	SD	MET	88	-4.397	11.362	51.354	1.00	22.70	B
3523	CE	MET	88	-4.716	13.026	51.897	1.00	14.99	B
3524	C	MET	88	-8.197	10.131	54.692	1.00	26.77	B
3525	O	MET	88	-8.272	11.161	55.368	1.00	24.35	B
3526	N	CYS	89	-9.275	9.430	54.355	1.00	28.86	B
3527	CA	CYS	89	-10.634	9.881	54.742	1.00	33.14	B
3528	CB	CYS	89	-11.652	9.565	53.651	1.00	33.44	B
3529	SG	CYS	89	-11.320	10.475	52.067	1.00	33.88	B
3530	C	CYS	89	-11.138	9.210	56.035	1.00	36.39	B
3531	O	CYS	89	-12.164	9.609	56.602	1.00	36.77	B
3532	N	GLU	90	-10.429	8.193	56.493	1.00	37.83	B
3533	CA	GLU	90	-10.822	7.464	57.722	1.00	39.76	B
3534	CB	GLU	90	-10.530	5.976	57.586	1.00	41.89	B
3535	CG	GLU	90	-10.914	5.423	56.221	1.00	47.23	B
3536	CD	GLU	90	-10.194	4.122	55.885	1.00	49.56	B
3537	OE1	GLU	90	-9.423	3.567	56.757	1.00	50.81	B
3538	OE2	GLU	90	-10.364	3.581	54.730	1.00	52.36	B
3539	C	GLU	90	-10.044	7.989	58.919	1.00	39.25	B
3540	O	GLU	90	-8.825	7.797	59.023	1.00	36.90	B
3541	N	PHE	91	-10.773	8.627	59.803	1.00	39.48	B
3542	CA	PHE	91	-10.181	9.247	60.980	1.00	41.22	B
3543	CB	PHE	91	-11.257	9.705	61.962	1.00	41.26	B
3544	CG	PHE	91	-10.731	10.830	62.846	1.00	41.77	B

3545	CD1	PHE	91	-10.719	12.152	62.378	1.00	41.67	B
3546	CD2	PHE	91	-10.241	10.529	64.114	1.00	41.52	B
3547	CE1	PHE	91	-10.197	13.171	63.185	1.00	42.64	B
3548	CE2	PHE	91	-9.712	11.544	64.918	1.00	41:82	B
3549	CZ	PHE	91	-9.689	12.865	64.454	1.00	43.06	B
3550	C	PHE	91	-9.181	8.298	61.674	1.00	40.11	B
3551	O	PHE	91	-9.541	7.203	62.137	1.00	38.76	B
3552	N	MET	92	-7.964	8.810	61.669	1.00	40.90	B
3553	CA	MET	92	-6.756	8.240	62.298	1.00	42.30	B
3554	CB	MET	92	-6.922	8.184	63.809	1.00	45.50	B
3555	CG	MET	92	-6.813	9.574	64.455	1.00	48.55	B
3556	SD	MET	92	-5.374	10.491	63.932	1.00	52.06	B
3557	CE	MET	92	-5.856	11.803	62.829	1.00	50.56	B
3558	C	MET	92	-6.344	6.844	61.774	1.00	39.48	B
3559	O	MET	92	-5.652	6.078	62.462	1.00	38.76	B
3560	N	ALA	93	-6.751	6.502	60.566	1.00	33.86	B
3561	CA	ALA	93	-6.259	5.267	59.929	1.00	28.92	B
3562	CB	ALA	93	-7.151	4.893	58.740	1.00	28.58	B
3563	C	ALA	93	-4.829	5.597	59.482	1.00	24.00	B
3564	O	ALA	93	-4.475	6.779	59.352	1.00	24.33	B
3565	N	PRO	94	-3.913	4.649	59.222	1.00	23.16	B
3566	CA	PRO	94	-2.555	5.007	58.805	1.00	24.97	B
3567	CD	PRO	94	-4.177	3.214	59.313	1.00	24.94	B
3568	CB	PRO	94	-1.853	3.683	58.656	1.00	24.03	B
3569	CG	PRO	94	-2.870	2.587	58.921	1.00	25.46	B
3570	C	PRO	94	-2.618	5.644	57.448	1.00	23.80	B
3571	O	PRO	94	-3.178	5.014	56.508	1.00	22.80	B
3572	N	SER	95	-2.070	6.836	57.278	1.00	20.76	B
3573	CA	SER	95	-2.154	7.500	55.953	1.00	21.62	B
3574	CB	SER	95	-3.448	8.307	55.863	1.00	19.16	B
3575	OG	SER	95	-3.519	9.222	56.949	1.00	22.28	B
3576	C	SER	95	-0.995	8.481	55.709	1.00	20.95	B
3577	O	SER	95	-1.043	9.263	54.758	1.00	16.39	B
3578	N	LEU	96	-0.046	8.552	56.654	1.00	17.56	B
3579	CA	LEU	96	1.080	9.424	56.446	1.00	17.73	B
3580	CB	LEU	96	2.103	9.253	57.589	1.00	16.08	B
3581	CG	LEU	96	3.280	10.249	57.467	1.00	17.92	B
3582	CD2	LEU	96	4.268	9.936	58.606	1.00	18.52	B
3583	CD1	LEU	96	2.838	11.689	57.558	1.00	17.61	B
3584	C	LEU	96	1.813	9.125	55.113	1.00	16.99	B
3585	O	LEU	96	2.327	10.088	54.586	1.00	16.66	B
3586	N	ASN	97	2.105	7.878	54.759	1.00	18.09	B
3587	CA	ASN	97	2.853	7.600	53.537	1.00	18.88	B
3588	CB	ASN	97	3.082	6.088	53.331	1.00	18.39	B
3589	CG	ASN	97	3.946	5.496	54.431	1.00	19.50	B
3590	OD1	ASN	97	4.562	6.212	55.213	1.00	18.63	B
3591	ND2	ASN	97	4.066	4.178	54.433	1.00	19.87	B
3592	C	ASN	97	2.176	8.190	52.295	1.00	18.30	B
3593	O	ASN	97	2.882	8.871	51.540	1.00	17.58	B
3594	N	ALA	98	0.878	8.102	52.167	1.00	19.70	B
3595	CA	ALA	98	0.097	8.722	51.085	1.00	20.62	B
3596	CB	ALA	98	-1.383	8.349	51.171	1.00	18.93	B

3597	C	ALA	98	0.178	10.236	51.134	1.00	20.78	B
3598	O	ALA	98	0.296	10.916	50.093	1.00	18.66	B
3599	N	ARG	99	0.082	10.825	52.357	1.00	16.74	B
3600	CA	ARG	99	0.260	12.255	52.446	1.00	16.82	B
3601	CB	ARG	99	0.044	12.787	53.895	1.00	16.52	B
3602	CG	ARG	99	-1.419	12.583	54.302	1.00	20.92	B
3603	CD	ARG	99	-1.621	12.631	55.803	1.00	19.06	B
3604	NE	ARG	99	-2.864	12.011	56.311	1.00	19.61	B
3605	CZ	ARG	99	-3.997	12.693	56.318	1.00	18.62	B
3606	NH1	ARG	99	-4.087	13.931	55.823	1.00	18.56	B
3607	NH2	ARG	99	-5.079	12.123	56.851	1.00	22.65	B
3608	C	ARG	99	1.647	12.710	51.977	1.00	16.01	B
3609	O	ARG	99	1.754	13.711	51.284	1.00	15.15	B
3610	N	GLN	100	2.689	12.074	52.483	1.00	15.37	B
3611	CA	GLN	100	4.052	12.421	52.139	1.00	16.70	B
3612	CB	GLN	100	4.998	11.468	52.858	1.00	15.63	B
3613	CG	GLN	100	5.091	11.699	54.391	1.00	16.85	B
3614	CD	GLN	100	6.155	12.731	54.679	1.00	14.79	B
3615	OE1	GLN	100	7.229	12.413	55.226	1.00	19.37	B
3616	NE2	GLN	100	5.894	13.950	54.297	1.00	13.40	B
3617	C	GLN	100	4.259	12.246	50.616	1.00	19.58	B
3618	O	GLN	100	4.960	13.028	49.977	1.00	19.18	B
3619	N	ASP	101	3.674	11.182	50.061	1.00	19.09	B
3620	CA	ASP	101	3.804	10.974	48.619	1.00	23.21	B
3621	CB	ASP	101	3.140	9.653	48.219	1.00	21.63	B
3622	CG	ASP	101	4.041	8.544	48.692	1.00	23.42	B
3623	OD1	ASP	101	5.237	8.713	49.026	1.00	23.05	B
3624	OD2	ASP	101	3.570	7.417	48.716	1.00	25.55	B
3625	C	ASP	101	3.272	12.181	47.866	1.00	23.52	B
3626	O	ASP	101	3.964	12.531	46.902	1.00	27.58	B
3627	N	LEU	102	2.221	12.858	48.283	1.00	21.41	B
3628	CA	LEU	102	1.773	14.076	47.645	1.00	21.13	B
3629	CB	LEU	102	0.365	14.429	48.148	1.00	22.49	B
3630	CG	LEU	102	-0.719	14.969	47.244	1.00	25.86	B
3631	CD2	LEU	102	-0.230	15.575	45.936	1.00	22.99	B
3632	CD1	LEU	102	-1.777	15.837	47.887	1.00	23.24	B
3633	C	LEU	102	2.661	15.269	47.949	1.00	18.50	B
3634	O	LEU	102	3.124	16.027	47.084	1.00	15.10	B
3635	N	VAL	103	2.771	15.633	49.228	1.00	16.27	B
3636	CA	VAL	103	3.469	16.877	49.594	1.00	15.16	B
3637	CB	VAL	103	3.174	17.330	51.057	1.00	16.22	B
3638	CG1	VAL	103	1.664	17.503	51.115	1.00	16.14	B
3639	CG2	VAL	103	3.685	16.265	52.039	1.00	17.61	B
3640	C	VAL	103	4.969	16.889	49.413	1.00	14.13	B
3641	O	VAL	103	5.475	18.019	49.242	1.00	16.57	B
3642	N	VAL	104	5.700	15.810	49.419	1.00	13.95	B
3643	CA	VAL	104	7.159	15.836	49.257	1.00	15.98	B
3644	CB	VAL	104	7.781	14.480	49.613	1.00	18.18	B
3645	CG1	VAL	104	9.208	14.278	49.122	1.00	18.90	B
3646	CG2	VAL	104	7.778	14.409	51.183	1.00	17.37	B
3647	C	VAL	104	7.551	16.307	47.837	1.00	18.14	B
3648	O	VAL	104	8.523	17.070	47.718	1.00	16.71	B

3649	N	THR	105	6.710	16.024	46.847	1.00	14.70	B
3650	CA	THR	105	7.037	16.606	45.508	1.00	18.73	B
3651	CB	THR	105	6.757	15.551	44.420	1.00	20.56	B
3652	OG1	THR	105	5.379	15.258	44.561	1.00	22.45	B
3653	CG2	THR	105	7.455	14.225	44.640	1.00	18.83	B
3654	C	THR	105	6.171	17.837	45.343	1.00	16.87	B
3655	O	THR	105	6.590	18.911	44.917	1.00	15.67	B
3656	N	GLY	106	4.926	17.804	45.845	1.00	17.08	B
3657	CA	GLY	106	4.009	18.958	45.686	1.00	15.04	B
3658	C	GLY	106	4.554	20.276	46.177	1.00	16.72	B
3659	O	GLY	106	4.402	21.388	45.604	1.00	14.12	B
3660	N	VAL	107	5.157	20.223	47.400	1.00	14.76	B
3661	CA	VAL	107	5.493	21.467	48.096	1.00	12.62	B
3662	CB	VAL	107	5.833	21.140	49.586	1.00	13.87	B
3663	CG1	VAL	107	6.694	22.259	50.147	1.00	12.26	B
3664	CG2	VAL	107	4.536	20.989	50.402	1.00	12.29	B
3665	C	VAL	107	6.582	22.191	47.332	1.00	8.49	B
3666	O	VAL	107	6.511	23.407	47.078	1.00	11.80	B
3667	N	PRO	108	7.674	21.564	46.995	1.00	11.13	B
3668	CA	PRO	108	8.738	22.249	46.244	1.00	13.03	B
3669	CD	PRO	108	8.030	20.167	47.314	1.00	11.98	B
3670	CB	PRO	108	9.881	21.276	46.221	1.00	14.96	B
3671	CG	PRO	108	9.373	19.937	46.672	1.00	14.09	B
3672	C	PRO	108	8.248	22.686	44.846	1.00	14.75	B
3673	O	PRO	108	8.700	23.764	44.357	1.00	14.99	B
3674	N	MET	109	7.454	21.855	44.195	1.00	15.61	B
3675	CA	MET	109	6.925	22.248	42.853	1.00	18.33	B
3676	CB	MET	109	6.203	21.093	42.175	1.00	20.39	B
3677	CG	MET	109	7.038	19.955	41.666	1.00	25.95	B
3678	SD	MET	109	7.845	20.136	40.010	1.00	32.81	B
3679	CE	MET	109	7.322	21.779	39.636	1.00	9.69	B
3680	C	MET	109	6.056	23.481	42.878	1.00	17.89	B
3681	O	MET	109	6.242	24.436	42.097	1.00	17.42	B
3682	N	LEU	110	5.114	23.641	43.826	1.00	17.16	B
3683	CA	LEU	110	4.337	24.836	44.023	1.00	16.55	B
3684	CB	LEU	110	3.398	24.742	45.228	1.00	18.81	B
3685	CG	LEU	110	1.993	25.234	45.279	1.00	22.87	B
3686	CD2	LEU	110	1.598	26.372	44.346	1.00	20.44	B
3687	CD1	LEU	110	1.416	25.406	46.675	1.00	18.22	B
3688	C	LEU	110	5.252	25.999	44.394	1.00	15.66	B
3689	O	LEU	110	5.045	27.150	43.989	1.00	17.04	B
3690	N	GLY	111	6.234	25.742	45.248	1.00	13.74	B
3691	CA	GLY	111	7.166	26.840	45.661	1.00	12.36	B
3692	C	GLY	111	7.929	27.331	44.384	1.00	13.67	B
3693	O	GLY	111	8.185	28.535	44.230	1.00	14.57	B
3694	N	LYS	112	8.380	26.429	43.534	1.00	13.85	B
3695	CA	LYS	112	9.083	26.871	42.300	1.00	15.97	B
3696	CB	LYS	112	9.404	25.577	41.506	1.00	17.11	B
3697	CG	LYS	112	10.259	25.800	40.255	1.00	19.11	B
3698	CD	LYS	112	9.866	24.819	39.132	1.00	22.92	B
3699	CE	LYS	112	8.518	25.307	38.571	1.00	25.00	B
3700	NZ	LYS	112	8.040	24.390	37.463	1.00	29.56	B

3701	C	LYS	112	8.194	27.809	41.497	1.00	14.17	B
3702	O	LYS	112	8.645	28.821	40.926	1.00	16.44	B
3703	N	GLU	113	6.905	27.506	41.360	1.00	16.44	B
3704	CA	GLU	113	5.999	28.347	40.568	1.00	18.98	B
3705	CB	GLU	113	4.598	27.718	40.523	1.00	20.29	B
3706	CG	GLU	113	4.716	26.355	39.814	1.00	26.33	B
3707	CD	GLU	113	3.450	25.543	39.850	1.00	30.51	B
3708	OE1	GLU	113	2.453	26.088	40.363	1.00	32.97	B
3709	OE2	GLU	113	3.469	24.372	39.401	1.00	32.07	B
3710	C	GLU	113	5.940	29.758	41.105	1.00	18.82	B
3711	O	GLU	113	5.968	30.776	40.398	1.00	14.21	B
3712	N	ALA	114	5.826	29.871	42.452	1.00	16.47	B
3713	CA	ALA	114	5.851	31.233	43.020	1.00	15.22	B
3714	CB	ALA	114	5.549	31.121	44.535	1.00	15.63	B
3715	C	ALA	114	7.223	31.849	42.825	1.00	10.70	B
3716	O	ALA	114	7.346	33.059	42.621	1.00	13.91	B
3717	N	ALA	115	8.294	31.104	43.001	1.00	11.13	B
3718	CA	ALA	115	9.627	31.678	42.960	1.00	11.73	B
3719	CB	ALA	115	10.620	30.551	43.272	1.00	11.44	B
3720	C	ALA	115	9.995	32.188	41.534	1.00	13.25	B
3721	O	ALA	115	10.562	33.247	41.379	1.00	12.18	B
3722	N	VAL	116	9.506	31.445	40.532	1.00	14.93	B
3723	CA	VAL	116	9.740	31.963	39.142	1.00	16.26	B
3724	CB	VAL	116	9.111	30.988	38.122	1.00	17.09	B
3725	CG1	VAL	116	9.033	31.537	36.668	1.00	17.13	B
3726	CG2	VAL	116	9.980	29.733	38.100	1.00	17.69	B
3727	C	VAL	116	9.129	33.334	38.971	1.00	17.01	B
3728	O	VAL	116	9.738	34.250	38.418	1.00	18.24	B
3729	N	LYS	117	7.908	33.529	39.490	1.00	18.30	B
3730	CA	LYS	117	7.255	34.835	39.360	1.00	19.80	B
3731	CB	LYS	117	5.810	34.793	39.887	1.00	16.76	B
3732	CG	LYS	117	4.990	33.768	39.096	1.00	17.71	B
3733	CD	LYS	117	3.540	33.813	39.556	1.00	20.14	B
3734	CE	LYS	117	2.755	32.582	39.050	1.00	21.53	B
3735	NZ	LYS	117	1.364	32.553	39.597	1.00	20.89	B
3736	C	LYS	117	8.012	35.925	40.102	1.00	19.46	B
3737	O	LYS	117	8.135	37.056	39.618	1.00	18.30	B
3738	N	ALA	118	8.482	35.601	41.311	1.00	18.05	B
3739	CA	ALA	118	9.255	36.602	42.058	1.00	17.77	B
3740	CB	ALA	118	9.626	36.045	43.456	1.00	18.31	B
3741	C	ALA	118	10.523	36.964	41.288	1.00	15.24	B
3742	O	ALA	118	10.868	38.122	41.231	1.00	14.63	B
3743	N	ILE	119	11.258	36.005	40.792	1.00	14.72	B
3744	CA	ILE	119	12.501	36.173	40.069	1.00	18.19	B
3745	CB	ILE	119	13.102	34.775	39.765	1.00	17.26	B
3746	CG2	ILE	119	14.281	34.889	38.784	1.00	17.26	B
3747	CG1	ILE	119	13.654	34.186	41.096	1.00	18.79	B
3748	CD1	ILE	119	14.055	32.715	40.937	1.00	17.54	B
3749	C	ILE	119	12.289	36.979	38.760	1.00	19.59	B
3750	O	ILE	119	13.059	37.877	38.470	1.00	20.21	B
3751	N	ASP	120	11.186	36.719	38.090	1.00	20.62	B
3752	CA	ASP	120	10.810	37.469	36.882	1.00	23.17	B

3753	CB	ASP	120	9.577	36.841	36.232	1.00	21.94	B
3754	CG	ASP	120	9.936	35.591	35.463	1.00	21.88	B
3755	OD1	ASP	120	9.058	34.818	35.026	1.00	25.46	B
3756	OD2	ASP	120	11.105	35.302	35.269	1.00	22.59	B
3757	C	ASP	120	10.485	38.895	37.254	1.00	22.73	B
3758	O	ASP	120	10.885	39.814	36.555	1.00	20.95	B
3759	N	GLU	121	9.724	39.123	38.369	1.00	18.54	B
3760	CA	GLU	121	9.479	40.507	38.702	1.00	17.30	B
3761	CB	GLU	121	8.466	40.604	39.888	1.00	17.31	B
3762	CG	GLU	121	8.541	41.968	40.550	1.00	18.93	B
3763	CD	GLU	121	7.682	42.145	41.799	1.00	18.71	B
3764	OE1	GLU	121	7.084	41.230	42.354	1.00	18.98	B
3765	OE2	GLU	121	7.474	43.302	42.175	1.00	20.98	B
3766	C	GLU	121	10.790	41.200	39.005	1.00	18.89	B
3767	O	GLU	121	11.038	42.381	38.667	1.00	18.49	B
3768	N	TRP	122	11.628	40.520	39.838	1.00	20.02	B
3769	CA	TRP	122	12.885	41.167	40.274	1.00	18.53	B
3770	CB	TRP	122	13.600	40.230	41.227	1.00	15.57	B
3771	CG	TRP	122	14.963	40.579	41.739	1.00	15.73	B
3772	CD2	TRP	122	16.105	39.697	41.830	1.00	17.08	B
3773	CD1	TRP	122	15.397	41.759	42.256	1.00	15.07	B
3774	NE1	TRP	122	16.706	41.665	42.632	1.00	16.21	B
3775	CE2	TRP	122	17.162	40.416	42.388	1.00	16.20	B
3776	CE3	TRP	122	16.328	38.365	41.459	1.00	18.05	B
3777	CZ2	TRP	122	18.442	39.883	42.586	1.00	18.57	B
3778	CZ3	TRP	122	17.576	37.828	41.663	1.00	20.98	B
3779	CH2	TRP	122	18.620	38.587	42.237	1.00	20.09	B
3780	C	TRP	122	13.725	41.503	39.025	1.00	21.21	B
3781	O	TRP	122	14.425	42.510	39.032	1.00	19.09	B
3782	N	GLY	123	13.902	40.536	38.089	1.00	20.57	B
3783	CA	GLY	123	14.458	40.851	36.771	1.00	21.40	B
3784	C	GLY	123	15.940	40.632	36.651	1.00	24.57	B
3785	O	GLY	123	16.522	40.777	35.566	1.00	25.85	B
3786	N	LEU	124	16.635	40.314	37.742	1.00	20.73	B
3787	CA	LEU	124	18.065	40.067	37.759	1.00	19.80	B
3788	CB	LEU	124	18.708	40.617	39.040	1.00	21.58	B
3789	CG	LEU	124	19.051	42.117	38.993	1.00	23.70	B
3790	CD2	LEU	124	19.563	42.678	40.330	1.00	23.32	B
3791	CD1	LEU	124	17.873	42.977	38.544	1.00	24.78	B
3792	C	LEU	124	18.354	38.592	37.589	1.00	19.77	B
3793	O	LEU	124	17.457	37.799	37.853	1.00	19.79	B
3794	N	PRO	125	19.570	38.236	37.228	1.00	20.42	B
3795	CA	PRO	125	19.936	36.861	37.051	1.00	22.86	B
3796	CD	PRO	125	20.662	39.172	36.902	1.00	23.62	B
3797	CB	PRO	125	21.363	36.893	36.550	1.00	22.60	B
3798	CG	PRO	125	21.722	38.309	36.274	1.00	26.47	B
3799	C	PRO	125	19.768	36.095	38.372	1.00	22.74	B
3800	O	PRO	125	20.269	36.477	39.430	1.00	21.45	B
3801	N	LYS	126	19.305	34.852	38.295	1.00	22.24	B
3802	CA	LYS	126	19.005	33.962	39.401	1.00	22.86	B
3803	CB	LYS	126	18.124	32.803	38.957	1.00	21.06	B
3804	CG	LYS	126	18.929	31.758	38.167	1.00	23.82	B

3805	CD	LYS	126	17.961	30.789	37.457	1.00	22.32	B
3806	CE	LYS	126	18.845	29.884	36.561	1.00	22.15	B
3807	NZ	LYS	126	17.961	28.791	36.027	1.00	24.49	B
3808	C	LYS	126	20.307	33.530	40.074	1.00	22.44	B
3809	O	LYS	126	20.382	33.087	41.219	1.00	21.24	B
3771	N	SER	127	21.377	33.758	39.322	0.50	22.04	B
3772	CA	SER	127	22.744	33.422	39.735	0.50	21.83	B
3773	CB	SER	127	23.690	33.643	38.551	0.50	22.82	B
3774	OG	SER	127	25.038	33.511	38.964	0.50	23.43	B
3775	C	SER	127	23.167	34.313	40.913	0.50	21.05	B
3776	O	SER	127	24.060	33.968	41.696	0.50	19.60	B
3771	N	2SER	127	21.411	33.697	39.339	0.50	19.47	B
3772	CA	2SER	127	22.756	33.339	39.826	0.50	17.14	B
3773	CB	2SER	127	23.775	33.421	38.687	0.50	14.50	B
3774	OG	2SER	127	23.950	34.771	38.291	0.50	7.29	B
3775	C	2SER	127	23.181	34.295	40.956	0.50	18.17	B
3776	O	2SER	127	24.097	34.012	41.735	0.50	16.66	B
3822	N	LYS	128	22.533	35.469	41.031	1.00	19.04	B
3823	CA	LYS	128	22.783	36.427	42.081	1.00	20.72	B
3824	CB	LYS	128	22.502	37.849	41.671	1.00	23.49	B
3825	CG	LYS	128	23.389	38.410	40.542	1.00	30.20	B
3826	CD	LYS	128	23.026	39.874	40.340	1.00	33.60	B
3827	CE	LYS	128	23.822	40.578	39.232	1.00	37.82	B
3828	NZ	LYS	128	25.202	40.880	39.721	1.00	39.55	B
3829	C	LYS	128	21.986	36.062	43.377	1.00	21.66	B
3830	O	LYS	128	22.241	36.770	44.382	1.00	20.03	B
3831	N	ILE	129	21.230	34.978	43.388	1.00	18.10	B
3832	CA	ILE	129	20.581	34.590	44.680	1.00	16.54	B
3833	CB	ILE	129	19.316	33.782	44.401	1.00	15.71	B
3834	CG2	ILE	129	18.718	33.127	45.663	1.00	11.23	B
3835	CG1	ILE	129	18.307	34.710	43.694	1.00	13.07	B
3836	CD1	ILE	129	17.061	33.962	43.180	1.00	15.51	B
3837	C	ILE	129	21.608	33.872	45.536	1.00	16.68	B
3838	O	ILE	129	22.165	32.871	45.084	1.00	15.39	B
3839	N	THR	130	21.957	34.462	46.705	1.00	15.34	B
3840	CA	THR	130	23.024	33.843	47.513	1.00	14.69	B
3841	CB	THR	130	23.876	34.966	48.174	1.00	14.81	B
3842	OG1	THR	130	23.019	35.931	48.807	1.00	13.89	B
3843	CG2	THR	130	24.706	35.623	47.041	1.00	17.84	B
3844	C	THR	130	22.560	32.969	48.666	1.00	14.07	B
3845	O	THR	130	23.308	32.122	49.204	1.00	16.08	B
3846	N	HIS	131	21.310	33.169	49.095	1.00	15.00	B
3847	CA	HIS	131	20.714	32.452	50.195	1.00	13.80	B
3848	ND1	HIS	131	22.691	34.795	51.389	1.00	13.62	B
3849	CG	HIS	131	21.955	33.803	52.010	1.00	13.18	B
3850	CB	HIS	131	20.636	33.364	51.471	1.00	10.47	B
3851	NE2	HIS	131	23.869	34.135	53.120	1.00	13.50	B
3852	CD2	HIS	131	22.700	33.398	53.113	1.00	12.01	B
3853	CE1	HIS	131	23.806	35.011	52.079	1.00	15.38	B
3854	C	HIS	131	19.298	32.060	49.795	1.00	12.63	B
3855	O	HIS	131	18.634	32.863	49.200	1.00	13.50	B
3856	N	LEU	132	18.831	30.924	50.313	1.00	13.69	B

3857	CA	LEU	132	17.473	30.501	50.116	1.00	13.61	B
3858	CB	LEU	132	17.465	29.221	49.300	1.00	10.62	B
3859	CG	LEU	132	16.188	28.382	49.191	1.00	14.13	B
3860	CD2	LEU	132	16.455	27.089	48.383	1.00	13.36	B
3861	CD1	LEU	132	15.047	29.149	48.528	1.00	13.56	B
3862	C	LEU	132	16.859	30.046	51.484	1.00	12.52	B
3863	O	LEU	132	17.454	29.195	52.156	1.00	12.11	B
3864	N	ILE	133	15.703	30.529	51.771	1.00	14.80	B
3865	CA	ILE	133	14.955	30.109	52.986	1.00	14.31	B
3866	CB	ILE	133	14.503	31.334	53.827	1.00	13.70	B
3867	CG2	ILE	133	13.588	30.819	54.982	1.00	12.52	B
3868	CG1	ILE	133	15.708	32.115	54.373	1.00	11.45	B
3869	CD1	ILE	133	15.251	33.498	54.892	1.00	11.04	B
3870	C	ILE	133	13.698	29.400	52.468	1.00	12.62	B
3871	O	ILE	133	12.926	30.087	51.772	1.00	13.96	B
3872	N	PHE	134	13.557	28.112	52.687	1.00	11.67	B
3873	CA	PHE	134	12.387	27.393	52.260	1.00	13.85	B
3874	CB	PHE	134	12.714	26.049	51.589	1.00	12.44	B
3875	CG	PHE	134	11.558	25.525	50.779	1.00	15.70	B
3876	CD1	PHE	134	11.633	25.605	49.361	1.00	15.31	B
3877	CD2	PHE	134	10.465	24.922	51.345	1.00	13.44	B
3878	CE1	PHE	134	10.524	25.216	48.602	1.00	13.92	B
3879	CE2	PHE	134	9.372	24.541	50.599	1.00	16.57	B
3880	CZ	PHE	134	9.395	24.662	49.177	1.00	15.48	B
3881	C	PHE	134	11.600	27.049	53.534	1.00	15.97	B
3882	O	PHE	134	12.189	26.468	54.472	1.00	17.75	B
3883	N	CYS	135	10.317	27.448	53.505	1.00	15.45	B
3884	CA	CYS	135	9.525	27.205	54.713	1.00	15.67	B
3885	CB	CYS	135	9.230	28.599	55.339	1.00	13.03	B
3886	SG	CYS	135	8.086	28.444	56.781	1.00	16.09	B
3887	C	CYS	135	8.214	26.506	54.398	1.00	15.14	B
3888	O	CYS	135	7.553	26.840	53.391	1.00	14.64	B
3889	N	THR	136	7.863	25.473	55.117	1.00	13.63	B
3890	CA	THR	136	6.561	24.815	54.979	1.00	12.82	B
3891	CB	THR	136	6.643	23.692	53.922	1.00	12.52	B
3892	OG1	THR	136	5.357	23.124	53.577	1.00	11.56	B
3893	CG2	THR	136	7.466	22.493	54.370	1.00	11.76	B
3894	C	THR	136	6.142	24.172	56.325	1.00	15.90	B
3895	O	THR	136	6.981	23.951	57.241	1.00	15.74	B
3896	N	THR	137	4.918	23.685	56.351	1.00	12.71	B
3897	CA	THR	137	4.337	22.970	57.499	1.00	15.88	B
3898	CB	THR	137	3.199	23.846	58.086	1.00	16.07	B
3899	OG1	THR	137	3.652	25.180	58.268	1.00	12.64	B
3900	CG2	THR	137	2.703	23.341	59.442	1.00	17.89	B
3901	C	THR	137	3.803	21.607	57.027	1.00	16.70	B
3902	O	THR	137	3.213	20.843	57.800	1.00	15.33	B
3903	N	ALA	138	4.045	21.306	55.754	1.00	14.66	B
3904	CA	ALA	138	3.515	20.073	55.135	1.00	16.54	B
3905	CB	ALA	138	2.639	20.440	53.934	1.00	16.96	B
3906	C	ALA	138	4.617	19.108	54.641	1.00	17.90	B
3907	O	ALA	138	5.237	19.333	53.590	1.00	18.24	B
3908	N	GLY	139	4.797	18.047	55.433	1.00	16.63	B

3909	CA	GLY	139	5.744	16.930	55.156	1.00	16.95	B
3910	C	GLY	139	7.213	17.318	55.420	1.00	14.53	B
3911	O	GLY	139	7.534	18.479	55.683	1.00	15.64	B
3912	N	VAL	140	8.063	16.293	55.362	1.00	11.63	B
3913	CA	VAL	140	9.539	16.427	55.474	1.00	13.84	B
3914	CB	VAL	140	10.068	16.286	56.910	1.00	13.57	B
3915	CG1	VAL	140	9.407	17.238	57.900	1.00	14.46	B
3916	CG2	VAL	140	9.903	14.878	57.479	1.00	13.38	B
3917	C	VAL	140	10.187	15.325	54.649	1.00	12.93	B
3918	O	VAL	140	9.553	14.310	54.338	1.00	17.79	B
3919	N	ASP	141	11.436	15.542	54.315	1.00	11.30	B
3920	CA	ASP	141	12.199	14.589	53.500	1.00	12.34	B
3921	CB	ASP	141	11.666	14.626	52.064	1.00	12.43	B
3922	CG	ASP	141	12.068	13.405	51.242	1.00	15.41	B
3923	OD1	ASP	141	12.095	12.240	51.790	1.00	16.79	B
3924	OD2	ASP	141	12.381	13.541	50.000	1.00	18.27	B
3925	C	ASP	141	13.674	14.980	53.510	1.00	10.73	B
3926	O	ASP	141	14.030	16.115	53.838	1.00	13.73	B
3927	N	MET	142	14.519	14.031	53.152	1.00	12.08	B
3928	CA	MET	142	15.977	14.258	53.095	1.00	12.54	B
3929	CB	MET	142	16.665	13.534	54.250	1.00	12.42	B
3930	CG	MET	142	16.027	13.847	55.607	1.00	14.21	B
3931	SD	MET	142	16.996	13.260	56.976	1.00	17.74	B
3932	CE	MET	142	18.395	14.329	57.212	1.00	14.81	B
3933	C	MET	142	16.518	13.753	51.747	1.00	14.99	B
3934	O	MET	142	16.298	12.575	51.633	1.00	13.32	B
3935	N	PRO	143	17.168	14.569	50.956	1.00	15.48	B
3936	CA	PRO	143	17.386	15.952	50.963	1.00	14.25	B
3937	CD	PRO	143	17.681	14.048	49.648	1.00	15.23	B
3938	CB	PRO	143	17.922	16.387	49.585	1.00	15.85	B
3939	CG	PRO	143	18.496	15.137	49.018	1.00	16.12	B
3940	C	PRO	143	16.059	16.669	51.159	1.00	13.65	B
3941	O	PRO	143	15.046	16.034	50.841	1.00	13.35	B
3942	N	GLY	144	16.011	17.906	51.657	1.00	12.74	B
3943	CA	GLY	144	14.736	18.559	51.848	1.00	14.31	B
3944	C	GLY	144	14.163	19.311	50.635	1.00	16.74	B
3945	O	GLY	144	14.744	19.323	49.539	1.00	15.00	B
3946	N	ALA	145	13.024	19.963	50.870	1.00	14.69	B
3947	CA	ALA	145	12.360	20.742	49.851	1.00	16.45	B
3948	CB	ALA	145	11.001	21.327	50.283	1.00	11.78	B
3949	C	ALA	145	13.284	21.862	49.365	1.00	19.61	B
3950	O	ALA	145	13.128	22.261	48.195	1.00	16.59	B
3951	N	ASP	146	14.180	22.370	50.228	1.00	17.60	B
3952	CA	ASP	146	15.134	23.390	49.763	1.00	18.57	B
3953	CB	ASP	146	16.007	23.868	50.924	1.00	18.75	B
3954	CG	ASP	146	16.880	22.821	51.582	1.00	17.58	B
3955	OD1	ASP	146	16.448	21.685	51.824	1.00	15.16	B
3956	OD2	ASP	146	18.073	23.072	51.863	1.00	16.33	B
3957	C	ASP	146	16.048	22.859	48.646	1.00	18.92	B
3958	O	ASP	146	16.314	23.574	47.647	1.00	17.71	B
3959	N	TYR	147	16.551	21.644	48.806	1.00	18.73	B
3960	CA	TYR	147	17.408	21.022	47.785	1.00	19.64	B

3961	CB	TYR	147	17.912	19.647	48.251	1.00	20.61	B
3962	CG	TYR	147	18.494	18.797	47.138	1.00	20.41	B
3963	CD1	TYR	147	19.822	18.953	46.757	1.00	21.27	B
3964	CD2	TYR	147	17.714	17.888	46.456	1.00	20.47	B
3965	CE1	TYR	147	20.376	18.182	45.758	1.00	23.19	B
3966	CE2	TYR	147	18.229	17.143	45.413	1.00	21.89	B
3967	CZ	TYR	147	19.566	17.297	45.083	1.00	24.50	B
3968	OH	TYR	147	20.091	16.548	44.065	1.00	27.67	B
3969	C	TYR	147	16.567	20.859	46.524	1.00	19.01	B
3970	O	TYR	147	17.125	21.097	45.442	1.00	16.71	B
3971	N	GLN	148	15.339	20.338	46.702	1.00	17.26	B
3972	CA	GLN	148	14.500	20.165	45.529	1.00	17.98	B
3973	CB	GLN	148	13.155	19.513	45.800	1.00	18.27	B
3974	CG	GLN	148	13.239	18.213	46.580	1.00	18.49	B
3975	CD	GLN	148	13.942	17.102	45.857	1.00	20.89	B
3976	OE1	GLN	148	14.271	17.217	44.645	1.00	19.88	B
3977	NE2	GLN	148	14.188	15.962	46.529	1.00	17.86	B
3978	C	GLN	148	14.258	21.474	44.775	1.00	19.24	B
3979	O	GLN	148	14.315	21.503	43.516	1.00	17.75	B
3980	N	LEU	149	14.073	22.586	45.489	1.00	16.00	B
3981	CA	LEU	149	13.885	23.879	44.884	1.00	16.60	B
3982	CB	LEU	149	13.565	24.981	45.874	1.00	19.06	B
3983	CG	LEU	149	12.552	26.080	45.648	1.00	22.52	B
3984	CD2	LEU	149	11.949	26.222	44.259	1.00	18.04	B
3985	CD1	LEU	149	13.010	27.450	46.157	1.00	19.02	B
3986	C	LEU	149	15.121	24.303	44.105	1.00	17.15	B
3987	O	LEU	149	14.996	24.881	42.998	1.00	14.65	B
3988	N	VAL	150	16.318	24.197	44.657	1.00	17.09	B
3989	CA	VAL	150	17.492	24.627	43.893	1.00	20.33	B
3990	CB	VAL	150	18.833	24.701	44.611	1.00	22.76	B
3991	CG1	VAL	150	18.725	24.838	46.133	1.00	19.08	B
3992	CG2	VAL	150	19.885	23.730	44.138	1.00	23.75	B
3993	C	VAL	150	17.620	23.854	42.558	1.00	20.24	B
3994	O	VAL	150	18.023	24.474	41.566	1.00	18.63	B
3995	N	LYS	151	17.357	22.565	42.591	1.00	18.77	B
3996	CA	LYS	151	17.432	21.733	41.387	1.00	23.02	B
3997	CB	LYS	151	17.289	20.272	41.809	1.00	26.22	B
3998	CG	LYS	151	17.340	19.281	40.655	1.00	31.92	B
3999	CD	LYS	151	17.313	17.833	41.158	1.00	35.35	B
4000	CE	LYS	151	17.095	16.899	39.977	1.00	38.72	B
4001	NZ	LYS	151	16.732	15.510	40.368	1.00	40.45	B
4002	C	LYS	151	16.347	22.157	40.397	1.00	22.83	B
4003	O	LYS	151	16.602	22.340	39.197	1.00	21.60	B
4004	N	LEU	152	15.135	22.388	40.901	1.00	18.66	B
4005	CA	LEU	152	14.031	22.838	40.101	1.00	20.27	B
4006	CB	LEU	152	12.710	22.942	40.869	1.00	18.41	B
4007	CG	LEU	152	12.055	21.606	41.224	1.00	20.69	B
4008	CD2	LEU	152	11.777	20.767	39.966	1.00	20.82	B
4009	CD1	LEU	152	10.743	21.748	41.980	1.00	20.71	B
4010	C	LEU	152	14.334	24.174	39.434	1.00	20.96	B
4011	O	LEU	152	13.898	24.429	38.289	1.00	17.97	B
4012	N	LEU	153	14.860	25.139	40.188	1.00	17.62	B

4013	CA	LEU	153	15.090	26.448	39.656	1.00	18.67	B
4014	CB	LEU	153	15.113	27.525	40.772	1.00	18.54	B
4015	CG	LEU	153	13.801	27.873	41.437	1.00	21.12	B
4016	CD2	LEU	153	12.835	28.385	40.361	1.00	21.73	B
4017	CD1	LEU	153	14.086	28.944	42.521	1.00	18.00	B
4018	C	LEU	153	16.448	26.607	38.957	1.00	18.37	B
4019	O	LEU	153	16.610	27.671	38.360	1.00	16.57	B
4020	N	GLY	154	17.373	25.682	39.144	1.00	16.87	B
4021	CA	GLY	154	18.735	25.830	38.659	1.00	19.10	B
4022	C	GLY	154	19.551	26.891	39.420	1.00	21.21	B
4023	O	GLY	154	20.314	27.728	38.876	1.00	17.48	B
4024	N	LEU	155	19.371	26.925	40.779	1.00	18.68	B
4025	CA	LEU	155	20.067	27.957	41.524	1.00	16.73	B
4026	CB	LEU	155	19.511	28.195	42.947	1.00	17.33	B
4027	CG	LEU	155	18.089	28.739	42.990	1.00	18.53	B
4028	CD2	LEU	155	17.948	30.088	42.289	1.00	14.57	B
4029	CD1	LEU	155	17.592	28.954	44.424	1.00	18.35	B
4030	C	LEU	155	21.502	27.466	41.709	1.00	15.61	B
4031	O	LEU	155	21.814	26.294	41.461	1.00	15.82	B
4032	N	SER	156	22.364	28.347	42.143	1.00	16.10	B
4033	CA	SER	156	23.761	27.979	42.394	1.00	17.10	B
4034	CB	SER	156	24.503	29.164	43.010	1.00	17.29	B
4035	OG	SER	156	25.755	28.741	43.526	1.00	19.70	B
4036	C	SER	156	23.809	26.790	43.369	1.00	19.78	B
4037	O	SER	156	23.096	26.770	44.387	1.00	19.11	B
4038	N	PRO	157	24.606	25.738	43.092	1.00	20.69	B
4039	CA	PRO	157	24.751	24.620	44.010	1.00	20.98	B
4040	CD	PRO	157	25.386	25.629	41.857	1.00	24.06	B
4041	CB	PRO	157	25.663	23.656	43.289	1.00	22.99	B
4042	CG	PRO	157	26.029	24.277	41.954	1.00	26.97	B
4043	C	PRO	157	25.367	25.061	45.321	1.00	18.59	B
4044	O	PRO	157	25.312	24.278	46.321	1.00	16.51	B
4045	N	SER	158	25.931	26.262	45.315	1.00	15.55	B
4046	CA	SER	158	26.589	26.829	46.508	1.00	15.78	B
4047	CB	SER	158	27.912	27.494	46.129	1.00	16.03	B
4048	OG	SER	158	28.903	26.496	45.929	1.00	19.38	B
4049	C	SER	158	25.698	27.871	47.210	1.00	14.51	B
4050	O	SER	158	26.160	28.654	48.048	1.00	15.60	B
4051	N	VAL	159	24.418	27.891	46.868	1.00	15.32	B
4052	CA	VAL	159	23.476	28.808	47.539	1.00	16.28	B
4053	CB	VAL	159	22.115	28.783	46.845	1.00	18.85	B
4054	CG1	VAL	159	21.381	27.456	47.026	1.00	18.11	B
4055	CG2	VAL	159	21.168	29.871	47.362	1.00	18.08	B
4056	C	VAL	159	23.358	28.337	49.028	1.00	14.43	B
4057	O	VAL	159	23.384	27.162	49.311	1.00	14.48	B
4058	N	LYS	160	23.404	29.274	49.965	1.00	15.01	B
4059	CA	LYS	160	23.265	28.918	51.398	1.00	14.62	B
4060	CB	LYS	160	23.819	30.055	52.286	1.00	12.92	B
4061	CG	LYS	160	25.364	29.932	52.258	1.00	16.86	B
4062	CD	LYS	160	25.946	31.113	53.073	1.00	19.51	B
4063	CE	LYS	160	27.425	30.781	53.328	1.00	22.56	B
4064	NZ	LYS	160	28.082	31.954	54.012	1.00	23.85	B

4065	C	LYS	160	21.809	28.709	51.739	1.00	11.89	B
4066	O	LYS	160	21.015	29.592	51.502	1.00	16.13	B
4067	N	ARG	161	21.442	27.560	52.268	1.00	13.89	B
4068	CA	ARG	161	20.056	27.201	52.491	1.00	13.32	B
4069	CB	ARG	161	19.838	25.813	51.845	1.00	15.41	B
4070	CG	ARG	161	20.039	25.987	50.298	1.00	14.72	B
4071	CD	ARG	161	19.982	24.565	49.751	1.00	17.76	B
4072	NE	ARG	161	21.232	23.881	49.799	1.00	18.42	B
4073	CZ	ARG	161	21.439	22.631	50.214	1.00	19.63	B
4074	NH1	ARG	161	20.545	21.803	50.732	1.00	19.49	B
4075	NH2	ARG	161	22.679	22.215	50.091	1.00	17.19	B
4076	C	ARG	161	19.645	27.069	53.960	1.00	15.16	B
4077	O	ARG	161	20.500	26.898	54.811	1.00	13.02	B
4078	N	TYR	162	18.384	27.386	54.235	1.00	14.69	B
4079	CA	TYR	162	17.778	27.412	55.579	1.00	15.19	B
4080	CB	TYR	162	17.548	28.876	56.044	1.00	12.87	B
4081	CG	TYR	162	18.884	29.590	56.047	1.00	17.46	B
4082	CD1	TYR	162	19.346	30.166	54.832	1.00	18.22	B
4083	CD2	TYR	162	19.743	29.587	57.114	1.00	15.37	B
4084	CE1	TYR	162	20.636	30.675	54.725	1.00	18.15	B
4085	CE2	TYR	162	20.998	30.152	57.047	1.00	18.00	B
4086	CZ	TYR	162	21.457	30.678	55.838	1.00	18.75	B
4087	OH	TYR	162	22.718	31.197	55.742	1.00	15.82	B
4088	C	TYR	162	16.477	26.633	55.469	1.00	12.63	B
4089	O	TYR	162	15.534	27.175	54.891	1.00	12.26	B
4090	N	MET	163	16.504	25.347	55.794	1.00	11.79	B
4091	CA	MET	163	15.323	24.518	55.566	1.00	10.61	B
4092	CB	MET	163	15.736	23.119	55.177	1.00	11.00	B
4093	CG	MET	163	14.681	22.041	54.967	1.00	13.38	B
4094	SD	MET	163	13.633	22.462	53.513	1.00	14.69	B
4095	CE	MET	163	12.076	22.822	54.259	1.00	15.70	B
4096	C	MET	163	14.426	24.539	56.819	1.00	13.04	B
4097	O	MET	163	14.803	23.911	57.803	1.00	10.67	B
4098	N	LEU	164	13.322	25.245	56.711	1.00	10.75	B
4099	CA	LEU	164	12.401	25.344	57.836	1.00	13.62	B
4100	CB	LEU	164	12.033	26.797	57.972	1.00	9.42	B
4101	CG	LEU	164	13.204	27.778	57.991	1.00	11.22	B
4102	CD2	LEU	164	14.160	27.441	59.168	1.00	11.90	B
4103	CD1	LEU	164	12.699	29.208	58.119	1.00	12.06	B
4104	C	LEU	164	11.181	24.457	57.667	1.00	13.25	B
4105	O	LEU	164	10.297	24.801	56.870	1.00	14.17	B
4106	N	TYR	165	11.170	23.345	58.378	1.00	11.58	B
4107	CA	TYR	165	10.071	22.417	58.360	1.00	12.91	B
4108	CB	TYR	165	10.715	21.024	58.356	1.00	14.17	B
4109	CG	TYR	165	10.993	20.431	56.983	1.00	16.40	B
4110	CD1	TYR	165	10.019	20.425	55.997	1.00	14.42	B
4111	CD2	TYR	165	12.233	19.860	56.727	1.00	15.87	B
4112	CE1	TYR	165	10.306	19.865	54.749	1.00	15.74	B
4113	CE2	TYR	165	12.515	19.284	55.511	1.00	17.46	B
4114	CZ	TYR	165	11.536	19.303	54.522	1.00	16.09	B
4115	OH	TYR	165	11.844	18.754	53.306	1.00	15.51	B
4116	C	TYR	165	9.179	22.465	59.639	1.00	15.72	B

4117	O	TYR	165	9.624	22.937	60.669	1.00	14.13	B
4118	N	GLN	166	7.953	22.041	59.464	1.00	15.27	B
4119	CA	GLN	166	6.925	21.948	60.475	1.00	16.47	B
4120	CB	GLN	166	7.300	20.779	61.448	1.00	17.57	B
4121	CG	GLN	166	6.035	20.172	62.121	1.00	15.02	B
4122	CD	GLN	166	5.209	19.481	61.039	1.00	19.41	B
4123	OE1	GLN	166	3.974	19.675	60.933	1.00	23.78	B
4124	NE2	GLN	166	5.823	18.751	60.159	1.00	14.10	B
4125	C	GLN	166	6.779	23.277	61.172	1.00	17.19	B
4126	O	GLN	166	6.732	23.328	62.400	1.00	17.83	B
4127	N	GLN	167	6.599	24.364	60.416	1.00	15.33	B
4128	CA	GLN	167	6.768	25.691	60.950	1.00	14.50	B
4129	CB	GLN	167	7.478	26.633	59.969	1.00	13.31	B
4130	CG	GLN	167	8.910	26.209	59.712	1.00	12.29	B
4131	CD	GLN	167	9.882	26.490	60.882	1.00	14.10	B
4132	OE1	GLN	167	9.991	27.627	61.346	1.00	16.04	B
4133	NE2	GLN	167	10.684	25.468	61.202	1.00	14.15	B
4134	C	GLN	167	5.469	26.312	61.429	1.00	17.24	B
4135	O	GLN	167	5.526	27.061	62.431	1.00	17.67	B
4136	N	GLY	168	4.351	26.064	60.787	1.00	14.58	B
4137	CA	GLY	168	3.075	26.597	61.180	1.00	13.86	B
4138	C	GLY	168	2.876	28.061	60.889	1.00	14.55	B
4139	O	GLY	168	3.556	28.794	60.162	1.00	14.79	B
4140	N	CSD	169	1.679	28.595	61.368	1.00	14.63	B
4141	CA	CSD	169	1.151	29.891	61.068	1.00	15.32	B
4142	CB	CSD	169	-0.314	30.034	61.451	1.00	15.26	B
4143	SG	CSD	169	-1.445	28.797	60.749	1.00	18.83	B
4144	C	CSD	169	1.842	31.150	61.523	1.00	16.05	B
4145	O	CSD	169	1.478	32.204	60.949	1.00	19.74	B
4146	OD1	CSD	169	-2.304	29.596	61.102	1.00	29.98	B
4147	OD2	CSD	169	-1.735	27.340	61.201	1.00	29.91	B
4148	N	ALA	170	2.841	31.159	62.375	1.00	14.11	B
4149	CA	ALA	170	3.557	32.429	62.584	1.00	15.04	B
4150	CB	ALA	170	4.094	32.429	64.055	1.00	12.79	B
4151	C	ALA	170	4.749	32.582	61.636	1.00	12.99	B
4152	O	ALA	170	5.405	33.630	61.710	1.00	12.65	B
4153	N	ALA	171	5.062	31.549	60.824	1.00	12.80	B
4154	CA	ALA	171	6.321	31.472	60.150	1.00	13.82	B
4155	CB	ALA	171	6.710	30.063	59.688	1.00	13.84	B
4156	C	ALA	171	6.520	32.369	58.919	1.00	12.96	B
4157	O	ALA	171	7.665	32.562	58.496	1.00	14.95	B
4158	N	GLY	172	5.494	33.072	58.472	1.00	13.38	B
4159	CA	GLY	172	5.613	34.140	57.526	1.00	14.64	B
4160	C	GLY	172	6.401	35.275	58.204	1.00	17.82	B
4161	O	GLY	172	7.195	35.990	57.566	1.00	15.56	B
4162	N	GLY	173	6.159	35.494	59.531	1.00	14.07	B
4163	CA	GLY	173	7.035	36.391	60.271	1.00	13.12	B
4164	C	GLY	173	8.426	35.844	60.453	1.00	13.41	B
4165	O	GLY	173	9.432	36.571	60.226	1.00	13.75	B
4166	N	THR	174	8.518	34.516	60.695	1.00	13.80	B
4167	CA	THR	174	9.851	33.931	60.889	1.00	16.34	B
4168	CB	THR	174	9.705	32.413	61.072	1.00	16.10	B

4169	OG1	THR	174	8.763	32.177	62.132	1.00	16.09	B
4170	CG2	THR	174	11.005	31.719	61.429	1.00	13.71	B
4171	C	THR	174	10.743	34.166	59.656	1.00	15.77	B
4172	O	THR	174	11.950	34.449	59.778	1.00	12.21	B
4173	N	VAL	175	10.135	33.979	58.440	1.00	14.73	B
4174	CA	VAL	175	11.040	34.031	57.264	1.00	12.67	B
4175	CB	VAL	175	10.428	33.481	55.984	1.00	9.99	B
4176	CG1	VAL	175	10.131	31.981	56.153	1.00	8.69	B
4177	CG2	VAL	175	9.074	34.126	55.663	1.00	7.67	B
4178	C	VAL	175	11.567	35.457	57.107	1.00	10.97	B
4179	O	VAL	175	12.715	35.616	56.683	1.00	14.18	B
4180	N	LEU	176	10.744	36.452	57.348	1.00	11.34	B
4181	CA	LEU	176	11.146	37.852	57.284	1.00	14.55	B
4182	CB	LEU	176	9.932	38.748	57.449	1.00	16.10	B
4183	CG	LEU	176	8.851	38.597	56.357	1.00	20.08	B
4184	CD2	LEU	176	9.477	38.939	55.004	1.00	20.87	B
4185	CD1	LEU	176	7.659	39.490	56.615	1.00	18.48	B
4186	C	LEU	176	12.204	38.154	58.334	1.00	14.60	B
4187	O	LEU	176	13.225	38.814	58.052	1.00	13.72	B
4188	N	ARG	177	11.989	37.637	59.562	1.00	14.11	B
4189	CA	ARG	177	13.035	37.819	60.615	1.00	11.32	B
4190	CB	ARG	177	12.440	37.125	61.879	1.00	11.84	B
4191	CG	ARG	177	13.463	37.052	63.039	1.00	10.17	B
4192	CD	ARG	177	12.575	36.798	64.308	1.00	10.62	B
4193	NE	ARG	177	11.849	35.547	64.299	1.00	9.67	B
4194	CZ	ARG	177	12.308	34.343	64.503	1.00	10.77	B
4195	NH1	ARG	177	13.600	34.147	64.768	1.00	14.32	B
4196	NH2	ARG	177	11.548	33.268	64.517	1.00	13.53	B
4197	C	ARG	177	14.384	37.265	60.283	1.00	10.45	B
4198	O	ARG	177	15.477	37.897	60.453	1.00	11.55	B
4199	N	LEU	178	14.432	36.029	59.766	1.00	12.38	B
4200	CA	LEU	178	15.626	35.379	59.269	1.00	13.93	B
4201	CB	LEU	178	15.389	33.915	58.876	1.00	13.12	B
4202	CG	LEU	178	16.561	33.133	58.286	1.00	13.30	B
4203	CD2	LEU	178	16.148	31.669	58.010	1.00	13.86	B
4204	CD1	LEU	178	17.777	33.097	59.247	1.00	13.76	B
4205	C	LEU	178	16.230	36.152	58.070	1.00	14.61	B
4206	O	LEU	178	17.436	36.374	58.000	1.00	11.90	B
4207	N	ALA	179	15.446	36.396	57.004	1.00	15.55	B
4208	CA	ALA	179	16.003	37.056	55.817	1.00	15.86	B
4209	CB	ALA	179	14.861	37.312	54.792	1.00	15.94	B
4210	C	ALA	179	16.606	38.423	56.114	1.00	16.96	B
4211	O	ALA	179	17.615	38.838	55.565	1.00	17.41	B
4212	N	LYS	180	15.988	39.189	57.028	1.00	17.85	B
4213	CA	LYS	180	16.568	40.453	57.494	1.00	15.94	B
4214	CB	LYS	180	15.667	41.086	58.560	1.00	19.01	B
4215	CG	LYS	180	16.295	42.352	59.178	1.00	17.50	B
4216	CD	LYS	180	15.147	43.189	59.748	1.00	18.63	B
4217	CE	LYS	180	15.715	44.188	60.760	1.00	17.33	B
4218	NZ	LYS	180	16.291	45.411	60.149	1.00	15.67	B
4219	C	LYS	180	17.996	40.304	57.985	1.00	16.75	B
4220	O	LYS	180	18.892	41.039	57.514	1.00	14.40	B

4221	N	ASP	181	18.322	39.325	58.833	1.00	15.83	B
4222	CA	ASP	181	19.697	39.191	59.317	1.00	14.80	B
4223	CB	ASP	181	19.735	38.260	60.541	1.00	17.26	B
4224	CG	ASP	181	19.301	38.908	61.876	1.00	16.08	B
4225	OD1	ASP	181	19.535	40.104	62.061	1.00	17.86	B
4226	OD2	ASP	181	18.712	38.258	62.743	1.00	15.80	B
4227	C	ASP	181	20.653	38.688	58.227	1.00	16.10	B
4228	O	ASP	181	21.795	39.120	58.095	1.00	16.73	B
4229	N	LEU	182	20.259	37.715	57.430	1.00	15.21	B
4230	CA	LEU	182	21.100	37.248	56.316	1.00	16.66	B
4231	CB	LEU	182	20.380	36.146	55.547	1.00	16.39	B
4232	CG	LEU	182	19.886	34.942	56.342	1.00	17.06	B
4233	CD2	LEU	182	21.100	34.312	57.009	1.00	17.01	B
4234	CD1	LEU	182	19.172	33.904	55.496	1.00	17.11	B
4235	C	LEU	182	21.434	38.389	55.353	1.00	14.47	B
4236	O	LEU	182	22.614	38.578	55.050	1.00	17.95	B
4237	N	ALA	183	20.461	39.166	54.954	1.00	15.14	B
4238	CA	ALA	183	20.652	40.215	53.938	1.00	17.15	B
4239	CB	ALA	183	19.292	40.789	53.562	1.00	17.03	B
4240	C	ALA	183	21.510	41.323	54.476	1.00	18.42	B
4241	O	ALA	183	22.395	41.831	53.811	1.00	16.11	B
4242	N	GLU	184	21.258	41.701	55.766	1.00	17.74	B
4243	CA	GLU	184	22.048	42.768	56.366	1.00	18.53	B
4244	CB	GLU	184	21.300	43.366	57.609	1.00	17.38	B
4245	CG	GLU	184	20.080	44.190	57.135	1.00	18.66	B
4246	CD	GLU	184	19.120	44.521	58.271	1.00	20.82	B
4247	OE1	GLU	184	19.502	44.277	59.444	1.00	19.61	B
4248	OE2	GLU	184	17.986	45.018	58.047	1.00	19.07	B
4249	C	GLU	184	23.441	42.360	56.778	1.00	16.95	B
4250	O	GLU	184	24.337	43.246	56.764	1.00	17.24	B
4251	N	ASN	185	23.699	41.086	57.024	1.00	13.32	B
4252	CA	ASN	185	25.053	40.743	57.464	1.00	15.62	B
4253	CB	ASN	185	25.065	39.580	58.508	1.00	14.79	B
4254	CG	ASN	185	26.403	39.531	59.220	1.00	14.88	B
4255	OD1	ASN	185	26.860	40.582	59.674	1.00	15.45	B
4256	ND2	ASN	185	27.144	38.441	59.247	1.00	15.11	B
4257	C	ASN	185	25.903	40.412	56.248	1.00	19.35	B
4258	O	ASN	185	27.106	40.302	56.402	1.00	17.69	B
4259	N	ASN	186	25.286	40.205	55.038	1.00	19.17	B
4260	CA	ASN	186	26.122	39.734	53.916	1.00	18.94	B
4261	CB	ASN	186	25.660	38.331	53.524	1.00	19.49	B
4262	CG	ASN	186	25.905	37.278	54.601	1.00	20.76	B
4263	OD1	ASN	186	26.931	36.628	54.616	1.00	19.30	B
4264	ND2	ASN	186	24.894	37.120	55.464	1.00	15.38	B
4265	C	ASN	186	26.069	40.686	52.728	1.00	20.75	B
4266	O	ASN	186	25.009	40.908	52.110	1.00	19.20	B
4267	N	LYS	187	27.113	41.511	52.646	1.00	21.83	B
4268	CA	LYS	187	27.157	42.526	51.601	1.00	25.25	B
4269	CB	LYS	187	28.511	43.248	51.653	1.00	29.81	B
4270	CG	LYS	187	28.575	44.332	50.603	1.00	36.57	B
4271	CD	LYS	187	29.598	45.433	50.924	1.00	41.20	B
4272	CE	LYS	187	29.104	46.675	50.149	1.00	43.93	B

4273	NZ	LYS	187	27.758	47.038	50.715	1.00	47.95	B
4274	C	LYS	187	26.917	41.925	50.215	1.00	21.96	B
4275	O	LYS	187	27.485	40.901	49.880	1.00	21.53	B
4276	N	GLY	188	25.966	42.457	49.477	1.00	24.02	B
4277	CA	GLY	188	25.673	42.019	48.104	1.00	22.40	B
4278	C	GLY	188	24.674	40.876	48.095	1.00	23.25	B
4279	O	GLY	188	24.196	40.436	47.028	1.00	20.66	B
4280	N	SER	189	24.256	40.404	49.313	1.00	17.56	B
4281	CA	SER	189	23.515	39.145	49.256	1.00	14.19	B
4282	CB	SER	189	23.551	38.426	50.639	1.00	13.25	B
4283	OG	SER	189	22.876	39.291	51.554	1.00	13.20	B
4284	C	SER	189	22.109	39.436	48.806	1.00	15.05	B
4285	O	SER	189	21.571	40.532	48.958	1.00	17.38	B
4286	N	ARG	190	21.487	38.445	48.182	1.00	14.62	B
4287	CA	ARG	190	20.096	38.511	47.766	1.00	15.71	B
4288	CB	ARG	190	19.897	38.718	46.217	1.00	13.97	B
4289	CG	ARG	190	20.434	40.137	45.851	1.00	13.63	B
4290	CD	ARG	190	19.361	41.172	46.158	1.00	14.77	B
4291	NE	ARG	190	19.686	42.563	45.843	1.00	17.01	B
4292	CZ	ARG	190	20.443	43.380	46.550	1.00	20.81	B
4293	NH1	ARG	190	21.162	42.937	47.632	1.00	19.67	B
4294	NH2	ARG	190	20.572	44.652	46.200	1.00	15.95	B
4295	C	ARG	190	19.454	37.199	48.194	1.00	14.14	B
4296	O	ARG	190	19.804	36.099	47.792	1.00	14.54	B
4297	N	VAL	191	18.414	37.349	49.012	1.00	15.36	B
4298	CA	VAL	191	17.760	36.199	49.639	1.00	12.79	B
4299	CB	VAL	191	17.461	36.518	51.153	1.00	14.80	B
4300	CG1	VAL	191	16.898	35.281	51.866	1.00	15.86	B
4301	CG2	VAL	191	18.744	37.016	51.804	1.00	12.63	B
4302	C	VAL	191	16.425	35.919	48.977	1.00	12.57	B
4303	O	VAL	191	15.569	36.765	48.870	1.00	15.60	B
4304	N	LEU	192	16.254	34.676	48.573	1.00	13.56	B
4305	CA	LEU	192	15.004	34.147	48.089	1.00	13.98	B
4306	CB	LEU	192	15.196	33.091	46.984	1.00	11.83	B
4307	CG	LEU	192	13.955	32.395	46.462	1.00	11.19	B
4308	CD2	LEU	192	14.314	31.376	45.351	1.00	12.26	B
4309	CD1	LEU	192	12.912	33.384	45.934	1.00	11.62	B
4310	C	LEU	192	14.313	33.410	49.255	1.00	12.76	B
4311	O	LEU	192	14.776	32.434	49.806	1.00	12.16	B
4312	N	ILE	193	13.131	33.883	49.540	1.00	14.99	B
4313	CA	ILE	193	12.253	33.305	50.553	1.00	14.26	B
4314	CB	ILE	193	11.539	34.395	51.365	1.00	15.44	B
4315	CG2	ILE	193	10.399	33.757	52.157	1.00	15.15	B
4316	CG1	ILE	193	12.573	35.095	52.283	1.00	15.62	B
4317	CD1	ILE	193	11.926	36.312	52.946	1.00	16.17	B
4318	C	ILE	193	11.136	32.571	49.790	1.00	15.15	B
4319	O	ILE	193	10.528	33.172	48.912	1.00	17.37	B
4320	N	VAL	194	10.932	31.311	50.091	1.00	14.25	B
4321	CA	VAL	194	9.762	30.613	49.656	1.00	13.35	B
4322	CB	VAL	194	10.191	29.433	48.700	1.00	14.38	B
4323	CG1	VAL	194	8.965	28.675	48.213	1.00	13.71	B
4324	CG2	VAL	194	10.993	29.982	47.503	1.00	12.10	B

4325	C	VAL	194	9.026	29.930	50.816	1.00	14.29	B
4326	O	VAL	194	9.570	29.017	51.418	1.00	15.09	B
4327	N	CYS	195	7.741	30.304	50.991	1.00	13.22	B
4328	CA	CYS	195	6.880	29.553	51.870	1.00	13.97	B
4329	CB	CYS	195	6.053	30.454	52.825	1.00	13.41	B
4330	SG	CYS	195	7.200	31.332	53.970	1.00	13.51	B
4331	C	CYS	195	5.940	28.750	50.981	1.00	12.18	B
4332	O	CYS	195	5.167	29.357	50.230	1.00	14.80	B
4333	N	SER	196	5.786	27.474	51.172	1.00	14.50	B
4334	CA	SER	196	4.895	26.697	50.348	1.00	13.53	B
4335	CB	SER	196	5.703	25.956	49.252	1.00	13.31	B
4336	OG	SER	196	4.731	25.204	48.538	1.00	15.99	B
4337	C	SER	196	4.115	25.682	51.194	1.00	14.19	B
4338	O	SER	196	4.712	24.852	51.890	1.00	12.43	B
4339	N	GLU	197	2.801	25.854	51.117	1.00	12.15	B
4340	CA	GLU	197	1.949	25.019	51.989	1.00	14.71	B
4341	CB	GLU	197	1.229	25.971	52.957	1.00	12.55	B
4342	CG	GLU	197	2.212	26.780	53.826	1.00	12.64	B
4343	CD	GLU	197	2.723	25.947	54.994	1.00	13.06	B
4344	OE1	GLU	197	2.769	24.708	54.939	1.00	12.15	B
4345	OE2	GLU	197	3.182	26.579	55.977	1.00	12.05	B
4346	C	GLU	197	0.907	24.245	51.209	1.00	15.35	B
4347	O	GLU	197	0.119	24.817	50.424	1.00	15.96	B
4348	N	ILE	198	0.849	22.954	51.481	1.00	14.10	B
4349	CA	ILE	198	-0.172	22.062	51.017	1.00	15.54	B
4350	CB	ILE	198	0.382	21.039	49.982	1.00	17.24	B
4351	CG2	ILE	198	-0.677	19.984	49.684	1.00	14.51	B
4352	CG1	ILE	198	0.746	21.854	48.680	1.00	17.38	B
4353	CD1	ILE	198	1.479	20.936	47.707	1.00	17.59	B
4354	C	ILE	198	-0.921	21.398	52.165	1.00	16.49	B
4355	O	ILE	198	-0.372	20.539	52.858	1.00	16.18	B
4356	N	THR	199	-2.205	21.756	52.307	1.00	17.00	B
4357	CA	THR	199	-2.983	21.232	53.431	1.00	19.19	B
4358	CB	THR	199	-4.254	22.122	53.649	1.00	19.78	B
4359	OG1	THR	199	-5.150	21.959	52.526	1.00	21.03	B
4360	CG2	THR	199	-3.805	23.546	53.817	1.00	18.34	B
4361	C	THR	199	-3.406	19.808	53.390	1.00	18.73	B
4362	O	THR	199	-3.991	19.378	54.389	1.00	20.23	B
4363	N	ALA	200	-3.032	18.966	52.437	1.00	17.18	B
4364	CA	ALA	200	-3.293	17.567	52.378	1.00	16.00	B
4365	CB	ALA	200	-2.716	16.854	51.158	1.00	16.69	B
4366	C	ALA	200	-2.722	16.809	53.619	1.00	19.26	B
4367	O	ALA	200	-3.231	15.757	53.967	1.00	12.21	B
4368	N	ILE	201	-1.612	17.337	54.180	1.00	16.68	B
4369	CA	ILE	201	-1.007	16.728	55.362	1.00	18.76	B
4370	CB	ILE	201	0.304	17.474	55.700	1.00	16.90	B
4371	CG2	ILE	201	0.016	18.875	56.251	1.00	18.55	B
4372	CG1	ILE	201	1.280	16.784	56.650	1.00	20.46	B
4373	CD1	ILE	201	1.753	15.422	56.130	1.00	18.57	B
4374	C	ILE	201	-1.960	16.730	56.559	1.00	15.39	B
4375	O	ILE	201	-1.810	15.844	57.397	1.00	16.53	B
4376	N	LEU	202	-2.902	17.650	56.652	1.00	16.21	B

4377	CA	LEU	202	-3.835	17.728	57.754	1.00	21.36	B
4378	CB	LEU	202	-3.592	19.031	58.485	1.00	23.96	B
4379	CG	LEU	202	-4.019	20.405	58.098	1.00	28.83	B
4380	CD2	LEU	202	-5.087	20.600	57.035	1.00	28.62	B
4381	CD1	LEU	202	-2.821	21.317	57.825	1.00	30.75	B
4382	C	LEU	202	-5.310	17.525	57.462	1.00	22.61	B
4383	O	LEU	202	-6.194	17.799	58.275	1.00	19.31	B
4384	N	PHE	203	-5.629	17.079	56.251	1.00	22.50	B
4385	CA	PHE	203	-6.982	16.715	55.860	1.00	20.37	B
4386	CB	PHE	203	-7.012	16.398	54.339	1.00	20.23	B
4387	CG	PHE	203	-8.352	15.853	53.883	1.00	20.06	B
4388	CD1	PHE	203	-8.609	14.510	53.948	1.00	18.64	B
4389	CD2	PHE	203	-9.284	16.690	53.311	1.00	20.57	B
4390	CE1	PHE	203	-9.842	13.981	53.547	1.00	21.29	B
4391	CE2	PHE	203	-10.503	16.156	52.883	1.00	22.67	B
4392	CZ	PHE	203	-10.795	14.783	52.990	1.00	19.78	B
4393	C	PHE	203	-7.402	15.465	56.633	1.00	18.11	B
4394	O	PHE	203	-6.679	14.478	56.768	1.00	19.21	B
4395	N	HIS	204	-8.612	15.480	57.181	1.00	18.25	B
4396	CA	HIS	204	-9.105	14.326	57.953	1.00	20.33	B
4397	ND1	HIS	204	-6.645	13.362	59.835	1.00	19.25	B
4398	CG	HIS	204	-7.412	14.477	59.880	1.00	20.81	B
4399	CB	HIS	204	-8.873	14.493	59.484	1.00	19.67	B
4400	NE2	HIS	204	-5.336	14.915	60.477	1.00	21.13	B
4401	CD2	HIS	204	-6.588	15.472	60.301	1.00	21.97	B
4402	CE1	HIS	204	-5.415	13.646	60.176	1.00	21.17	B
4403	C	HIS	204	-10.615	14.228	57.741	1.00	20.16	B
4404	O	HIS	204	-11.284	15.242	57.578	1.00	22.41	B
4405	N	GLY	205	-11.145	13.023	57.795	1.00	23.54	B
4406	CA	GLY	205	-12.584	12.827	57.732	1.00	24.24	B
4407	C	GLY	205	-13.205	13.258	59.062	1.00	26.72	B
4408	O	GLY	205	-12.514	13.592	60.020	1.00	25.43	B
4409	N	PRO	206	-14.533	13.398	59.071	1.00	29.13	B
4410	CA	PRO	206	-15.254	13.891	60.219	1.00	30.03	B
4411	CD	PRO	206	-15.440	13.080	57.932	1.00	29.68	B
4412	CB	PRO	206	-16.639	14.259	59.690	1.00	31.08	B
4413	CG	PRO	206	-16.819	13.450	58.454	1.00	32.10	B
4414	C	PRO	206	-15.313	12.905	61.364	1.00	31.36	B
4415	O	PRO	206	-15.395	11.692	61.190	1.00	33.66	B
4416	N	ASN	207	-15.222	13.421	62.582	1.00	32.19	B
4417	CA	ASN	207	-15.349	12.570	63.767	1.00	32.89	B
4418	CB	ASN	207	-14.021	11.922	64.099	1.00	35.19	B
4419	CG	ASN	207	-14.147	11.102	65.387	1.00	36.73	B
4420	OD1	ASN	207	-14.218	9.881	65.296	1.00	36.20	B
4421	ND2	ASN	207	-14.231	11.812	66.507	1.00	35.51	B
4422	C	ASN	207	-15.897	13.406	64.917	1.00	33.85	B
4423	O	ASN	207	-15.367	14.435	65.341	1.00	29.88	B
4424	N	ALA	208	-17.054	12.971	65.422	1.00	35.11	B
4425	CA	ALA	208	-17.849	13.627	66.447	1.00	36.05	B
4426	C	ALA	208	-17.072	13.998	67.693	1.00	35.44	B
4427	O	ALA	208	-17.409	14.992	68.318	1.00	37.83	B
4428	CB	ALA	208	-19.035	12.722	66.862	1.00	36.08	B

4429	N	ASN	209	-16.042	13.280	68.084	1.00	37.00	B
4430	CA	ASN	209	-15.220	13.565	69.233	1.00	39.36	B
4431	CB	ASN	209	-14.483	12.300	69.705	1.00	43.23	B
4432	CG	ASN	209	-15.411	11.124	69.843	1.00	47.10	B
4433	OD1	ASN	209	-16.521	11.246	70.386	1.00	48.34	B
4434	ND2	ASN	209	-15.021	9.956	69.351	1.00	50.28	B
4435	C	ASN	209	-14.106	14.582	68.963	1.00	39.10	B
4436	O	ASN	209	-13.268	14.824	69.859	1.00	36.18	B
4437	N	HIS	210	-13.946	14.940	67.682	1.00	36.31	B
4438	CA	HIS	210	-12.852	15.852	67.359	1.00	36.10	B
4439	ND1	HIS	210	-10.048	14.222	68.273	1.00	38.38	B
4440	CG	HIS	210	-11.110	14.011	67.418	1.00	37.24	B
4441	CB	HIS	210	-11.763	15.090	66.606	1.00	36.59	B
4442	NE2	HIS	210	-10.500	12.139	68.386	1.00	37.27	B
4443	CD2	HIS	210	-11.400	12.690	67.518	1.00	36.88	B
4444	CE1	HIS	210	-9.706	13.084	68.853	1.00	38.15	B
4445	C	HIS	210	-13.402	17.025	66.588	1.00	33.97	B
4446	O	HIS	210	-13.100	17.184	65.415	1.00	32.73	B
4447	N	LEU	211	-14.174	17.876	67.263	1.00	31.22	B
4448	CA	LEU	211	-14.756	19.025	66.584	1.00	30.65	B
4449	CB	LEU	211	-15.922	19.582	67.415	1.00	31.31	B
4450	CG	LEU	211	-16.990	18.529	67.788	1.00	33.04	B
4451	CD2	LEU	211	-17.760	18.036	66.566	1.00	32.52	B
4452	CD1	LEU	211	-17.972	19.040	68.848	1.00	31.68	B
4453	C	LEU	211	-13.696	20.046	66.181	1.00	29.64	B
4454	O	LEU	211	-13.918	20.865	65.279	1.00	26.09	B
4455	N	ASP	212	-12.556	20.106	66.903	1.00	28.39	B
4456	CA	ASP	212	-11.536	21.099	66.535	1.00	26.92	B
4457	CB	ASP	212	-10.460	21.241	67.600	1.00	27.92	B
4458	CG	ASP	212	-9.945	19.948	68.192	1.00	27.65	B
4459	OD1	ASP	212	-10.461	18.838	67.974	1.00	27.95	B
4460	OD2	ASP	212	-8.961	20.022	68.973	1.00	27.71	B
4461	C	ASP	212	-10.937	20.655	65.185	1.00	26.20	B
4462	O	ASP	212	-10.730	21.467	64.293	1.00	25.48	B
4463	N	SER	213	-10.739	19.365	65.008	1.00	25.13	B
4464	CA	SER	213	-10.322	18.789	63.751	1.00	27.51	B
4465	CB	SER	213	-10.133	17.276	63.869	1.00	26.98	B
4466	OG	SER	213	-9.376	16.834	62.750	1.00	32.33	B
4467	C	SER	213	-11.308	19.063	62.614	1.00	28.19	B
4468	O	SER	213	-10.856	19.339	61.484	1.00	26.21	B
4469	N	LEU	214	-12.609	19.062	62.939	1.00	27.08	B
4470	CA	LEU	214	-13.609	19.371	61.912	1.00	26.77	B
4471	CB	LEU	214	-15.053	19.166	62.403	1.00	28.10	B
4472	CG	LEU	214	-16.159	19.393	61.349	1.00	28.20	B
4473	CD2	LEU	214	-17.536	19.343	62.046	1.00	30.09	B
4474	CD1	LEU	214	-16.064	18.273	60.324	1.00	26.98	B
4475	C	LEU	214	-13.500	20.819	61.490	1.00	25.85	B
4476	O	LEU	214	-13.590	21.198	60.314	1.00	23.18	B
4477	N	VAL	215	-13.363	21.687	62.503	1.00	23.90	B
4478	CA	VAL	215	-13.231	23.111	62.261	1.00	23.37	B
4479	CB	VAL	215	-13.112	23.971	63.525	1.00	23.34	B
4480	CG1	VAL	215	-12.673	25.397	63.229	1.00	20.26	B

4481	CG2	VAL	215	-14.451	24.021	64.288	1.00	25.40	B
4482	C	VAL	215	-12.023	23.342	61.339	1.00	23.58	B
4483	O	VAL	215	-12.121	24.202	60.472	1.00	22.67	B
4484	N	ALA	216	-10.937	22.618	61.570	1.00	22.55	B
4485	CA	ALA	216	-9.715	22.759	60.797	1.00	22.68	B
4486	CB	ALA	216	-8.704	21.736	61.360	1.00	23.19	B
4487	C	ALA	216	-9.913	22.460	59.310	1.00	22.95	B
4488	O	ALA	216	-9.207	23.048	58.504	1.00	20.51	B
4489	N	GLN	217	-10.822	21.575	58.954	1.00	21.68	B
4490	CA	GLN	217	-11.191	21.251	57.572	1.00	24.69	B
4491	CB	GLN	217	-12.134	20.032	57.533	1.00	24.18	B
4492	CG	GLN	217	-11.556	18.851	58.303	1.00	25.26	B
4493	CD	GLN	217	-10.116	18.545	57.946	1.00	26.41	B
4494	OE1	GLN	217	-9.790	18.449	56.762	1.00	24.12	B
4495	NE2	GLN	217	-9.241	18.364	58.947	1.00	23.75	B
4496	C	GLN	217	-11.813	22.373	56.767	1.00	23.78	B
4497	O	GLN	217	-11.779	22.355	55.521	1.00	24.24	B
4498	N	ALA	218	-12.276	23.424	57.415	1.00	20.67	B
4499	CA	ALA	218	-12.817	24.588	56.748	1.00	21.53	B
4500	CB	ALA	218	-14.054	25.052	57.549	1.00	23.45	B
4501	C	ALA	218	-11.837	25.747	56.677	1.00	20.66	B
4502	O	ALA	218	-12.146	26.740	56.022	1.00	22.63	B
4503	N	LEU	219	-10.715	25.702	57.416	1.00	18.68	B
4504	CA	LEU	219	-9.909	26.882	57.570	1.00	19.47	B
4505	CB	LEU	219	-9.145	26.825	58.942	1.00	18.91	B
4506	CG	LEU	219	-10.037	26.789	60.198	1.00	21.08	B
4507	CD2	LEU	219	-10.925	28.016	60.331	1.00	20.43	B
4508	CD1	LEU	219	-9.132	26.792	61.458	1.00	20.16	B
4509	C	LEU	219	-8.833	27.161	56.511	1.00	19.17	B
4510	O	LEU	219	-8.508	28.323	56.309	1.00	21.06	B
4511	N	PHE	220	-8.145	26.148	56.049	1.00	19.83	B
4512	CA	PHE	220	-6.873	26.238	55.376	1.00	19.95	B
4513	CB	PHE	220	-5.901	25.187	55.953	1.00	18.15	B
4514	CG	PHE	220	-5.679	25.255	57.455	1.00	19.86	B
4515	CD1	PHE	220	-6.328	24.358	58.290	1.00	18.28	B
4516	CD2	PHE	220	-4.939	26.286	58.002	1.00	19.81	B
4517	CE1	PHE	220	-6.205	24.482	59.692	1.00	19.83	B
4518	CE2	PHE	220	-4.760	26.391	59.391	1.00	23.21	B
4519	CZ	PHE	220	-5.401	25.476	60.229	1.00	20.13	B
4520	C	PHE	220	-6.986	25.993	53.865	1.00	19.57	B
4521	O	PHE	220	-7.588	24.990	53.457	1.00	17.92	B
4522	N	GLY	221	-6.146	26.768	53.161	1.00	20.10	B
4523	CA	GLY	221	-6.032	26.501	51.716	1.00	18.64	B
4524	C	GLY	221	-4.550	26.418	51.354	1.00	20.22	B
4525	O	GLY	221	-3.693	26.584	52.246	1.00	14.78	B
4526	N	ASP	222	-4.303	26.051	50.080	1.00	17.81	B
4527	CA	ASP	222	-2.948	25.837	49.590	1.00	15.49	B
4528	CB	ASP	222	-2.864	24.580	48.675	1.00	15.81	B
4529	CG	ASP	222	-3.288	23.347	49.408	1.00	17.74	B
4530	OD1	ASP	222	-3.586	23.384	50.652	1.00	18.97	B
4531	OD2	ASP	222	-3.374	22.273	48.797	1.00	18.32	B
4532	C	ASP	222	-2.372	26.987	48.828	1.00	14.88	B

4533	O	ASP	222	-3.120	27.652	48.085	1.00	17.37	B
4534	N	GLY	223	-1.046	27.224	48.932	1.00	14.43	B
4535	CA	GLY	223	-0.490	28.359	48.200	1.00	15.06	B
4536	C	GLY	223	0.990	28.461	48.442	1.00	17.49	B
4537	O	GLY	223	1.432	27.950	49.507	1.00	15.78	B
4538	N	ALA	224	1.700	29.227	47.632	1.00	13.37	B
4539	CA	ALA	224	3.102	29.468	47.953	1.00	13.80	B
4540	CB	ALA	224	4.098	28.580	47.233	1.00	14.95	B
4541	C	ALA	224	3.401	30.902	47.587	1.00	16.27	B
4542	O	ALA	224	2.750	31.424	46.672	1.00	15.25	B
4543	N	ALA	225	4.222	31.521	48.423	1.00	14.47	B
4544	CA	ALA	225	4.677	32.875	48.161	1.00	15.02	B
4545	CB	ALA	225	4.129	33.882	49.156	1.00	16.77	B
4546	C	ALA	225	6.190	32.880	48.111	1.00	15.87	B
4547	O	ALA	225	6.859	32.196	48.926	1.00	14.87	B
4548	N	ALA	226	6.769	33.734	47.254	1.00	13.33	B
4549	CA	ALA	226	8.209	33.816	47.152	1.00	13.75	B
4550	CB	ALA	226	8.802	33.161	45.896	1.00	13.91	B
4551	C	ALA	226	8.598	35.280	47.167	1.00	15.62	B
4552	O	ALA	226	7.872	36.126	46.616	1.00	17.43	B
4553	N	LEU	227	9.677	35.596	47.892	1.00	14.60	B
4554	CA	LEU	227	10.089	36.990	47.945	1.00	14.38	B
4555	CB	LEU	227	9.963	37.569	49.368	1.00	17.61	B
4556	CG	LEU	227	8.613	38.091	49.833	1.00	17.91	B
4557	CD2	LEU	227	8.694	38.832	51.164	1.00	18.91	B
4558	CD1	LEU	227	7.665	36.907	49.927	1.00	18.08	B
4559	C	LEU	227	11.580	37.083	47.610	1.00	13.22	B
4560	O	LEU	227	12.295	36.151	47.952	1.00	13.64	B
4561	N	ILE	228	12.055	38.203	47.088	1.00	14.27	B
4562	CA	ILE	228	13.477	38.487	46.965	1.00	14.63	B
4563	CB	ILE	228	13.922	39.043	45.582	1.00	16.79	B
4564	CG2	ILE	228	15.381	39.487	45.613	1.00	15.68	B
4565	CG1	ILE	228	13.660	37.954	44.508	1.00	16.16	B
4566	CD1	ILE	228	14.595	36.753	44.642	1.00	17.11	B
4567	C	ILE	228	13.752	39.586	48.022	1.00	14.29	B
4568	O	ILE	228	13.008	40.554	48.078	1.00	14.75	B
4569	N	VAL	229	14.784	39.411	48.845	1.00	15.28	B
4570	CA	VAL	229	15.076	40.381	49.912	1.00	16.09	B
4571	CB	VAL	229	14.743	39.799	51.307	1.00	16.66	B
4572	CG1	VAL	229	15.267	40.706	52.425	1.00	16.72	B
4573	CG2	VAL	229	13.228	39.551	51.444	1.00	15.55	B
4574	C	VAL	229	16.559	40.717	49.872	1.00	14.72	B
4575	O	VAL	229	17.385	39.845	49.691	1.00	15.04	B
4576	N	GLY	230	16.891	41.990	50.035	1.00	14.63	B
4577	CA	GLY	230	18.323	42.287	50.038	1.00	15.35	B
4578	C	GLY	230	18.439	43.690	50.666	1.00	13.66	B
4579	O	GLY	230	17.498	44.456	50.586	1.00	14.33	B
4580	N	SER	231	19.645	44.041	51.070	1.00	13.97	B
4581	CA	SER	231	19.952	45.371	51.523	1.00	15.98	B
4582	CB	SER	231	20.991	45.316	52.687	1.00	14.94	B
4583	OG	SER	231	20.274	44.737	53.802	1.00	17.50	B
4584	C	SER	231	20.666	46.119	50.385	1.00	17.76	B

4585	O	SER	231	21.247	45.407	49.544	1.00	17.44	B
4586	N	GLY	232	20.668	47.439	50.443	1.00	17.64	B
4587	CA	GLY	232	21.461	48.143	49.423	1.00	21.35	B
4588	C	GLY	232	20.916	47.928	48.002	1.00	21.72	B
4589	O	GLY	232	21.655	47.442	47.155	1.00	22.80	B
4590	N	PRO	233	19.675	48.249	47.730	1.00	21.24	B
4591	CA	PRO	233	19.092	48.084	46.435	1.00	22.08	B
4592	CD	PRO	233	18.696	48.793	48.716	1.00	24.18	B
4593	CB	PRO	233	17.620	48.319	46.596	1.00	22.49	B
4594	CG	PRO	233	17.426	48.985	47.913	1.00	24.32	B
4595	C	PRO	233	19.731	48.966	45.358	1.00	23.61	B
4596	O	PRO	233	20.127	50.120	45.544	1.00	23.70	B
4597	N	HIS	234	19.912	48.360	44.185	1.00	23.26	B
4598	CA	HIS	234	20.456	49.160	43.035	1.00	25.59	B
4599	ND1	HIS	234	22.480	46.369	43.308	1.00	36.45	B
4600	CG	HIS	234	22.400	47.631	42.760	1.00	34.08	B
4601	CB	HIS	234	21.150	48.164	42.113	1.00	29.49	B
4602	NE2	HIS	234	24.413	47.262	43.570	1.00	37.58	B
4603	CD2	HIS	234	23.617	48.186	42.931	1.00	36.49	B
4604	CE1	HIS	234	23.691	46.180	43.802	1.00	37.67	B
4605	C	HIS	234	19.246	49.814	42.403	1.00	23.40	B
4606	O	HIS	234	18.578	49.156	41.574	1.00	21.79	B
4607	N	LEU	235	18.901	51.021	42.810	1.00	18.81	B
4608	CA	LEU	235	17.636	51.633	42.434	1.00	20.01	B
4609	CB	LEU	235	17.533	52.978	43.124	1.00	21.02	B
4610	CG	LEU	235	17.572	52.902	44.667	1.00	24.52	B
4611	CD2	LEU	235	16.400	52.135	45.242	1.00	22.44	B
4612	CD1	LEU	235	17.568	54.336	45.202	1.00	25.00	B
4613	C	LEU	235	17.338	51.823	40.943	1.00	20.03	B
4614	O	LEU	235	16.155	51.945	40.563	1.00	19.96	B
4615	N	ALA	236	18.360	51.915	40.105	1.00	19.87	B
4616	CA	ALA	236	17.982	52.005	38.653	1.00	21.88	B
4617	CB	ALA	236	19.244	52.318	37.890	1.00	22.39	B
4618	C	ALA	236	17.308	50.705	38.224	1.00	20.16	B
4619	O	ALA	236	16.498	50.743	37.287	1.00	21.64	B
4620	N	VAL	237	17.633	49.525	38.743	1.00	18.36	B
4621	CA	VAL	237	17.088	48.251	38.264	1.00	21.06	B
4622	CB	VAL	237	18.149	47.357	37.605	1.00	22.43	B
4623	CG1	VAL	237	18.923	48.123	36.501	1.00	22.33	B
4624	CG2	VAL	237	19.193	46.875	38.617	1.00	21.47	B
4625	C	VAL	237	16.320	47.409	39.274	1.00	23.18	B
4626	O	VAL	237	15.517	46.553	38.862	1.00	20.17	B
4627	N	GLU	238	16.532	47.678	40.575	1.00	23.12	B
4628	CA	GLU	238	15.717	46.968	41.592	1.00	24.28	B
4629	CB	GLU	238	16.573	46.412	42.756	1.00	20.87	B
4630	CG	GLU	238	17.547	45.322	42.328	1.00	22.37	B
4631	CD	GLU	238	18.508	44.782	43.383	1.00	21.53	B
4632	OE1	GLU	238	19.213	45.594	44.013	1.00	21.50	B
4633	OE2	GLU	238	18.638	43.542	43.508	1.00	20.73	B
4634	C	GLU	238	14.668	47.930	42.114	1.00	23.86	B
4635	O	GLU	238	14.928	49.131	42.206	1.00	26.30	B
4636	N	ARG	239	13.500	47.445	42.482	1.00	25.15	B

4637	CA	ARG	239	12.408	48.245	42.998	1.00	25.86	B
4638	CB	ARG	239	11.225	47.996	42.064	1.00	30.88	B
4639	CG	ARG	239	9.888	48.635	42.354	1.00	37.20	B
4640	CD	ARG	239	9.027	48.768	41.085	1.00	42.07	B
4641	NE	ARG	239	8.117	47.635	40.971	1.00	46.99	B
4642	CZ	ARG	239	7.975	46.768	39.976	1.00	49.94	B
4643	NH1	ARG	239	7.059	45.790	40.047	1.00	49.43	B
4644	NH2	ARG	239	8.743	46.867	38.874	1.00	51.54	B
4645	C	ARG	239	11.980	47.845	44.426	1.00	23.77	B
4646	O	ARG	239	11.099	46.999	44.587	1.00	20.90	B
4647	N	PRO	240	12.408	48.616	45.405	1.00	21.88	B
4648	CA	PRO	240	11.962	48.377	46.791	1.00	22.18	B
4649	CD	PRO	240	13.553	49.537	45.400	1.00	23.80	B
4650	CB	PRO	240	12.570	49.513	47.603	1.00	23.53	B
4651	CG	PRO	240	13.816	49.902	46.861	1.00	24.77	B
4652	C	PRO	240	10.458	48.477	46.877	1.00	22.38	B
4653	O	PRO	240	9.789	49.344	46.311	1.00	23.13	B
4654	N	ILE	241	9.883	47.575	47.635	1.00	21.04	B
4655	CA	ILE	241	8.470	47.539	47.964	1.00	18.55	B
4656	CB	ILE	241	7.865	46.177	47.673	1.00	18.72	B
4657	CG2	ILE	241	6.354	46.207	47.855	1.00	17.22	B
4658	CG1	ILE	241	8.257	45.697	46.248	1.00	17.91	B
4659	CD1	ILE	241	7.763	44.285	45.958	1.00	19.18	B
4660	C	ILE	241	8.327	47.861	49.467	1.00	21.37	B
4661	O	ILE	241	7.483	48.704	49.794	1.00	21.17	B
4662	N	PHE	242	9.103	47.245	50.366	1.00	19.00	B
4663	CA	PHE	242	9.008	47.549	51.777	1.00	21.33	B
4664	CB	PHE	242	8.031	46.667	52.600	1.00	19.86	B
4665	CG	PHE	242	6.569	46.842	52.271	1.00	19.00	B
4666	CD1	PHE	242	5.872	47.952	52.680	1.00	20.22	B
4667	CD2	PHE	242	5.902	45.898	51.512	1.00	19.55	B
4668	CE1	PHE	242	4.518	48.133	52.362	1.00	19.56	B
4669	CE2	PHE	242	4.563	46.078	51.186	1.00	19.20	B
4670	CZ	PHE	242	3.873	47.177	51.607	1.00	17.64	B
4671	C	PHE	242	10.376	47.282	52.401	1.00	21.54	B
4672	O	PHE	242	11.055	46.394	51.894	1.00	20.44	B
4673	N	GLU	243	10.699	48.070	53.433	1.00	20.95	B
4674	CA	GLU	243	11.948	47.754	54.148	1.00	20.26	B
4675	CB	GLU	243	12.557	49.082	54.594	1.00	23.58	B
4676	CG	GLU	243	13.077	49.907	53.400	1.00	26.69	B
4677	CD	GLU	243	13.781	51.146	53.920	1.00	30.46	B
4678	OE1	GLU	243	13.132	52.026	54.543	1.00	32.78	B
4679	OE2	GLU	243	14.999	51.197	53.750	1.00	30.83	B
4680	C	GLU	243	11.526	46.987	55.433	1.00	19.80	B
4681	O	GLU	243	10.442	47.304	55.920	1.00	18.51	B
4682	N	ILE	244	12.295	46.075	55.954	1.00	18.47	B
4683	CA	ILE	244	11.955	45.333	57.181	1.00	20.25	B
4684	CB	ILE	244	12.401	43.868	57.101	1.00	19.02	B
4685	CG2	ILE	244	11.838	43.071	58.309	1.00	17.85	B
4686	CG1	ILE	244	11.931	43.284	55.746	1.00	17.69	B
4687	CD1	ILE	244	12.590	41.934	55.415	1.00	16.92	B
4688	C	ILE	244	12.689	46.071	58.321	1.00	18.43	B

4689	O	ILE	244	13.909	46.028	58.391	1.00	19.97	B
4690	N	VAL	245	11.984	46.828	59.103	1.00	19.22	B
4691	CA	VAL	245	12.499	47.686	60.171	1.00	18.08	B
4692	CB	VAL	245	11.439	48.736	60.578	1.00	19.80	B
4693	CG1	VAL	245	11.979	49.666	61.669	1.00	18.28	B
4694	CG2	VAL	245	11.087	49.596	59.330	1.00	22.69	B
4695	C	VAL	245	12.924	46.920	61.412	1.00	18.38	B
4696	O	VAL	245	14.098	47.031	61.843	1.00	18.98	B
4697	N	SER	246	12.034	46.083	61.921	1.00	17.27	B
4698	CA	SER	246	12.373	45.309	63.145	1.00	18.32	B
4699	CB	SER	246	12.079	46.190	64.417	1.00	17.08	B
4700	OG	SER	246	10.656	46.389	64.402	1.00	16.05	B
4701	C	SER	246	11.497	44.099	63.232	1.00	15.69	B
4702	O	SER	246	10.431	43.979	62.604	1.00	15.37	B
4703	N	THR	247	11.944	43.067	63.969	1.00	17.49	B
4704	CA	THR	247	11.206	41.813	64.093	1.00	17.94	B
4705	CB	THR	247	11.874	40.706	63.264	1.00	18.33	B
4706	OG1	THR	247	13.257	40.548	63.674	1.00	18.76	B
4707	CG2	THR	247	11.887	41.109	61.776	1.00	16.41	B
4708	C	THR	247	11.215	41.411	65.587	1.00	21.08	B
4709	O	THR	247	12.203	41.716	66.268	1.00	21.65	B
4710	N	ASP	248	10.087	40.998	66.102	1.00	18.99	B
4711	CA	ASP	248	10.043	40.506	67.481	1.00	20.27	B
4712	CB	ASP	248	9.209	41.452	68.360	1.00	19.31	B
4713	CG	ASP	248	9.724	42.860	68.406	1.00	23.48	B
4714	OD1	ASP	248	10.953	42.990	68.662	1.00	25.47	B
4715	OD2	ASP	248	8.968	43.866	68.227	1.00	25.53	B
4716	C	ASP	248	9.447	39.119	67.406	1.00	18.31	B
4717	O	ASP	248	8.597	38.848	66.529	1.00	17.06	B
4718	N	GLN	249	9.811	38.250	68.355	1.00	15.25	B
4719	CA	GLN	249	9.058	37.000	68.484	1.00	14.33	B
4720	CB	GLN	249	9.920	35.822	68.053	1.00	14.91	B
4721	CG	GLN	249	9.131	34.535	67.927	1.00	14.29	B
4722	CD	GLN	249	10.002	33.361	67.594	1.00	15.87	B
4723	OE1	GLN	249	11.214	33.498	67.835	1.00	20.00	B
4724	NE2	GLN	249	9.452	32.259	67.103	1.00	14.13	B
4725	C	GLN	249	8.769	36.772	69.979	1.00	19.39	B
4726	O	GLN	249	9.706	37.032	70.759	1.00	19.23	B
4727	N	THR	250	7.561	36.367	70.339	1.00	19.32	B
4728	CA	THR	250	7.315	36.159	71.779	1.00	19.87	B
4729	CB	THR	250	6.773	37.389	72.527	1.00	21.59	B
4730	OG1	THR	250	7.683	38.481	72.307	1.00	28.35	B
4731	CG2	THR	250	6.983	37.166	74.051	1.00	18.89	B
4732	C	THR	250	6.319	35.038	71.977	1.00	18.75	B
4733	O	THR	250	5.428	34.865	71.142	1.00	20.02	B
4734	N	ILE	251	6.403	34.338	73.096	1.00	17.68	B
4735	CA	ILE	251	5.474	33.306	73.502	1.00	16.89	B
4736	CB	ILE	251	6.238	32.151	74.147	1.00	18.89	B
4737	CG2	ILE	251	5.264	31.172	74.834	1.00	18.52	B
4738	CG1	ILE	251	7.169	31.378	73.226	1.00	16.02	B
4739	CD1	ILE	251	8.288	30.632	74.067	1.00	15.23	B
4740	C	ILE	251	4.433	33.911	74.466	1.00	20.13	B

4741	O	ILE	251	4.769	34.618	75.425	1.00	17.32	B
4742	N	LEU	252	3.157	33.767	74.176	1.00	18.45	B
4743	CA	LEU	252	2.066	34.321	74.976	1.00	19.07	B
4744	CB	LEU	252	0.774	34.286	74.175	1.00	19.46	B
4745	CG	LEU	252	0.396	35.463	73.278	1.00	23.24	B
4746	CD2	LEU	252	-0.436	34.990	72.112	1.00	21.25	B
4747	CD1	LEU	252	1.508	36.394	72.882	1.00	23.75	B
4748	C	LEU	252	1.877	33.442	76.244	1.00	18.19	B
4749	O	LEU	252	1.836	32.204	76.181	1.00	17.28	B
4750	N	PRO	253	1.931	34.084	77.404	1.00	18.72	B
4751	CA	PRO	253	1.871	33.337	78.656	1.00	19.30	B
4752	CD	PRO	253	1.946	35.524	77.633	1.00	19.70	B
4753	CB	PRO	253	2.007	34.415	79.738	1.00	20.88	B
4754	CG	PRO	253	1.469	35.648	79.089	1.00	23.61	B
4755	C	PRO	253	0.618	32.514	78.761	1.00	18.39	B
4756	O	PRO	253	-0.418	32.946	78.274	1.00	20.01	B
4757	N	ASP	254	0.699	31.301	79.292	1.00	17.80	B
4758	CA	ASP	254	-0.433	30.459	79.586	1.00	19.42	B
4759	CB	ASP	254	-1.281	31.191	80.662	1.00	20.10	B
4760	CG	ASP	254	-0.420	31.437	81.902	1.00	21.35	B
4761	OD1	ASP	254	-0.125	32.573	82.229	1.00	24.83	B
4762	OD2	ASP	254	-0.004	30.451	82.485	1.00	23.09	B
4763	C	ASP	254	-1.326	30.155	78.392	1.00	21.18	B
4764	O	ASP	254	-2.512	29.857	78.582	1.00	18.72	B
4765	N	THR	255	-0.693	29.973	77.208	1.00	20.77	B
4766	CA	THR	255	-1.488	29.570	76.040	1.00	20.62	B
4767	CB	THR	255	-1.491	30.706	75.020	1.00	19.84	B
4768	OG1	THR	255	-0.108	30.933	74.638	1.00	22.29	B
4769	CG2	THR	255	-2.078	31.975	75.567	1.00	17.24	B
4770	C	THR	255	-0.914	28.333	75.379	1.00	23.88	B
4771	O	THR	255	-1.322	27.957	74.270	1.00	24.06	B
4772	N	GLU	256	-0.161	27.518	76.091	1.00	24.98	B
4773	CA	GLU	256	0.400	26.312	75.484	1.00	28.54	B
4774	CB	GLU	256	1.353	25.581	76.416	1.00	28.97	B
4775	CG	GLU	256	1.916	24.280	75.757	1.00	32.11	B
4776	CD	GLU	256	2.856	23.589	76.744	1.00	34.01	B
4777	OE1	GLU	256	3.578	24.233	77.533	1.00	34.39	B
4778	OE2	GLU	256	2.934	22.359	76.755	1.00	38.83	B
4779	C	GLU	256	-0.655	25.350	74.953	1.00	30.36	B
4780	O	GLU	256	-0.459	24.781	73.858	1.00	29.20	B
4781	N	LYS	257	-1.807	25.254	75.618	1.00	29.61	B
4782	CA	LYS	257	-2.880	24.389	75.134	1.00	31.41	B
4783	CB	LYS	257	-3.962	24.226	76.251	1.00	33.87	B
4784	CG	LYS	257	-4.745	25.533	76.410	1.00	37.41	B
4785	CD	LYS	257	-5.474	25.653	77.752	1.00	40.71	B
4786	CE	LYS	257	-6.368	26.895	77.668	1.00	42.65	B
4787	NZ	LYS	257	-7.353	26.923	78.786	1.00	44.31	B
4788	C	LYS	257	-3.592	24.923	73.907	1.00	28.64	B
4789	O	LYS	257	-4.535	24.304	73.415	1.00	30.31	B
4790	N	ALA	258	-3.389	26.174	73.532	1.00	26.22	B
4791	CA	ALA	258	-4.085	26.740	72.402	1.00	26.57	B
4792	CB	ALA	258	-3.496	28.091	72.058	1.00	25.14	B

4793	C	ALA	258	-3.971	25.820	71.162	1.00	25.74	B
4794	O	ALA	258	-4.987	25.614	70.519	1.00	23.24	B
4795	N	MET	259	-2.743	25.414	70.804	1.00	24.83	B
4796	CA	MET	259	-2.558	24.626	69.586	1.00	24.97	B
4797	C	MET	259	-1.424	23.629	69.654	1.00	22.87	B
4798	O	MET	259	-0.266	23.943	69.985	1.00	21.95	B
4799	CB	MET	259	-2.372	25.468	68.335	1.00	27.17	B
4800	CG	MET	259	-2.036	26.893	68.507	1.00	31.07	B
4801	SD	MET	259	-1.716	27.869	67.058	1.00	27.58	B
4802	CE	MET	259	-2.943	29.164	67.238	1.00	27.63	B
4803	N	LYS	260	-1.799	22.390	69.465	1.00	20.37	B
4804	CA	LYS	260	-0.861	21.301	69.406	1.00	22.25	B
4805	CB	LYS	260	-0.885	20.387	70.631	1.00	25.95	B
4806	CG	LYS	260	-0.545	21.132	71.927	1.00	29.48	B
4807	CD	LYS	260	-0.438	20.128	73.087	1.00	31.73	B
4808	CE	LYS	260	-0.473	20.914	74.395	1.00	34.61	B
4809	NZ	LYS	260	0.575	20.474	75.367	1.00	37.61	B
4810	C	LYS	260	-1.180	20.491	68.149	1.00	23.25	B
4811	O	LYS	260	-2.358	20.209	67.870	1.00	22.97	B
4812	N	LEU	261	-0.140	20.192	67.388	1.00	18.66	B
4813	CA	LEU	261	-0.314	19.380	66.160	1.00	19.19	B
4814	CB	LEU	261	-0.311	20.232	64.885	1.00	17.81	B
4815	CG	LEU	261	-1.332	21.363	64.779	1.00	19.40	B
4816	CD2	LEU	261	-1.651	21.592	63.295	1.00	20.42	B
4817	CD1	LEU	261	-0.745	22.621	65.381	1.00	19.17	B
4818	C	LEU	261	0.833	18.400	66.123	1.00	16.88	B
4819	O	LEU	261	1.988	18.807	66.270	1.00	14.68	B
4820	N	HIS	262	0.554	17.117	66.085	1.00	16.56	B
4821	CA	HIS	262	1.503	16.049	66.123	1.00	15.24	B
4822	ND1	HIS	262	1.625	16.568	69.085	1.00	19.24	B
4823	CG	HIS	262	0.770	15.663	68.504	1.00	19.32	B
4824	CB	HIS	262	1.044	15.004	67.169	1.00	17.45	B
4825	NE2	HIS	262	-0.141	16.475	70.325	1.00	19.03	B
4826	CD2	HIS	262	-0.390	15.677	69.229	1.00	20.60	B
4827	CE1	HIS	262	1.076	16.990	70.237	1.00	20.53	B
4828	C	HIS	262	1.577	15.306	64.756	1.00	18.43	B
4829	O	HIS	262	0.525	15.030	64.192	1.00	18.48	B
4830	N	LEU	263	2.791	14.947	64.349	1.00	17.35	B
4831	CA	LEU	263	2.932	14.217	63.051	1.00	18.01	B
4832	CB	LEU	263	4.127	14.711	62.235	1.00	18.24	B
4833	CG	LEU	263	4.232	14.166	60.785	1.00	20.07	B
4834	CD2	LEU	263	5.537	14.610	60.120	1.00	19.19	B
4835	CD1	LEU	263	3.068	14.736	59.968	1.00	18.51	B
4836	C	LEU	263	2.954	12.737	63.327	1.00	15.51	B
4837	O	LEU	263	3.868	12.177	63.915	1.00	18.64	B
4838	N	ARG	264	1.810	12.079	63.059	1.00	16.36	B
4839	CA	ARG	264	1.621	10.682	63.421	1.00	17.97	B
4840	CB	ARG	264	0.401	10.622	64.354	1.00	18.60	B
4841	CG	ARG	264	0.297	11.651	65.444	1.00	22.94	B
4842	CD	ARG	264	1.329	11.371	66.546	1.00	22.99	B
4843	NE	ARG	264	0.805	10.246	67.392	1.00	22.21	B
4844	CZ	ARG	264	1.569	9.755	68.375	1.00	23.91	B

4845	NH1	ARG	264	2.772	10.312	68.609	1.00	21.04	B
4846	NH2	ARG	264	1.170	8.752	69.133	1.00	23.70	B
4847	C	ARG	264	1.321	9.833	62.183	1.00	18.71	B
4848	O	ARG	264	1.180	10.358	61.045	1.00	19.40	B
4849	N	GLU	265	1.144	8.552	62.383	1.00	18.65	B
4850	CA	GLU	265	0.868	7.619	61.297	1.00	20.01	B
4851	CB	GLU	265	0.747	6.181	61.842	1.00	18.81	B
4852	CG	GLU	265	2.094	5.619	62.323	1.00	20.62	B
4853	CD	GLU	265	1.927	4.549	63.405	1.00	22.60	B
4854	OE1	GLU	265	0.932	3.802	63.364	1.00	22.66	B
4855	OE2	GLU	265	2.845	4.350	64.218	1.00	20.42	B
4856	C	GLU	265	-0.401	8.001	60.524	1.00	19.67	B
4857	O	GLU	265	-0.517	7.643	59.349	1.00	19.98	B
4858	N	GLY	266	-1.349	8.705	61.111	1.00	19.90	B
4859	CA	GLY	266	-2.585	9.157	60.528	1.00	19.35	B
4860	C	GLY	266	-2.557	10.572	59.965	1.00	19.40	B
4861	O	GLY	266	-3.581	11.135	59.554	1.00	19.85	B
4862	N	GLY	267	-1.365	11.167	59.892	1.00	19.43	B
4863	CA	GLY	267	-1.241	12.525	59.343	1.00	20.17	B
4864	C	GLY	267	-0.946	13.511	60.478	1.00	20.17	B
4865	O	GLY	267	-0.585	13.130	61.594	1.00	19.59	B
4866	N	LEU	268	-0.988	14.789	60.178	1.00	18.97	B
4867	CA	LEU	268	-0.762	15.841	61.152	1.00	21.63	B
4868	CB	LEU	268	-0.402	17.137	60.429	1.00	19.78	B
4869	CG	LEU	268	-0.074	18.357	61.290	1.00	20.29	B
4870	CD2	LEU	268	0.211	19.555	60.382	1.00	18.85	B
4871	CD1	LEU	268	1.119	18.054	62.234	1.00	16.00	B
4872	C	LEU	268	-2.057	16.011	61.959	1.00	22.49	B
4873	O	LEU	268	-3.049	16.446	61.351	1.00	23.93	B
4874	N	THR	269	-2.042	15.706	63.255	1.00	20.56	B
4875	CA	THR	269	-3.252	15.807	64.064	1.00	21.29	B
4876	CB	THR	269	-3.154	14.968	65.379	1.00	21.74	B
4877	OG1	THR	269	-2.214	15.681	66.180	1.00	20.22	B
4878	CG2	THR	269	-2.629	13.582	65.127	1.00	22.50	B
4879	C	THR	269	-3.500	17.219	64.544	1.00	24.25	B
4880	O	THR	269	-2.571	18.012	64.488	1.00	24.29	B
4881	N	PHE	270	-4.688	17.529	65.067	1.00	25.87	B
4882	CA	PHE	270	-5.070	18.864	65.476	1.00	31.34	B
4883	CB	PHE	270	-6.166	19.305	64.483	1.00	35.31	B
4884	CG	PHE	270	-5.748	20.288	63.453	1.00	37.32	B
4885	CD1	PHE	270	-5.602	19.976	62.109	1.00	41.39	B
4886	CD2	PHE	270	-5.516	21.582	63.840	1.00	38.00	B
4887	CE1	PHE	270	-5.182	20.955	61.208	1.00	41.19	B
4888	CE2	PHE	270	-5.119	22.571	62.989	1.00	39.05	B
4889	CZ	PHE	270	-4.930	22.227	61.676	1.00	41.09	B
4890	C	PHE	270	-5.676	18.977	66.873	1.00	34.01	B
4891	O	PHE	270	-6.331	18.047	67.412	1.00	35.09	B
4892	N	GLN	271	-5.144	19.903	67.662	1.00	32.32	B
4893	CA	GLN	271	-5.707	20.246	68.971	1.00	30.70	B
4894	CB	GLN	271	-4.865	19.770	70.136	1.00	34.37	B
4895	CG	GLN	271	-5.390	20.206	71.513	1.00	38.69	B
4896	CD	GLN	271	-4.616	19.515	72.638	1.00	39.85	B

4897	OE1	GLN	271	-4.175	18.365	72.522	1.00	40.73	B
4898	NE2	GLN	271	-4.417	20.204	73.761	1.00	40.59	B
4899	C	GLN	271	-5.804	21.760	68.944	1.00	29.55	B
4900	O	GLN	271	-4.772	22.432	68.988	1.00	30.22	B
4901	N	LEU	272	-6.971	22.329	68.747	1.00	26.55	B
4902	CA	LEU	272	-7.183	23.742	68.583	1.00	28.69	B
4903	CB	LEU	272	-7.720	24.105	67.203	1.00	31.23	B
4904	CG	LEU	272	-7.246	25.228	66.324	1.00	36.49	B
4905	CD2	LEU	272	-6.759	26.504	67.004	1.00	36.59	B
4906	CD1	LEU	272	-8.320	25.592	65.271	1.00	36.39	B
4907	C	LEU	272	-8.238	24.220	69.595	1.00	28.44	B
4908	O	LEU	272	-9.415	23.843	69.455	1.00	24.19	B
4909	N	HIS	273	-7.736	25.027	70.534	1.00	25.56	B
4910	CA	HIS	273	-8.663	25.539	71.542	1.00	26.63	B
4911	ND1	HIS	273	-8.590	25.102	74.753	1.00	34.69	B
4912	CG	HIS	273	-8.633	26.161	73.892	1.00	32.95	B
4913	CB	HIS	273	-7.797	26.215	72.646	1.00	28.30	B
4914	NE2	HIS	273	-10.052	26.478	75.526	1.00	35.08	B
4915	CD2	HIS	273	-9.561	27.046	74.366	1.00	33.09	B
4916	CE1	HIS	273	-9.453	25.329	75.739	1.00	34.70	B
4917	C	HIS	273	-9.624	26.565	71.014	1.00	24.27	B
4918	O	HIS	273	-9.253	27.528	70.305	1.00	21.53	B
4919	N	ARG	274	-10.897	26.506	71.421	1.00	26.35	B
4920	CA	ARG	274	-11.885	27.498	70.993	1.00	26.02	B
4921	CB	ARG	274	-13.299	27.078	71.470	1.00	30.33	B
4922	CG	ARG	274	-14.406	27.884	70.784	1.00	34.79	B
4923	CD	ARG	274	-15.809	27.333	71.119	1.00	37.50	B
4924	NE	ARG	274	-16.871	28.118	70.487	1.00	38.88	B
4925	CZ	ARG	274	-18.172	27.994	70.777	1.00	40.68	B
4926	NH1	ARG	274	-18.541	27.099	71.700	1.00	39.89	B
4927	NH2	ARG	274	-19.089	28.742	70.154	1.00	38.89	B
4928	C	ARG	274	-11.588	28.907	71.456	1.00	23.71	B
4929	O	ARG	274	-12.007	29.877	70.823	1.00	22.59	B
4930	N	ASP	275	-10.768	29.152	72.483	1.00	23.58	B
4931	CA	ASP	275	-10.497	30.501	72.936	1.00	24.04	B
4932	CB	ASP	275	-10.343	30.538	74.465	1.00	27.42	B
4933	CG	ASP	275	-11.632	30.300	75.239	1.00	31.03	B
4934	OD1	ASP	275	-12.743	30.473	74.687	1.00	32.66	B
4935	OD2	ASP	275	-11.456	29.933	76.422	1.00	33.99	B
4936	C	ASP	275	-9.237	31.107	72.328	1.00	22.28	B
4937	O	ASP	275	-8.887	32.239	72.671	1.00	20.30	B
4938	N	VAL	276	-8.754	30.506	71.227	1.00	21.31	B
4939	CA	VAL	276	-7.590	31.114	70.567	1.00	18.63	B
4940	CB	VAL	276	-7.141	30.306	69.325	1.00	19.27	B
4941	CG1	VAL	276	-6.304	31.145	68.349	1.00	21.02	B
4942	CG2	VAL	276	-6.400	29.081	69.808	1.00	18.70	B
4943	C	VAL	276	-7.785	32.552	70.267	1.00	15.46	B
4944	O	VAL	276	-6.921	33.346	70.606	1.00	16.12	B
4945	N	PRO	277	-8.904	33.001	69.692	1.00	17.02	B
4946	CA	PRO	277	-9.088	34.406	69.391	1.00	18.84	B
4947	CD	PRO	277	-10.016	32.159	69.207	1.00	17.63	B
4948	CB	PRO	277	-10.521	34.464	68.820	1.00	19.05	B

4949	CG	PRO	277	-10.718	33.106	68.215	1.00	18.29	B
4950	C	PRO	277	-8.906	35.279	70.621	1.00	19.45	B
4951	O	PRO	277	-8.372	36.389	70.553	1.00	18.40	B
4952	N	LEU	278	-9.543	34.876	71.735	1.00	19.69	B
4953	CA	LEU	278	-9.411	35.668	72.990	1.00	20.31	B
4954	CB	LEU	278	-10.361	35.068	74.035	1.00	22.50	B
4955	CG	LEU	278	-11.868	35.358	73.838	1.00	25.67	B
4956	CD2	LEU	278	-12.104	36.848	73.863	1.00	26.14	B
4957	CD1	LEU	278	-12.735	34.631	74.880	1.00	25.47	B
4958	C	LEU	278	-7.994	35.648	73.520	1.00	18.30	B
4959	O	LEU	278	-7.545	36.608	74.150	1.00	19.70	B
4960	N	MET	279	-7.252	34.541	73.319	1.00	19.49	B
4961	CA	MET	279	-5.837	34.574	73.740	1.00	19.53	B
4962	CB	MET	279	-5.202	33.205	73.600	1.00	19.87	B
4963	CG	MET	279	-5.986	32.085	74.264	1.00	19.95	B
4964	SD	MET	279	-5.197	30.502	73.968	1.00	22.16	B
4965	CE	MET	279	-6.496	29.371	74.455	1.00	22.34	B
4966	C	MET	279	-5.023	35.550	72.913	1.00	21.00	B
4967	O	MET	279	-4.159	36.294	73.426	1.00	20.65	B
4968	N	VAL	280	-5.405	35.759	71.635	1.00	20.55	B
4969	CA	VAL	280	-4.738	36.800	70.853	1.00	19.11	B
4970	CB	VAL	280	-5.061	36.677	69.321	1.00	20.89	B
4971	CG1	VAL	280	-4.516	37.881	68.551	1.00	19.38	B
4972	CG2	VAL	280	-4.493	35.369	68.775	1.00	18.88	B
4973	C	VAL	280	-5.214	38.144	71.374	1.00	20.36	B
4974	O	VAL	280	-4.408	39.065	71.561	1.00	18.34	B
4975	N	ALA	281	-6.507	38.281	71.737	1.00	19.24	B
4976	CA	ALA	281	-6.975	39.620	72.148	1.00	20.88	B
4977	CB	ALA	281	-8.491	39.556	72.402	1.00	22.00	B
4978	C	ALA	281	-6.293	40.164	73.395	1.00	20.35	B
4979	O	ALA	281	-5.938	41.340	73.517	1.00	22.71	B
4980	N	LYS	282	-6.003	39.261	74.326	1.00	20.86	B
4981	CA	LYS	282	-5.389	39.607	75.600	1.00	22.27	B
4982	CB	LYS	282	-5.374	38.346	76.506	1.00	21.78	B
4983	CG	LYS	282	-4.629	38.624	77.830	1.00	25.23	B
4984	CD	LYS	282	-4.444	37.340	78.625	1.00	24.84	B
4985	CE	LYS	282	-3.471	37.568	79.802	1.00	26.57	B
4986	NZ	LYS	282	-3.093	36.253	80.366	1.00	26.17	B
4987	C	LYS	282	-3.973	40.126	75.411	1.00	23.61	B
4988	O	LYS	282	-3.455	40.929	76.190	1.00	23.04	B
4989	N	ASN	283	-3.257	39.565	74.431	1.00	22.39	B
4990	CA	ASN	283	-1.846	39.928	74.252	1.00	21.71	B
4991	CB	ASN	283	-1.121	38.583	73.976	1.00	21.25	B
4992	CG	ASN	283	-1.243	37.725	75.255	1.00	23.44	B
4993	OD1	ASN	283	-0.471	37.967	76.191	1.00	23.77	B
4994	ND2	ASN	283	-2.088	36.721	75.343	1.00	21.55	B
4995	C	ASN	283	-1.552	40.913	73.151	1.00	21.06	B
4996	O	ASN	283	-0.396	41.341	73.072	1.00	21.73	B
4997	N	ILE	284	-2.472	41.229	72.245	1.00	20.12	B
4998	CA	ILE	284	-2.068	41.940	71.020	1.00	19.95	B
4999	CB	ILE	284	-3.168	41.791	69.926	1.00	20.33	B
5000	CG2	ILE	284	-4.349	42.702	70.204	1.00	19.28	B

5001	CG1	ILE	284	-2.545	42.172	68.551	1.00	22.20	B
5002	CD1	ILE	284	-1.701	41.017	68.025	1.00	19.74	B
5003	C	ILE	284	-1.685	43.374	71.172	1.00	18.24	B
5004	O	ILE	284	-0.680	43.802	70.567	1.00	17.37	B
5005	N	GLU	285	-2.223	44.176	72.104	1.00	19.63	B
5006	CA	GLU	285	-1.807	45.548	72.254	1.00	19.85	B
5007	CB	GLU	285	-2.656	46.404	73.204	1.00	23.34	B
5008	CG	GLU	285	-4.113	46.332	72.892	1.00	28.25	B
5009	CD	GLU	285	-4.950	46.886	74.064	1.00	30.04	B
5010	OE1	GLU	285	-5.555	46.026	74.748	1.00	30.75	B
5011	OE2	GLU	285	-4.905	48.109	74.215	1.00	28.37	B
5012	C	GLU	285	-0.371	45.610	72.760	1.00	20.50	B
5013	O	GLU	285	0.354	46.521	72.328	1.00	20.03	B
5014	N	ASN	286	0.000	44.672	73.635	1.00	20.12	B
5015	CA	ASN	286	1.409	44.689	74.075	1.00	20.92	B
5016	CB	ASN	286	1.631	43.638	75.167	1.00	23.97	B
5017	CG	ASN	286	0.951	43.931	76.494	1.00	27.46	B
5018	OD1	ASN	286	0.637	45.068	76.838	1.00	30.66	B
5019	ND2	ASN	286	0.716	42.905	77.291	1.00	30.06	B
5020	C	ASN	286	2.358	44.405	72.910	1.00	18.86	B
5021	O	ASN	286	3.454	44.955	72.867	1.00	18.21	B
5022	N	ALA	287	2.023	43.529	71.960	1.00	18.22	B
5023	CA	ALA	287	2.953	43.315	70.818	1.00	20.10	B
5024	CB	ALA	287	2.511	42.080	70.016	1.00	19.75	B
5025	C	ALA	287	3.021	44.544	69.926	1.00	18.86	B
5026	O	ALA	287	4.084	44.973	69.485	1.00	21.40	B
5027	N	ALA	288	1.931	45.242	69.672	1.00	19.69	B
5028	CA	ALA	288	1.877	46.486	68.906	1.00	20.76	B
5029	CB	ALA	288	0.407	46.944	68.814	1.00	18.71	B
5030	C	ALA	288	2.708	47.586	69.534	1.00	21.70	B
5031	O	ALA	288	3.608	48.189	68.957	1.00	21.81	B
5032	N	GLU	289	2.515	47.753	70.868	1.00	23.39	B
5033	CA	GLU	289	3.205	48.774	71.637	1.00	24.00	B
5034	CB	GLU	289	2.681	48.845	73.114	1.00	27.17	B
5035	CG	GLU	289	1.232	49.280	73.130	1.00	35.05	B
5036	CD	GLU	289	0.407	49.305	74.411	1.00	39.46	B
5037	OE1	GLU	289	0.395	48.320	75.195	1.00	41.32	B
5038	OE2	GLU	289	-0.305	50.327	74.642	1.00	40.70	B
5039	C	GLU	289	4.695	48.525	71.684	1.00	22.51	B
5040	O	GLU	289	5.466	49.478	71.569	1.00	22.73	B
5041	N	LYS	290	5.070	47.253	71.839	1.00	20.97	B
5042	CA	LYS	290	6.487	46.923	71.888	1.00	22.45	B
5043	CB	LYS	290	6.709	45.455	72.206	1.00	21.35	B
5044	CG	LYS	290	8.158	45.018	72.272	1.00	26.33	B
5045	CD	LYS	290	8.304	43.599	72.868	1.00	30.29	B
5046	CE	LYS	290	9.796	43.226	72.880	1.00	30.50	B
5047	NZ	LYS	290	9.952	41.875	73.506	1.00	31.52	B
5048	C	LYS	290	7.137	47.258	70.529	1.00	22.29	B
5049	O	LYS	290	8.279	47.671	70.537	1.00	20.37	B
5050	N	ALA	291	6.420	47.025	69.425	1.00	22.31	B
5051	CA	ALA	291	7.010	47.304	68.110	1.00	23.67	B
5052	CB	ALA	291	6.223	46.530	67.045	1.00	22.69	B

5053	C	ALA	291	7.015	48.776	67.683	1.00	22.63	B
5054	O	ALA	291	7.965	49.262	67.026	1.00	20.29	B
5055	N	LEU	292	5.959	49.466	68.074	1.00	21.09	B
5056	CA	LEU	292	5.778	50.862	67.678	1.00	22.30	B
5057	CB	LEU	292	4.285	51.008	67.371	1.00	20.82	B
5058	CG	LEU	292	3.811	50.103	66.212	1.00	22.17	B
5059	CD2	LEU	292	4.468	50.583	64.907	1.00	21.85	B
5060	CD1	LEU	292	2.295	50.171	66.117	1.00	23.60	B
5061	C	LEU	292	6.248	51.940	68.638	1.00	25.08	B
5062	O	LEU	292	6.779	53.007	68.223	1.00	21.43	B
5063	N	SER	293	6.298	51.610	69.948	1.00	24.60	B
5064	CA	SER	293	6.843	52.638	70.869	1.00	28.76	B
5065	CB	SER	293	6.729	52.236	72.353	1.00	27.81	B
5066	OG	SER	293	5.327	52.280	72.664	1.00	31.12	B
5067	C	SER	293	8.253	53.052	70.542	1.00	28.18	B
5068	O	SER	293	8.565	54.245	70.546	1.00	29.17	B
5069	N	PRO	294	9.184	52.185	70.179	1.00	30.83	B
5070	CA	PRO	294	10.532	52.588	69.789	1.00	32.60	B
5071	CD	PRO	294	9.014	50.707	70.150	1.00	30.64	B
5072	CB	PRO	294	11.221	51.289	69.374	1.00	33.07	B
5073	CG	PRO	294	10.446	50.226	70.086	1.00	32.36	B
5074	C	PRO	294	10.590	53.579	68.631	1.00	35.35	B
5075	O	PRO	294	11.626	54.234	68.415	1.00	34.68	B
5076	N	LEU	295	9.536	53.638	67.818	1.00	34.49	B
5077	CA	LEU	295	9.417	54.513	66.679	1.00	35.33	B
5078	CB	LEU	295	8.662	53.766	65.560	1.00	37.28	B
5079	CG	LEU	295	9.477	52.920	64.581	1.00	38.81	B
5080	CD2	LEU	295	8.746	51.638	64.198	1.00	39.17	B
5081	CD1	LEU	295	10.878	52.584	65.048	1.00	40.23	B
5082	C	LEU	295	8.625	55.766	67.031	1.00	34.72	B
5083	O	LEU	295	8.343	56.566	66.144	1.00	33.16	B
5084	N	GLY	296	8.207	55.888	68.297	1.00	32.08	B
5085	CA	GLY	296	7.417	57.025	68.714	1.00	30.94	B
5086	C	GLY	296	6.003	56.960	68.177	1.00	29.68	B
5087	O	GLY	296	5.339	57.979	68.025	1.00	30.58	B
5088	N	ILE	297	5.504	55.781	67.829	1.00	28.93	B
5089	CA	ILE	297	4.162	55.700	67.271	1.00	27.98	B
5090	CB	ILE	297	4.196	54.756	66.055	1.00	29.23	B
5091	CG2	ILE	297	2.770	54.493	65.608	1.00	28.73	B
5092	CG1	ILE	297	5.134	55.385	65.002	1.00	29.11	B
5093	CD1	ILE	297	5.184	54.647	63.667	1.00	29.61	B
5094	C	ILE	297	3.208	55.137	68.305	1.00	29.24	B
5095	O	ILE	297	3.448	54.026	68.774	1.00	26.04	B
5096	N	THR	298	2.129	55.872	68.586	1.00	28.94	B
5097	CA	THR	298	1.171	55.364	69.577	1.00	31.35	B
5098	CB	THR	298	1.160	56.274	70.828	1.00	33.69	B
5099	OG1	THR	298	1.076	57.636	70.377	1.00	34.34	B
5100	CG2	THR	298	2.431	56.102	71.635	1.00	34.41	B
5101	C	THR	298	-0.233	55.324	69.014	1.00	30.57	B
5102	O	THR	298	-1.145	54.760	69.629	1.00	32.05	B
5103	N	ASP	299	-0.438	55.922	67.857	1.00	29.91	B
5104	CA	ASP	299	-1.754	55.880	67.211	1.00	31.43	B

5105	CB	ASP	299	-2.025	57.228	66.540	1.00	32.66	B
5106	CG	ASP	299	-3.314	57.240	65.753	1.00	33.63	B
5107	OD1	ASP	299	-4.070	56.258	65.713	1.00	34.14	B
5108	OD2	ASP	299	-3.582	58.283	65.114	1.00	37.07	B
5109	C	ASP	299	-1.794	54.717	66.221	1.00	30.88	B
5110	O	ASP	299	-1.306	54.815	65.091	1.00	29.67	B
5111	N	TRP	300	-2.507	53.654	66.575	1.00	29.51	B
5112	CA	TRP	300	-2.663	52.451	65.798	1.00	29.64	B
5113	CB	TRP	300	-3.461	51.372	66.511	1.00	28.99	B
5114	CG	TRP	300	-3.030	51.004	67.903	1.00	32.00	B
5115	CD2	TRP	300	-1.724	51.098	68.469	1.00	31.35	B
5116	CD1	TRP	300	-3.848	50.537	68.900	1.00	30.36	B
5117	NE1	TRP	300	-3.124	50.326	70.052	1.00	30.99	B
5118	CE2	TRP	300	-1.816	50.637	69.801	1.00	33.33	B
5119	CE3	TRP	300	-0.484	51.486	67.982	1.00	33.69	B
5120	CZ2	TRP	300	-0.715	50.618	70.663	1.00	33.05	B
5121	CZ3	TRP	300	0.617	51.459	68.826	1.00	33.58	B
5122	CH2	TRP	300	0.480	51.026	70.145	1.00	34.60	B
5123	C	TRP	300	-3.291	52.646	64.410	1.00	30.15	B
5124	O	TRP	300	-3.070	51.810	63.516	1.00	27.40	B
5125	N	ASN	301	-4.042	53.738	64.235	1.00	28.62	B
5126	CA	ASN	301	-4.662	53.984	62.943	1.00	28.51	B
5127	CB	ASN	301	-5.999	54.705	63.081	1.00	29.21	B
5128	CG	ASN	301	-7.055	53.672	63.443	1.00	30.49	B
5129	OD1	ASN	301	-7.398	52.778	62.667	1.00	32.58	B
5130	ND2	ASN	301	-7.614	53.885	64.623	1.00	30.87	B
5131	C	ASN	301	-3.746	54.771	62.024	1.00	28.08	B
5132	O	ASN	301	-4.043	54.847	60.839	1.00	27.24	B
5133	N	SER	302	-2.611	55.230	62.548	1.00	27.38	B
5134	CA	SER	302	-1.657	55.926	61.691	1.00	28.99	B
5135	CB	SER	302	-0.871	56.918	62.534	1.00	29.19	B
5136	OG	SER	302	0.091	56.350	63.383	1.00	28.39	B
5137	C	SER	302	-0.742	54.941	60.948	1.00	27.37	B
5138	O	SER	302	0.178	55.410	60.274	1.00	28.02	B
5139	N	VAL	303	-0.938	53.638	61.044	1.00	26.60	B
5140	CA	VAL	303	-0.036	52.657	60.427	1.00	24.47	B
5141	CB	VAL	303	0.927	51.952	61.382	1.00	26.94	B
5142	CG1	VAL	303	1.838	52.902	62.175	1.00	26.73	B
5143	CG2	VAL	303	0.177	51.030	62.353	1.00	23.00	B
5144	C	VAL	303	-0.889	51.602	59.722	1.00	23.52	B
5145	O	VAL	303	-2.086	51.588	60.015	1.00	23.22	B
5146	N	PHE	304	-0.317	50.836	58.804	1.00	21.05	B
5147	CA	PHE	304	-1.087	49.856	58.039	1.00	22.26	B
5148	CB	PHE	304	-0.718	49.829	56.550	1.00	21.58	B
5149	CG	PHE	304	0.724	49.572	56.199	1.00	22.76	B
5150	CD1	PHE	304	1.655	50.599	56.139	1.00	22.21	B
5151	CD2	PHE	304	1.141	48.296	55.854	1.00	25.40	B
5152	CE1	PHE	304	2.966	50.345	55.832	1.00	22.11	B
5153	CE2	PHE	304	2.477	48.048	55.529	1.00	24.12	B
5154	CZ	PHE	304	3.393	49.072	55.509	1.00	23.69	B
5155	C	PHE	304	-0.838	48.507	58.695	1.00	23.31	B
5156	O	PHE	304	0.151	48.437	59.448	1.00	24.50	B

5157	N	TRP	305	-1.717	47.552	58.594	1.00	23.36	B
5158	CA	TRP	305	-1.655	46.298	59.330	1.00	24.97	B
5159	CB	TRP	305	-2.870	46.216	60.328	1.00	24.89	B
5160	CG	TRP	305	-2.765	47.319	61.334	1.00	25.03	B
5161	CD2	TRP	305	-2.010	47.280	62.562	1.00	25.82	B
5162	CD1	TRP	305	-3.232	48.600	61.221	1.00	25.61	B
5163	NE1	TRP	305	-2.827	49.342	62.298	1.00	24.83	B
5164	CE2	TRP	305	-2.106	48.538	63.149	1.00	24.79	B
5165	CE3	TRP	305	-1.288	46.258	63.219	1.00	24.79	B
5166	CZ2	TRP	305	-1.483	48.842	64.367	1.00	26.05	B
5167	CZ3	TRP	305	-0.721	46.562	64.445	1.00	24.46	B
5168	CH2	TRP	305	-0.777	47.838	64.998	1.00	25.19	B
5169	C	TRP	305	-1.787	45.096	58.424	1.00	24.85	B
5170	O	TRP	305	-2.672	45.104	57.578	1.00	26.94	B
5171	N	MET	306	-0.972	44.077	58.531	1.00	21.95	B
5172	CA	MET	306	-1.054	42.816	57.822	1.00	21.34	B
5173	CB	MET	306	0.209	42.563	56.995	1.00	21.09	B
5174	CG	MET	306	0.421	43.672	55.972	1.00	20.03	B
5175	SD	MET	306	2.139	44.089	55.648	1.00	22.51	B
5176	CE	MET	306	2.495	45.049	57.167	1.00	26.87	B
5177	C	MET	306	-1.211	41.711	58.880	1.00	20.66	B
5178	O	MET	306	-0.221	41.358	59.534	1.00	20.48	B
5179	N	VAL	307	-2.402	41.163	59.023	1.00	20.73	B
5180	CA	VAL	307	-2.707	40.294	60.137	1.00	18.05	B
5181	CB	VAL	307	-3.902	40.811	61.011	1.00	17.93	B
5182	CG1	VAL	307	-4.095	39.898	62.206	1.00	18.14	B
5183	CG2	VAL	307	-3.687	42.236	61.425	1.00	18.06	B
5184	C	VAL	307	-3.014	38.909	59.662	1.00	18.96	B
5185	O	VAL	307	-3.948	38.717	58.893	1.00	19.14	B
5186	N	HIS	308	-2.203	37.946	60.168	1.00	17.07	B
5187	CA	HIS	308	-2.425	36.566	59.814	1.00	17.63	B
5188	ND1	HIS	308	-1.407	33.596	58.952	1.00	17.99	B
5189	CG	HIS	308	-1.774	34.169	60.146	1.00	17.55	B
5190	CB	HIS	308	-1.500	35.594	60.541	1.00	16.64	B
5191	NE2	HIS	308	-2.452	32.080	60.105	1.00	19.33	B
5192	CD2	HIS	308	-2.392	33.200	60.862	1.00	16.86	B
5193	CE1	HIS	308	-1.784	32.330	58.955	1.00	20.71	B
5194	C	HIS	308	-3.862	36.171	60.146	1.00	20.15	B
5195	O	HIS	308	-4.196	36.218	61.336	1.00	20.31	B
5196	N	PRO	309	-4.609	35.703	59.157	1.00	19.60	B
5197	CA	PRO	309	-6.036	35.406	59.367	1.00	18.69	B
5198	CD	PRO	309	-4.216	35.666	57.711	1.00	17.25	B
5199	CB	PRO	309	-6.662	35.672	57.992	1.00	18.47	B
5200	CG	PRO	309	-5.542	35.330	57.035	1.00	19.57	B
5201	C	PRO	309	-6.227	34.020	59.848	1.00	17.62	B
5202	O	PRO	309	-6.848	33.191	59.186	1.00	20.03	B
5203	N	GLY	310	-5.701	33.632	61.041	1.00	18.19	B
5204	CA	GLY	310	-5.794	32.245	61.493	1.00	15.27	B
5205	C	GLY	310	-7.267	31.831	61.383	1.00	15.92	B
5206	O	GLY	310	-7.560	30.671	61.100	1.00	16.29	B
5207	N	GLY	311	-8.160	32.765	61.656	1.00	17.99	B
5208	CA	GLY	311	-9.596	32.551	61.436	1.00	20.00	B

5209	C	GLY	311	-10.183	33.951	61.373	1.00	19.56	B
5210	O	GLY	311	-9.534	34.864	61.873	1.00	20.74	B
5211	N	ARG	312	-11.407	34.144	60.868	1.00	20.47	B
5212	CA	ARG	312	-12.059	35.449	60.868	1.00	21.63	B
5213	CB	ARG	312	-13.527	35.256	60.375	1.00	24.00	B
5214	CG	ARG	312	-14.198	36.603	60.071	1.00	24.43	B
5215	CD	ARG	312	-15.709	36.524	60.340	1.00	28.53	B
5216	NE	ARG	312	-15.986	36.682	61.777	1.00	29.01	B
5217	CZ	ARG	312	-16.395	35.674	62.557	1.00	30.38	B
5218	NH1	ARG	312	-16.772	34.499	62.084	1.00	29.87	B
5219	NH2	ARG	312	-16.516	35.880	63.870	1.00	29.12	B
5220	C	ARG	312	-12.135	36.173	62.222	1.00	20.82	B
5221	O	ARG	312	-11.958	37.366	62.433	1.00	21.21	B
5222	N	ALA	313	-12.359	35.383	63.262	1.00	21.23	B
5223	CA	ALA	313	-12.522	35.849	64.666	1.00	22.59	B
5224	CB	ALA	313	-13.057	34.734	65.538	1.00	20.95	B
5225	C	ALA	313	-11.200	36.359	65.219	1.00	20.52	B
5226	O	ALA	313	-11.195	37.326	65.970	1.00	21.79	B
5227	N	ILE	314	-10.091	35.774	64.710	1.00	20.33	B
5228	CA	ILE	314	-8.813	36.388	65.138	1.00	20.36	B
5229	CB	ILE	314	-7.647	35.495	64.674	1.00	20.12	B
5230	CG2	ILE	314	-6.334	36.309	64.729	1.00	21.33	B
5231	CG1	ILE	314	-7.638	34.216	65.466	1.00	20.77	B
5232	CD1	ILE	314	-6.582	33.203	65.035	1.00	24.17	B
5233	C	ILE	314	-8.697	37.794	64.591	1.00	20.44	B
5234	O	ILE	314	-8.270	38.752	65.252	1.00	22.07	B
5235	N	LEU	315	-9.019	37.994	63.274	1.00	20.11	B
5236	CA	LEU	315	-8.984	39.339	62.709	1.00	18.16	B
5237	CB	LEU	315	-9.481	39.390	61.240	1.00	19.31	B
5238	CG	LEU	315	-8.629	38.553	60.225	1.00	18.63	B
5239	CD2	LEU	315	-7.183	38.975	60.278	1.00	16.29	B
5240	CD1	LEU	315	-9.181	38.712	58.804	1.00	19.25	B
5241	C	LEU	315	-9.871	40.276	63.539	1.00	18.51	B
5242	O	LEU	315	-9.550	41.443	63.803	1.00	20.92	B
5243	N	ASP	316	-11.070	39.827	63.846	1.00	17.94	B
5244	CA	ASP	316	-12.060	40.658	64.535	1.00	21.13	B
5245	CB	ASP	316	-13.352	39.852	64.669	1.00	22.57	B
5246	CG	ASP	316	-14.070	39.660	63.321	1.00	25.48	B
5247	OD1	ASP	316	-13.674	40.262	62.282	1.00	24.54	B
5248	OD2	ASP	316	-15.020	38.860	63.289	1.00	23.59	B
5249	C	ASP	316	-11.526	41.095	65.906	1.00	22.99	B
5250	O	ASP	316	-11.613	42.276	66.275	1.00	21.67	B
5251	N	GLN	317	-10.904	40.140	66.604	1.00	22.42	B
5252	CA	GLN	317	-10.360	40.506	67.953	1.00	22.73	B
5253	CB	GLN	317	-9.911	39.228	68.636	1.00	22.43	B
5254	CG	GLN	317	-11.056	38.391	69.222	1.00	23.87	B
5255	CD	GLN	317	-11.747	39.122	70.380	1.00	24.67	B
5256	OE1	GLN	317	-11.435	40.246	70.782	1.00	23.10	B
5257	NE2	GLN	317	-12.762	38.460	70.919	1.00	26.57	B
5258	C	GLN	317	-9.238	41.497	67.816	1.00	23.11	B
5259	O	GLN	317	-9.156	42.493	68.549	1.00	23.40	B
5260	N	VAL	318	-8.397	41.338	66.756	1.00	22.30	B

5261	CA	VAL	318	-7.305	42.320	66.610	1.00	21.68	B
5262	CB	VAL	318	-6.277	41.896	65.529	1.00	20.13	B
5263	CG1	VAL	318	-5.305	43.002	65.214	1.00	19.83	B
5264	CG2	VAL	318	-5.580	40.612	65.982	1.00	21.31	B
5265	C	VAL	318	-7.865	43.688	66.335	1.00	21.70	B
5266	O	VAL	318	-7.373	44.694	66.872	1.00	19.93	B
5267	N	GLU	319	-8.872	43.758	65.412	1.00	21.94	B
5268	CA	GLU	319	-9.491	45.053	65.091	1.00	23.27	B
5269	CB	GLU	319	-10.589	44.781	64.056	1.00	26.24	B
5270	CG	GLU	319	-11.395	45.943	63.519	1.00	29.12	B
5271	CD	GLU	319	-12.405	45.393	62.505	1.00	32.43	B
5272	OE1	GLU	319	-12.103	45.337	61.287	1.00	32.08	B
5273	OE2	GLU	319	-13.434	44.837	62.945	1.00	33.65	B
5274	C	GLU	319	-10.168	45.698	66.325	1.00	22.56	B
5275	O	GLU	319	-9.996	46.893	66.538	1.00	21.16	B
5276	N	ARG	320	-10.779	44.858	67.154	1.00	21.69	B
5277	CA	ARG	320	-11.410	45.381	68.390	1.00	23.35	B
5278	CB	ARG	320	-12.202	44.246	69.060	1.00	23.74	B
5279	CG	ARG	320	-12.782	44.760	70.420	1.00	25.66	B
5280	CD	ARG	320	-13.698	43.703	71.016	1.00	25.35	B
5281	NE	ARG	320	-12.941	42.596	71.621	1.00	26.01	B
5282	CZ	ARG	320	-12.502	42.520	72.886	1.00	25.36	B
5283	NH1	ARG	320	-12.793	43.513	73.735	1.00	22.52	B
5284	NH2	ARG	320	-11.849	41.417	73.296	1.00	22.41	B
5285	C	ARG	320	-10.374	45.888	69.365	1.00	24.31	B
5286	O	ARG	320	-10.303	47.082	69.618	1.00	25.73	B
5287	N	LYS	321	-9.399	45.049	69.751	1.00	24.51	B
5288	CA	LYS	321	-8.379	45.431	70.734	1.00	25.04	B
5289	CB	LYS	321	-7.697	44.101	71.190	1.00	26.27	B
5290	CG	LYS	321	-8.653	43.378	72.207	1.00	26.39	B
5291	CD	LYS	321	-8.195	43.887	73.557	1.00	30.28	B
5292	CE	LYS	321	-9.029	43.942	74.743	1.00	31.04	B
5293	NZ	LYS	321	-9.608	45.187	75.225	1.00	33.95	B
5294	C	LYS	321	-7.472	46.540	70.285	1.00	26.90	B
5295	O	LYS	321	-7.150	47.466	71.081	1.00	23.68	B
5296	N	LEU	322	-7.238	46.718	68.961	1.00	23.57	B
5297	CA	LEU	322	-6.435	47.852	68.517	1.00	24.43	B
5298	CB	LEU	322	-5.438	47.544	67.382	1.00	24.57	B
5299	CG	LEU	322	-4.381	46.474	67.731	1.00	25.26	B
5300	CD2	LEU	322	-3.464	46.950	68.854	1.00	25.41	B
5301	CD1	LEU	322	-3.551	46.075	66.505	1.00	25.95	B
5302	C	LEU	322	-7.332	49.018	68.132	1.00	23.91	B
5303	O	LEU	322	-6.806	50.057	67.724	1.00	22.61	B
5304	N	ASN	323	-8.653	48.845	68.240	1.00	25.03	B
5305	CA	ASN	323	-9.538	49.965	67.936	1.00	28.29	B
5306	CB	ASN	323	-9.422	51.126	68.954	1.00	31.89	B
5307	CG	ASN	323	-10.763	51.879	68.879	1.00	37.60	B
5308	OD1	ASN	323	-10.786	53.101	68.699	1.00	39.93	B
5309	ND2	ASN	323	-11.895	51.176	68.964	1.00	38.45	B
5310	C	ASN	323	-9.313	50.519	66.521	1.00	28.33	B
5311	O	ASN	323	-9.227	51.714	66.293	1.00	25.80	B
5312	N	LEU	324	-9.202	49.604	65.567	1.00	28.13	B

5313	CA	LEU	324	-8.933	49.902	64.180	1.00	29.48	B
5314	CB	LEU	324	-8.423	48.575	63.569	1.00	28.51	B
5315	CG	LEU	324	-6.923	48.372	63.396	1.00	30.27	B
5316	CD2	LEU	324	-6.565	46.882	63.341	1.00	28.32	B
5317	CD1	LEU	324	-6.002	49.137	64.326	1.00	27.79	B
5318	C	LEU	324	-10.181	50.368	63.448	1.00	29.19	B
5319	O	LEU	324	-11.238	49.776	63.601	1.00	27.17	B
5320	N	LYS	325	-10.039	51.350	62.562	1.00	33.48	B
5321	CA	LYS	325	-11.117	51.696	61.640	1.00	34.34	B
5322	CB	LYS	325	-10.679	52.796	60.698	1.00	36.67	B
5323	CG	LYS	325	-10.462	54.151	61.347	1.00	40.37	B
5324	CD	LYS	325	-10.216	55.199	60.259	1.00	43.88	B
5325	CE	LYS	325	-8.958	56.003	60.542	1.00	45.94	B
5326	NZ	LYS	325	-8.243	56.352	59.268	1.00	48.86	B
5327	C	LYS	325	-11.489	50.437	60.864	1.00	36.02	B
5328	O	LYS	325	-10.691	49.501	60.657	1.00	32.28	B
5329	N	GLU	326	-12.735	50.396	60.397	1.00	36.53	B
5330	CA	GLU	326	-13.322	49.268	59.705	1.00	38.57	B
5331	CB	GLU	326	-14.808	49.610	59.371	1.00	42.33	B
5332	CG	GLU	326	-15.651	49.277	60.588	1.00	48.46	B
5333	CD	GLU	326	-16.884	50.070	60.959	1.00	50.98	B
5334	OE1	GLU	326	-17.559	50.689	60.096	1.00	52.47	B
5335	OE2	GLU	326	-17.211	50.069	62.179	1.00	52.37	B
5336	C	GLU	326	-12.635	48.741	58.449	1.00	35.41	B
5337	O	GLU	326	-12.849	47.584	58.079	1.00	33.05	B
5338	N	ASP	327	-11.855	49.565	57.779	1.00	33.65	B
5339	CA	ASP	327	-11.150	49.105	56.597	1.00	36.31	B
5340	CB	ASP	327	-11.257	50.183	55.507	1.00	39.96	B
5341	CG	ASP	327	-10.669	51.502	55.930	1.00	45.67	B
5342	OD1	ASP	327	-10.291	51.751	57.100	1.00	48.30	B
5343	OD2	ASP	327	-10.657	52.409	55.062	1.00	49.05	B
5344	C	ASP	327	-9.693	48.777	56.864	1.00	32.45	B
5345	O	ASP	327	-9.055	48.309	55.915	1.00	30.64	B
5346	N	LYS	328	-9.167	49.007	58.082	1.00	28.05	B
5347	CA	LYS	328	-7.747	48.697	58.273	1.00	25.57	B
5348	CB	LYS	328	-7.294	49.051	59.709	1.00	25.04	B
5349	CG	LYS	328	-7.158	50.594	59.741	1.00	26.94	B
5350	CD	LYS	328	-5.687	50.955	59.478	1.00	26.71	B
5351	CE	LYS	328	-5.597	52.434	59.374	1.00	30.21	B
5352	NZ	LYS	328	-4.359	52.984	58.773	1.00	29.75	B
5353	C	LYS	328	-7.367	47.293	57.853	1.00	22.32	B
5354	O	LYS	328	-6.269	47.121	57.305	1.00	21.65	B
5355	N	LEU	329	-8.165	46.286	58.130	1.00	19.10	B
5356	CA	LEU	329	-7.811	44.905	57.824	1.00	20.35	B
5357	CB	LEU	329	-8.246	43.988	58.953	1.00	20.66	B
5358	CG	LEU	329	-7.625	44.367	60.337	1.00	22.03	B
5359	CD2	LEU	329	-6.111	44.528	60.248	1.00	22.71	B
5360	CD1	LEU	329	-8.061	43.297	61.325	1.00	23.16	B
5361	C	LEU	329	-8.349	44.383	56.493	1.00	20.28	B
5362	O	LEU	329	-8.392	43.197	56.280	1.00	19.00	B
5363	N	ARG	330	-8.760	45.279	55.610	1.00	23.20	B
5364	CA	ARG	330	-9.284	44.875	54.303	1.00	24.04	B

5365	CB	ARG	330	-9.453	46.132	53.424	1.00	26.77	B
5366	CG	ARG	330	-10.046	45.772	52.057	1.00	31.36	B
5367	CD	ARG	330	-9.558	46.633	50.901	1.00	33.97	B
5368	NE	ARG	330	-8.123	46.497	50.624	1.00	35.77	B
5369	CZ	ARG	330	-7.493	45.536	49.966	1.00	37.17	B
5370	NH1	ARG	330	-6.168	45.684	49.904	1.00	36.94	B
5371	NH2	ARG	330	-8.130	44.507	49.416	1.00	35.70	B
5372	C	ARG	330	-8.352	43.901	53.612	1.00	21.92	B
5373	O	ARG	330	-8.758	42.840	53.148	1.00	23.05	B
5374	N	ALA	331	-7.062	44.251	53.487	1.00	23.62	B
5375	CA	ALA	331	-6.152	43.396	52.711	1.00	22.13	B
5376	CB	ALA	331	-4.805	44.092	52.541	1.00	20.83	B
5377	C	ALA	331	-6.005	42.026	53.326	1.00	22.56	B
5378	O	ALA	331	-5.973	41.014	52.634	1.00	19.86	B
5379	N	SER	332	-6.054	41.933	54.683	1.00	20.56	B
5380	CA	SER	332	-5.993	40.664	55.376	1.00	18.63	B
5381	CB	SER	332	-5.796	40.926	56.918	1.00	19.54	B
5382	OG	SER	332	-4.538	41.563	57.076	1.00	21.55	B
5383	C	SER	332	-7.257	39.866	55.187	1.00	17.66	B
5384	O	SER	332	-7.263	38.648	54.994	1.00	17.37	B
5385	N	ARG	333	-8.407	40.587	55.268	1.00	17.66	B
5386	CA	ARG	333	-9.653	39.840	55.053	1.00	19.55	B
5387	CB	ARG	333	-10.859	40.731	55.411	1.00	22.26	B
5388	CG	ARG	333	-10.991	41.072	56.906	1.00	22.49	B
5389	CD	ARG	333	-12.232	41.922	57.195	1.00	23.61	B
5390	NE	ARG	333	-12.174	42.505	58.557	1.00	23.67	B
5391	CZ	ARG	333	-12.452	41.727	59.616	1.00	21.99	B
5392	NH1	ARG	333	-12.806	40.459	59.458	1.00	20.57	B
5393	NH2	ARG	333	-12.376	42.243	60.844	1.00	23.81	B
5394	C	ARG	333	-9.750	39.432	53.566	1.00	17.99	B
5395	O	ARG	333	-10.373	38.431	53.266	1.00	17.75	B
5396	N	HIS	334	-9.270	40.276	52.665	1.00	20.00	B
5397	CA	HIS	334	-9.342	39.895	51.221	1.00	21.81	B
5398	ND1	HIS	334	-9.552	41.251	48.032	1.00	29.33	B
5399	CG	HIS	334	-8.665	40.805	48.969	1.00	27.40	B
5400	CB	HIS	334	-8.819	41.098	50.436	1.00	24.11	B
5401	NE2	HIS	334	-8.080	40.166	46.964	1.00	29.21	B
5402	CD2	HIS	334	-7.713	40.103	48.291	1.00	27.91	B
5403	CE1	HIS	334	-9.180	40.853	46.829	1.00	29.04	B
5404	C	HIS	334	-8.591	38.606	50.922	1.00	20.31	B
5405	O	HIS	334	-9.089	37.653	50.282	1.00	18.30	B
5406	N	VAL	335	-7.370	38.457	51.474	1.00	18.88	B
5407	CA	VAL	335	-6.608	37.204	51.276	1.00	18.05	B
5408	CB	VAL	335	-5.172	37.361	51.835	1.00	16.25	B
5409	CG1	VAL	335	-4.408	36.038	51.905	1.00	14.81	B
5410	CG2	VAL	335	-4.370	38.358	51.024	1.00	17.43	B
5411	C	VAL	335	-7.352	36.022	51.845	1.00	18.69	B
5412	O	VAL	335	-7.462	34.911	51.264	1.00	16.92	B
5413	N	LEU	336	-7.857	36.177	53.089	1.00	18.84	B
5414	CA	LEU	336	-8.618	35.068	53.695	1.00	19.92	B
5415	CB	LEU	336	-9.112	35.538	55.092	1.00	18.93	B
5416	CG	LEU	336	-10.066	34.551	55.785	1.00	19.29	B

5417	CD2	LEU	336	-10.662	35.253	57.023	1.00	19.97	B
5418	CD1	LEU	336	-9.366	33.235	56.203	1.00	18.15	B
5419	C	LEU	336	-9.823	34.722	52.808	1.00	19.48	B
5420	O	LEU	336	-10.203	33.582	52.645	1.00	20.21	B
5421	N	SER	337	-10.528	35.740	52.296	1.00	20.81	B
5422	CA	SER	337	-11.673	35.416	51.431	1.00	23.18	B
5423	CB	SER	337	-12.370	36.729	51.034	1.00	24.45	B
5424	OG	SER	337	-13.518	36.378	50.302	1.00	26.44	B
5425	C	SER	337	-11.290	34.649	50.165	1.00	23.02	B
5426	O	SER	337	-11.873	33.600	49.897	1.00	22.24	B
5427	N	GLU	338	-10.259	35.081	49.455	1.00	22.57	B
5428	CA	GLU	338	-9.929	34.488	48.138	1.00	23.78	B
5429	CB	GLU	338	-9.131	35.534	47.340	1.00	25.65	B
5430	CG	GLU	338	-9.970	36.764	47.019	1.00	29.62	B
5431	CD	GLU	338	-11.085	36.437	46.034	1.00	33.44	B
5432	OE1	GLU	338	-11.086	35.397	45.350	1.00	34.88	B
5433	OE2	GLU	338	-12.028	37.240	45.911	1.00	35.93	B
5434	C	GLU	338	-9.093	33.245	48.215	1.00	23.79	B
5435	O	GLU	338	-9.026	32.430	47.283	1.00	22.08	B
5436	N	TYR	339	-8.427	32.976	49.366	1.00	20.54	B
5437	CA	TYR	339	-7.572	31.801	49.454	1.00	19.28	B
5438	CB	TYR	339	-6.097	32.268	49.464	1.00	20.25	B
5439	CG	TYR	339	-5.684	33.114	48.294	1.00	21.60	B
5440	CD1	TYR	339	-5.299	32.478	47.107	1.00	22.56	B
5441	CD2	TYR	339	-5.709	34.480	48.355	1.00	20.36	B
5442	CE1	TYR	339	-4.931	33.258	46.020	1.00	24.72	B
5443	CE2	TYR	339	-5.263	35.261	47.295	1.00	23.36	B
5444	CZ	TYR	339	-4.936	34.617	46.110	1.00	24.79	B
5445	OH	TYR	339	-4.534	35.348	45.019	1.00	27.21	B
5446	C	TYR	339	-7.681	30.965	50.745	1.00	19.15	B
5447	O	TYR	339	-7.009	29.946	50.763	1.00	16.70	B
5448	N	GLY	340	-8.364	31.454	51.773	1.00	19.15	B
5449	CA	GLY	340	-8.343	30.639	53.023	1.00	19.44	B
5450	C	GLY	340	-7.039	31.024	53.756	1.00	18.69	B
5451	O	GLY	340	-6.274	31.904	53.291	1.00	16.73	B
5452	N	ASN	341	-6.834	30.345	54.877	1.00	17.38	B
5453	CA	ASN	341	-5.644	30.512	55.712	1.00	17.00	B
5454	CB	ASN	341	-5.971	29.944	57.141	1.00	15.71	B
5455	CG	ASN	341	-4.786	29.996	58.098	1.00	22.10	B
5456	OD1	ASN	341	-3.607	30.225	57.760	1.00	20.41	B
5457	ND2	ASN	341	-5.035	29.790	59.417	1.00	18.04	B
5458	C	ASN	341	-4.531	29.705	55.073	1.00	12.66	B
5459	O	ASN	341	-4.573	28.497	55.103	1.00	13.74	B
5460	N	LEU	342	-3.480	30.293	54.531	1.00	13.87	B
5461	CA	LEU	342	-2.401	29.692	53.796	1.00	14.38	B
5462	CB	LEU	342	-1.947	30.703	52.713	1.00	13.53	B
5463	CG	LEU	342	-3.059	31.003	51.662	1.00	16.45	B
5464	CD2	LEU	342	-3.341	29.764	50.827	1.00	13.74	B
5465	CD1	LEU	342	-2.612	32.163	50.779	1.00	14.62	B
5466	C	LEU	342	-1.176	29.399	54.666	1.00	16.21	B
5467	O	LEU	342	-0.015	29.263	54.262	1.00	15.04	B
5468	N	ILE	343	-1.460	29.262	55.970	1.00	15.11	B

5469	CA	ILE	343	-0.383	28.954	56.925	1.00	12.87	B
5470	CB	ILE	343	-0.128	27.445	56.926	1.00	15.47	B
5471	CG2	ILE	343	0.552	27.109	58.289	1.00	17.57	B
5472	CG1	ILE	343	-1.420	26.625	56.838	1.00	14.46	B
5473	CD1	ILE	343	-1.178	25.109	56.887	1.00	16.26	B
5474	C	ILE	343	0.786	29.845	56.750	1.00	9.81	B
5475	O	ILE	343	0.620	31.104	56.721	1.00	12.86	B
5476	N	SER	344	2.035	29.387	56.667	1.00	12.79	B
5477	CA	SER	344	3.187	30.285	56.635	1.00	15.12	B
5478	CB	SER	344	4.537	29.588	56.676	1.00	17.57	B
5479	OG	SER	344	4.777	28.651	55.605	1.00	15.67	B
5480	C	SER	344	3.210	31.252	55.477	1.00	15.66	B
5481	O	SER	344	3.799	32.325	55.634	1.00	14.54	B
5482	N	ALA	345	2.565	30.927	54.352	1.00	16.70	B
5483	CA	ALA	345	2.555	31.866	53.226	1.00	18.03	B
5484	CB	ALA	345	2.162	31.047	51.946	1.00	15.91	B
5485	C	ALA	345	1.499	32.946	53.339	1.00	17.12	B
5486	O	ALA	345	1.627	33.940	52.626	1.00	17.06	B
5487	N	CYS	346	0.507	32.815	54.229	1.00	16.09	B
5488	CA	CYS	346	-0.582	33.775	54.299	1.00	16.82	B
5489	CB	CYS	346	-1.665	33.372	55.326	1.00	15.07	B
5490	SG	CYS	346	-3.346	33.982	54.889	1.00	16.25	B
5491	C	CYS	346	-0.234	35.239	54.412	1.00	16.79	B
5492	O	CYS	346	-0.687	36.081	53.561	1.00	13.66	B
5493	N	VAL	347	0.621	35.631	55.385	1.00	13.44	B
5494	CA	VAL	347	0.895	37.041	55.567	1.00	13.45	B
5495	CB	VAL	347	1.646	37.422	56.860	1.00	15.94	B
5496	CG1	VAL	347	0.748	37.144	58.075	1.00	13.87	B
5497	CG2	VAL	347	2.913	36.572	57.036	1.00	12.41	B
5498	C	VAL	347	1.700	37.559	54.355	1.00	14.78	B
5499	O	VAL	347	1.654	38.775	54.099	1.00	14.01	B
5500	N	LEU	348	2.447	36.691	53.694	1.00	15.03	B
5501	CA	LEU	348	3.216	37.183	52.508	1.00	14.71	B
5502	CB	LEU	348	4.233	36.090	52.165	1.00	13.20	B
5503	CG	LEU	348	5.101	35.645	53.362	1.00	14.08	B
5504	CD2	LEU	348	5.873	36.854	53.911	1.00	11.50	B
5505	CD1	LEU	348	6.129	34.629	52.878	1.00	13.45	B
5506	C	LEU	348	2.262	37.392	51.313	1.00	14.54	B
5507	O	LEU	348	2.382	38.426	50.654	1.00	16.63	B
5508	N	PHE	349	1.187	36.608	51.202	1.00	14.95	B
5509	CA	PHE	349	0.129	37.022	50.248	1.00	17.74	B
5510	CB	PHE	349	-1.008	36.024	50.119	1.00	15.15	B
5511	CG	PHE	349	-0.761	34.816	49.245	1.00	15.70	B
5512	CD1	PHE	349	-1.616	34.488	48.192	1.00	15.27	B
5513	CD2	PHE	349	0.314	33.972	49.493	1.00	14.11	B
5514	CE1	PHE	349	-1.368	33.348	47.444	1.00	16.03	B
5515	CE2	PHE	349	0.557	32.856	48.765	1.00	13.96	B
5516	CZ	PHE	349	-0.294	32.531	47.715	1.00	15.84	B
5517	C	PHE	349	-0.464	38.351	50.665	1.00	19.78	B
5518	O	PHE	349	-0.854	39.123	49.785	1.00	19.74	B
5519	N	ILE	350	-0.519	38.684	51.986	1.00	17.56	B
5520	CA	ILE	350	-1.132	39.939	52.372	1.00	17.74	B

5521	CB	ILE	350	-1.558	39.872	53.868	1.00	20.05	B
5522	CG2	ILE	350	-1.921	41.274	54.361	1.00	20.52	B
5523	CG1	ILE	350	-2.707	38.902	54.050	1.00	21.14	B
5524	CD1	ILE	350	-2.920	38.374	55.478	1.00	22.04	B
5525	C	ILE	350	-0.215	41.099	52.050	1.00	17.77	B
5526	O	ILE	350	-0.623	42.184	51.627	1.00	17.64	B
5527	N	ILE	351	1.112	40.911	52.209	1.00	15.39	B
5528	CA	ILE	351	2.041	41.992	51.833	1.00	17.61	B
5529	CB	ILE	351	3.483	41.508	52.029	1.00	17.55	B
5530	CG2	ILE	351	4.522	42.500	51.525	1.00	18.23	B
5531	CG1	ILE	351	3.766	41.162	53.517	1.00	19.15	B
5532	CD1	ILE	351	5.164	40.697	53.856	1.00	17.76	B
5533	C	ILE	351	1.785	42.294	50.322	1.00	18.50	B
5534	O	ILE	351	1.669	43.450	49.934	1.00	17.39	B
5535	N	ASP	352	1.656	41.234	49.549	1.00	13.85	B
5536	CA	ASP	352	1.474	41.464	48.063	1.00	19.00	B
5537	CB	ASP	352	1.548	40.106	47.393	1.00	16.36	B
5538	CG	ASP	352	1.879	40.216	45.870	1.00	17.87	B
5539	OD1	ASP	352	2.620	41.136	45.537	1.00	17.05	B
5540	OD2	ASP	352	1.552	39.234	45.190	1.00	17.08	B
5541	C	ASP	352	0.200	42.220	47.749	1.00	18.60	B
5542	O	ASP	352	0.182	43.149	46.939	1.00	21.09	B
5543	N	GLU	353	-0.875	41.885	48.453	1.00	19.67	B
5544	CA	GLU	353	-2.183	42.496	48.349	1.00	20.84	B
5545	CB	GLU	353	-3.252	41.729	49.160	1.00	17.41	B
5546	CG	GLU	353	-4.585	42.461	49.264	1.00	18.96	B
5547	CD	GLU	353	-5.299	42.580	47.896	1.00	20.82	B
5548	OE1	GLU	353	-4.986	41.788	46.991	1.00	22.39	B
5549	OE2	GLU	353	-6.170	43.442	47.721	1.00	18.42	B
5550	C	GLU	353	-2.148	43.966	48.707	1.00	21.56	B
5551	O	GLU	353	-2.645	44.865	47.990	1.00	19.49	B
5552	N	VAL	354	-1.529	44.254	49.870	1.00	21.53	B
5553	CA	VAL	354	-1.359	45.637	50.269	1.00	19.53	B
5554	CB	VAL	354	-0.630	45.761	51.630	1.00	19.84	B
5555	CG1	VAL	354	-0.323	47.206	51.960	1.00	17.36	B
5556	CG2	VAL	354	-1.557	45.178	52.690	1.00	19.82	B
5557	C	VAL	354	-0.627	46.433	49.197	1.00	20.27	B
5558	O	VAL	354	-1.080	47.545	48.852	1.00	20.16	B
5559	N	ARG	355	0.531	45.958	48.734	1.00	19.44	B
5560	CA	ARG	355	1.250	46.810	47.768	1.00	19.84	B
5561	CB	ARG	355	2.721	46.412	47.684	1.00	19.29	B
5562	CG	ARG	355	2.981	45.022	47.124	1.00	19.67	B
5563	CD	ARG	355	3.288	45.092	45.607	1.00	20.57	B
5564	NE	ARG	355	3.551	43.739	45.088	1.00	20.45	B
5565	CZ	ARG	355	4.488	43.429	44.194	1.00	21.00	B
5566	NH1	ARG	355	4.602	42.143	43.898	1.00	18.29	B
5567	NH2	ARG	355	5.350	44.316	43.658	1.00	20.14	B
5568	C	ARG	355	0.492	46.833	46.435	1.00	19.22	B
5569	O	ARG	355	0.418	47.907	45.844	1.00	20.61	B
5570	N	LYS	356	-0.157	45.763	46.019	1.00	20.34	B
5571	CA	LYS	356	-0.839	45.853	44.690	1.00	24.47	B
5572	CB	LYS	356	-1.229	44.485	44.141	1.00	21.60	B

5573	CG	LYS	356	0.070	43.739	43.786	1.00	22.62	B
5574	CD	LYS	356	-0.334	42.322	43.335	1.00	23.63	B
5575	CE	LYS	356	0.907	41.662	42.714	1.00	27.97	B
5576	NZ	LYS	356	0.502	40.324	42.167	1.00	30.54	B
5577	C	LYS	356	-2.022	46.810	44.746	1.00	25.59	B
5578	O	LYS	356	-2.201	47.685	43.892	1.00	23.97	B
5579	N	ARG	357	-2.798	46.682	45.837	1.00	25.23	B
5580	CA	ARG	357	-3.947	47.566	46.023	1.00	27.07	B
5581	CB	ARG	357	-4.781	47.087	47.204	1.00	29.98	B
5582	CG	ARG	357	-6.178	47.652	47.317	1.00	35.68	B
5583	CD	ARG	357	-7.002	47.478	46.029	1.00	38.99	B
5584	NE	ARG	357	-8.381	47.139	46.377	1.00	43.61	B
5585	CZ	ARG	357	-8.810	45.887	46.232	1.00	45.64	B
5586	NH1	ARG	357	-7.882	45.063	45.749	1.00	47.63	B
5587	NH2	ARG	357	-10.027	45.488	46.532	1.00	45.96	B
5588	C	ARG	357	-3.510	49.010	46.139	1.00	26.78	B
5589	O	ARG	357	-4.176	49.875	45.544	1.00	25.31	B
5590	N	SER	358	-2.412	49.299	46.835	1.00	22.91	B
5591	CA	SER	358	-1.967	50.678	46.985	1.00	24.66	B
5592	CB	SER	358	-0.732	50.694	47.910	1.00	23.49	B
5593	OG	SER	358	-1.166	50.289	49.224	1.00	24.21	B
5594	C	SER	358	-1.607	51.302	45.620	1.00	27.34	B
5595	O	SER	358	-1.985	52.457	45.341	1.00	26.59	B
5596	N	MET	359	-0.858	50.559	44.815	1.00	26.09	B
5597	CA	MET	359	-0.523	51.022	43.465	1.00	30.84	B
5598	CB	MET	359	0.399	50.042	42.754	1.00	33.37	B
5599	CG	MET	359	1.786	49.827	43.339	1.00	38.48	B
5600	SD	MET	359	2.611	51.373	43.748	1.00	45.78	B
5601	CE	MET	359	3.869	51.528	42.477	1.00	46.83	B
5602	C	MET	359	-1.805	51.181	42.632	1.00	30.24	B
5603	O	MET	359	-1.950	52.156	41.885	1.00	30.09	B
5604	N	ALA	360	-2.728	50.229	42.701	1.00	30.18	B
5605	CA	ALA	360	-3.943	50.276	41.910	1.00	32.29	B
5606	CB	ALA	360	-4.771	49.013	42.014	1.00	31.29	B
5607	C	ALA	360	-4.767	51.506	42.313	1.00	34.93	B
5608	O	ALA	360	-5.338	52.186	41.440	1.00	34.14	B
5609	N	GLU	361	-4.830	51.830	43.601	1.00	33.11	B
5610	CA	GLU	361	-5.603	52.981	44.033	1.00	33.75	B
5611	CB	GLU	361	-5.950	52.889	45.524	1.00	34.64	B
5612	CG	GLU	361	-7.009	51.862	45.846	1.00	38.36	B
5613	CD	GLU	361	-7.184	51.611	47.342	1.00	40.23	B
5614	OE1	GLU	361	-6.414	52.155	48.169	1.00	41.96	B
5615	OE2	GLU	361	-8.084	50.819	47.709	1.00	40.25	B
5616	C	GLU	361	-4.865	54.299	43.849	1.00	33.05	B
5617	O	GLU	361	-5.419	55.320	44.263	1.00	33.22	B
5618	N	GLY	362	-3.626	54.300	43.383	1.00	31.44	B
5619	CA	GLY	362	-2.840	55.498	43.290	1.00	32.90	B
5620	C	GLY	362	-2.459	56.088	44.636	1.00	32.35	B
5621	O	GLY	362	-2.209	57.290	44.693	1.00	31.88	B
5622	N	LYS	363	-2.171	55.284	45.668	1.00	31.50	B
5623	CA	LYS	363	-1.670	55.864	46.921	1.00	30.05	B
5624	CB	LYS	363	-1.644	54.791	48.023	1.00	30.86	B

5625	CG	LYS	363	-3.040	54.215	48.216	1.00	33.25	B
5626	CD	LYS	363	-3.979	55.369	48.550	1.00	35.05	B
5627	CE	LYS	363	-4.775	55.105	49.814	1.00	37.36	B
5628	NZ	LYS	363	-6.023	54.336	49.478	1.00	40.20	B
5629	C	LYS	363	-0.298	56.434	46.770	1.00	28.83	B
5630	O	LYS	363	0.489	55.922	45.979	1.00	26.37	B
5631	N	SER	364	0.114	57.272	47.729	1.00	26.81	B
5632	CA	SER	364	1.436	57.836	47.715	1.00	26.31	B
5633	CB	SER	364	1.553	59.069	48.633	1.00	28.44	B
5634	OG	SER	364	1.180	58.757	49.996	1.00	29.99	B
5635	C	SER	364	2.500	56.828	48.155	1.00	25.84	B
5636	O	SER	364	3.690	57.173	48.039	1.00	25.10	B
5637	N	THR	365	2.127	55.708	48.768	1.00	24.01	B
5638	CA	THR	365	3.170	54.793	49.260	1.00	23.87	B
5639	CB	THR	365	3.595	54.923	50.744	1.00	24.26	B
5640	OG1	THR	365	2.599	54.302	51.577	1.00	22.66	B
5641	CG2	THR	365	3.809	56.344	51.255	1.00	24.18	B
5642	C	THR	365	2.665	53.373	49.009	1.00	20.88	B
5643	O	THR	365	1.461	53.211	48.843	1.00	21.82	B
5644	N	THR	366	3.531	52.379	49.055	1.00	19.45	B
5645	CA	THR	366	3.127	50.989	48.920	1.00	19.21	B
5646	CB	THR	366	4.356	50.070	48.826	1.00	19.40	B
5647	OG1	THR	366	5.355	50.375	49.834	1.00	19.38	B
5648	CG2	THR	366	5.113	50.310	47.476	1.00	19.02	B
5649	C	THR	366	2.321	50.536	50.146	1.00	20.36	B
5650	O	THR	366	1.783	49.427	50.118	1.00	17.90	B
5651	N	GLY	367	2.373	51.274	51.261	1.00	20.93	B
5652	CA	GLY	367	1.638	50.740	52.463	1.00	22.97	B
5653	C	GLY	367	0.374	51.547	52.679	1.00	26.02	B
5654	O	GLY	367	0.262	52.285	53.679	1.00	27.99	B
5655	N	GLU	368	-0.571	51.492	51.742	1.00	23.43	B
5656	CA	GLU	368	-1.825	52.213	51.782	1.00	25.30	B
5657	CB	GLU	368	-2.740	51.605	52.867	1.00	25.99	B
5658	CG	GLU	368	-2.864	50.082	52.649	1.00	26.74	B
5659	CD	GLU	368	-3.660	49.375	53.720	1.00	27.59	B
5660	OE1	GLU	368	-3.896	49.979	54.799	1.00	28.76	B
5661	OE2	GLU	368	-4.129	48.229	53.528	1.00	28.71	B
5662	C	GLU	368	-1.687	53.709	51.963	1.00	25.50	B
5663	O	GLU	368	-2.570	54.337	52.557	1.00	27.62	B
5664	N	GLY	369	-0.681	54.348	51.399	1.00	23.87	B
5665	CA	GLY	369	-0.372	55.750	51.575	1.00	25.69	B
5666	C	GLY	369	0.250	56.102	52.936	1.00	26.59	B
5667	O	GLY	369	0.609	57.262	53.147	1.00	25.34	B
5668	N	LEU	370	0.505	55.138	53.818	1.00	26.36	B
5669	CA	LEU	370	1.065	55.425	55.134	1.00	27.96	B
5670	CB	LEU	370	0.305	54.613	56.159	1.00	28.99	B
5671	CG	LEU	370	-0.934	55.141	56.879	1.00	32.83	B
5672	CD2	LEU	370	-1.958	54.032	57.020	1.00	31.97	B
5673	CD1	LEU	370	-1.577	56.404	56.350	1.00	31.33	B
5674	C	LEU	370	2.549	55.042	55.156	1.00	28.04	B
5675	O	LEU	370	3.002	54.292	54.267	1.00	25.33	B
5676	N	ASP	371	3.284	55.512	56.155	1.00	25.78	B

5677	CA	ASP	371	4.693	55.240	56.240	1.00	28.14	B
5678	CB	ASP	371	5.406	56.400	56.980	1.00	31.72	B
5679	CG	ASP	371	5.397	57.639	56.081	1.00	35.24	B
5680	OD1	ASP	371	5.239	57.540	54.829	1.00	36.93	B
5681	OD2	ASP	371	5.612	58.738	56.641	1.00	37.53	B
5682	C	ASP	371	5.119	53.923	56.873	1.00	28.06	B
5683	O	ASP	371	6.097	53.374	56.357	1.00	27.73	B
5684	N	CYS	372	4.521	53.467	57.945	1.00	26.47	B
5685	CA	CYS	372	4.957	52.294	58.676	1.00	27.36	B
5686	CB	CYS	372	5.465	52.696	60.116	1.00	30.70	B
5687	SG	CYS	372	7.205	53.185	59.931	1.00	44.11	B
5688	C	CYS	372	3.823	51.329	58.851	1.00	23.53	B
5689	O	CYS	372	2.683	51.773	58.776	1.00	23.11	B
5690	N	GLY	373	4.083	50.033	58.853	1.00	23.03	B
5691	CA	GLY	373	3.019	49.047	58.989	1.00	18.94	B
5692	C	GLY	373	3.445	47.954	59.951	1.00	18.22	B
5693	O	GLY	373	4.647	47.710	60.134	1.00	19.54	B
5694	N	VAL	374	2.494	47.171	60.435	1.00	17.08	B
5695	CA	VAL	374	2.871	46.075	61.344	1.00	16.30	B
5696	CB	VAL	374	2.286	46.326	62.777	1.00	16.99	B
5697	CG1	VAL	374	2.416	45.059	63.638	1.00	20.31	B
5698	CG2	VAL	374	2.956	47.519	63.414	1.00	16.30	B
5699	C	VAL	374	2.280	44.782	60.849	1.00	14.24	B
5700	O	VAL	374	1.101	44.701	60.559	1.00	17.05	B
5701	N	LEU	375	3.081	43.754	60.803	1.00	15.98	B
5702	CA	LEU	375	2.644	42.427	60.368	1.00	16.70	B
5703	CB	LEU	375	3.564	42.006	59.272	1.00	15.92	B
5704	CG	LEU	375	4.091	40.684	58.767	1.00	22.02	B
5705	CD2	LEU	375	3.879	40.397	57.264	1.00	17.43	B
5706	CD1	LEU	375	3.941	39.445	59.608	1.00	19.27	B
5707	C	LEU	375	2.676	41.465	61.571	1.00	18.05	B
5708	O	LEU	375	3.693	41.521	62.292	1.00	16.00	B
5709	N	PHE	376	1.639	40.658	61.680	1.00	17.80	B
5710	CA	PHE	376	1.593	39.671	62.750	1.00	18.15	B
5711	CB	PHE	376	0.371	39.904	63.685	1.00	17.61	B
5712	CG	PHE	376	0.366	41.130	64.554	1.00	17.61	B
5713	CD1	PHE	376	-0.677	42.049	64.488	1.00	18.03	B
5714	CD2	PHE	376	1.379	41.351	65.481	1.00	18.64	B
5715	CE1	PHE	376	-0.708	43.188	65.298	1.00	18.81	B
5716	CE2	PHE	376	1.327	42.451	66.333	1.00	18.23	B
5717	CZ	PHE	376	0.315	43.380	66.256	1.00	17.54	B
5718	C	PHE	376	1.387	38.260	62.226	1.00	18.59	B
5719	O	PHE	376	0.529	38.023	61.355	1.00	20.07	B
5720	N	GLY	377	2.190	37.329	62.737	1.00	15.47	B
5721	CA	GLY	377	2.020	35.901	62.468	1.00	16.40	B
5722	C	GLY	377	1.637	35.252	63.842	1.00	18.96	B
5723	O	GLY	377	2.159	35.695	64.854	1.00	17.94	B
5724	N	PHE	378	0.750	34.276	63.879	1.00	17.37	B
5725	CA	PHE	378	0.330	33.615	65.119	1.00	18.50	B
5726	CB	PHE	378	-1.180	33.911	65.355	1.00	16.49	B
5727	CG	PHE	378	-1.543	35.378	65.328	1.00	17.95	B
5728	CD1	PHE	378	-1.008	36.232	66.285	1.00	19.64	B

5729	CD2	PHE	378	-2.473	35.897	64.464	1.00	19.18	B
5730	CE1	PHE	378	-1.360	37.565	66.364	1.00	19.64	B
5731	CE2	PHE	378	-2.837	37.233	64.522	1.00	18.80	B
5732	CZ	PHE	378	-2.295	38.100	65.467	1.00	19.16	B
5733	C	PHE	378	0.461	32.116	64.999	1.00	21.02	B
5734	O	PHE	378	-0.085	31.607	64.010	1.00	17.15	B
5735	N	GLY	379	1.195	31.419	65.870	1.00	18.50	B
5736	CA	GLY	379	1.310	29.967	65.746	1.00	16.05	B
5737	C	GLY	379	1.477	29.269	67.103	1.00	18.11	B
5738	O	GLY	379	1.224	29.923	68.128	1.00	13.64	B
5739	N	PRO	380	1.698	27.981	67.076	1.00	16.69	B
5740	CA	PRO	380	1.810	27.143	68.262	1.00	18.42	B
5741	CD	PRO	380	1.817	27.123	65.851	1.00	17.87	B
5742	CB	PRO	380	2.208	25.758	67.754	1.00	17.47	B
5743	CG	PRO	380	1.525	25.751	66.384	1.00	17.91	B
5744	C	PRO	380	2.873	27.669	69.228	1.00	17.32	B
5745	O	PRO	380	3.789	28.431	68.937	1.00	15.87	B
5746	N	GLY	381	2.380	27.682	70.496	1.00	17.73	B
5747	CA	GLY	381	3.330	28.035	71.601	1.00	15.93	B
5748	C	GLY	381	2.404	28.745	72.615	1.00	19.96	B
5749	O	GLY	381	2.433	28.322	73.753	1.00	16.38	B
5750	N	MET	382	1.457	29.648	72.505	1.00	17.53	B
5751	CA	MET	382	1.169	30.444	71.371	1.00	20.52	B
5752	CB	MET	382	-0.113	31.256	71.399	1.00	22.19	B
5753	CG	MET	382	-1.299	30.362	70.985	1.00	26.18	B
5754	SD	MET	382	-2.727	31.449	70.761	1.00	32.93	B
5755	CE	MET	382	-2.158	32.688	69.628	1.00	27.98	B
5756	C	MET	382	2.362	31.353	71.087	1.00	20.26	B
5757	O	MET	382	2.926	31.939	72.035	1.00	20.98	B
5758	N	THR	383	2.754	31.504	69.808	1.00	16.62	B
5759	CA	THR	383	3.776	32.487	69.441	1.00	16.94	B
5760	CB	THR	383	4.893	31.794	68.616	1.00	18.30	B
5761	OG1	THR	383	5.435	30.774	69.448	1.00	18.88	B
5762	CG2	THR	383	6.019	32.696	68.195	1.00	22.48	B
5763	C	THR	383	3.178	33.600	68.606	1.00	17.58	B
5764	O	THR	383	2.329	33.349	67.715	1.00	16.35	B
5765	N	VAL	384	3.645	34.824	68.789	1.00	15.64	B
5766	CA	VAL	384	3.293	35.954	67.931	1.00	15.95	B
5767	CB	VAL	384	2.706	37.166	68.658	1.00	16.79	B
5768	CG1	VAL	384	2.348	38.316	67.731	1.00	14.79	B
5769	CG2	VAL	384	1.437	36.785	69.437	1.00	20.42	B
5770	C	VAL	384	4.600	36.415	67.268	1.00	17.25	B
5771	O	VAL	384	5.590	36.546	67.986	1.00	15.34	B
5772	N	GLU	385	4.628	36.652	65.970	1.00	15.93	B
5773	CA	GLU	385	5.803	37.249	65.345	1.00	15.57	B
5774	CB	GLU	385	6.347	36.531	64.111	1.00	17.18	B
5775	CG	GLU	385	6.769	35.108	64.574	1.00	15.17	B
5776	CD	GLU	385	8.199	34.782	64.267	1.00	14.81	B
5777	OE1	GLU	385	8.997	35.669	63.884	1.00	17.65	B
5778	OE2	GLU	385	8.582	33.590	64.374	1.00	17.30	B
5779	C	GLU	385	5.312	38.639	64.968	1.00	14.54	B
5780	O	GLU	385	4.208	38.682	64.432	1.00	13.38	B

5781	N	THR	386	6.076	39.655	65.321	1.00	14.53	B
5782	CA	THR	386	5.612	41.011	65.010	1.00	15.70	B
5783	CB	THR	386	5.389	41.810	66.331	1.00	14.93	B
5784	OG1	THR	386	4.345	41.085	67.016	1.00	13.01	B
5785	CG2	THR	386	4.828	43.180	65.969	1.00	18.33	B
5786	C	THR	386	6.681	41.684	64.175	1.00	16.99	B
5787	O	THR	386	7.803	41.803	64.640	1.00	18.66	B
5788	N	VAL	387	6.425	41.983	62.916	1.00	17.17	B
5789	CA	VAL	387	7.424	42.576	62.036	1.00	15.47	B
5790	CB	VAL	387	7.542	41.744	60.737	1.00	17.25	B
5791	CG1	VAL	387	8.506	42.348	59.715	1.00	14.14	B
5792	CG2	VAL	387	7.871	40.298	61.076	1.00	16.11	B
5793	C	VAL	387	7.006	43.998	61.692	1.00	16.18	B
5794	O	VAL	387	5.859	44.154	61.228	1.00	18.67	B
5795	N	VAL	388	7.905	44.989	61.840	1.00	15.51	B
5796	CA	VAL	388	7.492	46.323	61.370	1.00	16.80	B
5797	CB	VAL	388	8.007	47.489	62.229	1.00	18.85	B
5798	CG1	VAL	388	7.739	48.850	61.608	1.00	18.96	B
5799	CG2	VAL	388	7.348	47.475	63.649	1.00	17.50	B
5800	C	VAL	388	8.054	46.524	59.936	1.00	17.03	B
5801	O	VAL	388	9.223	46.185	59.694	1.00	15.43	B
5802	N	LEU	389	7.204	47.053	59.075	1.00	17.33	B
5803	CA	LEU	389	7.663	47.282	57.679	1.00	21.43	B
5804	CB	LEU	389	6.629	46.538	56.807	1.00	19.43	B
5805	CG	LEU	389	6.944	45.190	56.210	1.00	20.03	B
5806	CD2	LEU	389	5.720	44.326	55.988	1.00	24.09	B
5807	CD1	LEU	389	8.107	44.417	56.764	1.00	18.41	B
5808	C	LEU	389	7.640	48.776	57.359	1.00	22.48	B
5809	O	LEU	389	6.684	49.409	57.842	1.00	23.82	B
5810	N	ARG	390	8.609	49.319	56.613	1.00	21.15	B
5811	CA	ARG	390	8.450	50.711	56.201	1.00	23.63	B
5812	CB	ARG	390	9.704	51.527	56.376	1.00	24.73	B
5813	CG	ARG	390	9.523	53.027	56.166	1.00	28.86	B
5814	CD	ARG	390	10.849	53.665	56.587	1.00	33.04	B
5815	NE	ARG	390	10.748	53.623	58.056	1.00	39.70	B
5816	CZ	ARG	390	11.635	53.406	59.003	1.00	41.83	B
5817	NH1	ARG	390	12.913	53.163	58.732	1.00	42.21	B
5818	NH2	ARG	390	11.191	53.429	60.265	1.00	43.28	B
5819	C	ARG	390	8.065	50.720	54.705	1.00	24.27	B
5820	O	ARG	390	8.725	50.052	53.923	1.00	22.53	B
5776	N	SER	391	7.049	51.498	54.388	0.60	24.71	B
5777	CA	SER	391	6.574	51.636	52.995	0.60	25.35	B
5778	CB	SER	391	5.341	52.544	52.900	0.60	25.10	B
5779	OG	SER	391	4.292	52.065	53.716	0.60	27.83	B
5780	C	SER	391	7.627	52.319	52.134	0.60	24.39	B
5781	O	SER	391	8.558	52.959	52.645	0.60	21.88	B
5776	N	2SER	391	7.051	51.444	54.373	0.40	23.03	B
5777	CA	2SER	391	6.591	51.532	52.978	0.40	22.31	B
5778	CB	2SER	391	5.260	52.277	52.904	0.40	19.63	B
5779	OG	2SER	391	5.425	53.608	53.370	0.40	16.14	B
5780	C	2SER	391	7.609	52.296	52.133	0.40	22.84	B
5781	O	2SER	391	8.490	52.991	52.661	0.40	21.30	B

5833	N	VAL	392	7.379	52.266	50.840	1.00	25.27	B
5834	CA	VAL	392	8.301	52.842	49.870	1.00	24.69	B
5835	CB	VAL	392	8.910	51.880	48.857	1.00	24.47	B
5836	CG1	VAL	392	9.681	52.695	47.782	1.00	25.05	B
5837	CG2	VAL	392	9.956	51.001	49.538	1.00	23.37	B
5838	C	VAL	392	7.443	53.929	49.183	1.00	28.14	B
5839	O	VAL	392	6.285	53.803	48.807	1.00	24.87	B
5840	N	ARG	393	8.071	55.076	49.196	1.00	33.33	B
5841	CA	ARG	393	7.439	56.253	48.669	1.00	41.36	B
5842	CB	ARG	393	8.174	57.532	49.050	1.00	44.63	B
5843	CG	ARG	393	7.379	58.740	48.576	1.00	48.73	B
5844	CD	ARG	393	7.291	59.792	49.682	1.00	52.29	B
5845	NE	ARG	393	5.910	60.250	49.820	1.00	54.82	B
5846	CZ	ARG	393	5.205	60.204	50.937	1.00	57.38	B
5847	NH1	ARG	393	5.726	59.726	52.067	1.00	57.43	B
5848	NH2	ARG	393	3.944	60.631	51.002	1.00	59.22	B
5849	C	ARG	393	7.382	56.113	47.147	1.00	44.23	B
5850	O	ARG	393	8.329	55.772	46.435	1.00	43.53	B
5851	N	VAL	394	6.168	56.338	46.646	1.00	46.97	B
5852	CA	VAL	394	5.966	56.264	45.214	1.00	50.68	B
5853	CB	VAL	394	5.165	55.055	44.684	1.00	50.32	B
5854	CG1	VAL	394	5.853	53.737	45.032	1.00	51.04	B
5855	CG2	VAL	394	3.721	55.066	45.118	1.00	49.56	B
5856	C	VAL	394	5.332	57.503	44.599	1.00	53.03	B
5857	OT	VAL	394	5.552	57.739	43.379	1.00	54.09	B
5858	OXT	VAL	394	5.105	58.606	45.112	1.00	55.26	B
5859	C8	AAC	395	-15.192	26.893	66.832	1.00	31.85	B
5860	N9	AAC	395	-15.934	25.758	67.103	1.00	32.08	B
5861	C4	AAC	395	-15.088	24.934	67.869	1.00	30.84	B
5862	C5	AAC	395	-13.832	25.530	67.809	1.00	30.43	B
5863	N7	AAC	395	-13.885	26.781	67.173	1.00	31.11	B
5864	N3	AAC	395	-15.294	23.593	68.102	1.00	30.53	B
5865	C2	AAC	395	-14.261	23.062	68.719	1.00	31.39	B
5866	N1	AAC	395	-12.944	23.490	68.590	1.00	30.31	B
5867	C6	AAC	395	-12.707	24.772	68.167	1.00	28.56	B
5868	N6	AAC	395	-11.444	25.259	68.054	1.00	27.76	B
5869	C1'	AAC	395	-17.565	25.621	67.019	1.00	33.80	B
5870	C2'	AAC	395	-18.568	26.410	67.757	1.00	33.92	B
5871	O2'	AAC	395	-18.460	25.742	68.939	1.00	35.53	B
5872	C3'	AAC	395	-19.659	26.490	66.695	1.00	34.93	B
5873	O3'	AAC	395	-20.567	25.398	66.547	1.00	37.60	B
5874	C4'	AAC	395	-19.026	26.473	65.246	1.00	34.24	B
5875	O4'	AAC	395	-17.686	25.823	65.578	1.00	31.70	B
5876	C5'	AAC	395	-18.654	27.909	64.805	1.00	34.89	B
5877	O5'	AAC	395	-18.589	28.914	66.006	1.00	36.12	B
5878	P1	AAC	395	-19.171	30.068	66.347	1.00	37.11	B
5879	O11	AAC	395	-18.851	30.453	67.744	1.00	36.83	B
5880	O12	AAC	395	-20.610	29.791	66.064	1.00	35.72	B
5881	O6	AAC	395	-18.515	31.021	65.274	1.00	34.92	B
5882	P2	AAC	395	-17.280	31.992	65.062	1.00	33.36	B
5883	O21	AAC	395	-16.471	31.770	66.293	1.00	30.55	B
5884	O22	AAC	395	-17.679	33.362	64.915	1.00	30.96	B

5885	O7	AAC	395	-16.646	31.579	63.771	1.00	32.38	B
5886	CPB	AAC	395	-16.080	30.192	63.750	1.00	31.68	B
5887	CPA	AAC	395	-14.542	30.319	63.372	1.00	30.89	B
5888	CP7	AAC	395	-13.888	31.248	64.422	1.00	31.27	B
5889	CP9	AAC	395	-14.489	30.884	61.936	1.00	30.17	B
5890	CP8	AAC	395	-13.807	28.985	63.475	1.00	30.74	B
5891	OP3	AAC	395	-14.107	30.729	65.756	1.00	32.31	B
5892	CP6	AAC	395	-12.343	31.291	64.332	1.00	31.20	B
5893	OP2	AAC	395	-11.876	32.045	63.433	1.00	29.03	B
5894	NP2	AAC	395	-11.624	30.543	65.153	1.00	32.06	B
5895	CP5	AAC	395	-10.533	29.754	64.393	1.00	33.24	B
5896	CP4	AAC	395	-9.228	30.266	64.907	1.00	33.51	B
5897	CP3	AAC	395	-8.159	29.225	64.583	1.00	33.61	B
5898	OP1	AAC	395	-7.893	28.716	65.682	1.00	32.17	B
5899	NP1	AAC	395	-7.229	29.455	63.650	1.00	30.09	B
5900	CP2	AAC	395	-5.812	29.049	64.048	1.00	28.37	B
5901	CP1	AAC	395	-5.272	27.710	63.569	1.00	30.17	B
5902	S	AAC	395	-3.497	27.744	63.958	1.00	34.21	B
5903	P3	AAC	395	-22.168	25.197	66.560	1.00	36.14	B
5904	O31	AAC	395	-22.761	25.893	65.401	1.00	35.36	B
5905	O32	AAC	395	-22.781	25.733	67.803	1.00	36.64	B
5906	O33	AAC	395	-22.188	23.595	66.448	1.00	36.54	B
5907	C51	AAC	395	-3.048	26.178	63.366	1.00	32.89	B
5908	C52	AAC	395	-1.642	25.785	63.820	1.00	34.16	B
5909	O51	AAC	395	-3.937	25.359	63.416	1.00	32.53	B
5910	C53	AAC	395	-0.644	25.743	62.664	1.00	34.31	B
5911	C54	AAC	395	-0.798	24.634	61.645	1.00	31.81	B
5912	O52	AAC	395	0.489	26.137	62.899	1.00	34.83	B
5913	OW0	WAT	1	34.833	42.831	79.558	1.00	24.60	W
5914	OW0	WAT	2	3.851	18.304	58.076	1.00	15.19	W
5915	OW0	WAT	3	10.671	17.830	49.206	1.00	12.89	W
5916	OW0	WAT	4	10.141	17.602	68.259	1.00	12.07	W
5917	OW0	WAT	5	32.698	32.703	80.877	1.00	22.54	W
5918	OW0	WAT	6	28.164	16.600	62.904	1.00	18.35	W
5919	OW0	WAT	7	-8.681	23.005	55.960	1.00	23.89	W
5920	OW0	WAT	8	18.659	24.304	57.009	1.00	14.47	W
5921	OW0	WAT	9	37.188	5.906	65.616	1.00	21.40	W
5922	OW0	WAT	10	9.584	18.395	70.986	1.00	16.40	W
5923	OW0	WAT	11	17.062	36.363	62.243	1.00	11.16	W
5924	OW0	WAT	12	13.451	23.284	60.136	1.00	10.89	W
5925	OW0	WAT	13	24.265	17.082	39.849	1.00	31.15	W
5926	OW0	WAT	14	4.587	15.225	66.740	1.00	16.62	W
5927	OW0	WAT	15	2.745	19.417	70.978	1.00	18.45	W
5928	OW0	WAT	16	2.872	55.277	59.456	1.00	21.70	W
5929	OW0	WAT	17	7.130	19.586	71.177	1.00	14.85	W
5930	OW0	WAT	18	23.610	32.233	58.057	1.00	10.85	W
5931	OW0	WAT	19	13.279	44.644	42.430	1.00	23.27	W
5932	OW0	WAT	20	-5.728	46.578	54.624	1.00	21.51	W
5933	OW0	WAT	21	31.220	-7.039	65.899	1.00	35.39	W
5934	OW0	WAT	22	11.942	28.570	63.201	1.00	15.27	W
5935	OW0	WAT	23	12.975	12.459	62.075	1.00	16.09	W
5936	OW0	WAT	24	27.265	29.217	41.221	1.00	45.85	W

5937	OW0	WAT	25	-4.415	43.306	73.997	1.00	21.65	W
5938	OW0	WAT	26	4.080	28.969	63.728	1.00	17.36	W
5939	OW0	WAT	27	-0.674	37.643	45.198	1.00	26.53	W
5940	OW0	WAT	28	-12.011	31.967	59.137	1.00	21.56	W
5941	OW0	WAT	29	9.814	17.806	52.000	1.00	11.02	W
5942	OW0	WAT	30	32.277	16.861	75.083	1.00	22.34	W
5943	OW0	WAT	31	-5.887	8.918	58.081	1.00	24.91	W
5944	OW0	WAT	32	14.641	12.037	49.335	1.00	20.01	W
5945	OW0	WAT	33	-5.901	28.682	48.527	1.00	15.15	W
5946	OW0	WAT	34	9.867	33.328	71.420	1.00	16.19	W
5947	OW0	WAT	35	7.243	23.184	65.189	1.00	12.89	W
5948	OW0	WAT	36	12.471	22.810	36.544	1.00	22.46	W
5949	OW0	WAT	37	-4.886	4.535	51.739	1.00	21.52	W
5950	OW0	WAT	38	7.963	25.910	67.738	1.00	18.53	W
5951	OW0	WAT	39	7.137	18.587	51.905	1.00	14.48	W
5952	OW0	WAT	40	15.459	40.211	62.055	1.00	17.02	W
5953	OW0	WAT	41	6.682	20.285	57.647	1.00	12.75	W
5954	OW0	WAT	42	18.453	17.014	54.016	1.00	17.42	W
5955	OW0	WAT	43	15.988	17.744	55.089	1.00	14.59	W
5956	OW0	WAT	44	9.657	27.916	66.070	1.00	21.06	W
5957	OW0	WAT	45	5.409	25.121	66.215	1.00	19.96	W
5958	OW0	WAT	46	1.102	33.642	57.497	1.00	14.88	W
5959	OW0	WAT	47	9.921	11.878	53.540	1.00	18.78	W
5960	OW0	WAT	48	-1.104	35.179	81.753	1.00	20.52	W
5961	OW0	WAT	49	-4.358	19.825	49.529	1.00	18.00	W
5962	OW0	WAT	50	32.742	32.506	77.847	1.00	19.42	W
5963	OW0	WAT	51	10.471	30.328	64.937	1.00	22.26	W
5964	OW0	WAT	52	29.066	-6.518	67.728	1.00	29.12	W
5965	OW0	WAT	53	23.893	38.780	44.707	1.00	22.24	W
5966	OW0	WAT	54	36.495	37.126	69.107	1.00	25.16	W
5967	OW0	WAT	55	27.620	4.330	52.694	1.00	26.50	W
5968	OW0	WAT	56	2.961	34.006	59.532	1.00	14.45	W
5969	OW0	WAT	57	25.883	33.854	55.114	1.00	18.60	W
5970	OW0	WAT	58	23.934	24.479	48.784	1.00	17.20	W
5971	OW0	WAT	59	-11.213	45.118	57.839	1.00	30.98	W
5972	OW0	WAT	60	-0.796	29.899	40.488	1.00	21.41	W
5973	OW0	WAT	61	9.058	44.419	65.396	1.00	16.69	W
5974	OW0	WAT	62	33.639	20.536	47.167	1.00	26.62	W
5975	OW0	WAT	63	17.361	46.985	62.113	1.00	28.80	W
5976	OW0	WAT	64	28.774	26.262	56.335	1.00	16.05	W
5977	OW0	WAT	65	8.319	17.938	74.501	1.00	29.07	W
5978	OW0	WAT	66	22.954	26.285	83.799	1.00	27.43	W
5979	OW0	WAT	67	26.549	36.290	50.427	1.00	25.74	W
5980	OW0	WAT	68	21.904	42.229	51.024	1.00	14.99	W
5981	OW0	WAT	69	11.885	15.625	68.435	1.00	16.06	W
5982	OW0	WAT	70	3.727	3.076	66.509	1.00	17.85	W
5983	OW0	WAT	71	27.566	41.917	69.685	1.00	25.81	W
5984	OW0	WAT	72	33.346	-2.248	71.890	1.00	32.26	W
5985	OW0	WAT	73	16.793	34.027	77.388	1.00	14.06	W
5986	OW0	WAT	74	3.307	30.509	80.393	1.00	26.64	W
5987	OW0	WAT	75	13.567	3.944	75.261	1.00	27.89	W
5988	OW0	WAT	76	9.592	38.551	63.829	1.00	17.98	W

5989	OW0	WAT	77	9.389	45.293	42.566	1.00	30.18	W
5990	OW0	WAT	78	-5.191	21.436	42.415	1.00	25.88	W
5991	OW0	WAT	79	21.648	31.139	42.786	1.00	17.08	W
5992	OW0	WAT	80	19.191	21.778	54.198	1.00	20.38	W
5993	OW0	WAT	81	26.780	39.147	69.085	1.00	17.18	W
5994	OW0	WAT	82	8.246	10.309	52.119	1.00	16.38	W
5995	OW0	WAT	83	3.964	12.812	68.057	1.00	14.72	W
5996	OW0	WAT	84	-9.721	27.929	67.632	1.00	32.83	W
5997	OW0	WAT	85	-4.054	15.227	45.174	1.00	24.29	W
5998	OW0	WAT	86	18.075	5.893	70.745	1.00	16.23	W
5999	OW0	WAT	87	22.585	17.373	56.517	1.00	18.76	W
6000	OW0	WAT	88	26.487	8.160	71.794	1.00	18.93	W
6001	OW0	WAT	89	6.429	43.196	69.535	1.00	19.11	W
6002	OW0	WAT	90	17.488	39.092	65.113	1.00	19.91	W
6003	OW0	WAT	91	16.700	42.492	65.311	1.00	25.17	W
6004	OW0	WAT	92	-7.482	22.305	53.597	1.00	35.05	W
6005	OW0	WAT	93	39.257	16.047	46.333	1.00	21.17	W
6006	OW0	WAT	94	36.318	43.091	76.325	1.00	25.27	W
6007	OW0	WAT	95	-12.497	37.547	54.922	1.00	21.19	W
6008	OW0	WAT	96	21.901	12.704	48.744	1.00	22.39	W
6009	OW0	WAT	97	-4.916	44.148	56.306	1.00	19.43	W
6010	OW0	WAT	98	21.194	31.992	84.275	1.00	35.72	W
6011	OW0	WAT	99	33.840	39.368	68.085	1.00	21.99	W
6012	OW0	WAT	100	8.893	-0.172	62.082	1.00	22.49	W
6013	OW0	WAT	101	18.453	-4.480	57.253	1.00	25.92	W
6014	OW0	WAT	102	13.569	16.019	62.639	1.00	13.04	W
6015	OW0	WAT	103	22.781	39.492	75.427	1.00	21.42	W
6016	OW0	WAT	104	-7.834	44.025	77.416	1.00	33.20	W
6017	OW0	WAT	105	29.427	5.861	61.950	1.00	20.36	W
6018	OW0	WAT	106	3.539	0.402	69.939	1.00	29.39	W
6019	OW0	WAT	107	18.155	19.548	52.456	1.00	16.41	W
6020	OW0	WAT	108	27.601	18.356	60.638	1.00	17.86	W
6021	OW0	WAT	109	2.260	40.202	73.144	1.00	20.92	W
6022	OW0	WAT	110	-9.554	18.969	50.641	1.00	32.12	W
6023	OW0	WAT	111	4.563	-1.441	68.389	1.00	19.23	W
6024	OW0	WAT	112	48.869	20.302	51.779	1.00	37.00	W
6025	OW0	WAT	113	-4.533	52.328	56.005	1.00	27.04	W
6026	OW0	WAT	114	5.063	37.094	76.058	1.00	29.92	W
6027	OW0	WAT	115	-0.474	5.884	53.613	1.00	20.80	W
6028	OW0	WAT	116	19.360	40.801	69.648	1.00	23.52	W
6029	OW0	WAT	117	20.908	23.658	55.291	1.00	25.91	W
6030	OW0	WAT	118	-6.751	15.614	64.282	1.00	30.02	W
6031	OW0	WAT	119	14.215	52.423	37.362	1.00	24.66	W
6032	OW0	WAT	120	17.895	-2.536	59.148	1.00	30.62	W
6033	OW0	WAT	121	33.040	37.124	58.297	1.00	27.56	W
6034	OW0	WAT	122	34.452	25.507	50.774	1.00	20.94	W
6035	OW0	WAT	123	17.664	41.847	62.811	1.00	21.31	W
6036	OW0	WAT	124	5.485	30.235	37.732	1.00	18.76	W
6037	OW0	WAT	125	-1.898	7.686	64.040	1.00	19.63	W
6038	OW0	WAT	126	19.019	48.698	52.195	1.00	20.04	W
6039	OW0	WAT	127	-3.037	31.394	63.373	1.00	18.81	W
6040	OW0	WAT	128	15.630	33.770	81.050	1.00	22.48	W

6041	OW0	WAT	129	23.983	44.352	50.610	1.00	25.96	W
6042	OW0	WAT	130	28.110	28.669	50.206	1.00	15.08	W
6043	OW0	WAT	131	-1.806	43.291	75.344	1.00	22.63	W
6044	OW0	WAT	132	28.287	-8.666	69.293	1.00	26.47	W
6045	OW0	WAT	133	7.361	31.080	64.997	1.00	25.48	W
6046	OW0	WAT	134	20.560	41.099	75.976	1.00	35.84	W
6047	OW0	WAT	135	-10.673	19.682	54.611	1.00	27.63	W
6048	OW0	WAT	136	12.764	16.066	49.078	1.00	18.12	W
6049	OW0	WAT	137	15.512	38.206	71.556	1.00	22.76	W
6050	OW0	WAT	138	2.289	29.709	76.361	1.00	20.87	W
6051	OW0	WAT	139	27.607	12.017	56.955	1.00	21.54	W
6052	OW0	WAT	140	43.717	10.364	62.596	1.00	29.34	W
6053	OW0	WAT	141	22.855	3.440	64.232	1.00	24.50	W
6054	OW0	WAT	142	39.489	28.943	75.323	1.00	25.73	W
6055	OW0	WAT	143	18.435	3.949	68.723	1.00	22.83	W
6056	OW0	WAT	144	22.017	29.915	39.105	1.00	26.92	W
6057	OW0	WAT	145	-13.904	15.849	62.886	1.00	23.40	W
6058	OW0	WAT	146	6.078	39.444	68.567	1.00	16.60	W
6059	OW0	WAT	147	-12.455	45.712	55.387	1.00	35.99	W
6060	OW0	WAT	148	3.763	16.311	71.884	1.00	23.06	W
6061	OW0	WAT	149	6.607	34.616	35.798	1.00	32.25	W
6062	OW0	WAT	150	37.996	18.102	44.945	1.00	29.62	W
6063	OW0	WAT	151	-18.165	30.197	48.373	1.00	25.75	W
6064	OW0	WAT	152	0.334	27.287	79.026	1.00	25.74	W
6065	OW0	WAT	153	10.426	48.456	66.152	1.00	21.45	W
6066	OW0	WAT	154	42.624	16.000	65.750	1.00	23.86	W
6067	OW0	WAT	155	21.994	18.147	53.858	1.00	33.50	W
6068	OW0	WAT	156	5.902	2.366	75.530	1.00	33.17	W
6069	OW0	WAT	157	5.376	32.084	35.797	1.00	24.80	W
6070	OW0	WAT	158	-8.651	40.561	76.072	1.00	26.15	W
6071	OW0	WAT	159	39.188	37.368	82.781	1.00	20.48	W
6072	OW0	WAT	160	22.782	13.672	41.336	1.00	30.01	W
6073	OW0	WAT	161	37.432	31.274	53.879	1.00	30.11	W
6074	OW0	WAT	162	0.115	26.377	71.555	1.00	21.49	W
6075	OW0	WAT	163	-9.279	30.393	58.466	1.00	20.71	W
6076	OW0	WAT	164	11.812	38.952	70.093	1.00	19.45	W
6077	OW0	WAT	165	2.458	36.524	41.602	1.00	17.20	W
6078	OW0	WAT	166	24.043	16.000	43.768	1.00	20.41	W
6079	OW0	WAT	167	-10.836	9.248	37.324	1.00	26.50	W
6080	OW0	WAT	168	34.158	28.322	54.719	1.00	19.03	W
6081	OW0	WAT	169	32.094	4.009	61.407	1.00	25.39	W
6082	OW0	WAT	170	26.257	22.100	84.514	1.00	31.25	W
6083	OW0	WAT	171	46.745	27.485	60.597	1.00	34.82	W
6084	OW0	WAT	172	25.950	43.206	60.062	1.00	20.37	W
6085	OW0	WAT	173	20.805	0.002	65.679	1.00	27.85	W
6086	OW0	WAT	174	25.880	31.658	48.636	1.00	24.24	W
6087	OW0	WAT	175	-13.506	30.648	68.700	1.00	27.76	W
6088	OW0	WAT	176	-27.081	17.078	52.775	1.00	39.62	W
6089	OW0	WAT	177	11.897	10.452	76.116	1.00	33.79	W
6090	OW0	WAT	178	31.984	20.596	77.502	1.00	21.81	W
6091	OW0	WAT	179	31.263	23.432	51.610	1.00	28.51	W
6092	OW0	WAT	180	-9.334	11.074	57.951	1.00	29.02	W

6093	OW0	WAT	181	-9.108	37.796	76.331	1.00	25.66	W
6094	OW0	WAT	182	13.322	22.309	83.725	1.00	31.25	W
6095	OW0	WAT	183	11.411	53.118	52.752	1.00	33.70	W
6096	OW0	WAT	184	31.449	33.237	54.875	1.00	21.50	W
6097	OW0	WAT	185	9.316	40.307	71.495	1.00	35.01	W
6098	OW0	WAT	186	-1.455	46.987	41.262	1.00	31.30	W
6099	OW0	WAT	187	10.799	16.341	45.718	1.00	27.73	W
6100	OW0	WAT	188	2.431	16.354	44.235	1.00	29.77	W
6101	OW0	WAT	189	40.154	15.788	64.071	1.00	22.73	W
6102	OW0	WAT	190	14.480	43.993	65.344	1.00	22.77	W
6103	OW0	WAT	191	-2.708	4.486	50.103	1.00	29.87	W
6104	OW0	WAT	192	16.266	34.225	83.895	1.00	29.68	W
6105	OW0	WAT	193	30.042	19.201	78.626	1.00	20.84	W
6106	OW0	WAT	194	6.162	2.780	56.188	1.00	19.96	W
6107	OW0	WAT	195	20.208	-4.100	49.927	1.00	28.83	W
6108	OW0	WAT	196	22.288	17.539	42.394	1.00	37.62	W
6109	OW0	WAT	197	-10.889	16.942	43.054	1.00	39.10	W
6110	OW0	WAT	198	19.697	5.855	78.027	1.00	28.62	W
6111	OW0	WAT	199	-3.070	17.530	67.970	1.00	26.17	W
6112	OW0	WAT	200	40.226	8.346	46.786	1.00	29.69	W
6113	OW0	WAT	201	5.142	47.390	43.700	1.00	39.12	W
6114	OW0	WAT	202	31.834	2.228	51.752	1.00	26.81	W
6115	OW0	WAT	203	-9.914	17.902	47.896	1.00	40.67	W
6116	OW0	WAT	204	-2.162	38.220	47.524	1.00	27.58	W
6117	OW0	WAT	205	44.805	12.169	60.199	1.00	26.37	W
6118	OW0	WAT	206	8.359	29.487	63.202	1.00	25.97	W
6119	OW0	WAT	207	16.840	40.422	70.542	1.00	29.25	W
6120	OW0	WAT	208	21.655	33.310	36.146	1.00	23.78	W
6121	OW0	WAT	209	3.445	20.123	73.634	1.00	35.71	W
6122	OW0	WAT	210	18.407	39.731	34.326	1.00	33.49	W
6123	OW0	WAT	211	3.255	52.496	71.113	1.00	33.73	W
6124	OW0	WAT	212	25.600	35.124	85.875	1.00	36.77	W
6125	OW0	WAT	213	-4.727	39.032	47.138	1.00	28.37	W
6126	OW0	WAT	214	21.172	21.454	57.118	1.00	25.17	W
6127	OW0	WAT	215	34.539	30.838	81.709	1.00	33.94	W
6128	OW0	WAT	216	-10.221	46.773	60.237	1.00	27.21	W
6129	OW0	WAT	217	38.172	2.762	68.914	1.00	40.44	W
6130	OW0	WAT	218	44.142	26.777	49.116	1.00	35.71	W
6131	OW0	WAT	219	-6.259	19.466	51.558	1.00	28.80	W
6132	OW0	WAT	220	47.174	19.165	64.417	1.00	34.12	W
6133	OW0	WAT	221	21.010	52.696	43.788	1.00	26.03	W
6134	OW0	WAT	222	41.521	34.528	67.480	1.00	38.90	W
6135	OW0	WAT	223	34.878	29.192	77.557	1.00	25.70	W
6136	OW0	WAT	224	-21.727	22.843	51.038	1.00	27.64	W
6137	OW0	WAT	225	15.307	1.674	55.892	1.00	37.01	W
6138	OW0	WAT	226	12.946	44.417	67.528	1.00	35.45	W
6139	OW0	WAT	227	2.765	38.991	42.902	1.00	28.20	W
6140	OW0	WAT	228	29.044	33.405	51.941	1.00	34.10	W
6141	OW0	WAT	229	52.147	25.423	67.839	1.00	41.44	W
6142	OW0	WAT	230	24.831	31.270	83.962	1.00	35.33	W
6143	OW0	WAT	231	-4.319	54.016	68.997	1.00	39.00	W
6144	OW0	WAT	232	-11.830	22.280	70.889	1.00	38.46	W

6145	OW0	WAT	233	-11.980	7.355	49.262	1.00	28.37	W
6146	OW0	WAT	234	17.583	51.329	54.796	1.00	30.01	W
6147	OW0	WAT	235	9.776	48.268	73.002	1.00	30.25	W
6148	OW0	WAT	236	-16.035	40.160	60.590	1.00	28.16	W
6149	OW0	WAT	237	-1.405	3.513	62.408	1.00	25.71	W
6150	OW0	WAT	238	-4.314	47.702	50.798	1.00	26.80	W
6151	OW0	WAT	239	22.355	30.748	36.279	1.00	30.92	W
6152	OW0	WAT	240	-1.966	20.655	42.218	1.00	32.05	W
6153	OW0	WAT	241	18.480	-1.429	76.956	1.00	29.78	W
6154	OW0	WAT	242	9.409	9.978	49.436	1.00	32.49	W
6155	OW0	WAT	243	27.641	32.376	58.093	1.00	21.72	W
6156	OW0	WAT	244	-20.176	24.730	52.508	1.00	26.25	W
6157	OW0	WAT	245	-5.446	55.757	58.325	1.00	41.56	W
6158	OW0	WAT	246	28.817	42.022	72.611	1.00	29.75	W
6159	OW0	WAT	247	14.247	36.114	80.912	1.00	30.87	W
6160	OW0	WAT	248	21.386	51.826	40.788	1.00	34.48	W
6161	OW0	WAT	249	-1.422	53.965	72.266	1.00	40.79	W
6162	OW0	WAT	250	28.196	35.091	57.452	1.00	25.63	W
6163	OW0	WAT	251	-6.712	56.104	66.234	1.00	36.33	W
6164	OW0	WAT	252	-0.371	2.660	55.086	1.00	29.48	W
6165	OW0	WAT	253	25.280	13.418	79.944	1.00	27.74	W
6166	OW0	WAT	254	-15.928	29.812	68.788	1.00	34.21	W
6167	OW0	WAT	255	4.853	41.410	72.878	1.00	29.51	W
6169	OW0	WAT	257	15.700	38.269	78.845	1.00	31.14	W
6170	OW0	WAT	258	-13.951	35.748	69.430	1.00	38.64	W
6171	OW0	WAT	259	-0.528	28.082	82.338	1.00	37.27	W
6172	OW0	WAT	260	11.005	45.170	39.407	1.00	35.77	W
6173	OW0	WAT	261	27.583	-3.213	76.354	1.00	35.29	W
6174	OW0	WAT	262	24.221	34.640	35.344	1.00	37.78	W
6176	OW0	WAT	264	-13.254	31.131	78.123	1.00	52.24	W
6177	OW0	WAT	265	-14.010	40.718	68.831	1.00	44.51	W
6178	OW0	WAT	266	-1.866	58.341	49.387	1.00	31.53	W
6179	OW0	WAT	267	34.994	-2.704	69.976	1.00	44.49	W
6180	OW0	WAT	268	18.804	35.034	84.016	1.00	22.70	W
6181	OW0	WAT	269	-7.103	10.995	59.608	1.00	32.43	W
6182	OW0	WAT	270	37.460	30.477	47.652	1.00	33.62	W
6183	OW0	WAT	271	-16.645	24.523	44.105	1.00	38.25	W
6184	OW0	WAT	272	1.623	1.123	65.050	1.00	36.59	W
6185	OW0	WAT	273	25.204	32.775	44.416	1.00	38.94	W
6186	OW0	WAT	274	-13.731	43.977	65.708	1.00	36.13	W
6187	OW0	WAT	275	2.990	13.777	70.756	1.00	31.65	W
6188	OW0	WAT	276	10.495	51.445	44.812	1.00	33.61	W
6189	OW0	WAT	277	23.022	18.900	82.573	1.00	23.37	W
6190	OW0	WAT	278	29.535	14.226	76.815	1.00	32.39	W
6191	OW0	WAT	279	9.656	32.798	33.321	1.00	46.33	W
6192	OW0	WAT	280	41.048	20.359	79.208	1.00	30.26	W
6193	OW0	WAT	281	24.589	30.011	39.558	1.00	36.63	W
6194	OW0	WAT	282	40.022	33.138	75.589	1.00	27.95	W
6195	OW0	WAT	283	13.000	18.212	42.451	1.00	34.13	W
6196	OW0	WAT	284	-10.548	42.137	75.750	1.00	23.51	W
6197	OW0	WAT	285	43.830	18.352	63.046	1.00	22.87	W
6198	OW0	WAT	286	-13.181	38.699	57.329	1.00	20.83	W

6199	OW0	WAT	287	-4.039	48.668	57.394	1.00	20.92	W
6200	OW0	WAT	288	-11.752	16.128	61.206	1.00	25.84	W
6201	OW0	WAT	289	24.307	43.914	53.706	1.00	25.66	W
6202	OW0	WAT	290	29.396	2.615	53.358	1.00	32.00	W
6203	OW0	WAT	291	46.029	16.371	65.925	1.00	47.24	W
6204	OW0	WAT	292	15.408	6.086	52.268	1.00	25.75	W
6205	OW0	WAT	293	25.890	32.042	41.458	1.00	33.89	W
6206	OW0	WAT	294	-21.759	8.749	52.215	1.00	35.49	W
6207	OW0	WAT	295	-22.534	28.343	64.578	1.00	39.76	W
6208	OW0	WAT	296	-9.629	14.160	40.844	1.00	39.41	W
6209	OW0	WAT	297	15.662	46.297	64.617	1.00	29.98	W
6210	OW0	WAT	298	47.452	23.009	48.142	1.00	37.05	W
6211	OW0	WAT	299	30.906	25.511	86.969	1.00	28.57	W
6212	OW0	WAT	300	29.458	34.520	54.929	1.00	28.09	W
6213	OW0	WAT	301	12.248	-2.398	62.389	1.00	23.37	W
6214	OW0	WAT	302	6.586	40.900	70.776	1.00	28.66	W
6215	OW0	WAT	303	26.731	-5.212	51.241	1.00	37.60	W
6216	OW0	WAT	304	-2.065	9.188	66.877	1.00	40.14	W
6217	OW0	WAT	305	33.333	15.587	72.760	1.00	31.54	W
6218	OW0	WAT	306	6.619	27.578	69.359	1.00	32.54	W
6219	OW0	WAT	307	-2.349	26.244	78.298	1.00	35.66	W
6220	OW0	WAT	308	52.161	11.033	59.127	1.00	43.46	W
6221	OW0	WAT	309	1.147	16.876	73.569	1.00	40.10	W
6222	OW0	WAT	310	42.839	17.626	69.680	1.00	33.57	W
6223	OW0	WAT	311	9.714	7.252	49.380	1.00	42.23	W
6224	OW0	WAT	312	4.967	28.723	66.279	1.00	35.79	W
6225	OW0	WAT	313	22.707	-8.021	75.301	1.00	42.23	W
6226	OW0	WAT	314	38.612	10.518	44.983	1.00	32.90	W
6227	OW0	WAT	315	35.206	13.781	73.124	1.00	32.15	W
6228	OW0	WAT	316	17.281	0.430	53.047	1.00	36.65	W
6229	OW0	WAT	317	13.378	44.865	39.537	1.00	27.59	W
6230	OW0	WAT	318	9.368	38.921	77.170	1.00	32.10	W
6231	OW0	WAT	319	-12.157	28.821	67.114	1.00	35.73	W
6232	OW0	WAT	320	49.055	20.121	66.102	1.00	34.26	W
6233	OW0	WAT	321	51.483	24.423	70.909	1.00	35.24	W
6234	OW0	WAT	322	38.833	5.939	63.218	1.00	28.09	W
6235	OW0	WAT	323	9.860	18.263	76.668	1.00	45.65	W
6236	OW0	WAT	324	20.261	18.981	50.680	1.00	30.83	W
6237	OW0	WAT	325	23.190	21.257	55.046	1.00	27.34	W
6238	OW0	WAT	326	27.260	42.057	66.647	1.00	26.66	W
6239	OW0	WAT	327	41.413	8.984	68.636	1.00	34.58	W
6240	OW0	WAT	328	43.883	34.723	70.681	1.00	34.47	W
6241	OW0	WAT	329	-1.961	7.539	44.617	1.00	33.01	W
6242	OW0	WAT	330	4.158	57.025	60.984	1.00	39.08	W
6244	OW0	WAT	332	0.127	22.354	42.728	1.00	39.89	W
6245	OW0	WAT	333	36.937	39.106	65.589	1.00	32.97	W
6246	OW0	WAT	334	-14.238	45.891	59.784	1.00	37.45	W
6247	OW0	WAT	335	24.653	19.852	84.466	1.00	30.48	W
6248	OW0	WAT	336	11.415	11.665	48.239	1.00	26.80	W
6249	OW0	WAT	337	-15.878	36.234	51.704	1.00	36.48	W
6250	OW0	WAT	338	2.066	1.236	57.713	1.00	35.34	W
6251	OW0	WAT	339	1.824	21.102	43.644	1.00	37.35	W

6252	OW0	WAT	340	12.771	9.948	46.645	1.00	32.82	W
6253	OW0	WAT	341	-4.647	54.375	54.379	1.00	30.72	W
6254	OW0	WAT	342	6.100	38.052	38.122	1.00	32.64	W
6255	OW0	WAT	343	17.546	34.296	36.005	1.00	32.50	W
6256	OW0	WAT	344	27.816	0.717	70.109	1.00	35.00	W
6257	OW0	WAT	345	18.540	-0.224	72.022	1.00	34.20	W
6258	OW0	WAT	346	33.678	-6.833	55.722	1.00	33.65	W
6259	OW0	WAT	347	15.061	12.931	46.581	1.00	33.22	W
6260	OW0	WAT	348	-22.692	16.145	50.080	1.00	37.41	W
6261	OW0	WAT	349	11.124	-0.578	60.734	1.00	33.64	W
6262	OW0	WAT	350	12.477	-6.964	72.013	1.00	35.64	W
6263	OW0	WAT	351	-11.684	42.426	52.043	1.00	35.79	W
6264	OW0	WAT	352	10.749	18.011	43.616	1.00	38.78	W
6265	OW0	WAT	353	10.695	46.256	69.179	1.00	42.67	W
6266	OW0	WAT	354	-8.853	16.832	67.349	1.00	34.74	W
6267	OW0	WAT	355	12.718	41.696	70.240	1.00	30.82	W
6268	OW0	WAT	356	-8.930	59.166	59.077	1.00	34.34	W
6269	OW0	WAT	357	20.857	-14.210	57.229	1.00	32.95	W
6270	OW0	WAT	358	14.519	4.631	49.796	1.00	44.66	W
6271	OW0	WAT	359	2.073	57.881	57.424	1.00	30.86	W
6272	OW0	WAT	360	45.440	8.237	60.801	1.00	36.34	W
6273	OW0	WAT	361	14.230	54.142	70.351	1.00	49.59	W
6274	OW0	WAT	362	41.300	3.844	59.740	1.00	38.05	W
6275	OW0	WAT	363	-12.931	40.320	51.355	1.00	35.66	W
6276	OW0	WAT	364	15.587	49.538	62.357	1.00	36.31	W
6277	OW0	WAT	365	2.582	38.475	75.494	1.00	40.42	W
6278	OW0	WAT	366	27.548	-6.502	49.377	1.00	67.95	W
6279	OW0	WAT	367	4.518	0.719	57.381	1.00	53.38	W
6280	OW0	WAT	368	10.164	31.136	79.624	1.00	36.75	W
6281	OW0	WAT	369	13.547	17.475	39.984	1.00	37.62	W
6282	OW0	WAT	370	-13.129	26.596	50.289	1.00	32.71	W
6283	OW0	WAT	371	14.417	6.722	47.829	1.00	36.03	W
6284	OW0	WAT	372	0.306	24.495	40.705	1.00	33.44	W
6285	OW0	WAT	373	48.962	16.693	63.882	1.00	52.26	W
6286	OW0	WAT	374	10.444	55.766	49.842	1.00	36.16	W
6287	OW0	WAT	375	-17.810	34.487	50.989	1.00	41.30	W
6288	OW0	WAT	376	30.138	23.191	81.873	1.00	33.16	W
6289	OW0	WAT	377	40.462	3.629	62.961	1.00	42.45	W
6290	OW0	WAT	378	-1.654	41.668	78.407	1.00	40.16	W
6291	OW0	WAT	379	26.203	36.571	38.774	1.00	46.13	W
6292	OW0	WAT	380	-11.749	44.049	48.503	1.00	58.07	W
6293	OW0	WAT	381	42.715	21.571	81.086	1.00	40.66	W
6294	OW0	WAT	382	-4.286	50.046	49.483	1.00	32.45	W
6295	OW0	WAT	383	38.125	27.017	76.389	1.00	40.31	W
6296	OW0	WAT	384	-25.988	13.692	54.676	1.00	36.33	W
6297	OW0	WAT	385	-21.590	26.317	54.434	1.00	34.29	W
6298	OW0	WAT	386	4.989	40.169	40.784	1.00	38.89	W
6299	OW0	WAT	387	15.117	-1.463	79.524	1.00	36.96	W
6300	OW0	WAT	388	-0.974	24.536	37.927	1.00	33.02	W
6301	OW0	WAT	389	22.450	-12.684	69.847	1.00	36.96	W
6302	OW0	WAT	390	33.210	35.282	55.745	1.00	37.80	W
6303	OW0	WAT	391	23.977	-15.440	70.811	1.00	55.29	W

6304	OW0	WAT	392	21.334	3.772	66.357	1.00	38.55	W
6305	OW0	WAT	393	30.244	15.090	38.226	1.00	41.68	W
6306	OW0	WAT	394	23.254	10.269	42.142	1.00	39.03	W
6307	OW0	WAT	395	22.318	45.619	66.182	1.00	35.89	W
6308	OW0	WAT	396	-18.640	18.477	45.035	1.00	35.67	W
6309	OW0	WAT	397	2.400	2.514	52.539	1.00	45.90	W
6310	OW0	WAT	398	18.907	44.629	62.294	1.00	37.92	W
6311	OW0	WAT	399	19.662	12.004	79.473	1.00	27.97	W
6312	OW0	WAT	400	-26.603	12.790	62.874	1.00	44.82	W
6313	OW0	WAT	401	32.383	-0.500	51.742	1.00	40.74	W
6314	OW0	WAT	402	49.790	27.368	53.659	1.00	45.32	W
6316	OW0	WAT	404	33.541	23.998	47.310	1.00	48.59	W
6317	OW0	WAT	405	-27.662	21.197	64.058	1.00	51.73	W
6318	OW0	WAT	406	-0.339	4.153	67.759	1.00	42.33	W
6319	OW0	WAT	407	24.102	12.203	37.676	1.00	46.14	W
6320	OW0	WAT	408	-14.157	17.556	70.142	1.00	31.93	W
6321	OW0	WAT	409	-23.772	23.390	49.235	1.00	43.79	W
6322	OW0	WAT	410	12.752	-8.490	57.666	1.00	46.09	W
6323	OW0	WAT	411	35.604	-7.850	57.694	1.00	42.78	W
6324	OW0	WAT	412	15.177	45.155	36.456	1.00	35.30	W
6325	OW0	WAT	413	44.585	9.274	65.094	1.00	32.90	W
6326	OW0	WAT	414	18.417	10.786	77.471	1.00	31.40	W
6327	OW0	WAT	415	18.832	-10.822	78.328	1.00	33.25	W
6328	OW0	WAT	416	19.308	40.195	81.294	1.00	39.51	W
6329	OW0	WAT	417	-14.525	39.134	72.943	1.00	39.02	W
6330	OW0	WAT	418	5.809	3.047	51.152	1.00	40.12	W
6331	OW0	WAT	419	18.978	43.478	67.054	1.00	48.35	W
6332	OW0	WAT	420	-6.116	50.154	71.782	1.00	50.58	W
6333	OW0	WAT	421	35.294	-6.916	60.117	1.00	37.54	W
6334	OW0	WAT	422	21.103	41.861	71.424	1.00	31.29	W
6335	OW0	WAT	423	5.611	32.606	78.029	1.00	48.39	W
6336	OW0	WAT	424	30.155	37.320	57.973	1.00	38.66	W
6337	OW0	WAT	425	42.663	10.046	71.467	1.00	45.60	W
6338	OW0	WAT	426	20.843	55.374	41.943	1.00	47.33	W
6339	OW0	WAT	427	33.849	-6.515	52.009	1.00	51.92	W
6340	OW0	WAT	428	39.602	5.110	66.807	1.00	31.12	W
6341	OW0	WAT	429	13.310	42.107	72.700	1.00	45.86	W
6342	OW0	WAT	430	15.435	41.736	68.476	1.00	39.15	W
6343	OW0	WAT	431	-14.455	39.203	53.503	1.00	36.54	W
6344	OW0	WAT	432	-12.893	9.554	38.543	1.00	39.54	W
6345	OW0	WAT	433	-27.689	24.945	60.863	1.00	36.39	W
6346	OW0	WAT	434	19.352	-4.834	76.947	1.00	50.49	W
6347	OW0	WAT	435	-4.457	58.132	59.848	1.00	44.39	W
6348	OW0	WAT	436	35.946	42.040	72.721	1.00	32.88	W
6349	OW0	WAT	437	-22.989	29.806	60.462	1.00	44.66	W
6350	OW0	WAT	438	16.404	11.978	76.652	1.00	37.94	W
6351	OW0	WAT	439	17.511	8.401	78.247	1.00	36.58	W
6352	OW0	WAT	440	-11.978	24.278	73.130	1.00	44.22	W
6353	OW0	WAT	441	25.379	0.872	47.157	1.00	35.40	W
6354	OW0	WAT	442	29.502	41.009	54.163	1.00	35.29	W
6355	OW0	WAT	443	9.666	22.319	37.019	1.00	35.65	W
6356	OW0	WAT	444	38.197	-1.983	55.446	1.00	36.65	W

6357	OW0	WAT	445	2.334	57.846	63.873	1.00	39.83	W
6358	OW0	WAT	446	10.150	-6.515	70.874	1.00	40.39	W
6359	OW0	WAT	447	4.644	42.725	39.903	1.00	45.20	W
6360	OW0	WAT	448	26.881	38.528	48.647	1.00	31.60	W
6361	OW0	WAT	449	9.031	20.773	77.665	1.00	37.57	W
6362	OW0	WAT	450	6.993	28.067	36.574	1.00	36.29	W
6363	OW0	WAT	451	-13.241	37.909	47.895	1.00	33.95	W
6364	OW0	WAT	452	7.509	3.326	53.116	1.00	43.55	W
6365	OW0	WAT	453	15.904	50.283	51.263	1.00	32.48	W
6367	OW0	WAT	455	35.670	30.907	51.394	1.00	50.15	W
6369	OW0	WAT	457	-3.674	49.995	72.941	1.00	51.56	W
6370	OW0	WAT	458	-1.876	18.327	43.172	1.00	34.13	W
6371	OW0	WAT	459	40.383	6.878	68.945	1.00	50.63	W
6372	OW0	WAT	460	45.906	24.778	47.259	1.00	41.29	W
6373	OW0	WAT	461	3.785	37.924	39.424	1.00	39.64	W
6374	OW0	WAT	462	1.292	58.070	66.860	1.00	37.08	W
6375	OW0	WAT	463	-4.643	42.723	44.332	1.00	53.12	W
6376	OW0	WAT	464	17.139	-8.893	79.247	1.00	38.42	W
6377	OW0	WAT	465	11.910	-4.645	82.933	1.00	38.95	W
6378	OW0	WAT	466	-24.232	22.740	68.547	1.00	46.16	W
6379	OW0	WAT	467	27.793	37.520	46.319	1.00	49.80	W
6380	OW0	WAT	468	7.117	49.493	44.707	1.00	43.74	W
6381	OW0	WAT	469	45.294	13.104	46.764	1.00	46.87	W
6382	OW0	WAT	470	9.424	16.793	79.089	1.00	37.97	W
6383	OW0	WAT	471	9.793	-1.720	82.356	1.00	35.04	W
6384	OW0	WAT	472	-1.389	20.063	39.098	1.00	43.34	W
6385	OW0	WAT	473	16.787	13.212	80.501	1.00	47.28	W
6386	OW0	WAT	474	41.533	36.135	69.647	1.00	43.73	W
6387	OW0	WAT	475	-5.170	56.784	55.948	1.00	44.97	W
6388	OW0	WAT	476	27.423	-12.833	55.835	1.00	37.01	W
6389	OW0	WAT	477	38.584	36.991	59.464	1.00	40.79	W
6390	OW0	WAT	478	-27.987	8.862	59.618	1.00	53.66	W
6391	OW0	WAT	479	20.230	51.861	47.577	1.00	40.83	W
6392	OW0	WAT	480	-2.196	45.838	77.392	1.00	50.14	W
6393	OW0	WAT	481	-29.703	18.549	57.301	1.00	32.79	W
6394	OW0	WAT	482	44.386	5.769	58.325	1.00	51.23	W
6395	OW0	WAT	483	-18.073	22.355	68.898	1.00	41.13	W
6396	OW0	WAT	484	40.081	36.439	71.933	1.00	34.48	W
6397	OW0	WAT	485	27.500	39.480	77.384	1.00	45.20	W
6398	OW0	WAT	486	28.735	35.934	52.078	1.00	53.74	W
6399	OW0	WAT	487	42.987	7.871	66.681	1.00	44.15	W
6400	OW0	WAT	488	27.401	24.527	88.235	1.00	39.98	W
6401	OW0	WAT	489	11.264	33.188	81.869	1.00	42.28	W
6403	OW0	WAT	491	-0.260	35.857	40.950	1.00	45.35	W
6404	OW0	WAT	492	-20.071	29.067	53.331	1.00	55.04	W
6405	OW0	WAT	493	32.688	24.529	44.418	1.00	44.22	W
6406	OW0	WAT	494	-2.749	28.055	39.216	1.00	44.69	W
6407	OW0	WAT	495	-20.243	23.515	69.911	1.00	43.24	W
6408	OW0	WAT	496	-7.782	46.922	76.436	1.00	44.94	W
6409	OW0	WAT	497	-14.142	31.967	73.149	1.00	45.00	W
6410	OW0	WAT	498	5.220	21.008	77.195	1.00	46.89	W
6411	OW0	WAT	499	18.449	52.543	49.223	1.00	44.94	W

6412	OW0	WAT	500	5.606	51.045	75.120	1.00	43.08	W
6413	OW0	WAT	501	0.585	7.734	46.905	1.00	40.04	W
6414	OW0	WAT	502	0.646	12.691	70.758	1.00	44.19	W
6415	OW0	WAT	503	0.587	58.251	59.482	1.00	37.44	W
6416	OW0	WAT	504	26.265	37.621	44.223	1.00	42.27	W
6417	OW0	WAT	505	2.799	20.132	41.418	1.00	49.03	W
6418	OW0	WAT	506	19.618	0.551	69.717	1.00	35.91	W
6419	OW0	WAT	507	4.617	28.787	77.968	1.00	32.85	W
6420	OW0	WAT	508	40.487	36.867	63.836	1.00	33.53	W
6421	OW0	WAT	509	40.536	13.697	75.399	1.00	46.10	W
6422	OW0	WAT	510	-7.126	43.053	45.104	1.00	41.77	W
6423	OW0	WAT	511	36.064	28.929	82.495	1.00	64.61	W
6424	OW0	WAT	512	16.095	6.640	44.452	1.00	55.92	W
6425	OW0	WAT	513	12.402	32.185	83.832	1.00	56.64	W
6426	OW0	WAT	514	3.804	17.973	42.165	1.00	38.55	W
6427	OW0	WAT	515	15.129	14.995	43.155	1.00	34.59	W
6428	OW0	WAT	516	-12.895	48.759	65.920	1.00	46.55	W
6429	OW0	WAT	517	7.814	30.918	77.806	1.00	43.13	W
6430	OW0	WAT	518	15.378	44.589	68.748	1.00	47.42	W
6431	OW0	WAT	519	23.423	48.687	52.464	1.00	51.53	W
6432	OW0	WAT	520	8.730	28.031	34.552	1.00	45.00	W
6433	OW0	WAT	521	-5.694	45.025	43.601	1.00	52.66	W
6434	OW0	WAT	522	-13.465	9.596	59.350	1.00	46.34	W
6435	OW0	WAT	523	40.029	-0.641	57.082	1.00	59.65	W
6436	OW0	WAT	524	-16.093	33.826	74.072	1.00	34.99	W
6437	OW0	WAT	525	36.464	39.863	68.565	1.00	43.68	W
6438	OW0	WAT	526	51.637	13.562	55.466	1.00	49.68	W
6439	OW0	WAT	527	-1.692	33.877	43.605	1.00	45.70	W
6440	OW0	WAT	528	26.307	40.989	75.070	1.00	45.20	W
6441	OW0	WAT	529	21.836	43.211	42.723	1.00	33.95	W
6442	OW0	WAT	530	37.472	40.460	71.382	1.00	47.53	W
6443	OW0	WAT	531	26.392	44.450	65.042	1.00	37.05	W
6444	OW0	WAT	532	9.807	19.244	37.207	1.00	37.60	W
6445	OW0	WAT	533	-1.839	49.077	39.508	1.00	42.70	W
6446	OW0	WAT	534	40.926	35.494	74.588	1.00	44.27	W
6447	OW0	WAT	535	21.981	23.595	40.662	1.00	49.79	W
6448	OW0	WAT	536	12.398	50.065	65.683	1.00	39.01	W
6449	OW0	WAT	537	23.603	42.961	45.081	1.00	49.97	W
6450	OW0	WAT	538	-10.352	47.740	76.915	1.00	46.80	W
6451	OW0	WAT	539	-15.806	39.195	57.947	1.00	39.96	W
6452	OW0	WAT	541	14.503	-5.582	79.614	1.00	53.05	W
6453	OW0	WAT	542	0.684	18.258	44.653	1.00	33.50	W
6454	OW0	WAT	543	5.269	23.624	37.419	1.00	46.63	W
6455	OW0	WAT	544	14.440	-9.982	79.496	1.00	51.43	W
6456	OW0	WAT	545	13.044	-10.837	56.679	1.00	52.73	W
6457	OW0	WAT	546	-13.064	43.674	53.671	1.00	45.82	W
6458	OW0	WAT	547	24.822	10.978	80.940	1.00	44.36	W
6459	OW0	WAT	548	-12.481	48.719	70.168	1.00	41.45	W
6460	OW0	WAT	549	-3.052	4.179	44.889	1.00	58.63	W

TABLE 4

Complex	PDB Accession No.
CHS-coA complex	1BQ6
CHS-malonyl-CoA complex	1CM1
CHS-hexanoyl-CoA comlex	1CHW
CHS-naringenin complex	1CGK
CHS-resveratrol complex	1CGZ

The crystals of the present invention belong to the tetragonal space group. The unit cell dimensions vary by a few angstroms between crystals but on average, chalcone synthase native crystals belong to space group $P3_221$ with unit cell dimensions of $a = b = 97.54$ Å; $c = 65.52$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$ with a single monomer per asymmetric unit. Stilbene synthase crystals belong to space group C222 with unit cell dimensions of $a = 74.94$ Å , $b = 86.63$ Å , $c = 364.18$ Å , $\alpha = \beta = \gamma = 90°$. Pyrone synthase crystals belong to space group P3121 with unit cell dimensions of $a = 82.15$ Å, $b = 241.33$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$ with one PS dimer per asymmetric unit.

Crystal structures are preferably obtained at a resolution of about 1.56 angstroms to about 3 angstroms for a polyketide synthase in the presence and in the absence of bound substrate or substrate analog. Coordinates for a polyketide synthase in the absence of a substrate bound in the active site have been deposited at the Brookhaven National Laboratory Protein Data Bank, accession number 1CGK. Those skilled in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. Therefore, for the purpose of this invention, any set of structure coordinates wherein the active site α-carbons of a polyketide synthase, synthase homologue, or mutants thereof, have a root mean square deviation less than ± 2.3 angstroms when superimposed using the structural coordinates listed in Table 1 and PDB Accession No. 1BI5, shall be considered

identical.

A schematic representation of the three-dimensional shape of a CHS homodimer is shown in Figure 2a, which was prepared by MOLSCRIPT (Kraulis, J. Appl. Crystallogr. 24:946-950, 1991). CHS functions as a homodimer of two 42 kDa polypeptides. The structure of CHS reveals that the enzyme forms a symmetric dimer with each monomer related by a 2-fold crystallographic axis. The dimer interface buries approximately 1580 angstroms with interactions occurring along a fairly flat surface. Two distinct structural features delineate the ends of this interface. First, the N-terminal helix of monomer A entwines with the corresponding helix of monomer B. Second, a tight loop containing a cis-peptide bond between Met_{137} and Pro_{138} exposes the methionine sidechain as a knob on the monomer surface. Across the interface, Met_{137} protrudes into a hole found in the surface of the adjoining monomer to form part of the cyclization pocket (discussed below).

The CHS homodimer contains two functionally independent active sites (Tropf, et al, J. Biol. Chem. 270:7922-7928, 1995). Consistent with this information, bound CoA thioesters and product analogs occupy both active sites of the homodimer in the CHS complex structures. These structures identify the location of the active site at the cleft between the upper and lower domains of each monomer. Each active site consists almost entirely of residues from a single monomer, with Met_{137} from the adjoining monomer being the only exception. A detailed description of the active site structure is presented in the Examples section, below.

An isolated, polyketide synthase of the invention comprises at least fourteen active site α-carbons having the structural coordinates of Table 1 ±2.3 angstroms. The active site α-carbons of Table 1 generally are not all contiguous, i.e., are not adjacent to one another in the primary amino acid sequence of a polyketide synthase due to intervening amino acid residues between various active site α-carbons. Nevertheless, it should be appreciated that certain active site α-carbons can be adjacent to one another in some instances. Active site α-carbons are numbered in Table 1 for convenience only and may be situated in any suitable order in the primary amino acid

sequence that achieves the structural coordinates given in Table 1.

An appropriate combination of R-groups, linked to active site α-carbons, can facilitate the formation of one or more desired reaction products. The combination of R-groups selected for use in a synthase can be any combination other than the ordered arrangements of R-groups found in known native isolated polyketide synthases. Typically, R-groups found on active site α-carbons are those found in naturally occurring amino acids. In some embodiments, however, R-groups other than those found in naturally occurring amino acids can be used.

The present invention permits the use of molecular design techniques to design, select, and synthesize genes encoding mutant polyketide synthases that produce different and/or novel polyketide compounds using substrates. Mutant proteins of the present invention and nucleic acids encoding the same can be designed by genetic manipulation based on structural information about polyketide synthases. For example, one or more R-groups associated with the active site α-carbon atoms of CHS can be changed by altering the nucleotide sequence of the corresponding CHS gene, thus making one or more mutant polyketide synthases. Such genetic manipulations can be guided by structural information concerning the R-groups found in the active site α-carbons when substrate is bound to the protein upon crystallization.

Mutant proteins of the present invention may be prepared in a number of ways available to the skilled artisan. For example, the gene encoding wild-type CHS may be mutated at those sites identified herein as corresponding to amino acid residues identified in the active site by means currently available to the artisan skilled in molecular biology techniques. Said techniques include oligonucleotide-directed mutagenesis, deletion, chemical mutagenesis, and the like. The protein encoded by the mutant gene is then produced by expressing the gene in, for example, a bacterial or plant expression system.

Alternatively, polyketide synthase mutants may be generated by site specific-replacement of a particular amino acid with an unnaturally occurring amino acid. As such, polyketide synthase mutants may be generated through replacement of an amino

acid residue or a particular cysteine or methionine residue with selenocysteine or selenomethionine. This may be achieved by growing a host organism capable of expressing either the wild-type or mutant polypeptide on a growth medium depleted of natural cysteine or methionine or both and growing on medium enriched with either selenocysteine, selenomethionine, or both. These and similar techniques are described in Sambrook et al., (Molecular Cloning, A Laboratory Manual, 2nd Ed. (1989) Cold Spring Harbor Laboratory Press).

Another suitable method of creating mutant synthases of the present invention is based on a procedure described in Noel and Tsal (1989) J. Cell. Biochem., 40:309-320. In so doing, the nucleic acids encoding said polyketide synthase can be synthetically produced using oligonucleotides having overlapping regions, said oligonucleotides being degenerate at specific bases so that mutations are induced.

According to the present invention, nucleic acid sequences encoding a mutated polyketide synthase can be produced by the methods described herein, or any alternative methods available to the skilled artisan. In designing the nucleic acid sequence of interest, it may be desirable to reengineer said gene for improved expression in a particular expression system. For example, it has been shown that many bacterially derived genes do not express well in plant systems. In some cases, plant-derived genes do not express well in bacteria. This phenomenon may be due to the non-optimal G+C content and/or A+T content of said gene relative to the expression system being used. For example, the very low G+C content of many bacterial genes results in the generation of sequences mimicking or duplicating plant gene control sequences that are highly A+T rich. The presence of A+T rich sequences within the genes introduced into plants (e.g., TATA box regions normally found in promoters) may result in aberrant transcription of the gene(s). In addition, the presence of other regulatory sequences residing in the transcribed mRNA (e.g. polyadenylation signal sequences (AAUAAA) or sequences complementary to small nuclear RNAs involved in pre-mRNA splicing) may lead to RNA instability. Therefore, one goal in the design of genes is to generate nucleic acid sequences that have a G+C content that affords mRNA stability and translation accuracy for a

particular expression system.

Due to the plasticity afforded by the redundancy of the genetic code (i.e., some amino acids are specified by more than one codon), evolution of the genomes of different organisms or classes of organisms has resulted in differential usage of redundant codons. This "codon bias" is reflected in the mean base composition of protein coding regions. For example, organisms with relatively low G+C contents utilize codons having A or T in the third position of redundant codons, whereas those having higher G+C contents utilize codons having G or C in the third position. Therefore, in reengineering genes for expression, one may wish to determine the codon bias of the organism in which the gene is to be expressed. Looking at the usage of the codons as determined for genes of a particular organism deposited in GenBank can provide this information. After determining the bias thereof, the new gene sequence can be analyzed for restriction enzyme sites as well as other sites that could affect transcription such as exon:intron junctions, polyA addition signals, or RNA polymerase termination signals.

Genes encoding polyketide synthases can be placed in an appropriate vector, depending on the artisan's interest, and can be expressed using a suitable expression system. An expression vector, as is well known in the art, typically includes elements that permit replication of said vector within the host cell and may contain one or more phenotypic markers for selection of cells containing said gene. The expression vector will typically contain sequences that control expression such as promoter sequences, ribosome binding sites, and translational initiation and termination sequences. Expression vectors may also contain elements such as subgenomic promoters, a repressor gene or various activator genes. The artisan may also choose to include nucleic acid sequences that result in secretion of the gene product, movement of said product to a particular organelle such as a plant plastid (see U.S. Patent Nos. 4,762,785; 5,451,513 and 5,545,817, which are incorporated herein by reference) or other sequences that increase the ease of peptide purification, such as an affinity tag.

A wide variety of expression control sequences are useful in expressing the

mutated polyketide synthases when operably linked thereto. Such expression control sequences include, for example, the early and late promoters of SV40 for animal cells, the lac system, the trp system, major operator and promoter systems of phage S, and the control regions of coat proteins, particularly those from RNA viruses in plants. In *E. coli*, a useful transcriptional control sequence is the T7 RNA polymerase binding promoter, which can be incorporated into a pET vector as described by Studier et al., (1990) Methods Enzymology, 185:60-89, which is incorporated herein by reference.

For expression, a desired gene should be operably linked to the expression control sequence and maintain the appropriate reading frame to permit production of the desired polyketide synthase. Any of a wide variety of well-known expression vectors are of use to the present invention. These include, for example, vectors comprising segments of chromosomal, non-chromosomal and synthetic DNA sequences such as those derived from SV40, bacterial plasmids including those from *E. coli* such as col E1, pCR1, pBR322 and derivatives thereof, pMB9), wider host range plasmids such as RP4, phage DNA such as phage S, NM989, M13, and other such systems as described by Sambrook et al., (Molecular Cloning, A Laboratory Manual, 2nd Ed. (1989) Cold Spring Harbor Laboratory Press), which is incorporated herein by reference.

A wide variety of host cells are available for expressing synthase mutants of the present invention. Such host cells include, for example, bacteria such as *E. coli*, *Bacillus* and *Streptomyces*, fungi, yeast, animal cells, plant cells, insect cells, and the like. Preferred embodiments of the present invention include chalcone synthase mutants that are expressed in *E. coli* or in plant cells. Said plant cells can either be in suspension culture or a transgenic plant as further described herein.

As stated previously, genes encoding synthases of the present invention can be expressed in transgenic plant cells. In order to produce transgenic plants, vectors containing the nucleic acid construct encoding polyketide synthases and mutants thereof are inserted into the plant genome. Preferably, these recombinant vectors are

capable of stable integration into the plant genome. One variable in making a transgenic plant is the choice of a selectable marker. A selectable marker is used to identify transformed cells against a high background of untransformed cells. The preference for a particular marker is at the discretion of the artisan, but any of the selectable markers may be used along with any other gene not listed herein that could function as a selectable marker. Such selectable markers include aminoglycoside phosphotransferase gene of transposon Tn5 (Aph 11) (which encodes resistance to the antibiotics kanamycin), neomycin, G418, as well as those genes which code for resistance or tolerance to glyphosate, hygromycin, methotrexate, phosphinothricin, imidazolinones, sulfonylureas, triazolophyrimidine herbicides, such as chlorosulfuron, bromoxynil, dalapon, and the like. In addition to a selectable marker, it may be desirable to use a reporter gene. In some instances a reporter gene may be used with a selectable marker. Reporter genes allow the detection of transformed cells and may be used at the discretion of the artisan. A list of these reporter genes is provided in K. Wolsing et al., 1988, Ann. Rev. Genetics, 22:421.

Said genes are expressed either by promoters expressing in all tissues at all times (constitutive promoters), by promoters expressing in specific tissues (tissue-specific promoters), promoters expressing at specific stages of development (developmental promoters), and/or promoter expression in response to a stimulus or stimuli (inducible promoters). The choice of these is at the discretion of the artisan.

Several techniques exist for introducing foreign genes into plant cells, and for obtaining plants that stably maintain and express the introduced gene. Such techniques include acceleration of genetic material coated on a substrate directly into cells (U.S. Patents 4,945,050 to Comell): Plant cells may also be transformed using *Agrobacterium* technology (see, for example, U.S. Patents 5,177,010 to University of Toledo, 5,104,310 to Texas A&M, U. S. Patents 5,149,645, 5,469,976, 5,464,763, 4,940,838, and 4,693,976 to Schilperoot, European Patent Applications 116718, 290799, 320500 to Max Planck, European Patent Applications 604662,627752 and U.S. Patent 5,591,616 to Japan Tobacco, European Patent Applications 0267159, 0292435 and U.S. Patent 5,231,01.q to Ciba-Geigy, U.S. Patents 5,463,174 and

4,762,785 to Calgene, and U.S. Patents 5,004,863 and 5,159,135 to Agracetus). Other transformation technologies include whiskers technology (see U. S. Patents 5,302,523 and 5,464,765 to Zeneca). Electroporation technology has also been used to transform plants (see WO 87106614 to Boyce Thompson Institute, 5,472,869 and 5,384,253 to Dakalb, and WO 92/09696 and WO 93/21335 to Plant Genetic Systems, all which are incorporated by reference). Viral vector expression systems can also be used such as those described in U.S, Patent 5,316,931, 5,589,367, 5,811,653, and 5,866,785 to BioSource, which are incorporated herein by reference.

In addition to numerous technologies for transforming plants, the type of tissue that is contacted with the genes of interest may vary as well. Suitable tissue includes, for example, embryonic tissue, callus tissue, hypocotyl, meristem, and the like. Almost all plant tissues may be transformed during de-differentiation using the appropriate techniques described herein.

Regardless of the transformation system used, a gene encoding a mutant polyketide synthase is preferably incorporated into a gene transfer vector adapted to express said gene in a plant cell by including in the vector an expression control sequence (plant promoter regulatory element). In addition to plant promoter regulatory elements, promoter regulatory elements from a variety of sources can be used efficiently in plant cells to express foreign genes. For example, promoter regulatory elements of bacterial origin, such as the octopine synthase promoter, the nopaline synthase promoter, the mannopine synthase promoter, and the like, may be used. Promoters of viral origin, such as the cauliflower mosaic virus (35S and 198) are also desirable. Plant promoter regulatory elements also include ribulose-1,6-bisphosphate carboxylase small subunit promoter, beta-conglycinin promoter, phaseolin promoter, ADH promoter, heat-shock promoters, tissue specific promoters, and the like. Numerous promoters are available to skilled artisans for use at their discretion.

It should be understood that not all expression vectors and expression systems function in the same way to express the mutated gene sequences of the present

invention. Neither do all host cells function equally well with the same expression system. However, one skilled in the art may make a selection among these vectors, expression control sequences, and host without undue experimentation and without departing from the scope of this invention.

Once a synthase of the present invention is expressed, the protein obtained therefrom can be purified so that structural analysis, modeling, and/or biochemical analysis can be performed, as exemplified herein. The nature of the protein obtained can be dependent on the expression system used. For example, genes, when expressed in mammalian or other eukaryotic cells, may contain latent signal sequences that may result in glycosylation, phosphorylation, or other post-translational modifications, which may or may not alter function. Therefore, a preferred embodiment of the present invention is the expression of mutant synthase genes in *E. coli* calls. Once said proteins are expressed, they can be easily purified using techniques common to the person having ordinary skill in the art of protein biochemistry, such as, for example, techniques described in Colligan at al., (1997) Current Protocols in Protein Science, Chanda, V. B., Ed., John Wiley & Sons, Inc., which is incorporated herein by reference. Such techniques often include the use of cation-exchange or anion-exchange chromatography, gel filtration-size exclusion chromatography, and the like. Another technique that may be commonly used is affinity chromatography. Affinity chromatography can include the use of antibodies, substrate analogs, or histidine residues (His-tag technology).

Once purified, mutants of the present invention may be characterized by any of several different properties. For example, such mutants may have altered active site surface charges of one or more charge units. In addition, said mutants may have altered substrate specificity or product capability relative to a non-mutated polyketide synthase.

The present invention allows for the characterization of polyketide synthase mutants by crystallization followed by X-ray diffraction. Polypeptide crystallization occurs in solutions where the polypeptide concentration exceeds it solubility

maximum (i.e., the polypeptide solution is supersaturated). Such solutions may be restored to equilibrium by reducing the polypeptide concentration, preferably through precipitation of the polypeptide crystals. Often polypeptides may be induced to crystallize from supersaturated solutions by adding agents that alter the polypeptide surface charges or perturb the interaction between the polypeptide and bulk water to promote associations that lead to crystallization.

Compounds known as "precipitants" are often used to decrease the solubility of the polypeptide in a concentrated solution by forming an energetically unfavorable precipitating layer around the polypeptide molecules (Weber, Advances in Protein Chemistry, 41:1-36, 1991). In addition to precipitants, other materials are sometimes added to the polypeptide crystallization solution. These include buffers to adjust the pH of the solution and salts to reduce the solubility of the polypeptide. Various precipitants are known in the art and include the following: ethanol, 3-ethyl-2-4 pentanediol, and many of the polyglycols, such as polyethylene glycol.

Commonly used polypeptide crystallization methods include the following techniques: batch, hanging drop, seed initiation, and dialysis. In each of these methods, it is important to promote continued crystallization after nucleation by maintaining a supersaturated solution. In the batch method, polypeptide is mixed with precipitants to achieve supersaturation, the vessel is sealed, and set aside until crystals appear. In the dialysis method, polypeptide is retained in a sealed dialysis membrane that is placed into a solution containing precipitant. Equilibration across the membrane increases the polypeptide and precipitant concentrations thereby causing the polypeptide to reach supersaturation levels.

In the preferred hanging drop technique (McPherson, J. Biot Chem, 6300-6306, 1976), an initial polypeptide mixture is created by adding a precipitant to a concentrated polypeptide solution. The concentrations of the polypeptide and precipitants are such that in this initial form, the polypeptide does not crystallize. A small drop of this mixture is placed on a glass slide that is inverted and suspended

over a reservoir of a second solution. The system is then sealed. Typically, the second solution contains a higher concentration of precipitant or other dehydrating agent. The difference in the precipitant concentrations causes the protein solution to have a higher vapor pressure than the solution. Since the system containing the two solutions is sealed, an equilibrium is established, and water from the polypeptide mixture transfers to the second solution. This equilibrium increases the polypeptide and precipitant concentration in the polypeptide solution. At the critical concentration of polypeptide and precipitant, a crystal of the polypeptide will form.

Another method of crystallization introduces a nucleation site into a concentrated polypeptide solution. Generally, a concentrated polypeptide solution is prepared and a seed crystal of the polypeptide is introduced into this solution. If the concentration of the polypeptide and any precipitants are correct, the seed crystal will provide a nucleation site around which a larger crystal forms. In preferred embodiments, the crystals of the present invention are formed in hanging drops with (15% PEG 8000; 200 rnM magnesium acetate or magnesium chloride, 100 mM 3-(N-morpholino)-2-hydroxypropanesulfonic acid (pH 7.0), 1 mM dithiothreitol as precipitant).

Some proteins may be recalcitrant to crystallization. However, several techniques are available to the skilled artisan. Quite often the removal of polypeptide segments at the amino or caroxy terminal end of the protein is necessary to produce crystalline protein samples. Said procedures involve either the treatment of the protein with one of several proteases including trypsin, chymotrypsin, substilisin, and the like. This treatment often results in the removal of flexible polypeptide segments that are likely to negatively affect crystallization. Alternatively, the removal of coding sequences from the protein's gene facilitates the recombinant expression of shortened proteins that can be screened for crystallization.

The crystals so produced have a wide range of uses. For example, high quality crystals are suitable for X-ray or neutron diffraction analysis to determine the three-dimensional structure of a mutant polyketide synthase and to design additional

mutants thereof. In addition, crystallization can serve as a further purification method. In some instances, a polypeptide or protein will crystallize from a heterogeneous mixture into crystals. Isolation of such crystals by filtration, centrifugation, etc., followed by redissolving the polypeptide affords a purified solution suitable for use in growing the high-quality crystals needed for diffraction studies. The high-quality crystals may also be dissolved in water and then formulated to provide an aqueous solution having other uses as desired.

Because synthases may crystallize in more than one crystal form, the structural coordinates of α-carbons of an active site determined from a synthase or portions thereof, as provided by this invention, are particularly useful to solve the structure of other crystal forms of synthases. Said structural coordinates, as provided herein, may also be used to solve the structure of synthases having α-carbons positioned within the active sites in a manner similar to the wild-type, yet having R-groups that may or may not be identical.

Furthermore, the structural coordinates disclosed herein may be used to determine the structure of the crystalline form of other proteins with significant amino acid or structural homology to any functional domain of a synthase. One method that may be employed for such purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of a synthase, a synthase having a mutated active site, or the crystal of some other protein with significant sequence and/or structural homology to a polyketide synthase may be determined using the coordinates given in Table 1. This method provides sufficient structural form for the unknown crystal more efficiently than attempting to determine such information *ab initio*. In addition, this method can be used to determine whether or not a given polyketide synthase in question falls within the scope of this invention.

As further disclosed herein, polyketide synthases and mutants thereof may be crystallized in the presence or absence of substrates and substrate analogs. The crystal structures of a series of complexes may then be solved by molecular replacement and compared to that of the wild-type to assist in determination of suitable replacements

for R-groups within the active site, thus making synthase mutants according to the present invention.

All mutants of the present inventions may be modeled using the information disclosed herein without necessarily having to crystallize and solve the structure for each and every mutant. For example, one skilled in the art may use one of several specialized computer programs to assist in the process of designing synthases having mutated active sites relative to the wild-type. Examples of such programs include: GRID (Goodford, 1985, J. Mod. Chem., 28:849-857), MCSS (Miranker and Karplus, 1991, Proteins: Structure, Function and Genetics, 11:29-34); AUTODOCK (Goodsell and Olsen, 1990, Proteins. Structure, Fumtion, and Genetics, 8:195-202); and DOCK (Kuntz et al., 1982, J. Mot BioL, 161:269-288), and the like, as well as those discussed in the Examples below. In addition, specific computer programs are also available to evaluate specific substrate-active site interactions and the deformation energies and electrostatic interactions resulting therefrom. MODELLER is a computer program often used for homology or comparative modeling of the three-dimensional structure of a protein. A. Saii & T.L. Blundell. J. Mol.Biol. 234:779-815, 1993. A sequence to be modeled is aligned with one or more known related structures and the MODELLER program is used to calculate a full-atom model, based on optimum satisfaction of spatial restraints. Such restraints can include, inter alia, homologous structures, site-directed mutagenesis, fluorescence spectroscopy, NMR experiments, or atom-atom potentials of mean force.

The present invention enables polyketide synthase mutants to be made and the crystal structure thereof to be solved. Moreover, by virtue of the present invention, the location of the active site and the interface of substrate therewith permit the identification of desirable R-groups for mutagenesis.

The three-dimensional coordinates of the polyketide synthase provided herein may additionally be used to predict the activity and or substrate specificity of a protein whose primary amino acid sequence suggests that it may have polyketide synthase activity. The family of CHS-related enzymes is defined, in part, by the presence of

four highly conserved amino acid residues, Cys_{164}, Phe_{215}, His_{303}, and Asn_{336}. More than 150 enzymes having these conserved residues have been identified to date, including several bacterial proteins. The functions, substrates, and products of many of these enzymes remains unknown. However, by employing the three-dimensional coordinates disclosed herein and computer modeling programs, structural comparisons of CHS can be made with a putative enzyme. Differences between the two would provide the skilled artisan with information regarding the activity and/or substrate specificity of the putative enzyme. This procedure is demonstrated in the Examples section below.

Thus, in another embodiment of the invention, there is provided a method of predicting the activity and/or substrate specificity of a putative polyketide synthase comprising (a) generating a three-dimentional representation of a known polyketide synthase using three-dimentional coordinate data, (b) generating a predicted three-dimentional representation of a putative polyketide synthase, and (c) comparing the representation of the known polyketide synthase with the representation of the putative polyketide synthase, wherein the differences between the two representations are predictive of activity and/or substrate specificity of the putative polyketide synthase.

In a further embodiment of the present invention, there is also provided a method of identifying a potential substrate of a polyketide synthase comprising (a) defining the active site of the polyketide synthase based on the atomic coordinates of said polyketide synthase, (b) identifying a potential substrate that fits the defined active site, and (c) contacting the polyketide synthase with the potential substrate of (b) and determining the activity thereon. Techniques for computer modeling and structural comparisons similar to those described herein for predicting putative polyketide synthase activity and/or substrate specificity can be used to identify novel substrates for polyketide synthases.

In addition, the structural coordinates and three-dimensional models disclosed herein can be used to design or identify polyketide synthase inhibitors. Using the

modeling techniques disclosed herein, potential inhibitor structures can be modeled with the polyketide synthase active site and those that appear to interact therewith can subsequently be tested in activity assays in the presence of substrate.

Methods of using crystal structure data to design binding agents or substrates are known in the art. Thus, the crystal structure data provided herein can be used in the design of new or improved inhibitors, substrates or binding agents. For example, the synthase polypeptide coordinates can be superimposed onto other available coordinates of similar enzymes to identify modifications in the active sites of the enzymes to create novel byproducts of enzymatic activity or to modulate polyketide synthesis. Alternatively, the synthase polypeptide coordinates can be superimposed onto other available coordinates of similar enzymes which have substrates or inhibitors bound to them to give an approximation of the way these and related substrates or inhibitors might bind to a synthase. Alternatively, computer programs employed in the practice of rational drug design can be used to identify compounds that reproduce interaction characteristics similar to those found between a synthase polypeptide and a co-crystalized substrate. Furthermore, detailed knowledge of the nature of binding site interactions allows for the modification of compounds to alter or improve solubility, pharmacokinetics, *etc.* without affecting binding activity.

Computer programs are widely available that are capable of carrying out the activities necessary to design agents using the crystal structure information provided herein. Examples include, but are not limited to, the computer programs listed below:

Catalyst Databases™ - an information retrieval program accessing chemical databases such as BioByte Master File, Derwent WDI and ACD;

Catalyst/HYPO™ - generates models of compounds and hypotheses to explain variations of activity with the structure of drug candidates;

Ludi™ - fits molecules into the active site of a protein by identifying and matching complementary polar and hydrophobic groups;

Leapfrog™ - "grows" new ligands using a genetic algorithm with parameters under the control of the user.

In addition, various general purpose machines may be used with programs written in accordance with the teachings herein, or it may be more convenient to construct more specialized apparatus to perform the operations. However, preferably the embodiment is implemented in one or more computer programs executing on programmable systems each comprising at least one processor, at least one data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. The program is executed on the processor to perform the functions described herein.

Each such program may be implemented in any desired computer language (including machine, assembly, high level procedural, object oriented programming languages, or the like) to communicate with a computer system. In any case, the language may be a compiled or interpreted language. The computer program will typically be stored on a storage media or device (*e.g.*, ROM, CD-ROM, or magnetic or optical media) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

Embodiments of the invention include systems (*e.g.*, internet based systems), particularly computer systems which store and manipulate the coordinate and sequence information described herein. One example of a computer system **100** is illustrated in block diagram form in Figure 9. As used herein, "a computer system" refers to the hardware components, software components, and data storage components used to analyze the coordinates and sequences as set forth in Accession Nos. 1BI5, 1D6F, 1D6I, 1D6H, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ, Table 1, and Table 3. The computer system **100** typically includes a processor for processing, accessing and manipulating

the sequence data. The processor **105** can be any well-known type of central processing unit, such as, for example, the Pentium III from Intel Corporation, or similar processor from Sun, Motorola, Compaq, AMD or International Business Machines.

Typically the computer system **100** is a general purpose system that comprises the processor **105** and one or more internal data storage components **110** for storing data, and one or more data retrieving devices for retrieving the data stored on the data storage components. A skilled artisan can readily appreciate that any one of the currently available computer systems are suitable.

In one particular embodiment, the computer system **100** includes a processor **105** connected to a bus which is connected to a main memory **115** (preferably implemented as RAM) and one or more internal data storage devices **110**, such as a hard drive and/or other computer readable media having data recorded thereon. In some embodiments, the computer system **100** further includes one or more data retrieving device **118** for reading the data stored on the internal data storage devices **110**.

The data retrieving device **118** may represent, for example, a floppy disk drive, a compact disk drive, a magnetic tape drive, or a modem capable of connection to a remote data storage system (*e.g.*, via the internet) etc. In some embodiments, the internal data storage device **110** is a removable computer readable medium such as a floppy disk, a compact disk, a magnetic tape, etc. containing control logic and/or data recorded thereon. The computer system **100** may advantageously include or be programmed by appropriate software for reading the control logic and/or the data from the data storage component once inserted in the data retrieving device.

The computer system **100** includes a display **120** which is used to display output to a computer user. It should also be noted that the computer system **100** can be linked to other computer systems **125a-c** in a network or wide area network to provide centralized access to the computer system **100**.

Software for accessing and processing the coordinate and sequences described herein, (such as search tools, compare tools, and modeling tools etc.) may reside in main memory **115** during execution.

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize novel enzymes, chemical entities and compounds, including inhibitory compounds, capable of binding to a polyketide synthase polypeptide (*e.g.*, a chalcone synthase polypeptide), in whole or in part.

One approach enabled by this invention, is to use the structure coordinates as set forth in Accession Nos. 1BI5, 1D6F, 1D6I, 1D6H, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ, Table 1, and Table 3 to design new enzymes capable of synthesizing novel polyketides. For example, polyketide synthases (PKSs) generate molecular diversity in their products by utilizing different starter molecule sand by varying the final size of the polyketide chain. The structural coordinates disclosed herein allowed the elucidation of the nature by which PKSs achieve starter molecule selectivity and control polyketide chain length. By comparing the structure of chalcone synthase, which yields a tetraketide product to 2-pyrone synthases which forms a triketide product the invention demonstrated that 2-pyrone synthase maintains a smaller initiation/elongation cavity. Accordingly, generation of a chalcone synthase mutant with an active site sterically analogous to 2-pyrone synthase resulted in the synthesis of a polyketide product of a different size. As discussed more fully below, this invention allows for the strategic development and biosynthesis of more diverse polyketides and demonstrates a structural basis for control of polyketide chain length in other PKSs. In addition, the structural coordinates allow for the development of substrates or binding agents that bind to the polypeptide and alter the physical properties of the compounds in different ways, *e.g.*, solubility.

In another approach a polyketide synthase polypeptide crystal is probed with molecules composed of a variety of different chemical entities to determine optimal sites

for interaction between candidate binding molecules (*e.g.*, substrates) and the polyketide synthase (*e.g.*, chalcone synthase).

In another embodiment, an approach made possible and enabled by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to a polyketide synthase polypeptide or fragment thereof. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng, E. C. *et al.*, J. Comp. Chem., 13, pp. 505-524 (1992).

Because chalcone synthase is one member of a family of polyketide synthase polypeptides, many of which have similar functional activity, many polyketide synthase polypeptides may crystallize in more than one crystal form, the structure coordinates of chalcone synthase, or portions thereof, as provided by this invention are particularly useful to solve the structure, function or activity of other crystal forms of polyketide synthase molecules. They may also be used to solve the structure of a polyketide synthase or a chalcone synthase mutant.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another polyketide synthase crystal form, a polyketide synthase or chalcone synthase mutant, or a polyketide synthase complexed with a substrate or other molecule, or the crystal of some other protein with significant amino acid sequence homology to any polyketide synthase polypeptide, may be determined using the structure coordinates as provided in Accession Nos. 1BI5, 1D6F, 1D6I, 1D6H, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ, Table 1, or Table 3. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

In addition, in accordance with the present invention, a polyketide synthase or chalcone synthase polypeptide mutant may be crystallized in association or complex with known polyketide synthase binding agents, substrates, or inhibitors. The crystal

structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type polyketide synthase molecules. Potential sites for modification within the synthase molecule may thus be identified. This information provides an additional tool for determining the most efficient binding interactions between a polyketide synthase and a chemical entity, substrate or compound.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined to 2-3 Å resolution X-ray data to an R value of about 0.20 or less using computer software, such as X-PLOR (Yale University, 1992, distributed by Molecular Simulations, Inc.). See, *e.g.*, Blundel & Johnson, *supra*; Methods in Enzymology, vol. 114 and 115, H. W. Wyckoff *et al.*, eds., Academic Press (1985). This information may thus be used to optimize known classes of polyketide synthase substrates or binding agents (*e.g.*, inhibitors), and to design and synthesize novel classes of polyketide synthases, substrates, and binding agents (*e.g.*, inhibitors).

The design of substrates, compounds or binding agents that bind to or inhibit a polyketide synthase polypeptide according to the invention generally involves consideration of two factors. First, the substrate, compound or binding agent must be capable of physically and structurally associating with a polyketide synthase molecule. Non-covalent molecular interactions important in the association of a polyketide synthase with a substrate include hydrogen bonding, van der Waals and hydrophobic interactions, and the like.

Second, the substrate, compound or binding agent must be able to assume a conformation that allows it to associate with a polyketide synthase molecule. Although certain portions of the substrate, compound or binding agent will not directly participate in this association, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, *e.g.*, active site or accessory binding site of a polyketide synthase (*e.g.*, a chalcone synthase

polypeptide), or the spacing between functional groups of a substrate or compound comprising several chemical entities that directly interact with a polyketide synthase.

The potential binding effect of a substrate or chemical compound on a polyketide synthase or the activity a newly synthesized or mutated polyketide synthase might have on a known substrate may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. For example, if the theoretical structure of the given substrate or compound suggests insufficient interaction and association between it and a polyketide synthase, synthesis and testing of the compound may be obviated. However, if computer modeling indicates a strong interaction, the molecule may then be tested for its ability to bind to, initiate catalysis or elongation of a polyketide by a polyketide synthase. Methods of assaying for polyketide synthase activity are known in the art (as identified and discussed herein). Methods for assaying the effect of a newly created polyketide synthase or a potential substrate or binding agent can be performed in the presence of a known binding agent or polyketide synthase. For example, the effect of the potential binding agent can be assayed by measuring the ability of the potential binding agent to compete with a known substrate.

A mutagenized synthase, novel synthase, substrate or other binding compound of an polyketide synthase may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of the polyketide synthase.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a polyketide synthase and more particularly with the individual binding pockets of a chalcone synthase polypeptide. This process may begin by visual inspection of, for example, the active site on the computer screen based on the coordinates in Accession Nos. 1BI5, 1D6F, 1D6I, 1D6H, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ, Table 1, or Table 3. Selected fragments or substrates or chemical entities may then be positioned in a variety of orientations, or docked, within an individual binding pocket of a polyketide synthase. Docking may be

accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure. Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, Mass.

3. AUTODOCK (Goodsell, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure. Function, and Genetics, 8, pp. 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.

4. DOCK (Kuntz, I. D. *et al.*, "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable substrates, chemical entities or fragments have been selected, they can be assembled into a single polypeptide, compound or binding agent (*e.g.*, an inhibitor). Assembly may be performed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of the molecules as set forth in Accession Nos. 1BI5, 1D6F, 1D6I, 1D6H, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ, Table 1, or Table 3.

This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (Bartlett, P. A. et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In "Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989)). CAVEAT is available from the University of California, Berkeley, Calif.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif.). This area is reviewed in Martin, Y. C., "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992)).

3. HOOK (available from Molecular Simulations, Burlington, Mass.).

In addition to the method of building or identifying novel enzymes or a polyketide synthase substrate or binding agent in a step-wise fashion one fragment or chemical entity at a time as described above, substrates, inhibitors or other polyketide synthase interactions may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of known substrates, binding agents or inhibitors. These methods include:

1. LUDI (Bohm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, Calif.

2. LEGEND (Nishibata, Y. and A. Itai, Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, Mass.

3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).

Other molecular modeling techniques may also be employed in accordance with this invention. See, *e.g.*, Cohen, N. C. *et al.*, "Molecular Modeling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33, pp. 883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once a substrate, compound or binding agent has been designed or selected by the above methods, the efficiency with which that substrate, compound or binding agent may bind to a polyketide synthase may be tested and optimized by computational evaluation.

A substrate or compound designed or selected as a polyketide binding agent may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target site. Such non-complementary (*e.g.*, electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the binding agent and the polyketide synthase when the binding agent is bound to the polyketide synthase, preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa., 1992); AMBER, version 4.0 (P. A. Kollman, University of California at San Francisco, 1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, Mass. 1994); and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif., 1994). These programs may be implemented, for example, using a Silicon Graphics workstation, IRIS 4D/35 or IBM RISC/6000 workstation model 550. Other hardware systems and software packages will be known to those skilled in the art of which the speed and capacity are continually modified

Once a polyketide synthase, polyketide synthase substrate or polyketide synthase binding agent has been selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, *e.g.*, the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analyzed for efficiency of fit to a polyketide synthase substrate or fit of a modifed substrate to a polyketide synthase having a structure defined by the coordinates in Accession Nos. 1BI5, 1D6F, 1D6I, 1D6H, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ, Table 1, or Table 3, by the same computer methods described, above.

Conserved regions of the polyketide family synthases lend themselves to the methods and compositions of the invention. For example, pyrone synthase and chalcone synthase have conserved residues present within their active sites (as described more fully below). Accordingly, modification to the active site of chalcone synthase or a chalcone synthase substrate can be extrapolated to other conserved members of the polyketide family of synthases such as, for example, pyrone synthase.

Functional fragments of polyketide synthase polypeptides such as, for example, fragments of chalcone synthase can be designed based on the crystal structure and atomic coordinates described herein. Fragments of a chalcone synthase polypeptide and the fragment's corresponding atomic coordinates can be used in the modeling described herein. In addition, such fragments may be used to design novel substrates or modified active sites to create new diverse polyketides.

In one embodiment of the present invention, the crystal structure and atomic coordinates allow for the design of novel polyketide synthases and novel polyketide synthase substrates. The development of new polyketide synthases will lead to the development a biodiverse repetoir of polyketides for use as antibiotics, anti-cancer agents, anti-fungal agents and other therapeutic agents as described herein or known in the art. In vitro assay systems for production and determination of activity are

known in the art. For example, antibiotic activities of novel polyketides can be measured by any number of anti-microbial techniques currently used in hospitals and laboratories. In addition, anticancer activity can be determined by contacting cells having a cell proliferative disorder with a newly synthesized polyketide and measuring the proliferation or apoptosis of the cells before and after contact with the polyketide. Specific examples of apoptosis assays are provided in the following references: Lymphocyte: C. J. Li *et al.*, Science, 268:429-431, 1995; D. Gibellini *et al.*, Br. J. Haematol. 89:24-33, 1995; S. J. Martin *et al.*, J. Immunol. 152:330-42, 1994; C. Terai *et al.*, J. Clin Invest. 87:1710-5, 1991; J. Dhein *et al.*, Nature 373:438-441, 1995; P. D. Katsikis *et al.*, J. Exp. Med. 1815:2029-2036, 1995; Michael O. Westendorp *et al.*, Nature 375:497, 1995; DeRossi *et al.*, Virology 198:234-44, 1994. Fibroblasts: H. Vossbeck *et al.*, Int. J. Cancer 61:92-97, 1995; S. Goruppi *et al.*, Oncogene 9:1537-44, 1994; A. Fernandez *et al.*, Oncogene 9:2009-17, 1994; E. A. Harrington *et al.*, Embo J. 13:3286-3295, 1994; N. Itoh *et al.*, J. Biol. Chem. 268:10932-7, 1993. Neuronal Cells: G. Melino *et al.*, Mol. Cell. Biol. 14:6584-6596, 1994; D. M. Rosenbaum *et al.*, Ann. Neurol. 36:864-870, 1994; N. Sato *et al.*, J. Neurobiol 25:1227-1234, 1994; G. Ferrari *et al.*, J. Neurosci. 1516:2857-2866, 1995; A. K. Talley *et al.*, Mol. Cell Biol. 1585:2359-2366, 1995; A. K. Talley *et al.*, Mol. and Cell. Biol. 15:2359-2366, 1995; G. Walkinshaw *et al.*, J. Clin. Invest. 95:2458-2464, 1995. Insect Cells: R. J. Clem *et al.*, Science 254:1388-90, 1991; N. E. Crook *et al.*, J. Virol. 67:2168-74, 1993; S. Rabizadeh *et al.*, J. Neurochem. 61:2318-21, 1993; M. J. Birnbaum *et al.*, J. Virol 68:2521-8, 1994; R. J. Clem *et al.*, Mol. Cell. Biol. 14:5212-5222, (1994). Other assays are well within the ability of those of skill in the art.

Product of novel polyketides or polyketide synthases can be carried out in culture. For example, mammalian expression constructs carrying polyketide synthases can be introduced into various cell lines such as CHO, 3T3, HL60, Rat-1, or Jurkart cells, for example. In addition, SF21 insect cells may be used in which case the polyketide synthase gene is expressed using an insect heat shock promotor.

In another embodiment of the present invention, once a novel substrate or binding agent is developed by the computer methodology discussed above, the invention provides a method for determining the ability of the substrate or agent to be acted upon by a polyketide synthase. The method includes contacting components comprising the substrate or agent and a polyketide synthase polypeptide, or a recombinant cell expressing a polyketide synthase polypeptide, under conditions sufficient to allow the substrate or agent to interact and determining the affect of the agent on the activity of the polypeptide. The term "affect", as used herein, encompasses any means by which protein activity can be modulated, and includes measuring the interaction of the agent with the polyketide synthase molecule by physical means including, for example, fluorescence detection of the binding of an agent to the polypeptide. Such agents can include, for example, polypeptides, peptidomimetics, chemical compounds, small molecules, substrates and biologic agents as described herein. Examples of small molecules include but are not limited to small peptides or peptide-like molecules.

Contacting or incubating includes conditions which allow contact between the test agent or substrate and a polyketide synthase or modified polyketide synthase polypeptide or a cell expressing a polyketide synthase or modified polyketide synthase polypeptide. Contacting includes in solution and in solid phase. The substrate or test agent may optionally be a combinatorial library for screening a plurality of substrates or test agents. Agents identified in the method of the invention can be further evaluated by chromatography, cloning, sequencing, and the like.

Although methods and materials similar or equivalent to those described herein can be used to practice the invention, suitable methods and materials are described below. All publications, patent applications, patents and other references mentioned herein are incorporated by reference in their entirety. The invention will now be described in greater detail by reference to the following non-limiting examples.

EXAMPLES

Mutagenesis, expression, and purification. Alfalfa CHS2 cDNA (Junghans, H., et al, Plant Mol. Biol. 22:239-253, 1993) was subcloned into pHIS8 plasmid vector derived from pET-28a(+) (Novagen). PCR-based mutagenesis using the QuikChange system (Stratagene) generated the various mutants including $C_{164}S$, $C_{164}D$, $H_{303}A$, $H_{303}Q$, $H_{303}D$, $H_{303}T$, $N_{336}A$, $N_{336}D$, $N_{336}Q$, $N_{336}H$, $F_{215}S$, $F_{215}Y$ and $F_{215}W$. N-teminal His8-tagged CHS was expressed in BL21(DE3) *E. coli* cells. Cells were harvested and lysed by sonication. His-tagged CHS was purified from bacterial sonicates using a NI-NTA (Qiagen) column. Thrombin digest removed the His-tag and the protein was passed over another NI-NTA column and a benzamidine-Sepharose (Pharmacia) column. The final purification step used a Superdex 200 16/60 (Pharmacia) column.

Crystallization. CHS crystals (wild-type and $C_{164}S$ mutant) were grown by vapor diffusion at 4° C in 2 µl drops containing a 1:1 mixture of 25 mg/ml protein and crystallization buffer (2.2-2.4 M ammonium sulfate and 0.1 M PIPES, pH 6.5) in the presence or absence of 5 mM DTT. Prior to freezing at 105° K, crystals were stabilized in 40% (v/v) PEG400, 0.1 M PIPES (pH 6.5), and 0.050-0.075 M ammonium sulfate. This cryoprotectant was used for heavy atom soaks. Likewise, all substrate and product analog complexes were obtained by soaking crystals in cryoprotectant containing 10-20 mM of the compound.

Data Collection and Processing. X-ray diffraction data were collected at 105° K using a DIP2000 imaging plate system (Mac-Science Corporation, Japan) and CuK radiation produced by a rotating anode operated at 45 kV and 100 mA and equipped with double focusing Pt/Ni coated mirrors. Native CHS crystals belong to space group $P3_221$ with unit cell dimensions of $a = b = 97.54$ Å; c = 65.52 Å with a single monomer per asymmetric unit. Data were indexed and integrated using DENZO (Otwinowski & Minor, Meth. Enzymol. 276:307-326, 1997) and scaled with SCALEPACK (Otwinowski & Minor, Meth. Enzymol. 276:307-326, 1997). The

heavy atom derivative datasets were scaled against the native dataset with SCALEIT (CCP4 Suite: Programs for protein crystallography, Acta Crystallogr. D 50:760-763, 1994).

Structure determination. MIRAS was used to solve the structure of native CHS using native data set 1 (1.8 Å). Initial phasing was performed with derivative datasets including reflections to 2.3 Å resolution. Heavy atom positions for the $Hg(OAc)_2$ derivative were estimated by inspection of difference Patterson maps using the program XTALVIEW (McRee, J. Mol. Graph. 10:44-46, 1992) and initially refined with MLPHARE (Otwinowski, Z. in CCP4 Proc. *80-88,* Daresbury Laboratory, Warrington, UK, 1991). Heavy atom positions for the additional derivative data sets were determined by difference Fourier analysis using phases calculated from the $Hg(OAc)_2$ data set and the Hg positions. These sites were confirmed by inspection of difference Patterson maps. Final refinement of heavy atom parameters, identification of minor heavy atom binding sites, and phase-angle calculations were performed with the program SHARP (de La Fortelle, & Bricogne, Meth. Enzymol. 276:472-494, 1997). MIRAS phases were improved and extended to 1.8 Å by solvent flipping using the CCP4 program SOLOMON (Abrahams, & Leslie, Acta Crystallogr. D 52:30-42, 1996).

Model building and refinement. The program O (Jones, et al, Acta Crystallogr. D 49:148-157, 1993) was used for model building and graphical display of the molecules and electron-density maps. The experimental map for the native 1 dataset at 1.8 Å was of high quality and allowed unambiguous modeling of residues 3 to 389. The model was first refined with REFMAC (Murshudov, et al, Acta Crystallogr. D 53:240-255, 1997) and ARP (Lamzin & Wilson, Acta Crystallogr. D 49:129-147, 1993) against the native 1 dataset. This was followed by manual adjustments using $|2F_o-F_c|$ difference maps. Water molecules introduced by ARP were edited using the $|2F_o-F_c|$ and $|F_o-F_c|$ maps. A second refinement with SHELX-97 (Sheldrick & Schneider, Meth. Enzymol. 277:319-343, 1997) was then carried out against the native 2 data set to 1.56 Å resolution. Structures of CHS complexed with naringenin and resveratrol and the $C_{164}S$ mutant complexed with malonyl- and

hexanoyl-CoA were obtained using difference Fourier methods and were refined with REFMAC and ARP. All structures were checked with PROCHECK (Laskowski, et al, J. AppL Crystallogr. 26:283-291, 1993). 91.3 % of the residues in CHS are in the most favored regions of the Ramachandran plot, 8.4% in the additional allowed region, and 0.3% in the generously allowed region.

Three dimensional structure determination and description

Recombinant alfalfa CHS2 was expressed in *E. coli,* affinity purified using an N-terminal poly-His linker, and crystallized. The structure of wild-type CHS was determined using multiple isomorphous replacement supplemented with anomalous scattering (MIRAS) (Table X). The final 1.56 Å resolution apoenzyme model of CHS included 2982 protein atoms and 355 water molecules. In addition, the structures of a series of complexes were obtained by difference Fourier analysis. First, a crystal of a mutant ($C_{164}S$) was soaked with malonyl-CoA. This mutant retains limited catalytic activity, and the resulting acetyl-CoA complex yields insight on the decarboxylation reaction. The same mutant was also complexed with hexanoyl-CoA to mimic the structure of a linear polyketide-CoA reaction intermediate. Finally, two product analogs, naringenin and resveratrol (see Figure 1) were complexed with CHS to provide information on how the enzyme governs sequential addition of acetates to the coumaroyl moiety and how CHS controls the stereochemistry of the polyketide cyclization reaction. In plants, chalcone isomerase rapidly and stereospecifically converts chalcone to naringenin ((-)(2S)-5,7,4'-trihydroxyflavanone) through an additional ring closure. This reaction also occurs at a slower rate and non-stereospecifically in solution. As such, naringenin provides a suitable mimic of the CHS reaction product. Finally, since STS uses the same substrates as CHS but a different cyclization pathway for the biosynthesis of resveratrol, resveratrol was also soaked into CHS to investigate the structural features governing cyclization of the same substrates into two different products.

CHS functions as a homodimer of two 42 kDa polypeptides. The structure of CHS revealed that the enzyme forms a symmetric dimer with each monomer related

by a 2-fold crystallographic axis (See Figures 2a and 2b). The dimer interface buries approximately 1580 $Å^2$ with interactions occurring along a fairly flat surface. Two distinct structural features delineate the ends of this interface. First, the N-terminal helix of monomer A entwines with the corresponding helix of monomer B. Second, a tight loop containing a cis-peptide bond between Met_{137} and Pro_{138} exposes the methionine sidechain as a knob on the monomer surface. Across the interface, Met_{137} protrudes into a hole found in the surface of the adjoining monomer to form part of the cyclization pocket.

Each CHS monomer consists of two structural domains (see Figure 3). The upper domain exhibits an xBxBx pseudo-symmetric motif originally observed in thiolase from *Saccharomyces cerevisiae* (Mathieu, et al, Structure 2:797-808, 1994). The upper domains of CHS and thiolase are superimposeable with a r.m.s. deviation of 3.3 Å for 266 equivalent C-atoms. Both enzymes use a cysteine as a nucleophile and shuttle reaction intermediates via CoA molecules. However, CHS condenses a p-coumaroyl- and three malonyl-CoA molecules through an iterative series of reactions, whereas thiolase generates two acetyl-CoA molecules from acetoacetyl-CoA and free CoA. The drastic structural differences in the lower domain of CHS create a larger active site than that of thiolase and provide space for the polyketide reaction intermediates required for chalcone formation.

The CHS homodimer contains two functionally independent active sites. Consistent with this information, bound CoA thioesters and product analogs occupy both active sites of the homodimer in the CHS complex structures. These structures identify the location of the active site at the cleft between the upper and lower domains of each monomer. Each active site consists almost entirely of residues from a single monomer with Met_{137} from the adjoining monomer being the only exception. There are remarkably few chemically reactive residues in the active site. Four residues conserved in all the known CHS-related enzymes (Cys_{164}, Phe_{215}, His_{303}, and Asn_{336}) define the active site. Cys_{164} apparently serves as the nucleophile and as the attachment site for polyketide intermediates as previously suggested for both CHS and STS (Lanz, et al, J. Biol. Chem. 266:9971-9976, 1991). His_{303} most likely acts as a

general base during the generation of a nucleophilic thiolate anion from Cys_{164}, since the N of His_{303} is within hydrogen bonding distance of the sulfur of Cys_{164}. Phe_{215} and Asn_{336} may function in the decarboxylation reaction, as discussed below. Topologically, three interconnected cavities intersect with these four residues and form the active site architecture of CHS. These cavities include a CoA-binding tunnel, a coumaroyl-binding pocket, and a cyclization pocket.

The CoA-binding tunnel is 16 angstroms long and links the surrounding solvent with the buried active site. Binding of the CoA moiety in this tunnel positions substrates at the active site, as observed in the $C_{164}S$ mutant (described in greater detail below) complexed with malonyl- or hexanoyl-CoA. The conformation of the CoA molecules bound to CHS resembles that observed in other CoA binding enzymes. The adenosine nucleoside is in the 2'-endo conformation with an anti-glycosidic bond torsion angle. At the tunnel entrance, Lys_{55}, Arg_{58}, and Lys_{62} hydrogen bond with two phosphates of CoA. Apart from these interactions, and an additional hydrogen bond between the backbone amide nitrogen of Ala_{308} and the first carbonyl of the pantetheine moiety, van der Waals contacts dominate the remaining interactions between CHS and CoA. The pantetheine arm of the CoA extends into the enzyme positioning the terminally bound thioester-linked substrates near Cys_{164}.

Both naringenin and resveratrol bind at the active site end of the CoA-binding tunnel. The interactions observed in the naringenin and resveratrol complexes define the coumaroyl-binding and cyclization pockets (see Figure 5). The space to the lower left of the CoA-binding tunnel's end serves as the coumaroyl-binding pocket. Residues of this pocket (Ser_{133}, Glu_{192}, Thr_{194}, Thr_{197}, and Ser_{338}) surround the coumaroyl-derived portion of the bound naringenin and resveratrol molecules and interact primarily through van der Waals contacts. However, the carbonyl oxygen of Gly_{216} hydrogen bonds to the phenolic oxygen of both naringenin and resveratrol and the hydroxyl of Thr_{197} interacts with the carbonyl of naringenin derived from coumaroyl-CoA. The identity of the residues in this pocket likely contributes to the preference for coumaroyl-CoA as a substrate for parsley CHS over other cinnamoyl-CoA starter molecules, like caffeoyl- or feruloyl-CoA.

In both the naringenin and resveratrol complexes, the malonyl-derived portion of each molecule occupies a large pocket adjacent to Cys164 suggesting this is where the polyketide reaction intermediate cyclizes into the new ring system and where aromatization of the ring occurs. The six-carbon chain of hexanoyl-CoA also binds in this pocket. Physically, the size of the pocket limits the number of acetate additions to three. Phe_{265} separates the coumaroyl-binding site from the cyclization pocket and may function as a mobile steric gate during successive rounds of polyketide elongation. Although a polyketide possesses a number of hydrogen bond acceptors through which specific interactions could aid in proper folding for the cyclization reaction, the residues of the cyclization pocket, including Thr_{132}, Met_{137}, Phe_{215}, Ile_{254}, Gly_{256}, Phe_{265}, and Pro_{375}, provide few potential hydrogen bond donors. As in the coumaroyl-binding pocket, van der Waals contacts dominate the interaction between CHS and both naringenin and resveratrol. Thus, the surface topology of the cyclization pocket dictates how the malonyl-derived portion of the polyketide is folded and how the stereochemistry of the cyclization reaction leading to chalcone formation in CHS and resveratrol formation in STS is controlled.

Reaction mechanism

The position of the CoA thioesters and product analogs in the CHS active site suggest binding modes for substrates and intermediates in the polyketide elongation mechanism that are consistent with the known product specificity of CHS. In addition, the stereochemical features of the substrate and product analog complexes elucidate the roles of Cys_{164}, Phe_{215}, His_{303}, and Asn_{336} in the reaction mechanism. Utilizing structural constraints derived from the available complexes, the following reaction sequence is proposed (see Figure 6).

In the mechanism, binding of p-coumaroyl-CoA initiates the CHS reaction. Functional and structural evidence supports a coumaroyl-first mechanism over a malonyl-first one. Cerulenin, a potent irreversible inhibitor of CHS, covalently modifies Cys_{164} in CHS (Lanz, et al., J. Biol. Chem. 266:9971-9976, 1991). Preincubation of CHS with coumaroyl-CoA prevents inactivation by cerulenin, but

pre-incubation with malonyl-CoA does not (Preisig-Mueller, et al., Biochemistry 36:8349-8358, 1997). Also, the location of the coumaroyl-derived portion of naringenin and resveratrol in the CHS complexes agrees with a coumaroyl first mechanism, since the presence of a triketide reaction intermediate attached to Cys_{164} would limit access to the coumaroyl-binding pocket.

After p-coumaroyl-CoA binds to CHS, Cys_{164}, activated by His_{303}, attacks the thioester linkage, transferring the coumaroyl moiety to Cys_{164} (Monoketide Intermediate). Asn_{336} hydrogen bonds with the carbonyl oxygen of the thioester further stabilizing formation of the tetrahedral reaction intermediate. CoA then dissociates from the enzyme, leaving a coumaroyl-thioester at Cys_{164}. Binding of the first malonyl-CoA positions the bridging methylene carbon of the malonyl moiety near the carbonyl carbon of the covalently attached coumaroyl-thioester. Decarboxylation of malonyl-CoA leads to carbanion formation. Resonance between the keto and enol species stabilizes the carbanion. Attack of this carbanion on the coumaroyl-thioester releases the thiolate anion of Cys_{164} and transfers the coumaroyl group to the acetyl moiety of the CoA thioester (Diketide CoA Thioester). Capture of this elongated diketide-CoA by Cys_{164} and release of CoA sets the stage for two additional rounds of elongation resulting in formation of the tetraketide reaction intermediate.

Asn_{336} appears to play a crucial role in the decarboxylation reaction. Structural evidence shows that the decarboxylation reaction does not require transfer of the malonyl moiety to Cys_{164} as originally indicated by $C0_2$ exchange assays. Decarboxylation occurs without Cys_{164}, since the $C_{164}S$ mutant produces acetyl-CoA as determined crystallographically and confirmed by a functional assay. In the hexanoyl-CoA complex, the side chain amide of Asn_{336} provides a hydrogen bond to the carbonyl oxygen of the thioester. This interaction would stabilize the enolate anion resulting from decarboxylation of malonyl-CoA (see Figure 6). At the same time, the lack of formal positive charge at Asn_{336} may preserve the partial carbanion character of this resonance-stabilized anion, and thus the nucleophilicity of the carbanion form.

The role of Phe_{215} in the catalytic mechanism is subtler than that of Asn_{336}. Its position in both CoA complexes suggests that it provide van der Waals interactions for substrate binding. However, its conservation in bacterial enzymes related to CHS that do not make flavonoids or stilbenes may indicate a more general catalytic role for Phe_{215}. Its position near the acetyl moiety of the malonyl-CoA complex suggests that it participates in decarboxylation by favoring conversion of the negatively charged carboxyl group to a neutral carbon dioxide molecule.

Figure 7A depicts the addition of the third malonyl-CoA molecule as a three-dimensional model. The position of the coumaroyl ring in the modeled triketide intermediate is as observed in the naringenin and resveratrol complexes. The coumaroyl-binding pocket locks this moiety in position, while the acetate units added in subsequent chain extension steps bend to fill the cyclization pocket. The backbone of bound hexanoyl-CoA provides a guide for modeling the triketide reaction intermediate attached to Cys_{164}. Based on the observed acetyl-CoA complex, a rotation of the acetyl group would place the terminal methylene of the decarboxylated malonyl-CoA in position for nucleophilic attack on the triketide thioester linkage resulting in formation of a tetraketide CoA thioester.

The cyclization reaction catalyzed by CHS is an intramolecular Claisen condensation encompassing the three acetate units derived from three malonyl-CoAs. During cyclization, the nucleophilic methylene group nearest the coumaroyl moiety attacks the carbonyl carbon of the thioester linked to Cys_{164}. Ring closure proceeds through an internal proton transfer from the nucleophilic carbon to the carbonyl oxygen. Modeling of the tetraketide intermediate in a conformation leading to chalcone formation places one of the acidic protons of the nucleophilic carbon (C6) proximal to the target carbonyl (C1) (see Figure 7B). Since there is no base capable of proton abstraction from the tetraketide, it is proposed that the intermediate itself provides the driving force for carbanion formation. Protonation of the carbonyl oxygen would also stabilize the negative charge on the tetrahedral intermediate. Breakdown of this tetrahedral intermediate expels the newly cyclized ring system from Cys_{164}. Subsequent aromatization of the trione ring through a second series of

facile internal proton transfers yields chalcone.

Although the cyclization reaction has been modeled as occurring via a polyketide intermediate attached to Cys_{164}, it is possible that the reaction proceeds when the polyketide is attached to CoA. The rate of cyclization versus the rate of reattachment to Cys_{164} would dictate which of the two cyclization alternatives is mechanistically preferred.

An important question in the biosynthesis of chalcones concerns the exchangeability of the polyketide reaction intermediates. In the presence of chalcone reductase (CHR), CHS produces 6-deoxychalcone (Welle & Grisebach, FEBS Lett. 236:22-225, 1988). Mechanistically, CHR must reduce a ketone on the polyketide intermediate before cyclization occurs. Based on the CHS structure, any polyketide attached to Cys_{164} would be inaccessible to CHR unless a drastic structural change occurs in CHS upon interaction with CHR. While this conformational change is possible, such a change is difficult to imagine given the buried nature of the CHS active site. This would argue for the presence of moderately exchangeable polyketide-CoA reaction intermediates. Consistent with this idea, a recently identified CHS-like enzyme from *Pinus strobus* involved in the biosynthesis of C-methylated chalcones is active only with a starter molecule that is sterically analogous to the diketide-CoA intermediate postulated to be formed after the first condensation reaction in CHS30. These results suggest that the enzymes involved in the biosynthesis of plant polyketides may require specific localization in the plant cell to allow efficient channeling of intermediates from one enzyme to another during the production of particular products.

Cyclization specificity of CHS and STS

Both CHS and STS use the same precursor molecules and reaction mechanism to create a common tetraketide intermediate. Each enzyme must then impart a different folded conformation on this intermediate to facilitate the different cyclization reactions that yield chalcone and resveratrol. Although the three-dimensional structure of STS remains unknown, determination of the CHS structure allows

speculation about the basis for the intramolecular aldol condensation and cyclization reaction catalyzed by STS. This alternate pathway involves nucleophilic attack of the methylene group (C2) nearest the thioester linkage to Cys_{164} on the carbonyl carbon (C7) of the coumaroyl moiety (see Figure 7c). Again, modeling of the tetraketide intermediate in a conformation leading to cyclization suggests an internal proton transfer mechanism. Unlike CHS, this cyclization intermediate remains covalently attached to STS. Completion of the reaction sequence requires hydrolysis from Cys_{164} and an additional decarboxylation step prior to formation of resveratrol. These extra steps may account for the lower ,product formation rates observed with STS than with CHS (Schroeder J., et al., Biochemistry 37:8417-8425, 1998). Alternatively, the cyclization reaction may use a tetraketide-CoA thioester reaction intermediate, and subsequent hydrolysis and decarboxylation in solution.

The identity of the residue or residues involved in modulating between the intramolecular Claisen condensation in CHS and the aldol condensation in STS remains equivocal. The known CHS and STS enzymes exhibit no consistent differences in the residues lining the active site, although sequence variability between the CHS and STS enzymes does occur in the solvent exposed residues of strands ß1d (residues 253 to 259) and ß2d (residues 262-268) lining the cyclization pocket (see Figures 5b and 5c). Comparison of the naringenin and resveratrol complexes provides a possible explanation for modulation of the cyclization stereochemistry.

The cyclization pocket of CHS accommodates the newly cyclized ring of naringenin more easily than that of resveratrol. Strand ß1d (residues 253 to 259) moves slightly to enlarge the cyclization pocket in the resveratrol complex compared to the naringenin complex. Two residues that consistently vary between CHS-like and STS-like enzymes, Asp_{255} and Leu_{268}, move closer together in the resveratrol complex as ßld shifts position. Sequence variations of the solvent exposed residues of strands ß1d and ß2d may determine the conformation of the tetraketide intermediate before ring formation. Therefore, alterations in the surface topology of the cyclization pocket, mediated partially by the position of strand ßld, may affect the stereochemistry of the cyclization reaction and modulate product selectivity.

Structural basis for functionally novel CHS-like enzymes

Absolute conservation of Cys_{164}, Phe_{215}, His_{303}, and Asn_{336} occurs in CHS-like sequences, including several bacterial proteins possessing very low (typically 20-30%) amino acid sequence identity. Moreover, all CHS-like proteins exhibit strong conservation of residues shaping the geometry of the active site (Pro_{138}, Gly_{163}, Gly_{167}, Leu_{214}, Asp_{217}, Gly_{262}, Pro_{304}, Gly_{305}, Gly_{306}, Gly_{335}, Gly_{374}, Pro_{375}, and Gly_{376}). Although the functions of the bacterial CHS-like proteins remain unknown, these enzymes likely form polyketides or polyketide-CoA thioesters in a manner resembling CHS. However, steric differences resulting from sequence variation in both the coumaroyl-binding pocket and the cyclization pocket strongly suggest alternate substrate and product specificity in the bacterial enzymes.

The sequence databases include approximately 150 plant enzyme sequences classified as CHSlike proteins. The substrate and product specificity of a majority of these sequences remains to be determined. In addition, the high sequence similarity of all plant sequences complicates classification of these sequences as authentic CHS, STS, ACS, or BBS enzymes. The information provided by the three-dimensional structure of CHS should make new substrate and product specificity more readily discernible from sequence information.

To illustrate the usefulness of structural information in identifying potentially new activities, a CHS-related sequence from *Gerbera hybrids* (GCHS2)32 that is 74% identical with alfalfa CHS2 was examined. Modeling the active site architecture of GCHS2 using the structure of alfalfa CHS2 as a template indicates that GCHS2 will not catalyze either the CHS-like or STS-like reaction (see Figure 8). This variation in reaction specificity results from striking steric differences in the coumaroyl binding and cyclization pockets that substantially reduce the volume of both pockets from 923 $Å^3$ in CHS to 269 $Å^3$ in GCHS2. Side chain variation at positions 197 and 338 alter the coumaroyl binding pocket, while the identity of residue 256 dictates major steric changes in the cychzation pocket. The reduced size of these pockets in GCHS2 suggests that fewer than three acetate additions will occur, and that a CoA thioester

with an acyl moiety smaller than p-coumaroyl initiates the reaction. Recent functional characterization of GCHS2 confirms this prediction and demonstrates that this enzyme uses acetyl-CoA or benzoyl-CoA and two condensation reactions with malonyl-CoA to form pyrone products (Eckermann, et al., Nature 396:397-396, 1998).

Crystallization of Additional Polyketide Synthases

Stilbene synthase from *Pinus strubus* was overexpressed in *E. coli* as an octahistidyl N-terminal fusion protein, purified to >90% homogeneity by metal affinity and gel filtration chromatography, and crystallized in the preparation lacking the N-terminal polyhistidine tag (removed by thrombin cleavage) from 13% (w/v) polyethylene glycol (PEG8000), 0.05 M MOPSO, 0.3 M ammonium acetate at pH 7.0. This STS is 396 amino acids in length and, like alfalfa CHS exists as a homodimer in solution. A partial data set on a frozen crystal (!))K) has been collected to 2.7 Å. The crystals belong to space group C222 with with unit cell dimensions of a = 74.94 Å , b = 86.63 Å , c = 364.18 Å , $\alpha = \beta = \gamma = 90°$.

2-Pyrone synthase (2-PS) from *Gerbera hybrida* was expressed and purified from *E. coli* in a similar manner to CHS and STS. Crystals were obtained from 1.5 M ammonium sulfate, 011 M Na^+ - succinate, 0.002 M DTT at pH 5.5.

2-Pyrone synthase (2-PS) from *Gerbera hybrida* forms a triketide from an acetyl-CoA initiator and two acetyl-CoA α-carbanions derived from decarboxylation of two malonyl-CoAs that cyclizes into the 6-methyl-4-hydroxy-2-pyrone. In comparison, alfalfa chalcone synthase 2 (CHS2; 74% amino acid sequence identity to 2-PS), condenses *p*-coumaroyl-CoA and three acetyl-CoA α-carbanions derived from decarboxylation of three malonyl-CoAs into a tetraketide that cyclizes into chalcone. A homology model of 2-PS based on the structure of CHS suggested that the 2-PS initiation/elongation cavity is smaller than that of CHS. A smaller cavity would account for the terminal formation of a triketide intermediate prior to cyclization by 2-PS.

Expression, Purification and Crystallization of 2-PS.

2-PS was expressed in *E. coli*, purified and crystallized as described above. *Gerbera hybrida* 2-PS was expressed in *E. coli* using the pHIS8 vector and was purified as described for CHS. 2-PS crystals grew at 4 °C in hanging-drops containing a 1:1 mixture of 25 mg ml^{-1} protein and crystallization buffer (1.5 M ammonium sulfate, 50 mM succinic acid (pH 5.5), and 5 mM DTT). Before freezing at 105 K, crystals ($P3_121$; unit cell dimensions a = 82.15 Å, c = 241.33 Å; one 2-PS dimer per asymmetric unit) were stepped through stabilizer (50 mM succinic acid (pH 5.5), 50 mM ammonium sulfate, and 5 mM DTT) containing 5 mM acetoacetyl-CoA and increasing concentrations of glycerol (30% (v/v) final). Diffraction data were collected using a DIP2030 imaging plate system and CuK radiation produced by a rotating anode (wavelength 1.54 Å). All images were processed with DENZO/SCALEPACK (Z. Otwinowski, W. Minor, *Methods Enzymol.* 276:307 (1997)). A total of 179,623 reflections were merged to give 60,824 unique reflections (98.2% complete overall to 2.05 Å and 98.1% complete in the highest resolution shell) with an R_{sym} = 0.042 (0.206 in the highest resolution shell) and an I/_of 21.7 (4.5 in the highest resolution shell). The structure of 2-PS complexed with acetoacetyl-CoA was determined by molecular replacement using CHS as a search model and was refined to 2.05 Å resolution. The overall fold of 2-PS is the αβαβα motif found in CHS and β-ketoacyl synthase II (KAS II). In addition, the positions of the catalytic residues of 2-PS (Cys_{169}, His_{308}, and Asn_{341}), CHS (Cys_{163}, His_{303}, Asn_{336}), and KAS II (Cys_{163}, His_{303}, and His_{340}) are structurally analogous. As expected from sequence homology, the structures of 2-PS and CHS are nearly identical and superimpose with a r.m.s. deviation of 0.64 Å for the two proteins' α-carbon atoms. Similar to CHS, the 2-PS dimerization surface buries 1805 $Å^2$ of surface area per monomer and a loop containing a *cis*-peptide bond between Met_{142} and Pro_{143} allows

the methionine of one monomer to protrude into the adjoining monomer's active site. Thus, dimerization allows formation of the complete 2-PS active site.

Acetoacetyl-CoA is a reaction intermediate of 2-PS. Electron density for the ligand is well defined in the 2-PS active site and shows that the acetoacetyl moiety extends from the CoA pantetheine arm into a large internal cavity. The electron density also reveals oxidation of the catalytic cysteine's (Cys_{169}) sulfhydryl to sulfinic acid (-SO_2H). This oxidation state prevents formation of a covalent acetoacetyl-enzyme complex but allows trapping of the bound acetoacetyl-CoA intermediate. Extensive protein-ligand contacts position CoA at the entrance to the active site and orient the acetoacetyl moiety at the end of a 15 Å long tunnel that opens into a cavity that defines the initiation and elongation steps of polyketide formation.

The 2-PS active site cavity consists of twenty-seven residues from one monomer and Met_{142} from the adjoining monomer. Phe_{220} and Phe_{270} mark the boundary between the CoA binding site and the initiation/elongation cavity. Near the CoA thioester, Cys_{169}, His_{308}, and Asn_{341} form the catalytic center of 2-PS. These residues are conserved in all homodimeric iterative PKSs. Based on this, catalytic roles were proposed for each residue that are analogous to the corresponding residues in CHS. Cys_{169} acts as the nucleophile in the reaction and as the attachment site for the elongating polyketide chain. Interaction between His_{308} and Cys_{169} maintains the thiolate required for condensation of the starter molecule. His_{308} and Asn_{341} catalyze malonyl-CoA decarboxylation and stabilize the transition states during the condensation steps by forming an oxyanion hole that accommodates the negatively charged tetravalent transition state. Following the first condensation reaction, a diketide remains attached to Cys_{169}. The second malonyl-CoA then binds, undergoes decarboxylation, and the resulting nucleophilic acetyl-coA α-carbanion performs a

second condensation reaction with the enzyme bound diketide, ultimately generating the triketide that cyclizes into methylpyrone.

Comparison of the initiation/elongation cavities of 2-PS and CHS reveal four amino acid differences. In 2-PS, Leu_{202}, Met_{259}, Leu_{261}, and Ile_{343} replace Thr_{197}, Ile_{254}, Gly_{256}, and Ser_{338}, respectively, of CHS. These four substitutions reduce cavity volume from 923 $Å^3$ in CHS to 274 $Å^3$ in 2-PS. A model of methylpyrone in the 2-PS cavity, based on the position of acetoacetyl-CoA, emphasizes the volume change compared to the CHS-naringenin complex (Accession No. 1CGK). Leu_{202} and Ile_{343} occlude the portion of the 2-PS cavity corresponding to the coumaroyl-binding site of CHS. Replacement of Gly_{256} in CHS by Leu_{261} in 2-PS severely reduces the size of the active site cavity. Substitution of Met_{259} in 2-PS for Ile_{254} in CHS produces a modest alteration in cavity volume. To examine the functional importance of these amino acid differences, the initiation/elongation cavity of CHS was altered by mutagenesis to resemble that of 2-PS. The resulting mutant proteins were screened for activity using either *p*-coumaroyl-CoA or acetyl-CoA as starter molecules. Activities of 2-PS, CHS, and the CHS mutants were determined by monitoring product formation using a TLC-based radiometric assay. Assay conditions were 100 mM Hepes (pH 7.0), 30 μM starter-CoA (either *p*-coumaroyl-CoA or acetyl-CoA), and 60 μM [^{14}C]-malonyl-CoA (50,000 cpm) in 100 μl at 25 °C. Reactions were quenched with 5% acetic acid, extracted with ethyl acetate, and applied to TLC plates and developed. Due to the spontaneous cyclization of chalcone into the flavanone naringenin, activities of CHS are referenced to naringenin formation.

The x-ray crystal structures of 2-PS and CHS imply that the size of the active site cavity limits polyketide length and modulates folding of the polyketide chain. Wild-type CHS generates the tetraketide chalcone and 2-PS produces the triketide methylpyrone. Likewise, the CHS I254M mutant also yields chalcone. Interestingly,

the T197L, G256L, and S338I mutants do not form chalcone. Crystallographic analysis of the G256L and S338I mutants demonstrates that the substituted side-chains adopt conformations similar to the corresponding residues in 2-PS without altering the position of the protein backbone. Since the T197L, G256L, and S338I mutants altered product formation, a CHS triple mutant was generated. Consistent with the proposal that cavity volume dictates polyketide length, the T197L/G256L/S338I mutant produces only methylpyrone, as confirmed by liquid chromatography/mass spectroscopy (LC/MS). LC/MS/MS analysis was performed by the Mass Spectroscopy facility of the Scripps Research Institute. Scaled-up assays (2 ml reaction volume) with the CHS T197L/G256L/S338I mutant and 2-PS were performed. Extracts were analyzed on a Hewlett-Packard HP1100 MSD single quadrupole mass spectrometer coupled to a Zorbax SB-C_{18} column (5 μm, 2.1 mm x 150 mm). HPLC conditions were as follows: gradient system from 0 to 100% methanol in water (each containing 0.2% acetic acid) within 10 min; flow rate 0.25 ml min^{-1}. LC/MS/MS data from both reactions were identical: 6-methyl-4-hydroxy-2-pyrone, R_t = 5.068 min; $[M-H]^-$ 125 (41); $[M-H-CO_2]^-$ 81 (100). The numbers show *m/z* values with relative intensities in parenthesis. The observed fragmentation matches previously published data.

In addition, the size of the cavity in 2-PS and CHS confers starter molecule specificity. 2-PS accepts acetyl-CoA but does not use *p*-coumaroyl-CoA. Structurally, the constricted 2-PS active site excludes the bulky coumaroyl group. As such, incubation of 2-PS in the presence of coumaroyl-CoA and malonyl-CoA yields methylpyrone produced from three malonyl-CoA molecules. In comparison, the larger initiation/elongation cavity of CHS allows for different sized aliphatic and aromatic starter molecules to be used *in vitro* with varying efficiencies. CHS exhibits a 230-fold preference for *p*-coumaroyl-CoA versus acetyl-CoA. Alterations in the

active site cavity of CHS, affect starter molecule preference. The CHS I254M mutant is functionally comparable to wild-type enzyme with a modest reduction in specific activity. The T197L and S338I mutants exhibit 10-fold and 3-fold preferences, respectively, for coumaroyl-CoA. Moreover, both form a distinct product using coumaroyl-CoA as a starter molecule. In contrast, the G256L mutant favors acetyl-CoA 3-fold. Like 2-PS, the CHS T197L/G256L/S338I (3x) mutant only accepts acetyl-CoA (or malonyl-CoA) as the starter molecule.

Functional diversity among other homodimeric iterative PKSs, like *p*-coumaroyltriacetic acid synthase (CTAS), acridone synthase (ACS), and the *rppA* protein from *Streptomyces griseus*, likely results from variations of residues lining the initiation/elongation cavity. As demonstrated, positions 197, 256, and 338 distinguish between tetraketide products derived from a final Claisen condensation in wild-type CHS and triketide products derived from an enolate-directed condensation in the CHS triple mutant. Although CHS, CTAS, and ACS generate tetraketides, each enzyme differs in either the cyclization reaction or in the identity of the starter molecule. CTAS forms the same enzyme-bound tetraketide as CHS but does not catalyze the final cyclization reaction. Comparison of these two enzymes reveals that substitution of Thr 197 in CHS with an asparagine in CTAS may prevent the covalently-bound tetraketide intermediate from undergoing cyclization into chalcone. ACS uses N-methylanthranoyl-CoA as a starting substrate to produce the alkaloid acridone. Three differences between CHS (Thr_{132}, Ser_{133}, and Phe_{265}) and ACS (Ser_{132}, Ala_{133}, and Val_{265}) may alter starter molecule specificity. In ACS, these changes likely widen the portion of the cavity corresponding to the *p*-coumaroyl-binding site in CHS to accommodate N-methylanthranoyl-CoA binding. Comparative changes in the active site cavity allow formation of longer polyketides. The *rppA* protein forms a pentaketide from five acetates derived from malonyl-CoA decarboxylation. Thr_{137}, Ala_{138}, Thr_{199}, Leu_{202}, Met_{259}, Leu_{261}, Leu_{268}, Pro_{304}, and Ile_{343} of 2-PS are replaced by

Cys_{106}, Thr_{107}, Cys_{168}, Cys_{171}, Ile_{228}, Tyr_{230}, Phe_{237}, Ala_{261}, and Ala_{295}, respectively, in the *rppA* protein. Models of the *rppA* protein based on the 2-PS and CHS structures show that cavity volume is 1145 $Å^3$ in the *rppA* protein versus 274 $Å^3$ in 2-PS (or 923 Å in CHS). Manipulation of the active site through amino acid substitutions offers a strategy for increasing the molecular diversity of polyketide formation through both the choice of starter molecule and the number of subsequent condensation steps.

The reaction mechanism for polyketide formation and the structural basis for controlling polyketide length described here may be shared with other more complex iterative (*e.g.*, actinorhodin (*act*) PKS and tetracenomycin (*tcm*) PKS) and modular PKSs (*e.g.*, 6-deoxyerythronolide B synthase (DEBS)). The structural similarity of the 2-PS, CHS, and KAS II active sites, the sequence homology of KAS II and the ketosynthases of *act* PKS, *tcm* PKS, and DEBS, and mutagenesis studies of CHS and *act* PKS demonstrating similar roles for the catalytic residues of each protein indicate that a conserved active site architecture catalyzes similar reactions in these enzymes.

As in 2-PS and CHS, the volume of the active site cavities in other PKSs likely limits the size of the final polyketide. For example, *act* PKS and *tcm* PKS generate octaketide and decaketide products, respectively, at a single active site. This suggests that the active site cavities of these PKSs differ in size, and are larger than those of 2-PS or CHS. Similarly, the ketosynthases of different DEBS modules accept polyketide intermediates ranging in length from five to twelve carbons. Modular PKSs, like DEBS, use an assembly-line system in which an individual module catalyzes one elongation reaction and passes the growing polyketide to the next module. Although the ketosynthase domains of DEBS are functionally permissive, modulation of active site volume in each module's ketosynthase would provide selectivity for the proper sized intermediate at each elongation step.

Structural differences among PKSs alter the volume of the initiation/elongation cavity to allow discrimination between starter molecules and to vary the number of elongation steps to ultimately direct the nature and length of the polyketide product.

While the foregoing has been presented with reference to particular embodiments of the invention, it will be appreciated by those skilled in the art that changes in these embodiments may be made without departing from the principles and spirit of the invention, the scope of which is defined by the appended claims.

That which is claimed:

1. An isolated polyketide synthase comprising at least fourteen active site α-carbons having the structural coordinates of Table 1.

2. The isolated polyketide synthase of claim 1, wherein the amino acid located at position 164 is alanine or serine.

3. The isolated polyketide synthase of claim 1, wherein the amino acid located at position 303 is alanine, asparagine, glutamine, aspartic acid, or threonine.

4. The isolated polyketide synthase of claim 1, wherein the amino acid located at position 336 is a lysine, alanine, aspartic acid, glutamine, or histidine.

5. The isolated polyketide synthase of claim 1, wherein the amino acid located at position 215 is serine, tyrosine, or tryptophan.

6. The isolated polyketide synthase of claim 1, wherein the polyketide synthase has atomic coordinates as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ. 1D6F, 1D6I, or 1D6H.

7. A nucleic acid encoding the synthase of claim 1.

8. A nucleic acid encoding the synthase of claim 2.

9. A nucleic acid encoding the synthase of claim 3.

10. A nucleic acid encoding the synthase of claim 4.

11. A nucleic acid encoding the synthase of claim 5.

12. A method of predicting the activity and/or substrate specificity of a putative polyketide synthase, said method comprising:

comparing the representation of a known polyketide synthase and the representation of a putative polyketide synthase, wherein differences between the two

representations are predictive of polyketide synthase activity and/or substrate specificity.

13. The method of claim 12, wherein the known polyketide synthase is chalcone synthase, stilbene synthase, or pyrone synthase.

14. The method of claim 13, wherein the known chalcone synthase has strucutral coordinants as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, or 1CGZ.

15. The method of claim 13, wherein the known pyrone synthase has atomic coordinates as set forth in Table 3.

16. The method of claim 12, wherein the putative synthase is a mutant of a known polyketide synthase.

17. A crystalline form of the polyketide synthase of claim 1.

18. A crystalline form of the polyketide synthase of claim 2.

19. A crystalline form of the polyketide synthase of claim 3.

20. A crystalline form of the polyketide synthase of claim 4.

21. A crystalline form of the polyketide synthase of claim 5.

22. A crystalline chalcone synthase, stilbene synthase, or pyrone synthase..

23. A crystalline complex comprising chalcone synthase and a chalcone synthase substrate.

24. The crystalline complex of claim 23, wherein the chalcone synthase is native chalcone synthase.

25. The crystalline complex of claim 23, wherein the chalcone synthase is a non-native chalcone synthase.

26. The crystalline complex of claim 23, wherein the chalcone synthase substrate is selected from the group consisting of chalcone, naringenin, resveratrol, cerulenin, acyl-CoA, malonyl-CoA, and hexanoyl-CoA.

27. The crystalline complex of claim 23, wherein the complex has atomic coordinates as set forth in PDB Accession Nos: 1BQ6, 1CML, 1CHW, 1CGK or 1CGZ.

28. A method of identifying a potential substrate of a polyketide synthase, said method comprising:

(a) defining the active site of said polyketide synthase based on a plurality of atomic coordinates of said polyketide synthase,

(b) identifying a potential substrate that fits the active site of (a) with the polyketide synthase, and

(c) contacting the polyketide synthase with the potential substrate and determining its activity thereon.

29. The method of claim 28, wherein the polyketide synthase is chalcone synthase, stilbene synthase, or pyrone synthase.

30. The method of claim 28, wherein the polyketide synthase is a mutant of a known polyketide synthase.

31. The method of claim 30, wherein the known polyketide synthase is chalcone synthase, stilbene synthase, or pyrone synthase.

32. The method of claim 28, wherein the plurality of atomic coordinates are as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ. 1D6F, 1D6I, 1D6H, or portions thereof.

33. A method of identifying a potential inhibitor of a polyketide synthase, said method comprising:

(a) defining the active site of said polyketide synthase based on a plurality of atomic coordinates of said polyketide synthase,

(b) contacting a potential compound that fits the active site of (a) with the polyketide synthase in the presence of a substrate, and

(c) determining the ability of said compound to inhibit the activity of said polyketide synthase on said substrate.

34. The method of claim 33, wherein the polyketide synthase is chalcone synthase, stilbene synthase, or pyrone synthase.

35. The method of claim 33, wherein the polyketide synthase is a mutant of a known polyketide synthase.

36. The method of claim 35, wherein the mutant polyketide synthase is a mutant of chalcone synthase, stilbene synthase, and pyrone synthase.

37. The method of claim 33, wherein the plurality of atomic coordinates are as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ. 1D6F, 1D6I, 1D6H, or portions thereof.

38. A computer program on a computer readable medium, said computer program comprising instructions to cause a computer to:

define a polyketide synthase or fragment thereof based on a plurality of atomic coordinates of the polyketide synthase.

39. The computer program of claim 38, wherein the plurality of atomic coordinates are as set forth in PDB Accession Nos: 1BI5, 1BQ6, 1CML, 1CHW, 1CGK, 1CGZ. 1D6F, 1D6I, 1D6H, Table 3, or portions thereof.

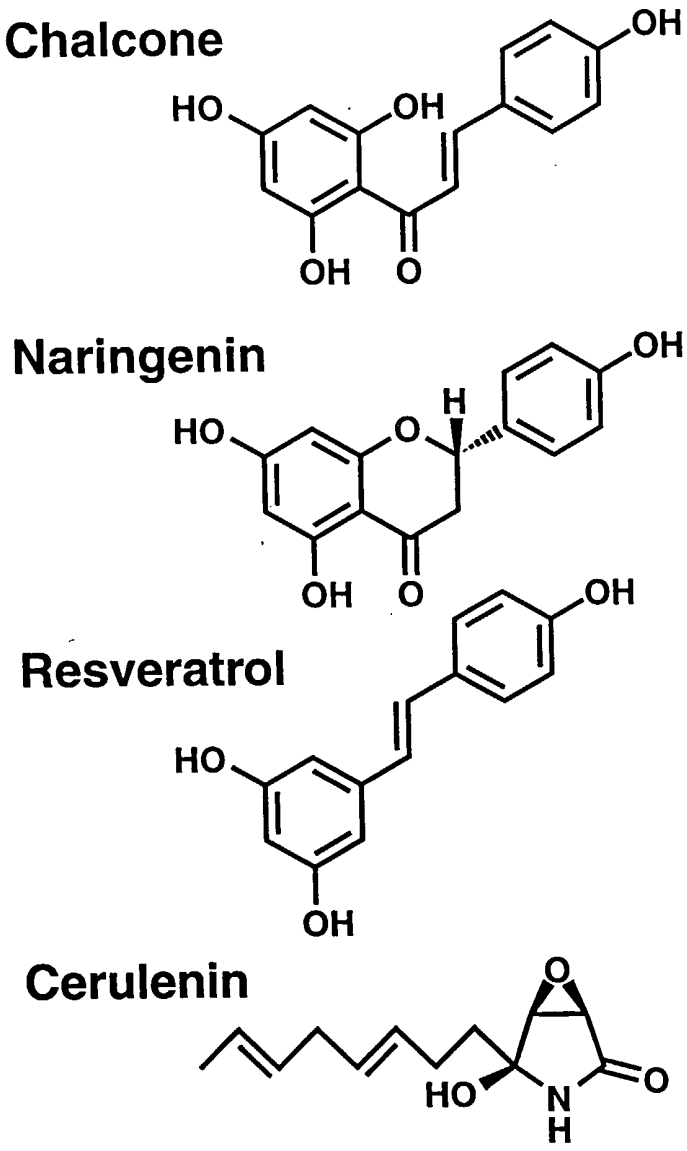

Chalcone
HO
OH
OH
OH
O
Naringenin
HO
O
H
OH
OH
O
Resveratrol
HO
OH
OH
Cerulenin
O
HO
N
H
O

FIGURE 1A

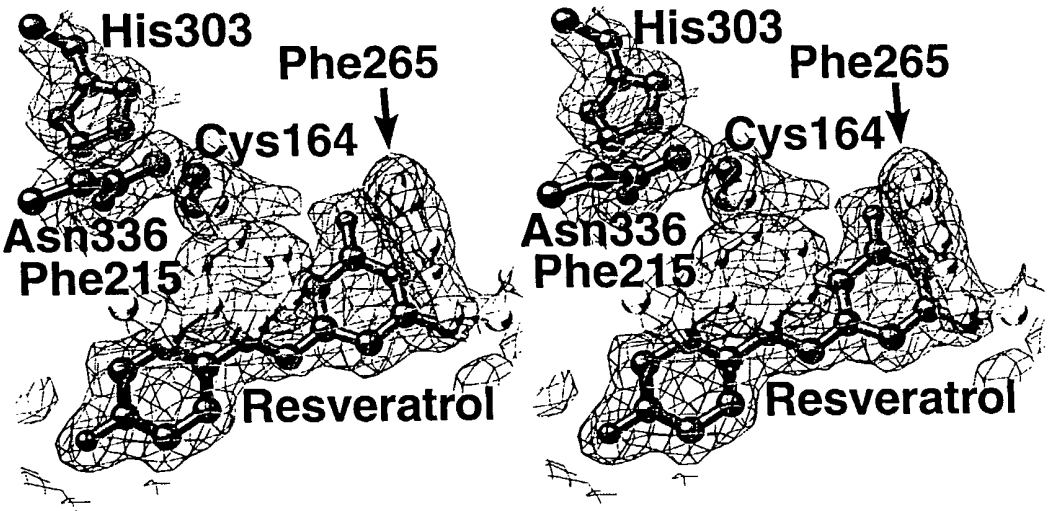

His303
Phe265
Cys164
Asn336
Phe215
Resveratrol
His303
Phe265
Cys164
Asn336
Phe215
Resveratrol

FIGURE 1B

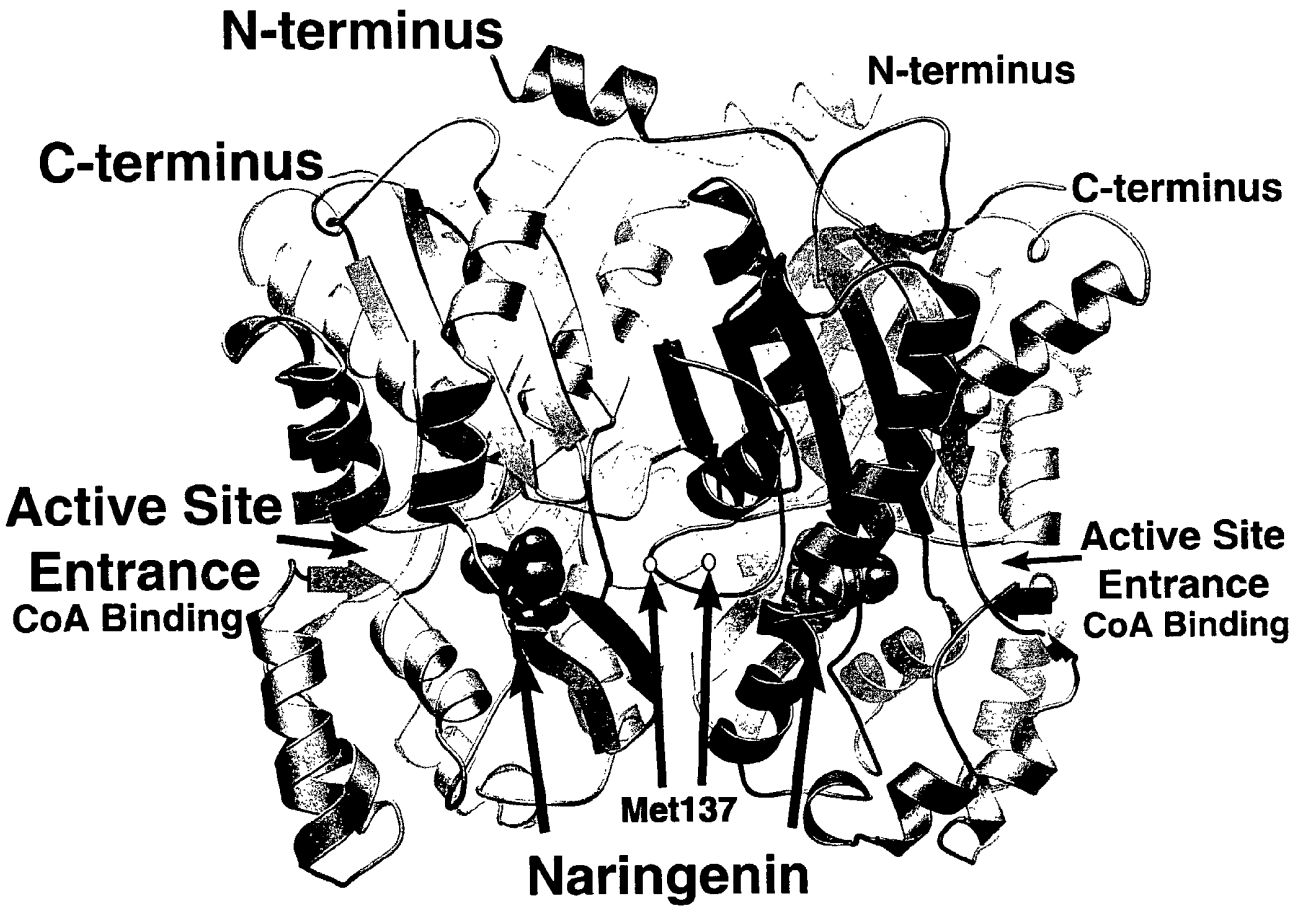

N-terminus
N-terminus
C-terminus
C-terminus
Active Site
Entrance
CoA Binding
Active Site
Entrance
CoA Binding
Met137
Naringenin

Figure 2A

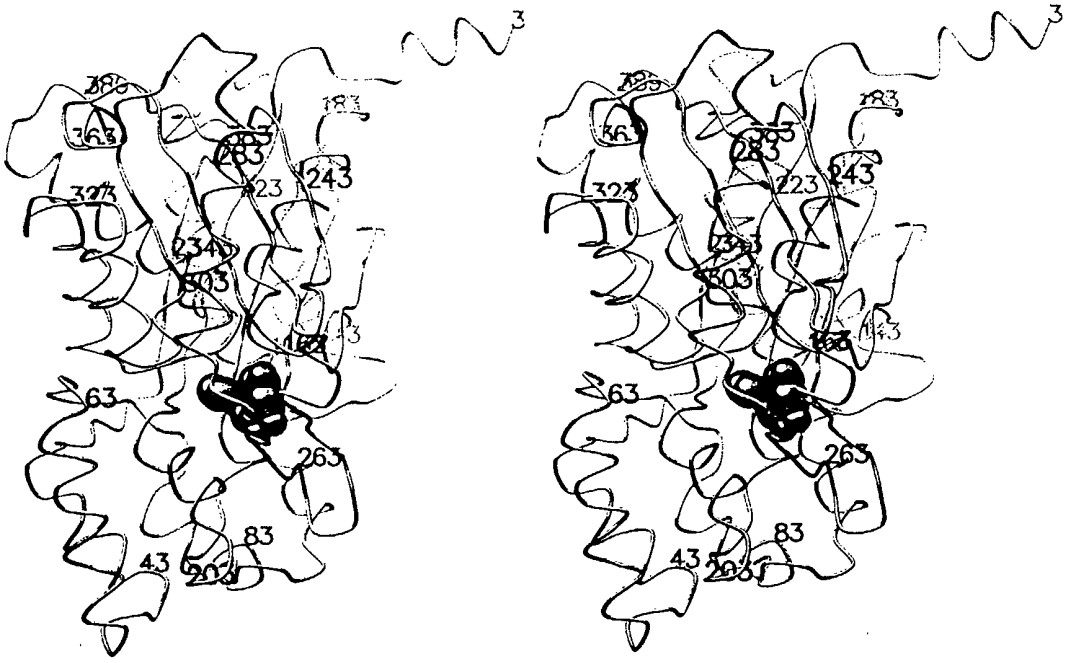


FIGURE 2B

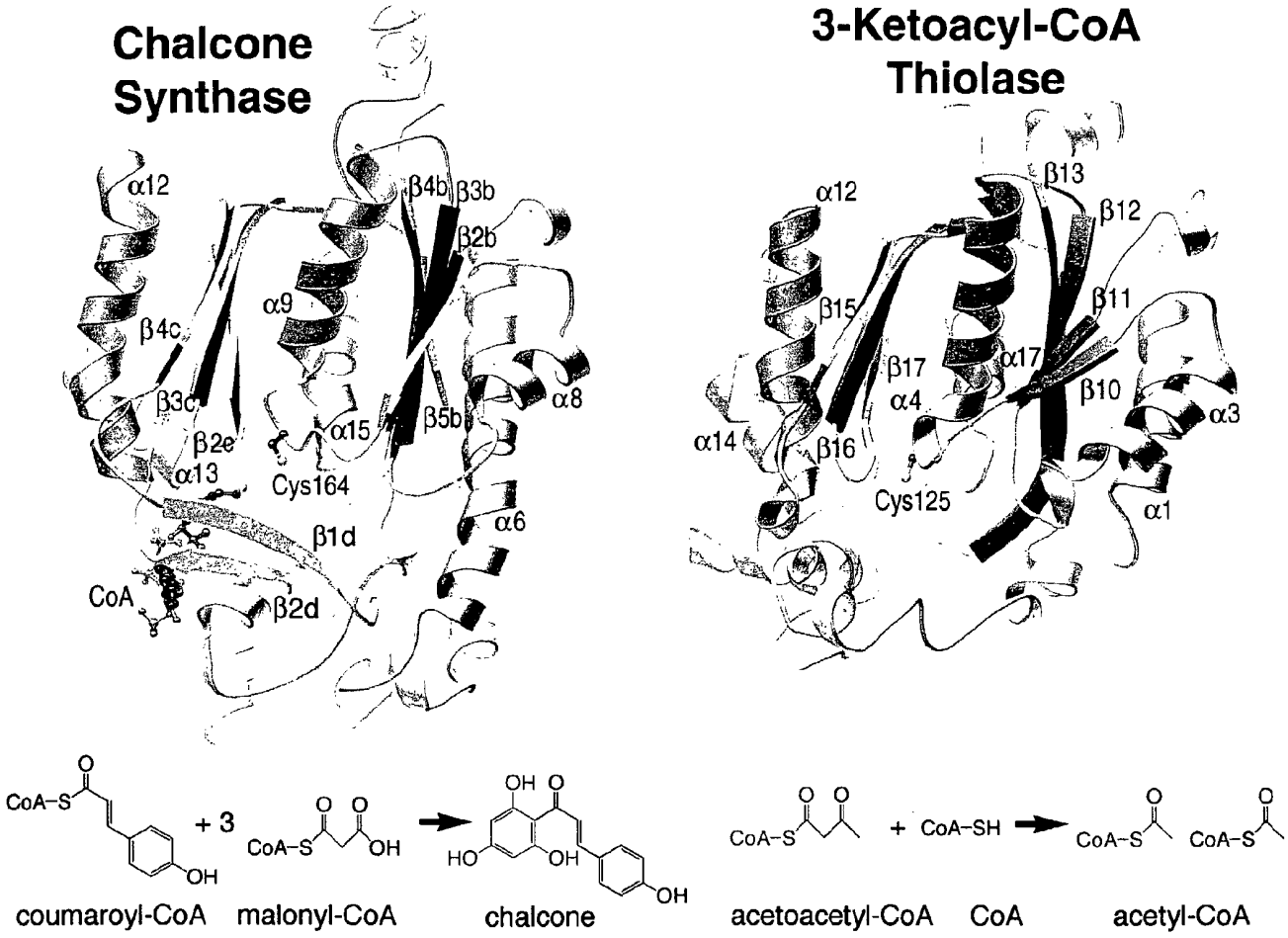

Chalcone Synthase
α12
β4b
β3b
β2b
α9
β4c
β3c
β2e
α13
α15
Cys164
β5b
α8
α6
β1d
CoA
β2d
3-Ketoacyl-CoA Thiolase
α12
β13
β12
β15
β11
β17
α17
α4
β10
α3
α14
β16
Cys125
α1
CoA–S
OH
+ 3
CoA–S
OH
HO
OH
OH
coumaroyl-CoA
malonyl-CoA
chalcone
CoA–S
+ CoA–SH
CoA–S
CoA–S
acetoacetyl-CoA
CoA
acetyl-CoA

FIGURE 3

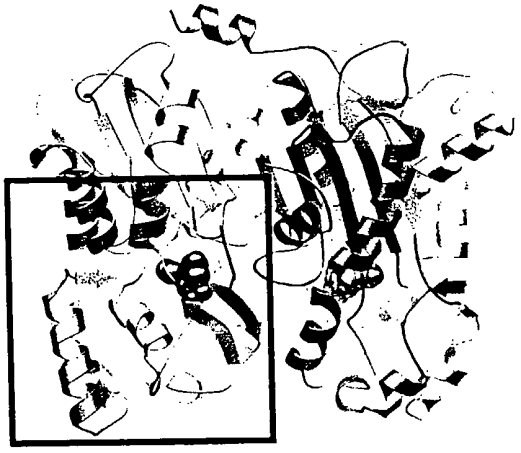
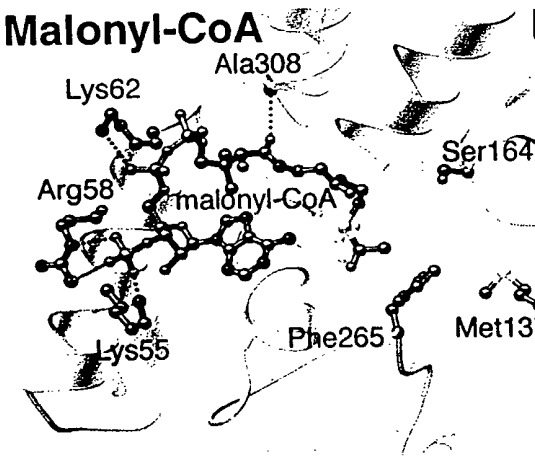


FIGURE 4A



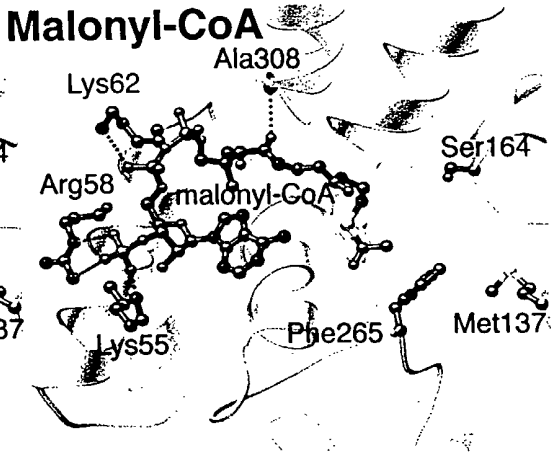
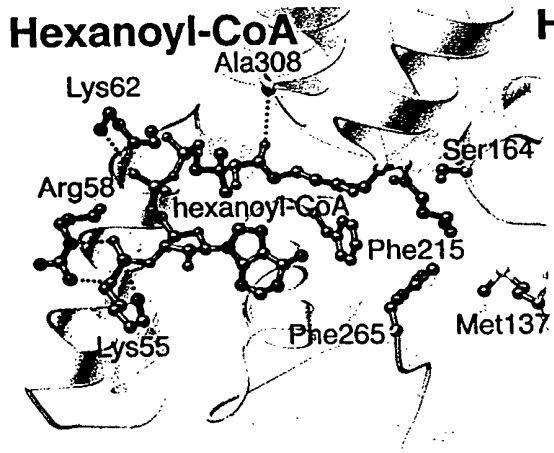


FIGURE 4B



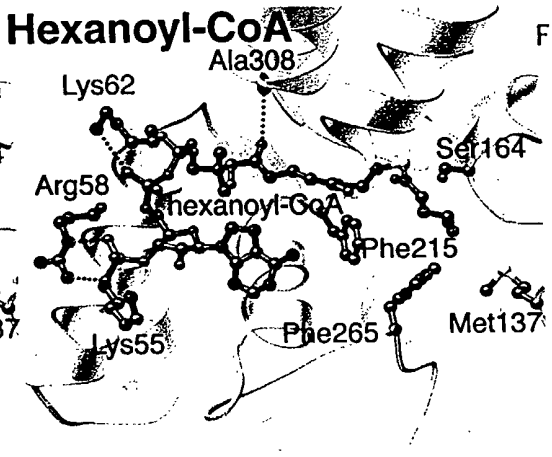


FIGURE 4C

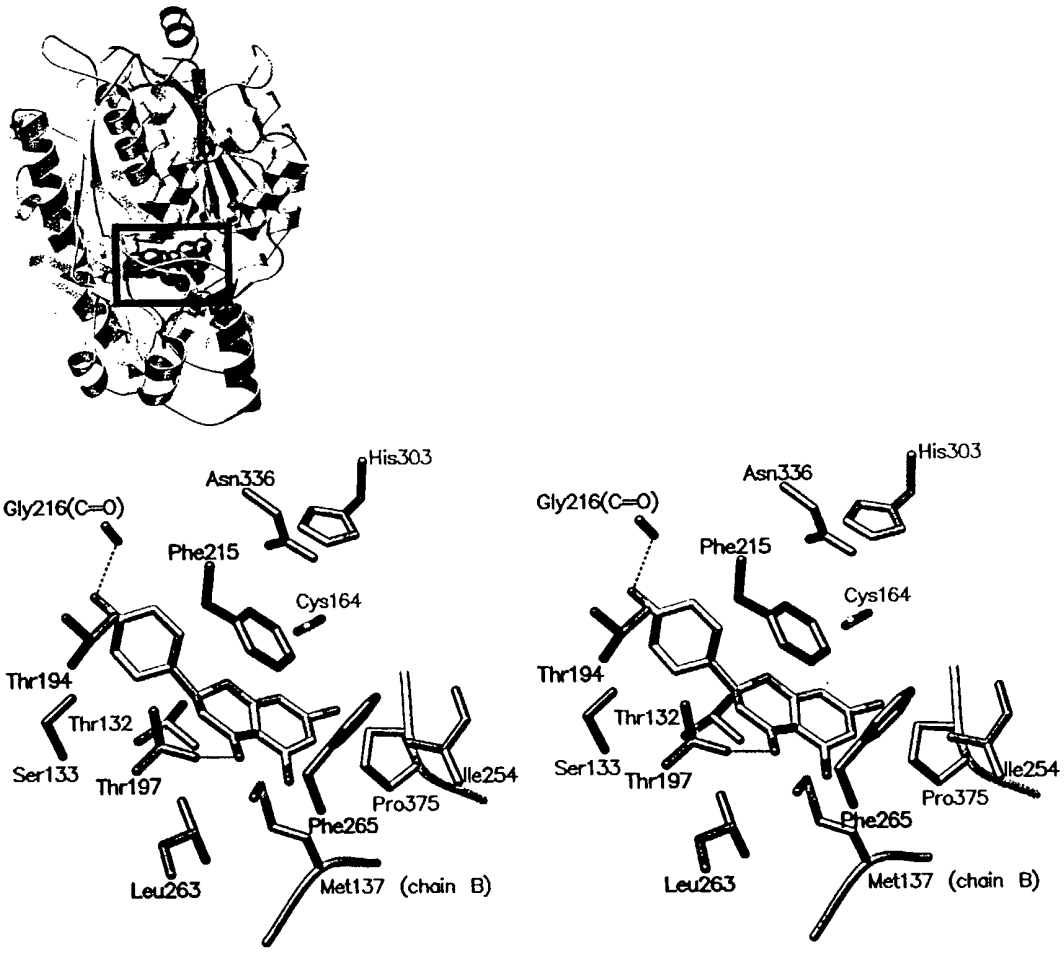

Gly216(C=O)
Asn336
His303
Phe215
Cys164
Thr194
Thr132
Ser133
Thr197
Ile254
Pro375
Phe265
Leu263
Met137 (chain B)
Gly216(C=O)
Asn336
His303
Phe215
Cys164
Thr194
Thr132
Ser133
Thr197
Ile254
Pro375
Phe265
Leu263
Met137 (chain B)

FIGURE 5A

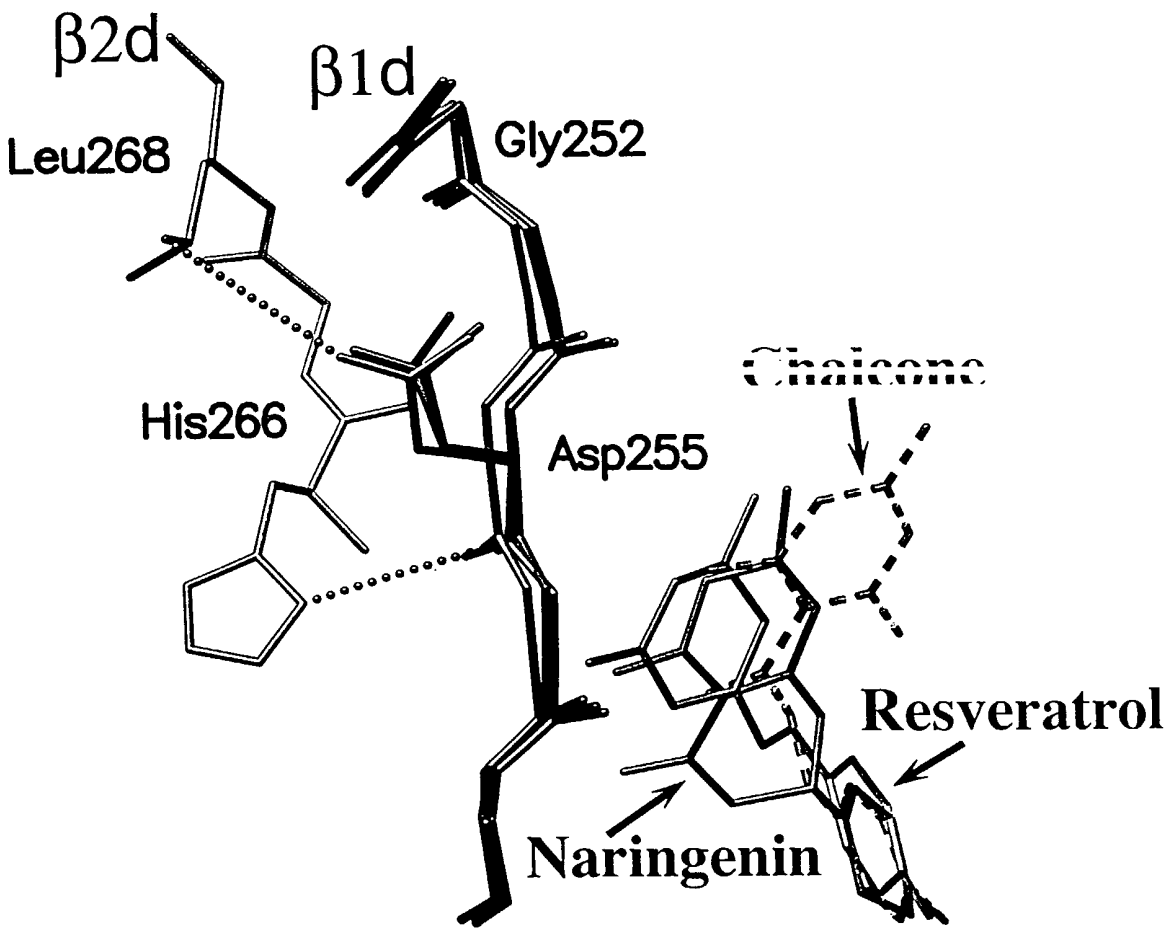

β2d
β1d
Leu268
Gly252
His266
Asp255
Chalcone
Resveratrol
Naringenin

FIGURE 5B

```
                          250        260        270
chs2 (alfalfa)          ...SEGAIDGHLREAGLTFHLLKDVPG...
chs2 (barley)           ...SEGAIDGHLTEAGLTIHLLKDVPG...
acs (Ruta graveolens)   ...SDGAIEGHIREEGLTVHLKKDVPA...
sts1 (peanut)           ...SHGAIGGLLREVGLTFYLNKSVPD...
sts1 (pine)             ...SDGAISGKLREVGLTFQLKGAVPD...
bbs (Phalaenopsis sp)   ...SAGAIGGHVSEGGLLATLHRDVPQ...
```

FIGURE 5C

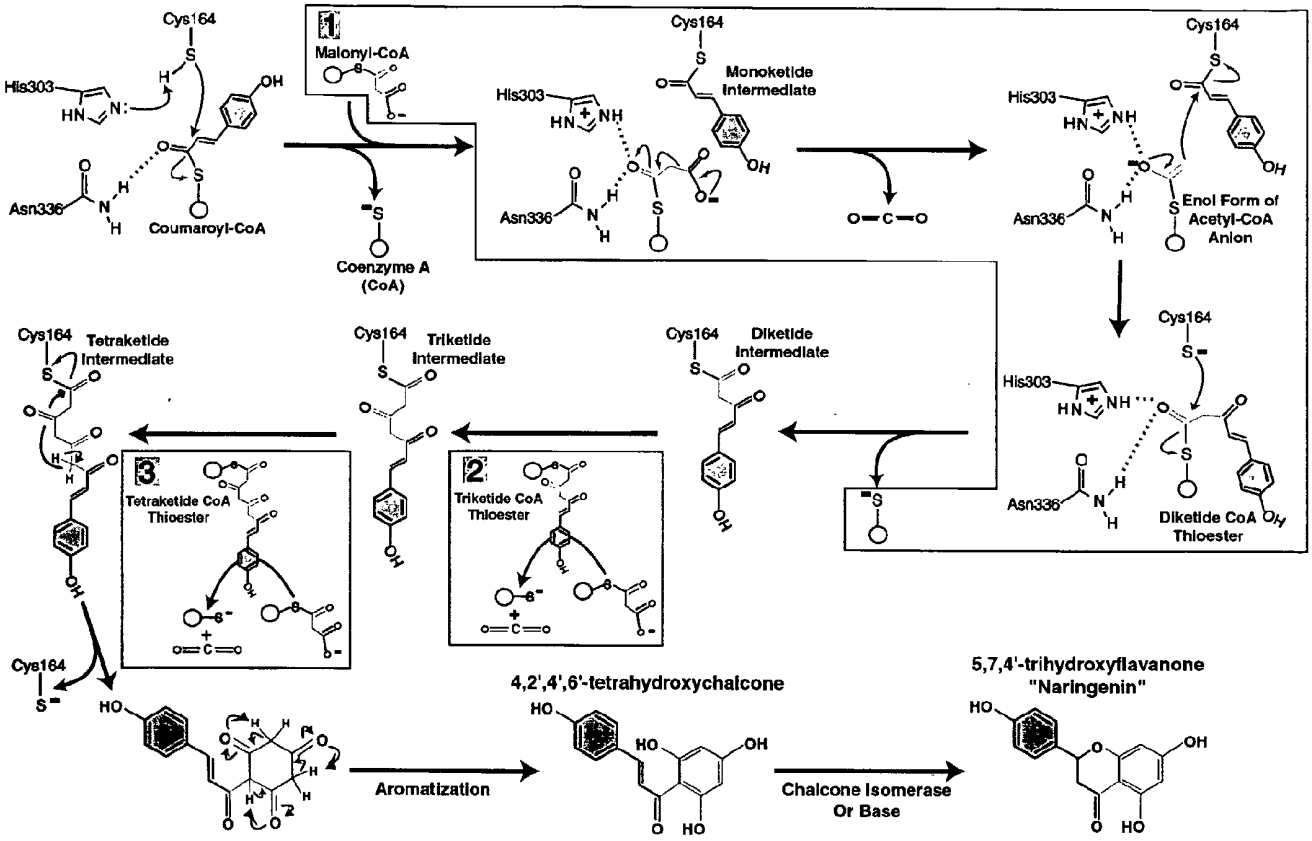

Cys164
His303
Asn336
Coumaroyl-CoA
1
Malonyl-CoA
Coenzyme A (CoA)
Monoketide Intermediate
Enol Form of Acetyl-CoA Anion
Diketide CoA Thioester
Diketide Intermediate
Triketide Intermediate
Tetraketide Intermediate
2
Triketide CoA Thioester
3
Tetraketide CoA Thioester
Aromatization
4,2',4',6'-tetrahydroxychalcone
Chalcone Isomerase Or Base
5,7,4'-trihydroxyflavanone "Naringenin"

FIGURE 6

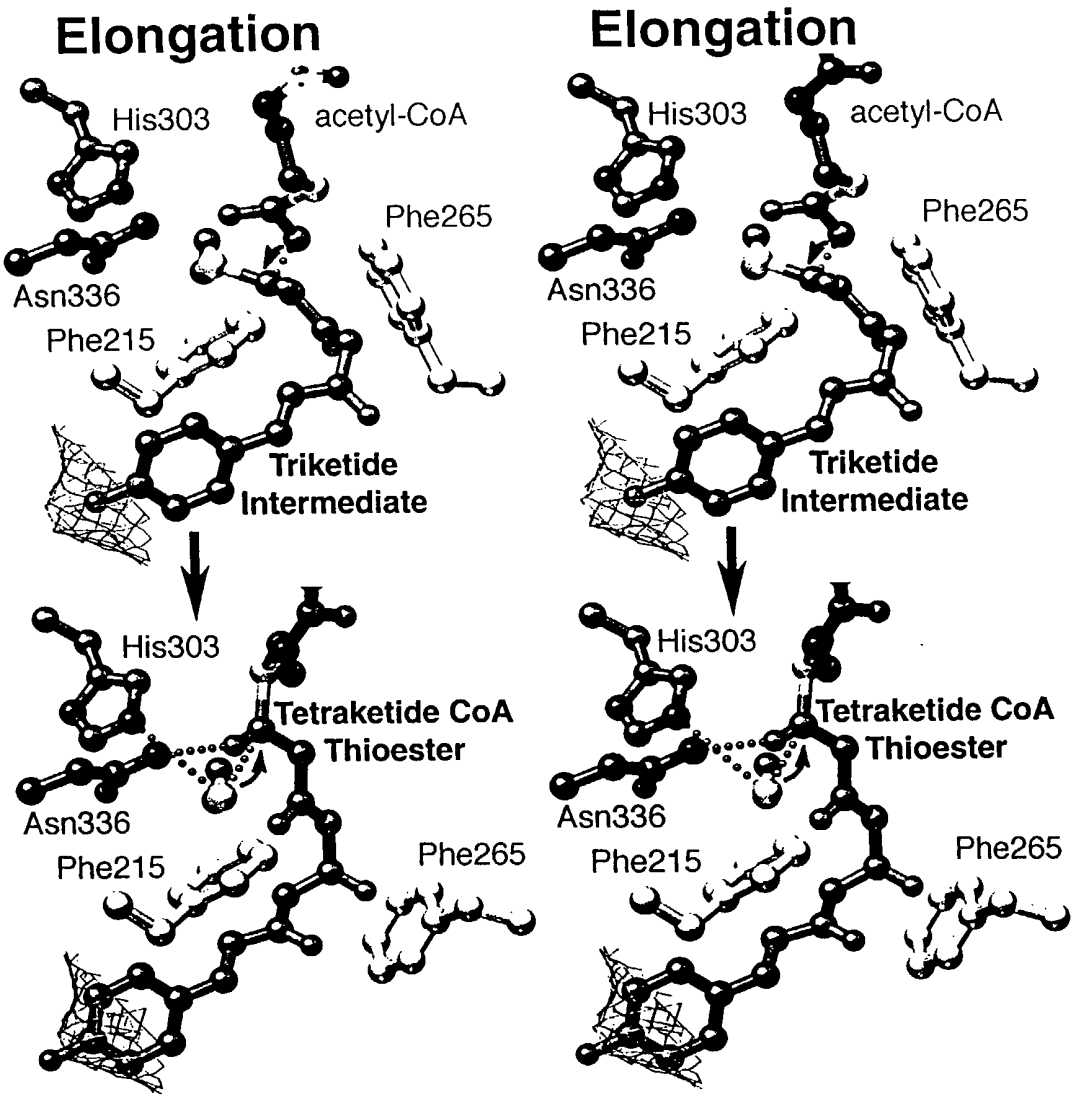

Elongation
His303
acetyl-CoA
Phe265
Asn336
Phe215
Triketide
Intermediate
His303
Tetraketide CoA
Thioester
Asn336
Phe215
Phe265
Elongation
His303
acetyl-CoA
Phe265
Asn336
Phe215
Triketide
Intermediate
His303
Tetraketide CoA
Thioester
Asn336
Phe215
Phe265

FIGURE 7A

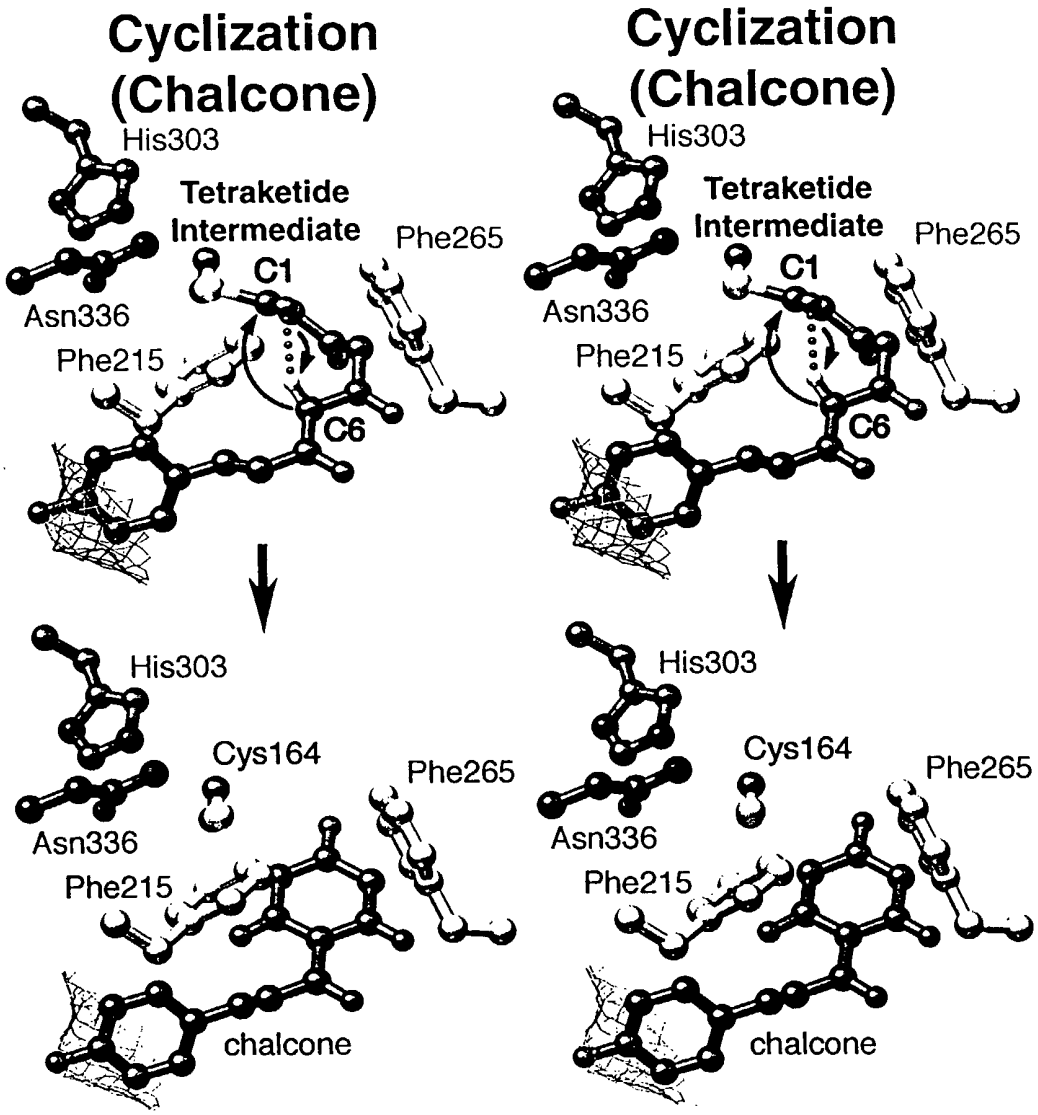

Cyclization
(Chalcone)
His303
Tetraketide
Intermediate
Phe265
C1
Asn336
Phe215
C6
His303
Cys164
Phe265
Asn336
Phe215
chalcone
Cyclization
(Chalcone)
His303
Tetraketide
Intermediate
Phe265
C1
Asn336
Phe215
C6
His303
Cys164
Phe265
Asn336
Phe215
chalcone

FIGURE 7B

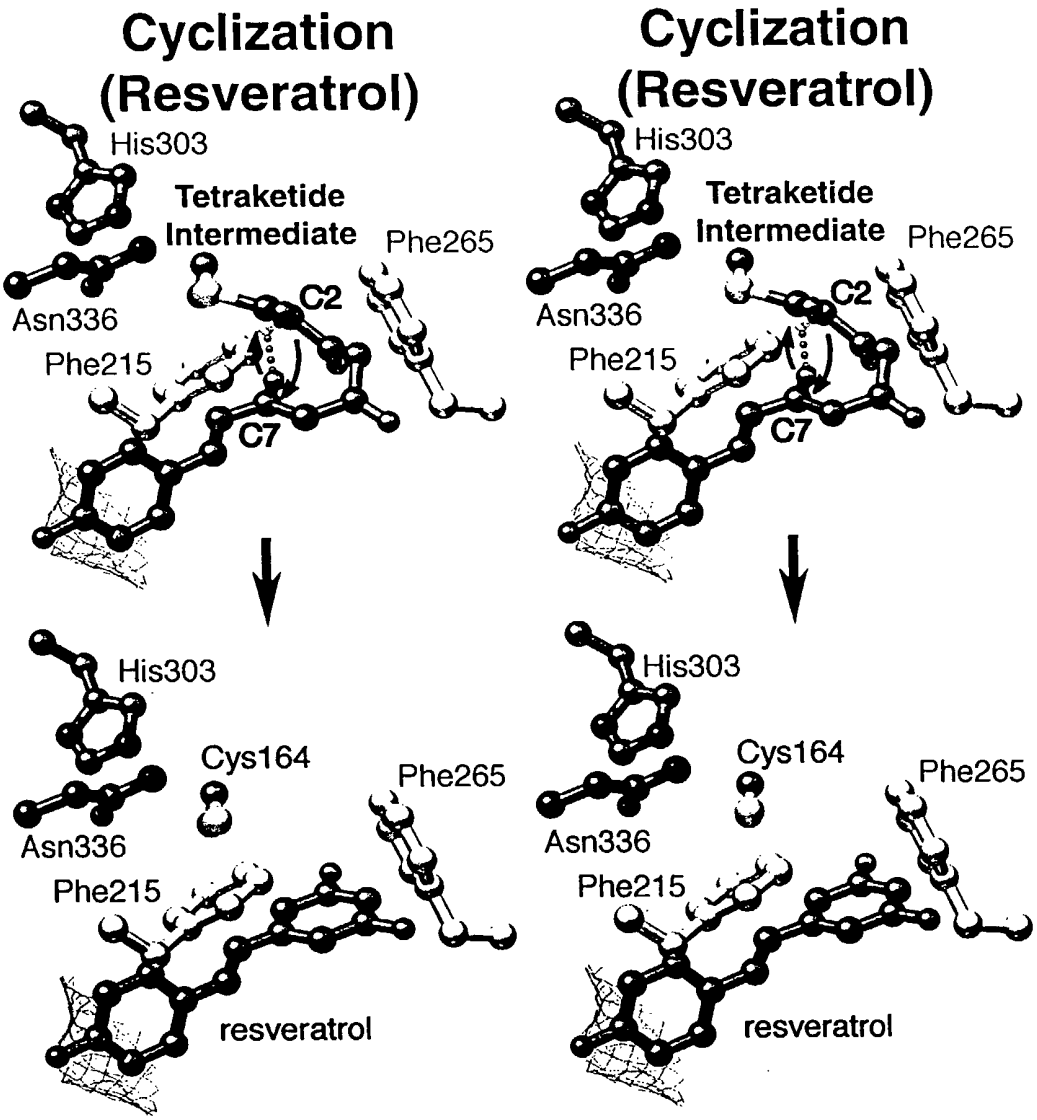

Cyclization
(Resveratrol)
His303
Tetraketide
Intermediate
Phe265
C2
Asn336
Phe215
C7
His303
Cys164
Phe265
Asn336
Phe215
resveratrol
Cyclization
(Resveratrol)
His303
Tetraketide
Intermediate
Phe265
C2
Asn336
Phe215
C7
His303
Cys164
Phe265
Asn336
Phe215
resveratrol

FIGURE 7C

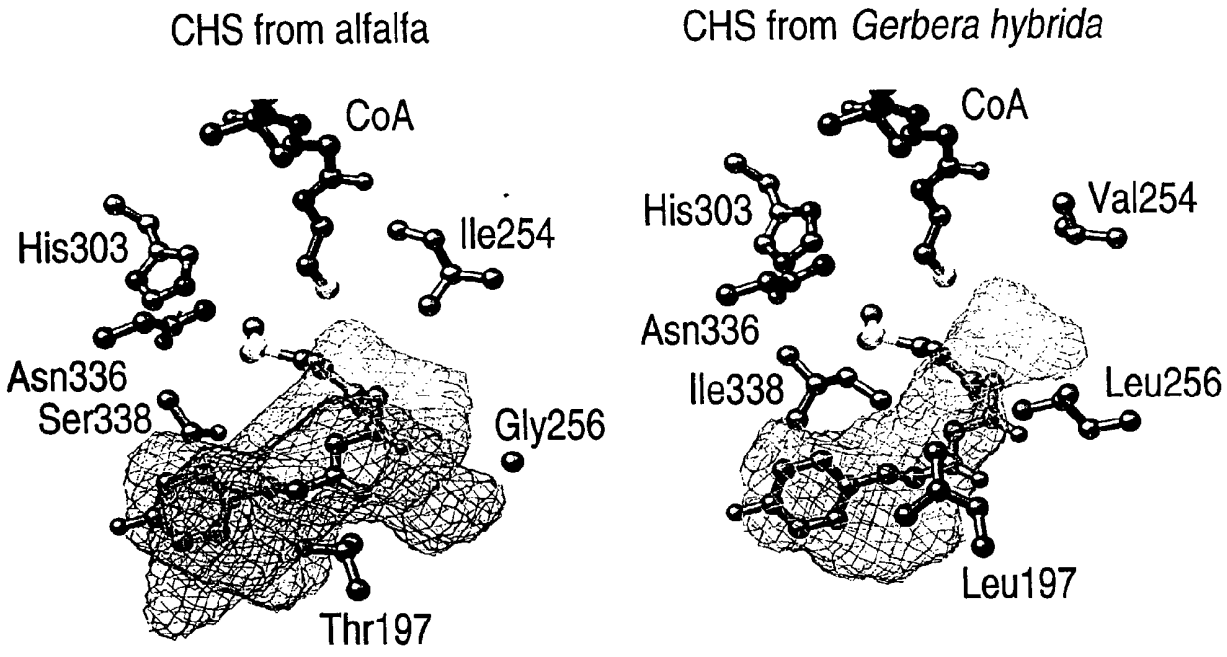

CHS from alfalfa
CoA
His303
Ile254
Asn336
Ser338
Gly256
Thr197
CHS from *Gerbera hybrida*
CoA
His303
Val254
Asn336
Ile338
Leu256
Leu197

FIGURE 8

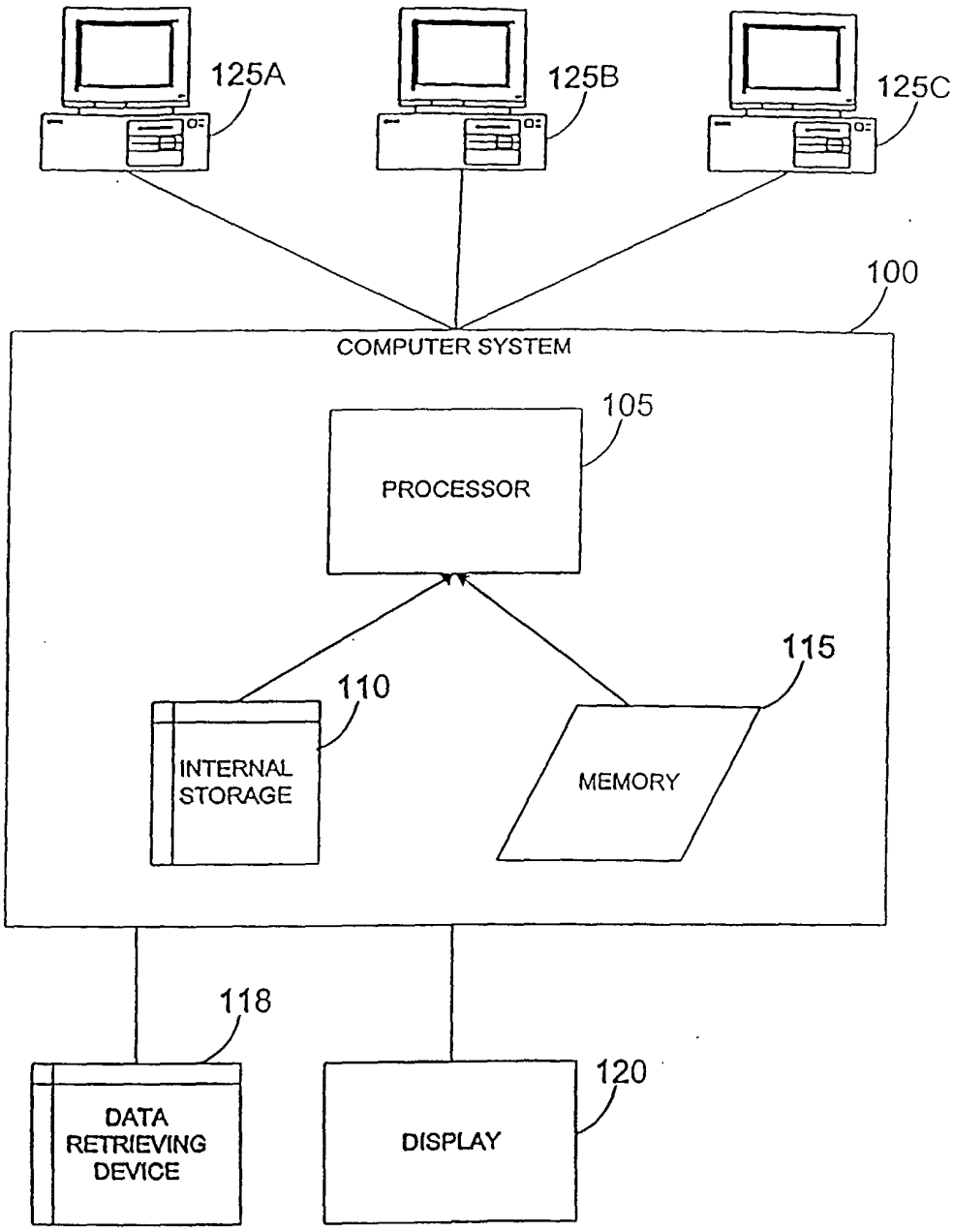

125A
125B
125C
100
COMPUTER SYSTEM
105
PROCESSOR
110
INTERNAL STORAGE
115
MEMORY
118
DATA RETRIEVING DEVICE
120
DISPLAY

FIGURE 9