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(54) Title: CRYSTAL STRUCTURE OF AMPK AND USES THEREOF

(57) Abstract: The invention provides the crystal structure of the gamma subunit of an AMPK protein molecule. The structure is set out in Table 1 and Table 2. The structure may be used in to model the interaction of compounds such as pharmaceuticals with this protein, and to determine the structure of related protein molecules.

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CRYSTAL STRUCTURE OF AMPK AND USES THEREOF

Field of the Invention.

The present invention relates to crystals and co-crystals of adenosine monophosphate-activated protein kinase (AMPK) and their 3-dimensional structures, and uses thereof.

Background to the Invention.

AMPK

AMP-activated protein kinase (AMPK) regulates cellular metabolism in response to the availability of energy. The enzyme is therefore a target for type II diabetes treatment[1]. It senses changes in the ratio of AMP/ATP by binding both species in a competitive manner[2]. Thus increases in the concentration of AMP, activate AMPK resulting in the phosphorylation and differential regulation of a series of downstream targets that control anabolic and catabolic pathways[1-3].

AMPK has been described as a cellular fuel gauge[4]. As early as 1980, the phosphorylation and inactivation of acetyl-CoA carboxylase was shown to depend on the relative levels of ATP and AMP[5], although at that time it was not known that the kinase responsible was AMPK. It is now becoming clear that AMPK plays a central role in controlling whole body metabolism in response to nutrients and hormonal signals[1]. AMPK is involved in the regulation of lipid metabolism [6], feeding and body weight[7], glucose homeostasis[8], and mitochondrial biogenesis[9]. In addition to metabolic stress, AMPK is activated by hormones, including leptin[10], adiponectin[11] and ciliary neurotrophic factor[12]. AMPK is also activated by metformin[13], one of the most widely used drugs for the treatment of type 2 diabetes, prescribed to over 120 million people worldwide. Moreover, a recent study suggests that AMPK activation is essential for the therapeutic effects of this drug in the liver[14]. In mammalian cells AMPK is activated by increases in intracellular AMP by an allosteric mechanism and by regulating the level of AMPK phosphorylation by inhibiting the dephosphorylation of Thr-172 in the activation loop of the kinase domain[15]. AMPK is a heterotrimeric complex, consisting of an alpha catalytic subunit (2 isoforms) with beta (2 isoforms) and gamma (3 isoforms) regulatory subunits[3]. The beta subunit acts as a scaffold binding both the alpha and gamma subunits[16] and the C-terminal 85 residues of beta is sufficient to form a functional AMP-dependent heterotrimer[17]. Recently, the structure of the AMPK homologue from *S. pombe* has revealed the architecture of the heterotrimer subunit interactions[18] but appears to be fundamentally different from the mammalian enzyme in the way that it senses AMP/ATP. The yeast structure showed AMP binding to only one site.

The three isoforms of the gamma subunit are highly homologous in the C-terminal region. The gamma-2 and gamma-3 isoforms have N-terminal extensions which are different from each other and not present in the gamma-1 subunit. The gamma-1 subunit is distributed throughout the body whereas the distribution of the other two subunits varies. The homologous C-terminal regions of all three isoforms of the gamma subunit are composed of four cystathionine β-synthase domains, termed CBS domains. These are numbered, in the N- to C- terminal direction as CBS-1 to CBS-4 respectively. These domains are paired to form two Bateman

domains (CBS1+2 and CBS3+4), and it is believed that these Bateman domains form AMP binding pockets.

The gamma subunit of AMPK is known to bind AMP and ATP. However, it is still not known in detail how AMP and ATP interact with this subunit of AMPK to provide regulation of the enzyme.

In another recent study, a Bateman fragment of the human AMPK gamma subunit was crystallised with AMP and the structure of this fragment resolved, to show binding of the fragment with a single AMP molecule.

WO2003/03945 describes an AMPK inhibitor screening assay. The publication proposes that tandem pairs of CBS domains from AMPK form allosteric binding sites for two molecules of AMP or ATP.

Despite the above studies, key questions remain as to the mechanism and regulation of the mammalian enzyme.

Background to Crystallisation

It is well-known in the art of protein chemistry, that crystallising a protein is a chancy and difficult process without any clear expectation of success. It is now evident that protein crystallization is the main hurdle in protein structure determination. For this reason, protein crystallization has become a research subject in and of itself, and is not simply an extension of the protein crystallographer's laboratory. There are many references which describe the difficulties associated with growing protein crystals. For example, Kierzek, A.M. and Zielenkiewicz, P., (2001), Biophysical Chemistry, 91, 1-20, *Models of protein crystal* growth, and Wiencek, J.M. (1999) Annu. Rev. Biomed. Eng., 1, 505-534, *New Strategies for crystal growth*.

It is commonly held that crystallization of protein molecules from solution is the major obstacle in the process of determining protein structures. The reasons for this are many; proteins are complex molecules, and the delicate balance involving specific and non-specific interactions with other protein molecules and small molecules in solution, is difficult to predict.

Each protein crystallizes under a unique set of conditions, which cannot be predicted in advance. Simply supersaturating the protein to bring it out of solution may not work, the result would, in most cases, be an amorphous precipitate. Many precipitating agents are used, common ones are different salts, and polyethylene glycols, but others are known. In addition, additives such as metals and detergents can be added to modulate the behaviour of the protein in solution. Many kits are available (e.g. from Hampton Research), which attempt to cover as many parameters in crystallization space as possible, but in many cases these are just a starting point to optimise crystalline precipitates and crystals which are unsuitable for diffraction analysis. Successful crystallization is aided by a knowledge of the proteins behaviour in terms of solubility, dependence on metal ions for correct folding or activity, interactions with other

molecules and any other information that is available. Even so, crystallization of proteins is often regarded as a time-consuming process, whereby subsequent experiments build on observations of past trials.

In cases where protein crystals are obtained, these are not necessarily always suitable for diffraction analysis; they may be limited in resolution, and it may subsequently be difficult to improve them to the point at which they will diffract to the resolution required for analysis. Limited resolution in a crystal can be due to several things. It may be due to intrinsic mobility of the protein within the crystal, which can be difficult to overcome, even with other crystal forms. It may be due to high solvent content within the crystal, which consequently results in weak scattering. Alternatively, it could be due to defects within the crystal lattice which mean that the diffracted x-rays will not be completely in phase from unit to unit within the lattice. Any one of these or a combination of these could mean that the crystals are not suitable for structure determination.

Some proteins never crystallize, and after a reasonable attempt it is necessary to examine the protein itself and consider whether it is possible to make individual domains, different N or C-terminal truncations, or point mutations. It is often hard to predict how a protein could be re-engineered in such a manner as to improve crystallisability. Our understanding of crystallisation mechanisms are still incomplete and the factors of protein structure which are involved in crystallisation are poorly understood.

Disclosure of the Invention.

We have now crystallised a full length gamma subunit of mammalian AMPK. We have found that AMPK contains not, as commonly believed, two nucleotide binding sites, but three AMP binding sites. Surprisingly, one of these sites (which we refer to as "AMP3") binds AMP very tightly whereas the other two sites appear ("AMP1" and "AMP2") to be capable of exchanging AMP for ATP.

Thus, unlike the previously published structures mentioned above, we have now found that three-binding sites are present and these sites have different characteristics from each other to explain how the enzyme is regulated.

We also propose a model to explain how relatively small changes in AMP concentrations can cause activation or inactivation of AMPK.

These new insights into the structure and function of AMPK open new avenues to the development of new compounds which are activators or inhibitors of AMPK. One such avenue is in the use of the new crystal structures disclosed herein for modelling new chemical structures or remodelling existing structures to bind AMPK. Another avenue is in the provision of assays which utilise a fluorescently labelled nucleotide to identify potential modulators of AMPK.

In one aspect, the present invention provides a three dimensional structure of the gamma subunit set out in Table 1 or Table 2, and uses, described further herein below of the three dimensional structure of the gamma subunit of AMPK set out in Table 1 or Table 2. Thus there is provided a computer-based method for the analysis of the interaction of a molecular structure with an AMPK gamma subunit structure, which comprises:

providing an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof;

providing a molecular structure to be fitted to said AMPK structure or selected coordinates thereof; and

fitting the molecular structure to said AMPK structure.

In general aspects, the present invention is concerned with the provision of an AMPK structure and its use in modelling the interaction of molecular structures, e.g. potential and existing pharmaceutical compounds, including inhibitors or activators, with this AMPK structure. These and other aspects and embodiments of the present invention are discussed below.

In further aspects, the invention is defined by the accompanying claims.

Brief Description of the Tables

Table 1a (Figure 1) sets out the coordinate data of the gamma subunit of AMPK, derived from a co-crystal of AMPK and three AMP molecules.
Table 1b (Figure 1) is a further refinement of the structure of Table 1a.
Table 2a (Figure 2) sets out data of the gamma subunit of AMPK, derived from a co-crystal of AMPK and one AMP with two ATP molecules.
Table 2b (Figure 2) is a further refinement of the structure of Table 2a.
Table 3 sets out binding site residues of the AMP1 pocket which bind AMP and ATP.
Table 4 sets out binding site residues of the AMP2 pocket which bind AMP and ATP
Table 5 sets out binding site residues of the AMP3 pocket which bind AMP.

Brief Description of the Drawings

Figure 1 sets out Tables 1a and 1b
Figure 2 sets out Tables 2a and 2b.
Figure 3 sets out an alignment of rat (SEQ ID NO:1) and human (SEQ ID NO:2) AMPK gamma 1 sequences.
Figure 4 illustrates the location of AMP binding in the AMP-1 binding pocket of AMPK.
Figure 5 illustrates the location of ATP binding in the AMP-1 binding pocket of AMPK.
Figure 6 illustrates the location of AMP binding in the AMP-2 binding pocket of AMPK.
Figure 7 illustrates the location of ATP binding in the AMP-2 binding pocket of AMPK.
Figure 8 illustrates the location of AMP binding in the AMP-3 binding pocket of AMPK.

Detailed Description of the Invention

The present invention is based upon the use, e.g. in crystals and assay methods, of a mammalian gamma subunit comprising both Bateman domains, together with, in some aspects, at least a C-terminal domain of a mammalian beta subunit and/or at least a C-terminal domain of a mammalian alpha subunit. These proteins are readily obtainable in the prior art and the production of the protein complex that has been crystallized in the accompanying examples was obtained as described by Neumann *et al* (Ref: 31). To provide further guidance to those of skill in the art the proteins for use in the invention may be further characterised by the following definitions.

Sequences referred to below by their database accession number are hereby incorporated by reference in their entirety in the form as entered onto the database at the filing date of the present application.

In the description below, where reference is made to Table 1, a structure of Table 1, or the like, then it will be understood that unless explicitly stated to the contrary, this may be read as reference to either Table 1a or Table 1b. Likewise, where reference is made to Table 2, a structure of Table 2, or the like, then it will be understood that unless explicitly stated to the contrary, this may be read as reference to either Table 2a or Table 2b.

In one aspect of the invention, reference to Table 1 or a structure of Table 1, or the like, may be read as a reference to Table 1a or a structure of Table 1a. In another aspect of the invention, reference to Table 1 or a structure of Table 1, or the like, may be read as a reference to Table 1b or a structure of Table 1b.

In one aspect of the invention, reference to Table 2 or a structure of Table 2, or the like, may be read as a reference to Table 2a or a structure of Table 2a. In another aspect of the invention, reference to Table 2 or a structure of Table 2, or the like, may be read as a reference to Table 2b or a structure of Table 2b.

A mammalian AMPK gamma subunit comprising both Bateman domains

This may be any isoform of any mammalian AMPK gamma subunit. In the accompanying examples, we have used the rat gamma isoform whose sequence is shown as SEQ ID NO:1 (Genbank X95578). However, other mammalian forms have a high degree of homology and may equally be used. For example, the human gamma 1 isoform of SEQ ID NO:2 (Genbank NP_002724) may also be used. As can be seen from the alignment of Figure 3, the sequences are identical apart from eight, mainly conserved, changes in the N-terminal region. Other mammalian gamma-1 subunits are of a similar level of homology, including bovine or murine forms.

Thus in one embodiment the gamma subunit may be that of SEQ ID NO:1 or SEQ ID NO:2 (or a fragment thereof as defined in the following paragraph), or a protein in which from 1 to 10, for example from 1 to 8, e.g. from 1 to 5, such as 1 or 2 amino acid substitutions, deletions or

insertions are present. (In the case of deletions or insertions, the numbers recited herein relate to the numbers of amino acids deleted or substituted). Combinations of substitutions, deletions or insertions may be present, as illustrated by the alignment of Figure 3.

Further, although it is preferred that the full-length gamma 1 subunit is used, small N- and/or C-terminal truncations are not excluded from the scope of the invention provided that the protein retains both Bateman domains which include the CBS 1+2 pair and the CBS 3+4 pair.

Alternatively, the gamma subunit may be a gamma-2 or gamma-3 subunit C-terminal fragment corresponding to the gamma-1 region. These C-terminal fragments are highly conserved and also contain four CBS domains folded into two Bateman domains. Thus the C-terminal 330 amino acid region of any mammalian AMPK gamma-2 or AMPK gamma-3 protein may be used in place of the AMPK gamma-1 protein, or a fragment thereof retaining both Bateman domains.

Suitable gamma-2 proteins include the human gamma-2 (long form) (Genbank AJ249976), the human (short form) (Genbank NP_077747), the rat (short form) (Genbank (NP_908940) and the mouse (long form) (Genbank Q91WG5).

Suitable gamma-3 proteins include the human gamma-3 (Genbank AJ249977) or the corresponding murine (Genbank NP_714966), bovine (Genbank Q2LL38) or porcine (Genbank Q9MYP4) forms.

Gamma-2 and gamma-3 C-terminal regions also include variants of wild-type sequences in which from 1 to 10, for example from 1 to 8, e.g. from 1 to 5, such as 1 or 2 amino acid substitutions, deletions or insertions are present. (In the case of deletions or insertions, the numbers recited herein relate to the numbers of amino acids deleted or substituted). Combinations of substitutions, deletions or insertions may be present.

C-terminal domain of a mammalian beta subunit

The beta subunit of AMPK exists in two mammalian isoforms. In the accompanying examples the use of the beta-2 isoform is illustrated, though the beta-1 isoform may also be used.

The following beta-1 and beta-2 isoforms are available by reference to the following Genbank accession numbers:

Beta-1		Beta-2	
Species	**Accession No.**	**Species**	**Accession No.**
Human	AJ224525	Human	AJ224538
Rat	X95577	Rat	Q9QZH4
Bovine	Q5BIS9	Mouse	Q6PAM0
Mouse	Q9R078		

The C-terminal domain of the beta isoform contains an alpha/gamma binding domain (in yeast, the equivalent region is termed the ASC domain).

Thus the C-terminal domain will usually include about 100 or fewer amino acids of a beta subunit, e.g. such as a fragment having residues 187-272 of the human beta 2 domain or the corresponding regions of any other mammalian beta domain. The corresponding region of such beta domains may be determined by conventional alignment of protein sequences. Fragments of this portion comprising at least 60, for example at least 70, e.g. at least 80 amino acids may be used.

Beta-1 and Beta-2 C-terminal domains also include variants of wild-type sequences in which from 1 to 10, for example from 1 to 8, e.g. from 1 to 5, such as 1 or 2 amino acid substitutions, deletions or insertions are present. (In the case of deletions or insertions, the numbers recited herein relate to the numbers of amino acids deleted or substituted). Combinations of substitutions, deletions or insertions may be present.

The C-terminal domains, fragments and variant thereof as defined above will retain the ability to form a complex with a C-terminal domain of an AMPK subunit comprising both Bateman domains.

C-terminal domain of a mammalian alpha subunit

The alpha subunit of AMPK exists in two mammalian isoforms. In the accompanying examples the use of the alpha -1 isoform is illustrated, though the alpha -2 isoform may also be used.

The following alpha -1 and alpha -2 isoforms are available by reference to the following Genbank accession numbers:

Alpha-1		Alpha-2	
Species	**Accession No.**	**Species**	**Accession No.**
Human (long form)	NP_006242	Human	NP_006243
Human (short form)	AAH37303	Rat	Q09137
Mouse (short form)	NP_001013385		
Rat (short form)	U40819		

The C-terminal domain of the alpha isoform contains a beta binding domain and accordingly the C-terminal domain will usually include about 200 or fewer amino acids of a alpha subunit, e.g. such as a fragment having residues 396-548 of the rat alpha 1 domain or the corresponding regions of any other mammalian alpha domain, or such as a fragment having residues 396-544 of the rat alpha 1 domain or the corresponding region of any other mammalian alpha domain. The corresponding region of such alpha domains may be determined by conventional alignment of protein sequences. Fragments of this portion comprising at least 60, for example at least 70, e.g. at least 80 amino acids may be used.

Alpha-1 and alpha-2 C-terminal domains also include variants of wild-type sequences in which from 1 to 10, for example from 1 to 8, e.g. from 1 to 5, such as 1 or 2 amino acid substitutions, deletions or insertions are present. (In the case of deletions or insertions, the numbers recited

herein relate to the numbers of amino acids deleted or substituted). Combinations of substitutions, deletions or insertions may be present. A variant of the rat alpha 1 subunit was used for crystallisation as described in the accompanying examples.

The C-terminal domains, fragments and variant thereof as defined above will retain the ability to form a complex with a C-terminal domain of an AMPK subunit comprising both Bateman domains.

Protein Crystals.

The present invention provides a co-crystal of AMPK complex of a mammalian gamma subunit comprising both Bateman domains bound to three nucleotides, C-terminal domains of a mammalian beta and alpha subunits. In one aspect, the co-crystal have a space group $P2_12_12$ with cell dimensions of about a=49, b=120, c=128 Å, 90°, 90°, 90°. Unit cell variability of 5% may be observed in all dimensions.

Two specific examples of a crystal of the invention are the co-crystal comprising three AMP nucleotides having a=48.52, b=119.39, c=129.31, and a co-crystal comprising two ATP nucleotides and an AMP nucleotide having a=48.79, b=120.69, c=127.07.

Other nucleotides which may be co-crystallized or obtained by soaking, used, analysed or modified either *in silico* or chemically as a result of the use of methods of the invention include adenosine diphosphate (ADP) and synthetic adenosine nucleotide analogues including 5-Aminoimidazole-4-carboxamide ribonucleoside (AICAR) or ZMP, the monophosphorylated derivative of AICAR as well as adenosine analogues including thiophosphate or phosphoramidate analogues.

Alternatively the co-crystal could comprise a compound whose interaction with AMPK is unknown.

Such crystals may be obtained using the methods described in the accompanying examples. Generally, such methods include co-crystallization and soaking. Since AMPK has three separate nucleotide binding pockets, co-crystals may comprise a mixture of two or three different nucleotides or other compounds located in such pockets.

The present invention is believed to be the first time that a complete gamma domain of a mammalian AMPK domain has been crystallized and its structure resolved. The successful crystallization of the gamma domain is believed to have been achieved through the use of the presence of the C-terminal regions of mammalian alpha and beta subunits to stabilize the folding of the gamma subunit.

This methodology is generally applicable to the provision of other crystals of mammalian AMPK gamma subunits. Thus crystals of the invention may be formed from the following components:

The methodology used to provide a crystal illustrated herein may be used generally to provide an AMPK crystal resolvable at a resolution of at least about 2.4 Å.

In a further aspect, the invention provides a method for making a protein crystal, particularly of an AMPK protein comprising a mammalian gamma subunit comprising both Bateman domains in association with a C-terminal domain of a mammalian AMPK beta subunit and a C-terminal domain of a mammalian AMPK alpha subunit, which method comprises growing a crystal by vapor diffusion. Protein stock solution comprising 5-30mg/ml, e.g. about 15mg/ml in 50mM Tris, pH 7.0, 100mM NaCl and 1mM TCEP (Tris(2-carboxyethyl)phosphine hydrochloride) is mixed with an excess of nucleotide from 1.1 to 5 times e.g. 3-fold excess. Vapour diffusion is done by mixing protein stock solution with a reservoir buffer in the ratio 0.3 to 3.0 to one, e.g. 1 to 1, where the reservoir solution contains from 6-22% isopropanol e.g. about 15%. Crystals are prepared for data collection by replacing the crystallisation mixture with crystallisation mixture with 25-35% ethylene glycol e.g. about 30%.

Crystals may be prepared in the presence of a nucleotide, particularly AMP, ADP or ATP, or a mixture of two or more of these nucleotides.

Crystal Coordinates.

Overview

In one aspect, the invention utilizes the novel crystal coordinates set out in Table 1 and Table 2. The uses of the coordinates are described further herein below and include various methods relating to the computer modelling of ligands that may interact with AMPK, the delivery of the coordinates through computer systems for use by those of skill in the art, and the use of the coordinates in constructing homology models of related proteins or in interpreting X-ray or nmr data of other proteins in order provide a structure of such other proteins. These uses are not exhaustive and other uses are set out herein below.

Format of Table 1 and Table 2

Table 1 and Table 2 give atomic coordinate data for the structures of AMPK. In these Tables the first column is the identifier "ATOM", the second column a contiguous number to uniquely refer to an atom of a particular row, the third column denotes the atom and its location within an amino acid residue, the fourth the residue type, the fifth the chain identification, the sixth the residue number (the atom numbering is with respect to the full length wild type protein), the seventh, eighth and ninth columns are the X, Y, Z coordinates respectively of the atom in question, the tenth column the occupancy of the atom, and the eleventh the temperature factor of the atom, the twelfth the atom type.

Table 1 and Table 2 are set out in an internally consistent format. For example the coordinates of the atoms of each amino acid residue are listed such that the backbone nitrogen atom is first, followed by the C-alpha backbone carbon atom, designated CA, followed by side chain residues (designated according to one standard convention) and finally the carbon and oxygen of the protein backbone. Alternative file formats (e.g. such as a format consistent with that of

the EBI Macromolecular Structure Database (Hinxton, UK)) which may include a different ordering of these atoms, or a different designation of the side-chain residues, ligand or water, may be used or preferred by others of skill in the art. However it will be apparent that the use of a different file format to present or manipulate the coordinates of the Table is within the scope of the present invention.

Thus the coordinates of Table 1 and Table 2 provide a measure of atomic location in Angstroms, given to 3 decimal places. The coordinates are a relative set of positions that define a shape in three dimensions, but the skilled person would understand that an entirely different set of coordinates having a different origin and/or axes could define a similar or identical shape. Thus for the purposes described herein as being aspects of the present invention, it is within the scope of the invention if: the coordinates of any of Table 1 and Table 2 are transposed to a different origin and/or axes.

AMPK gamma subunit structure

Tables 1 and 2 contain not only the structure of the AMPK gamma subunit, but also include the coordinate data the C-terminal AMPK alpha and AMPK beta domains, the nucleotide molecules present in the gamma subunit, water molecules, and in the case of Table 2, Magnesium ions. Thus in Table 1a, the gamma subunit is identified as chain "E", in the rows numbered 1444-3884 of the Table. In Table 2a, the gamma subunit is identified as chain "C", in the rows numbered 1438-3878. In Table 1b and Table 2b, the gamma subunit is identified as chain "E", in the rows numbered 1458-3898 of the Table.

In the present invention, reference to the "AMPK gamma subunit structure of Table 1 or Table 2", or the like, is to be taken as reference to those coordinates in the Tables which relate to this subunit alone. However, unless explicitly set out to the contrary, or otherwise clear from the context, reference throughout the present specification to the use of all or selected coordinates of or from Table 1 or Table 2 does not exclude the use of additional coordinates, particularly some or all of the coordinate of alpha or beta subunit domains, the nucleotides, water molecules or magnesium ions.

RMSD

Protein structure similarity is routinely expressed and measured by the root mean square deviation (rmsd), which measures the difference in positioning in space between two sets of atoms, based on the square root of the arithmetic mean of the squares of the deviations from the mean. The rmsd measures distance between equivalent atoms after their optimal superposition. The rmsd can be calculated over all atoms, over residue backbone atoms (i.e. the nitrogen-carbon-carbon backbone atoms of the protein amino acid residues), main chain atoms only (i.e. the nitrogen-carbon-oxygen-carbon backbone atoms of the protein amino acid residues), side chain atoms only or more usually over C-alpha atoms only. For the purposes of this invention, the rmsd can be calculated over any of these, using any of the methods outlined below. In one embodiment, rmsd is measured by reference to the C-alpha atoms.

For the purposes of the present invention, the skilled person would understand that varying the relative atomic positions of the atoms of the structure so that the root mean square deviation of the C-alpha atoms is less than 1.5 Å, preferably less than 1.0 Å, more preferably less than 0.5 Å, more preferably less than 0.3 Å, such as less than 0.25 Å, or less than 0.2 Å, and most preferably less than 0.1 Å, when superimposed on the coordinates of AMPK gamma subunit structure of Table 1 or Table 2 for the residue backbone atoms, will generally result in a structure which is substantially the same as the structure of Table 1 and Table 2 in terms of both its structural characteristics and usefulness for structure-based analysis of -interactivity molecular structures.

Reference herein to the AMPK gamma subunit structure of Table 1 or Table 2 and the like thus includes the AMPK gamma subunit coordinate data of these Tables in which one or more individual values of either Table are varied within an rmsd of less than 1.5 Å or any of the narrower values identified above.

Methods of comparing protein structures are discussed in Methods of Enzymology, vol 115, pg 397-420. The necessary least-squares algebra to calculate rmsd has been given by Rossman and Argos (J. Biol. Chem. , vol 250, pp7525 (1975)) although faster methods have been described by Kabsch (Acta Crystallogr., Section A, A92, 922 (1976)); Acta Cryst. A34, 827-828 (1978)), Hendrickson (Acta Crystallogr., Section A, A35, 158 (1979)); McLachan (J. Mol. Biol., vol 128, pp49 (1979)) and Kearsley (Acta Crystallogr., Section A, A45, 208 (1989)). Some algorithms use an iterative procedure in which the one molecule is moved relative to the other, such as that described by Ferro and Hermans (Ferro and Hermans, Acta Crystallographic, A33, 345-347 (1977)). Other methods e.g. Kabsch's algorithm locate the best fit directly.

Programs for determining rmsd include MNYFIT (part of a collection of programs called COMPOSER, Sutcliffe, M.J., Haneef, I., Carney, D. and Blundell, T.L. (1987) Protein Engineering, 1, 377-384), MAPS (Lu, G. An Approach for Multiple Alignment of Protein Structures (1998, in manuscript and on http://bioinfo1.mbfys.lu.se/TOP/maps.html)).

It is usual to consider C-alpha atoms and the rmsd can then be calculated using programs such as LSQKAB (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763), QUANTA (Jones et al., Acta Crystallography A47 (1991), 110-119 and commercially available from Accelerys, San Diego, CA), Insight (commercially available from Accelerys, San Diego, CA), Sybyl® (commercially available from Tripos, Inc., St Louis), O (Jones et al., *Acta Crystallographica*, A47, (1991), 110-119), and other coordinate fitting programs.

In, for example the programs LSQKAB and O, the user can define the residues in the two proteins that are to be paired for the purpose of the calculation. Alternatively, the pairing of residues can be determined by generating a sequence alignment of the two proteins. Programs for sequence alignment are well known in the art, e.g. the BLAST package of alignment programs. The atomic coordinates can then be superimposed according to this alignment and an rmsd value calculated. The program Sequoia (C.M. Bruns, I. Hubatsch, M.

Ridderström, B. Mannervik, and J.A. Tainer (1999) Human Glutathione Transferase A4-4 Crystal Structures and Mutagenesis Reveal the Basis of High Catalytic Efficiency with Toxic Lipid Peroxidation Products, *Journal of Molecular Biology* 288(3): 427-439) performs the alignment of homologous protein sequences, and the superposition of homologous protein atomic coordinates. Once aligned, the rmsd can be calculated using programs detailed above. For sequence identical, or highly identical, the structural alignment of proteins can be done manually or automatically as outlined above. Another approach would be to generate a superposition of protein atomic coordinates without considering the sequence.

Selected coordinates

Those of skill in the art will appreciate that in many applications of the invention, it is not necessary to utilise all the coordinates of Table 1 and Table 2, but merely a portion of them. For example, as described below, in methods of modelling candidate compounds, selected coordinates of the AMPK gamma subunit structure of Table 1 or Table 2 may be used.

By "selected coordinates" it is meant for example at least 5, preferably at least 10, more preferably at least 50 and even more preferably at least 100, for example at least 500 or at least 1000 atoms of the AMPK gamma subunit structure of Table 1 or Table 2. Likewise, the other applications of the invention described herein, including homology modelling and structure solution, and data storage and computer assisted manipulation of the coordinates, may also utilise all or a portion of the coordinates (i.e. selected coordinates) of Table 1 and Table 2.

The structures of Tables 1 and 2 have allowed us to identify particular residues of AMPK which are involved in the interaction with AMP or ATP at the AMP-1, 2 and 3 regions of the protein. Figures 4, 6 and 8 illustrate the binding of AMP to the AMP-1, 2 and 3 sites respectively, Figures 5 and 7 illustrate the binding of ATP to the AMP-1 and 2 sites respectively. Thus the residues at these regions are thus of particular interest, and are as set out in Tables 3 to 5 below:

Table 3: "AMP-1" region:

Arg 69	Lys 169	Ser 225	Ala 226	Asp 238	Ile 239
Tyr 240	Ser 241	Lys 242	Phe 243	Asp 244	His 270
Tyr 271	Phe 272	Glu 273	Gly 274	Val 275	Leu 276
His 297	Arg 298	Leu 299	Val 300		

Table 4: "AMP-2" region:

Ala 70	Met 84	Leu 85	Thr 86	Ile 87	Thr 88
Asp 89	Lys 126	Pro 127	Leu 128	Val 129	Ile 149
His 150	Arg 151	Leu 152	Pro 153	Lys 242	

Table 5: "AMP-3" region

His 150	Thr 199	Tyr 200	Ala 201	Asn 202	Ile 203
Ala 204	Ser 225	Ala 226	Leu 227	Pro 228	His 297
Arg 298	Ile 311	Val 312	Ser 313	Leu 314	Ser 315
Asp 316					

In some aspects of the invention, the selected coordinates may include one or more coordinates of an atom from an amino acid set out in any one of Tables 3 to 5.

Preferably the selected coordinates include one or more, such as at least 5, preferably at least 10, more preferably at least 50 and even more preferably at least 100, coordinates of atoms of the amino acids set out in any one of Tables 3 to 5. More preferably the selected coordinates are of atoms of residues of Table 3 or Table 4. When the selected coordinates are of atoms of residues of either of Tables 3 or 4, the coordinates are desirably derived from at least 2, more preferably at least 4, such as at least 10 different amino acids. Likewise, when the selected coordinates are of atoms of residues of Table 5, the coordinates are desirably derived from at least 2, more preferably at least 4, such as at least 10 different amino acids.

In one embodiment the invention uses at least 10 selected coordinates from at least 4 different amino acids in any one of Tables 3 or 4. In another embodiment the invention uses at least 50 selected coordinates from at least 10 different amino acids in any one of Tables 3 or 4.

In one embodiment the invention uses at least 10 selected coordinates from at least 4 different amino acids in Table 5. In another embodiment the invention uses at least 50 selected coordinates from at least 10 different amino acids in Table 5.

In another embodiment the invention uses at least 10 selected coordinates from at least 4 different amino acids in Table 3 and at least 10 selected coordinates from at least 4 different amino acids in Table 4. In this embodiment, optionally at least a further 10 selected coordinates from at least 4 different amino acids in Table 5 may also be used.

In another embodiment the invention uses at least 50 selected coordinates from at least 10 different amino acids in Table 3 and at least 50 selected coordinates from at least 10 different amino acids in Table 4. In this embodiment, optionally at least a further 10 selected coordinates from at least 4 different amino acids in Table 5 may also be used.

In embodiments of the invention in which some or all of the coordinates of atoms of the amino acids in Table 5 are used, the coordinates of some (e.g. at least 5, such as at least 10) or all of the AMP atoms of Table 1 or 2 may also be used.

Residues in the above tables whose mutation is implicated in Wolff-Parkinson-White syndrome are Arg 69, His 150, Thr 167 and Arg 298. The equivalent residues in γ2 are: Arg-69≡Arg-302,

His-150≡His-383, Thr-167≡Thr-400, Arg-298≡Arg-531. Atoms from these resides, when the relevant tables are being used, may be included in the methods of the present invention.

Description of Structure.

The overall structure of the enzyme can be regarded as being made up of two components: an α+β module at the bottom interacting with one shoulder of the γ domain module at the top. Whilst the α subunit is composed of both helices and strands, and has a recognisable hydrophobic core, the β chain consists of beta structure and generates most of its hydrophobic contacts via interactions with the α subunit.

However, the interface between the α+β and γ modules is mediated by the last two strands of the β subunit forming an interdomain beta sheet with a beta-strand from γ. Thus it appears that although the C-terminal domain of β relies for its folding on the structure of α, it is responsible for mediating complex formation. The γ subunit, made up of four cystathionine β-synthase (CBS) domains, is shaped like a flattened disk about 60 Å across and 30 Å deep. These CBS domains, packing together to generate two Bateman domains, obey approximate 2,2,2 point group symmetry. Each Bateman domain (CBS1+2 and CBS3+4) arises from the packing of a pair of anti-parallel strands from each CBS domain according to a local dyad axis. It is this interaction that generates the adenyl binding sites. The two Bateman domains pack around a second dyad axis through an interface dominated by a pair of α-helices from each CBS domain. Passing through the centre of the γ domain there is a small solvent accessible channel.

Comparison of the structure of mammalian AMPK with its homologue from yeast reveals three striking differences. Firstly, the mammalian enzyme, both in the crystal and in solution, is a monomer whereas the yeast enzyme has been reported to be a dimer. Secondly, there is hinging movement between the α+β and γ modules such that there is about a 12° difference in their relative orientations between the two species. Thirdly, mammalian AMPK binds three AMP molecules; one does not exchange but the other two compete for binding with Mg.ATP and are responsible for the adenyl sensing properties of the mammalian enzyme. In the case of the yeast homologue the structure shows one adenyl-binding site, equivalent to the non-exchangeable site in our structure, which seems to bind either AMP or non Mg^{2+}-bound ATP[18].

The symmetry relating the CBS domains of γ means that there are four potential adenyl binding sites. There is well-defined electron density for AMP in three of these sites but not the fourth. In these three sites, the nucleotide binds in a surface pocket at the interface of the two CBS domains, within each Bateman domain. The adenine moiety sits in a hydrophobic pocket making hydrogen bonds with main chain groups from two different strands. The phosphate group interacts with the basic side chains of a number of different residues (including Arg-69, His-150, Arg-151, Lys-169, His-297 & Arg-298) and with the hydroxyl groups of either serine or threonine residues.

Importantly, there are some interactions of the bound AMP molecules with protein residues from the alternate Bateman to which the binding site is predominantly generated (for example

Lys-169 and His-150). The 2' and 3' hydroxyl groups of the ribose group make a bi-dentate interaction with an aspartic acid residue located on the first turn of a α-helix adjacent to the site (Asp-244 with AMP-1, Asp-89 with AMP-2 & Asp-316 with AMP-3). In the fourth potential adenyl binding site there is an arginine residue, at position 170, instead of this aspartic acid that likely accounts for the fact that AMP does not bind at this fourth site.

Only small crystals were obtained from co-crystallisation of AMPK with ATP so we soaked ATP into our AMPK/AMP_3 crystals. To test the results of our solution studies we carried out soaking experiments with Mg.ATP and with Mg^{2+}-free ATP. In both cases the resulting electron density maps revealed that ATP replaced two out of the three molecules of AMP and that the metal-bound and metal-free forms of the ATP adopted very similar conformations. Consistent with the results of our binding studies, that showed no difference in affinity between the two forms, the magnesium ions complexed between the β and γ phosphate oxygens of the ATP do not interact with the protein. Two views of the structure of the γ subunit with bound nucleotide from both the AMPK/AMP_3 and AMPK/$AMP_1(MgATP)_2$ complexes were compared. The two molecules of ATP bind in a similar manner to the AMP molecules that they replace. The β- and γ-phosphates adopt an extended conformation within the binding channel necessitating the rearrangement of the side-chains of a few basic residues; otherwise there are no significant differences in the two different complexes.

Comparison of the AMP and ATP structures suggests that AMP-3, which does not exchange for ATP, represents the tightly bound adenyl moiety that co-purifies with the protein and, as noted above, AMP-3 occupies the equivalent site to the single molecule of AMP seen bound to the yeast homologue[18]. All three adenyl binding sites are structurally related but comparison suggests that the positioning of two serine residues (225 & 315), that interact with the phosphate group, and a threonine residue (199), that interacts with the ribose, which does not occur in the other two sites, may account for the enhanced affinity of this site. Interestingly, the only one of these residues not conserved in the *S. pombe* sequence is Ser-315 which is an alanine residue in that sequence (residues 307 of the C chain in PDB file 2OOX). At least for mammalian AMPK our results show that AMP binding at this non-exchangeable site is not involved in AMP/ATP sensing. Clearly mutagenic and biophysical/biochemical studies will be required to elucidate the role of this tightly bound adenyl species.

A glycogen storage cardiomyopathy associated with an electrical conductance disorder in humans (Refs 26-28) has been attributed to naturally occurring mutations in the γ2 isoform of AMPK. These mutations generally interfere with the normal activation of AMPK by AMP. The corresponding residues mapped onto the γ1 structure reveals that eight out of the ten mutations that have been characterised involve amino acids whose side-chains are in proximity to the adenyl binding sites (Table 6). The remaining two (Tyr-254 & Asn-255) are located towards the periphery of the gamma domain and may affect protein stability/aggregation rather than enzymatic activity directly.

Six of the remaining eight are seen to be contacting the phosphate groups of the AMP/ATP. The structure also shows how small changes in the side-chain conformations of these residues

accommodate either AMP or ATP in the binding site. All the mutations tested for adenyl binding have been shown to reduce the enzyme's affinity for both AMP and ATP, in some cases quite substantially. All but one of these mutations is identified here as contacting the adenyl phosphate groups and the remaining one (a leucine insertion) is close to this site and may well affect binding also. Once the molecular basis for signal propagation by AMP binding to AMPK is further elucidated additional insights into the actions of these mutations may be revealed.

Table 6:

Mutation in human γ2	Equivalent residue in γ1	Effect on AMP/ATP binding (from in vitro studies: Ref: 1; Ref: 2; Ref: 3)	Close to the nucleotide binding sites (and interacting) from structure
Arg-302-Gln	Arg-69	Yes	Yes (Yes)
Leu-351 insertion	Insertion between Arg-117 and Glu-118	Yes	Yes (NA)
His-383-Arg	His-150	Yes	Yes (Yes)
Thr-400-Asn	Thr-167	Yes	Yes (Yes)
Tyr-487-His	Tyr-254	ND	No (No)
Asn-488-Ile	Asn-255	No	No (No)
Glu-506-Lys	Glu-273	ND	Yes (No)
Arg-531-Gly/Gln	Arg-298	Yes	Yes (Yes)
Ser-548-Pro	Ser-315	ND	Yes (Yes)

Homology Modelling.

The invention also provides a means for homology modelling of other proteins (referred to below as target proteins). By "homology modelling", it is meant the prediction of related structures based either on X-ray crystallographic data or computer-assisted *de novo* prediction of structure, based upon manipulation of the coordinate data derivable from any one of Table 1 and Table 2 or selected portions thereof.

"Homology modelling" extends to target proteins which are analogues or homologues of the AMPK gamma subunit structure that has been determined herein. It also extends to protein mutants of AMPK gamma subunit protein itself.

The term "homologous regions" describes amino acid residues in two sequences that are identical or have similar (e.g. aliphatic, aromatic, polar, negatively charged, or positively charged) side-chain chemical groups. Identical and similar residues in homologous regions are sometimes described as being respectively "invariant" and "conserved" by those skilled in the art.

In general, the method involves comparing the amino acid sequences of the AMPK gamma subunit of SEQ ID NO:1 with a target protein by aligning the amino acid sequences. Amino acids in the sequences are then compared and groups of amino acids that are homologous (conveniently referred to as "corresponding regions") are grouped together. This method detects conserved regions of the polypeptides and accounts for amino acid insertions or deletions.

Homology between amino acid sequences can be determined using commercially available algorithms. The programs *BLAST*, *gapped BLAST*, *BLASTN*, *PSI-BLAST* and *BLAST 2* (provided by the National Center for Biotechnology Information) are widely used in the art for this purpose, and can align homologous regions of two amino acid sequences. These may be used with default parameters to determine the degree of homology between the amino acid sequence of the SEQ ID NO:1 protein and other target proteins which are to be modelled.

Analogues are defined as proteins with similar three-dimensional structures and/or functions with little evidence of a common ancestor at a sequence level.

Homologues are defined as proteins with evidence of a common ancestor, i.e. likely to be the result of evolutionary divergence and are divided into remote, medium and close sub-divisions based on the degree (usually expressed as a percentage) of sequence identity.

A homologue is defined here as a protein with at least 15%, preferably at least 40%, more preferably at least 70%, sequence identity or which has at least one functional domain, which is characteristic of the AMPK gamma subunit.

The homlogues could also be polymorphic forms of the AMPK gamma subunit such as alleles or mutants.

Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in a computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.

The structures of amino acids located in non-conserved regions may be assigned manually by using standard peptide geometries or by molecular simulation techniques, such as molecular dynamics. The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or energy minimization.

Homology modelling as such is a technique that is well known to those skilled in the art (see e.g. Greer, *Science*, Vol. 228, (1985), 1055, and Blundell *et al.*, *Eur. J. Biochem*, Vol. 172, (1988), 513). The techniques described in these references, as well as other homology

modelling techniques, generally available in the art, may be used in performing the present invention.

Thus the invention provides a method of homology modelling comprising the steps of:

(a) aligning a representation of an amino acid sequence of a target protein of unknown three-dimensional structure with the amino acid sequence of SEQ ID NO:1 to match homologous regions of the amino acid sequences;

(b) modelling the structure of the matched homologous regions of said target of unknown structure on the corresponding regions of the AMPK gamma subunit structure of Table 1 or Table 2, or selected coordinates thereof; and

(c) determining a conformation (e.g. so that favourable interactions are formed within the target of unknown structure and/or so that a low energy conformation is formed) for said target of unknown structure which substantially preserves the structure of said matched homologous regions.

Preferably one or all of steps (a) to (c) are performed by computer modelling.

The co-ordinate data of Table 1 and Table 2 or selected coordinates thereof, will be particularly advantageous for homology modelling of other mammalian proteins, in particular the C-terminal Bateman domains of AMPK gamma-2 or AMPK gamma-3, including the human forms thereof.

The aspects of the invention described herein which utilise the structure *in silico* may be equally applied to homologue models of obtained by the above aspect of the invention, and this application forms a further aspect of the present invention. Thus having determined a conformation of a by the method described above, such a conformation may be used in a computer-based method of rational drug design as described herein.

Structure Solution

The atomic coordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 can also be used to solve the crystal structure of other target proteins including other crystal forms of AMPK, mutants, co-complexes of AMPK gamma, where X-ray diffraction data or NMR spectroscopic data of these target proteins has been generated and requires interpretation in order to provide a structure.

In the case of AMPK gamma, this protein may crystallize in more than one crystal form. The data of Table 1 and Table 2, or portions thereof, as provided by this invention, are particularly useful to solve the structure of those other crystal forms of AMPK. It may also be used to solve the structure of AMPK mutants, AMPK co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of AMPK.

In the case of other target proteins, particularly the human proteins referred to above, the present invention allows the structures of such targets to be obtained more readily where raw X-ray diffraction data is generated.

Thus, where X-ray crystallographic or NMR spectroscopic data is provided for a target of unknown three-dimensional structure, the atomic coordinate data derived from any one of AMPK gamma subunit structure of Table 1 or Table 2, may be used to interpret that data to provide a likely structure for the other by techniques which are well known in the art, e.g. phasing in the case of X-ray crystallography and assisting peak assignments in NMR spectra.

One method that may be employed for these purposes is molecular replacement. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio.* Examples of computer programs known in the art for performing molecular replacement are CNX (Brunger A.T.; Adams P.D.; Rice L.M., Current Opinion in Structural Biology, Volume 8, Issue 5, October 1998, Pages 606-611 (also commercially available from Accelrys San Diego, CA), MOLREP (A.Vagin, A.Teplyakov, MOLREP: an automated program for molecular replacement, J. Appl. Cryst. (1997) 30, 1022-1025, part of the CCP4 suite) or AMoRe (Navaza, J. (1994). AMoRe: an automated package for molecular replacement. Acta Cryst. A50, 157-163).

Thus, in a further aspect of the invention provides a method for determining the structure of a protein, which method comprises;

providing an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof, and

positioning the coordinates in the crystal unit cell of said protein so as to provide a structure for said protein.

The invention may also be used to assign peaks of NMR spectra of such proteins, by manipulation of the data of any one of Table 1 and Table 2.

In a preferred aspect of this invention the co-ordinates are used to solve the structure of target AMPK gamma subunits, particularly the gamma-2 and gamma-3 subunits.

Computer Systems

In another aspect, the present invention provides systems, particularly a computer system, intended to generate structures and/or perform optimisation of compounds which interact with an AMPK gamma subunit, the system containing computer-readable data comprising one or more of:

(a) AMPK co-ordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof, said data defining the three-dimensional structure of the gamma subunit of AMPK or said selected coordinates thereof;

(b) atomic coordinate data of a target protein generated by homology modelling of the target based on the coordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof; or

(c) atomic coordinate data of a target protein generated by interpreting X-ray crystallographic data or NMR data by reference to the co-ordinate data of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof.

For example the computer system may comprise: (i) a computer-readable data storage medium comprising data storage material encoded with the computer-readable data; (ii) a working memory for storing instructions for processing said computer-readable data; and (iii) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-readable data and thereby generating structures and/or performing rational drug design. The computer system may further comprise a display coupled to said central-processing unit for displaying said structures.

The instructions for processing said computer-readable data may include instructions for constructing a model of the AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof, for constructing a model of an AMPK gamma subunit structure based on homology modelling or structure solution using the data derived from said Tables, or performing the computer-based modelling methods of the invention described herein.

The display may be used to provide an output in which an AMPK gamma subunit structure of the invention, optionally including one or more molecular structures fitted said AMPK gamma subunit structure is displayed in the form of a model. Such a model may be (a) a wire-frame model; (b) a chicken-wire model; (c) a ball-and-stick model; (d) a space-filling model; (e) a stick-model; (f) a ribbon model; (g) a snake model; (h) an arrow and cylinder model; (i) an electron density map; (j) a molecular surface model.

The invention also provides such systems containing atomic coordinate data of target proteins wherein such data has been generated according to the methods of the invention described herein based on the starting data provided the data of Table 1 or Table 2 or selected coordinates thereof.

Such data is useful for a number of purposes, including the generation of structures to analyse the mechanisms of action of, and/or to perform rational drug design of compounds, which interact with, AMPK and are potential activators or inhibitors of the enzyme.

In a further aspect, the present invention provides a computer-readable storage medium, comprising a data storage material encoded with computer readable data, wherein the data are defined by all or a portion of the structure coordinates of the AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof.

As used herein, "computer readable media" refers to any medium or media, which can be read and accessed directly by a computer. Such media include, but are not limited to: magnetic

storage media such as floppy discs, hard disc storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM and ROM; and hybrids of these categories such as magnetic/optical storage media.

By providing such computer readable media, the atomic coordinate data of the invention can be routinely accessed to model s or selected coordinates thereof. For example, RASMOL (Sayle et al., *TIBS*, Vol. 20, (1995), 374) is a publicly available computer software package, which allows access and analysis of atomic coordinate data for structure determination and/or rational drug design.

As used herein, "a computer system" refers to the hardware means, software means and data storage means used to analyse the atomic coordinate data of the invention. The minimum hardware means of the computer-based systems of the present invention comprises a central processing unit (CPU), input means, output means and data storage means. Desirably a monitor is provided to visualize structure data. The data storage means may be RAM or means for accessing computer readable media of the invention. Examples of such systems are microcomputer workstations available from Silicon Graphics Incorporated and Sun Microsystems running Unix based, Windows NT or IBM OS/2 operating systems.

The invention also provides a computer-readable data storage medium comprising a data storage material encoded with a first set of computer-readable data comprising the AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof, which, when combined with a second set of machine readable data comprising an X-ray diffraction pattern of a molecule or molecular complex of unknown structure, using a machine programmed with the instructions for using said first set of data and said second set of data, can determine at least a portion of the electron density corresponding to the second set of machine readable data.

A further aspect of the invention provides a method of providing data for generating structures and/or performing optimisation of compounds which interact with an AMPK gamma subunit the method comprising:

(i) establishing communication with a remote device containing

(a) AMPK co-ordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof, said data defining the three-dimensional structure of the gamma subunit of AMPK or said selected coordinates thereof;

(b) atomic coordinate data of a target protein generated by homology modelling of the target based on the coordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof; or

(c) atomic coordinate data of a target protein generated by interpreting X-ray crystallographic data or NMR data by reference to the co-ordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof; and

(ii) receiving said computer-readable data from said remote device.

When such data is received it may be utilised in the various methods of the invention described herein, including computer-based methods of the analysis of the interaction of a molecular structure with an AMPK gamma subunit structure. The atomic coordinate data may include coordinates of amino acids set out in Table 3, Table 4 and/or Table 5.

Thus the remote device may comprise e.g. a computer system or computer readable media of one of the previous aspects of the invention. The device may be in a different country or jurisdiction from where the computer-readable data is received.

The communication may be via the internet, intranet, e-mail etc, transmitted through wires or by wireless means such as by terrestrial radio or by satellite. Typically the communication will be electronic in nature, but some or all of the communication pathway may be optical, for example, over optical fibres.

The data received from said remote device may be used to perform the methods of the invention described herein, including but not limited to the computer based methods for the analysis of the interaction of a molecular structure with an AMPK gamma subunit structure.

Uses of the Structures of the Invention.

The crystal structures obtained according to the present invention as well as the structures of target proteins obtained in accordance with the methods described herein), may be used in several ways for drug design.

In particular, the finding that AMPK is activated by binding of AMP into two of the three AMP binding sites of AMPK allows the rational drug design of potential activator compounds specifically directed to one or other of these sites. Similarly, potential inhibitors of AMPK that binds at the "AMP-1" and "AMP-2" but not the AMP-3 sites allows the development of compounds which interact with AMPK in novel ways. Alternatively, the high-affinity AMP-3 provides a further novel target for drug development.

(i) Obtaining and analysing crystal complexes.

In one approach, the structure of a compound bound to a may be determined by experiment. This will provide a starting point in the analysis of the compound bound to , thus providing those of skill in the art with a detailed insight as to how that particular compound interacts with AMPK.

Many of the techniques and approaches to structure-based drug design described above rely at some stage on X-ray analysis to identify the binding position of a ligand in a ligand-protein complex. A common way of doing this is to perform X-ray crystallography on the complex, produce a difference Fourier electron density map, and associate a particular pattern of electron density with the ligand. However, in order to produce the map (as explained e.g. by Blundell et al., in *Protein Crystallography*, Academic Press, New York, London and San

Francisco, (1976)), it is necessary to know beforehand the protein 3D structure (or at least the protein structure factors). Therefore, determination of the structure also allows difference Fourier electron density maps of -compound complexes to be produced, determination of the binding position of the drug and hence may greatly assist the process of rational drug design.

Accordingly, the invention provides a method for determining the structure of a compound bound to an AMPK gamma subunit, said method comprising:

providing a crystal of an AMPK gamma subunit according to the invention;

soaking the crystal with said compounds; and

determining the structure of said compound complex by employing the coordinate data of any one of Table 1 and Table 2 or selected coordinates thereof.

Alternatively, an AMPK gamma subunit and compound may be co-crystallized. Thus the invention provides a method for determining the structure of a compound bound to an AMPK gamma subunit, said method comprising;

mixing the protein with the compound(s), crystallizing the protein-compound(s) complex; and determining the structure of said -compound(s) complex by reference to the coordinate data of Table 1 or Table 2, or selected coordinates thereof.

The analysis of such structures may employ (i) X-ray crystallographic diffraction data from the complex and (ii) a three-dimensional structure of an AMPK gamma subunit, or at least selected coordinates thereof, to generate a difference Fourier electron density map of the complex, the three-dimensional structure being defined by atomic coordinate data of Table 1 or Table 2, or selected coordinates thereof. The difference Fourier electron density map may then be analysed.

Therefore, such complexes can be crystallized and analysed using X-ray diffraction methods, e.g. according to the approach described by Greer et al., *J. of Medicinal Chemistry*, Vol. 37, (1994), 1035-1054, and difference Fourier electron density maps can be calculated based on X-ray diffraction patterns of soaked or co-crystallized and the solved structure of uncomplexed. These maps can then be analysed e.g. to determine whether and where a particular compound binds to an AMPK gamma subunit and/or changes the conformation of an AMPK gamma subunit.

Electron density maps can be calculated using programs such as those from the CCP4 computing package (Collaborative Computational Project 4. The CCP4 Suite: Programs for Protein Crystallography, *Acta Crystallographica*, D50, (1994), 760-763.). For map visualization and model building programs such as "O" (Jones et al., *Acta Crystallographica*, A47, (1991), 110-119) can be used.

In addition, in accordance with this invention, an AMPK gamma subunit variants or isoforms may be crystallized in co-complex with known an AMPK gamma subunit substrates or inhibitors or novel compounds. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of the an AMPK gamma subunit structure of

Table 1 or Table 2, or selected coordinates thereof. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between an AMPK gamma subunit and a chemical entity or compound.

(ii) In silico analysis and design

Although the invention will facilitate the determination of actual crystal structures comprising a and a compound, which interacts with an AMPK gamma subunit, current computational techniques provide a powerful alternative to the need to generate such crystals and generate and analyse diffraction date. Accordingly, a particularly preferred aspect of the invention relates to "i*n silico*" methods directed to the analysis and development of compounds which interact with structures of the present invention.

Determination of the three-dimensional structure of an AMPK gamma subunit provides important information about the binding sites of this protein. This information may then be used for rational design and modification of AMPK ligands including activators or inhibitors, e.g. by computational techniques which identify possible binding ligands for the binding sites, by enabling linked-fragment approaches to drug design, and by enabling the identification and location of bound ligands (e.g. including those ligands mentioned herein above) using X-ray crystallographic analysis. These techniques are discussed in more detail below.

Thus as a result of the determination of the three-dimensional structures provided by the present invention, more purely computational techniques for rational drug design may also be used to design structures whose interaction with AMPK is better understood (for an overview of these techniques see e.g. Walters et al (*Drug Discovery Today*, Vol.3, No.4, (1998), 160-178; Abagyan, R.; Totrov, M. *Curr. Opin. Chem. Biol.* **2001**, *5*, 375-382). For example, automated ligand-receptor docking programs (discussed e.g. by Jones et al. in *Current Opinion in Biotechnology*, Vol.6, (1995), 652-656 and Halperin, I.; Ma, B.; Wolfson, H.; Nussinov, R. *Proteins* **2002**, *47*, 409-443), which require accurate information on the atomic coordinates of target receptors may be used.

The aspects of the invention described herein which utilize the structures of the present invention *in silico* may be equally applied to both the an AMPK gamma subunit structure of Table 1 or Table 2, or selected coordinates thereof, and the models of target proteins obtained by other aspects of the invention. Thus having determined a conformation of an AMPK gamma subunit by the method described above, such a conformation may be used in a computer-based method of rational drug design as described herein. In addition the availability of the structure of an AMPK gamma subunit will allow the generation of highly predictive pharmacophore models for virtual library screening or compound design.

Accordingly, the invention provides a computer-based method for the analysis of the interaction of a molecular structure with an AMPK gamma subunit structure, which comprises:

providing an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof;

providing a molecular structure to be fitted to said AMPK structure or selected coordinates thereof; and

fitting the molecular structure to said AMPK structure.

By "fitting", it is meant determining at least one interaction between an atom of said AMPK structure and said molecular structure.

Interactions may be determined by automatic, semi-automatic or manual means. Computer programs can be employed to estimate interactions including the attraction, repulsion, and steric hindrance of the two binding partners (i.e. the AMPK structure and a molecular structure). Various computer-based methods for fitting are described further herein. Generally the process involves calculating the extent to which such an interaction is present or stable.

In practice, it will be desirable to model a sufficient number of atoms of the as defined by the coordinates of any one of Table 1 and Table 2, or selected coordinates thereof, which represent a binding pocket. Thus preferred numbers and/or locations of selected coordinates as defined above may be used in the present invention.

In order to provide a three-dimensional structure of compounds to be fitted to a structure of the invention, the compound structure may be modelled in three dimensions using commercially available software for this purpose or, if its crystal structure of a compound is available, the coordinates of the structure may be used to provide a representation of the compound for fitting to a structure of the invention.

More specifically, the interaction of a compound or compounds with can be examined through the use of computer modelling using a docking program such as GOLD (Jones et al., *J. Mol. Biol.*, 245, 43-53 (1995), Jones et al., *J. Mol. Biol.,* 267, 727-748 (1997)), GRAMM (Vakser, I.A., *Proteins* , Suppl., 1:226-230 (1997)), DOCK (Kuntz et al, *J.Mol.Biol.* **1982** , *161*, 269-288, Makino et al, *J.Comput.Chem.* **1997**, *18*, 1812-1825), AUTODOCK (Goodsell et al, *Proteins* **1990**, *8*, 195-202, Morris et al, *J.Comput.Chem.* **1998**, *19*, 1639-1662.), FlexX, (Rarey et al, *J.Mol.Biol.* **1996**, *261*, 470-489) or ICM (Abagyan et al, *J.Comput.Chem.* **1994**, *15*, 488-506). This procedure can include computer fitting of compounds to an AMPK gamma subunit structure of the invention to ascertain how well the shape and the chemical structure of the compound will bind to AMPK.

In one aspect, the invention provides a method of identifying a potential ligand of an AMPK gamma subunit protein comprising a nucleotide binding pocket, said method comprising the steps of:

(a) using the atomic coordinates of Table 1 or Table 2 to generate a three-dimensional model;

(b) identifying said binding pocket residues which comprises at least one or more of the residues set out in any one of Tables 3 to 5, and using said residues to generate a specific three-dimensional (3-D) target;

(c) employing said 3-D target of (b) to design or select said potential ligand;

(d) synthesizing said potential ligand; and

(e) contacting said potential ligand with said AMPK gamma subunit protein in vitro to determine the ability of said potential inhibitor to interact with said AMPK gamma subunit protein; whereby the ability to interact is an indication that said potential ligand of said AMPK gamma subunit protein is identified.

The above method may use any of the AMPK subunit proteins described herein, for example an AMPK gamma subunit protein selected from the group consisting of a gamma 1 subunit or fragment thereof comprising both Bateman domains which include the CBS 1+2 pair and the CBS 3+4 pair; a gamma-2 subunit or C-terminal fragment thereof retaining both Bateman domains; and a gamma-3 subunit retaining both Bateman domains. Suitable subunit proteins include those of SEQ ID NO:1 and SEQ ID NO:2.

The invention further provides a method of designing a compound which binds to a nucleotide binding pocket of an AMPK gamma subunit protein, wherein said protein is characterized by:

(i) the atomic coordinates of amino acids 23-326 of SEQ ID No: 1 shown in Table 1, optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å;

(ii) the atomic coordinates of amino acids 23-326 of SEQ ID No: 1 shown in Table 2, optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å; and/or

(iii) the atomic coordinates of a nucleotide binding pocket defined by amino acids of any one of Tables 3, 4 and 5, optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å;

said method comprising the steps of:

(a) using the atomic coordinates of Table 1 or Table 2 to build a 3-D computer model of a compound interaction region of said protein comprising at least one of (i), (ii) and (iii);

(b) assessing the stereochemical complementarity between a compound and said interaction region;

(c) optimizing said stereochemical complementarity in an iterative approach by observing changes in the protein or compound that affect the protein/compound associations; and

(d) designing a compound which optimizes said protein/compound stereochemical complementarity.

Also computer-assisted, manual examination of the active site structure of may be performed. The use of programs such as GRID (Goodford, *J. Med. Chem.*, 28, (1985), 849-857) - a program that determines probable interaction sites between molecules with various functional groups and an enzyme surface - may also be used to analyse the active site to predict, for example, the types of modifications which will alter the rate of metabolism of a compound.

Since AMPK has been found to contain three nucleotide binding pockets a plurality of molecular structures, e.g. two or three, may be provided in the modelling methods of the invention and the interactions between each of said structures and an AMPK gamma subunit structure of the invention may be determined. In addition, the interactions between two or more of such molecular structures may be examined.

It is also envisaged that two or more such structures may be assembled to form a single larger structure. For example, the binding of one or more molecular fragments can be determined in the protein binding pocket by X-ray crystallography. Molecular fragments are typically compounds with a molecular weight between 100 and 200 Da. This can then provide a starting point for medicinal chemistry to optimise the interactions using a structure-based approach. The fragments can be combined onto a template or used as the starting point for 'growing out' an inhibitor into other pockets of the protein (Blundell *et al,* 2002, *Nat Rev Drug Discov.* Jan;1(1):45-54). The fragments can be positioned in the binding pocket of the and then 'grown' to fill the space available, exploring the electrostatic, van der Waals or hydrogen-bonding interactions that are involved in molecular recognition. The potency of the original weakly binding fragment thus can be rapidly improved using iterative structure-based chemical synthesis.

At one or more stages in the fragment growing approach, the compound may be synthesized and tested in a biological system for its activity. This can be used to guide the further growing out of the fragment.

As indicated above, where two fragment-binding regions are identified, a linked fragment approach may be based upon attempting to link the two fragments directly, or growing one or both fragments in the manner described above in order to obtain a larger, linked structure, which may have the desired properties.

Where the binding site of two or more ligands are determined they may be connected to form a potential lead compound that can be further refined using e.g. the iterative technique of *Greer* et al. For a virtual linked-fragment approach see Verlinde et al., *J. of Computer-Aided Molecular Design*, 6, (1992), 131-147, and for NMR and X-ray approaches see Shuker et al., *Science*, 274, (1996), 1531-1534 and Stout et al., *Structure*, 6, (1998), 839-848. The use of these approaches to design inhibitors is made possible by the determination of the structure.

The various computer-based methods of analysis described herein may be performed using computer systems such as those described in the preceding section. Generally, the computer systems used will be configured to display or transmit a model of the structure of Table 1 or 2, or selected coordinates thereof and a molecular structure so as to indicate one or more interactions between the two. A variety of formats of display are known in the art and may be selected by a person of ordinary skill in the art dependent upon a variety of factors including, for example, the nature of the interactions being determined.

By using the present invention, detailed structural information can be obtained about the binding of compounds to AMPK, and in the light of this information adjustments can be made to the structure or functionality of the compound, e.g. to alter its interaction with AMPK. The above steps may be repeated and re-repeated as necessary. For example, Greer *et al.* (*J. of Medicinal Chemistry*, Vol. 37, (1994), 1035-1054) describes an iterative approach to ligand design based on repeated sequences of computer modelling, protein-ligand complex formation and X-ray crystallographic or NMR spectroscopic analysis. Thus novel thymidylate synthase inhibitor series were designed *de novo* by Greer *et al.*, and ligands may also be designed or modified in the this way. More specifically, using e.g. GRID on the solved structure of AMPK, a ligand may be designed that complements the functionalities of the protein's binding sites. Alternatively a ligand may be modified such that it complements the functionalities of protein's binding sites better or less well. The ligand can then be synthesised, formed into a complex with an AMPK gamma subunit, and the complex then analysed by X-ray crystallography to identify the actual position of the bound ligand. The structure and/or functional groups of the ligand can then be adjusted, if necessary, in view of the results of the X-ray analysis, and the synthesis and analysis sequence repeated until an optimised ligand is obtained. Related approaches to structure-based drug design are also discussed in Bohacek *et al.*, Medicinal Research Reviews, Vol.16, (1996), 3-50. Design of a compound with alternative properties using structure based drug design may also take into account the requirements for high affinity to a second, target protein. Gschwend *et al.,* (Bioorganic & Medicinal Chemistry Letters, Vol 9, (1999), 307-312) and Bayley *et al.,* (Proteins: Structure, Function and Genetics, Vol 29, (1997) 29-67) describe approaches where structure based drug design is used to reduce affinity to one protein whilst maintaining affinity for a target protein.

Modification will be those conventional in the art known to the skilled medicinal chemist, and will include, for example, substitutions or removal of groups containing residues which interact with the amino acid side chain groups of a structure of the invention. For example, the replacements may include the addition or removal of groups in order to decrease or increase the charge of a group in a test compound, the replacement of a group to increase or decrease the size of the group in a test compound, the replacement of a charge group with a group of the opposite charge, or the replacement of a hydrophobic group with a hydrophilic group or vice versa. It will be understood that these are only examples of the type of substitutions considered by medicinal chemists in the development of new pharmaceutical compounds and other modifications may be made, depending upon the nature of the starting compound and its activity.

As indicated above, molecular structures, which may be fitted to an AMPK structure of the invention, include compounds under development as potential pharmaceutical agents. The agents may be fitted in order to determine how they bind to AMPK and to provide, for example, a basis for modelling further candidate modulators of AMPK activity, particularly activators.

Molecular structures, which may be used in the present invention, will usually be compounds under development for pharmaceutical use. Generally such compounds will be organic molecules, which are typically from about 100 to 2000 Da, more preferably from about 100 to

1000 Da in molecular weight. Such compounds include nucleotide analogues such as AICAR and ZMP. In principle, any compound under development in the field of pharmacy can be used in the present invention in order to facilitate its development or to allow further rational drug design to improve its properties.

Where a potential modified compound has been developed by fitting a starting compound to the structure of the invention and predicting from this a modified compound with an altered activity, the invention further includes the step of synthesizing the modified compound and testing it in a in vivo or in vitro biological system in order to determine its activity.

The above-described processes of the invention may be iterated in that the modified compound may itself be the basis for further compound design.

Assay Methods

In one aspect of the invention, there is provided an assay method for a modulator of AMPK, which method comprises:

providing a candidate AMPK modulator compound;

bringing said compound into contact with a mammalian AMPK gamma subunit or fragment thereof having two Bateman domains; and

determining the binding of said candidate compound for said gamma subunit or fragment thereof in competition with an adenosine nucleotide;

wherein said adenosine nucleotide is labelled with a fluorescent label.

Although the exact assay format may be varied according to the preferences of any individual practitioner of ordinary skill in the art, the method can conveniently be performed in a multi-well format, allowing different candidate modulators and/or different concentrations of such candidate modulators to be assayed simultaneously. Such a format will also permit automation of the method using standard robotic technology.

The candidate modulator compound may be any compound available to those of skill in the art. For example, commercially available combinatorial chemical libraries may be used. Candidate compounds which are nucleotide analogues may be used.

In performing the assay of the invention, the mammalian AMPK gamma subunit or fragment thereof having two Bateman domains may be used alone or in combination with either or both of an AMPK gamma alpha subunit or C-terminal fragment thereof, and/or an AMPK beta subunit or C-terminal fragment thereof. Any mammalian alpha, beta and gamma subunit may be used, given the high degree of conservation between these subunits. This is evidenced by the present examples in which a rat gamma subunit is co-expressed and forms an active AMPK with a human beta subunit and rat alpha subunit. In view of this, it is believed that other mammalian subunits may be used interchangeably in the present invention without loss of assay function.

The mammalian AMPK gamma subunit or fragment thereof is preferably a gamma-1 subunit, though the use of a gamma-2 or gamma-3 subunit is also contemplated.

Any method for measuring the binding of the candidate compound in competition an adenosine nucleotide, particularly AMP or ATP, may be used. ADP may also be used. Generally, this will involve labelling one or other, or both, of the candidate compound or the adenosine nucleotide with a detectable label, such that the amount of label that can be detected either bound to or free of the AMPK gamma subunit is altered when or if the candidate compound binds to the subunit in place of ATP/AMP, or vice versa.

In one currently preferred aspect the fluorescent label is N-methylanthraniloyl ("mant").

The concentrations of the protein, candidate compound and adenosine nucleotide may be varied according to the particular format of the assay. Suitably, 300 µl of from 1 to 100 µm mant-AXP (where "AXP" may be AMP, ADP or ATP), e.g. 10 µM mant-AXP, titrated up to 5-200 µM AMPK, e.g. about 15 µm AMPK, in the presence of a fixed concentration of the candidate compound which might be in the range of 10nM up to 1mM.

Compounds of the invention

Where a potential compound has been developed by the computer based methods or assay methods described above, the invention provides such a compound, which may be manufactured and/or used in the preparation, i.e. manufacture or formulation, of a composition such as a medicament, pharmaceutical composition or drug. These formulations or compositions may be administered to individuals, e.g. to an individual with a metabolic syndrome. Such a condition includes a disease selected from the group of diabetes, obesity, insulin-resistance, hypertension, cardiovascular disease, and dyslipidaemia.

Thus, the present invention extends in various aspects not only to a compound as provided by the invention, but also a pharmaceutical composition, medicament, drug or other composition comprising such a compound. The compositions may be used. for treatment (which may include preventative treatment) of disease such as those mentioned above. Such a treatment may comprise administration of such a composition to a patient, e.g. for treatment of disease; the use of such an inhibitor in the manufacture of a composition for administration, e.g. for treatment of disease; and a method of making a pharmaceutical composition comprising admixing such an inhibitor with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

Thus a further aspect of the present invention provides a method for preparing a medicament, pharmaceutical composition or drug, the method comprising:
(a) identifying or modifying a compound by a method of any one of the other aspects of the invention disclosed herein; (b) optimising the structure of the molecule; and (c) preparing a medicament, pharmaceutical composition or drug containing the optimised compound.

The above-described processes of the invention may be iterated in that the modified compound may itself be the basis for further compound design.

By "optimising the structure" we mean e.g. adding molecular scaffolding, adding or varying functional groups, or connecting the molecule with other molecules (e.g. using a fragment linking approach) such that the chemical structure of the modulator molecule is changed while its original modulating functionality is maintained or enhanced. Such optimisation is regularly undertaken during drug development programmes to e.g. enhance potency, promote pharmacological acceptability, increase chemical stability etc. of lead compounds.

Modification will be those conventional in the art known to the skilled medicinal chemist, and will include, for example, substitutions or removal of groups containing residues which interact with the amino acid side chain groups of a structure of the invention. For example, the replacements may include the addition or removal of groups in order to decrease or increase the charge of a group in a test compound, the replacement of a charge group with a group of the opposite charge, or the replacement of a hydrophobic group with a hydrophilic group or vice versa. It will be understood that these are only examples of the type of substitutions considered by medicinal chemists in the development of new pharmaceutical compounds and other modifications may be made, depending upon the nature of the starting compound and its activity.

Compositions may be formulated for any suitable route and means of administration. Pharmaceutically acceptable carriers or diluents include those used in formulations suitable for oral, rectal, nasal, topical (including buccal and sublingual), vaginal or parenteral (including subcutaneous, intramuscular, intravenous, intradermal, intrathecal and epidural) administration. The formulations may conveniently be presented in unit dosage form and may be prepared by any of the methods well known in the art of pharmacy.

For solid compositions, conventional non-toxic solid carriers include, for example, pharmaceutical grades of mannitol, lactose, cellulose, cellulose derivatives, starch, magnesium stearate, sodium saccharin, talcum, glucose, sucrose, magnesium carbonate, and the like may be used. Liquid pharmaceutically administrable compositions can, for example, be prepared by dissolving, dispersing, etc, an active compound as defined above and optional pharmaceutical adjuvants in a carrier, such as, for example, water, saline aqueous dextrose, glycerol, ethanol, and the like, to thereby form a solution or suspension. If desired, the pharmaceutical composition to be administered may also contain minor amounts of non-toxic auxiliary substances such as wetting or emulsifying agents, pH buffering agents and the like, for example, sodium acetate, sorbitan monolaurate, triethanolamine sodium acetate, sorbitan monolaurate, triethanolamine oleate, etc. Actual methods of preparing such dosage forms are known, or will be apparent, to those skilled in this art; for example, see Remington's Pharmaceutical Sciences, Mack Publishing Company, Easton, Pennsylvania, 15th Edition, 1975.

Examples

The invention is illustrated by the following examples. In summary, the examples show that truncated AMPK was cloned into a tricistronic vector and expressed in *E.coli*. Proteins were initially purified by Nickel affinity chromatography. Crystals were grown by vapour diffusion in hanging drops using iospropanol as precipitant and were cryo-protected with 28% ethylene glycol. Crystals were soaked in ATP or MgATP made up in reservoir solution. Diffraction data were collected at 100K and processed using Denzo and Scalepack. The structures were solved by molecular replacement and refined using Refmac5 with manual model building using O. Bound nucleotide analysis was carried out by denaturation of samples, removal of protein and analysis by hplc. *N*-methylanthraniloyl (mant) nucleotides were prepared according to published methods. Uncorrected fluorescence emission spectra of the mant nucleotides and their complexes with AMPK were recorded at 20° C using a SPEX FluoroMax fluorimeter. Binding of mant-AXPs was monitored by titrating 10μM of the nucleotides with AMPK. Dissociation constants for AMP and ATP were determined using competition assays.

Expression and crystallization of AMPK

Using a tri-cistronic expression system we were able to express and purify full-length mammalian AMPK. Truncated AMPK, $\gamma1_{(rat)}\beta2_{(human)}$(187-272)His-$\alpha1_{(rat)}$(396-548), was cloned into a tricistronic vector and subsequently expressed in *E.coli* BL21 (BL21-CodonPlus-RIL, stratagene)[31]. Proteins were purified using a Nickel affinity chromatography (His-Trap, GE Healthcare), anion exchange (Mono Q, GE Healthcare), and gel filtration (Superdex 200, GE Healthcare).

As a result of cloning the sequence of the alpha subunit fragment into the vector, residues 545-548 (ILAQ) of the alpha chain were replaced by NSCT and two additional residues, V549 and N550, were incorporated.

We measured diffraction data extending to 2.1 Å Bragg spacing from crystals obtained from the trimeric complex of the C-terminal domains of the α fragment and β (187-272) with full-length γ.

Protein complex stock solution was prepared at 15 mg/ml in 50 mM Tris, pH 7.0, 100 mM NaCl and 1 mM TCEP, and then mixed with a three-fold molar excess of AMP. Crystals were grown by vapour diffusion technique at 18°C in hanging drops. Drops were prepared by mixing equal volumes of protein complex with reservoir solution containing 15% isopropanol. Crystals were first transferred into mother liquor with an additional 25% ethylene glycol, prior to plunging into liquid nitrogen. For crystal soaking experiments 1mM ATP/0.1mM EDTA and 0.5mM ATP/0.6 mM $MgCl_2$ were made up in reservoir buffer, crystals were soaked for 1-5 hours prior to flash cooling. Diffraction data were collected on an in-house MicroMax 007HF rotating anode coupled to a RaxisIV^{++} detector. Data were integrated using Denzo and scaled with Scalepack[32]. The structure was solved by molecular replacement using Amore[33] using 2OOX.pdb as the search model, because of the differences in domain orientation between the yeast and mammalian enzyme the calculations were first performed with the gamma domain, which was then fixed, and the search repeated with the combined alpha and beta domains.

Standard refinement was carried out with Refmac5[34] and CNS[35] together with manual model building with O[36]. Figures were created with Pymol (http://pymol.sourceforge.net/) and Grasp. The structure was solved by molecular replacement and relevant crystallographic statistics are given in Table 7.

Table 7:

	$AMPK/AMP_3$ complex	$AMPK/(ATP.Mg)_2AMP$ complex	$AMPK/ATP_2AMP$ complex
Data collection			
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Cell dimensions			
a, *b*, *c* (Å)	48.5, 119.4, 129.2	48.8, 120.8, 126.8	49.0, 121.4, 127.1
α, β, γ (°)	90, 90, 90		
Resolution (Å)	20–2.1 (2.18–2.1)*	25-2.6 (2.7-2.6)	20–2.3 (2.4–2.3)
R_{sym} or R_{merge}	5.9 (41.6)	9.9 (48.0)	9.8 (44.3)
$I/\sigma I$	18.7 (2.2)	12.0 (1.7)	16.5 (1.9)
Completeness (%)	99.0 (98.4)	95.8 (87.9)	99.1 (95.2)
Redundancy	5.6 (5.1)	6.0 (2.1)	7.3 (2.5)
Refinement			
Resolution (Å)	20-2.1	25-2.6	20-2.3
No. reflections	42054	21913	31118
R_{work}/ R_{free}	21.4/24.6	24.8/27.1	23.4/28.4
No. atoms			
Protein	3884	3884	3884
Ligand/ion	69	87	85
Water	442	-	176
B-factors			
Protein	44.6	56.9	53.1
Ligand/ion	35.0	37.6	45.7
Water	62.1	-	59.2
R.m.s deviations			
Bond lengths (Å)	0.009	0.010	0.010
Bond angles (°)	1.44	1.52	1.47

One crystal was used for each of the two datasets.
*Highest resolution shell is shown in parenthesis.

Further refinement

The $AMPK/AMP_3$ structure of Table 1a and $AMPK/(ATP.Mg)_2AMP$ structure of Table 2a were subject to further refinement to produce the structures of Tables 1b and 2b respectively.

The structures of Table 1a and Table 2a were determined as for a complex including the native sequence of the rat alpha subunit fragment 396-548.

The structures of Table 1b and Table 2b were determined as for a complex including the rat alpha subunit fragment 396-548 in which wild type residues 545 to 548 were replaced by NSCT and with an additional two C terminal residues VN as residues 549 and 550. As noted above, the fragment used for crystallisation consisted of residues 396 to 544 of the rat α1 subunit, fused at the C terminus to NSCTVN.
The co-ordinates in Table 1b and Table 2b also reflect the rebuilding of some loop residues as a further refinement of the structure of Table 1a and Table 2a respectively.

Binding Studies

To understand better the regulation of AMPK by changes in AMP/ATP ratio we carried out a series of binding studies.

N-methylanthraniloyl (mant) nucleotides were synthesised, purified and characterised as described elsewhere[37]. Uncorrected fluorescence emission spectra of the mant nucleotides and their complexes with AMPK were recorded at 20° C in 25mM Tris, 1mM TCEP (pH 7.5) using a SPEX FluoroMax fluorimeter with lambda ex =366 or 380 nm (bandwidth 1.7 nm) and emission scanned from 400 to 550 nm (bandwidth 5 nm). Binding of mant-AXPs was monitored by titrating 10μM of the nucleotides with AMPK. Dissociation constants for AMP and ATP were determined using two different types of competition assay.

The uncomplexed mant-nucleotides have an emission maximum at 446 nm. In the presence of saturating AMPK the emission maximum is blue-shifted and the fluorescence intensity is increased. The emission maxima and intensity ratios (Complexed/Free) for total integrated fluorescence (400-550 nm) are: 429 nm and 5.25 for mant-AMP; 436 nm and 5.35 for mant-ADP; 437 nm and 5.55 for mant-ATP. These fluorescence changes were used to determine apparent dissociation constants by titrating ~ 10 μM mant-nuceotides with AMPK in 25 mM Tris (pH 8) at 20°C. Titrations of mant-ATP with the full-length protein and with the crystallization fragment clearly indicated that the two proteins bind mant-ATP with similar affinity and show that binding cannot be described using a simple 1:1 binding model (the dashed line is the best fit attainable with such a model). The K_ds were therefore determined using standard methods with the assumptions that there are two identical, non-interacting sites for nucleotide binding and that the binding at each site generates the same change in the fluorescence spectrum of the mant-nucleotide. The observation that the intensity ratios are closely similar for all three nucleotides is consistent with the view that the same number of nucleotides is bound in all cases. Binding data for mant-AMP were therefore analysed with the same two-site model.

Dissociation constants were determined to be 4 ± 0.5 μM for mant-ATP and 10 ± 2 μM for mant-AMP. Increasing the salt concentration to 100 mM increased the K_d by a factor of ~ 4 for both nucleotides, to 14 ± 3 μM for mant-ATP and to 38 ± 7 μM for mant-AMP. Increasing the magnesium concentration to 125 μM slightly increased the K_d for mant-ATP (to 5.5 ± 0.8 μM) but had no effect on the affinity for mant-AMP. Much higher concentrations of magnesium led to significant decreases in the affinity for mant-ATP but had relatively little effect on the affinity for mant-AMP. Since the effect of, for example, 1.25 mM $MgCl_2$ is significantly greater than the

effect of 100 mM NaCl the magnesium effect is not related to ionic strength changes. In the low salt buffer used in these measurements the K_d for mant-ATP binding to Mg^{2+} was determined using ITC to be 5.3 ± 1 μM (cf. 15 ± 2 μM for ATP itself) in 25 mM Tris (pH 8) at 20°C. Therefore, the mant-ATP is largely Mg^{2+} saturated at 125 μM Mg^{2+} and the observed effects cannot be attributed to changes in the saturation of the nucleotide by Mg^{2+}. We do not know whether this phenomenon is a result of a weak-binding site for the metal on the enzyme, or on the nucleotide itself, but we conclude that the effect is not physiologically relevant to AMPK regulation.

Dissociation constants for unlabelled nucleotides were determined by using the mant-nucleotides as reporters for the binding of unlabelled nucleotides. Competition assays were performed in which the mant-nucleotide plus unlabelled nucleotide (with and without magnesium) was titrated with AMPK. These data were then analyzed with the previously determined K_d for the mant-nucleotide held constant in the analysis using methods described elsewhere (Ref 41).

From the titration studies described in the next paragraph we observed two AMP binding sites on AMPK, apparently in contradiction to the three molecules seen in our crystal structure. We therefore analysed our purified, over-expressed protein by high-pressure-liquid-chromatography for bound nucleotides and discovered that for both the crystallisation fragment, and full-length protein, there was approximately one adenyl molecule present for every molecule of AMPK. Most of the adenyl species (85%) was present as AMP with a small amount of ADP (15%). As yet we have not managed to displace this co-purifying adenyl moiety and are therefore unable to determine its binding affinity. However, the fact that it persists through the various stages of protein purification, including gel filtration, suggests that the binding is very tight.

We synthesised *N*-methylanthraniloyl (mant) labelled analogues of AMP and ATP to use as probes for determining the affinity of the unlabelled nucleotides. AMPK binds two mant-nucleotides with dissociation constants of 4 ± 0.5 μM (mant-ATP) and 10 ± 2 μM (mant-AMP). Dissociation constants for the unlabelled nucleotides were determined using competition assays in which a mant-nucleotide plus unlabelled nucleotide (either AMP or ATP) was titrated with AMPK. The values determined were 12.5 ± 4 μM for ATP and 24.5 ± 4.5 μM for AMP. We also obtained very similar results from titrations carried out with full-length AMPK. Given the recent description of the structure of the AMPK homologue from *S. pombe* in complex with Mg^{2+}-free ATP we investigated the effect of the metal ion on nucleotide binding with mammalian AMPK. Initial experiments indicated that Mg^{2+} reduced the apparent affinity of AMPK for ATP, however, this effect is only observed at very high concentrations of the metal ion that are not physiologically relevant. Titrations of ATP carried out in the presence of 125 μM Mg^{2+} (which will saturate most of the ATP) are the same as those done in the absence of the metal ion. Therefore, at least for mammalian AMPK, the enzyme binds ATP or Mg.ATP with the same affinity. This means that under physiological conditions (where nearly all ATP is complexed with Mg^{2+} and there is about 0.4mM free Mg^{2+}[20]) the majority of the enzyme will be in complex with two Mg.ATP moieties. Mammalian AMPK is therefore different to proteins, like

kinases and small GTPases, whose affinity for the nucleotide is strongly dependent on Mg^{2+} binding but it is also different to its homolgue from *S. pombe* where it is inferred that ATP-bound metal counter ions must be stripped before binding to AMPK. Our results are consistent with earlier studies of adenyl binding to AMPK γ domain[21], which concluded that the affinity of the protein for ATP was independent of Mg^{2+}.

Taken together, our studies indicate that under physiological conditions the majority of AMPK will contain Mg.ATP and only a small proportion of the enzyme will have AMP bound at the two regulatory binding sites.

Modelling AMPK activity

AMPK has substantial basal activity once phosphorylated that can be modestly enhanced by the allosteric effect of AMP binding. However, AMP binding also significantly decreases the rate of dephosphorylation of activated AMPK. Any molecular model of AMPK action must account for both of these phenomena. We think the lack of any significant conformational change in the γ subunit between the AMP and ATP bound forms implies that the activation signal, initiated by AMP binding, is not propagated via the limited rearrangements of some basic side-chains at the binding site. Instead, we hypothesise that AMP binding triggers the formation of inter-subunit interactions that are not possible when ATP is bound. Such changes in the quaternary structure of the heterotrimer then influence the activity of the kinase domain and its susceptibility to dephosphorylation. Given the structure and charge associated with the ATP binding sites, a plausible binding partner for AMP would be a phosphorylated residue from either the α and/or β subunits (at least eight such phosphorylation sites have been identified). The fact that our structure shows there are two exchangeable AMP/ATP sites, on opposite faces of the γ subunit, suggests the possibility that two distinct inter-subunit interactions with γ occur, perhaps providing for separate mechanisms for the allosteric activation and dephosphorylation protection activities of AMP.

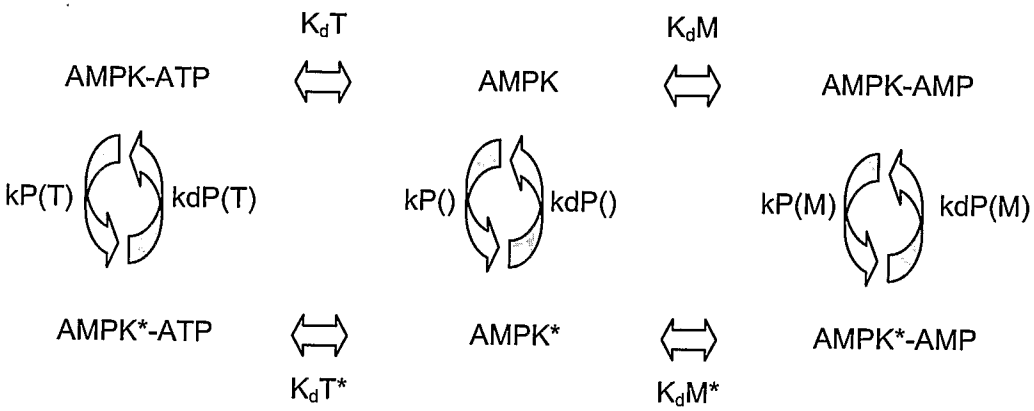
To describe how changes in the cellular ATP/AMP ratio affect AMPK activity we set up a simple model to simulate the enzyme's activity using the binding constants determined here together with data from the literature concerning AMPK activation and adenyl concentrations. Key assumptions of the model are that AMP binding to the enzyme causes allosteric activation as well as inhibiting de-phosphorylation of the enzyme's T-loop and that the non-phosphorylated form has negligible activity. The model shows that 2-3 fold increases in the low micromolar concentrations of AMP bring about a similar fold enhancement in the proportion of AMP-bound enzyme in the presence of a much higher, and essentially unchanging, concentration of Mg.ATP. Importantly, this change in AMP-bound AMPK accounts for the 2-3 fold enhancement of muscle AMPK activity observed following moderate exercise[22, 23]. A key prediction of this model is that only a small proportion of AMPK is active at any one time. This notion, of a large pool of essentially inactive AMPK, is supported by studies using prolonged exercise[24] or non-physiologic methods to activate AMPK, e.g. respiratory uncouplers, that generate a large increase in AMP and lead to increases in enzyme activity at least 5-10 fold greater than that stimulated by moderate exercise[25].

The model is set forth as follows:

1. Under physiological conditions the majority of AMPK will contain Mg.ATP at the two regulatory sites and only a very small proportion (<1%) will have AMP bound at these sites because the nucleotides bind with similar affinity and Mg.ATP is in large excess over AMP.

2. How then do changes in the cellular ATP/AMP ratio affect AMPK activity?

3. To address this issue we set up the following highly simplified model. In this model the asterisk indicates that the enzyme is phosphorylated, the K_d (and K_d*) values are for binding of AMP and ATP to the non-phosphorylated (and phosphorylated) states, and the kP (and kdP) values are rates of phosphorylation (and de-phosphorylation) for the ATP-bound, AMP-bound, and apo (nucleotide free) forms of the enzyme.



4. Two key features of the model are that all the non-phosphorylated forms have negligible activity and that AMP binding to the enzyme causes allosteric activation, with AMPK*-AMP being 2-5 times more active than AMPK*-ATP, depending on the isoform composition of the complex (Ref 42).

5. The experimental finding is that a doubling of the low micromolar AMP concentration in the presence of say 5 mM Mg.ATP produces a 2-3 fold enhancement of muscle AMPK activity following exercise (Ref 43). If phosphorylation does not affect the affinity of AMPK for the nucleotides (see below) then doubling the amount of AMP will effectively double the concentration of enzyme with AMP bound (Note: This will still only result in a small proportion of the total enzyme being in the AMP-bound form).

6. At low [AMP] the 'activity' will be:

$$A_{AMPK^*\text{-}ATP}[AMPK^*\text{-}ATP] + A_{AMPK^*\text{-}AMP}[AMPK^*\text{-}AMP]$$

where $A_{AMPK^*\text{-}ATP}$ and $A_{AMPK^*\text{-}AMP}$ are the activities of the ATP and AMP bound forms.

If we assume that doubling the AMP concentration doubles the concentration of AMPK*-AMP but leaves the concentration of AMPK*-ATP unchanged then the 'activity' at high AMP will be:

$A_{AMPK^*\text{-}ATP}[AMPK^*\text{-}ATP] + 2 \times A_{AMPK^*\text{-}AMP}[AMPK^*\text{-}AMP]$

The activity ratio (activity at high [AMP] divided by activity at low [AMP] will then be:

$$\frac{A_{AMPK^*\text{-}ATP}[AMPK^*\text{-}ATP] + 2 \times A_{AMPK^*\text{-}AMP}[AMPK^*\text{-}AMP]}{A_{AMPK^*\text{-}ATP}[AMPK^*\text{-}ATP] + A_{AMPK^*\text{-}AMP}[AMPK^*\text{-}AMP]}$$

Let $A_{AMPK^*\text{-}ATP} = 0.33 \times A_{AMPK^*\text{-}AMP}$, divide top and bottom by [AMPK*-ATP] and let β = [AMPK*-AMP]/[AMPK*-ATP] gives the activity ratio as:

$$\frac{0.33 \times A_{AMPK^*\text{-}AMP} + 2\beta \times A_{AMPK^*\text{-}AMP}}{0.33 * A_{AMPK^*\text{-}AMP} + \beta \times A_{AMPK^*\text{-}AMP}}$$

7. This relationship clearly shows that a doubling in activity can only be observed if β (i.e., [AMPK*-AMP] divided by [AMPK*-ATP]) is close to or greater than one. However, if nucleotide binding is not affected by phosphorylation then R would be < 0.002 (see (1)) under physiological conditions.

8. Because most of the AMPK will have Mg.ATP bound at the regulatory sites (see (1)) the ratio β can only approach 1 if the concentration of AMPK*-ATP is very much smaller than the concentration of AMPK-ATP. If it is not then [AMPK*-ATP] would always remain much greater than [AMPK*-AMP] (assuming that the rates of phosphorylation and de-phosphorylation are unaffected by nucleotide content – see below). Thus, a key prediction of this model is that only a very small proportion of the total AMPK is active at any one time.

9. The third key assumption of this model is then that the binding of AMP inhibits de-phosphorylation of the enzyme's T-loop (i.e. kdP(M) is much smaller than kdP(T) or kdP()). With this assumption, a large fraction of the enzyme with AMP bound could be in the phosphorylated (active) state whereas almost all of the enzyme with Mg.ATP bound would be in the non-phosphorylated (inactive) state, and the concentrations of AMPK*-ATP and AMPK*-AMP would be similar (β close to 1).

10. Another factor that could contribute to maintaining β close to 1 would be if phosphorylation reduced the affinity of the enzyme for ATP (i.e. $K_d(T^*) > K_d(T)$).

11. Although many much more complex models are possible (we have not included cooperativity in nucleotide binding, or the possibility that mixed nucleotide species might have different activity etc.) this model provides a working explanation as to the activation of AMPK and is consistent with the presence of the three nucleotide biding sites described herein.

All publications and patents mentioned in the above specification are herein incorporated by reference. Various modifications and variations of the described invention will be apparent to those of skill in the art without departing from the scope and spirit of the invention. Although the invention has been described in connection with specific preferred embodiments, it should be understood that the invention as claimed should not be unduly limited to such specific embodiments.

Sequences:

SEQ ID NO:1 - Rat AMPK Gamma Subunit (Genbank X95578)

MESVAAESAP APENEHSQET PESNSSVYTT FMKSHRCYDL IPTSSKLVVF DTSLQVKKAF
FALVTNGVRA APLWDSKKQS FVGMLTITDF INILHRYYKS ALVQIYELEE HKIETWREVY
LQDSFKPLVC ISPNASLFDA VSSLIRNKIH RLPVIDPESG NTLYILTHKR ILKFLKLFIT
EFPKPEFMSK SLEELQIGTY ANIAMVRTTT PVYVALGIFV QHRVSALPVV DEKGRVVDIY
SKFDVINLAA EKTYNNLDVS VTKALQHRSH YFEGVLKCYL HETLEAIINR LVEAEVHRLV
VVDEHDVVKG IVSLSDILQA LVLTGGEKKP

SEQ ID NO:2 - Human AMPK Gamma Subunit (Genbank NP_002724)

METVISSDSS PAVENEHPQE TPESNNSVYT SFMKSHRCYD LIPTSSKLVV FDTSLQVKKA
FFALVTNGVR AAPLWDSKKQ SFVGMLTITD FINILHRYYK SALVQIYELE EHKIETWREV
YLQDSFKPLV CISPNASLFD AVSSLIRNKI HRLPVIDPES GNTLYILTHK RILKFLKLFI
TEFPKPEFMS KSLEELQIGT YANIAMVRTT TPVYVALGIF VQHRVSALPV VDEKGRVVDI
YSKFDVINLA AEKTYNNLDV SVTKALQHRS HYFEGVLKCY LHETLETIIN RLVEAEVHRL
VVVDENDVVK GIVSLSDILQ ALVLTGGEKK P

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Claims:

1. A computer-based method for the analysis of the interaction of a molecular structure with an AMPK gamma subunit structure, which comprises:

providing an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof;

providing a molecular structure to be fitted to said AMPK structure or selected coordinates thereof; and

fitting the molecular structure to said AMPK structure.

2. The method of claim 1 wherein said selected coordinates include atoms from one or more of the residues of Tables 3, 4 or 5.

3 The method of claim 1 or 2 wherein the selected coordinates are of at least 5, 10, 50, 100, 500 or 1000 atoms.

4. The method of any one of the claims 1 to 3 which further comprises the steps of:

(a) obtaining or synthesising a compound which has said molecular structure; and

(b) contacting said compound with an AMPK gamma subunit protein to determine the ability of said compound to interact with said protein.

5. The method of any one of claims 1 to 3 which further comprises the steps of:

(a) obtaining or synthesising a compound which has said molecular structure;

(b) forming a complex of an AMPK gamma subunit protein and said compound; and

(c) analysing said complex by X-ray crystallography.

6. The method of any one of claims 1 to 3 which further comprises the steps of:

(a) obtaining or synthesising a compound which has said molecular structure; and

(b) determining or predicting how said compound is bound to an AMPK gamma subunit; and

(c) modifying the compound structure so as to alter the interaction between it and an AMPK gamma subunit.

7. The method of claim 6 wherein the compound is modified to alter its interaction with one or more atoms of the residues of any one of Tables 3, 4 or 5.

8. The method of any one of claims 1 to 7 wherein a plurality of molecular structures are fitted to said AMPK gamma subunit structure are assembled into a single molecule to form a candidate modulator molecule.

9. A method of identifying a potential ligand of an AMPK gamma subunit protein comprising a nucleotide binding pocket, said method comprising the steps of:

(a) using the atomic coordinates of Table 1 or Table 2 to generate a three-dimensional model;

(b) identifying said binding pocket residues which comprises at least one or more of the residues set out in any one of Tables 3 to 5, and using said residues to generate a specific three-dimensional (3-D) target;

(c) employing said 3-D target of (b) to design or select said potential ligand;

(d) synthesizing said potential ligand; and

(e) contacting said potential ligand with said AMPK gamma subunit protein in vitro to determine the ability of said potential inhibitor to interact with said AMPK gamma subunit protein; whereby the ability to interact is an indication that said potential ligand of said AMPK gamma subunit protein is identified.

10. The method of claim 9 wherein said AMPK gamma subunit protein is selected from the group consisting of a gamma 1 subunit or fragment thereof comprising both Bateman domains which include the CBS 1+2 pair and the CBS 3+4 pair; a gamma-2 subunit or C-terminal fragment thereof retaining both Bateman domains; and a gamma-3 subunit retaining both Bateman domains.

11. The method of claim 9 wherein said AMPK gamma subunit protein is selected from the group of SEQ ID NO:1 and SEQ ID NO:2.

12. A method of designing a compound which binds to a nucleotide binding pocket of an AMPK gamma subunit protein, wherein said protein is characterized by:

(i) the atomic coordinates of amino acids 23-326 of SEQ ID No: 1 shown in Table 1, optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å;

(ii) the atomic coordinates of amino acids 23-326 of SEQ ID No: 1 shown in Table 2, optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å; and/or

(iii) the atomic coordinates of a nucleotide binding pocket defined by amino acids of any one of Tables 3, 4 and 5, optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å;

said method comprising the steps of:

(a) using the atomic coordinates of Table 1 or Table 2 to build a 3-D computer model of a compound interaction region of said protein comprising at least one of (i), (ii) and (iii);

(b) assessing the stereochemical complementarity between a compound and said interaction region;

(c) optimizing said stereochemical complementarity in an iterative approach by observing changes in the protein or compound that affect the protein/compound associations; and

(d) designing a compound which optimizes said protein/compound stereochemical complementarity.

13. A method of obtaining a structure of an AMPK gamma subunit protein, the method comprises the steps of:

providing a crystal of said protein;

obtaining an X-ray diffraction pattern of said crystal,

calculating a three-dimensional atomic coordinate structure of said protein, by modelling its structure on the AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof.

14. The method of claim 9 wherein said target protein is a mammalian AMPK gamma-2 or a mammalian AMPK gamma-3 protein.

15. A method for determining the structure of a compound bound to an AMPK gamma subunit protein, said method comprising:

(a) providing a crystal of said protein;

(b) soaking the crystal with the compound to form a complex; and

(c) determining the structure of the complex by employing the data of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof.

16. A method for determining the structure of a compound bound to an AMPK gamma subunit protein, said method comprising:

(a) mixing protein with the compound;

(b) crystallizing a protein-compound complex; and

(c) determining the structure of the complex by employing the data of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof.

17. A method of obtaining a representation of the three dimensional structure of a crystal of the AMPK gamma subunit, which method comprises providing the data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof, and constructing a three-dimensional structure representing said coordinates.

18. A computer system, intended to generate structures and/or perform optimisation of compounds which interact with an AMPK gamma subunit, the system containing computer-readable data comprising one or more of:

(a) AMPK co-ordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof, said data defining the three-dimensional structure of the gamma subunit of AMPK or said selected coordinates thereof;

(b) atomic coordinate data of a target protein generated by homology modelling of the target based on the coordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof; or

(c) atomic coordinate data of a target protein generated by interpreting X-ray crystallographic data or NMR data by reference to the co-ordinate data of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof.

19. A computer system according to claim 18, wherein said atomic coordinate data is for at least one of the atoms of any one of Tables 3, 4 or 5.

20. A computer system according to any one of claims 18 or 19 comprising:

a computer-readable data storage medium comprising data storage material encoded with said computer-readable data;

a working memory for storing instructions for processing said computer-readable data; and

a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-readable data and thereby generating structures and/or performing rational drug design.

21. A computer system according to claim 20 further comprising a display coupled to said central-processing unit for displaying said structures.

22. A method of providing data for generating structures and/or performing optimisation of compounds which interact with an AMPK gamma subunit the method comprising:

(i) establishing communication with a remote device containing

(a) AMPK co-ordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof, said data defining the three-dimensional structure of the gamma subunit of AMPK or said selected coordinates thereof;

(b) atomic coordinate data of a target protein generated by homology modelling of the target based on the coordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof; or

(c) atomic coordinate data of a target protein generated by interpreting X-ray crystallographic data or NMR data by reference to the co-ordinate data of an AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof; and

(ii) receiving said computer-readable data from said remote device.

23. The method of claim 22 which further comprises use of the computer readable data to perform the method of any one of claims 1 to 17.

24 A computer-readable storage medium, comprising a data storage material encoded with computer readable data, wherein the data are defined by all or a portion of the structure coordinates of the AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof.

25. Use of a computer-readable storage medium, comprising a data storage material encoded with computer readable data, wherein the data are defined by the structure coordinates of the AMPK gamma subunit structure of Table 1 or Table 2 optionally varied by a root mean square deviation of residue C-α atoms of less than 1.5 Å, or selected coordinates thereof in a method of performing a computer-based method of any one of claims 1 to 17.

26 A co-crystal of AMPK gamma subunit protein and a ligand, wherein said crystal further comprises a C-terminal portion of an AMPK alpha subunit protein and a C-terminal portion of an AMPK beta subunit protein.

27. The crystal of claim 26 with cell dimensions a=49, b=120, c=128 Å, 90°, 90°, 90°.with a unit cell variability of 5% in all dimensions.

28. An assay method for a modulator of AMPK activity, which method comprises:
providing a candidate AMPK modulator compound;
bringing said compound into contact with a mammalian AMPK gamma subunit or fragment thereof having two Bateman domains; and
determining the binding of said candidate compound for said gamma subunit or fragment thereof in competition with an adenosine nucleotide;
wherein said adenosine nucleotide is labelled with a fluorescent label.

29. The method of claim 28 wherein the fluorescent label is N-methylanthraniloyl.

30. The method of claim 28 wherein said adenosine nucleotide is mant-AMP or mant-ATP.

Figure 1 - Table 1a

ATOM	1	N	SER A 393	24.265	73.867	34.077	1.00	56.26	N
ATOM	2	CA	SER A 393	23.145	73.807	33.092	1.00	56.00	C
ATOM	3	CB	SER A 393	22.698	72.366	32.891	1.00	55.69	C
ATOM	4	OG	SER A 393	22.093	71.882	34.069	1.00	56.49	O
ATOM	5	C	SER A 393	21.982	74.676	33.572	1.00	55.67	C
ATOM	6	O	SER A 393	20.877	74.177	33.834	1.00	56.10	O
ATOM	7	N	MET A 394	22.253	75.975	33.702	1.00	54.85	N
ATOM	8	CA	MET A 394	21.287	76.933	34.233	1.00	53.58	C
ATOM	9	CB	MET A 394	21.959	77.896	35.219	1.00	54.24	C
ATOM	10	CG	MET A 394	21.591	77.647	36.673	1.00	56.90	C
ATOM	11	SD	MET A 394	20.403	78.845	37.354	1.00	62.60	S
ATOM	12	CE	MET A 394	21.447	79.839	38.432	1.00	60.62	C
ATOM	13	C	MET A 394	20.526	77.680	33.137	1.00	51.81	C
ATOM	14	O	MET A 394	19.302	77.571	33.071	1.00	51.86	O
ATOM	15	N	ALA A 395	21.237	78.417	32.281	1.00	49.68	N
ATOM	16	CA	ALA A 395	20.590	79.254	31.247	1.00	47.42	C
ATOM	17	CB	ALA A 395	21.146	80.675	31.275	1.00	47.28	C
ATOM	18	C	ALA A 395	20.641	78.670	29.825	1.00	45.85	C
ATOM	19	O	ALA A 395	21.676	78.700	29.151	1.00	45.88	O
ATOM	20	N	TRP A 396	19.498	78.160	29.381	1.00	43.82	N
ATOM	21	CA	TRP A 396	19.359	77.536	28.069	1.00	41.93	C
ATOM	22	CB	TRP A 396	18.362	76.387	28.152	1.00	41.29	C
ATOM	23	CG	TRP A 396	18.845	75.243	29.013	1.00	40.25	C
ATOM	24	CD1	TRP A 396	18.465	74.958	30.289	1.00	39.39	C
ATOM	25	NE1	TRP A 396	19.125	73.833	30.742	1.00	39.04	N
ATOM	26	CE2	TRP A 396	19.950	73.372	29.750	1.00	38.76	C
ATOM	27	CD2	TRP A 396	19.804	74.242	28.644	1.00	38.84	C
ATOM	28	CE3	TRP A 396	20.550	73.990	27.480	1.00	38.54	C
ATOM	29	CZ3	TRP A 396	21.414	72.892	27.462	1.00	38.11	C
ATOM	30	CH2	TRP A 396	21.536	72.047	28.581	1.00	38.30	C
ATOM	31	CZ2	TRP A 396	20.817	72.272	29.732	1.00	38.36	C
ATOM	32	C	TRP A 396	18.890	78.550	27.036	1.00	41.43	C
ATOM	33	O	TRP A 396	17.921	79.271	27.260	1.00	41.53	O
ATOM	34	N	HIS A 397	19.584	78.605	25.907	1.00	40.43	N
ATOM	35	CA	HIS A 397	19.231	79.541	24.847	1.00	40.09	C
ATOM	36	CB	HIS A 397	20.459	80.348	24.424	1.00	40.02	C
ATOM	37	CG	HIS A 397	21.096	81.087	25.560	1.00	41.19	C
ATOM	38	ND1	HIS A 397	22.205	80.611	26.230	1.00	42.68	N
ATOM	39	CE1	HIS A 397	22.521	81.447	27.202	1.00	42.35	C
ATOM	40	NE2	HIS A 397	21.649	82.440	27.198	1.00	42.91	N
ATOM	41	CD2	HIS A 397	20.744	82.235	26.182	1.00	41.47	C
ATOM	42	C	HIS A 397	18.631	78.795	23.671	1.00	39.64	C
ATOM	43	O	HIS A 397	19.133	77.747	23.281	1.00	39.21	O
ATOM	44	N	LEU A 398	17.545	79.333	23.124	1.00	39.11	N
ATOM	45	CA	LEU A 398	16.933	78.765	21.931	1.00	38.72	C
ATOM	46	CB	LEU A 398	15.529	79.342	21.730	1.00	39.15	C
ATOM	47	CG	LEU A 398	14.727	78.853	20.510	1.00	38.97	C
ATOM	48	CD1	LEU A 398	14.185	77.455	20.720	1.00	37.90	C
ATOM	49	CD2	LEU A 398	13.584	79.829	20.222	1.00	37.40	C
ATOM	50	C	LEU A 398	17.823	79.072	20.721	1.00	38.81	C
ATOM	51	O	LEU A 398	18.079	80.250	20.402	1.00	37.86	O
ATOM	52	N	GLY A 399	18.292	78.011	20.059	1.00	38.58	N
ATOM	53	CA	GLY A 399	19.193	78.126	18.907	1.00	38.24	C
ATOM	54	C	GLY A 399	20.343	79.087	19.147	1.00	38.52	C
ATOM	55	O	GLY A 399	20.904	79.140	20.250	1.00	38.41	O
ATOM	56	N	ILE A 400	20.686	79.865	18.118	1.00	38.36	N
ATOM	57	CA	ILE A 400	21.832	80.775	18.171	1.00	38.76	C
ATOM	58	CB	ILE A 400	23.062	80.212	17.396	1.00	39.15	C
ATOM	59	CG1	ILE A 400	22.719	79.941	15.922	1.00	38.85	C
ATOM	60	CD1	ILE A 400	23.950	79.819	15.017	1.00	40.18	C
ATOM	61	CG2	ILE A 400	23.607	78.911	18.085	1.00	39.33	C
ATOM	62	C	ILE A 400	21.439	82.141	17.619	1.00	38.92	C
ATOM	63	O	ILE A 400	20.574	82.230	16.760	1.00	38.55	O
ATOM	64	N	ARG A 401	22.064	83.195	18.136	1.00	38.79	N
ATOM	65	CA	ARG A 401	21.745	84.561	17.739	1.00	39.65	C

Figure 1 Table 1a - 2

ATOM	66	CB	ARG A 401	21.408	85.438	18.954	1.00	39.51	C
ATOM	67	CG	ARG A 401	20.098	85.043	19.642	1.00	42.06	C
ATOM	68	CD	ARG A 401	19.768	85.901	20.860	1.00	44.19	C
ATOM	69	NE	ARG A 401	20.703	85.746	21.980	1.00	51.96	N
ATOM	70	CZ	ARG A 401	20.611	84.820	22.945	1.00	54.89	C
ATOM	71	NH1	ARG A 401	19.626	83.916	22.953	1.00	55.53	N
ATOM	72	NH2	ARG A 401	21.518	84.793	23.917	1.00	55.42	N
ATOM	73	C	ARG A 401	22.854	85.190	16.905	1.00	39.08	C
ATOM	74	O	ARG A 401	24.022	84.800	16.992	1.00	38.99	O
ATOM	75	N	SER A 402	22.473	86.164	16.087	1.00	38.83	N
ATOM	76	CA	SER A 402	23.400	86.824	15.186	1.00	39.02	C
ATOM	77	CB	SER A 402	23.465	86.062	13.857	1.00	39.09	C
ATOM	78	OG	SER A 402	24.429	86.618	12.980	1.00	38.37	O
ATOM	79	C	SER A 402	22.946	88.258	14.941	1.00	39.49	C
ATOM	80	O	SER A 402	21.744	88.555	14.937	1.00	39.18	O
ATOM	81	N	GLN A 403	23.908	89.153	14.752	1.00	39.68	N
ATOM	82	CA	GLN A 403	23.577	90.499	14.317	1.00	40.65	C
ATOM	83	CB	GLN A 403	24.176	91.554	15.271	1.00	40.73	C
ATOM	84	CG	GLN A 403	23.793	91.278	16.742	1.00	41.97	C
ATOM	85	CD	GLN A 403	24.288	92.326	17.725	1.00	43.16	C
ATOM	86	OE1	GLN A 403	25.472	92.679	17.755	1.00	45.04	O
ATOM	87	NE2	GLN A 403	23.378	92.810	18.561	1.00	44.97	N
ATOM	88	C	GLN A 403	23.983	90.696	12.852	1.00	40.53	C
ATOM	89	O	GLN A 403	23.993	91.815	12.356	1.00	40.75	O
ATOM	90	N	SER A 404	24.289	89.591	12.165	1.00	40.34	N
ATOM	91	CA	SER A 404	24.568	89.602	10.727	1.00	40.24	C
ATOM	92	CB	SER A 404	25.151	88.259	10.276	1.00	40.08	C
ATOM	93	OG	SER A 404	26.305	87.907	11.025	1.00	40.64	O
ATOM	94	C	SER A 404	23.291	89.903	9.941	1.00	40.14	C
ATOM	95	O	SER A 404	22.195	89.699	10.450	1.00	39.83	O
ATOM	96	N	ARG A 405	23.428	90.401	8.713	1.00	40.00	N
ATOM	97	CA	ARG A 405	22.256	90.690	7.888	1.00	40.78	C
ATOM	98	CB	ARG A 405	22.654	91.384	6.577	1.00	40.91	C
ATOM	99	CG	ARG A 405	23.029	92.883	6.708	1.00	41.36	C
ATOM	100	CD	ARG A 405	23.157	93.539	5.315	1.00	42.72	C
ATOM	101	NE	ARG A 405	22.811	94.965	5.293	1.00	46.48	N
ATOM	102	CZ	ARG A 405	23.322	95.871	4.448	1.00	47.83	C
ATOM	103	NH1	ARG A 405	24.231	95.519	3.543	1.00	48.70	N
ATOM	104	NH2	ARG A 405	22.933	97.146	4.508	1.00	47.00	N
ATOM	105	C	ARG A 405	21.519	89.365	7.620	1.00	41.04	C
ATOM	106	O	ARG A 405	22.172	88.359	7.348	1.00	40.84	O
ATOM	107	N	PRO A 406	20.189	89.375	7.709	1.00	41.34	N
ATOM	108	CA	PRO A 406	19.399	88.148	7.548	1.00	42.27	C
ATOM	109	CB	PRO A 406	17.956	88.647	7.656	1.00	42.38	C
ATOM	110	CG	PRO A 406	18.048	89.876	8.480	1.00	41.74	C
ATOM	111	CD	PRO A 406	19.357	90.518	8.125	1.00	41.61	C
ATOM	112	C	PRO A 406	19.626	87.498	6.188	1.00	42.64	C
ATOM	113	O	PRO A 406	19.679	86.274	6.092	1.00	43.16	O
ATOM	114	N	ASN A 407	19.764	88.320	5.151	1.00	43.24	N
ATOM	115	CA	ASN A 407	20.136	87.834	3.828	1.00	43.79	C
ATOM	116	CB	ASN A 407	20.227	88.998	2.833	1.00	44.58	C
ATOM	117	CG	ASN A 407	20.512	90.329	3.514	1.00	47.73	C
ATOM	118	OD1	ASN A 407	19.890	90.673	4.521	1.00	50.60	O
ATOM	119	ND2	ASN A 407	21.452	91.089	2.958	1.00	50.17	N
ATOM	120	C	ASN A 407	21.447	87.051	3.850	1.00	42.90	C
ATOM	121	O	ASN A 407	21.585	86.033	3.172	1.00	42.42	O
ATOM	122	N	ASP A 408	22.406	87.533	4.637	1.00	41.92	N
ATOM	123	CA	ASP A 408	23.713	86.890	4.736	1.00	41.24	C
ATOM	124	CB	ASP A 408	24.736	87.853	5.338	1.00	41.16	C
ATOM	125	CG	ASP A 408	25.032	89.031	4.429	1.00	41.80	C
ATOM	126	OD1	ASP A 408	24.579	89.015	3.264	1.00	40.40	O
ATOM	127	OD2	ASP A 408	25.719	89.972	4.881	1.00	42.56	O
ATOM	128	C	ASP A 408	23.643	85.607	5.560	1.00	40.86	C
ATOM	129	O	ASP A 408	24.352	84.637	5.281	1.00	40.37	O
ATOM	130	N	ILE A 409	22.784	85.604	6.574	1.00	40.41	N
ATOM	131	CA	ILE A 409	22.563	84.401	7.388	1.00	40.34	C
ATOM	132	CB	ILE A 409	21.671	84.675	8.621	1.00	40.11	C

Figure 1 Table 1a - 3

ATOM	133	CG1	ILE	A	409	22.310	85.764	9.499	1.00	39.63	C
ATOM	134	CD1	ILE	A	409	21.452	86.234	10.644	1.00	39.88	C
ATOM	135	CG2	ILE	A	409	21.456	83.393	9.433	1.00	39.77	C
ATOM	136	C	ILE	A	409	22.016	83.258	6.523	1.00	40.64	C
ATOM	137	O	ILE	A	409	22.571	82.162	6.525	1.00	40.23	O
ATOM	138	N	MET	A	410	20.963	83.536	5.758	1.00	41.02	N
ATOM	139	CA	MET	A	410	20.332	82.514	4.929	1.00	41.70	C
ATOM	140	CB	MET	A	410	18.999	82.999	4.359	1.00	41.77	C
ATOM	141	CG	MET	A	410	17.997	83.441	5.411	1.00	43.41	C
ATOM	142	SD	MET	A	410	17.478	82.145	6.547	1.00	46.29	S
ATOM	143	CE	MET	A	410	18.732	82.147	7.818	1.00	49.54	C
ATOM	144	C	MET	A	410	21.248	82.023	3.817	1.00	42.06	C
ATOM	145	O	MET	A	410	21.383	80.817	3.626	1.00	42.54	O
ATOM	146	N	ALA	A	411	21.883	82.953	3.099	1.00	42.28	N
ATOM	147	CA	ALA	A	411	22.870	82.599	2.077	1.00	42.44	C
ATOM	148	CB	ALA	A	411	23.538	83.850	1.505	1.00	42.46	C
ATOM	149	C	ALA	A	411	23.919	81.639	2.633	1.00	42.50	C
ATOM	150	O	ALA	A	411	24.168	80.596	2.043	1.00	42.55	O
ATOM	151	N	GLU	A	412	24.512	81.988	3.773	1.00	42.28	N
ATOM	152	CA	GLU	A	412	25.525	81.140	4.407	1.00	42.59	C
ATOM	153	CB	GLU	A	412	26.251	81.873	5.541	1.00	42.46	C
ATOM	154	CG	GLU	A	412	27.254	82.916	5.035	1.00	44.12	C
ATOM	155	CD	GLU	A	412	28.400	82.288	4.262	1.00	44.68	C
ATOM	156	OE1	GLU	A	412	29.261	81.622	4.883	1.00	45.40	O
ATOM	157	OE2	GLU	A	412	28.440	82.464	3.032	1.00	45.49	O
ATOM	158	C	GLU	A	412	25.022	79.771	4.876	1.00	42.33	C
ATOM	159	O	GLU	A	412	25.726	78.776	4.699	1.00	41.74	O
ATOM	160	N	VAL	A	413	23.826	79.706	5.460	1.00	42.83	N
ATOM	161	CA	VAL	A	413	23.301	78.394	5.869	1.00	43.38	C
ATOM	162	CB	VAL	A	413	22.100	78.419	6.891	1.00	43.68	C
ATOM	163	CG1	VAL	A	413	22.306	79.445	7.992	1.00	43.80	C
ATOM	164	CG2	VAL	A	413	20.780	78.622	6.221	1.00	46.07	C
ATOM	165	C	VAL	A	413	23.022	77.506	4.643	1.00	43.64	C
ATOM	166	O	VAL	A	413	23.347	76.318	4.665	1.00	43.21	O
ATOM	167	N	CYS	A	414	22.476	78.093	3.567	1.00	43.64	N
ATOM	168	CA	CYS	A	414	22.285	77.359	2.314	1.00	44.18	C
ATOM	169	CB	CYS	A	414	21.520	78.198	1.292	1.00	44.41	C
ATOM	170	SG	CYS	A	414	19.784	78.328	1.713	1.00	47.57	S
ATOM	171	C	CYS	A	414	23.600	76.865	1.718	1.00	43.99	C
ATOM	172	O	CYS	A	414	23.658	75.747	1.203	1.00	43.32	O
ATOM	173	N	ARG	A	415	24.641	77.703	1.795	1.00	44.04	N
ATOM	174	CA	ARG	A	415	25.994	77.322	1.383	1.00	44.40	C
ATOM	175	CB	ARG	A	415	26.975	78.495	1.507	1.00	44.60	C
ATOM	176	CG	ARG	A	415	28.388	78.180	0.981	1.00	45.02	C
ATOM	177	CD	ARG	A	415	29.458	79.207	1.407	1.00	46.24	C
ATOM	178	NE	ARG	A	415	29.513	79.443	2.853	1.00	48.15	N
ATOM	179	CZ	ARG	A	415	29.858	78.536	3.773	1.00	49.74	C
ATOM	180	NH1	ARG	A	415	30.185	77.289	3.431	1.00	49.22	N
ATOM	181	NH2	ARG	A	415	29.864	78.877	5.055	1.00	49.50	N
ATOM	182	C	ARG	A	415	26.510	76.124	2.188	1.00	44.30	C
ATOM	183	O	ARG	A	415	27.046	75.177	1.607	1.00	44.44	O
ATOM	184	N	ALA	A	416	26.353	76.178	3.513	1.00	43.96	N
ATOM	185	CA	ALA	A	416	26.780	75.086	4.401	1.00	44.08	C
ATOM	186	CB	ALA	A	416	26.649	75.488	5.856	1.00	43.63	C
ATOM	187	C	ALA	A	416	26.017	73.793	4.148	1.00	43.98	C
ATOM	188	O	ALA	A	416	26.609	72.711	4.166	1.00	44.02	O
ATOM	189	N	ILE	A	417	24.712	73.913	3.913	1.00	44.05	N
ATOM	190	CA	ILE	A	417	23.866	72.752	3.634	1.00	44.67	C
ATOM	191	CB	ILE	A	417	22.366	73.147	3.496	1.00	44.96	C
ATOM	192	CG1	ILE	A	417	21.765	73.435	4.877	1.00	44.28	C
ATOM	193	CD1	ILE	A	417	20.555	74.359	4.852	1.00	45.00	C
ATOM	194	CG2	ILE	A	417	21.570	72.037	2.779	1.00	45.41	C
ATOM	195	C	ILE	A	417	24.361	72.038	2.377	1.00	44.71	C
ATOM	196	O	ILE	A	417	24.539	70.814	2.377	1.00	44.18	O
ATOM	197	N	LYS	A	418	24.604	72.826	1.326	1.00	44.78	N
ATOM	198	CA	LYS	A	418	25.137	72.328	0.065	1.00	45.13	C
ATOM	199	CB	LYS	A	418	25.172	73.457	-0.975	1.00	45.04	C

Figure 1

Table 1a - 4

ATOM	200	CG	LYS	A	418	25.235	72.969	-2.406	1.00	45.77	C
ATOM	201	CD	LYS	A	418	25.706	74.050	-3.361	1.00	46.98	C
ATOM	202	CE	LYS	A	418	25.952	73.459	-4.737	1.00	47.95	C
ATOM	203	NZ	LYS	A	418	26.611	74.430	-5.658	1.00	49.27	N
ATOM	204	C	LYS	A	418	26.532	71.711	0.241	1.00	45.57	C
ATOM	205	O	LYS	A	418	26.836	70.676	-0.354	1.00	45.58	O
ATOM	206	N	GLN	A	419	27.364	72.347	1.065	1.00	45.99	N
ATOM	207	CA	GLN	A	419	28.714	71.860	1.362	1.00	46.63	C
ATOM	208	CB	GLN	A	419	29.469	72.891	2.204	1.00	46.97	C
ATOM	209	CG	GLN	A	419	30.982	72.869	2.018	1.00	49.21	C
ATOM	210	CD	GLN	A	419	31.445	73.738	0.857	1.00	51.70	C
ATOM	211	OE1	GLN	A	419	30.967	74.866	0.670	1.00	53.27	O
ATOM	212	NE2	GLN	A	419	32.385	73.222	0.076	1.00	53.35	N
ATOM	213	C	GLN	A	419	28.708	70.517	2.101	1.00	46.59	C
ATOM	214	O	GLN	A	419	29.596	69.692	1.899	1.00	46.73	O
ATOM	215	N	LEU	A	420	27.708	70.310	2.956	1.00	46.36	N
ATOM	216	CA	LEU	A	420	27.584	69.085	3.747	1.00	46.28	C
ATOM	217	CB	LEU	A	420	26.889	69.394	5.078	1.00	46.13	C
ATOM	218	CG	LEU	A	420	27.723	69.931	6.247	1.00	46.78	C
ATOM	219	CD1	LEU	A	420	28.900	70.763	5.762	1.00	47.58	C
ATOM	220	CD2	LEU	A	420	26.850	70.724	7.215	1.00	44.79	C
ATOM	221	C	LEU	A	420	26.835	67.967	3.020	1.00	46.29	C
ATOM	222	O	LEU	A	420	26.675	66.866	3.560	1.00	46.49	O
ATOM	223	N	ASP	A	421	26.377	68.261	1.807	1.00	46.42	N
ATOM	224	CA	ASP	A	421	25.583	67.332	0.990	1.00	46.89	C
ATOM	225	CB	ASP	A	421	26.384	66.074	0.636	1.00	46.88	C
ATOM	226	CG	ASP	A	421	27.465	66.354	-0.355	1.00	48.69	C
ATOM	227	OD1	ASP	A	421	27.151	66.929	-1.426	1.00	50.33	O
ATOM	228	OD2	ASP	A	421	28.632	65.996	-0.068	1.00	50.96	O
ATOM	229	C	ASP	A	421	24.235	66.963	1.607	1.00	46.70	C
ATOM	230	O	ASP	A	421	23.727	65.848	1.413	1.00	46.61	O
ATOM	231	N	TYR	A	422	23.665	67.892	2.365	1.00	46.55	N
ATOM	232	CA	TYR	A	422	22.292	67.738	2.806	1.00	46.47	C
ATOM	233	CB	TYR	A	422	22.007	68.567	4.066	1.00	46.62	C
ATOM	234	CG	TYR	A	422	22.836	68.227	5.294	1.00	47.62	C
ATOM	235	CD1	TYR	A	422	22.707	68.980	6.468	1.00	48.09	C
ATOM	236	CE1	TYR	A	422	23.459	68.685	7.601	1.00	49.52	C
ATOM	237	CZ	TYR	A	422	24.367	67.637	7.564	1.00	50.15	C
ATOM	238	OH	TYR	A	422	25.118	67.341	8.680	1.00	51.71	O
ATOM	239	CE2	TYR	A	422	24.523	66.881	6.411	1.00	49.39	C
ATOM	240	CD2	TYR	A	422	23.758	67.179	5.286	1.00	47.65	C
ATOM	241	C	TYR	A	422	21.394	68.188	1.652	1.00	46.06	C
ATOM	242	O	TYR	A	422	21.803	69.001	0.818	1.00	46.04	O
ATOM	243	N	GLU	A	423	20.191	67.635	1.580	1.00	45.50	N
ATOM	244	CA	GLU	A	423	19.188	68.187	0.692	1.00	45.41	C
ATOM	245	CB	GLU	A	423	18.357	67.088	0.004	1.00	46.27	C
ATOM	246	CG	GLU	A	423	17.661	66.123	0.928	1.00	49.05	C
ATOM	247	CD	GLU	A	423	17.691	64.673	0.434	1.00	52.29	C
ATOM	248	OE1	GLU	A	423	17.252	64.407	-0.705	1.00	52.61	O
ATOM	249	OE2	GLU	A	423	18.140	63.789	1.209	1.00	54.70	O
ATOM	250	C	GLU	A	423	18.350	69.208	1.472	1.00	44.61	C
ATOM	251	O	GLU	A	423	18.298	69.171	2.707	1.00	44.12	O
ATOM	252	N	TRP	A	424	17.759	70.159	0.754	1.00	43.29	N
ATOM	253	CA	TRP	A	424	16.904	71.164	1.382	1.00	42.74	C
ATOM	254	CB	TRP	A	424	17.724	72.334	1.963	1.00	43.19	C
ATOM	255	CG	TRP	A	424	18.191	73.331	0.934	1.00	44.40	C
ATOM	256	CD1	TRP	A	424	17.698	74.597	0.726	1.00	45.41	C
ATOM	257	NE1	TRP	A	424	18.380	75.208	-0.305	1.00	45.43	N
ATOM	258	CE2	TRP	A	424	19.333	74.344	-0.778	1.00	46.38	C
ATOM	259	CD2	TRP	A	424	19.244	73.149	-0.021	1.00	45.46	C
ATOM	260	CE3	TRP	A	424	20.120	72.091	-0.315	1.00	46.05	C
ATOM	261	CZ3	TRP	A	424	21.054	72.261	-1.330	1.00	45.91	C
ATOM	262	CH2	TRP	A	424	21.116	73.461	-2.069	1.00	46.22	C
ATOM	263	CZ2	TRP	A	424	20.271	74.512	-1.806	1.00	46.49	C
ATOM	264	C	TRP	A	424	15.861	71.696	0.419	1.00	41.57	C
ATOM	265	O	TRP	A	424	16.002	71.578	-0.800	1.00	40.84	O
ATOM	266	N	LYS	A	425	14.810	72.268	0.997	1.00	40.26	N

Figure 1 Table 1a - 5

ATOM	267	CA	LYS	A	425	13.816	73.024	0.257	1.00	39.44	C
ATOM	268	CB	LYS	A	425	12.528	72.220	0.096	1.00	39.55	C
ATOM	269	CG	LYS	A	425	12.776	70.924	-0.672	1.00	41.43	C
ATOM	270	CD	LYS	A	425	11.553	70.131	-1.014	1.00	43.55	C
ATOM	271	CE	LYS	A	425	12.007	68.839	-1.691	1.00	43.38	C
ATOM	272	NZ	LYS	A	425	10.887	67.919	-1.947	1.00	49.08	N
ATOM	273	C	LYS	A	425	13.552	74.328	1.003	1.00	38.49	C
ATOM	274	O	LYS	A	425	13.546	74.359	2.234	1.00	37.61	O
ATOM	275	N	VAL	A	426	13.329	75.385	0.237	1.00	37.51	N
ATOM	276	CA	VAL	A	426	13.006	76.704	0.766	1.00	37.37	C
ATOM	277	CB	VAL	A	426	13.595	77.803	-0.154	1.00	37.08	C
ATOM	278	CG1	VAL	A	426	13.292	79.205	0.374	1.00	37.17	C
ATOM	279	CG2	VAL	A	426	15.099	77.596	-0.296	1.00	36.99	C
ATOM	280	C	VAL	A	426	11.491	76.847	0.848	1.00	37.46	C
ATOM	281	O	VAL	A	426	10.808	76.943	-0.181	1.00	37.13	O
ATOM	282	N	VAL	A	427	10.964	76.847	2.071	1.00	37.26	N
ATOM	283	CA	VAL	A	427	9.526	77.041	2.265	1.00	37.18	C
ATOM	284	CB	VAL	A	427	9.018	76.483	3.638	1.00	37.25	C
ATOM	285	CG1	VAL	A	427	7.500	76.631	3.731	1.00	37.05	C
ATOM	286	CG2	VAL	A	427	9.414	75.012	3.837	1.00	37.22	C
ATOM	287	C	VAL	A	427	9.185	78.531	2.144	1.00	37.08	C
ATOM	288	O	VAL	A	427	8.310	78.889	1.370	1.00	37.02	O
ATOM	289	N	ASN	A	428	9.870	79.353	2.951	1.00	37.43	N
ATOM	290	CA	ASN	A	428	9.829	80.828	2.979	1.00	37.99	C
ATOM	291	CB	ASN	A	428	9.477	81.345	4.400	1.00	39.13	C
ATOM	292	CG	ASN	A	428	8.088	81.027	4.807	1.00	41.24	C
ATOM	293	OD1	ASN	A	428	7.155	81.120	4.010	1.00	49.49	O
ATOM	294	ND2	ASN	A	428	7.922	80.650	6.048	1.00	43.07	N
ATOM	295	C	ASN	A	428	11.264	81.289	2.804	1.00	37.89	C
ATOM	296	O	ASN	A	428	12.186	80.488	3.016	1.00	37.98	O
ATOM	297	N	PRO	A	429	11.474	82.594	2.512	1.00	37.09	N
ATOM	298	CA	PRO	A	429	12.831	83.150	2.583	1.00	37.27	C
ATOM	299	CB	PRO	A	429	12.607	84.653	2.339	1.00	37.09	C
ATOM	300	CG	PRO	A	429	11.381	84.680	1.443	1.00	36.94	C
ATOM	301	CD	PRO	A	429	10.497	83.605	2.058	1.00	36.99	C
ATOM	302	C	PRO	A	429	13.571	82.910	3.920	1.00	37.34	C
ATOM	303	O	PRO	A	429	14.803	82.937	3.944	1.00	37.51	O
ATOM	304	N	TYR	A	430	12.835	82.654	5.002	1.00	36.91	N
ATOM	305	CA	TYR	A	430	13.456	82.451	6.304	1.00	37.57	C
ATOM	306	CB	TYR	A	430	13.065	83.578	7.276	1.00	37.73	C
ATOM	307	CG	TYR	A	430	13.309	84.958	6.731	1.00	40.22	C
ATOM	308	CD1	TYR	A	430	12.242	85.791	6.396	1.00	42.38	C
ATOM	309	CE1	TYR	A	430	12.462	87.075	5.890	1.00	42.90	C
ATOM	310	CZ	TYR	A	430	13.764	87.526	5.710	1.00	42.80	C
ATOM	311	OH	TYR	A	430	13.993	88.795	5.221	1.00	43.00	O
ATOM	312	CE2	TYR	A	430	14.837	86.715	6.027	1.00	42.67	C
ATOM	313	CD2	TYR	A	430	14.606	85.433	6.538	1.00	41.84	C
ATOM	314	C	TYR	A	430	13.145	81.103	6.929	1.00	36.84	C
ATOM	315	O	TYR	A	430	13.287	80.938	8.136	1.00	36.66	O
ATOM	316	N	TYR	A	431	12.741	80.144	6.102	1.00	36.89	N
ATOM	317	CA	TYR	A	431	12.253	78.850	6.576	1.00	36.91	C
ATOM	318	CB	TYR	A	431	10.728	78.915	6.724	1.00	37.37	C
ATOM	319	CG	TYR	A	431	10.035	77.665	7.240	1.00	39.49	C
ATOM	320	CD1	TYR	A	431	10.720	76.687	7.967	1.00	41.92	C
ATOM	321	CE1	TYR	A	431	10.057	75.543	8.440	1.00	42.30	C
ATOM	322	CZ	TYR	A	431	8.698	75.407	8.189	1.00	42.30	C
ATOM	323	OH	TYR	A	431	8.001	74.308	8.635	1.00	43.54	O
ATOM	324	CE2	TYR	A	431	8.007	76.378	7.491	1.00	41.18	C
ATOM	325	CD2	TYR	A	431	8.669	77.490	7.028	1.00	40.27	C
ATOM	326	C	TYR	A	431	12.693	77.736	5.625	1.00	36.92	C
ATOM	327	O	TYR	A	431	12.222	77.656	4.489	1.00	36.39	O
ATOM	328	N	LEU	A	432	13.608	76.896	6.094	1.00	36.70	N
ATOM	329	CA	LEU	A	432	14.110	75.784	5.299	1.00	37.80	C
ATOM	330	CB	LEU	A	432	15.625	75.861	5.156	1.00	37.62	C
ATOM	331	CG	LEU	A	432	16.242	77.192	4.724	1.00	37.46	C
ATOM	332	CD1	LEU	A	432	17.720	77.024	4.751	1.00	38.75	C
ATOM	333	CD2	LEU	A	432	15.779	77.624	3.344	1.00	36.57	C

Figure 1 Table 1a - 6

ATOM	334	C	LEU	A	432	13.777	74.451	5.942	1.00	38.57	C
ATOM	335	O	LEU	A	432	13.757	74.332	7.168	1.00	38.16	O
ATOM	336	N	ARG	A	433	13.533	73.454	5.099	1.00	39.38	N
ATOM	337	CA	ARG	A	433	13.376	72.084	5.538	1.00	40.95	C
ATOM	338	CB	ARG	A	433	12.041	71.537	5.031	1.00	40.97	C
ATOM	339	CG	ARG	A	433	10.965	71.584	6.114	1.00	44.41	C
ATOM	340	CD	ARG	A	433	9.692	72.330	5.741	1.00	48.44	C
ATOM	341	NE	ARG	A	433	8.689	71.517	5.062	1.00	52.74	N
ATOM	342	CZ	ARG	A	433	7.386	71.817	4.992	1.00	55.18	C
ATOM	343	NH1	ARG	A	433	6.904	72.908	5.579	1.00	55.20	N
ATOM	344	NH2	ARG	A	433	6.555	71.016	4.326	1.00	55.49	N
ATOM	345	C	ARG	A	433	14.570	71.324	4.988	1.00	41.28	C
ATOM	346	O	ARG	A	433	14.867	71.425	3.792	1.00	41.50	O
ATOM	347	N	VAL	A	434	15.296	70.625	5.855	1.00	41.94	N
ATOM	348	CA	VAL	A	434	16.519	69.944	5.424	1.00	43.08	C
ATOM	349	CB	VAL	A	434	17.841	70.631	5.935	1.00	43.33	C
ATOM	350	CG1	VAL	A	434	17.607	72.086	6.327	1.00	43.80	C
ATOM	351	CG2	VAL	A	434	18.460	69.877	7.076	1.00	45.73	C
ATOM	352	C	VAL	A	434	16.493	68.447	5.724	1.00	43.42	C
ATOM	353	O	VAL	A	434	15.849	67.997	6.674	1.00	43.16	O
ATOM	354	N	ARG	A	435	17.183	67.690	4.882	1.00	43.74	N
ATOM	355	CA	ARG	A	435	17.214	66.249	4.978	1.00	44.39	C
ATOM	356	CB	ARG	A	435	16.203	65.655	3.999	1.00	44.45	C
ATOM	357	CG	ARG	A	435	16.011	64.163	4.064	1.00	47.16	C
ATOM	358	CD	ARG	A	435	14.869	63.777	3.135	1.00	49.35	C
ATOM	359	NE	ARG	A	435	14.719	62.337	3.014	1.00	52.43	N
ATOM	360	CZ	ARG	A	435	14.918	61.646	1.894	1.00	53.74	C
ATOM	361	NH1	ARG	A	435	15.286	62.258	0.770	1.00	53.53	N
ATOM	362	NH2	ARG	A	435	14.748	60.330	1.902	1.00	54.91	N
ATOM	363	C	ARG	A	435	18.635	65.776	4.678	1.00	44.61	C
ATOM	364	O	ARG	A	435	19.307	66.294	3.775	1.00	44.05	O
ATOM	365	N	ARG	A	436	19.073	64.790	5.453	1.00	44.72	N
ATOM	366	CA	ARG	A	436	20.427	64.272	5.429	1.00	45.61	C
ATOM	367	CB	ARG	A	436	21.178	64.798	6.671	1.00	46.31	C
ATOM	368	CG	ARG	A	436	22.569	64.226	6.908	1.00	48.99	C
ATOM	369	CD	ARG	A	436	22.554	63.024	7.818	1.00	53.37	C
ATOM	370	NE	ARG	A	436	22.913	63.362	9.191	1.00	56.60	N
ATOM	371	CZ	ARG	A	436	22.548	62.653	10.260	1.00	57.32	C
ATOM	372	NH1	ARG	A	436	21.781	61.577	10.120	1.00	57.45	N
ATOM	373	NH2	ARG	A	436	22.934	63.040	11.471	1.00	57.79	N
ATOM	374	C	ARG	A	436	20.348	62.744	5.480	1.00	45.37	C
ATOM	375	O	ARG	A	436	19.583	62.188	6.274	1.00	45.10	O
ATOM	376	N	LYS	A	437	21.128	62.069	4.637	1.00	44.98	N
ATOM	377	CA	LYS	A	437	21.316	60.626	4.764	1.00	44.79	C
ATOM	378	CB	LYS	A	437	21.491	59.968	3.391	1.00	45.04	C
ATOM	379	CG	LYS	A	437	21.470	58.439	3.412	1.00	45.15	C
ATOM	380	CD	LYS	A	437	21.760	57.876	2.035	1.00	46.20	C
ATOM	381	CE	LYS	A	437	21.714	56.352	2.018	1.00	46.25	C
ATOM	382	NZ	LYS	A	437	21.925	55.819	0.634	1.00	46.99	N
ATOM	383	C	LYS	A	437	22.534	60.362	5.652	1.00	44.67	C
ATOM	384	O	LYS	A	437	23.626	60.878	5.400	1.00	44.73	O
ATOM	385	N	ASN	A	438	22.344	59.587	6.710	1.00	44.47	N
ATOM	386	CA	ASN	A	438	23.461	59.211	7.562	1.00	44.80	C
ATOM	387	CB	ASN	A	438	22.964	58.542	8.844	1.00	44.57	C
ATOM	388	CG	ASN	A	438	24.058	58.384	9.873	1.00	43.84	C
ATOM	389	OD1	ASN	A	438	25.087	57.771	9.610	1.00	42.77	O
ATOM	390	ND2	ASN	A	438	23.840	58.939	11.050	1.00	42.67	N
ATOM	391	C	ASN	A	438	24.441	58.293	6.818	1.00	45.23	C
ATOM	392	O	ASN	A	438	24.048	57.227	6.354	1.00	45.15	O
ATOM	393	N	PRO	A	439	25.716	58.719	6.687	1.00	45.87	N
ATOM	394	CA	PRO	A	439	26.726	57.919	5.973	1.00	46.37	C
ATOM	395	CB	PRO	A	439	27.998	58.778	6.068	1.00	46.50	C
ATOM	396	CG	PRO	A	439	27.744	59.747	7.189	1.00	46.37	C
ATOM	397	CD	PRO	A	439	26.271	59.995	7.179	1.00	45.87	C
ATOM	398	C	PRO	A	439	26.970	56.531	6.578	1.00	46.76	C
ATOM	399	O	PRO	A	439	27.138	55.561	5.836	1.00	47.01	O
ATOM	400	N	VAL	A	440	26.974	56.439	7.907	1.00	47.01	N

Figure 1 Table 1a - 7

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ATOM    401  CA  VAL A 440      27.280  55.185   8.601  1.00 47.37      C
ATOM    402  CB  VAL A 440      27.767  55.440  10.062  1.00 47.25      C
ATOM    403  CG1 VAL A 440      28.098  54.130  10.767  1.00 47.02      C
ATOM    404  CG2 VAL A 440      28.978  56.373  10.076  1.00 47.12      C
ATOM    405  C   VAL A 440      26.062  54.257   8.613  1.00 47.68      C
ATOM    406  O   VAL A 440      26.165  53.065   8.305  1.00 47.77      O
ATOM    407  N   THR A 441      24.914  54.838   8.943  1.00 47.86      N
ATOM    408  CA  THR A 441      23.679  54.113   9.219  1.00 48.37      C
ATOM    409  CB  THR A 441      22.881  54.854  10.325  1.00 48.79      C
ATOM    410  OG1 THR A 441      23.669  54.901  11.527  1.00 50.85      O
ATOM    411  CG2 THR A 441      21.579  54.129  10.631  1.00 50.27      C
ATOM    412  C   THR A 441      22.790  53.930   7.984  1.00 47.73      C
ATOM    413  O   THR A 441      21.994  52.991   7.924  1.00 47.39      O
ATOM    414  N   SER A 442      22.929  54.840   7.019  1.00 47.39      N
ATOM    415  CA  SER A 442      22.092  54.899   5.809  1.00 47.29      C
ATOM    416  CB  SER A 442      22.096  53.570   5.026  1.00 47.40      C
ATOM    417  OG  SER A 442      23.411  53.196   4.644  1.00 46.83      O
ATOM    418  C   SER A 442      20.659  55.401   6.045  1.00 47.41      C
ATOM    419  O   SER A 442      19.828  55.333   5.139  1.00 47.76      O
ATOM    420  N   THR A 443      20.368  55.916   7.238  1.00 47.05      N
ATOM    421  CA  THR A 443      19.027  56.449   7.508  1.00 46.74      C
ATOM    422  CB  THR A 443      18.572  56.243   8.973  1.00 46.89      C
ATOM    423  OG1 THR A 443      19.495  56.886   9.860  1.00 46.65      O
ATOM    424  CG2 THR A 443      18.451  54.750   9.311  1.00 46.50      C
ATOM    425  C   THR A 443      18.909  57.932   7.158  1.00 46.62      C
ATOM    426  O   THR A 443      19.910  58.629   6.993  1.00 46.33      O
ATOM    427  N   PHE A 444      17.670  58.392   7.039  1.00 46.39      N
ATOM    428  CA  PHE A 444      17.392  59.774   6.740  1.00 46.80      C
ATOM    429  CB  PHE A 444      16.407  59.904   5.576  1.00 47.03      C
ATOM    430  CG  PHE A 444      17.015  59.622   4.232  1.00 47.90      C
ATOM    431  CD1 PHE A 444      16.969  58.342   3.688  1.00 48.28      C
ATOM    432  CE1 PHE A 444      17.528  58.074   2.429  1.00 49.84      C
ATOM    433  CZ  PHE A 444      18.146  59.096   1.710  1.00 49.61      C
ATOM    434  CE2 PHE A 444      18.192  60.391   2.249  1.00 49.82      C
ATOM    435  CD2 PHE A 444      17.633  60.639   3.508  1.00 48.99      C
ATOM    436  C   PHE A 444      16.842  60.469   7.972  1.00 46.64      C
ATOM    437  O   PHE A 444      16.001  59.909   8.693  1.00 46.51      O
ATOM    438  N   SER A 445      17.352  61.674   8.204  1.00 45.76      N
ATOM    439  CA  SER A 445      16.857  62.567   9.236  1.00 45.81      C
ATOM    440  CB  SER A 445      17.899  62.736  10.335  1.00 45.45      C
ATOM    441  OG  SER A 445      17.930  61.582  11.142  1.00 47.92      O
ATOM    442  C   SER A 445      16.483  63.933   8.648  1.00 45.57      C
ATOM    443  O   SER A 445      17.111  64.412   7.701  1.00 45.03      O
ATOM    444  N   LYS A 446      15.451  64.542   9.226  1.00 45.18      N
ATOM    445  CA  LYS A 446      14.907  65.797   8.748  1.00 45.07      C
ATOM    446  CB  LYS A 446      13.509  65.586   8.175  1.00 45.34      C
ATOM    447  CG  LYS A 446      13.416  64.629   6.991  1.00 46.41      C
ATOM    448  CD  LYS A 446      11.964  64.406   6.584  1.00 47.86      C
ATOM    449  CE  LYS A 446      11.151  63.733   7.703  1.00 50.57      C
ATOM    450  NZ  LYS A 446       9.772  63.347   7.269  1.00 52.27      N
ATOM    451  C   LYS A 446      14.830  66.810   9.888  1.00 44.45      C
ATOM    452  O   LYS A 446      14.567  66.458  11.038  1.00 43.74      O
ATOM    453  N   MET A 447      15.060  68.073   9.555  1.00 44.10      N
ATOM    454  CA  MET A 447      14.863  69.167  10.500  1.00 44.01      C
ATOM    455  CB  MET A 447      16.129  69.401  11.327  1.00 43.79      C
ATOM    456  CG  MET A 447      17.378  69.756  10.531  1.00 45.43      C
ATOM    457  SD  MET A 447      18.684  70.298  11.652  1.00 49.58      S
ATOM    458  CE  MET A 447      20.030  70.654  10.534  1.00 48.09      C
ATOM    459  C   MET A 447      14.416  70.435   9.766  1.00 43.15      C
ATOM    460  O   MET A 447      14.490  70.497   8.535  1.00 42.26      O
ATOM    461  N   SER A 448      13.916  71.409  10.530  1.00 42.04      N
ATOM    462  CA  SER A 448      13.527  72.716  10.020  1.00 42.34      C
ATOM    463  CB  SER A 448      12.117  73.073  10.470  1.00 42.06      C
ATOM    464  OG  SER A 448      11.177  72.291   9.773  1.00 46.65      O
ATOM    465  C   SER A 448      14.461  73.772  10.573  1.00 41.67      C
ATOM    466  O   SER A 448      14.918  73.662  11.716  1.00 41.12      O
ATOM    467  N   LEU A 449      14.738  74.783   9.755  1.00 41.36      N
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Figure 1 Table 1a - 8

ATOM	468	CA	LEU	A	449	15.450	75.978	10.194	1.00 41.00 C
ATOM	469	CB	LEU	A	449	16.744	76.153	9.409	1.00 41.21 C
ATOM	470	CG	LEU	A	449	17.986	75.472	9.979	1.00 43.83 C
ATOM	471	CD1	LEU	A	449	18.104	74.064	9.456	1.00 46.00 C
ATOM	472	CD2	LEU	A	449	19.225	76.260	9.617	1.00 46.86 C
ATOM	473	C	LEU	A	449	14.558	77.188	9.977	1.00 40.58 C
ATOM	474	O	LEU	A	449	14.006	77.357	8.892	1.00 40.59 O
ATOM	475	N	GLN	A	450	14.433	78.029	11.003	1.00 39.26 N
ATOM	476	CA	GLN	A	450	13.622	79.225	10.921	1.00 38.94 C
ATOM	477	CB	GLN	A	450	12.289	79.034	11.652	1.00 39.27 C
ATOM	478	CG	GLN	A	450	11.467	80.331	11.794	1.00 37.46 C
ATOM	479	CD	GLN	A	450	10.772	80.754	10.507	1.00 37.60 C
ATOM	480	OE1	GLN	A	450	9.923	80.024	9.989	1.00 38.04 O
ATOM	481	NE2	GLN	A	450	11.111	81.963	9.995	1.00 37.29 N
ATOM	482	C	GLN	A	450	14.377	80.423	11.501	1.00 39.01 C
ATOM	483	O	GLN	A	450	14.794	80.401	12.666	1.00 38.44 O
ATOM	484	N	LEU	A	451	14.562	81.451	10.678	1.00 38.42 N
ATOM	485	CA	LEU	A	451	15.114	82.721	11.145	1.00 38.64 C
ATOM	486	CB	LEU	A	451	15.906	83.442	10.037	1.00 38.55 C
ATOM	487	CG	LEU	A	451	16.820	84.609	10.488	1.00 38.83 C
ATOM	488	CD1	LEU	A	451	17.921	84.105	11.429	1.00 38.56 C
ATOM	489	CD2	LEU	A	451	17.455	85.343	9.306	1.00 37.77 C
ATOM	490	C	LEU	A	451	14.024	83.635	11.705	1.00 39.21 C
ATOM	491	O	LEU	A	451	12.997	83.869	11.055	1.00 39.38 O
ATOM	492	N	TYR	A	452	14.292	84.168	12.900	1.00 39.57 N
ATOM	493	CA	TYR	A	452	13.420	85.094	13.614	1.00 40.24 C
ATOM	494	CB	TYR	A	452	13.029	84.518	14.972	1.00 40.60 C
ATOM	495	CG	TYR	A	452	12.050	83.375	14.941	1.00 41.22 C
ATOM	496	CD1	TYR	A	452	12.456	82.078	15.261	1.00 41.67 C
ATOM	497	CE1	TYR	A	452	11.546	81.020	15.241	1.00 41.96 C
ATOM	498	CZ	TYR	A	452	10.219	81.266	14.899	1.00 42.28 C
ATOM	499	OH	TYR	A	452	9.312	80.238	14.873	1.00 44.16 O
ATOM	500	CE2	TYR	A	452	9.802	82.542	14.580	1.00 42.20 C
ATOM	501	CD2	TYR	A	452	10.713	83.590	14.610	1.00 41.43 C
ATOM	502	C	TYR	A	452	14.145	86.410	13.890	1.00 40.66 C
ATOM	503	O	TYR	A	452	15.373	86.448	13.948	1.00 40.34 O
ATOM	504	N	GLN	A	453	13.379	87.484	14.063	1.00 41.09 N
ATOM	505	CA	GLN	A	453	13.939	88.761	14.514	1.00 42.03 C
ATOM	506	CB	GLN	A	453	13.371	89.943	13.714	1.00 41.72 C
ATOM	507	CG	GLN	A	453	14.060	91.287	14.029	1.00 43.39 C
ATOM	508	CD	GLN	A	453	13.584	92.448	13.159	1.00 42.92 C
ATOM	509	OE1	GLN	A	453	13.267	92.279	11.991	1.00 45.01 O
ATOM	510	NE2	GLN	A	453	13.540	93.629	13.734	1.00 45.06 N
ATOM	511	C	GLN	A	453	13.624	88.907	15.993	1.00 42.02 C
ATOM	512	O	GLN	A	453	12.472	88.740	16.389	1.00 42.21 O
ATOM	513	N	VAL	A	454	14.645	89.189	16.804	1.00 42.63 N
ATOM	514	CA	VAL	A	454	14.449	89.355	18.252	1.00 43.18 C
ATOM	515	CB	VAL	A	454	15.270	88.344	19.107	1.00 43.38 C
ATOM	516	CG1	VAL	A	454	14.746	86.922	18.918	1.00 42.82 C
ATOM	517	CG2	VAL	A	454	16.760	88.434	18.806	1.00 43.35 C
ATOM	518	C	VAL	A	454	14.642	90.781	18.789	1.00 43.79 C
ATOM	519	O	VAL	A	454	14.050	91.118	19.806	1.00 43.95 O
ATOM	520	N	ASP	A	455	15.481	91.577	18.123	1.00 44.09 N
ATOM	521	CA	ASP	A	455	15.660	93.016	18.406	1.00 45.70 C
ATOM	522	CB	ASP	A	455	17.083	93.335	18.895	1.00 45.30 C
ATOM	523	CG	ASP	A	455	17.259	93.136	20.368	1.00 47.09 C
ATOM	524	OD1	ASP	A	455	16.615	92.240	20.957	1.00 50.30 O
ATOM	525	OD2	ASP	A	455	18.076	93.874	20.954	1.00 50.11 O
ATOM	526	C	ASP	A	455	15.468	93.746	17.097	1.00 45.69 C
ATOM	527	O	ASP	A	455	15.016	93.167	16.123	1.00 46.61 O
ATOM	528	N	SER	A	456	15.851	95.013	17.065	1.00 46.14 N
ATOM	529	CA	SER	A	456	16.003	95.719	15.802	1.00 46.21 C
ATOM	530	CB	SER	A	456	15.772	97.210	16.013	1.00 46.16 C
ATOM	531	OG	SER	A	456	16.223	97.586	17.305	1.00 47.35 O
ATOM	532	C	SER	A	456	17.390	95.459	15.192	1.00 45.98 C
ATOM	533	O	SER	A	456	17.637	95.800	14.035	1.00 46.59 O
ATOM	534	N	ARG	A	457	18.287	94.862	15.978	1.00 45.55 N

Figure 1 Table 1a - 9

ATOM	535	CA	ARG	A	457	19.652	94.532	15.533	1.00 45.08	C
ATOM	536	CB	ARG	A	457	20.685	95.226	16.432	1.00 45.17	C
ATOM	537	CG	ARG	A	457	20.263	96.607	16.955	1.00 46.40	C
ATOM	538	CD	ARG	A	457	21.419	97.409	17.603	1.00 48.47	C
ATOM	539	NE	ARG	A	457	22.495	97.667	16.646	1.00 50.88	N
ATOM	540	CZ	ARG	A	457	23.674	97.048	16.656	1.00 51.48	C
ATOM	541	NH1	ARG	A	457	23.960	96.153	17.595	1.00 51.75	N
ATOM	542	NH2	ARG	A	457	24.577	97.338	15.733	1.00 52.73	N
ATOM	543	C	ARG	A	457	19.943	93.010	15.516	1.00 44.11	C
ATOM	544	O	ARG	A	457	20.999	92.576	15.037	1.00 44.18	O
ATOM	545	N	THR	A	458	19.023	92.204	16.042	1.00 42.47	N
ATOM	546	CA	THR	A	458	19.376	90.832	16.406	1.00 40.89	C
ATOM	547	CB	THR	A	458	19.500	90.654	17.952	1.00 40.60	C
ATOM	548	OG1	THR	A	458	20.219	91.757	18.521	1.00 41.61	O
ATOM	549	CG2	THR	A	458	20.225	89.356	18.304	1.00 40.96	C
ATOM	550	C	THR	A	458	18.426	89.784	15.818	1.00 39.83	C
ATOM	551	O	THR	A	458	17.201	89.931	15.865	1.00 39.07	O
ATOM	552	N	TYR	A	459	19.024	88.726	15.278	1.00 39.03	N
ATOM	553	CA	TYR	A	459	18.283	87.596	14.714	1.00 38.45	C
ATOM	554	CB	TYR	A	459	18.516	87.487	13.201	1.00 38.57	C
ATOM	555	CG	TYR	A	459	18.327	88.839	12.541	1.00 39.13	C
ATOM	556	CD1	TYR	A	459	19.410	89.691	12.336	1.00 38.40	C
ATOM	557	CE1	TYR	A	459	19.232	90.956	11.780	1.00 39.87	C
ATOM	558	CZ	TYR	A	459	17.955	91.373	11.446	1.00 39.61	C
ATOM	559	OH	TYR	A	459	17.766	92.602	10.890	1.00 38.85	O
ATOM	560	CE2	TYR	A	459	16.858	90.540	11.658	1.00 39.48	C
ATOM	561	CD2	TYR	A	459	17.053	89.295	12.215	1.00 38.99	C
ATOM	562	C	TYR	A	459	18.644	86.304	15.435	1.00 38.35	C
ATOM	563	O	TYR	A	459	19.730	86.184	16.004	1.00 37.87	O
ATOM	564	N	LEU	A	460	17.707	85.361	15.407	1.00 37.78	N
ATOM	565	CA	LEU	A	460	17.839	84.081	16.069	1.00 37.63	C
ATOM	566	CB	LEU	A	460	16.978	84.076	17.346	1.00 37.80	C
ATOM	567	CG	LEU	A	460	16.275	82.938	18.117	1.00 38.26	C
ATOM	568	CD1	LEU	A	460	16.551	81.516	17.660	1.00 39.20	C
ATOM	569	CD2	LEU	A	460	16.487	83.084	19.618	1.00 36.34	C
ATOM	570	C	LEU	A	460	17.489	82.964	15.079	1.00 37.40	C
ATOM	571	O	LEU	A	460	16.418	82.975	14.452	1.00 37.33	O
ATOM	572	N	LEU	A	461	18.426	82.038	14.907	1.00 37.14	N
ATOM	573	CA	LEU	A	461	18.215	80.870	14.064	1.00 36.92	C
ATOM	574	CB	LEU	A	461	19.501	80.490	13.313	1.00 36.74	C
ATOM	575	CG	LEU	A	461	19.467	79.339	12.285	1.00 38.05	C
ATOM	576	CD1	LEU	A	461	18.527	79.648	11.086	1.00 37.96	C
ATOM	577	CD2	LEU	A	461	20.882	79.102	11.790	1.00 38.41	C
ATOM	578	C	LEU	A	461	17.731	79.740	14.963	1.00 36.93	C
ATOM	579	O	LEU	A	461	18.418	79.343	15.908	1.00 36.80	O
ATOM	580	N	ASP	A	462	16.517	79.277	14.687	1.00 36.77	N
ATOM	581	CA	ASP	A	462	15.864	78.234	15.448	1.00 38.01	C
ATOM	582	CB	ASP	A	462	14.423	78.668	15.749	1.00 38.40	C
ATOM	583	CG	ASP	A	462	13.592	77.569	16.361	1.00 40.81	C
ATOM	584	OD1	ASP	A	462	14.051	76.909	17.314	1.00 42.83	O
ATOM	585	OD2	ASP	A	462	12.468	77.345	15.878	1.00 45.66	O
ATOM	586	C	ASP	A	462	15.897	76.912	14.652	1.00 37.73	C
ATOM	587	O	ASP	A	462	15.624	76.904	13.451	1.00 37.79	O
ATOM	588	N	PHE	A	463	16.243	75.814	15.330	1.00 37.69	N
ATOM	589	CA	PHE	A	463	16.344	74.471	14.724	1.00 38.01	C
ATOM	590	CB	PHE	A	463	17.714	73.831	14.985	1.00 38.21	C
ATOM	591	CG	PHE	A	463	18.888	74.658	14.565	1.00 38.84	C
ATOM	592	CD1	PHE	A	463	19.281	75.776	15.310	1.00 39.14	C
ATOM	593	CE1	PHE	A	463	20.383	76.545	14.926	1.00 40.05	C
ATOM	594	CZ	PHE	A	463	21.120	76.174	13.808	1.00 39.67	C
ATOM	595	CE2	PHE	A	463	20.751	75.056	13.070	1.00 40.60	C
ATOM	596	CD2	PHE	A	463	19.645	74.285	13.466	1.00 39.52	C
ATOM	597	C	PHE	A	463	15.323	73.557	15.378	1.00 38.53	C
ATOM	598	O	PHE	A	463	15.226	73.520	16.605	1.00 37.67	O
ATOM	599	N	ARG	A	464	14.584	72.801	14.570	1.00 38.61	N
ATOM	600	CA	ARG	A	464	13.570	71.913	15.106	1.00 39.97	C
ATOM	601	CB	ARG	A	464	12.191	72.532	14.935	1.00 40.35	C

Figure 1 Table 1a - 10

ATOM	602	CG	ARG A 464	11.089	71.780	15.652	1.00	43.11	C
ATOM	603	CD	ARG A 464	9.714	72.250	15.193	1.00	48.08	C
ATOM	604	NE	ARG A 464	8.639	71.567	15.915	1.00	52.69	N
ATOM	605	CZ	ARG A 464	8.202	70.337	15.644	1.00	54.47	C
ATOM	606	NH1	ARG A 464	8.746	69.616	14.666	1.00	55.20	N
ATOM	607	NH2	ARG A 464	7.217	69.821	16.366	1.00	55.51	N
ATOM	608	C	ARG A 464	13.633	70.572	14.388	1.00	40.01	C
ATOM	609	O	ARG A 464	13.662	70.532	13.164	1.00	39.63	O
ATOM	610	N	SER A 465	13.666	69.476	15.139	1.00	40.10	N
ATOM	611	CA	SER A 465	13.698	68.175	14.504	1.00	40.86	C
ATOM	612	CB	SER A 465	14.256	67.087	15.442	1.00	40.88	C
ATOM	613	OG	SER A 465	13.389	66.851	16.525	1.00	41.05	O
ATOM	614	C	SER A 465	12.296	67.806	14.034	1.00	41.63	C
ATOM	615	O	SER A 465	11.291	68.234	14.611	1.00	40.81	O
ATOM	616	N	ILE A 466	12.251	67.010	12.976	1.00	42.91	N
ATOM	617	CA	ILE A 466	11.001	66.572	12.395	1.00	44.82	C
ATOM	618	CB	ILE A 466	10.925	66.933	10.906	1.00	44.31	C
ATOM	619	CG1	ILE A 466	10.871	68.452	10.751	1.00	43.93	C
ATOM	620	CD1	ILE A 466	11.180	68.933	9.356	1.00	46.16	C
ATOM	621	CG2	ILE A 466	9.713	66.224	10.234	1.00	43.91	C
ATOM	622	C	ILE A 466	10.908	65.074	12.577	1.00	46.89	C
ATOM	623	O	ILE A 466	11.792	64.335	12.136	1.00	46.86	O
ATOM	624	N	ASP A 467	9.837	64.644	13.239	1.00	49.88	N
ATOM	625	CA	ASP A 467	9.641	63.252	13.595	1.00	52.88	C
ATOM	626	CB	ASP A 467	8.450	63.102	14.555	1.00	53.14	C
ATOM	627	CG	ASP A 467	8.651	63.856	15.874	1.00	54.97	C
ATOM	628	OD1	ASP A 467	9.771	63.823	16.426	1.00	56.42	O
ATOM	629	OD2	ASP A 467	7.681	64.474	16.367	1.00	57.25	O
ATOM	630	C	ASP A 467	9.410	62.414	12.354	1.00	54.68	C
ATOM	631	O	ASP A 467	8.783	62.869	11.395	1.00	55.00	O
ATOM	632	N	ASP A 468	9.921	61.188	12.392	1.00	57.16	N
ATOM	633	CA	ASP A 468	9.672	60.187	11.355	1.00	59.32	C
ATOM	634	CB	ASP A 468	10.291	58.850	11.762	1.00	59.57	C
ATOM	635	CG	ASP A 468	11.754	58.741	11.385	1.00	60.88	C
ATOM	636	OD1	ASP A 468	12.168	57.624	10.991	1.00	63.04	O
ATOM	637	OD2	ASP A 468	12.484	59.753	11.483	1.00	61.14	O
ATOM	638	C	ASP A 468	8.184	59.976	11.077	1.00	60.34	C
ATOM	639	O	ASP A 468	7.435	59.549	11.961	1.00	60.58	O
ATOM	640	N	GLU A 469	7.778	60.304	9.850	1.00	61.59	N
ATOM	641	CA	GLU A 469	6.454	59.966	9.297	1.00	62.68	C
ATOM	642	CB	GLU A 469	5.962	58.613	9.819	1.00	62.71	C
ATOM	643	CG	GLU A 469	5.686	57.590	8.734	1.00	64.23	C
ATOM	644	CD	GLU A 469	6.149	56.194	9.127	1.00	65.81	C
ATOM	645	OE1	GLU A 469	7.246	56.081	9.724	1.00	66.63	O
ATOM	646	OE2	GLU A 469	5.424	55.212	8.835	1.00	66.11	O
ATOM	647	C	GLU A 469	5.410	61.054	9.543	1.00	62.99	C
ATOM	648	O	GLU A 469	4.460	61.198	8.764	1.00	63.51	O
ATOM	649	N	VAL A 524	20.824	41.664	24.854	1.00	55.34	N
ATOM	650	CA	VAL A 524	20.148	42.552	23.914	1.00	55.24	C
ATOM	651	CB	VAL A 524	18.664	42.749	24.287	1.00	55.29	C
ATOM	652	CG1	VAL A 524	18.149	44.076	23.743	1.00	55.06	C
ATOM	653	CG2	VAL A 524	17.826	41.588	23.757	1.00	54.93	C
ATOM	654	C	VAL A 524	20.843	43.910	23.836	1.00	55.28	C
ATOM	655	O	VAL A 524	21.082	44.557	24.859	1.00	55.13	O
ATOM	656	N	ALA A 525	21.163	44.333	22.615	1.00	55.14	N
ATOM	657	CA	ALA A 525	22.159	45.378	22.398	1.00	55.16	C
ATOM	658	CB	ALA A 525	23.554	44.771	22.320	1.00	55.05	C
ATOM	659	C	ALA A 525	21.852	46.177	21.134	1.00	55.05	C
ATOM	660	O	ALA A 525	21.448	45.613	20.117	1.00	55.30	O
ATOM	661	N	PRO A 526	22.050	47.495	21.201	1.00	54.81	N
ATOM	662	CA	PRO A 526	21.414	48.413	20.251	1.00	54.62	C
ATOM	663	CB	PRO A 526	21.428	49.749	20.998	1.00	54.45	C
ATOM	664	CG	PRO A 526	22.602	49.655	21.898	1.00	54.50	C
ATOM	665	CD	PRO A 526	22.700	48.213	22.313	1.00	54.97	C
ATOM	666	C	PRO A 526	22.188	48.533	18.942	1.00	54.37	C
ATOM	667	O	PRO A 526	23.383	48.833	18.953	1.00	54.76	O
ATOM	668	N	ARG A 527	21.505	48.280	17.828	1.00	53.90	N

Figure 1 Table 1a - 11

ATOM	669	CA	ARG	A	527	21.242	49.322	16.843	1.00 53.25	C
ATOM	670	CB	ARG	A	527	21.073	48.758	15.439	1.00 53.99	C
ATOM	671	CG	ARG	A	527	20.614	47.301	15.397	1.00 55.93	C
ATOM	672	CD	ARG	A	527	19.295	47.148	14.645	1.00 59.52	C
ATOM	673	NE	ARG	A	527	18.685	48.435	14.314	1.00 61.89	N
ATOM	674	CZ	ARG	A	527	17.547	48.881	14.839	1.00 62.89	C
ATOM	675	NH1	ARG	A	527	16.889	48.147	15.727	1.00 63.41	N
ATOM	676	NH2	ARG	A	527	17.065	50.062	14.476	1.00 63.45	N
ATOM	677	C	ARG	A	527	22.174	50.524	16.874	1.00 51.89	C
ATOM	678	O	ARG	A	527	22.239	51.247	17.871	1.00 51.69	O
ATOM	679	N	PRO	A	528	22.907	50.732	15.780	1.00 50.61	N
ATOM	680	CA	PRO	A	528	23.360	52.077	15.411	1.00 49.22	C
ATOM	681	CB	PRO	A	528	24.195	51.828	14.152	1.00 49.04	C
ATOM	682	CG	PRO	A	528	24.704	50.435	14.316	1.00 50.19	C
ATOM	683	CD	PRO	A	528	23.610	49.681	15.021	1.00 50.52	C
ATOM	684	C	PRO	A	528	22.188	53.005	15.093	1.00 47.84	C
ATOM	685	O	PRO	A	528	21.203	52.574	14.489	1.00 48.05	O
ATOM	686	N	GLY	A	529	22.299	54.263	15.503	1.00 45.75	N
ATOM	687	CA	GLY	A	529	21.221	55.219	15.337	1.00 44.01	C
ATOM	688	C	GLY	A	529	20.733	55.800	16.650	1.00 42.09	C
ATOM	689	O	GLY	A	529	20.533	55.078	17.624	1.00 42.20	O
ATOM	690	N	SER	A	530	20.550	57.116	16.672	1.00 40.45	N
ATOM	691	CA	SER	A	530	19.538	57.742	17.518	1.00 39.05	C
ATOM	692	CB	SER	A	530	20.094	58.022	18.916	1.00 38.66	C
ATOM	693	OG	SER	A	530	19.323	59.009	19.581	1.00 38.16	O
ATOM	694	C	SER	A	530	19.040	59.034	16.885	1.00 38.08	C
ATOM	695	O	SER	A	530	19.813	59.968	16.672	1.00 37.87	O
ATOM	696	N	HIS	A	531	17.746	59.081	16.586	1.00 37.29	N
ATOM	697	CA	HIS	A	531	17.154	60.237	15.928	1.00 37.63	C
ATOM	698	CB	HIS	A	531	15.637	60.070	15.811	1.00 38.55	C
ATOM	699	CG	HIS	A	531	14.989	61.064	14.897	1.00 41.89	C
ATOM	700	ND1	HIS	A	531	14.413	62.231	15.354	1.00 45.23	N
ATOM	701	CE1	HIS	A	531	13.924	62.909	14.331	1.00 45.28	C
ATOM	702	NE2	HIS	A	531	14.162	62.225	13.226	1.00 46.33	N
ATOM	703	CD2	HIS	A	531	14.826	61.067	13.552	1.00 45.25	C
ATOM	704	C	HIS	A	531	17.487	61.529	16.673	1.00 36.51	C
ATOM	705	O	HIS	A	531	17.802	62.547	16.057	1.00 35.91	O
ATOM	706	N	THR	A	532	17.421	61.479	17.999	1.00 35.50	N
ATOM	707	CA	THR	A	532	17.683	62.663	18.829	1.00 34.85	C
ATOM	708	CB	THR	A	532	17.223	62.481	20.287	1.00 34.77	C
ATOM	709	OG1	THR	A	532	15.792	62.474	20.325	1.00 35.86	O
ATOM	710	CG2	THR	A	532	17.720	63.635	21.173	1.00 35.80	C
ATOM	711	C	THR	A	532	19.146	63.080	18.790	1.00 34.52	C
ATOM	712	O	THR	A	532	19.446	64.253	18.622	1.00 34.52	O
ATOM	713	N	ILE	A	533	20.065	62.131	18.940	1.00 34.20	N
ATOM	714	CA	ILE	A	533	21.475	62.510	18.949	1.00 33.90	C
ATOM	715	CB	ILE	A	533	22.382	61.381	19.455	1.00 32.96	C
ATOM	716	CG1	ILE	A	533	22.003	60.983	20.898	1.00 32.44	C
ATOM	717	CD1	ILE	A	533	22.001	62.132	21.948	1.00 30.05	C
ATOM	718	CG2	ILE	A	533	23.854	61.793	19.336	1.00 33.01	C
ATOM	719	C	ILE	A	533	21.924	62.994	17.560	1.00 34.20	C
ATOM	720	O	ILE	A	533	22.715	63.947	17.441	1.00 33.75	O
ATOM	721	N	GLU	A	534	21.418	62.326	16.525	1.00 34.13	N
ATOM	722	CA	GLU	A	534	21.661	62.726	15.142	1.00 35.28	C
ATOM	723	CB	GLU	A	534	21.065	61.695	14.190	1.00 35.18	C
ATOM	724	CG	GLU	A	534	21.858	60.424	14.182	1.00 37.32	C
ATOM	725	CD	GLU	A	534	21.211	59.363	13.363	1.00 38.09	C
ATOM	726	OE1	GLU	A	534	20.976	59.610	12.165	1.00 41.88	O
ATOM	727	OE2	GLU	A	534	20.942	58.289	13.919	1.00 39.02	O
ATOM	728	C	GLU	A	534	21.139	64.117	14.798	1.00 35.46	C
ATOM	729	O	GLU	A	534	21.764	64.831	14.016	1.00 35.79	O
ATOM	730	N	PHE	A	535	19.999	64.500	15.375	1.00 35.61	N
ATOM	731	CA	PHE	A	535	19.494	65.875	15.222	1.00 35.31	C
ATOM	732	CB	PHE	A	535	18.103	66.021	15.875	1.00 34.73	C
ATOM	733	CG	PHE	A	535	17.689	67.456	16.150	1.00 35.08	C
ATOM	734	CD1	PHE	A	535	17.426	68.350	15.096	1.00 34.15	C
ATOM	735	CE1	PHE	A	535	17.043	69.666	15.354	1.00 32.87	C

Figure 1 Table 1a - 12

ATOM	736	CZ	PHE A 535	16.907	70.107	16.663	1.00	32.72	C
ATOM	737	CE2	PHE A 535	17.178	69.232	17.723	1.00	34.39	C
ATOM	738	CD2	PHE A 535	17.555	67.907	17.453	1.00	33.31	C
ATOM	739	C	PHE A 535	20.518	66.872	15.779	1.00	35.80	C
ATOM	740	O	PHE A 535	20.856	67.880	15.123	1.00	35.11	O
ATOM	741	N	PHE A 536	21.046	66.571	16.969	1.00	35.81	N
ATOM	742	CA	PHE A 536	22.088	67.413	17.585	1.00	35.81	C
ATOM	743	CB	PHE A 536	22.517	66.866	18.957	1.00	35.11	C
ATOM	744	CG	PHE A 536	21.449	66.963	20.033	1.00	35.21	C
ATOM	745	CD1	PHE A 536	21.390	66.021	21.050	1.00	32.48	C
ATOM	746	CE1	PHE A 536	20.409	66.093	22.049	1.00	34.45	C
ATOM	747	CZ	PHE A 536	19.469	67.113	22.026	1.00	32.56	C
ATOM	748	CE2	PHE A 536	19.509	68.053	20.997	1.00	34.86	C
ATOM	749	CD2	PHE A 536	20.494	67.972	20.009	1.00	35.32	C
ATOM	750	C	PHE A 536	23.330	67.548	16.685	1.00	36.07	C
ATOM	751	O	PHE A 536	23.880	68.646	16.518	1.00	35.59	O
ATOM	752	N	GLU A 537	23.773	66.424	16.129	1.00	36.50	N
ATOM	753	CA	GLU A 537	24.967	66.408	15.291	1.00	37.26	C
ATOM	754	CB	GLU A 537	25.432	64.983	15.005	1.00	37.41	C
ATOM	755	CG	GLU A 537	26.024	64.300	16.258	1.00	37.17	C
ATOM	756	CD	GLU A 537	26.735	63.006	15.958	1.00	39.02	C
ATOM	757	OE1	GLU A 537	26.344	62.312	14.988	1.00	40.47	O
ATOM	758	OE2	GLU A 537	27.675	62.665	16.714	1.00	39.73	O
ATOM	759	C	GLU A 537	24.746	67.184	14.008	1.00	38.13	C
ATOM	760	O	GLU A 537	25.633	67.936	13.599	1.00	38.28	O
ATOM	761	N	MET A 538	23.571	67.005	13.390	1.00	38.54	N
ATOM	762	CA	MET A 538	23.175	67.784	12.212	1.00	40.39	C
ATOM	763	CB	MET A 538	21.744	67.472	11.788	1.00	39.60	C
ATOM	764	CG	MET A 538	21.591	66.281	10.864	1.00	44.34	C
ATOM	765	SD	MET A 538	20.054	66.424	9.914	1.00	46.49	S
ATOM	766	CE	MET A 538	18.907	65.867	11.173	1.00	48.06	C
ATOM	767	C	MET A 538	23.270	69.282	12.496	1.00	39.62	C
ATOM	768	O	MET A 538	23.848	70.034	11.700	1.00	39.63	O
ATOM	769	N	CYS A 539	22.669	69.707	13.611	1.00	39.25	N
ATOM	770	CA	CYS A 539	22.711	71.109	14.041	1.00	39.46	C
ATOM	771	CB	CYS A 539	21.911	71.315	15.327	1.00	39.42	C
ATOM	772	SG	CYS A 539	20.132	71.082	15.165	1.00	41.36	S
ATOM	773	C	CYS A 539	24.128	71.598	14.262	1.00	39.58	C
ATOM	774	O	CYS A 539	24.510	72.661	13.760	1.00	39.59	O
ATOM	775	N	ALA A 540	24.911	70.834	15.018	1.00	39.57	N
ATOM	776	CA	ALA A 540	26.273	71.229	15.312	1.00	40.22	C
ATOM	777	CB	ALA A 540	26.932	70.254	16.285	1.00	40.16	C
ATOM	778	C	ALA A 540	27.082	71.346	14.020	1.00	40.72	C
ATOM	779	O	ALA A 540	27.874	72.273	13.876	1.00	40.41	O
ATOM	780	N	ASN A 541	26.871	70.406	13.096	1.00	40.99	N
ATOM	781	CA	ASN A 541	27.575	70.383	11.826	1.00	41.94	C
ATOM	782	CB	ASN A 541	27.284	69.089	11.054	1.00	42.15	C
ATOM	783	CG	ASN A 541	27.921	67.861	11.689	1.00	44.38	C
ATOM	784	OD1	ASN A 541	28.768	67.969	12.583	1.00	46.59	O
ATOM	785	ND2	ASN A 541	27.513	66.678	11.227	1.00	45.19	N
ATOM	786	C	ASN A 541	27.203	71.591	10.968	1.00	42.18	C
ATOM	787	O	ASN A 541	28.074	72.239	10.382	1.00	41.58	O
ATOM	788	N	LEU A 542	25.909	71.891	10.898	1.00	42.46	N
ATOM	789	CA	LEU A 542	25.467	73.054	10.143	1.00	43.41	C
ATOM	790	CB	LEU A 542	23.948	73.114	10.037	1.00	43.92	C
ATOM	791	CG	LEU A 542	23.455	72.477	8.742	1.00	46.28	C
ATOM	792	CD1	LEU A 542	21.960	72.346	8.786	1.00	49.10	C
ATOM	793	CD2	LEU A 542	23.888	73.339	7.540	1.00	46.96	C
ATOM	794	C	LEU A 542	26.034	74.349	10.707	1.00	43.25	C
ATOM	795	O	LEU A 542	26.518	75.173	9.947	1.00	42.69	O
ATOM	796	N	ILE A 543	25.992	74.498	12.030	1.00	43.35	N
ATOM	797	CA	ILE A 543	26.535	75.672	12.710	1.00	43.79	C
ATOM	798	CB	ILE A 543	26.233	75.635	14.231	1.00	43.83	C
ATOM	799	CG1	ILE A 543	24.726	75.851	14.475	1.00	43.94	C
ATOM	800	CD1	ILE A 543	24.257	75.521	15.906	1.00	43.15	C
ATOM	801	CG2	ILE A 543	27.068	76.691	14.982	1.00	43.28	C
ATOM	802	C	ILE A 543	28.040	75.847	12.438	1.00	44.27	C

Figure 1 Table 1a - 13

ATOM	803	O	ILE	A	543	28.487	76.913	12.000	1.00	44.02	O
ATOM	804	N	LYS	A	544	28.814	74.791	12.680	1.00	44.70	N
ATOM	805	CA	LYS	A	544	30.256	74.831	12.458	1.00	45.23	C
ATOM	806	CB	LYS	A	544	30.875	73.450	12.698	1.00	44.95	C
ATOM	807	CG	LYS	A	544	32.366	73.390	12.431	1.00	45.61	C
ATOM	808	CD	LYS	A	544	33.012	72.110	12.936	1.00	47.04	C
ATOM	809	CE	LYS	A	544	34.546	72.222	12.850	1.00	48.65	C
ATOM	810	NZ	LYS	A	544	35.250	71.080	13.524	1.00	50.34	N
ATOM	811	C	LYS	A	544	30.593	75.326	11.047	1.00	45.31	C
ATOM	812	O	LYS	A	544	31.544	76.088	10.850	1.00	44.79	O
ATOM	813	N	ILE	A	545	29.803	74.889	10.072	1.00	45.67	N
ATOM	814	CA	ILE	A	545	30.213	74.947	8.674	1.00	46.46	C
ATOM	815	CB	ILE	A	545	29.886	73.634	7.935	1.00	46.42	C
ATOM	816	CG1	ILE	A	545	30.154	72.432	8.846	1.00	47.52	C
ATOM	817	CD1	ILE	A	545	31.127	71.427	8.273	1.00	48.78	C
ATOM	818	CG2	ILE	A	545	30.700	73.522	6.659	1.00	47.24	C
ATOM	819	C	ILE	A	545	29.574	76.129	7.951	1.00	46.43	C
ATOM	820	O	ILE	A	545	29.478	76.141	6.722	1.00	46.75	O
ATOM	821	N	LEU	A	546	29.148	77.127	8.721	1.00	46.29	N
ATOM	822	CA	LEU	A	546	28.364	78.230	8.178	1.00	46.45	C
ATOM	823	CB	LEU	A	546	26.921	77.783	7.939	1.00	46.57	C
ATOM	824	CG	LEU	A	546	25.888	78.124	9.012	1.00	47.48	C
ATOM	825	CD1	LEU	A	546	24.705	77.179	8.927	1.00	51.48	C
ATOM	826	CD2	LEU	A	546	26.500	78.067	10.390	1.00	48.82	C
ATOM	827	C	LEU	A	546	28.389	79.458	9.092	1.00	46.03	C
ATOM	828	O	LEU	A	546	27.996	80.552	8.685	1.00	45.61	O
ATOM	829	N	ALA	A	547	28.851	79.264	10.324	1.00	45.37	N
ATOM	830	CA	ALA	A	547	28.694	80.263	11.376	1.00	44.92	C
ATOM	831	CB	ALA	A	547	27.782	79.728	12.491	1.00	43.79	C
ATOM	832	C	ALA	A	547	30.045	80.665	11.950	1.00	45.09	C
ATOM	833	O	ALA	A	547	30.984	79.867	11.962	1.00	45.34	O
ATOM	834	N	GLN	A	548	30.133	81.906	12.424	1.00	44.98	N
ATOM	835	CA	GLN	A	548	31.288	82.375	13.183	1.00	44.77	C
ATOM	836	CB	GLN	A	548	30.948	82.483	14.674	1.00	44.06	C
ATOM	837	CG	GLN	A	548	32.085	82.104	15.604	1.00	44.78	C
ATOM	838	CD	GLN	A	548	32.125	82.957	16.860	1.00	47.07	C
ATOM	839	OE1	GLN	A	548	32.446	84.149	16.809	1.00	45.39	O
ATOM	840	NE2	GLN	A	548	31.808	82.349	17.998	1.00	47.60	N
ATOM	841	C	GLN	A	548	32.518	81.494	12.975	1.00	45.00	C
ATOM	842	O	GLN	A	548	33.538	81.959	12.456	1.00	44.62	O
ATOM	843	N	GLY	B	190	-0.498	94.476	-28.920	1.00	47.53	N
ATOM	844	CA	GLY	B	190	0.180	93.607	-27.911	1.00	47.38	C
ATOM	845	C	GLY	B	190	1.004	94.399	-26.910	1.00	47.23	C
ATOM	846	O	GLY	B	190	2.232	94.507	-27.046	1.00	47.78	O
ATOM	847	N	GLN	B	191	0.327	94.935	-25.895	1.00	46.36	N
ATOM	848	CA	GLN	B	191	0.945	95.820	-24.907	1.00	45.15	C
ATOM	849	CB	GLN	B	191	-0.154	96.544	-24.118	1.00	44.94	C
ATOM	850	CG	GLN	B	191	0.309	97.677	-23.209	1.00	43.91	C
ATOM	851	CD	GLN	B	191	-0.819	98.207	-22.328	1.00	44.11	C
ATOM	852	OE1	GLN	B	191	-1.685	97.450	-21.883	1.00	43.56	O
ATOM	853	NE2	GLN	B	191	-0.810	99.511	-22.072	1.00	41.51	N
ATOM	854	C	GLN	B	191	1.878	95.073	-23.958	1.00	44.77	C
ATOM	855	O	GLN	B	191	1.640	93.911	-23.623	1.00	44.99	O
ATOM	856	N	GLU	B	192	2.942	95.751	-23.532	1.00	44.23	N
ATOM	857	CA	GLU	B	192	3.814	95.248	-22.473	1.00	44.00	C
ATOM	858	CB	GLU	B	192	4.984	96.215	-22.225	1.00	44.05	C
ATOM	859	CG	GLU	B	192	4.636	97.529	-21.475	1.00	43.25	C
ATOM	860	CD	GLU	B	192	3.913	98.584	-22.321	1.00	42.99	C
ATOM	861	OE1	GLU	B	192	3.953	98.534	-23.571	1.00	42.68	O
ATOM	862	OE2	GLU	B	192	3.295	99.482	-21.714	1.00	41.53	O
ATOM	863	C	GLU	B	192	3.005	95.027	-21.189	1.00	43.99	C
ATOM	864	O	GLU	B	192	2.072	95.784	-20.895	1.00	43.52	O
ATOM	865	N	MET	B	193	3.355	93.985	-20.446	1.00	43.98	N
ATOM	866	CA	MET	B	193	2.668	93.657	-19.196	1.00	44.34	C
ATOM	867	CB	MET	B	193	2.291	92.173	-19.144	1.00	44.54	C
ATOM	868	CG	MET	B	193	1.160	91.814	-20.114	1.00	45.77	C
ATOM	869	SD	MET	B	193	-0.003	90.606	-19.446	1.00	47.31	S

Figure 1 Table 1a - 14

ATOM	870	CE	MET	B	193	-1.241	90.639	-20.736	1.00	45.99	C
ATOM	871	C	MET	B	193	3.480	94.049	-17.968	1.00	43.70	C
ATOM	872	O	MET	B	193	4.710	93.986	-17.975	1.00	43.92	O
ATOM	873	N	TYR	B	194	2.772	94.437	-16.913	1.00	42.80	N
ATOM	874	CA	TYR	B	194	3.392	95.000	-15.726	1.00	41.95	C
ATOM	875	CB	TYR	B	194	2.737	96.349	-15.381	1.00	41.37	C
ATOM	876	CG	TYR	B	194	2.981	97.392	-16.445	1.00	40.39	C
ATOM	877	CD1	TYR	B	194	2.281	97.356	-17.653	1.00	39.29	C
ATOM	878	CE1	TYR	B	194	2.508	98.296	-18.644	1.00	39.23	C
ATOM	879	CZ	TYR	B	194	3.447	99.293	-18.439	1.00	39.56	C
ATOM	880	OH	TYR	B	194	3.667	100.224	-19.425	1.00	40.80	O
ATOM	881	CE2	TYR	B	194	4.161	99.357	-17.248	1.00	40.04	C
ATOM	882	CD2	TYR	B	194	3.928	98.400	-16.259	1.00	40.12	C
ATOM	883	C	TYR	B	194	3.336	94.055	-14.540	1.00	42.06	C
ATOM	884	O	TYR	B	194	2.372	93.310	-14.369	1.00	42.13	O
ATOM	885	N	ALA	B	195	4.385	94.090	-13.731	1.00	42.02	N
ATOM	886	CA	ALA	B	195	4.483	93.243	-12.564	1.00	42.42	C
ATOM	887	CB	ALA	B	195	5.775	92.450	-12.589	1.00	42.24	C
ATOM	888	C	ALA	B	195	4.387	94.068	-11.287	1.00	42.74	C
ATOM	889	O	ALA	B	195	5.082	95.071	-11.126	1.00	41.89	O
ATOM	890	N	PHE	B	196	3.524	93.616	-10.386	1.00	43.60	N
ATOM	891	CA	PHE	B	196	3.319	94.266	-9.104	1.00	45.06	C
ATOM	892	CB	PHE	B	196	1.830	94.512	-8.861	1.00	43.51	C
ATOM	893	CG	PHE	B	196	1.220	95.516	-9.802	1.00	41.72	C
ATOM	894	CD1	PHE	B	196	0.880	95.160	-11.104	1.00	38.53	C
ATOM	895	CE1	PHE	B	196	0.310	96.100	-11.980	1.00	38.54	C
ATOM	896	CZ	PHE	B	196	0.083	97.397	-11.550	1.00	37.40	C
ATOM	897	CE2	PHE	B	196	0.413	97.764	-10.257	1.00	37.43	C
ATOM	898	CD2	PHE	B	196	0.983	96.825	-9.384	1.00	38.63	C
ATOM	899	C	PHE	B	196	3.908	93.368	-8.030	1.00	47.33	C
ATOM	900	O	PHE	B	196	3.414	92.260	-7.782	1.00	46.82	O
ATOM	901	N	ARG	B	197	4.980	93.847	-7.411	1.00	50.72	N
ATOM	902	CA	ARG	B	197	5.746	93.039	-6.469	1.00	54.44	C
ATOM	903	CB	ARG	B	197	7.249	93.138	-6.755	1.00	54.59	C
ATOM	904	CG	ARG	B	197	7.721	92.177	-7.822	1.00	56.22	C
ATOM	905	CD	ARG	B	197	9.026	92.638	-8.469	1.00	59.31	C
ATOM	906	NE	ARG	B	197	9.231	92.078	-9.814	1.00	61.19	N
ATOM	907	CZ	ARG	B	197	8.750	90.907	-10.236	1.00	61.91	C
ATOM	908	NH1	ARG	B	197	8.024	90.142	-9.424	1.00	61.43	N
ATOM	909	NH2	ARG	B	197	9.001	90.491	-11.473	1.00	62.02	N
ATOM	910	C	ARG	B	197	5.462	93.482	-5.057	1.00	56.68	C
ATOM	911	O	ARG	B	197	6.013	94.490	-4.594	1.00	56.67	O
ATOM	912	N	SER	B	198	4.588	92.723	-4.393	1.00	59.70	N
ATOM	913	CA	SER	B	198	4.282	92.884	-2.969	1.00	62.76	C
ATOM	914	CB	SER	B	198	3.808	91.549	-2.383	1.00	62.73	C
ATOM	915	OG	SER	B	198	4.723	90.509	-2.695	1.00	63.64	O
ATOM	916	C	SER	B	198	5.529	93.341	-2.232	1.00	64.55	C
ATOM	917	O	SER	B	198	5.479	94.209	-1.352	1.00	65.10	O
ATOM	918	N	GLU	B	199	6.648	92.739	-2.637	1.00	66.79	N
ATOM	919	CA	GLU	B	199	7.980	93.066	-2.157	1.00	68.74	C
ATOM	920	CB	GLU	B	199	8.353	94.528	-2.443	1.00	68.90	C
ATOM	921	CG	GLU	B	199	9.783	94.703	-2.948	1.00	70.67	C
ATOM	922	CD	GLU	B	199	10.373	96.064	-2.609	1.00	73.05	C
ATOM	923	OE1	GLU	B	199	9.606	96.999	-2.286	1.00	73.66	O
ATOM	924	OE2	GLU	B	199	11.617	96.194	-2.660	1.00	74.36	O
ATOM	925	C	GLU	B	199	8.040	92.746	-0.681	1.00	69.57	C
ATOM	926	O	GLU	B	199	8.541	91.678	-0.299	1.00	70.09	O
ATOM	927	N	GLU	B	200	7.513	93.634	0.160	1.00	70.45	N
ATOM	928	CA	GLU	B	200	7.656	93.371	1.551	1.00	71.06	C
ATOM	929	CB	GLU	B	200	8.881	94.003	2.195	1.00	71.38	C
ATOM	930	CG	GLU	B	200	10.166	93.205	1.829	1.00	72.72	C
ATOM	931	CD	GLU	B	200	10.918	93.758	0.625	1.00	74.70	C
ATOM	932	OE1	GLU	B	200	10.384	94.664	-0.054	1.00	75.28	O
ATOM	933	OE2	GLU	B	200	12.053	93.277	0.357	1.00	75.72	O
ATOM	934	C	GLU	B	200	6.687	92.622	2.454	1.00	70.98	C
ATOM	935	O	GLU	B	200	5.997	93.223	3.284	1.00	71.26	O
ATOM	936	N	ARG	B	201	6.631	91.310	2.258	1.00	70.62	N

Figure 1 Table 1a - 15

ATOM	937	CA	ARG	B	201	5.979	90.408	3.188	1.00	70.28	C
ATOM	938	CB	ARG	B	201	5.216	89.327	2.430	1.00	70.57	C
ATOM	939	CG	ARG	B	201	4.599	89.739	1.088	1.00	71.54	C
ATOM	940	CD	ARG	B	201	4.096	88.488	0.337	1.00	72.77	C
ATOM	941	NE	ARG	B	201	3.915	87.344	1.238	1.00	74.51	N
ATOM	942	CZ	ARG	B	201	2.970	87.254	2.177	1.00	75.34	C
ATOM	943	NH1	ARG	B	201	2.096	88.243	2.355	1.00	75.70	N
ATOM	944	NH2	ARG	B	201	2.905	86.179	2.951	1.00	75.91	N
ATOM	945	C	ARG	B	201	7.071	89.732	4.007	1.00	69.36	C
ATOM	946	O	ARG	B	201	6.868	89.344	5.164	1.00	69.19	O
ATOM	947	N	PHE	B	202	8.224	89.576	3.362	1.00	68.17	N
ATOM	948	CA	PHE	B	202	9.405	88.988	3.964	1.00	66.95	C
ATOM	949	CB	PHE	B	202	9.784	87.697	3.225	1.00	66.56	C
ATOM	950	CG	PHE	B	202	8.735	86.621	3.301	1.00	65.46	C
ATOM	951	CD1	PHE	B	202	7.875	86.396	2.233	1.00	64.25	C
ATOM	952	CE1	PHE	B	202	6.904	85.397	2.296	1.00	64.07	C
ATOM	953	CZ	PHE	B	202	6.787	84.609	3.442	1.00	64.39	C
ATOM	954	CE2	PHE	B	202	7.641	84.823	4.514	1.00	64.18	C
ATOM	955	CD2	PHE	B	202	8.613	85.827	4.438	1.00	64.44	C
ATOM	956	C	PHE	B	202	10.541	90.007	3.902	1.00	66.50	C
ATOM	957	O	PHE	B	202	11.655	89.684	3.469	1.00	66.38	O
ATOM	958	N	LYS	B	203	10.240	91.244	4.309	1.00	65.74	N
ATOM	959	CA	LYS	B	203	11.251	92.293	4.455	1.00	65.02	C
ATOM	960	CB	LYS	B	203	10.614	93.603	4.939	1.00	65.09	C
ATOM	961	CG	LYS	B	203	11.517	94.827	4.800	1.00	65.31	C
ATOM	962	CD	LYS	B	203	10.952	96.031	5.540	1.00	66.09	C
ATOM	963	CE	LYS	B	203	9.993	96.841	4.677	1.00	65.81	C
ATOM	964	NZ	LYS	B	203	9.576	98.087	5.388	1.00	66.94	N
ATOM	965	C	LYS	B	203	12.269	91.823	5.471	1.00	64.28	C
ATOM	966	O	LYS	B	203	13.462	91.706	5.180	1.00	64.44	O
ATOM	967	N	SER	B	204	11.767	91.536	6.666	1.00	63.13	N
ATOM	968	CA	SER	B	204	12.582	91.042	7.752	1.00	62.18	C
ATOM	969	CB	SER	B	204	12.591	92.066	8.881	1.00	62.13	C
ATOM	970	OG	SER	B	204	11.268	92.418	9.234	1.00	61.92	O
ATOM	971	C	SER	B	204	12.017	89.712	8.243	1.00	61.45	C
ATOM	972	O	SER	B	204	10.827	89.438	8.051	1.00	61.03	O
ATOM	973	N	PRO	B	205	12.870	88.876	8.869	1.00	60.80	N
ATOM	974	CA	PRO	B	205	12.387	87.664	9.513	1.00	60.62	C
ATOM	975	CB	PRO	B	205	13.600	87.191	10.314	1.00	60.42	C
ATOM	976	CG	PRO	B	205	14.756	87.708	9.581	1.00	60.15	C
ATOM	977	CD	PRO	B	205	14.335	89.009	8.985	1.00	60.64	C
ATOM	978	C	PRO	B	205	11.217	87.952	10.449	1.00	60.83	C
ATOM	979	O	PRO	B	205	11.149	89.040	11.030	1.00	60.71	O
ATOM	980	N	PRO	B	206	10.299	86.985	10.599	1.00	61.25	N
ATOM	981	CA	PRO	B	206	9.172	87.178	11.501	1.00	61.94	C
ATOM	982	CB	PRO	B	206	8.471	85.813	11.485	1.00	61.65	C
ATOM	983	CG	PRO	B	206	9.477	84.860	10.948	1.00	61.16	C
ATOM	984	CD	PRO	B	206	10.278	85.646	9.982	1.00	61.01	C
ATOM	985	C	PRO	B	206	9.638	87.496	12.914	1.00	62.97	C
ATOM	986	O	PRO	B	206	10.712	87.052	13.329	1.00	62.73	O
ATOM	987	N	ILE	B	207	8.836	88.264	13.643	1.00	64.37	N
ATOM	988	CA	ILE	B	207	9.099	88.484	15.060	1.00	65.95	C
ATOM	989	CB	ILE	B	207	8.236	89.619	15.677	1.00	65.86	C
ATOM	990	CG1	ILE	B	207	6.733	89.323	15.553	1.00	66.53	C
ATOM	991	CD1	ILE	B	207	6.114	88.656	16.784	1.00	66.66	C
ATOM	992	CG2	ILE	B	207	8.598	90.957	15.048	1.00	66.08	C
ATOM	993	C	ILE	B	207	8.891	87.169	15.785	1.00	66.75	C
ATOM	994	O	ILE	B	207	8.142	86.306	15.320	1.00	66.70	O
ATOM	995	N	LEU	B	208	9.562	87.017	16.917	1.00	68.12	N
ATOM	996	CA	LEU	B	208	9.691	85.707	17.538	1.00	69.22	C
ATOM	997	CB	LEU	B	208	10.702	85.745	18.700	1.00	69.30	C
ATOM	998	CG	LEU	B	208	11.021	84.445	19.451	1.00	68.85	C
ATOM	999	CD1	LEU	B	208	11.583	83.378	18.526	1.00	68.37	C
ATOM	1000	CD2	LEU	B	208	11.993	84.732	20.573	1.00	68.98	C
ATOM	1001	C	LEU	B	208	8.371	85.031	17.946	1.00	70.24	C
ATOM	1002	O	LEU	B	208	7.900	84.143	17.235	1.00	70.49	O
ATOM	1003	N	PRO	B	209	7.754	85.479	19.055	1.00	71.23	N

Figure 1 Table 1a - 16

ATOM	1004	CA	PRO	B	209	7.010	84.522	19.881	1.00	72.06	C
ATOM	1005	CB	PRO	B	209	6.958	85.221	21.251	1.00	72.12	C
ATOM	1006	CG	PRO	B	209	6.997	86.676	20.940	1.00	71.58	C
ATOM	1007	CD	PRO	B	209	7.700	86.847	19.610	1.00	71.32	C
ATOM	1008	C	PRO	B	209	5.597	84.095	19.431	1.00	72.82	C
ATOM	1009	O	PRO	B	209	4.632	84.859	19.608	1.00	72.91	O
ATOM	1010	N	PRO	B	210	5.479	82.874	18.854	1.00	73.31	N
ATOM	1011	CA	PRO	B	210	4.223	82.130	19.005	1.00	73.74	C
ATOM	1012	CB	PRO	B	210	4.445	80.867	18.157	1.00	73.73	C
ATOM	1013	CG	PRO	B	210	5.916	80.754	17.979	1.00	73.57	C
ATOM	1014	CD	PRO	B	210	6.465	82.141	18.039	1.00	73.22	C
ATOM	1015	C	PRO	B	210	4.097	81.811	20.499	1.00	74.01	C
ATOM	1016	O	PRO	B	210	3.338	82.483	21.206	1.00	74.16	O
ATOM	1017	N	HIS	B	211	4.827	80.791	20.959	1.00	74.16	N
ATOM	1018	CA	HIS	B	211	5.428	80.826	22.266	1.00	74.36	C
ATOM	1019	CB	HIS	B	211	4.566	81.183	23.438	1.00	74.53	C
ATOM	1020	CG	HIS	B	211	4.968	82.489	24.053	1.00	75.49	C
ATOM	1021	ND1	HIS	B	211	5.459	82.590	25.338	1.00	76.52	N
ATOM	1022	CE1	HIS	B	211	5.766	83.853	25.589	1.00	76.84	C
ATOM	1023	NE2	HIS	B	211	5.523	84.569	24.503	1.00	76.92	N
ATOM	1024	CD2	HIS	B	211	5.038	83.737	23.523	1.00	76.11	C
ATOM	1025	C	HIS	B	211	6.880	80.661	22.584	1.00	74.09	C
ATOM	1026	O	HIS	B	211	7.245	80.242	23.689	1.00	74.16	O
ATOM	1027	N	LEU	B	212	7.719	80.964	21.603	1.00	73.72	N
ATOM	1028	CA	LEU	B	212	9.124	80.611	21.682	1.00	73.13	C
ATOM	1029	CB	LEU	B	212	9.751	80.571	20.288	1.00	73.21	C
ATOM	1030	CG	LEU	B	212	9.501	79.268	19.524	1.00	72.55	C
ATOM	1031	CD1	LEU	B	212	9.971	79.408	18.091	1.00	72.35	C
ATOM	1032	CD2	LEU	B	212	10.177	78.078	20.210	1.00	71.50	C
ATOM	1033	C	LEU	B	212	9.904	81.511	22.625	1.00	72.78	C
ATOM	1034	O	LEU	B	212	10.089	82.701	22.365	1.00	72.88	O
ATOM	1035	N	LEU	B	213	10.336	80.924	23.736	1.00	72.39	N
ATOM	1036	CA	LEU	B	213	11.158	81.623	24.712	1.00	71.93	C
ATOM	1037	CB	LEU	B	213	10.937	81.055	26.119	1.00	72.09	C
ATOM	1038	CG	LEU	B	213	9.681	81.505	26.873	1.00	72.22	C
ATOM	1039	CD1	LEU	B	213	9.403	80.567	28.042	1.00	72.88	C
ATOM	1040	CD2	LEU	B	213	9.809	82.952	27.354	1.00	72.56	C
ATOM	1041	C	LEU	B	213	12.629	81.541	24.327	1.00	71.49	C
ATOM	1042	O	LEU	B	213	13.174	80.446	24.126	1.00	71.53	O
ATOM	1043	N	GLN	B	214	13.251	82.714	24.212	1.00	70.82	N
ATOM	1044	CA	GLN	B	214	14.675	82.845	23.916	1.00	70.35	C
ATOM	1045	CB	GLN	B	214	15.074	84.319	23.911	1.00	70.31	C
ATOM	1046	CG	GLN	B	214	14.959	85.011	22.582	1.00	70.44	C
ATOM	1047	CD	GLN	B	214	15.609	86.370	22.599	1.00	70.03	C
ATOM	1048	OE1	GLN	B	214	16.825	86.485	22.749	1.00	70.05	O
ATOM	1049	NE2	GLN	B	214	14.804	87.413	22.449	1.00	70.46	N
ATOM	1050	C	GLN	B	214	15.547	82.134	24.938	1.00	69.94	C
ATOM	1051	O	GLN	B	214	16.578	81.568	24.589	1.00	69.57	O
ATOM	1052	N	VAL	B	215	15.129	82.203	26.201	1.00	69.80	N
ATOM	1053	CA	VAL	B	215	15.916	81.719	27.327	1.00	69.88	C
ATOM	1054	CB	VAL	B	215	16.563	82.896	28.130	1.00	69.85	C
ATOM	1055	CG1	VAL	B	215	17.431	82.371	29.271	1.00	69.65	C
ATOM	1056	CG2	VAL	B	215	17.395	83.801	27.220	1.00	69.78	C
ATOM	1057	C	VAL	B	215	15.039	80.890	28.263	1.00	70.12	C
ATOM	1058	O	VAL	B	215	13.935	81.298	28.616	1.00	69.95	O
ATOM	1059	N	ILE	B	216	15.536	79.718	28.643	1.00	70.61	N
ATOM	1060	CA	ILE	B	216	14.926	78.922	29.704	1.00	71.30	C
ATOM	1061	CB	ILE	B	216	14.585	77.475	29.240	1.00	71.15	C
ATOM	1062	CG1	ILE	B	216	13.745	77.476	27.950	1.00	71.03	C
ATOM	1063	CD1	ILE	B	216	12.367	78.123	28.049	1.00	70.69	C
ATOM	1064	CG2	ILE	B	216	13.913	76.681	30.366	1.00	71.00	C
ATOM	1065	C	ILE	B	216	15.907	78.876	30.867	1.00	71.97	C
ATOM	1066	O	ILE	B	216	17.058	78.469	30.697	1.00	71.81	O
ATOM	1067	N	LEU	B	217	15.453	79.309	32.039	1.00	73.05	N
ATOM	1068	CA	LEU	B	217	16.285	79.295	33.240	1.00	74.30	C
ATOM	1069	CB	LEU	B	217	16.136	80.605	34.018	1.00	74.24	C
ATOM	1070	CG	LEU	B	217	16.754	81.847	33.364	1.00	74.67	C

Figure 1

Table 1a - 17

ATOM	1071	CD1	LEU	B	217	16.066	83.130	33.828	1.00	74.86	C
ATOM	1072	CD2	LEU	B	217	18.261	81.907	33.613	1.00	75.05	C
ATOM	1073	C	LEU	B	217	15.967	78.090	34.124	1.00	75.06	C
ATOM	1074	O	LEU	B	217	14.868	77.985	34.671	1.00	75.20	O
ATOM	1075	N	ASN	B	218	16.936	77.183	34.244	1.00	76.12	N
ATOM	1076	CA	ASN	B	218	16.771	75.948	35.013	1.00	77.21	C
ATOM	1077	CB	ASN	B	218	16.899	74.718	34.101	1.00	77.27	C
ATOM	1078	CG	ASN	B	218	15.696	74.530	33.189	1.00	78.04	C
ATOM	1079	OD1	ASN	B	218	14.680	75.212	33.327	1.00	78.99	O
ATOM	1080	ND2	ASN	B	218	15.808	73.595	32.254	1.00	78.85	N
ATOM	1081	C	ASN	B	218	17.741	75.826	36.187	1.00	77.76	C
ATOM	1082	O	ASN	B	218	18.890	75.412	36.020	1.00	77.90	O
ATOM	1083	N	LYS	B	219	17.269	76.188	37.374	1.00	78.56	N
ATOM	1084	CA	LYS	B	219	18.044	75.995	38.596	1.00	79.36	C
ATOM	1085	CB	LYS	B	219	17.925	77.218	39.517	1.00	79.29	C
ATOM	1086	CG	LYS	B	219	18.647	77.102	40.869	1.00	79.52	C
ATOM	1087	CD	LYS	B	219	20.169	77.164	40.731	1.00	79.76	C
ATOM	1088	CE	LYS	B	219	20.852	77.477	42.062	1.00	79.81	C
ATOM	1089	NZ	LYS	B	219	20.860	76.321	43.010	1.00	79.65	N
ATOM	1090	C	LYS	B	219	17.585	74.727	39.318	1.00	79.89	C
ATOM	1091	O	LYS	B	219	16.391	74.554	39.579	1.00	80.03	O
ATOM	1092	N	ASP	B	220	18.534	73.838	39.616	1.00	80.48	N
ATOM	1093	CA	ASP	B	220	18.297	72.752	40.558	1.00	81.06	C
ATOM	1094	CB	ASP	B	220	19.475	71.765	40.576	1.00	81.08	C
ATOM	1095	CG	ASP	B	220	19.658	71.023	39.254	1.00	81.37	C
ATOM	1096	OD1	ASP	B	220	19.907	69.797	39.295	1.00	81.05	O
ATOM	1097	OD2	ASP	B	220	19.568	71.659	38.177	1.00	81.62	O
ATOM	1098	C	ASP	B	220	18.139	73.436	41.914	1.00	81.39	C
ATOM	1099	O	ASP	B	220	19.120	73.638	42.638	1.00	81.48	O
ATOM	1100	N	THR	B	221	16.898	73.810	42.233	1.00	81.77	N
ATOM	1101	CA	THR	B	221	16.594	74.672	43.383	1.00	82.16	C
ATOM	1102	CB	THR	B	221	15.061	74.812	43.614	1.00	82.21	C
ATOM	1103	OG1	THR	B	221	14.414	75.159	42.380	1.00	82.27	O
ATOM	1104	CG2	THR	B	221	14.757	75.892	44.658	1.00	82.28	C
ATOM	1105	C	THR	B	221	17.301	74.225	44.667	1.00	82.35	C
ATOM	1106	O	THR	B	221	17.898	75.046	45.369	1.00	82.43	O
ATOM	1107	N	ASN	B	222	17.241	72.924	44.954	1.00	82.52	N
ATOM	1108	CA	ASN	B	222	17.948	72.346	46.097	1.00	82.65	C
ATOM	1109	CB	ASN	B	222	17.106	71.247	46.766	1.00	82.70	C
ATOM	1110	CG	ASN	B	222	17.152	69.921	46.013	1.00	82.92	C
ATOM	1111	OD1	ASN	B	222	16.933	69.864	44.799	1.00	83.30	O
ATOM	1112	ND2	ASN	B	222	17.431	68.844	46.740	1.00	82.91	N
ATOM	1113	C	ASN	B	222	19.331	71.814	45.711	1.00	82.69	C
ATOM	1114	O	ASN	B	222	19.567	71.427	44.560	1.00	82.70	O
ATOM	1115	N	PRO	B	233	3.129	72.117	31.238	1.00	71.35	N
ATOM	1116	CA	PRO	B	233	4.321	72.967	31.258	1.00	71.17	C
ATOM	1117	CB	PRO	B	233	5.479	71.962	31.097	1.00	71.35	C
ATOM	1118	CG	PRO	B	233	4.882	70.605	31.375	1.00	71.53	C
ATOM	1119	CD	PRO	B	233	3.457	70.713	30.934	1.00	71.47	C
ATOM	1120	C	PRO	B	233	4.305	73.967	30.101	1.00	70.84	C
ATOM	1121	O	PRO	B	233	3.257	74.554	29.805	1.00	71.03	O
ATOM	1122	N	ASN	B	234	5.458	74.168	29.465	1.00	70.22	N
ATOM	1123	CA	ASN	B	234	5.534	74.947	28.231	1.00	69.43	C
ATOM	1124	CB	ASN	B	234	6.949	75.486	27.999	1.00	69.82	C
ATOM	1125	CG	ASN	B	234	7.362	76.556	29.017	1.00	70.32	C
ATOM	1126	OD1	ASN	B	234	7.954	77.576	28.649	1.00	71.34	O
ATOM	1127	ND2	ASN	B	234	7.069	76.319	30.292	1.00	70.64	N
ATOM	1128	C	ASN	B	234	5.095	74.056	27.073	1.00	68.50	C
ATOM	1129	O	ASN	B	234	5.746	73.048	26.764	1.00	68.47	O
ATOM	1130	N	HIS	B	235	3.988	74.439	26.440	1.00	67.17	N
ATOM	1131	CA	HIS	B	235	3.252	73.558	25.520	1.00	65.65	C
ATOM	1132	CB	HIS	B	235	2.060	74.296	24.879	1.00	65.99	C
ATOM	1133	CG	HIS	B	235	1.095	74.868	25.876	1.00	66.94	C
ATOM	1134	ND1	HIS	B	235	0.533	74.115	26.888	1.00	67.97	N
ATOM	1135	CE1	HIS	B	235	-0.274	74.878	27.605	1.00	68.17	C
ATOM	1136	NE2	HIS	B	235	-0.262	76.096	27.093	1.00	68.24	N
ATOM	1137	CD2	HIS	B	235	0.587	76.116	26.010	1.00	67.66	C

Figure 1 Table 1a - 18

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ATOM   1138  C   HIS B 235      4.118  72.846  24.464  1.00 63.95      C
ATOM   1139  O   HIS B 235      4.225  71.613  24.482  1.00 63.82      O
ATOM   1140  N   VAL B 236      4.735  73.617  23.566  1.00 61.65      N
ATOM   1141  CA  VAL B 236      5.553  73.026  22.501  1.00 59.27      C
ATOM   1142  CB  VAL B 236      4.684  72.586  21.277  1.00 59.71      C
ATOM   1143  CG1 VAL B 236      4.307  73.774  20.369  1.00 59.82      C
ATOM   1144  CG2 VAL B 236      5.372  71.485  20.495  1.00 60.04      C
ATOM   1145  C   VAL B 236      6.828  73.823  22.103  1.00 57.26      C
ATOM   1146  O   VAL B 236      6.939  74.406  21.004  1.00 57.00      O
ATOM   1147  N   MET B 237      7.780  73.839  23.034  1.00 54.02      N
ATOM   1148  CA  MET B 237      9.185  74.009  22.695  1.00 50.87      C
ATOM   1149  CB  MET B 237      9.968  74.622  23.855  1.00 51.12      C
ATOM   1150  CG  MET B 237      9.348  74.451  25.231  1.00 52.67      C
ATOM   1151  SD  MET B 237      9.845  75.804  26.352  1.00 56.27      S
ATOM   1152  CE  MET B 237      9.123  77.233  25.537  1.00 55.68      C
ATOM   1153  C   MET B 237      9.737  72.634  22.326  1.00 47.46      C
ATOM   1154  O   MET B 237     10.953  72.449  22.206  1.00 46.01      O
ATOM   1155  N   LEU B 238      8.818  71.679  22.154  1.00 44.04      N
ATOM   1156  CA  LEU B 238      9.151  70.315  21.755  1.00 41.34      C
ATOM   1157  CB  LEU B 238      7.893  69.457  21.575  1.00 41.41      C
ATOM   1158  CG  LEU B 238      7.248  68.819  22.799  1.00 42.05      C
ATOM   1159  CD1 LEU B 238      6.084  67.915  22.361  1.00 42.59      C
ATOM   1160  CD2 LEU B 238      8.268  68.035  23.613  1.00 41.28      C
ATOM   1161  C   LEU B 238      9.940  70.300  20.464  1.00 39.28      C
ATOM   1162  O   LEU B 238      9.610  71.026  19.524  1.00 37.87      O
ATOM   1163  N   ASN B 239     10.994  69.486  20.451  1.00 37.20      N
ATOM   1164  CA  ASN B 239     11.805  69.236  19.261  1.00 36.09      C
ATOM   1165  CB  ASN B 239     10.926  68.868  18.063  1.00 35.98      C
ATOM   1166  CG  ASN B 239     10.314  67.479  18.160  1.00 38.01      C
ATOM   1167  OD1 ASN B 239     10.169  66.897  19.239  1.00 37.53      O
ATOM   1168  ND2 ASN B 239      9.941  66.937  16.998  1.00 39.39      N
ATOM   1169  C   ASN B 239     12.723  70.404  18.856  1.00 35.20      C
ATOM   1170  O   ASN B 239     13.444  70.285  17.878  1.00 34.78      O
ATOM   1171  N   HIS B 240     12.688  71.507  19.600  1.00 33.83      N
ATOM   1172  CA  HIS B 240     13.527  72.672  19.316  1.00 34.34      C
ATOM   1173  CB  HIS B 240     12.858  73.971  19.783  1.00 34.26      C
ATOM   1174  CG  HIS B 240     11.708  74.404  18.923  1.00 35.93      C
ATOM   1175  ND1 HIS B 240     11.834  75.355  17.933  1.00 37.38      N
ATOM   1176  CE1 HIS B 240     10.665  75.529  17.340  1.00 38.07      C
ATOM   1177  NE2 HIS B 240      9.782  74.735  17.919  1.00 38.45      N
ATOM   1178  CD2 HIS B 240     10.409  74.017  18.909  1.00 36.41      C
ATOM   1179  C   HIS B 240     14.870  72.538  20.000  1.00 34.10      C
ATOM   1180  O   HIS B 240     14.957  71.979  21.101  1.00 33.14      O
ATOM   1181  N   LEU B 241     15.912  73.050  19.342  1.00 34.09      N
ATOM   1182  CA  LEU B 241     17.263  73.030  19.895  1.00 34.15      C
ATOM   1183  CB  LEU B 241     18.342  73.112  18.802  1.00 34.73      C
ATOM   1184  CG  LEU B 241     19.824  73.071  19.231  1.00 34.32      C
ATOM   1185  CD1 LEU B 241     20.255  71.616  19.601  1.00 33.83      C
ATOM   1186  CD2 LEU B 241     20.689  73.618  18.127  1.00 34.71      C
ATOM   1187  C   LEU B 241     17.480  74.162  20.886  1.00 34.03      C
ATOM   1188  O   LEU B 241     17.206  75.354  20.596  1.00 33.05      O
ATOM   1189  N   TYR B 242     17.997  73.766  22.046  1.00 33.56      N
ATOM   1190  CA  TYR B 242     18.483  74.688  23.057  1.00 34.05      C
ATOM   1191  CB  TYR B 242     17.689  74.530  24.359  1.00 34.29      C
ATOM   1192  CG  TYR B 242     16.314  75.118  24.273  1.00 33.97      C
ATOM   1193  CD1 TYR B 242     15.249  74.378  23.760  1.00 34.66      C
ATOM   1194  CE1 TYR B 242     13.981  74.928  23.665  1.00 34.60      C
ATOM   1195  CZ  TYR B 242     13.774  76.229  24.086  1.00 35.05      C
ATOM   1196  OH  TYR B 242     12.524  76.788  23.989  1.00 37.47      O
ATOM   1197  CE2 TYR B 242     14.812  76.988  24.593  1.00 34.40      C
ATOM   1198  CD2 TYR B 242     16.074  76.426  24.688  1.00 34.99      C
ATOM   1199  C   TYR B 242     19.957  74.390  23.296  1.00 34.32      C
ATOM   1200  O   TYR B 242     20.422  73.293  22.994  1.00 34.42      O
ATOM   1201  N   ALA B 243     20.683  75.368  23.838  1.00 34.42      N
ATOM   1202  CA  ALA B 243     22.104  75.208  24.113  1.00 34.62      C
ATOM   1203  CB  ALA B 243     22.936  75.513  22.861  1.00 34.93      C
ATOM   1204  C   ALA B 243     22.536  76.112  25.247  1.00 34.86      C
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Figure 1

Table 1a - 19

ATOM	1205	O	ALA	B	243	21.939	77.165	25.478	1.00	34.18	O
ATOM	1206	N	LEU	B	244	23.568	75.684	25.964	1.00	35.40	N
ATOM	1207	CA	LEU	B	244	24.245	76.549	26.921	1.00	36.09	C
ATOM	1208	CB	LEU	B	244	24.916	75.727	28.025	1.00	35.66	C
ATOM	1209	CG	LEU	B	244	24.046	74.840	28.917	1.00	37.13	C
ATOM	1210	CD1	LEU	B	244	24.936	74.003	29.842	1.00	37.02	C
ATOM	1211	CD2	LEU	B	244	23.032	75.672	29.725	1.00	38.06	C
ATOM	1212	C	LEU	B	244	25.302	77.346	26.180	1.00	36.48	C
ATOM	1213	O	LEU	B	244	25.732	76.951	25.097	1.00	36.00	O
ATOM	1214	N	SER	B	245	25.722	78.463	26.768	1.00	37.83	N
ATOM	1215	CA	SER	B	245	26.902	79.173	26.303	1.00	39.03	C
ATOM	1216	CB	SER	B	245	27.279	80.288	27.281	1.00	39.28	C
ATOM	1217	OG	SER	B	245	26.376	81.377	27.206	1.00	41.15	O
ATOM	1218	C	SER	B	245	28.056	78.186	26.215	1.00	39.56	C
ATOM	1219	O	SER	B	245	28.208	77.329	27.084	1.00	39.87	O
ATOM	1220	N	ILE	B	246	28.861	78.289	25.169	1.00	40.10	N
ATOM	1221	CA	ILE	B	246	30.043	77.446	25.074	1.00	40.87	C
ATOM	1222	CB	ILE	B	246	30.714	77.565	23.694	1.00	40.87	C
ATOM	1223	CG1	ILE	B	246	29.877	76.828	22.646	1.00	40.83	C
ATOM	1224	CD1	ILE	B	246	30.237	77.207	21.224	1.00	41.79	C
ATOM	1225	CG2	ILE	B	246	32.146	77.031	23.729	1.00	40.15	C
ATOM	1226	C	ILE	B	246	31.019	77.770	26.214	1.00	41.55	C
ATOM	1227	O	ILE	B	246	31.339	78.936	26.456	1.00	41.30	O
ATOM	1228	N	LYS	B	247	31.452	76.725	26.916	1.00	42.52	N
ATOM	1229	CA	LYS	B	247	32.398	76.834	28.029	1.00	43.99	C
ATOM	1230	CB	LYS	B	247	31.705	76.613	29.377	1.00	44.13	C
ATOM	1231	CG	LYS	B	247	31.660	77.840	30.272	1.00	45.58	C
ATOM	1232	CD	LYS	B	247	31.476	77.439	31.729	1.00	47.03	C
ATOM	1233	CE	LYS	B	247	31.501	78.658	32.650	1.00	48.67	C
ATOM	1234	NZ	LYS	B	247	31.927	78.286	34.042	1.00	48.90	N
ATOM	1235	C	LYS	B	247	33.521	75.820	27.881	1.00	44.32	C
ATOM	1236	O	LYS	B	247	33.262	74.636	27.673	1.00	44.28	O
ATOM	1237	N	ASP	B	248	34.761	76.301	27.979	1.00	44.92	N
ATOM	1238	CA	ASP	B	248	35.957	75.453	27.951	1.00	45.30	C
ATOM	1239	CB	ASP	B	248	36.128	74.707	29.282	1.00	45.57	C
ATOM	1240	CG	ASP	B	248	36.605	75.611	30.416	1.00	47.17	C
ATOM	1241	OD1	ASP	B	248	37.391	76.557	30.168	1.00	48.33	O
ATOM	1242	OD2	ASP	B	248	36.203	75.356	31.574	1.00	49.09	O
ATOM	1243	C	ASP	B	248	35.970	74.462	26.791	1.00	44.96	C
ATOM	1244	O	ASP	B	248	36.331	73.298	26.973	1.00	45.10	O
ATOM	1245	N	SER	B	249	35.564	74.935	25.615	1.00	44.45	N
ATOM	1246	CA	SER	B	249	35.552	74.143	24.378	1.00	44.41	C
ATOM	1247	CB	SER	B	249	36.967	73.658	24.023	1.00	44.55	C
ATOM	1248	OG	SER	B	249	37.855	74.752	23.818	1.00	45.47	O
ATOM	1249	C	SER	B	249	34.531	72.983	24.356	1.00	44.10	C
ATOM	1250	O	SER	B	249	34.692	72.015	23.604	1.00	43.78	O
ATOM	1251	N	VAL	B	250	33.482	73.089	25.170	1.00	43.58	N
ATOM	1252	CA	VAL	B	250	32.377	72.126	25.129	1.00	43.24	C
ATOM	1253	CB	VAL	B	250	32.359	71.125	26.368	1.00	43.40	C
ATOM	1254	CG1	VAL	B	250	33.067	71.704	27.591	1.00	43.41	C
ATOM	1255	CG2	VAL	B	250	30.943	70.651	26.716	1.00	42.77	C
ATOM	1256	C	VAL	B	250	31.007	72.763	24.835	1.00	42.96	C
ATOM	1257	O	VAL	B	250	30.571	73.703	25.504	1.00	42.53	O
ATOM	1258	N	MET	B	251	30.383	72.250	23.780	1.00	42.79	N
ATOM	1259	CA	MET	B	251	28.993	72.494	23.453	1.00	43.72	C
ATOM	1260	CB	MET	B	251	28.730	72.063	22.023	1.00	43.79	C
ATOM	1261	CG	MET	B	251	29.004	73.058	20.969	1.00	47.62	C
ATOM	1262	SD	MET	B	251	28.470	72.259	19.449	1.00	51.99	S
ATOM	1263	CE	MET	B	251	29.748	71.005	19.254	1.00	51.41	C
ATOM	1264	C	MET	B	251	28.076	71.631	24.313	1.00	42.11	C
ATOM	1265	O	MET	B	251	28.359	70.449	24.539	1.00	41.57	O
ATOM	1266	N	VAL	B	252	26.973	72.219	24.769	1.00	40.73	N
ATOM	1267	CA	VAL	B	252	25.908	71.447	25.392	1.00	39.60	C
ATOM	1268	CB	VAL	B	252	25.738	71.726	26.895	1.00	39.62	C
ATOM	1269	CG1	VAL	B	252	24.753	70.736	27.500	1.00	39.20	C
ATOM	1270	CG2	VAL	B	252	27.075	71.635	27.620	1.00	39.98	C
ATOM	1271	C	VAL	B	252	24.623	71.752	24.649	1.00	38.79	C

Figure 1

Table 1a - 20

ATOM	1272	O	VAL	B	252	24.096	72.866	24.724	1.00	38.47	O
ATOM	1273	N	LEU	B	253	24.162	70.754	23.905	1.00	37.50	N
ATOM	1274	CA	LEU	B	253	22.949	70.842	23.113	1.00	37.38	C
ATOM	1275	CB	LEU	B	253	23.187	70.257	21.720	1.00	37.09	C
ATOM	1276	CG	LEU	B	253	24.327	70.912	20.940	1.00	38.69	C
ATOM	1277	CD1	LEU	B	253	24.503	70.263	19.595	1.00	39.38	C
ATOM	1278	CD2	LEU	B	253	24.083	72.424	20.787	1.00	37.78	C
ATOM	1279	C	LEU	B	253	21.835	70.084	23.802	1.00	37.40	C
ATOM	1280	O	LEU	B	253	22.064	69.038	24.405	1.00	37.17	O
ATOM	1281	N	SER	B	254	20.623	70.613	23.704	1.00	37.23	N
ATOM	1282	CA	SER	B	254	19.495	70.021	24.395	1.00	37.10	C
ATOM	1283	CB	SER	B	254	19.302	70.709	25.748	1.00	37.38	C
ATOM	1284	OG	SER	B	254	18.544	69.872	26.587	1.00	40.15	O
ATOM	1285	C	SER	B	254	18.214	70.121	23.597	1.00	36.41	C
ATOM	1286	O	SER	B	254	18.019	71.067	22.816	1.00	36.05	O
ATOM	1287	N	ALA	B	255	17.332	69.146	23.798	1.00	35.34	N
ATOM	1288	CA	ALA	B	255	15.989	69.205	23.226	1.00	34.75	C
ATOM	1289	CB	ALA	B	255	15.995	68.859	21.715	1.00	34.58	C
ATOM	1290	C	ALA	B	255	15.102	68.257	23.985	1.00	34.44	C
ATOM	1291	O	ALA	B	255	15.591	67.302	24.589	1.00	34.61	O
ATOM	1292	N	THR	B	256	13.816	68.517	23.952	1.00	34.02	N
ATOM	1293	CA	THR	B	256	12.835	67.654	24.539	1.00	33.87	C
ATOM	1294	CB	THR	B	256	11.910	68.439	25.448	1.00	33.66	C
ATOM	1295	OG1	THR	B	256	12.677	69.146	26.404	1.00	34.72	O
ATOM	1296	CG2	THR	B	256	10.972	67.530	26.147	1.00	34.63	C
ATOM	1297	C	THR	B	256	12.026	66.963	23.474	1.00	33.64	C
ATOM	1298	O	THR	B	256	11.477	67.613	22.616	1.00	33.12	O
ATOM	1299	N	HIS	B	257	11.971	65.647	23.532	1.00	32.78	N
ATOM	1300	CA	HIS	B	257	11.182	64.853	22.601	1.00	33.12	C
ATOM	1301	CB	HIS	B	257	12.064	63.998	21.692	1.00	33.51	C
ATOM	1302	CG	HIS	B	257	12.954	64.773	20.781	1.00	35.40	C
ATOM	1303	ND1	HIS	B	257	14.213	65.183	21.145	1.00	37.12	N
ATOM	1304	CE1	HIS	B	257	14.769	65.826	20.142	1.00	37.50	C
ATOM	1305	NE2	HIS	B	257	13.917	65.851	19.142	1.00	37.27	N
ATOM	1306	CD2	HIS	B	257	12.774	65.201	19.515	1.00	37.67	C
ATOM	1307	C	HIS	B	257	10.170	63.938	23.291	1.00	32.99	C
ATOM	1308	O	HIS	B	257	10.304	63.630	24.429	1.00	31.69	O
ATOM	1309	N	ARG	B	258	9.170	63.512	22.546	1.00	32.77	N
ATOM	1310	CA	ARG	B	258	8.025	62.796	23.052	1.00	33.53	C
ATOM	1311	CB	ARG	B	258	6.774	63.444	22.512	1.00	34.51	C
ATOM	1312	CG	ARG	B	258	5.481	63.174	23.203	1.00	36.75	C
ATOM	1313	CD	ARG	B	258	4.309	63.479	22.269	1.00	42.75	C
ATOM	1314	NE	ARG	B	258	3.679	62.218	21.969	1.00	49.03	N
ATOM	1315	CZ	ARG	B	258	3.463	61.704	20.775	1.00	50.61	C
ATOM	1316	NH1	ARG	B	258	3.749	62.371	19.672	1.00	52.65	N
ATOM	1317	NH2	ARG	B	258	2.922	60.510	20.712	1.00	51.26	N
ATOM	1318	C	ARG	B	258	8.098	61.373	22.563	1.00	33.05	C
ATOM	1319	O	ARG	B	258	8.348	61.145	21.415	1.00	32.73	O
ATOM	1320	N	TYR	B	259	7.906	60.421	23.456	1.00	32.34	N
ATOM	1321	CA	TYR	B	259	7.644	59.040	23.089	1.00	31.81	C
ATOM	1322	CB	TYR	B	259	8.766	58.104	23.534	1.00	31.88	C
ATOM	1323	CG	TYR	B	259	8.542	56.631	23.215	1.00	31.61	C
ATOM	1324	CD1	TYR	B	259	8.875	56.117	21.990	1.00	32.53	C
ATOM	1325	CE1	TYR	B	259	8.672	54.798	21.691	1.00	31.61	C
ATOM	1326	CZ	TYR	B	259	8.122	53.961	22.617	1.00	31.50	C
ATOM	1327	OH	TYR	B	259	7.927	52.653	22.294	1.00	30.16	O
ATOM	1328	CE2	TYR	B	259	7.781	54.444	23.844	1.00	31.29	C
ATOM	1329	CD2	TYR	B	259	7.988	55.771	24.139	1.00	31.21	C
ATOM	1330	C	TYR	B	259	6.343	58.619	23.715	1.00	32.18	C
ATOM	1331	O	TYR	B	259	6.215	58.560	24.917	1.00	31.18	O
ATOM	1332	N	LYS	B	260	5.361	58.326	22.866	1.00	32.14	N
ATOM	1333	CA	LYS	B	260	3.980	58.178	23.309	1.00	32.65	C
ATOM	1334	CB	LYS	B	260	3.780	56.829	24.002	1.00	32.20	C
ATOM	1335	CG	LYS	B	260	4.251	55.640	23.185	1.00	33.09	C
ATOM	1336	CD	LYS	B	260	3.700	54.343	23.747	1.00	36.51	C
ATOM	1337	CE	LYS	B	260	3.963	53.176	22.810	1.00	37.68	C
ATOM	1338	NZ	LYS	B	260	3.804	51.869	23.506	1.00	40.49	N

Figure 1

Table 1a - 21

ATOM	1339	C	LYS	B	260	3.583	59.319	24.239	1.00	32.81	C
ATOM	1340	O	LYS	B	260	3.375	60.448	23.795	1.00	32.99	O
ATOM	1341	N	LYS	B	261	3.486	59.022	25.531	1.00	33.14	N
ATOM	1342	CA	LYS	B	261	3.023	60.007	26.500	1.00	33.62	C
ATOM	1343	CB	LYS	B	261	1.817	59.471	27.272	1.00	33.64	C
ATOM	1344	CG	LYS	B	261	0.591	59.238	26.404	1.00	36.41	C
ATOM	1345	CD	LYS	B	261	-0.661	59.806	27.050	1.00	40.03	C
ATOM	1346	CE	LYS	B	261	-1.753	60.043	26.017	1.00	42.01	C
ATOM	1347	NZ	LYS	B	261	-3.023	60.485	26.655	1.00	43.69	N
ATOM	1348	C	LYS	B	261	4.132	60.425	27.465	1.00	33.27	C
ATOM	1349	O	LYS	B	261	3.869	61.042	28.496	1.00	33.78	O
ATOM	1350	N	LYS	B	262	5.370	60.086	27.122	1.00	32.68	N
ATOM	1351	CA	LYS	B	262	6.514	60.420	27.963	1.00	32.76	C
ATOM	1352	CB	LYS	B	262	7.274	59.153	28.370	1.00	32.50	C
ATOM	1353	CG	LYS	B	262	6.377	57.975	28.732	1.00	31.74	C
ATOM	1354	CD	LYS	B	262	6.145	57.885	30.229	1.00	28.85	C
ATOM	1355	CE	LYS	B	262	4.934	57.024	30.552	1.00	26.20	C
ATOM	1356	NZ	LYS	B	262	5.137	56.225	31.785	1.00	25.51	N
ATOM	1357	C	LYS	B	262	7.449	61.382	27.241	1.00	33.06	C
ATOM	1358	O	LYS	B	262	7.590	61.321	26.021	1.00	32.80	O
ATOM	1359	N	TYR	B	263	8.085	62.266	28.003	1.00	32.80	N
ATOM	1360	CA	TYR	B	263	8.957	63.285	27.434	1.00	33.67	C
ATOM	1361	CB	TYR	B	263	8.397	64.682	27.703	1.00	34.04	C
ATOM	1362	CG	TYR	B	263	6.994	64.887	27.175	1.00	36.15	C
ATOM	1363	CD1	TYR	B	263	5.885	64.499	27.920	1.00	36.50	C
ATOM	1364	CE1	TYR	B	263	4.601	64.682	27.440	1.00	37.75	C
ATOM	1365	CZ	TYR	B	263	4.413	65.260	26.200	1.00	37.67	C
ATOM	1366	OH	TYR	B	263	3.138	65.446	25.715	1.00	37.57	O
ATOM	1367	CE2	TYR	B	263	5.498	65.653	25.443	1.00	37.25	C
ATOM	1368	CD2	TYR	B	263	6.778	65.464	25.931	1.00	35.46	C
ATOM	1369	C	TYR	B	263	10.367	63.171	27.995	1.00	33.15	C
ATOM	1370	O	TYR	B	263	10.553	62.985	29.200	1.00	32.90	O
ATOM	1371	N	VAL	B	264	11.356	63.276	27.114	1.00	32.63	N
ATOM	1372	CA	VAL	B	264	12.753	63.195	27.526	1.00	32.24	C
ATOM	1373	CB	VAL	B	264	13.428	61.905	27.005	1.00	32.30	C
ATOM	1374	CG1	VAL	B	264	13.600	61.967	25.497	1.00	32.30	C
ATOM	1375	CG2	VAL	B	264	14.767	61.695	27.688	1.00	32.52	C
ATOM	1376	C	VAL	B	264	13.534	64.413	27.044	1.00	31.68	C
ATOM	1377	O	VAL	B	264	13.598	64.687	25.847	1.00	31.71	O
ATOM	1378	N	THR	B	265	14.123	65.140	27.986	1.00	31.50	N
ATOM	1379	CA	THR	B	265	15.002	66.248	27.667	1.00	31.77	C
ATOM	1380	CB	THR	B	265	14.866	67.345	28.714	1.00	31.63	C
ATOM	1381	OG1	THR	B	265	13.492	67.753	28.760	1.00	32.82	O
ATOM	1382	CG2	THR	B	265	15.779	68.557	28.393	1.00	32.27	C
ATOM	1383	C	THR	B	265	16.401	65.664	27.684	1.00	32.05	C
ATOM	1384	O	THR	B	265	16.927	65.261	28.741	1.00	32.81	O
ATOM	1385	N	THR	B	266	16.972	65.556	26.498	1.00	31.89	N
ATOM	1386	CA	THR	B	266	18.287	64.953	26.318	1.00	32.13	C
ATOM	1387	CB	THR	B	266	18.327	64.101	25.043	1.00	31.96	C
ATOM	1388	OG1	THR	B	266	17.223	63.181	25.053	1.00	33.08	O
ATOM	1389	CG2	THR	B	266	19.645	63.314	24.957	1.00	30.44	C
ATOM	1390	C	THR	B	266	19.312	66.071	26.211	1.00	32.36	C
ATOM	1391	O	THR	B	266	19.075	67.050	25.504	1.00	32.34	O
ATOM	1392	N	LEU	B	267	20.435	65.925	26.907	1.00	32.24	N
ATOM	1393	CA	LEU	B	267	21.573	66.819	26.724	1.00	33.88	C
ATOM	1394	CB	LEU	B	267	21.986	67.444	28.058	1.00	33.70	C
ATOM	1395	CG	LEU	B	267	20.959	68.347	28.747	1.00	34.40	C
ATOM	1396	CD1	LEU	B	267	19.768	67.538	29.232	1.00	34.05	C
ATOM	1397	CD2	LEU	B	267	21.604	69.096	29.905	1.00	33.83	C
ATOM	1398	C	LEU	B	267	22.753	66.072	26.112	1.00	34.21	C
ATOM	1399	O	LEU	B	267	23.119	64.990	26.572	1.00	35.70	O
ATOM	1400	N	LEU	B	268	23.339	66.653	25.072	1.00	34.36	N
ATOM	1401	CA	LEU	B	268	24.588	66.146	24.521	1.00	34.38	C
ATOM	1402	CB	LEU	B	268	24.499	66.033	22.998	1.00	33.94	C
ATOM	1403	CG	LEU	B	268	25.687	65.379	22.290	1.00	33.02	C
ATOM	1404	CD1	LEU	B	268	25.934	63.978	22.829	1.00	32.88	C
ATOM	1405	CD2	LEU	B	268	25.469	65.354	20.783	1.00	33.26	C

Figure 1 Table 1a - 22

ATOM	1406	C	LEU	B	268	25.761	67.036	24.914	1.00 35.01 C
ATOM	1407	O	LEU	B	268	25.792	68.223	24.579	1.00 35.37 O
ATOM	1408	N	TYR	B	269	26.720	66.453	25.628	1.00 35.61 N
ATOM	1409	CA	TYR	B	269	28.011	67.092	25.855	1.00 36.16 C
ATOM	1410	CB	TYR	B	269	28.542	66.756	27.250	1.00 35.41 C
ATOM	1411	CG	TYR	B	269	27.891	67.553	28.356	1.00 34.49 C
ATOM	1412	CD1	TYR	B	269	26.574	67.311	28.729	1.00 33.96 C
ATOM	1413	CE1	TYR	B	269	25.972	68.038	29.736	1.00 34.60 C
ATOM	1414	CZ	TYR	B	269	26.685	69.024	30.386	1.00 33.83 C
ATOM	1415	OH	TYR	B	269	26.085	69.747	31.389	1.00 35.22 O
ATOM	1416	CE2	TYR	B	269	27.996	69.286	30.036	1.00 35.41 C
ATOM	1417	CD2	TYR	B	269	28.591	68.550	29.025	1.00 34.66 C
ATOM	1418	C	TYR	B	269	29.017	66.663	24.796	1.00 37.48 C
ATOM	1419	O	TYR	B	269	29.247	65.472	24.592	1.00 37.28 O
ATOM	1420	N	LYS	B	270	29.616	67.644	24.132	1.00 39.12 N
ATOM	1421	CA	LYS	B	270	30.326	67.407	22.881	1.00 41.36 C
ATOM	1422	CB	LYS	B	270	29.344	67.435	21.707	1.00 41.82 C
ATOM	1423	CG	LYS	B	270	29.960	67.085	20.365	1.00 44.48 C
ATOM	1424	CD	LYS	B	270	29.047	67.488	19.213	1.00 45.12 C
ATOM	1425	CE	LYS	B	270	29.535	66.904	17.896	1.00 45.95 C
ATOM	1426	NZ	LYS	B	270	28.945	67.608	16.723	1.00 49.89 N
ATOM	1427	C	LYS	B	270	31.419	68.455	22.672	1.00 41.90 C
ATOM	1428	O	LYS	B	270	31.125	69.634	22.476	1.00 42.20 O
ATOM	1429	N	PRO	B	271	32.679	68.020	22.712	1.00 42.45 N
ATOM	1430	CA	PRO	B	271	33.793	68.863	22.260	1.00 43.27 C
ATOM	1431	CB	PRO	B	271	34.944	67.865	22.106	1.00 42.98 C
ATOM	1432	CG	PRO	B	271	34.616	66.770	23.052	1.00 43.07 C
ATOM	1433	CD	PRO	B	271	33.120	66.658	23.060	1.00 42.58 C
ATOM	1434	C	PRO	B	271	33.496	69.521	20.916	1.00 43.97 C
ATOM	1435	O	PRO	B	271	32.859	68.909	20.058	1.00 43.92 O
ATOM	1436	N	ILE	B	272	33.954	70.755	20.740	1.00 45.11 N
ATOM	1437	CA	ILE	B	272	33.852	71.433	19.440	1.00 46.48 C
ATOM	1438	CB	ILE	B	272	33.579	72.958	19.566	1.00 46.56 C
ATOM	1439	CG1	ILE	B	272	32.902	73.303	20.897	1.00 47.40 C
ATOM	1440	CD1	ILE	B	272	32.973	74.775	21.248	1.00 47.04 C
ATOM	1441	CG2	ILE	B	272	32.722	73.449	18.387	1.00 47.73 C
ATOM	1442	C	ILE	B	272	35.113	71.191	18.605	1.00 46.72 C
ATOM	1443	O	ILE	B	272	35.245	71.696	17.478	1.00 47.85 O
ATOM	1444	N	SER	E	23	5.709	32.051	49.885	1.00 65.02 N
ATOM	1445	CA	SER	E	23	4.553	31.361	49.248	1.00 65.09 C
ATOM	1446	CB	SER	E	23	3.357	32.326	49.177	1.00 65.11 C
ATOM	1447	OG	SER	E	23	2.117	31.650	49.037	1.00 65.03 O
ATOM	1448	C	SER	E	23	4.935	31.006	47.825	1.00 64.89 C
ATOM	1449	O	SER	E	23	6.126	30.934	47.479	1.00 65.33 O
ATOM	1450	N	ASN	E	24	3.897	30.698	47.046	1.00 64.06 N
ATOM	1451	CA	ASN	E	24	3.672	31.360	45.761	1.00 63.02 C
ATOM	1452	CB	ASN	E	24	3.483	32.870	46.044	1.00 62.87 C
ATOM	1453	CG	ASN	E	24	2.260	33.472	45.354	1.00 63.18 C
ATOM	1454	OD1	ASN	E	24	2.151	34.699	45.232	1.00 62.43 O
ATOM	1455	ND2	ASN	E	24	1.337	32.619	44.906	1.00 63.30 N
ATOM	1456	C	ASN	E	24	4.713	31.209	44.646	1.00 62.15 C
ATOM	1457	O	ASN	E	24	5.925	31.369	44.869	1.00 62.12 O
ATOM	1458	N	SER	E	25	4.212	30.924	43.439	1.00 60.88 N
ATOM	1459	CA	SER	E	25	4.773	31.535	42.236	1.00 59.39 C
ATOM	1460	CB	SER	E	25	3.941	31.213	40.995	1.00 59.71 C
ATOM	1461	OG	SER	E	25	4.162	32.183	39.980	1.00 60.40 O
ATOM	1462	C	SER	E	25	4.599	32.986	42.619	1.00 57.97 C
ATOM	1463	O	SER	E	25	4.405	33.284	43.789	1.00 58.46 O
ATOM	1464	N	SER	E	26	4.660	33.937	41.721	1.00 55.61 N
ATOM	1465	CA	SER	E	26	4.563	35.228	42.333	1.00 53.45 C
ATOM	1466	CB	SER	E	26	5.937	35.900	42.429	1.00 53.61 C
ATOM	1467	OG	SER	E	26	6.091	36.528	43.682	1.00 53.32 O
ATOM	1468	C	SER	E	26	3.514	36.137	41.766	1.00 51.71 C
ATOM	1469	O	SER	E	26	3.405	36.310	40.563	1.00 51.71 O
ATOM	1470	N	VAL	E	27	2.739	36.700	42.679	1.00 49.56 N
ATOM	1471	CA	VAL	E	27	2.105	37.981	42.473	1.00 48.33 C
ATOM	1472	CB	VAL	E	27	1.550	38.520	43.815	1.00 48.24 C

Figure 1

Table 1a - 23

ATOM	1473	CG1	VAL	E	27	1.052	39.924	43.661	1.00	49.45	C
ATOM	1474	CG2	VAL	E	27	0.418	37.621	44.336	1.00	48.71	C
ATOM	1475	C	VAL	E	27	3.152	38.951	41.858	1.00	46.97	C
ATOM	1476	O	VAL	E	27	2.831	39.730	40.959	1.00	46.87	O
ATOM	1477	N	TYR	E	28	4.403	38.857	42.321	1.00	45.24	N
ATOM	1478	CA	TYR	E	28	5.516	39.668	41.799	1.00	44.17	C
ATOM	1479	CB	TYR	E	28	6.713	39.623	42.751	1.00	43.44	C
ATOM	1480	CG	TYR	E	28	6.464	40.357	44.040	1.00	42.96	C
ATOM	1481	CD1	TYR	E	28	6.053	39.673	45.187	1.00	41.38	C
ATOM	1482	CE1	TYR	E	28	5.819	40.350	46.376	1.00	41.80	C
ATOM	1483	CZ	TYR	E	28	5.982	41.727	46.423	1.00	42.16	C
ATOM	1484	OH	TYR	E	28	5.754	42.403	47.595	1.00	43.34	O
ATOM	1485	CE2	TYR	E	28	6.385	42.428	45.301	1.00	42.22	C
ATOM	1486	CD2	TYR	E	28	6.620	41.742	44.114	1.00	42.09	C
ATOM	1487	C	TYR	E	28	5.970	39.283	40.393	1.00	43.67	C
ATOM	1488	O	TYR	E	28	6.083	40.138	39.523	1.00	43.01	O
ATOM	1489	N	THR	E	29	6.243	37.997	40.189	1.00	43.29	N
ATOM	1490	CA	THR	E	29	6.720	37.481	38.907	1.00	43.49	C
ATOM	1491	CB	THR	E	29	7.087	35.979	39.017	1.00	44.11	C
ATOM	1492	OG1	THR	E	29	8.073	35.805	40.049	1.00	46.02	O
ATOM	1493	CG2	THR	E	29	7.665	35.469	37.725	1.00	45.37	C
ATOM	1494	C	THR	E	29	5.675	37.720	37.812	1.00	42.80	C
ATOM	1495	O	THR	E	29	6.011	38.133	36.701	1.00	42.92	O
ATOM	1496	N	THR	E	30	4.410	37.478	38.153	1.00	42.23	N
ATOM	1497	CA	THR	E	30	3.275	37.693	37.255	1.00	41.47	C
ATOM	1498	CB	THR	E	30	1.951	37.242	37.915	1.00	41.42	C
ATOM	1499	OG1	THR	E	30	2.003	35.836	38.165	1.00	41.67	O
ATOM	1500	CG2	THR	E	30	0.755	37.546	37.028	1.00	41.56	C
ATOM	1501	C	THR	E	30	3.176	39.159	36.856	1.00	40.93	C
ATOM	1502	O	THR	E	30	3.097	39.472	35.667	1.00	40.58	O
ATOM	1503	N	PHE	E	31	3.174	40.039	37.860	1.00	40.39	N
ATOM	1504	CA	PHE	E	31	3.185	41.490	37.642	1.00	39.94	C
ATOM	1505	CB	PHE	E	31	3.287	42.235	38.981	1.00	39.65	C
ATOM	1506	CG	PHE	E	31	3.154	43.730	38.852	1.00	39.80	C
ATOM	1507	CD1	PHE	E	31	4.273	44.524	38.595	1.00	39.26	C
ATOM	1508	CE1	PHE	E	31	4.155	45.908	38.465	1.00	39.41	C
ATOM	1509	CZ	PHE	E	31	2.905	46.514	38.593	1.00	39.05	C
ATOM	1510	CE2	PHE	E	31	1.784	45.732	38.865	1.00	40.48	C
ATOM	1511	CD2	PHE	E	31	1.912	44.343	38.981	1.00	39.79	C
ATOM	1512	C	PHE	E	31	4.314	41.947	36.713	1.00	39.80	C
ATOM	1513	O	PHE	E	31	4.091	42.769	35.822	1.00	39.52	O
ATOM	1514	N	MET	E	32	5.519	41.427	36.943	1.00	39.65	N
ATOM	1515	CA	MET	E	32	6.698	41.823	36.172	1.00	40.61	C
ATOM	1516	CB	MET	E	32	7.978	41.311	36.828	1.00	40.66	C
ATOM	1517	CG	MET	E	32	8.336	42.035	38.117	1.00	41.00	C
ATOM	1518	SD	MET	E	32	9.969	41.552	38.686	1.00	45.16	S
ATOM	1519	CE	MET	E	32	9.642	41.023	40.366	1.00	45.50	C
ATOM	1520	C	MET	E	32	6.617	41.383	34.715	1.00	40.23	C
ATOM	1521	O	MET	E	32	6.994	42.127	33.806	1.00	39.65	O
ATOM	1522	N	LYS	E	33	6.102	40.177	34.508	1.00	40.49	N
ATOM	1523	CA	LYS	E	33	5.863	39.640	33.170	1.00	40.79	C
ATOM	1524	CB	LYS	E	33	5.634	38.117	33.229	1.00	40.97	C
ATOM	1525	CG	LYS	E	33	6.908	37.328	33.505	1.00	40.64	C
ATOM	1526	CD	LYS	E	33	6.619	35.856	33.722	1.00	42.61	C
ATOM	1527	CE	LYS	E	33	7.907	35.093	33.965	1.00	43.00	C
ATOM	1528	NZ	LYS	E	33	7.651	33.710	34.434	1.00	45.68	N
ATOM	1529	C	LYS	E	33	4.715	40.353	32.438	1.00	41.19	C
ATOM	1530	O	LYS	E	33	4.724	40.414	31.211	1.00	40.97	O
ATOM	1531	N	SER	E	34	3.755	40.911	33.178	1.00	41.63	N
ATOM	1532	CA	SER	E	34	2.590	41.566	32.555	1.00	42.74	C
ATOM	1533	CB	SER	E	34	1.316	41.320	33.374	1.00	43.00	C
ATOM	1534	OG	SER	E	34	1.318	42.073	34.581	1.00	45.00	O
ATOM	1535	C	SER	E	34	2.773	43.064	32.270	1.00	42.78	C
ATOM	1536	O	SER	E	34	1.938	43.683	31.602	1.00	43.61	O
ATOM	1537	N	HIS	E	35	3.867	43.645	32.758	1.00	42.55	N
ATOM	1538	CA	HIS	E	35	4.129	45.070	32.568	1.00	41.89	C
ATOM	1539	CB	HIS	E	35	4.235	45.778	33.918	1.00	42.36	C

Figure 1 Table 1a - 24

ATOM	1540	CG	HIS	E	35	2.913	45.973	34.580	1.00	43.15	C
ATOM	1541	ND1	HIS	E	35	2.278	44.966	35.275	1.00	43.65	N
ATOM	1542	CE1	HIS	E	35	1.114	45.407	35.717	1.00	44.84	C
ATOM	1543	NE2	HIS	E	35	0.974	46.667	35.342	1.00	44.57	N
ATOM	1544	CD2	HIS	E	35	2.080	47.041	34.617	1.00	43.78	C
ATOM	1545	C	HIS	E	35	5.355	45.352	31.710	1.00	41.32	C
ATOM	1546	O	HIS	E	35	6.350	44.627	31.784	1.00	41.08	O
ATOM	1547	N	ARG	E	36	5.252	46.397	30.889	1.00	40.44	N
ATOM	1548	CA	ARG	E	36	6.338	46.855	30.022	1.00	40.32	C
ATOM	1549	CB	ARG	E	36	5.787	47.534	28.763	1.00	40.24	C
ATOM	1550	CG	ARG	E	36	4.918	46.645	27.903	1.00	42.73	C
ATOM	1551	CD	ARG	E	36	4.468	47.323	26.607	1.00	44.15	C
ATOM	1552	NE	ARG	E	36	3.498	46.475	25.908	1.00	51.27	N
ATOM	1553	CZ	ARG	E	36	3.798	45.375	25.210	1.00	53.09	C
ATOM	1554	NH1	ARG	E	36	5.058	44.969	25.083	1.00	53.67	N
ATOM	1555	NH2	ARG	E	36	2.830	44.668	24.632	1.00	53.95	N
ATOM	1556	C	ARG	E	36	7.225	47.861	30.743	1.00	39.24	C
ATOM	1557	O	ARG	E	36	6.753	48.630	31.583	1.00	38.73	O
ATOM	1558	N	CYS	E	37	8.505	47.876	30.387	1.00	38.75	N
ATOM	1559	CA	CYS	E	37	9.433	48.907	30.862	1.00	38.22	C
ATOM	1560	CB	CYS	E	37	10.771	48.751	30.159	1.00	38.02	C
ATOM	1561	SG	CYS	E	37	11.637	47.301	30.813	1.00	42.51	S
ATOM	1562	C	CYS	E	37	8.894	50.332	30.706	1.00	37.62	C
ATOM	1563	O	CYS	E	37	9.080	51.175	31.591	1.00	37.07	O
ATOM	1564	N	TYR	E	38	8.200	50.588	29.594	1.00	36.91	N
ATOM	1565	CA	TYR	E	38	7.547	51.877	29.358	1.00	36.48	C
ATOM	1566	CB	TYR	E	38	6.633	51.775	28.130	1.00	36.98	C
ATOM	1567	CG	TYR	E	38	5.783	53.007	27.895	1.00	36.83	C
ATOM	1568	CD1	TYR	E	38	4.455	53.052	28.319	1.00	36.98	C
ATOM	1569	CE1	TYR	E	38	3.674	54.184	28.111	1.00	37.33	C
ATOM	1570	CZ	TYR	E	38	4.235	55.294	27.482	1.00	37.66	C
ATOM	1571	OH	TYR	E	38	3.487	56.432	27.274	1.00	36.84	O
ATOM	1572	CE2	TYR	E	38	5.552	55.267	27.063	1.00	38.75	C
ATOM	1573	CD2	TYR	E	38	6.320	54.130	27.281	1.00	36.68	C
ATOM	1574	C	TYR	E	38	6.741	52.383	30.565	1.00	36.26	C
ATOM	1575	O	TYR	E	38	6.736	53.586	30.853	1.00	36.65	O
ATOM	1576	N	ASP	E	39	6.058	51.461	31.247	1.00	35.67	N
ATOM	1577	CA	ASP	E	39	5.148	51.778	32.350	1.00	35.58	C
ATOM	1578	CB	ASP	E	39	4.446	50.506	32.858	1.00	35.53	C
ATOM	1579	CG	ASP	E	39	3.483	49.908	31.845	1.00	37.75	C
ATOM	1580	OD1	ASP	E	39	3.084	50.612	30.893	1.00	38.42	O
ATOM	1581	OD2	ASP	E	39	3.103	48.728	32.012	1.00	39.43	O
ATOM	1582	C	ASP	E	39	5.833	52.449	33.529	1.00	34.84	C
ATOM	1583	O	ASP	E	39	5.181	53.144	34.299	1.00	34.98	O
ATOM	1584	N	LEU	E	40	7.130	52.212	33.699	1.00	34.53	N
ATOM	1585	CA	LEU	E	40	7.859	52.781	34.832	1.00	34.21	C
ATOM	1586	CB	LEU	E	40	8.961	51.837	35.344	1.00	34.41	C
ATOM	1587	CG	LEU	E	40	8.948	50.321	35.514	1.00	36.38	C
ATOM	1588	CD1	LEU	E	40	9.446	49.986	36.930	1.00	35.42	C
ATOM	1589	CD2	LEU	E	40	7.637	49.660	35.251	1.00	37.44	C
ATOM	1590	C	LEU	E	40	8.514	54.113	34.511	1.00	33.36	C
ATOM	1591	O	LEU	E	40	9.109	54.735	35.393	1.00	33.38	O
ATOM	1592	N	ILE	E	41	8.443	54.545	33.257	1.00	33.08	N
ATOM	1593	CA	ILE	E	41	9.073	55.813	32.870	1.00	32.84	C
ATOM	1594	CB	ILE	E	41	9.263	55.899	31.327	1.00	32.90	C
ATOM	1595	CG1	ILE	E	41	10.076	54.694	30.816	1.00	33.03	C
ATOM	1596	CD1	ILE	E	41	10.199	54.657	29.288	1.00	34.43	C
ATOM	1597	CG2	ILE	E	41	9.917	57.262	30.890	1.00	31.92	C
ATOM	1598	C	ILE	E	41	8.225	56.993	33.385	1.00	32.95	C
ATOM	1599	O	ILE	E	41	7.002	57.007	33.194	1.00	33.17	O
ATOM	1600	N	PRO	E	42	8.863	57.990	34.039	1.00	32.77	N
ATOM	1601	CA	PRO	E	42	8.096	59.141	34.478	1.00	32.75	C
ATOM	1602	CB	PRO	E	42	9.086	59.933	35.347	1.00	32.78	C
ATOM	1603	CG	PRO	E	42	10.426	59.541	34.857	1.00	32.49	C
ATOM	1604	CD	PRO	E	42	10.289	58.103	34.399	1.00	33.14	C
ATOM	1605	C	PRO	E	42	7.667	59.968	33.267	1.00	32.67	C
ATOM	1606	O	PRO	E	42	8.223	59.802	32.166	1.00	32.50	O

Figure 1 Table 1a - 25

ATOM	1607	N	THR	E	43	6.671	60.820	33.472	1.00	32.12	N
ATOM	1608	CA	THR	E	43	6.120	61.644	32.396	1.00	32.90	C
ATOM	1609	CB	THR	E	43	4.894	62.442	32.877	1.00	32.42	C
ATOM	1610	OG1	THR	E	43	3.847	61.512	33.185	1.00	32.76	O
ATOM	1611	CG2	THR	E	43	4.405	63.435	31.818	1.00	32.88	C
ATOM	1612	C	THR	E	43	7.193	62.553	31.809	1.00	33.34	C
ATOM	1613	O	THR	E	43	7.279	62.701	30.597	1.00	32.90	O
ATOM	1614	N	SER	E	44	8.021	63.125	32.679	1.00	34.46	N
ATOM	1615	CA	SER	E	44	9.123	63.970	32.250	1.00	36.36	C
ATOM	1616	CB	SER	E	44	8.795	65.433	32.548	1.00	36.48	C
ATOM	1617	OG	SER	E	44	9.885	66.253	32.178	1.00	42.39	O
ATOM	1618	C	SER	E	44	10.434	63.527	32.914	1.00	36.55	C
ATOM	1619	O	SER	E	44	10.463	63.207	34.106	1.00	36.16	O
ATOM	1620	N	SER	E	45	11.507	63.468	32.131	1.00	36.90	N
ATOM	1621	CA	SER	E	45	12.837	63.149	32.665	1.00	37.20	C
ATOM	1622	CB	SER	E	45	13.069	61.630	32.736	1.00	37.20	C
ATOM	1623	OG	SER	E	45	13.043	61.008	31.460	1.00	37.88	O
ATOM	1624	C	SER	E	45	13.921	63.822	31.839	1.00	37.05	C
ATOM	1625	O	SER	E	45	13.651	64.302	30.742	1.00	36.97	O
ATOM	1626	N	LYS	E	46	15.128	63.899	32.397	1.00	36.83	N
ATOM	1627	CA	LYS	E	46	16.286	64.322	31.648	1.00	36.43	C
ATOM	1628	CB	LYS	E	46	16.917	65.602	32.221	1.00	37.52	C
ATOM	1629	CG	LYS	E	46	17.639	65.457	33.531	1.00	41.00	C
ATOM	1630	CD	LYS	E	46	18.416	66.729	33.832	1.00	44.04	C
ATOM	1631	CE	LYS	E	46	18.606	66.878	35.319	1.00	47.57	C
ATOM	1632	NZ	LYS	E	46	18.681	68.318	35.719	1.00	48.60	N
ATOM	1633	C	LYS	E	46	17.309	63.211	31.483	1.00	35.54	C
ATOM	1634	O	LYS	E	46	17.387	62.251	32.273	1.00	35.18	O
ATOM	1635	N	LEU	E	47	18.103	63.358	30.440	1.00	34.35	N
ATOM	1636	CA	LEU	E	47	19.088	62.366	30.095	1.00	33.93	C
ATOM	1637	CB	LEU	E	47	18.551	61.452	28.991	1.00	33.60	C
ATOM	1638	CG	LEU	E	47	19.466	60.309	28.559	1.00	33.85	C
ATOM	1639	CD1	LEU	E	47	19.393	59.161	29.603	1.00	32.22	C
ATOM	1640	CD2	LEU	E	47	19.045	59.858	27.186	1.00	31.85	C
ATOM	1641	C	LEU	E	47	20.327	63.092	29.626	1.00	33.76	C
ATOM	1642	O	LEU	E	47	20.280	63.899	28.699	1.00	32.81	O
ATOM	1643	N	VAL	E	48	21.432	62.817	30.298	1.00	33.78	N
ATOM	1644	CA	VAL	E	48	22.704	63.380	29.919	1.00	34.22	C
ATOM	1645	CB	VAL	E	48	23.547	63.778	31.156	1.00	34.74	C
ATOM	1646	CG1	VAL	E	48	24.902	64.326	30.713	1.00	33.14	C
ATOM	1647	CG2	VAL	E	48	22.790	64.802	32.030	1.00	34.48	C
ATOM	1648	C	VAL	E	48	23.442	62.325	29.094	1.00	34.20	C
ATOM	1649	O	VAL	E	48	23.593	61.190	29.536	1.00	33.89	O
ATOM	1650	N	VAL	E	49	23.887	62.720	27.902	1.00	34.08	N
ATOM	1651	CA	VAL	E	49	24.659	61.843	27.024	1.00	34.38	C
ATOM	1652	CB	VAL	E	49	23.907	61.588	25.678	1.00	34.68	C
ATOM	1653	CG1	VAL	E	49	24.765	60.758	24.711	1.00	33.84	C
ATOM	1654	CG2	VAL	E	49	22.540	60.904	25.941	1.00	33.33	C
ATOM	1655	C	VAL	E	49	26.026	62.464	26.741	1.00	34.64	C
ATOM	1656	O	VAL	E	49	26.123	63.659	26.429	1.00	35.12	O
ATOM	1657	N	PHE	E	50	27.085	61.665	26.856	1.00	34.58	N
ATOM	1658	CA	PHE	E	50	28.412	62.145	26.499	1.00	35.23	C
ATOM	1659	CB	PHE	E	50	29.446	61.832	27.590	1.00	35.08	C
ATOM	1660	CG	PHE	E	50	29.085	62.348	28.962	1.00	35.02	C
ATOM	1661	CD1	PHE	E	50	29.168	61.510	30.067	1.00	34.75	C
ATOM	1662	CE1	PHE	E	50	28.851	61.978	31.363	1.00	35.46	C
ATOM	1663	CZ	PHE	E	50	28.441	63.292	31.542	1.00	33.95	C
ATOM	1664	CE2	PHE	E	50	28.369	64.151	30.436	1.00	36.23	C
ATOM	1665	CD2	PHE	E	50	28.696	63.674	29.154	1.00	35.55	C
ATOM	1666	C	PHE	E	50	28.898	61.559	25.175	1.00	35.47	C
ATOM	1667	O	PHE	E	50	28.862	60.340	24.968	1.00	35.24	O
ATOM	1668	N	ASP	E	51	29.369	62.435	24.295	1.00	35.10	N
ATOM	1669	CA	ASP	E	51	30.192	62.002	23.187	1.00	35.86	C
ATOM	1670	CB	ASP	E	51	30.485	63.185	22.253	1.00	35.93	C
ATOM	1671	CG	ASP	E	51	31.171	62.758	20.974	1.00	37.40	C
ATOM	1672	OD1	ASP	E	51	30.513	62.783	19.906	1.00	40.26	O
ATOM	1673	OD2	ASP	E	51	32.359	62.370	21.031	1.00	37.75	O

Figure 1

Table 1a - 26

ATOM	1674	C	ASP	E	51	31.487	61.413	23.779	1.00	36.28	C
ATOM	1675	O	ASP	E	51	32.057	61.975	24.722	1.00	35.95	O
ATOM	1676	N	THR	E	52	31.934	60.276	23.239	1.00	36.70	N
ATOM	1677	CA	THR	E	52	33.111	59.568	23.768	1.00	36.95	C
ATOM	1678	CB	THR	E	52	33.244	58.130	23.191	1.00	37.15	C
ATOM	1679	OG1	THR	E	52	33.265	58.178	21.761	1.00	36.96	O
ATOM	1680	CG2	THR	E	52	32.084	57.233	23.670	1.00	36.57	C
ATOM	1681	C	THR	E	52	34.451	60.306	23.606	1.00	37.48	C
ATOM	1682	O	THR	E	52	35.461	59.884	24.167	1.00	37.58	O
ATOM	1683	N	SER	E	53	34.452	61.403	22.853	1.00	37.34	N
ATOM	1684	CA	SER	E	53	35.634	62.237	22.701	1.00	37.73	C
ATOM	1685	CB	SER	E	53	35.691	62.845	21.295	1.00	37.65	C
ATOM	1686	OG	SER	E	53	34.589	63.706	21.083	1.00	37.16	O
ATOM	1687	C	SER	E	53	35.709	63.335	23.770	1.00	38.18	C
ATOM	1688	O	SER	E	53	36.686	64.071	23.833	1.00	38.21	O
ATOM	1689	N	LEU	E	54	34.688	63.427	24.621	1.00	38.72	N
ATOM	1690	CA	LEU	E	54	34.699	64.373	25.737	1.00	39.43	C
ATOM	1691	CB	LEU	E	54	33.364	64.324	26.479	1.00	39.28	C
ATOM	1692	CG	LEU	E	54	32.635	65.568	27.002	1.00	40.24	C
ATOM	1693	CD1	LEU	E	54	31.890	65.229	28.290	1.00	37.69	C
ATOM	1694	CD2	LEU	E	54	33.487	66.828	27.178	1.00	39.89	C
ATOM	1695	C	LEU	E	54	35.790	63.998	26.735	1.00	40.01	C
ATOM	1696	O	LEU	E	54	35.990	62.812	27.020	1.00	39.98	O
ATOM	1697	N	GLN	E	55	36.480	65.007	27.270	1.00	40.42	N
ATOM	1698	CA	GLN	E	55	37.409	64.796	28.373	1.00	41.31	C
ATOM	1699	CB	GLN	E	55	38.140	66.086	28.736	1.00	40.95	C
ATOM	1700	CG	GLN	E	55	39.247	66.455	27.760	1.00	43.70	C
ATOM	1701	CD	GLN	E	55	40.123	67.610	28.244	1.00	45.57	C
ATOM	1702	OE1	GLN	E	55	40.025	68.053	29.396	1.00	50.14	O
ATOM	1703	NE2	GLN	E	55	41.002	68.086	27.369	1.00	47.20	N
ATOM	1704	C	GLN	E	55	36.685	64.235	29.600	1.00	40.88	C
ATOM	1705	O	GLN	E	55	35.609	64.706	29.976	1.00	40.50	O
ATOM	1706	N	VAL	E	56	37.295	63.227	30.207	1.00	40.86	N
ATOM	1707	CA	VAL	E	56	36.756	62.551	31.374	1.00	41.23	C
ATOM	1708	CB	VAL	E	56	37.705	61.382	31.796	1.00	41.83	C
ATOM	1709	CG1	VAL	E	56	37.729	61.188	33.276	1.00	42.71	C
ATOM	1710	CG2	VAL	E	56	37.312	60.101	31.079	1.00	41.58	C
ATOM	1711	C	VAL	E	56	36.427	63.502	32.534	1.00	40.86	C
ATOM	1712	O	VAL	E	56	35.370	63.403	33.145	1.00	40.63	O
ATOM	1713	N	LYS	E	57	37.319	64.445	32.805	1.00	40.72	N
ATOM	1714	CA	LYS	E	57	37.106	65.421	33.870	1.00	40.70	C
ATOM	1715	CB	LYS	E	57	38.336	66.309	33.997	1.00	41.22	C
ATOM	1716	CG	LYS	E	57	38.649	66.774	35.401	1.00	44.48	C
ATOM	1717	CD	LYS	E	57	39.645	67.953	35.338	1.00	49.52	C
ATOM	1718	CE	LYS	E	57	40.463	68.104	36.619	1.00	51.21	C
ATOM	1719	NZ	LYS	E	57	41.375	69.290	36.489	1.00	54.21	N
ATOM	1720	C	LYS	E	57	35.866	66.285	33.635	1.00	39.83	C
ATOM	1721	O	LYS	E	57	35.150	66.626	34.581	1.00	39.46	O
ATOM	1722	N	LYS	E	58	35.622	66.647	32.379	1.00	38.77	N
ATOM	1723	CA	LYS	E	58	34.435	67.429	32.028	1.00	38.61	C
ATOM	1724	CB	LYS	E	58	34.558	68.006	30.611	1.00	38.50	C
ATOM	1725	CG	LYS	E	58	35.741	68.964	30.437	1.00	39.79	C
ATOM	1726	CD	LYS	E	58	36.038	69.195	28.962	1.00	42.00	C
ATOM	1727	CE	LYS	E	58	37.356	69.944	28.749	1.00	43.66	C
ATOM	1728	NZ	LYS	E	58	37.099	71.300	28.210	1.00	44.99	N
ATOM	1729	C	LYS	E	58	33.154	66.595	32.173	1.00	37.88	C
ATOM	1730	O	LYS	E	58	32.133	67.100	32.625	1.00	37.23	O
ATOM	1731	N	ALA	E	59	33.232	65.326	31.781	1.00	37.47	N
ATOM	1732	CA	ALA	E	59	32.121	64.386	31.905	1.00	38.19	C
ATOM	1733	CB	ALA	E	59	32.489	63.027	31.291	1.00	38.07	C
ATOM	1734	C	ALA	E	59	31.676	64.215	33.355	1.00	37.94	C
ATOM	1735	O	ALA	E	59	30.495	64.312	33.660	1.00	37.29	O
ATOM	1736	N	PHE	E	60	32.622	64.001	34.259	1.00	38.47	N
ATOM	1737	CA	PHE	E	60	32.243	63.831	35.656	1.00	39.32	C
ATOM	1738	CB	PHE	E	60	33.364	63.184	36.450	1.00	40.32	C
ATOM	1739	CG	PHE	E	60	33.621	61.770	36.043	1.00	42.10	C
ATOM	1740	CD1	PHE	E	60	34.836	61.404	35.495	1.00	43.56	C

Figure 1 Table 1a - 27

ATOM	1741	CE1	PHE	E	60	35.072	60.087	35.115	1.00	44.70	C
ATOM	1742	CZ	PHE	E	60	34.075	59.132	35.259	1.00	44.91	C
ATOM	1743	CE2	PHE	E	60	32.844	59.488	35.798	1.00	46.58	C
ATOM	1744	CD2	PHE	E	60	32.622	60.807	36.178	1.00	45.20	C
ATOM	1745	C	PHE	E	60	31.696	65.076	36.329	1.00	39.15	C
ATOM	1746	O	PHE	E	60	30.771	64.990	37.132	1.00	38.62	O
ATOM	1747	N	PHE	E	61	32.239	66.238	35.974	1.00	39.33	N
ATOM	1748	CA	PHE	E	61	31.685	67.493	36.460	1.00	39.56	C
ATOM	1749	CB	PHE	E	61	32.578	68.676	36.077	1.00	40.25	C
ATOM	1750	CG	PHE	E	61	32.153	69.976	36.694	1.00	42.16	C
ATOM	1751	CD1	PHE	E	61	32.048	70.104	38.075	1.00	44.33	C
ATOM	1752	CE1	PHE	E	61	31.646	71.313	38.650	1.00	45.96	C
ATOM	1753	CZ	PHE	E	61	31.356	72.408	37.844	1.00	44.56	C
ATOM	1754	CE2	PHE	E	61	31.461	72.291	36.464	1.00	45.76	C
ATOM	1755	CD2	PHE	E	61	31.855	71.075	35.896	1.00	44.21	C
ATOM	1756	C	PHE	E	61	30.255	67.704	35.955	1.00	38.78	C
ATOM	1757	O	PHE	E	61	29.400	68.239	36.671	1.00	38.29	O
ATOM	1758	N	ALA	E	62	30.001	67.269	34.725	1.00	38.31	N
ATOM	1759	CA	ALA	E	62	28.680	67.396	34.123	1.00	38.23	C
ATOM	1760	CB	ALA	E	62	28.738	67.066	32.656	1.00	38.19	C
ATOM	1761	C	ALA	E	62	27.636	66.520	34.835	1.00	38.37	C
ATOM	1762	O	ALA	E	62	26.465	66.892	34.901	1.00	38.21	O
ATOM	1763	N	LEU	E	63	28.060	65.369	35.368	1.00	38.58	N
ATOM	1764	CA	LEU	E	63	27.172	64.516	36.185	1.00	39.10	C
ATOM	1765	CB	LEU	E	63	27.851	63.196	36.586	1.00	38.65	C
ATOM	1766	CG	LEU	E	63	28.228	62.139	35.545	1.00	38.55	C
ATOM	1767	CD1	LEU	E	63	28.751	60.926	36.269	1.00	39.11	C
ATOM	1768	CD2	LEU	E	63	27.045	61.739	34.664	1.00	39.44	C
ATOM	1769	C	LEU	E	63	26.740	65.252	37.442	1.00	39.24	C
ATOM	1770	O	LEU	E	63	25.566	65.260	37.784	1.00	39.50	O
ATOM	1771	N	VAL	E	64	27.703	65.856	38.133	1.00	39.79	N
ATOM	1772	CA	VAL	E	64	27.418	66.663	39.322	1.00	40.61	C
ATOM	1773	CB	VAL	E	64	28.715	67.180	39.981	1.00	40.71	C
ATOM	1774	CG1	VAL	E	64	28.400	68.170	41.104	1.00	42.39	C
ATOM	1775	CG2	VAL	E	64	29.505	66.024	40.522	1.00	41.41	C
ATOM	1776	C	VAL	E	64	26.512	67.838	38.986	1.00	40.46	C
ATOM	1777	O	VAL	E	64	25.478	68.035	39.631	1.00	41.14	O
ATOM	1778	N	THR	E	65	26.899	68.598	37.961	1.00	40.24	N
ATOM	1779	CA	THR	E	65	26.156	69.786	37.526	1.00	40.28	C
ATOM	1780	CB	THR	E	65	26.819	70.407	36.284	1.00	40.12	C
ATOM	1781	OG1	THR	E	65	28.103	70.918	36.660	1.00	41.50	O
ATOM	1782	CG2	THR	E	65	25.987	71.551	35.725	1.00	41.94	C
ATOM	1783	C	THR	E	65	24.692	69.480	37.233	1.00	39.90	C
ATOM	1784	O	THR	E	65	23.803	70.252	37.587	1.00	40.16	O
ATOM	1785	N	ASN	E	66	24.450	68.343	36.593	1.00	39.35	N
ATOM	1786	CA	ASN	E	66	23.101	67.951	36.212	1.00	39.00	C
ATOM	1787	CB	ASN	E	66	23.152	67.247	34.859	1.00	38.52	C
ATOM	1788	CG	ASN	E	66	23.480	68.212	33.729	1.00	37.68	C
ATOM	1789	OD1	ASN	E	66	22.655	69.037	33.368	1.00	38.59	O
ATOM	1790	ND2	ASN	E	66	24.694	68.127	33.188	1.00	34.98	N
ATOM	1791	C	ASN	E	66	22.344	67.118	37.254	1.00	39.24	C
ATOM	1792	O	ASN	E	66	21.167	66.820	37.064	1.00	38.96	O
ATOM	1793	N	GLY	E	67	23.017	66.758	38.345	1.00	39.58	N
ATOM	1794	CA	GLY	E	67	22.408	65.924	39.398	1.00	40.73	C
ATOM	1795	C	GLY	E	67	21.989	64.559	38.876	1.00	41.12	C
ATOM	1796	O	GLY	E	67	20.871	64.112	39.096	1.00	41.65	O
ATOM	1797	N	VAL	E	68	22.905	63.910	38.172	1.00	41.26	N
ATOM	1798	CA	VAL	E	68	22.640	62.654	37.491	1.00	41.46	C
ATOM	1799	CB	VAL	E	68	22.515	62.955	35.966	1.00	41.79	C
ATOM	1800	CG1	VAL	E	68	23.302	62.001	35.087	1.00	42.41	C
ATOM	1801	CG2	VAL	E	68	21.035	63.122	35.552	1.00	40.89	C
ATOM	1802	C	VAL	E	68	23.771	61.673	37.857	1.00	41.26	C
ATOM	1803	O	VAL	E	68	24.908	62.096	38.085	1.00	41.32	O
ATOM	1804	N	ARG	E	69	23.462	60.380	37.927	1.00	40.73	N
ATOM	1805	CA	ARG	E	69	24.442	59.373	38.365	1.00	40.63	C
ATOM	1806	CB	ARG	E	69	23.848	58.463	39.446	1.00	41.17	C
ATOM	1807	CG	ARG	E	69	23.045	59.207	40.496	1.00	44.78	C

Figure 1 Table 1a - 28

ATOM	1808	CD	ARG	E	69	23.329	58.675	41.862	1.00	49.16	C
ATOM	1809	NE	ARG	E	69	22.403	57.624	42.264	1.00	54.66	N
ATOM	1810	CZ	ARG	E	69	22.621	56.783	43.276	1.00	56.09	C
ATOM	1811	NH1	ARG	E	69	23.733	56.859	43.983	1.00	56.65	N
ATOM	1812	NH2	ARG	E	69	21.729	55.851	43.575	1.00	58.61	N
ATOM	1813	C	ARG	E	69	24.991	58.502	37.242	1.00	39.77	C
ATOM	1814	O	ARG	E	69	25.860	57.666	37.482	1.00	39.23	O
ATOM	1815	N	ALA	E	70	24.478	58.691	36.028	1.00	38.50	N
ATOM	1816	CA	ALA	E	70	24.848	57.848	34.895	1.00	37.96	C
ATOM	1817	CB	ALA	E	70	24.151	56.505	34.967	1.00	37.35	C
ATOM	1818	C	ALA	E	70	24.489	58.541	33.602	1.00	37.33	C
ATOM	1819	O	ALA	E	70	23.512	59.286	33.548	1.00	37.55	O
ATOM	1820	N	ALA	E	71	25.282	58.274	32.569	1.00	36.77	N
ATOM	1821	CA	ALA	E	71	25.113	58.883	31.256	1.00	36.41	C
ATOM	1822	CB	ALA	E	71	26.008	60.102	31.154	1.00	36.33	C
ATOM	1823	C	ALA	E	71	25.451	57.884	30.150	1.00	36.17	C
ATOM	1824	O	ALA	E	71	26.535	57.324	30.158	1.00	36.75	O
ATOM	1825	N	PRO	E	72	24.528	57.653	29.192	1.00	36.52	N
ATOM	1826	CA	PRO	E	72	24.921	56.871	27.992	1.00	36.60	C
ATOM	1827	CB	PRO	E	72	23.671	56.902	27.089	1.00	36.31	C
ATOM	1828	CG	PRO	E	72	22.522	57.311	27.980	1.00	36.88	C
ATOM	1829	CD	PRO	E	72	23.118	58.104	29.137	1.00	36.65	C
ATOM	1830	C	PRO	E	72	26.094	57.505	27.238	1.00	36.50	C
ATOM	1831	O	PRO	E	72	26.325	58.721	27.336	1.00	36.54	O
ATOM	1832	N	LEU	E	73	26.818	56.671	26.492	1.00	36.26	N
ATOM	1833	CA	LEU	E	73	27.998	57.102	25.748	1.00	36.29	C
ATOM	1834	CB	LEU	E	73	29.252	56.316	26.177	1.00	36.17	C
ATOM	1835	CG	LEU	E	73	29.657	56.487	27.647	1.00	37.03	C
ATOM	1836	CD1	LEU	E	73	30.887	55.650	27.997	1.00	37.18	C
ATOM	1837	CD2	LEU	E	73	29.898	57.958	27.991	1.00	37.26	C
ATOM	1838	C	LEU	E	73	27.748	56.946	24.272	1.00	36.10	C
ATOM	1839	O	LEU	E	73	27.383	55.859	23.800	1.00	35.61	O
ATOM	1840	N	TRP	E	74	27.900	58.054	23.552	1.00	35.54	N
ATOM	1841	CA	TRP	E	74	27.684	58.068	22.121	1.00	35.94	C
ATOM	1842	CB	TRP	E	74	26.795	59.246	21.727	1.00	35.84	C
ATOM	1843	CG	TRP	E	74	26.576	59.437	20.236	1.00	35.77	C
ATOM	1844	CD1	TRP	E	74	27.258	60.289	19.413	1.00	34.56	C
ATOM	1845	NE1	TRP	E	74	26.771	60.206	18.136	1.00	35.63	N
ATOM	1846	CE2	TRP	E	74	25.741	59.302	18.108	1.00	35.13	C
ATOM	1847	CD2	TRP	E	74	25.592	58.791	19.418	1.00	34.92	C
ATOM	1848	CE3	TRP	E	74	24.587	57.843	19.667	1.00	35.39	C
ATOM	1849	CZ3	TRP	E	74	23.775	57.426	18.601	1.00	35.28	C
ATOM	1850	CH2	TRP	E	74	23.959	57.950	17.299	1.00	35.06	C
ATOM	1851	CZ2	TRP	E	74	24.930	58.886	17.037	1.00	34.22	C
ATOM	1852	C	TRP	E	74	29.037	58.110	21.404	1.00	36.31	C
ATOM	1853	O	TRP	E	74	29.860	59.012	21.628	1.00	36.40	O
ATOM	1854	N	ASP	E	75	29.273	57.094	20.580	1.00	36.49	N
ATOM	1855	CA	ASP	E	75	30.432	57.056	19.702	1.00	36.94	C
ATOM	1856	CB	ASP	E	75	30.919	55.618	19.534	1.00	36.88	C
ATOM	1857	CG	ASP	E	75	32.234	55.522	18.767	1.00	38.46	C
ATOM	1858	OD1	ASP	E	75	33.042	54.625	19.087	1.00	39.48	O
ATOM	1859	OD2	ASP	E	75	32.463	56.333	17.844	1.00	39.12	O
ATOM	1860	C	ASP	E	75	30.027	57.661	18.357	1.00	36.91	C
ATOM	1861	O	ASP	E	75	29.252	57.063	17.604	1.00	36.37	O
ATOM	1862	N	SER	E	76	30.556	58.849	18.066	1.00	37.44	N
ATOM	1863	CA	SER	E	76	30.161	59.592	16.868	1.00	38.19	C
ATOM	1864	CB	SER	E	76	30.680	61.026	16.919	1.00	38.17	C
ATOM	1865	OG	SER	E	76	30.007	61.820	15.956	1.00	39.07	O
ATOM	1866	C	SER	E	76	30.598	58.916	15.558	1.00	38.58	C
ATOM	1867	O	SER	E	76	29.847	58.908	14.582	1.00	38.53	O
ATOM	1868	N	LYS	E	77	31.808	58.355	15.540	1.00	39.34	N
ATOM	1869	CA	LYS	E	77	32.296	57.631	14.355	1.00	39.96	C
ATOM	1870	CB	LYS	E	77	33.735	57.151	14.543	1.00	40.45	C
ATOM	1871	CG	LYS	E	77	34.760	58.264	14.506	1.00	42.99	C
ATOM	1872	CD	LYS	E	77	36.036	57.822	13.813	1.00	46.66	C
ATOM	1873	CE	LYS	E	77	37.238	58.625	14.306	1.00	48.56	C
ATOM	1874	NZ	LYS	E	77	37.673	58.168	15.671	1.00	49.19	N

Figure 1

Table 1a - 29

ATOM	1875	C	LYS	E	77	31.395	56.451	14.009	1.00	39.64	C
ATOM	1876	O	LYS	E	77	31.049	56.252	12.847	1.00	39.76	O
ATOM	1877	N	LYS	E	78	31.017	55.684	15.030	1.00	39.27	N
ATOM	1878	CA	LYS	E	78	30.160	54.515	14.870	1.00	39.06	C
ATOM	1879	CB	LYS	E	78	30.371	53.544	16.034	1.00	39.43	C
ATOM	1880	CG	LYS	E	78	31.716	52.856	16.008	1.00	40.46	C
ATOM	1881	CD	LYS	E	78	31.923	52.034	17.258	1.00	43.16	C
ATOM	1882	CE	LYS	E	78	33.196	51.208	17.157	1.00	44.03	C
ATOM	1883	NZ	LYS	E	78	33.439	50.479	18.436	1.00	45.96	N
ATOM	1884	C	LYS	E	78	28.683	54.862	14.778	1.00	38.77	C
ATOM	1885	O	LYS	E	78	27.882	54.034	14.334	1.00	38.88	O
ATOM	1886	N	GLN	E	79	28.320	56.075	15.200	1.00	38.05	N
ATOM	1887	CA	GLN	E	79	26.921	56.518	15.211	1.00	37.46	C
ATOM	1888	CB	GLN	E	79	26.355	56.620	13.787	1.00	37.41	C
ATOM	1889	CG	GLN	E	79	26.915	57.777	12.968	1.00	36.97	C
ATOM	1890	CD	GLN	E	79	26.396	59.108	13.473	1.00	36.31	C
ATOM	1891	OE1	GLN	E	79	25.219	59.420	13.309	1.00	35.15	O
ATOM	1892	NE2	GLN	E	79	27.264	59.884	14.112	1.00	35.60	N
ATOM	1893	C	GLN	E	79	26.054	55.594	16.074	1.00	37.18	C
ATOM	1894	O	GLN	E	79	24.978	55.176	15.659	1.00	36.61	O
ATOM	1895	N	SER	E	80	26.549	55.265	17.266	1.00	37.22	N
ATOM	1896	CA	SER	E	80	25.770	54.496	18.225	1.00	37.42	C
ATOM	1897	CB	SER	E	80	25.752	53.001	17.886	1.00	37.34	C
ATOM	1898	OG	SER	E	80	27.050	52.474	17.892	1.00	39.95	O
ATOM	1899	C	SER	E	80	26.219	54.684	19.654	1.00	37.05	C
ATOM	1900	O	SER	E	80	27.331	55.143	19.936	1.00	37.18	O
ATOM	1901	N	PHE	E	81	25.301	54.352	20.551	1.00	36.75	N
ATOM	1902	CA	PHE	E	81	25.598	54.176	21.958	1.00	36.24	C
ATOM	1903	CB	PHE	E	81	24.301	53.984	22.739	1.00	35.67	C
ATOM	1904	CG	PHE	E	81	23.436	55.198	22.761	1.00	35.58	C
ATOM	1905	CD1	PHE	E	81	22.217	55.206	22.093	1.00	34.72	C
ATOM	1906	CE1	PHE	E	81	21.403	56.327	22.114	1.00	36.00	C
ATOM	1907	CZ	PHE	E	81	21.820	57.477	22.798	1.00	36.00	C
ATOM	1908	CE2	PHE	E	81	23.043	57.482	23.458	1.00	35.70	C
ATOM	1909	CD2	PHE	E	81	23.843	56.347	23.441	1.00	34.42	C
ATOM	1910	C	PHE	E	81	26.492	52.959	22.127	1.00	36.28	C
ATOM	1911	O	PHE	E	81	26.224	51.905	21.544	1.00	36.59	O
ATOM	1912	N	VAL	E	82	27.547	53.111	22.926	1.00	35.96	N
ATOM	1913	CA	VAL	E	82	28.528	52.043	23.117	1.00	36.12	C
ATOM	1914	CB	VAL	E	82	29.923	52.422	22.547	1.00	35.99	C
ATOM	1915	CG1	VAL	E	82	29.880	52.516	21.018	1.00	36.32	C
ATOM	1916	CG2	VAL	E	82	30.455	53.716	23.175	1.00	35.59	C
ATOM	1917	C	VAL	E	82	28.688	51.595	24.576	1.00	36.14	C
ATOM	1918	O	VAL	E	82	29.396	50.628	24.849	1.00	36.08	O
ATOM	1919	N	GLY	E	83	28.052	52.305	25.505	1.00	36.36	N
ATOM	1920	CA	GLY	E	83	28.234	52.014	26.929	1.00	36.35	C
ATOM	1921	C	GLY	E	83	27.686	53.100	27.825	1.00	36.62	C
ATOM	1922	O	GLY	E	83	26.958	53.993	27.364	1.00	36.24	O
ATOM	1923	N	MET	E	84	28.056	53.018	29.102	1.00	36.61	N
ATOM	1924	CA	MET	E	84	27.626	53.958	30.128	1.00	37.31	C
ATOM	1925	CB	MET	E	84	26.720	53.259	31.149	1.00	37.74	C
ATOM	1926	CG	MET	E	84	25.428	52.686	30.562	1.00	39.90	C
ATOM	1927	SD	MET	E	84	24.187	53.954	30.249	1.00	41.85	S
ATOM	1928	CE	MET	E	84	23.595	53.384	28.692	1.00	45.60	C
ATOM	1929	C	MET	E	84	28.828	54.552	30.854	1.00	37.37	C
ATOM	1930	O	MET	E	84	29.898	53.950	30.915	1.00	37.72	O
ATOM	1931	N	LEU	E	85	28.653	55.747	31.393	1.00	37.44	N
ATOM	1932	CA	LEU	E	85	29.599	56.269	32.362	1.00	37.41	C
ATOM	1933	CB	LEU	E	85	30.278	57.544	31.851	1.00	37.46	C
ATOM	1934	CG	LEU	E	85	31.546	58.009	32.591	1.00	38.11	C
ATOM	1935	CD1	LEU	E	85	32.745	57.126	32.246	1.00	37.72	C
ATOM	1936	CD2	LEU	E	85	31.858	59.455	32.237	1.00	37.51	C
ATOM	1937	C	LEU	E	85	28.826	56.516	33.650	1.00	37.24	C
ATOM	1938	O	LEU	E	85	27.865	57.290	33.681	1.00	37.54	O
ATOM	1939	N	THR	E	86	29.231	55.828	34.706	1.00	36.80	N
ATOM	1940	CA	THR	E	86	28.516	55.888	35.976	1.00	36.13	C
ATOM	1941	CB	THR	E	86	27.875	54.531	36.344	1.00	36.22	C

Figure 1 Table 1a - 30

ATOM	1942	OG1	THR	E	86	28.873	53.646	36.880	1.00	34.96	O
ATOM	1943	CG2	THR	E	86	27.162	53.890	35.137	1.00	33.71	C
ATOM	1944	C	THR	E	86	29.510	56.318	37.052	1.00	36.57	C
ATOM	1945	O	THR	E	86	30.697	56.536	36.756	1.00	35.93	O
ATOM	1946	N	ILE	E	87	29.027	56.446	38.285	1.00	36.48	N
ATOM	1947	CA	ILE	E	87	29.881	56.826	39.412	1.00	36.65	C
ATOM	1948	CB	ILE	E	87	29.087	57.098	40.720	1.00	36.67	C
ATOM	1949	CG1	ILE	E	87	27.954	58.115	40.505	1.00	38.09	C
ATOM	1950	CD1	ILE	E	87	28.293	59.266	39.603	1.00	41.99	C
ATOM	1951	CG2	ILE	E	87	30.038	57.533	41.859	1.00	36.12	C
ATOM	1952	C	ILE	E	87	30.949	55.771	39.690	1.00	36.35	C
ATOM	1953	O	ILE	E	87	32.022	56.108	40.164	1.00	36.39	O
ATOM	1954	N	THR	E	88	30.649	54.507	39.394	1.00	36.08	N
ATOM	1955	CA	THR	E	88	31.630	53.435	39.536	1.00	36.10	C
ATOM	1956	CB	THR	E	88	31.038	52.070	39.166	1.00	36.12	C
ATOM	1957	OG1	THR	E	88	30.064	51.698	40.151	1.00	34.90	O
ATOM	1958	CG2	THR	E	88	32.133	50.994	39.098	1.00	35.38	C
ATOM	1959	C	THR	E	88	32.883	53.729	38.701	1.00	36.73	C
ATOM	1960	O	THR	E	88	34.010	53.581	39.197	1.00	36.62	O
ATOM	1961	N	ASP	E	89	32.676	54.171	37.456	1.00	36.34	N
ATOM	1962	CA	ASP	E	89	33.767	54.561	36.560	1.00	37.03	C
ATOM	1963	CB	ASP	E	89	33.219	54.882	35.163	1.00	37.21	C
ATOM	1964	CG	ASP	E	89	32.465	53.707	34.563	1.00	36.96	C
ATOM	1965	OD1	ASP	E	89	31.267	53.853	34.264	1.00	37.45	O
ATOM	1966	OD2	ASP	E	89	33.062	52.623	34.425	1.00	37.12	O
ATOM	1967	C	ASP	E	89	34.562	55.747	37.089	1.00	37.30	C
ATOM	1968	O	ASP	E	89	35.780	55.790	36.935	1.00	37.23	O
ATOM	1969	N	PHE	E	90	33.870	56.704	37.717	1.00	37.52	N
ATOM	1970	CA	PHE	E	90	34.536	57.835	38.367	1.00	37.38	C
ATOM	1971	CB	PHE	E	90	33.515	58.793	38.983	1.00	37.76	C
ATOM	1972	CG	PHE	E	90	34.131	59.975	39.673	1.00	38.87	C
ATOM	1973	CD1	PHE	E	90	34.948	60.873	38.968	1.00	39.12	C
ATOM	1974	CE1	PHE	E	90	35.524	61.976	39.604	1.00	40.27	C
ATOM	1975	CZ	PHE	E	90	35.266	62.199	40.965	1.00	40.99	C
ATOM	1976	CE2	PHE	E	90	34.453	61.306	41.675	1.00	40.59	C
ATOM	1977	CD2	PHE	E	90	33.890	60.205	41.024	1.00	39.87	C
ATOM	1978	C	PHE	E	90	35.469	57.326	39.447	1.00	37.21	C
ATOM	1979	O	PHE	E	90	36.598	57.779	39.565	1.00	36.89	O
ATOM	1980	N	ILE	E	91	34.984	56.375	40.234	1.00	36.21	N
ATOM	1981	CA	ILE	E	91	35.782	55.819	41.309	1.00	36.71	C
ATOM	1982	CB	ILE	E	91	34.919	54.966	42.240	1.00	36.36	C
ATOM	1983	CG1	ILE	E	91	33.938	55.877	42.991	1.00	36.26	C
ATOM	1984	CD1	ILE	E	91	32.797	55.151	43.637	1.00	35.28	C
ATOM	1985	CG2	ILE	E	91	35.787	54.136	43.197	1.00	36.44	C
ATOM	1986	C	ILE	E	91	37.009	55.044	40.796	1.00	36.79	C
ATOM	1987	O	ILE	E	91	38.098	55.182	41.359	1.00	37.01	O
ATOM	1988	N	ASN	E	92	36.825	54.245	39.747	1.00	36.82	N
ATOM	1989	CA	ASN	E	92	37.930	53.528	39.109	1.00	37.77	C
ATOM	1990	CB	ASN	E	92	37.449	52.669	37.939	1.00	37.78	C
ATOM	1991	CG	ASN	E	92	36.451	51.605	38.350	1.00	40.57	C
ATOM	1992	OD1	ASN	E	92	36.399	51.182	39.508	1.00	41.67	O
ATOM	1993	ND2	ASN	E	92	35.638	51.171	37.392	1.00	41.45	N
ATOM	1994	C	ASN	E	92	38.992	54.507	38.601	1.00	37.93	C
ATOM	1995	O	ASN	E	92	40.192	54.281	38.790	1.00	37.23	O
ATOM	1996	N	ILE	E	93	38.527	55.590	37.966	1.00	37.94	N
ATOM	1997	CA	ILE	E	93	39.407	56.641	37.445	1.00	38.73	C
ATOM	1998	CB	ILE	E	93	38.645	57.590	36.469	1.00	38.86	C
ATOM	1999	CG1	ILE	E	93	38.233	56.799	35.231	1.00	39.76	C
ATOM	2000	CD1	ILE	E	93	37.077	57.377	34.435	1.00	42.98	C
ATOM	2001	CG2	ILE	E	93	39.521	58.787	36.044	1.00	40.29	C
ATOM	2002	C	ILE	E	93	40.127	57.428	38.544	1.00	38.88	C
ATOM	2003	O	ILE	E	93	41.340	57.634	38.453	1.00	38.76	O
ATOM	2004	N	LEU	E	94	39.385	57.876	39.562	1.00	39.29	N
ATOM	2005	CA	LEU	E	94	39.966	58.615	40.692	1.00	40.15	C
ATOM	2006	CB	LEU	E	94	38.902	59.014	41.713	1.00	40.03	C
ATOM	2007	CG	LEU	E	94	38.314	60.421	41.787	1.00	42.70	C
ATOM	2008	CD1	LEU	E	94	37.669	60.602	43.157	1.00	43.64	C

Figure 1 Table 1a - 31

ATOM	2009	CD2	LEU	E	94	39.340	61.535	41.529	1.00	44.14	C
ATOM	2010	C	LEU	E	94	41.025	57.798	41.424	1.00	40.17	C
ATOM	2011	O	LEU	E	94	42.055	58.325	41.837	1.00	40.18	O
ATOM	2012	N	HIS	E	95	40.746	56.515	41.616	1.00	40.42	N
ATOM	2013	CA	HIS	E	95	41.683	55.636	42.295	1.00	40.82	C
ATOM	2014	CB	HIS	E	95	41.062	54.272	42.569	1.00	40.39	C
ATOM	2015	CG	HIS	E	95	41.936	53.371	43.385	1.00	41.69	C
ATOM	2016	ND1	HIS	E	95	42.376	52.146	42.929	1.00	42.36	N
ATOM	2017	CE1	HIS	E	95	43.128	51.582	43.856	1.00	42.35	C
ATOM	2018	NE2	HIS	E	95	43.205	52.403	44.889	1.00	43.04	N
ATOM	2019	CD2	HIS	E	95	42.466	53.527	44.622	1.00	41.76	C
ATOM	2020	C	HIS	E	95	42.964	55.501	41.469	1.00	41.28	C
ATOM	2021	O	HIS	E	95	44.061	55.620	42.008	1.00	40.62	O
ATOM	2022	N	ARG	E	96	42.807	55.266	40.167	1.00	42.01	N
ATOM	2023	CA	ARG	E	96	43.938	55.209	39.243	1.00	43.95	C
ATOM	2024	CB	ARG	E	96	43.458	54.929	37.826	1.00	44.43	C
ATOM	2025	CG	ARG	E	96	43.675	53.508	37.381	1.00	48.99	C
ATOM	2026	CD	ARG	E	96	45.139	53.276	37.062	1.00	53.75	C
ATOM	2027	NE	ARG	E	96	45.395	51.893	36.685	1.00	57.94	N
ATOM	2028	CZ	ARG	E	96	45.325	51.427	35.440	1.00	60.04	C
ATOM	2029	NH1	ARG	E	96	44.996	52.232	34.438	1.00	60.71	N
ATOM	2030	NH2	ARG	E	96	45.583	50.145	35.201	1.00	61.69	N
ATOM	2031	C	ARG	E	96	44.760	56.493	39.244	1.00	43.74	C
ATOM	2032	O	ARG	E	96	45.984	56.444	39.276	1.00	44.52	O
ATOM	2033	N	TYR	E	97	44.067	57.626	39.217	1.00	43.40	N
ATOM	2034	CA	TYR	E	97	44.676	58.947	39.269	1.00	43.47	C
ATOM	2035	CB	TYR	E	97	43.587	60.029	39.138	1.00	44.75	C
ATOM	2036	CG	TYR	E	97	44.001	61.426	39.568	1.00	46.77	C
ATOM	2037	CD1	TYR	E	97	44.598	62.306	38.661	1.00	48.87	C
ATOM	2038	CE1	TYR	E	97	44.981	63.589	39.047	1.00	50.36	C
ATOM	2039	CZ	TYR	E	97	44.760	64.005	40.358	1.00	50.90	C
ATOM	2040	OH	TYR	E	97	45.138	65.283	40.740	1.00	52.46	O
ATOM	2041	CE2	TYR	E	97	44.165	63.150	41.278	1.00	50.34	C
ATOM	2042	CD2	TYR	E	97	43.779	61.870	40.875	1.00	48.44	C
ATOM	2043	C	TYR	E	97	45.487	59.138	40.547	1.00	42.26	C
ATOM	2044	O	TYR	E	97	46.614	59.631	40.502	1.00	41.73	O
ATOM	2045	N	TYR	E	98	44.909	58.756	41.683	1.00	40.90	N
ATOM	2046	CA	TYR	E	98	45.588	58.916	42.962	1.00	39.72	C
ATOM	2047	CB	TYR	E	98	44.671	58.547	44.139	1.00	39.77	C
ATOM	2048	CG	TYR	E	98	45.388	58.602	45.465	1.00	40.48	C
ATOM	2049	CD1	TYR	E	98	45.524	59.807	46.156	1.00	40.99	C
ATOM	2050	CE1	TYR	E	98	46.204	59.862	47.374	1.00	41.30	C
ATOM	2051	CZ	TYR	E	98	46.762	58.713	47.895	1.00	41.64	C
ATOM	2052	OH	TYR	E	98	47.436	58.768	49.100	1.00	43.98	O
ATOM	2053	CE2	TYR	E	98	46.654	57.505	47.220	1.00	40.62	C
ATOM	2054	CD2	TYR	E	98	45.969	57.457	46.014	1.00	39.36	C
ATOM	2055	C	TYR	E	98	46.911	58.128	43.009	1.00	38.81	C
ATOM	2056	O	TYR	E	98	47.962	58.682	43.364	1.00	37.99	O
ATOM	2057	N	LYS	E	99	46.850	56.852	42.636	1.00	37.83	N
ATOM	2058	CA	LYS	E	99	48.035	55.992	42.631	1.00	37.34	C
ATOM	2059	CB	LYS	E	99	47.654	54.517	42.425	1.00	37.49	C
ATOM	2060	CG	LYS	E	99	46.791	53.911	43.548	1.00	37.85	C
ATOM	2061	CD	LYS	E	99	47.546	53.824	44.872	1.00	38.62	C
ATOM	2062	CE	LYS	E	99	46.854	52.883	45.870	1.00	39.50	C
ATOM	2063	NZ	LYS	E	99	47.649	52.804	47.134	1.00	39.63	N
ATOM	2064	C	LYS	E	99	49.070	56.443	41.595	1.00	36.51	C
ATOM	2065	O	LYS	E	99	50.259	56.493	41.895	1.00	36.01	O
ATOM	2066	N	SER	E	100	48.607	56.794	40.397	1.00	35.40	N
ATOM	2067	CA	SER	E	100	49.488	57.234	39.313	1.00	34.36	C
ATOM	2068	CB	SER	E	100	48.687	57.438	38.024	1.00	35.10	C
ATOM	2069	OG	SER	E	100	48.112	56.221	37.579	1.00	35.67	O
ATOM	2070	C	SER	E	100	50.250	58.524	39.654	1.00	33.86	C
ATOM	2071	O	SER	E	100	51.424	58.677	39.284	1.00	32.60	O
ATOM	2072	N	ALA	E	101	49.579	59.440	40.353	1.00	32.88	N
ATOM	2073	CA	ALA	E	101	50.186	60.701	40.783	1.00	32.47	C
ATOM	2074	CB	ALA	E	101	49.151	61.604	41.429	1.00	32.25	C
ATOM	2075	C	ALA	E	101	51.380	60.477	41.719	1.00	32.39	C

Figure 1 Table 1a - 32

ATOM	2076	O	ALA	E	101	52.380	61.198	41.640	1.00	32.06	O
ATOM	2077	N	LEU	E	102	51.279	59.455	42.571	1.00	32.01	N
ATOM	2078	CA	LEU	E	102	52.355	59.074	43.495	1.00	32.25	C
ATOM	2079	CB	LEU	E	102	51.862	57.998	44.480	1.00	32.42	C
ATOM	2080	CG	LEU	E	102	50.801	58.418	45.511	1.00	33.49	C
ATOM	2081	CD1	LEU	E	102	50.317	57.219	46.324	1.00	32.90	C
ATOM	2082	CD2	LEU	E	102	51.340	59.501	46.444	1.00	35.63	C
ATOM	2083	C	LEU	E	102	53.611	58.597	42.762	1.00	32.24	C
ATOM	2084	O	LEU	E	102	54.710	58.522	43.331	1.00	31.84	O
ATOM	2085	N	VAL	E	103	53.434	58.317	41.476	1.00	32.33	N
ATOM	2086	CA	VAL	E	103	54.493	57.819	40.617	1.00	31.86	C
ATOM	2087	CB	VAL	E	103	54.138	56.353	40.223	1.00	32.57	C
ATOM	2088	CG1	VAL	E	103	53.578	56.234	38.831	1.00	32.80	C
ATOM	2089	CG2	VAL	E	103	55.305	55.428	40.471	1.00	33.21	C
ATOM	2090	C	VAL	E	103	54.697	58.827	39.460	1.00	31.48	C
ATOM	2091	O	VAL	E	103	55.338	58.548	38.436	1.00	30.85	O
ATOM	2092	N	GLN	E	104	54.163	60.029	39.673	1.00	31.17	N
ATOM	2093	CA	GLN	E	104	54.318	61.170	38.758	1.00	31.30	C
ATOM	2094	CB	GLN	E	104	55.774	61.691	38.739	1.00	30.94	C
ATOM	2095	CG	GLN	E	104	56.369	62.020	40.119	1.00	30.63	C
ATOM	2096	CD	GLN	E	104	56.810	60.769	40.895	1.00	31.22	C
ATOM	2097	OE1	GLN	E	104	57.478	59.894	40.355	1.00	30.93	O
ATOM	2098	NE2	GLN	E	104	56.426	60.690	42.161	1.00	30.48	N
ATOM	2099	C	GLN	E	104	53.804	60.878	37.335	1.00	31.91	C
ATOM	2100	O	GLN	E	104	54.375	61.333	36.340	1.00	31.17	O
ATOM	2101	N	ILE	E	105	52.721	60.112	37.257	1.00	33.20	N
ATOM	2102	CA	ILE	E	105	52.012	59.905	35.999	1.00	34.91	C
ATOM	2103	CB	ILE	E	105	51.801	58.405	35.703	1.00	35.05	C
ATOM	2104	CG1	ILE	E	105	53.138	57.732	35.378	1.00	34.28	C
ATOM	2105	CD1	ILE	E	105	53.071	56.221	35.348	1.00	34.37	C
ATOM	2106	CG2	ILE	E	105	50.809	58.217	34.560	1.00	34.32	C
ATOM	2107	C	ILE	E	105	50.664	60.615	36.027	1.00	36.82	C
ATOM	2108	O	ILE	E	105	49.766	60.234	36.778	1.00	36.58	O
ATOM	2109	N	TYR	E	106	50.531	61.653	35.206	1.00	39.00	N
ATOM	2110	CA	TYR	E	106	49.364	62.526	35.256	1.00	41.77	C
ATOM	2111	CB	TYR	E	106	49.778	63.952	35.632	1.00	40.80	C
ATOM	2112	CG	TYR	E	106	50.704	64.030	36.823	1.00	40.15	C
ATOM	2113	CD1	TYR	E	106	52.072	64.204	36.652	1.00	39.45	C
ATOM	2114	CE1	TYR	E	106	52.924	64.277	37.739	1.00	38.58	C
ATOM	2115	CZ	TYR	E	106	52.412	64.175	39.015	1.00	38.36	C
ATOM	2116	OH	TYR	E	106	53.258	64.246	40.095	1.00	38.39	O
ATOM	2117	CE2	TYR	E	106	51.056	64.001	39.212	1.00	38.17	C
ATOM	2118	CD2	TYR	E	106	50.212	63.930	38.119	1.00	38.34	C
ATOM	2119	C	TYR	E	106	48.630	62.531	33.921	1.00	44.32	C
ATOM	2120	O	TYR	E	106	48.526	63.566	33.268	1.00	45.40	O
ATOM	2121	N	GLU	E	107	48.126	61.369	33.519	1.00	47.49	N
ATOM	2122	CA	GLU	E	107	47.371	61.253	32.277	1.00	50.44	C
ATOM	2123	CB	GLU	E	107	47.595	59.879	31.642	1.00	50.59	C
ATOM	2124	CG	GLU	E	107	49.051	59.490	31.480	1.00	51.07	C
ATOM	2125	CD	GLU	E	107	49.230	58.016	31.172	1.00	51.57	C
ATOM	2126	OE1	GLU	E	107	48.492	57.191	31.752	1.00	54.15	O
ATOM	2127	OE2	GLU	E	107	50.109	57.682	30.351	1.00	51.67	O
ATOM	2128	C	GLU	E	107	45.884	61.458	32.527	1.00	52.18	C
ATOM	2129	O	GLU	E	107	45.259	62.340	31.936	1.00	52.60	O
ATOM	2130	N	LEU	E	108	45.327	60.635	33.409	1.00	54.13	N
ATOM	2131	CA	LEU	E	108	43.936	60.217	33.295	1.00	55.67	C
ATOM	2132	CB	LEU	E	108	43.505	59.445	34.542	1.00	55.83	C
ATOM	2133	CG	LEU	E	108	44.080	58.038	34.713	1.00	56.77	C
ATOM	2134	CD1	LEU	E	108	43.401	57.339	35.871	1.00	57.51	C
ATOM	2135	CD2	LEU	E	108	43.933	57.225	33.435	1.00	58.44	C
ATOM	2136	C	LEU	E	108	43.010	61.404	33.072	1.00	56.51	C
ATOM	2137	O	LEU	E	108	42.013	61.298	32.359	1.00	57.10	O
ATOM	2138	N	GLU	E	109	43.344	62.534	33.688	1.00	57.22	N
ATOM	2139	CA	GLU	E	109	42.388	63.625	33.831	1.00	58.32	C
ATOM	2140	CB	GLU	E	109	42.714	64.465	35.068	1.00	58.91	C
ATOM	2141	CG	GLU	E	109	41.534	64.662	36.011	1.00	60.44	C
ATOM	2142	CD	GLU	E	109	41.013	63.356	36.590	1.00	62.95	C

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ATOM	2143	OE1	GLU	E	109	40.633	63.341	37.781	1.00	63.63	O
ATOM	2144	OE2	GLU	E	109	40.981	62.345	35.857	1.00	63.82	O
ATOM	2145	C	GLU	E	109	42.336	64.497	32.580	1.00	58.05	C
ATOM	2146	O	GLU	E	109	41.443	65.332	32.434	1.00	58.93	O
ATOM	2147	N	GLU	E	110	43.293	64.292	31.679	1.00	57.53	N
ATOM	2148	CA	GLU	E	110	43.191	64.807	30.315	1.00	56.74	C
ATOM	2149	CB	GLU	E	110	44.499	65.477	29.891	1.00	57.17	C
ATOM	2150	CG	GLU	E	110	44.562	66.967	30.200	1.00	59.53	C
ATOM	2151	CD	GLU	E	110	43.732	67.346	31.413	1.00	62.30	C
ATOM	2152	OE1	GLU	E	110	42.493	67.447	31.278	1.00	63.97	O
ATOM	2153	OE2	GLU	E	110	44.317	67.542	32.501	1.00	62.97	O
ATOM	2154	C	GLU	E	110	42.814	63.706	29.325	1.00	55.58	C
ATOM	2155	O	GLU	E	110	42.599	63.970	28.141	1.00	55.30	O
ATOM	2156	N	HIS	E	111	42.740	62.474	29.820	1.00	54.03	N
ATOM	2157	CA	HIS	E	111	42.042	61.400	29.122	1.00	52.96	C
ATOM	2158	CB	HIS	E	111	41.854	60.194	30.047	1.00	53.46	C
ATOM	2159	CG	HIS	E	111	42.879	59.119	29.861	1.00	55.11	C
ATOM	2160	ND1	HIS	E	111	44.061	59.323	29.182	1.00	57.63	N
ATOM	2161	CE1	HIS	E	111	44.765	58.205	29.180	1.00	57.53	C
ATOM	2162	NE2	HIS	E	111	44.082	57.282	29.835	1.00	57.40	N
ATOM	2163	CD2	HIS	E	111	42.900	57.829	30.272	1.00	56.45	C
ATOM	2164	C	HIS	E	111	40.682	61.871	28.616	1.00	51.75	C
ATOM	2165	O	HIS	E	111	39.952	62.568	29.324	1.00	51.05	O
ATOM	2166	N	LYS	E	112	40.351	61.488	27.388	1.00	50.36	N
ATOM	2167	CA	LYS	E	112	38.961	61.448	26.955	1.00	49.61	C
ATOM	2168	CB	LYS	E	112	38.849	61.804	25.472	1.00	49.84	C
ATOM	2169	CG	LYS	E	112	39.357	60.727	24.530	1.00	50.18	C
ATOM	2170	CD	LYS	E	112	40.148	61.332	23.376	1.00	50.41	C
ATOM	2171	CE	LYS	E	112	39.592	62.686	22.965	1.00	50.36	C
ATOM	2172	NZ	LYS	E	112	40.376	63.292	21.852	1.00	51.26	N
ATOM	2173	C	LYS	E	112	38.350	60.075	27.227	1.00	48.82	C
ATOM	2174	O	LYS	E	112	39.065	59.110	27.508	1.00	48.41	O
ATOM	2175	N	ILE	E	113	37.026	59.996	27.142	1.00	47.68	N
ATOM	2176	CA	ILE	E	113	36.294	58.807	27.564	1.00	46.82	C
ATOM	2177	CB	ILE	E	113	34.770	59.016	27.460	1.00	46.55	C
ATOM	2178	CG1	ILE	E	113	34.295	60.008	28.526	1.00	45.37	C
ATOM	2179	CD1	ILE	E	113	32.894	60.529	28.300	1.00	44.45	C
ATOM	2180	CG2	ILE	E	113	34.038	57.690	27.591	1.00	45.06	C
ATOM	2181	C	ILE	E	113	36.704	57.588	26.742	1.00	47.24	C
ATOM	2182	O	ILE	E	113	36.965	56.515	27.292	1.00	46.36	O
ATOM	2183	N	GLU	E	114	36.757	57.763	25.425	1.00	47.87	N
ATOM	2184	CA	GLU	E	114	37.413	56.805	24.542	1.00	49.19	C
ATOM	2185	CB	GLU	E	114	37.801	57.476	23.224	1.00	49.20	C
ATOM	2186	CG	GLU	E	114	36.755	57.358	22.138	1.00	51.71	C
ATOM	2187	CD	GLU	E	114	37.295	57.732	20.772	1.00	54.44	C
ATOM	2188	OE1	GLU	E	114	38.035	58.736	20.676	1.00	55.30	O
ATOM	2189	OE2	GLU	E	114	36.979	57.020	19.795	1.00	55.19	O
ATOM	2190	C	GLU	E	114	38.652	56.204	25.192	1.00	49.47	C
ATOM	2191	O	GLU	E	114	38.718	54.997	25.427	1.00	49.28	O
ATOM	2192	N	THR	E	115	39.632	57.054	25.480	1.00	50.41	N
ATOM	2193	CA	THR	E	115	40.962	56.595	25.843	1.00	51.95	C
ATOM	2194	CB	THR	E	115	42.003	57.737	25.826	1.00	51.79	C
ATOM	2195	OG1	THR	E	115	41.607	58.768	26.737	1.00	53.22	O
ATOM	2196	CG2	THR	E	115	42.104	58.327	24.435	1.00	51.93	C
ATOM	2197	C	THR	E	115	40.960	55.874	27.185	1.00	52.62	C
ATOM	2198	O	THR	E	115	41.694	54.901	27.360	1.00	52.64	O
ATOM	2199	N	TRP	E	116	40.130	56.324	28.123	1.00	53.82	N
ATOM	2200	CA	TRP	E	116	39.987	55.570	29.360	1.00	55.35	C
ATOM	2201	CB	TRP	E	116	39.248	56.341	30.460	1.00	56.12	C
ATOM	2202	CG	TRP	E	116	39.229	55.532	31.734	1.00	58.16	C
ATOM	2203	CD1	TRP	E	116	40.272	55.345	32.604	1.00	59.04	C
ATOM	2204	NE1	TRP	E	116	39.889	54.514	33.629	1.00	61.05	N
ATOM	2205	CE2	TRP	E	116	38.585	54.135	33.432	1.00	60.36	C
ATOM	2206	CD2	TRP	E	116	38.138	54.751	32.245	1.00	60.03	C
ATOM	2207	CE3	TRP	E	116	36.826	54.517	31.813	1.00	60.86	C
ATOM	2208	CZ3	TRP	E	116	36.007	53.689	32.576	1.00	60.94	C
ATOM	2209	CH2	TRP	E	116	36.476	53.095	33.762	1.00	60.76	C

Figure 1 Table 1a - 34

ATOM	2210	CZ2	TRP	E	116	37.761	53.305	34.203	1.00	61.47	C
ATOM	2211	C	TRP	E	116	39.347	54.199	29.115	1.00	55.62	C
ATOM	2212	O	TRP	E	116	39.792	53.198	29.670	1.00	55.57	O
ATOM	2213	N	ARG	E	117	38.311	54.166	28.282	1.00	56.18	N
ATOM	2214	CA	ARG	E	117	37.610	52.923	27.984	1.00	56.96	C
ATOM	2215	CB	ARG	E	117	36.376	53.195	27.123	1.00	56.48	C
ATOM	2216	CG	ARG	E	117	35.169	53.680	27.910	1.00	55.44	C
ATOM	2217	CD	ARG	E	117	34.076	54.200	26.990	1.00	52.92	C
ATOM	2218	NE	ARG	E	117	33.625	53.188	26.037	1.00	51.27	N
ATOM	2219	CZ	ARG	E	117	32.884	52.133	26.358	1.00	50.54	C
ATOM	2220	NH1	ARG	E	117	32.504	51.940	27.615	1.00	49.92	N
ATOM	2221	NH2	ARG	E	117	32.523	51.267	25.421	1.00	50.53	N
ATOM	2222	C	ARG	E	117	38.526	51.916	27.294	1.00	58.06	C
ATOM	2223	O	ARG	E	117	38.481	50.721	27.586	1.00	57.83	O
ATOM	2224	N	GLU	E	118	39.356	52.407	26.380	1.00	59.60	N
ATOM	2225	CA	GLU	E	118	40.353	51.572	25.719	1.00	61.59	C
ATOM	2226	CB	GLU	E	118	41.032	52.347	24.589	1.00	61.65	C
ATOM	2227	CG	GLU	E	118	41.953	51.505	23.719	1.00	63.81	C
ATOM	2228	CD	GLU	E	118	41.213	50.786	22.606	1.00	66.48	C
ATOM	2229	OE1	GLU	E	118	40.398	51.434	21.914	1.00	67.14	O
ATOM	2230	OE2	GLU	E	118	41.451	49.572	22.422	1.00	66.99	O
ATOM	2231	C	GLU	E	118	41.396	51.069	26.712	1.00	62.53	C
ATOM	2232	O	GLU	E	118	41.957	49.987	26.542	1.00	62.51	O
ATOM	2233	N	VAL	E	119	41.647	51.861	27.750	1.00	64.07	N
ATOM	2234	CA	VAL	E	119	42.746	51.600	28.676	1.00	65.42	C
ATOM	2235	CB	VAL	E	119	43.160	52.879	29.437	1.00	65.35	C
ATOM	2236	CG1	VAL	E	119	43.508	52.558	30.883	1.00	65.32	C
ATOM	2237	CG2	VAL	E	119	44.328	53.557	28.735	1.00	65.24	C
ATOM	2238	C	VAL	E	119	42.392	50.500	29.674	1.00	66.49	C
ATOM	2239	O	VAL	E	119	43.278	49.865	30.247	1.00	66.67	O
ATOM	2240	N	TYR	E	120	41.097	50.278	29.875	1.00	67.95	N
ATOM	2241	CA	TYR	E	120	40.635	49.149	30.676	1.00	69.42	C
ATOM	2242	CB	TYR	E	120	39.668	49.613	31.766	1.00	69.94	C
ATOM	2243	CG	TYR	E	120	39.205	48.498	32.679	1.00	71.50	C
ATOM	2244	CD1	TYR	E	120	40.119	47.763	33.428	1.00	72.65	C
ATOM	2245	CE1	TYR	E	120	39.702	46.740	34.264	1.00	72.95	C
ATOM	2246	CZ	TYR	E	120	38.356	46.441	34.359	1.00	72.98	C
ATOM	2247	OH	TYR	E	120	37.936	45.426	35.190	1.00	73.06	O
ATOM	2248	CE2	TYR	E	120	37.429	47.156	33.625	1.00	72.92	C
ATOM	2249	CD2	TYR	E	120	37.856	48.178	32.791	1.00	72.81	C
ATOM	2250	C	TYR	E	120	39.983	48.072	29.814	1.00	69.96	C
ATOM	2251	O	TYR	E	120	40.416	46.920	29.815	1.00	70.44	O
ATOM	2252	N	LEU	E	121	38.940	48.450	29.082	1.00	70.56	N
ATOM	2253	CA	LEU	E	121	38.050	47.476	28.455	1.00	71.13	C
ATOM	2254	CB	LEU	E	121	36.861	48.182	27.797	1.00	71.15	C
ATOM	2255	CG	LEU	E	121	35.752	48.689	28.724	1.00	71.10	C
ATOM	2256	CD1	LEU	E	121	34.501	49.015	27.925	1.00	71.09	C
ATOM	2257	CD2	LEU	E	121	35.443	47.674	29.815	1.00	71.09	C
ATOM	2258	C	LEU	E	121	38.781	46.614	27.425	1.00	71.55	C
ATOM	2259	O	LEU	E	121	38.150	45.988	26.571	1.00	71.82	O
ATOM	2260	N	GLN	E	122	40.108	46.577	27.521	1.00	71.84	N
ATOM	2261	CA	GLN	E	122	40.967	46.312	26.366	1.00	72.08	C
ATOM	2262	CB	GLN	E	122	42.373	45.905	26.818	1.00	72.26	C
ATOM	2263	CG	GLN	E	122	42.767	46.420	28.194	1.00	73.16	C
ATOM	2264	CD	GLN	E	122	42.546	45.393	29.291	1.00	74.36	C
ATOM	2265	OE1	GLN	E	122	42.919	45.609	30.444	1.00	74.89	O
ATOM	2266	NE2	GLN	E	122	41.934	44.268	28.934	1.00	74.59	N
ATOM	2267	C	GLN	E	122	40.380	45.239	25.451	1.00	71.91	C
ATOM	2268	O	GLN	E	122	39.576	45.536	24.566	1.00	71.98	O
ATOM	2269	N	ASP	E	123	40.790	43.993	25.668	1.00	71.65	N
ATOM	2270	CA	ASP	E	123	40.138	42.849	25.039	1.00	71.37	C
ATOM	2271	CB	ASP	E	123	41.014	41.600	25.156	1.00	71.53	C
ATOM	2272	CG	ASP	E	123	42.355	41.759	24.468	1.00	72.16	C
ATOM	2273	OD1	ASP	E	123	43.208	42.510	24.990	1.00	72.92	O
ATOM	2274	OD2	ASP	E	123	42.560	41.130	23.408	1.00	72.68	O
ATOM	2275	C	ASP	E	123	38.778	42.587	25.676	1.00	70.92	C
ATOM	2276	O	ASP	E	123	37.938	41.891	25.104	1.00	71.02	O

Figure 1 Table 1a - 35

ATOM	2277	N	SER	E	124	38.567	43.157	26.860	1.00	70.17	N
ATOM	2278	CA	SER	E	124	37.598	42.626	27.814	1.00	69.24	C
ATOM	2279	CB	SER	E	124	37.989	43.010	29.244	1.00	69.38	C
ATOM	2280	OG	SER	E	124	38.306	44.389	29.334	1.00	69.76	O
ATOM	2281	C	SER	E	124	36.183	43.106	27.505	1.00	68.28	C
ATOM	2282	O	SER	E	124	35.493	43.638	28.376	1.00	68.35	O
ATOM	2283	N	PHE	E	125	35.763	42.913	26.257	1.00	67.03	N
ATOM	2284	CA	PHE	E	125	34.352	42.990	25.891	1.00	65.73	C
ATOM	2285	CB	PHE	E	125	33.921	41.719	25.150	1.00	66.16	C
ATOM	2286	CG	PHE	E	125	34.576	41.545	23.808	1.00	67.14	C
ATOM	2287	CD1	PHE	E	125	35.157	40.334	23.459	1.00	67.89	C
ATOM	2288	CE1	PHE	E	125	35.760	40.166	22.223	1.00	67.73	C
ATOM	2289	CZ	PHE	E	125	35.786	41.214	21.321	1.00	67.71	C
ATOM	2290	CE2	PHE	E	125	35.210	42.427	21.656	1.00	67.62	C
ATOM	2291	CD2	PHE	E	125	34.608	42.587	22.894	1.00	67.62	C
ATOM	2292	C	PHE	E	125	33.454	43.208	27.108	1.00	64.30	C
ATOM	2293	O	PHE	E	125	33.204	42.281	27.881	1.00	64.17	O
ATOM	2294	N	LYS	E	126	32.977	44.438	27.270	1.00	62.13	N
ATOM	2295	CA	LYS	E	126	31.706	44.685	27.945	1.00	60.06	C
ATOM	2296	CB	LYS	E	126	31.934	45.281	29.338	1.00	60.29	C
ATOM	2297	CG	LYS	E	126	32.892	44.485	30.213	1.00	61.19	C
ATOM	2298	CD	LYS	E	126	32.229	43.238	30.779	1.00	62.40	C
ATOM	2299	CE	LYS	E	126	33.221	42.404	31.572	1.00	63.21	C
ATOM	2300	NZ	LYS	E	126	32.801	40.977	31.655	1.00	64.34	N
ATOM	2301	C	LYS	E	126	30.827	45.613	27.112	1.00	58.02	C
ATOM	2302	O	LYS	E	126	30.910	46.835	27.233	1.00	58.29	O
ATOM	2303	N	PRO	E	127	29.987	45.026	26.260	1.00	55.77	N
ATOM	2304	CA	PRO	E	127	29.102	45.810	25.395	1.00	53.66	C
ATOM	2305	CB	PRO	E	127	28.525	44.757	24.447	1.00	53.70	C
ATOM	2306	CG	PRO	E	127	28.553	43.497	25.236	1.00	54.86	C
ATOM	2307	CD	PRO	E	127	29.792	43.575	26.083	1.00	55.63	C
ATOM	2308	C	PRO	E	127	27.977	46.472	26.185	1.00	51.46	C
ATOM	2309	O	PRO	E	127	27.668	46.044	27.298	1.00	50.88	O
ATOM	2310	N	LEU	E	128	27.376	47.506	25.608	1.00	49.21	N
ATOM	2311	CA	LEU	E	128	26.210	48.147	26.202	1.00	47.00	C
ATOM	2312	CB	LEU	E	128	25.794	49.369	25.381	1.00	46.57	C
ATOM	2313	CG	LEU	E	128	24.511	50.072	25.826	1.00	46.70	C
ATOM	2314	CD1	LEU	E	128	24.699	50.730	27.186	1.00	46.20	C
ATOM	2315	CD2	LEU	E	128	24.071	51.093	24.792	1.00	46.59	C
ATOM	2316	C	LEU	E	128	25.042	47.173	26.314	1.00	45.50	C
ATOM	2317	O	LEU	E	128	24.638	46.558	25.326	1.00	45.37	O
ATOM	2318	N	VAL	E	129	24.502	47.038	27.522	1.00	43.41	N
ATOM	2319	CA	VAL	E	129	23.264	46.295	27.723	1.00	41.79	C
ATOM	2320	CB	VAL	E	129	23.363	45.327	28.922	1.00	41.88	C
ATOM	2321	CG1	VAL	E	129	24.812	44.955	29.191	1.00	41.50	C
ATOM	2322	CG2	VAL	E	129	22.724	45.931	30.154	1.00	42.08	C
ATOM	2323	C	VAL	E	129	22.085	47.248	27.916	1.00	40.71	C
ATOM	2324	O	VAL	E	129	22.120	48.136	28.769	1.00	40.32	O
ATOM	2325	N	CYS	E	130	21.044	47.060	27.113	1.00	39.38	N
ATOM	2326	CA	CYS	E	130	19.876	47.933	27.156	1.00	38.79	C
ATOM	2327	CB	CYS	E	130	19.920	48.943	26.008	1.00	38.28	C
ATOM	2328	SG	CYS	E	130	19.922	48.195	24.362	1.00	40.53	S
ATOM	2329	C	CYS	E	130	18.589	47.119	27.094	1.00	38.39	C
ATOM	2330	O	CYS	E	130	18.624	45.886	27.038	1.00	38.06	O
ATOM	2331	N	ILE	E	131	17.456	47.816	27.099	1.00	37.52	N
ATOM	2332	CA	ILE	E	131	16.155	47.161	27.052	1.00	37.14	C
ATOM	2333	CB	ILE	E	131	15.615	46.874	28.470	1.00	37.13	C
ATOM	2334	CG1	ILE	E	131	14.465	45.869	28.409	1.00	37.92	C
ATOM	2335	CD1	ILE	E	131	14.662	44.662	29.289	1.00	40.34	C
ATOM	2336	CG2	ILE	E	131	15.170	48.165	29.150	1.00	36.40	C
ATOM	2337	C	ILE	E	131	15.141	48.002	26.283	1.00	37.21	C
ATOM	2338	O	ILE	E	131	15.116	49.226	26.404	1.00	36.84	O
ATOM	2339	N	SER	E	132	14.308	47.334	25.492	1.00	36.89	N
ATOM	2340	CA	SER	E	132	13.222	47.999	24.793	1.00	37.07	C
ATOM	2341	CB	SER	E	132	12.595	47.036	23.783	1.00	36.98	C
ATOM	2342	OG	SER	E	132	11.491	47.650	23.141	1.00	38.54	O
ATOM	2343	C	SER	E	132	12.154	48.480	25.780	1.00	37.23	C

Figure 1 Table 1a - 36

ATOM	2344	O	SER	E	132	11.894	47.800	26.780	1.00	36.94	O
ATOM	2345	N	PRO	E	133	11.516	49.641	25.499	1.00	37.07	N
ATOM	2346	CA	PRO	E	133	10.368	50.071	26.313	1.00	37.25	C
ATOM	2347	CB	PRO	E	133	9.954	51.407	25.671	1.00	37.03	C
ATOM	2348	CG	PRO	E	133	10.516	51.359	24.274	1.00	37.60	C
ATOM	2349	CD	PRO	E	133	11.807	50.597	24.412	1.00	37.45	C
ATOM	2350	C	PRO	E	133	9.205	49.059	26.278	1.00	37.64	C
ATOM	2351	O	PRO	E	133	8.391	49.017	27.208	1.00	37.53	O
ATOM	2352	N	ASN	E	134	9.147	48.245	25.222	1.00	37.67	N
ATOM	2353	CA	ASN	E	134	8.111	47.224	25.084	1.00	38.49	C
ATOM	2354	CB	ASN	E	134	7.728	47.022	23.614	1.00	38.60	C
ATOM	2355	CG	ASN	E	134	7.033	48.227	23.039	1.00	40.84	C
ATOM	2356	OD1	ASN	E	134	6.198	48.851	23.702	1.00	43.00	O
ATOM	2357	ND2	ASN	E	134	7.387	48.584	21.809	1.00	43.28	N
ATOM	2358	C	ASN	E	134	8.443	45.877	25.719	1.00	38.26	C
ATOM	2359	O	ASN	E	134	7.591	45.002	25.744	1.00	38.45	O
ATOM	2360	N	ALA	E	135	9.664	45.714	26.228	1.00	38.08	N
ATOM	2361	CA	ALA	E	135	10.040	44.480	26.919	1.00	38.03	C
ATOM	2362	CB	ALA	E	135	11.540	44.313	26.924	1.00	38.05	C
ATOM	2363	C	ALA	E	135	9.503	44.482	28.346	1.00	37.96	C
ATOM	2364	O	ALA	E	135	9.228	45.545	28.912	1.00	37.95	O
ATOM	2365	N	SER	E	136	9.382	43.291	28.931	1.00	37.62	N
ATOM	2366	CA	SER	E	136	8.800	43.146	30.258	1.00	37.23	C
ATOM	2367	CB	SER	E	136	8.456	41.685	30.547	1.00	37.20	C
ATOM	2368	OG	SER	E	136	9.638	40.906	30.594	1.00	36.97	O
ATOM	2369	C	SER	E	136	9.718	43.677	31.348	1.00	37.36	C
ATOM	2370	O	SER	E	136	10.943	43.716	31.193	1.00	36.94	O
ATOM	2371	N	LEU	E	137	9.098	44.080	32.455	1.00	37.32	N
ATOM	2372	CA	LEU	E	137	9.805	44.439	33.663	1.00	37.31	C
ATOM	2373	CB	LEU	E	137	8.796	44.935	34.702	1.00	37.23	C
ATOM	2374	CG	LEU	E	137	9.263	45.370	36.096	1.00	39.14	C
ATOM	2375	CD1	LEU	E	137	10.408	46.414	36.042	1.00	38.19	C
ATOM	2376	CD2	LEU	E	137	8.056	45.925	36.870	1.00	38.99	C
ATOM	2377	C	LEU	E	137	10.631	43.261	34.192	1.00	37.08	C
ATOM	2378	O	LEU	E	137	11.730	43.451	34.725	1.00	36.70	O
ATOM	2379	N	PHE	E	138	10.103	42.044	34.026	1.00	36.54	N
ATOM	2380	CA	PHE	E	138	10.806	40.819	34.409	1.00	36.78	C
ATOM	2381	CB	PHE	E	138	9.919	39.586	34.149	1.00	36.25	C
ATOM	2382	CG	PHE	E	138	10.487	38.292	34.681	1.00	36.97	C
ATOM	2383	CD1	PHE	E	138	10.216	37.877	35.984	1.00	36.98	C
ATOM	2384	CE1	PHE	E	138	10.737	36.660	36.476	1.00	38.64	C
ATOM	2385	CZ	PHE	E	138	11.536	35.851	35.653	1.00	37.44	C
ATOM	2386	CE2	PHE	E	138	11.812	36.262	34.349	1.00	38.30	C
ATOM	2387	CD2	PHE	E	138	11.284	37.474	33.869	1.00	37.93	C
ATOM	2388	C	PHE	E	138	12.130	40.705	33.655	1.00	36.93	C
ATOM	2389	O	PHE	E	138	13.152	40.349	34.242	1.00	37.18	O
ATOM	2390	N	ASP	E	139	12.108	41.018	32.361	1.00	37.39	N
ATOM	2391	CA	ASP	E	139	13.323	40.984	31.537	1.00	38.07	C
ATOM	2392	CB	ASP	E	139	12.999	41.151	30.050	1.00	38.36	C
ATOM	2393	CG	ASP	E	139	12.542	39.849	29.383	1.00	41.08	C
ATOM	2394	OD1	ASP	E	139	12.536	38.775	30.035	1.00	43.74	O
ATOM	2395	OD2	ASP	E	139	12.196	39.903	28.182	1.00	42.90	O
ATOM	2396	C	ASP	E	139	14.331	42.050	31.977	1.00	37.87	C
ATOM	2397	O	ASP	E	139	15.545	41.806	31.954	1.00	37.70	O
ATOM	2398	N	ALA	E	140	13.819	43.219	32.373	1.00	37.20	N
ATOM	2399	CA	ALA	E	140	14.656	44.300	32.914	1.00	36.84	C
ATOM	2400	CB	ALA	E	140	13.823	45.563	33.165	1.00	35.89	C
ATOM	2401	C	ALA	E	140	15.377	43.867	34.187	1.00	36.41	C
ATOM	2402	O	ALA	E	140	16.593	44.023	34.297	1.00	36.26	O
ATOM	2403	N	VAL	E	141	14.623	43.315	35.139	1.00	36.45	N
ATOM	2404	CA	VAL	E	141	15.190	42.867	36.410	1.00	36.43	C
ATOM	2405	CB	VAL	E	141	14.104	42.378	37.428	1.00	36.70	C
ATOM	2406	CG1	VAL	E	141	14.752	41.809	38.701	1.00	36.01	C
ATOM	2407	CG2	VAL	E	141	13.199	43.514	37.807	1.00	36.71	C
ATOM	2408	C	VAL	E	141	16.248	41.792	36.165	1.00	36.40	C
ATOM	2409	O	VAL	E	141	17.344	41.874	36.719	1.00	36.43	O
ATOM	2410	N	SER	E	142	15.925	40.813	35.320	1.00	36.23	N

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ATOM	2411	CA	SER	E	142	16.857	39.742	34.969	1.00	36.71	C
ATOM	2412	CB	SER	E	142	16.181	38.740	34.028	1.00	36.92	C
ATOM	2413	OG	SER	E	142	15.015	38.201	34.634	1.00	38.86	O
ATOM	2414	C	SER	E	142	18.150	40.256	34.329	1.00	36.60	C
ATOM	2415	O	SER	E	142	19.235	39.752	34.611	1.00	37.02	O
ATOM	2416	N	SER	E	143	18.025	41.242	33.454	1.00	36.22	N
ATOM	2417	CA	SER	E	143	19.185	41.880	32.845	1.00	36.57	C
ATOM	2418	CB	SER	E	143	18.741	42.827	31.737	1.00	35.99	C
ATOM	2419	OG	SER	E	143	19.864	43.455	31.175	1.00	37.48	O
ATOM	2420	C	SER	E	143	20.073	42.622	33.852	1.00	36.66	C
ATOM	2421	O	SER	E	143	21.304	42.557	33.755	1.00	37.02	O
ATOM	2422	N	LEU	E	144	19.465	43.336	34.803	1.00	36.56	N
ATOM	2423	CA	LEU	E	144	20.238	44.012	35.851	1.00	36.46	C
ATOM	2424	CB	LEU	E	144	19.338	44.853	36.768	1.00	36.57	C
ATOM	2425	CG	LEU	E	144	18.786	46.185	36.236	1.00	36.34	C
ATOM	2426	CD1	LEU	E	144	17.682	46.658	37.152	1.00	37.75	C
ATOM	2427	CD2	LEU	E	144	19.865	47.264	36.123	1.00	36.14	C
ATOM	2428	C	LEU	E	144	21.041	43.010	36.676	1.00	36.73	C
ATOM	2429	O	LEU	E	144	22.239	43.184	36.874	1.00	36.41	O
ATOM	2430	N	ILE	E	145	20.374	41.952	37.133	1.00	37.29	N
ATOM	2431	CA	ILE	E	145	21.024	40.891	37.920	1.00	38.23	C
ATOM	2432	CB	ILE	E	145	19.983	39.872	38.459	1.00	38.57	C
ATOM	2433	CG1	ILE	E	145	18.919	40.598	39.288	1.00	39.91	C
ATOM	2434	CD1	ILE	E	145	17.621	39.824	39.423	1.00	42.84	C
ATOM	2435	CG2	ILE	E	145	20.652	38.785	39.304	1.00	38.90	C
ATOM	2436	C	ILE	E	145	22.128	40.186	37.123	1.00	38.28	C
ATOM	2437	O	ILE	E	145	23.291	40.188	37.535	1.00	38.28	O
ATOM	2438	N	ARG	E	146	21.768	39.626	35.971	1.00	38.41	N
ATOM	2439	CA	ARG	E	146	22.694	38.821	35.166	1.00	38.98	C
ATOM	2440	CB	ARG	E	146	21.971	38.237	33.935	1.00	39.42	C
ATOM	2441	CG	ARG	E	146	22.876	37.912	32.738	1.00	41.09	C
ATOM	2442	CD	ARG	E	146	22.119	37.313	31.556	1.00	41.52	C
ATOM	2443	NE	ARG	E	146	21.373	38.314	30.796	1.00	45.63	N
ATOM	2444	CZ	ARG	E	146	20.057	38.488	30.872	1.00	45.46	C
ATOM	2445	NH1	ARG	E	146	19.324	37.721	31.668	1.00	45.99	N
ATOM	2446	NH2	ARG	E	146	19.475	39.421	30.135	1.00	45.66	N
ATOM	2447	C	ARG	E	146	23.963	39.581	34.763	1.00	38.41	C
ATOM	2448	O	ARG	E	146	25.056	39.024	34.764	1.00	37.79	O
ATOM	2449	N	ASN	E	147	23.813	40.859	34.433	1.00	38.03	N
ATOM	2450	CA	ASN	E	147	24.951	41.666	34.016	1.00	37.73	C
ATOM	2451	CB	ASN	E	147	24.519	42.641	32.917	1.00	37.71	C
ATOM	2452	CG	ASN	E	147	24.035	41.911	31.684	1.00	37.84	C
ATOM	2453	OD1	ASN	E	147	24.814	41.237	31.022	1.00	37.44	O
ATOM	2454	ND2	ASN	E	147	22.739	42.004	31.394	1.00	36.44	N
ATOM	2455	C	ASN	E	147	25.669	42.377	35.157	1.00	37.57	C
ATOM	2456	O	ASN	E	147	26.663	43.071	34.930	1.00	37.47	O
ATOM	2457	N	LYS	E	148	25.160	42.195	36.378	1.00	37.36	N
ATOM	2458	CA	LYS	E	148	25.751	42.792	37.581	1.00	36.92	C
ATOM	2459	CB	LYS	E	148	27.051	42.075	37.950	1.00	37.04	C
ATOM	2460	CG	LYS	E	148	26.803	40.664	38.419	1.00	37.83	C
ATOM	2461	CD	LYS	E	148	28.090	39.929	38.768	1.00	42.16	C
ATOM	2462	CE	LYS	E	148	27.775	38.498	39.214	1.00	43.32	C
ATOM	2463	NZ	LYS	E	148	29.009	37.752	39.540	1.00	46.79	N
ATOM	2464	C	LYS	E	148	25.920	44.310	37.403	1.00	36.57	C
ATOM	2465	O	LYS	E	148	26.996	44.879	37.568	1.00	35.81	O
ATOM	2466	N	ILE	E	149	24.796	44.939	37.092	1.00	36.30	N
ATOM	2467	CA	ILE	E	149	24.745	46.319	36.689	1.00	36.95	C
ATOM	2468	CB	ILE	E	149	24.580	46.318	35.141	1.00	37.18	C
ATOM	2469	CG1	ILE	E	149	25.671	47.131	34.491	1.00	39.03	C
ATOM	2470	CD1	ILE	E	149	26.983	46.413	34.502	1.00	39.29	C
ATOM	2471	CG2	ILE	E	149	23.145	46.516	34.648	1.00	37.83	C
ATOM	2472	C	ILE	E	149	23.644	47.053	37.484	1.00	36.58	C
ATOM	2473	O	ILE	E	149	22.729	46.402	38.006	1.00	36.21	O
ATOM	2474	N	HIS	E	150	23.765	48.384	37.593	1.00	36.39	N
ATOM	2475	CA	HIS	E	150	22.818	49.247	38.336	1.00	35.92	C
ATOM	2476	CB	HIS	E	150	23.555	50.007	39.456	1.00	35.43	C
ATOM	2477	CG	HIS	E	150	24.145	49.113	40.504	1.00	34.84	C

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ATOM	2478	ND1	HIS	E	150	25.404	48.566	40.389	1.00	34.90	N
ATOM	2479	CE1	HIS	E	150	25.655	47.812	41.446	1.00	35.15	C
ATOM	2480	NE2	HIS	E	150	24.605	47.862	42.249	1.00	34.99	N
ATOM	2481	CD2	HIS	E	150	23.643	48.658	41.678	1.00	34.23	C
ATOM	2482	C	HIS	E	150	22.038	50.259	37.473	1.00	36.11	C
ATOM	2483	O	HIS	E	150	21.196	50.998	37.992	1.00	35.93	O
ATOM	2484	N	ARG	E	151	22.322	50.286	36.172	1.00	36.16	N
ATOM	2485	CA	ARG	E	151	21.745	51.280	35.251	1.00	37.26	C
ATOM	2486	CB	ARG	E	151	22.755	52.393	34.931	1.00	36.64	C
ATOM	2487	CG	ARG	E	151	23.470	52.997	36.152	1.00	38.68	C
ATOM	2488	CD	ARG	E	151	22.624	54.067	36.852	1.00	41.29	C
ATOM	2489	NE	ARG	E	151	22.905	54.110	38.287	1.00	43.84	N
ATOM	2490	CZ	ARG	E	151	22.250	54.860	39.173	1.00	44.06	C
ATOM	2491	NH1	ARG	E	151	21.260	55.670	38.789	1.00	41.86	N
ATOM	2492	NH2	ARG	E	151	22.593	54.796	40.454	1.00	44.74	N
ATOM	2493	C	ARG	E	151	21.335	50.577	33.972	1.00	36.88	C
ATOM	2494	O	ARG	E	151	22.176	50.016	33.270	1.00	37.94	O
ATOM	2495	N	LEU	E	152	20.044	50.569	33.678	1.00	36.19	N
ATOM	2496	CA	LEU	E	152	19.583	49.904	32.478	1.00	35.75	C
ATOM	2497	CB	LEU	E	152	18.693	48.699	32.825	1.00	35.79	C
ATOM	2498	CG	LEU	E	152	18.214	47.818	31.676	1.00	35.48	C
ATOM	2499	CD1	LEU	E	152	19.370	47.132	30.938	1.00	36.51	C
ATOM	2500	CD2	LEU	E	152	17.268	46.784	32.231	1.00	35.82	C
ATOM	2501	C	LEU	E	152	18.869	50.906	31.575	1.00	35.39	C
ATOM	2502	O	LEU	E	152	17.720	51.266	31.833	1.00	35.81	O
ATOM	2503	N	PRO	E	153	19.552	51.364	30.509	1.00	34.97	N
ATOM	2504	CA	PRO	E	153	18.914	52.303	29.589	1.00	34.94	C
ATOM	2505	CB	PRO	E	153	20.054	52.726	28.656	1.00	35.21	C
ATOM	2506	CG	PRO	E	153	20.989	51.556	28.666	1.00	35.44	C
ATOM	2507	CD	PRO	E	153	20.921	51.023	30.089	1.00	34.53	C
ATOM	2508	C	PRO	E	153	17.806	51.642	28.795	1.00	34.73	C
ATOM	2509	O	PRO	E	153	17.980	50.529	28.272	1.00	34.74	O
ATOM	2510	N	VAL	E	154	16.665	52.318	28.741	1.00	34.73	N
ATOM	2511	CA	VAL	E	154	15.526	51.870	27.971	1.00	34.67	C
ATOM	2512	CB	VAL	E	154	14.201	52.239	28.670	1.00	35.21	C
ATOM	2513	CG1	VAL	E	154	13.006	51.889	27.802	1.00	34.57	C
ATOM	2514	CG2	VAL	E	154	14.095	51.552	30.042	1.00	33.78	C
ATOM	2515	C	VAL	E	154	15.655	52.570	26.620	1.00	35.27	C
ATOM	2516	O	VAL	E	154	15.596	53.802	26.541	1.00	34.02	O
ATOM	2517	N	ILE	E	155	15.863	51.776	25.563	1.00	35.10	N
ATOM	2518	CA	ILE	E	155	16.152	52.331	24.237	1.00	35.31	C
ATOM	2519	CB	ILE	E	155	17.585	51.949	23.739	1.00	35.73	C
ATOM	2520	CG1	ILE	E	155	18.657	52.430	24.733	1.00	34.86	C
ATOM	2521	CD1	ILE	E	155	20.105	52.163	24.286	1.00	35.17	C
ATOM	2522	CG2	ILE	E	155	17.837	52.472	22.305	1.00	35.03	C
ATOM	2523	C	ILE	E	155	15.081	51.890	23.241	1.00	35.86	C
ATOM	2524	O	ILE	E	155	14.854	50.688	23.045	1.00	35.45	O
ATOM	2525	N	ASP	E	156	14.405	52.880	22.656	1.00	36.03	N
ATOM	2526	CA	ASP	E	156	13.376	52.662	21.646	1.00	36.75	C
ATOM	2527	CB	ASP	E	156	12.658	53.989	21.356	1.00	37.12	C
ATOM	2528	CG	ASP	E	156	11.659	53.892	20.208	1.00	38.16	C
ATOM	2529	OD1	ASP	E	156	11.150	52.796	19.931	1.00	39.99	O
ATOM	2530	OD2	ASP	E	156	11.369	54.928	19.588	1.00	39.54	O
ATOM	2531	C	ASP	E	156	14.017	52.107	20.372	1.00	36.95	C
ATOM	2532	O	ASP	E	156	14.817	52.804	19.734	1.00	36.58	O
ATOM	2533	N	PRO	E	157	13.670	50.852	19.991	1.00	37.25	N
ATOM	2534	CA	PRO	E	157	14.281	50.277	18.782	1.00	37.41	C
ATOM	2535	CB	PRO	E	157	13.748	48.835	18.741	1.00	37.38	C
ATOM	2536	CG	PRO	E	157	12.551	48.828	19.616	1.00	37.45	C
ATOM	2537	CD	PRO	E	157	12.735	49.914	20.644	1.00	37.10	C
ATOM	2538	C	PRO	E	157	13.946	51.039	17.495	1.00	37.95	C
ATOM	2539	O	PRO	E	157	14.774	51.091	16.589	1.00	38.29	O
ATOM	2540	N	GLU	E	158	12.766	51.645	17.414	1.00	38.24	N
ATOM	2541	CA	GLU	E	158	12.379	52.354	16.196	1.00	39.09	C
ATOM	2542	CB	GLU	E	158	10.871	52.629	16.170	1.00	39.79	C
ATOM	2543	CG	GLU	E	158	10.015	51.346	16.365	1.00	44.01	C
ATOM	2544	CD	GLU	E	158	8.669	51.391	15.648	1.00	49.27	C

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ATOM	2545	OE1	GLU	E	158	8.279	52.473	15.138	1.00	52.92	O
ATOM	2546	OE2	GLU	E	158	8.000	50.331	15.581	1.00	51.84	O
ATOM	2547	C	GLU	E	158	13.192	53.635	15.980	1.00	38.75	C
ATOM	2548	O	GLU	E	158	13.675	53.884	14.882	1.00	38.91	O
ATOM	2549	N	SER	E	159	13.355	54.406	17.051	1.00	38.01	N
ATOM	2550	CA	SER	E	159	14.083	55.684	17.074	1.00	37.92	C
ATOM	2551	CB	SER	E	159	13.577	56.510	18.262	1.00	37.65	C
ATOM	2552	OG	SER	E	159	12.552	57.375	17.830	1.00	43.08	O
ATOM	2553	C	SER	E	159	15.576	55.535	17.292	1.00	36.36	C
ATOM	2554	O	SER	E	159	16.366	56.342	16.806	1.00	36.05	O
ATOM	2555	N	GLY	E	160	15.937	54.546	18.103	1.00	34.83	N
ATOM	2556	CA	GLY	E	160	17.281	54.422	18.622	1.00	33.68	C
ATOM	2557	C	GLY	E	160	17.511	55.346	19.811	1.00	33.38	C
ATOM	2558	O	GLY	E	160	18.630	55.411	20.323	1.00	34.41	O
ATOM	2559	N	ASN	E	161	16.460	56.050	20.243	1.00	31.82	N
ATOM	2560	CA	ASN	E	161	16.535	57.010	21.340	1.00	31.17	C
ATOM	2561	CB	ASN	E	161	15.357	58.008	21.291	1.00	31.02	C
ATOM	2562	CG	ASN	E	161	15.420	58.968	20.107	1.00	30.38	C
ATOM	2563	OD1	ASN	E	161	14.393	59.515	19.688	1.00	34.55	O
ATOM	2564	ND2	ASN	E	161	16.601	59.176	19.566	1.00	26.12	N
ATOM	2565	C	ASN	E	161	16.536	56.329	22.712	1.00	31.45	C
ATOM	2566	O	ASN	E	161	15.699	55.472	22.996	1.00	30.85	O
ATOM	2567	N	THR	E	162	17.467	56.727	23.569	1.00	31.15	N
ATOM	2568	CA	THR	E	162	17.393	56.353	24.966	1.00	31.34	C
ATOM	2569	CB	THR	E	162	18.745	56.547	25.657	1.00	31.72	C
ATOM	2570	OG1	THR	E	162	19.700	55.690	25.024	1.00	32.87	O
ATOM	2571	CG2	THR	E	162	18.656	56.173	27.129	1.00	31.59	C
ATOM	2572	C	THR	E	162	16.306	57.212	25.611	1.00	30.93	C
ATOM	2573	O	THR	E	162	16.289	58.430	25.457	1.00	30.16	O
ATOM	2574	N	LEU	E	163	15.394	56.561	26.327	1.00	31.05	N
ATOM	2575	CA	LEU	E	163	14.232	57.245	26.884	1.00	30.97	C
ATOM	2576	CB	LEU	E	163	12.971	56.403	26.678	1.00	30.57	C
ATOM	2577	CG	LEU	E	163	12.687	55.946	25.245	1.00	30.40	C
ATOM	2578	CD1	LEU	E	163	11.484	55.016	25.215	1.00	29.63	C
ATOM	2579	CD2	LEU	E	163	12.477	57.141	24.319	1.00	28.95	C
ATOM	2580	C	LEU	E	163	14.419	57.544	28.364	1.00	31.31	C
ATOM	2581	O	LEU	E	163	13.839	58.491	28.891	1.00	31.21	O
ATOM	2582	N	TYR	E	164	15.228	56.725	29.031	1.00	31.88	N
ATOM	2583	CA	TYR	E	164	15.187	56.628	30.483	1.00	32.32	C
ATOM	2584	CB	TYR	E	164	13.767	56.293	30.954	1.00	33.57	C
ATOM	2585	CG	TYR	E	164	13.596	56.332	32.457	1.00	33.90	C
ATOM	2586	CD1	TYR	E	164	13.720	57.526	33.159	1.00	33.84	C
ATOM	2587	CE1	TYR	E	164	13.567	57.563	34.536	1.00	35.60	C
ATOM	2588	CZ	TYR	E	164	13.285	56.394	35.220	1.00	35.59	C
ATOM	2589	OH	TYR	E	164	13.129	56.419	36.586	1.00	36.71	O
ATOM	2590	CE2	TYR	E	164	13.156	55.199	34.542	1.00	34.46	C
ATOM	2591	CD2	TYR	E	164	13.313	55.175	33.169	1.00	34.69	C
ATOM	2592	C	TYR	E	164	16.162	55.574	30.981	1.00	32.01	C
ATOM	2593	O	TYR	E	164	16.470	54.617	30.269	1.00	32.24	O
ATOM	2594	N	LEU	E	165	16.647	55.752	32.206	1.00	32.03	N
ATOM	2595	CA	LEU	E	165	17.616	54.830	32.785	1.00	31.86	C
ATOM	2596	CB	LEU	E	165	18.889	55.574	33.194	1.00	32.30	C
ATOM	2597	CG	LEU	E	165	19.565	56.411	32.106	1.00	32.61	C
ATOM	2598	CD1	LEU	E	165	20.703	57.221	32.688	1.00	33.77	C
ATOM	2599	CD2	LEU	E	165	20.066	55.518	30.985	1.00	34.74	C
ATOM	2600	C	LEU	E	165	17.030	54.098	33.985	1.00	32.26	C
ATOM	2601	O	LEU	E	165	16.821	54.690	35.045	1.00	31.57	O
ATOM	2602	N	LEU	E	166	16.779	52.804	33.813	1.00	33.10	N
ATOM	2603	CA	LEU	E	166	16.105	52.009	34.833	1.00	34.35	C
ATOM	2604	CB	LEU	E	166	15.562	50.717	34.221	1.00	34.84	C
ATOM	2605	CG	LEU	E	166	14.087	50.393	34.468	1.00	38.15	C
ATOM	2606	CD1	LEU	E	166	13.261	51.658	34.589	1.00	38.37	C
ATOM	2607	CD2	LEU	E	166	13.539	49.495	33.364	1.00	37.59	C
ATOM	2608	C	LEU	E	166	17.044	51.689	35.990	1.00	34.01	C
ATOM	2609	O	LEU	E	166	18.232	51.435	35.785	1.00	33.51	O
ATOM	2610	N	THR	E	167	16.505	51.704	37.207	1.00	34.08	N
ATOM	2611	CA	THR	E	167	17.284	51.377	38.396	1.00	33.62	C

Figure 1 Table 1a - 40

ATOM	2612	CB	THR	E	167	17.639	52.639	39.206	1.00	33.39	C
ATOM	2613	OG1	THR	E	167	16.436	53.264	39.672	1.00	33.34	O
ATOM	2614	CG2	THR	E	167	18.426	53.629	38.348	1.00	34.56	C
ATOM	2615	C	THR	E	167	16.524	50.409	39.297	1.00	33.04	C
ATOM	2616	O	THR	E	167	15.299	50.315	39.224	1.00	32.69	O
ATOM	2617	N	HIS	E	168	17.257	49.698	40.149	1.00	32.77	N
ATOM	2618	CA	HIS	E	168	16.648	48.903	41.215	1.00	32.92	C
ATOM	2619	CB	HIS	E	168	17.722	48.344	42.151	1.00	32.61	C
ATOM	2620	CG	HIS	E	168	18.638	47.352	41.502	1.00	33.70	C
ATOM	2621	ND1	HIS	E	168	19.693	47.727	40.698	1.00	34.31	N
ATOM	2622	CE1	HIS	E	168	20.323	46.647	40.269	1.00	35.42	C
ATOM	2623	NE2	HIS	E	168	19.720	45.585	40.772	1.00	34.50	N
ATOM	2624	CD2	HIS	E	168	18.663	45.997	41.547	1.00	34.99	C
ATOM	2625	C	HIS	E	168	15.645	49.729	42.016	1.00	32.92	C
ATOM	2626	O	HIS	E	168	14.502	49.316	42.214	1.00	32.83	O
ATOM	2627	N	LYS	E	169	16.081	50.900	42.473	1.00	33.11	N
ATOM	2628	CA	LYS	E	169	15.253	51.754	43.319	1.00	34.60	C
ATOM	2629	CB	LYS	E	169	16.027	53.043	43.612	1.00	34.18	C
ATOM	2630	CG	LYS	E	169	15.582	53.858	44.831	1.00	38.73	C
ATOM	2631	CD	LYS	E	169	16.567	55.055	45.099	1.00	37.98	C
ATOM	2632	CE	LYS	E	169	17.991	54.527	45.353	1.00	42.38	C
ATOM	2633	NZ	LYS	E	169	18.976	55.484	45.971	1.00	43.92	N
ATOM	2634	C	LYS	E	169	13.876	52.049	42.697	1.00	33.70	C
ATOM	2635	O	LYS	E	169	12.841	51.881	43.344	1.00	34.04	O
ATOM	2636	N	ARG	E	170	13.882	52.472	41.442	1.00	33.46	N
ATOM	2637	CA	ARG	E	170	12.659	52.772	40.701	1.00	33.49	C
ATOM	2638	CB	ARG	E	170	12.999	53.245	39.281	1.00	32.87	C
ATOM	2639	CG	ARG	E	170	11.788	53.628	38.447	1.00	32.91	C
ATOM	2640	CD	ARG	E	170	11.167	54.942	38.937	1.00	33.28	C
ATOM	2641	NE	ARG	E	170	10.150	55.414	37.994	1.00	33.00	N
ATOM	2642	CZ	ARG	E	170	9.420	56.519	38.133	1.00	31.41	C
ATOM	2643	NH1	ARG	E	170	9.584	57.327	39.181	1.00	29.10	N
ATOM	2644	NH2	ARG	E	170	8.523	56.816	37.198	1.00	29.66	N
ATOM	2645	C	ARG	E	170	11.738	51.556	40.607	1.00	33.01	C
ATOM	2646	O	ARG	E	170	10.525	51.658	40.808	1.00	32.61	O
ATOM	2647	N	ILE	E	171	12.335	50.429	40.254	1.00	33.33	N
ATOM	2648	CA	ILE	E	171	11.624	49.181	40.083	1.00	33.46	C
ATOM	2649	CB	ILE	E	171	12.574	48.076	39.549	1.00	33.64	C
ATOM	2650	CG1	ILE	E	171	13.013	48.436	38.114	1.00	34.23	C
ATOM	2651	CD1	ILE	E	171	14.108	47.557	37.508	1.00	32.73	C
ATOM	2652	CG2	ILE	E	171	11.902	46.684	39.678	1.00	33.53	C
ATOM	2653	C	ILE	E	171	10.970	48.740	41.401	1.00	33.54	C
ATOM	2654	O	ILE	E	171	9.788	48.423	41.415	1.00	33.83	O
ATOM	2655	N	LEU	E	172	11.717	48.723	42.504	1.00	33.08	N
ATOM	2656	CA	LEU	E	172	11.097	48.288	43.765	1.00	33.00	C
ATOM	2657	CB	LEU	E	172	12.099	48.127	44.912	1.00	32.97	C
ATOM	2658	CG	LEU	E	172	11.524	47.411	46.151	1.00	33.28	C
ATOM	2659	CD1	LEU	E	172	11.175	45.942	45.863	1.00	33.62	C
ATOM	2660	CD2	LEU	E	172	12.449	47.515	47.374	1.00	32.78	C
ATOM	2661	C	LEU	E	172	9.975	49.231	44.173	1.00	32.88	C
ATOM	2662	O	LEU	E	172	8.936	48.777	44.667	1.00	31.62	O
ATOM	2663	N	LYS	E	173	10.171	50.536	43.944	1.00	33.06	N
ATOM	2664	CA	LYS	E	173	9.108	51.504	44.268	1.00	34.01	C
ATOM	2665	CB	LYS	E	173	9.554	52.942	44.033	1.00	34.17	C
ATOM	2666	CG	LYS	E	173	8.518	53.964	44.513	1.00	36.38	C
ATOM	2667	CD	LYS	E	173	9.055	55.383	44.408	1.00	39.95	C
ATOM	2668	CE	LYS	E	173	8.133	56.372	45.127	1.00	41.96	C
ATOM	2669	NZ	LYS	E	173	8.875	57.629	45.478	1.00	43.18	N
ATOM	2670	C	LYS	E	173	7.826	51.212	43.472	1.00	34.12	C
ATOM	2671	O	LYS	E	173	6.719	51.174	44.029	1.00	33.47	O
ATOM	2672	N	PHE	E	174	7.994	51.001	42.171	1.00	34.58	N
ATOM	2673	CA	PHE	E	174	6.876	50.697	41.287	1.00	35.29	C
ATOM	2674	CB	PHE	E	174	7.392	50.529	39.865	1.00	35.26	C
ATOM	2675	CG	PHE	E	174	6.324	50.531	38.821	1.00	36.92	C
ATOM	2676	CD1	PHE	E	174	5.829	49.326	38.316	1.00	37.95	C
ATOM	2677	CE1	PHE	E	174	4.832	49.325	37.324	1.00	38.06	C
ATOM	2678	CZ	PHE	E	174	4.339	50.534	36.835	1.00	37.98	C

Figure 1 Table 1a - 41

ATOM	2679	CE2	PHE	E	174	4.832	51.739	37.328	1.00	37.98	C
ATOM	2680	CD2	PHE	E	174	5.830	51.731	38.311	1.00	36.43	C
ATOM	2681	C	PHE	E	174	6.141	49.435	41.759	1.00	35.48	C
ATOM	2682	O	PHE	E	174	4.908	49.418	41.834	1.00	35.36	O
ATOM	2683	N	LEU	E	175	6.907	48.393	42.071	1.00	35.67	N
ATOM	2684	CA	LEU	E	175	6.348	47.125	42.565	1.00	36.29	C
ATOM	2685	CB	LEU	E	175	7.456	46.096	42.836	1.00	35.94	C
ATOM	2686	CG	LEU	E	175	8.191	45.512	41.624	1.00	36.62	C
ATOM	2687	CD1	LEU	E	175	9.338	44.597	42.034	1.00	34.69	C
ATOM	2688	CD2	LEU	E	175	7.242	44.800	40.662	1.00	36.47	C
ATOM	2689	C	LEU	E	175	5.516	47.320	43.822	1.00	36.75	C
ATOM	2690	O	LEU	E	175	4.385	46.853	43.891	1.00	36.86	O
ATOM	2691	N	LYS	E	176	6.083	48.024	44.804	1.00	37.46	N
ATOM	2692	CA	LYS	E	176	5.427	48.307	46.084	1.00	38.21	C
ATOM	2693	CB	LYS	E	176	6.393	49.063	47.021	1.00	38.28	C
ATOM	2694	CG	LYS	E	176	5.733	49.836	48.186	1.00	39.20	C
ATOM	2695	CD	LYS	E	176	5.223	48.912	49.287	1.00	41.06	C
ATOM	2696	CE	LYS	E	176	4.319	49.655	50.277	1.00	41.15	C
ATOM	2697	NZ	LYS	E	176	3.866	48.731	51.360	1.00	44.82	N
ATOM	2698	C	LYS	E	176	4.134	49.094	45.895	1.00	38.59	C
ATOM	2699	O	LYS	E	176	3.119	48.813	46.540	1.00	39.09	O
ATOM	2700	N	LEU	E	177	4.166	50.066	44.994	1.00	39.11	N
ATOM	2701	CA	LEU	E	177	3.022	50.930	44.774	1.00	39.42	C
ATOM	2702	CB	LEU	E	177	3.435	52.184	44.000	1.00	39.38	C
ATOM	2703	CG	LEU	E	177	4.092	53.265	44.853	1.00	40.50	C
ATOM	2704	CD1	LEU	E	177	4.668	54.357	43.977	1.00	39.29	C
ATOM	2705	CD2	LEU	E	177	3.064	53.827	45.831	1.00	42.67	C
ATOM	2706	C	LEU	E	177	1.867	50.259	44.059	1.00	39.40	C
ATOM	2707	O	LEU	E	177	0.713	50.488	44.413	1.00	39.15	O
ATOM	2708	N	PHE	E	178	2.174	49.463	43.043	1.00	39.72	N
ATOM	2709	CA	PHE	E	178	1.138	48.978	42.126	1.00	40.69	C
ATOM	2710	CB	PHE	E	178	1.560	49.164	40.664	1.00	40.41	C
ATOM	2711	CG	PHE	E	178	1.434	50.586	40.189	1.00	40.21	C
ATOM	2712	CD1	PHE	E	178	2.530	51.445	40.224	1.00	39.75	C
ATOM	2713	CE1	PHE	E	178	2.418	52.767	39.810	1.00	38.44	C
ATOM	2714	CZ	PHE	E	178	1.196	53.247	39.355	1.00	38.68	C
ATOM	2715	CE2	PHE	E	178	0.085	52.399	39.324	1.00	39.78	C
ATOM	2716	CD2	PHE	E	178	0.207	51.079	39.748	1.00	39.50	C
ATOM	2717	C	PHE	E	178	0.677	47.557	42.394	1.00	41.65	C
ATOM	2718	O	PHE	E	178	-0.241	47.059	41.737	1.00	42.10	O
ATOM	2719	N	ILE	E	179	1.294	46.905	43.368	1.00	42.35	N
ATOM	2720	CA	ILE	E	179	0.831	45.590	43.751	1.00	43.36	C
ATOM	2721	CB	ILE	E	179	1.979	44.580	43.909	1.00	43.32	C
ATOM	2722	CG1	ILE	E	179	2.692	44.395	42.565	1.00	43.59	C
ATOM	2723	CD1	ILE	E	179	3.860	43.431	42.598	1.00	44.19	C
ATOM	2724	CG2	ILE	E	179	1.430	43.252	44.411	1.00	44.03	C
ATOM	2725	C	ILE	E	179	-0.024	45.670	45.008	1.00	43.91	C
ATOM	2726	O	ILE	E	179	0.398	46.187	46.039	1.00	43.68	O
ATOM	2727	N	THR	E	180	-1.247	45.173	44.874	1.00	45.02	N
ATOM	2728	CA	THR	E	180	-2.169	44.995	45.978	1.00	46.67	C
ATOM	2729	CB	THR	E	180	-3.350	44.128	45.539	1.00	46.27	C
ATOM	2730	OG1	THR	E	180	-3.837	44.589	44.276	1.00	48.97	O
ATOM	2731	CG2	THR	E	180	-4.420	44.255	46.507	1.00	47.48	C
ATOM	2732	C	THR	E	180	-1.493	44.291	47.149	1.00	47.20	C
ATOM	2733	O	THR	E	180	-0.665	43.400	46.950	1.00	47.64	O
ATOM	2734	N	GLU	E	181	-1.843	44.687	48.368	1.00	47.98	N
ATOM	2735	CA	GLU	E	181	-1.258	44.066	49.543	1.00	48.67	C
ATOM	2736	CB	GLU	E	181	-1.555	44.884	50.807	1.00	48.73	C
ATOM	2737	CG	GLU	E	181	-1.101	44.203	52.105	1.00	49.60	C
ATOM	2738	CD	GLU	E	181	-1.378	45.024	53.357	1.00	50.66	C
ATOM	2739	OE1	GLU	E	181	-0.998	44.567	54.458	1.00	51.28	O
ATOM	2740	OE2	GLU	E	181	-1.970	46.121	53.248	1.00	52.27	O
ATOM	2741	C	GLU	E	181	-1.730	42.619	49.712	1.00	48.96	C
ATOM	2742	O	GLU	E	181	-0.912	41.731	49.951	1.00	48.89	O
ATOM	2743	N	PHE	E	182	-3.035	42.382	49.552	1.00	49.08	N
ATOM	2744	CA	PHE	E	182	-3.653	41.231	50.210	1.00	49.70	C
ATOM	2745	CB	PHE	E	182	-4.639	41.682	51.291	1.00	49.84	C

Figure 1

Table 1a - 42

ATOM	2746	CG	PHE	E	182	-4.065	41.639	52.664	1.00	50.36	C
ATOM	2747	CD1	PHE	E	182	-3.479	40.467	53.143	1.00	50.38	C
ATOM	2748	CE1	PHE	E	182	-2.938	40.413	54.408	1.00	50.63	C
ATOM	2749	CZ	PHE	E	182	-2.981	41.538	55.223	1.00	51.67	C
ATOM	2750	CE2	PHE	E	182	-3.565	42.715	54.758	1.00	51.68	C
ATOM	2751	CD2	PHE	E	182	-4.101	42.761	53.482	1.00	50.66	C
ATOM	2752	C	PHE	E	182	-4.236	40.053	49.425	1.00	49.69	C
ATOM	2753	O	PHE	E	182	-5.163	39.385	49.913	1.00	50.13	O
ATOM	2754	N	PRO	E	183	-3.745	39.820	48.199	1.00	49.19	N
ATOM	2755	CA	PRO	E	183	-3.257	38.477	47.881	1.00	48.42	C
ATOM	2756	CB	PRO	E	183	-3.550	38.337	46.376	1.00	48.72	C
ATOM	2757	CG	PRO	E	183	-4.295	39.617	45.982	1.00	48.90	C
ATOM	2758	CD	PRO	E	183	-3.889	40.645	46.994	1.00	48.91	C
ATOM	2759	C	PRO	E	183	-1.746	38.468	48.194	1.00	47.52	C
ATOM	2760	O	PRO	E	183	-0.921	38.837	47.347	1.00	46.84	O
ATOM	2761	N	LYS	E	184	-1.404	38.093	49.427	1.00	46.24	N
ATOM	2762	CA	LYS	E	184	-0.034	38.248	49.929	1.00	45.38	C
ATOM	2763	CB	LYS	E	184	-0.027	38.941	51.298	1.00	45.23	C
ATOM	2764	CG	LYS	E	184	1.370	39.251	51.840	1.00	45.55	C
ATOM	2765	CD	LYS	E	184	1.324	39.872	53.238	1.00	45.18	C
ATOM	2766	CE	LYS	E	184	0.758	41.288	53.211	1.00	44.18	C
ATOM	2767	NZ	LYS	E	184	0.640	41.879	54.570	1.00	43.76	N
ATOM	2768	C	LYS	E	184	0.725	36.920	50.000	1.00	44.40	C
ATOM	2769	O	LYS	E	184	0.280	35.976	50.661	1.00	44.29	O
ATOM	2770	N	PRO	E	185	1.917	36.869	49.352	1.00	43.52	N
ATOM	2771	CA	PRO	E	185	2.754	35.667	49.383	1.00	42.82	C
ATOM	2772	CB	PRO	E	185	3.969	36.070	48.545	1.00	42.92	C
ATOM	2773	CG	PRO	E	185	3.457	37.111	47.619	1.00	43.09	C
ATOM	2774	CD	PRO	E	185	2.420	37.869	48.393	1.00	43.15	C
ATOM	2775	C	PRO	E	185	3.189	35.317	50.804	1.00	42.18	C
ATOM	2776	O	PRO	E	185	3.489	36.211	51.597	1.00	41.56	O
ATOM	2777	N	GLU	E	186	3.214	34.025	51.115	1.00	41.30	N
ATOM	2778	CA	GLU	E	186	3.629	33.553	52.432	1.00	41.27	C
ATOM	2779	CB	GLU	E	186	3.597	32.020	52.492	1.00	41.28	C
ATOM	2780	CG	GLU	E	186	2.194	31.423	52.504	1.00	43.34	C
ATOM	2781	CD	GLU	E	186	2.150	30.004	51.955	1.00	46.37	C
ATOM	2782	OE1	GLU	E	186	2.484	29.813	50.766	1.00	49.81	O
ATOM	2783	OE2	GLU	E	186	1.775	29.080	52.711	1.00	48.12	O
ATOM	2784	C	GLU	E	186	5.022	34.064	52.786	1.00	40.05	C
ATOM	2785	O	GLU	E	186	5.303	34.370	53.946	1.00	39.40	O
ATOM	2786	N	PHE	E	187	5.887	34.165	51.781	1.00	39.15	N
ATOM	2787	CA	PHE	E	187	7.279	34.589	52.003	1.00	38.71	C
ATOM	2788	CB	PHE	E	187	8.184	34.308	50.785	1.00	38.92	C
ATOM	2789	CG	PHE	E	187	7.892	35.155	49.559	1.00	39.54	C
ATOM	2790	CD1	PHE	E	187	8.267	36.494	49.505	1.00	39.37	C
ATOM	2791	CE1	PHE	E	187	8.017	37.261	48.368	1.00	40.57	C
ATOM	2792	CZ	PHE	E	187	7.407	36.675	47.259	1.00	41.10	C
ATOM	2793	CE2	PHE	E	187	7.053	35.329	47.297	1.00	40.36	C
ATOM	2794	CD2	PHE	E	187	7.304	34.582	48.435	1.00	39.63	C
ATOM	2795	C	PHE	E	187	7.433	36.027	52.518	1.00	38.26	C
ATOM	2796	O	PHE	E	187	8.440	36.354	53.148	1.00	38.02	O
ATOM	2797	N	MET	E	188	6.431	36.869	52.267	1.00	37.50	N
ATOM	2798	CA	MET	E	188	6.464	38.266	52.726	1.00	37.57	C
ATOM	2799	CB	MET	E	188	5.270	39.061	52.168	1.00	37.65	C
ATOM	2800	CG	MET	E	188	5.351	39.333	50.669	1.00	38.90	C
ATOM	2801	SD	MET	E	188	6.746	40.356	50.193	1.00	43.25	S
ATOM	2802	CE	MET	E	188	6.176	41.967	50.734	1.00	44.37	C
ATOM	2803	C	MET	E	188	6.500	38.382	54.253	1.00	36.88	C
ATOM	2804	O	MET	E	188	7.045	39.341	54.787	1.00	36.24	O
ATOM	2805	N	SER	E	189	5.909	37.401	54.932	1.00	36.43	N
ATOM	2806	CA	SER	E	189	5.888	37.346	56.397	1.00	37.15	C
ATOM	2807	CB	SER	E	189	4.554	36.760	56.870	1.00	37.27	C
ATOM	2808	OG	SER	E	189	3.484	37.504	56.297	1.00	40.35	O
ATOM	2809	C	SER	E	189	7.052	36.542	57.000	1.00	36.95	C
ATOM	2810	O	SER	E	189	7.077	36.276	58.203	1.00	36.85	O
ATOM	2811	N	LYS	E	190	7.989	36.129	56.150	1.00	36.71	N
ATOM	2812	CA	LYS	E	190	9.192	35.433	56.595	1.00	36.06	C

Figure 1 Table 1a - 43

ATOM	2813	CB	LYS	E	190	9.534	34.315	55.615	1.00	36.21	C
ATOM	2814	CG	LYS	E	190	8.595	33.126	55.733	1.00	37.98	C
ATOM	2815	CD	LYS	E	190	8.971	32.048	54.754	1.00	42.38	C
ATOM	2816	CE	LYS	E	190	8.065	30.826	54.921	1.00	45.06	C
ATOM	2817	NZ	LYS	E	190	8.301	29.867	53.812	1.00	47.30	N
ATOM	2818	C	LYS	E	190	10.358	36.402	56.721	1.00	35.66	C
ATOM	2819	O	LYS	E	190	10.443	37.378	55.980	1.00	35.19	O
ATOM	2820	N	SER	E	191	11.272	36.116	57.641	1.00	35.65	N
ATOM	2821	CA	SER	E	191	12.383	37.019	57.922	1.00	35.66	C
ATOM	2822	CB	SER	E	191	12.900	36.776	59.336	1.00	35.51	C
ATOM	2823	OG	SER	E	191	13.525	35.507	59.439	1.00	36.66	O
ATOM	2824	C	SER	E	191	13.528	36.910	56.905	1.00	35.72	C
ATOM	2825	O	SER	E	191	13.614	35.936	56.152	1.00	34.72	O
ATOM	2826	N	LEU	E	192	14.401	37.916	56.894	1.00	36.50	N
ATOM	2827	CA	LEU	E	192	15.641	37.894	56.098	1.00	37.49	C
ATOM	2828	CB	LEU	E	192	16.495	39.124	56.392	1.00	37.16	C
ATOM	2829	CG	LEU	E	192	15.992	40.475	55.883	1.00	39.25	C
ATOM	2830	CD1	LEU	E	192	17.003	41.572	56.206	1.00	40.71	C
ATOM	2831	CD2	LEU	E	192	15.689	40.439	54.374	1.00	39.92	C
ATOM	2832	C	LEU	E	192	16.455	36.654	56.422	1.00	38.12	C
ATOM	2833	O	LEU	E	192	17.011	36.014	55.535	1.00	38.34	O
ATOM	2834	N	GLU	E	193	16.540	36.357	57.714	1.00	38.43	N
ATOM	2835	CA	GLU	E	193	17.157	35.146	58.237	1.00	39.62	C
ATOM	2836	CB	GLU	E	193	16.898	35.089	59.747	1.00	39.66	C
ATOM	2837	CG	GLU	E	193	17.258	33.773	60.424	1.00	43.97	C
ATOM	2838	CD	GLU	E	193	18.716	33.697	60.760	1.00	47.94	C
ATOM	2839	OE1	GLU	E	193	19.547	34.124	59.929	1.00	51.45	O
ATOM	2840	OE2	GLU	E	193	19.031	33.214	61.859	1.00	50.79	O
ATOM	2841	C	GLU	E	193	16.659	33.860	57.547	1.00	39.37	C
ATOM	2842	O	GLU	E	193	17.443	33.098	56.989	1.00	39.21	O
ATOM	2843	N	GLU	E	194	15.354	33.626	57.575	1.00	39.58	N
ATOM	2844	CA	GLU	E	194	14.833	32.400	57.002	1.00	39.79	C
ATOM	2845	CB	GLU	E	194	13.459	32.039	57.556	1.00	40.64	C
ATOM	2846	CG	GLU	E	194	12.483	33.166	57.668	1.00	43.94	C
ATOM	2847	CD	GLU	E	194	11.303	32.826	58.577	1.00	48.60	C
ATOM	2848	OE1	GLU	E	194	11.012	31.609	58.746	1.00	50.77	O
ATOM	2849	OE2	GLU	E	194	10.671	33.771	59.117	1.00	48.17	O
ATOM	2850	C	GLU	E	194	14.841	32.386	55.481	1.00	39.33	C
ATOM	2851	O	GLU	E	194	15.022	31.329	54.874	1.00	38.95	O
ATOM	2852	N	LEU	E	195	14.666	33.552	54.861	1.00	38.27	N
ATOM	2853	CA	LEU	E	195	14.703	33.634	53.414	1.00	38.15	C
ATOM	2854	CB	LEU	E	195	13.959	34.875	52.911	1.00	38.11	C
ATOM	2855	CG	LEU	E	195	12.457	34.871	53.213	1.00	38.40	C
ATOM	2856	CD1	LEU	E	195	11.836	36.212	52.868	1.00	39.48	C
ATOM	2857	CD2	LEU	E	195	11.724	33.725	52.497	1.00	38.52	C
ATOM	2858	C	LEU	E	195	16.121	33.599	52.859	1.00	38.05	C
ATOM	2859	O	LEU	E	195	16.315	33.323	51.679	1.00	37.84	O
ATOM	2860	N	GLN	E	196	17.098	33.881	53.720	1.00	37.98	N
ATOM	2861	CA	GLN	E	196	18.507	34.034	53.341	1.00	38.83	C
ATOM	2862	CB	GLN	E	196	19.150	32.676	53.028	1.00	38.35	C
ATOM	2863	CG	GLN	E	196	18.903	31.669	54.176	1.00	40.73	C
ATOM	2864	CD	GLN	E	196	19.685	30.382	54.049	1.00	42.86	C
ATOM	2865	OE1	GLN	E	196	20.109	30.012	52.955	1.00	44.95	O
ATOM	2866	NE2	GLN	E	196	19.868	29.678	55.171	1.00	44.66	N
ATOM	2867	C	GLN	E	196	18.704	35.092	52.247	1.00	38.48	C
ATOM	2868	O	GLN	E	196	19.259	34.847	51.165	1.00	38.40	O
ATOM	2869	N	ILE	E	197	18.214	36.285	52.550	1.00	38.67	N
ATOM	2870	CA	ILE	E	197	18.339	37.414	51.646	1.00	38.53	C
ATOM	2871	CB	ILE	E	197	16.961	38.087	51.396	1.00	38.57	C
ATOM	2872	CG1	ILE	E	197	15.996	37.101	50.721	1.00	38.73	C
ATOM	2873	CD1	ILE	E	197	14.563	37.645	50.543	1.00	37.79	C
ATOM	2874	CG2	ILE	E	197	17.109	39.362	50.554	1.00	38.28	C
ATOM	2875	C	ILE	E	197	19.323	38.387	52.288	1.00	38.76	C
ATOM	2876	O	ILE	E	197	19.127	38.810	53.440	1.00	39.29	O
ATOM	2877	N	GLY	E	198	20.383	38.713	51.553	1.00	38.22	N
ATOM	2878	CA	GLY	E	198	21.406	39.653	52.016	1.00	37.31	C
ATOM	2879	C	GLY	E	198	22.800	39.046	51.966	1.00	36.70	C

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ATOM	2880	O	GLY	E	198	22.968	37.897	51.574	1.00	36.19	O
ATOM	2881	N	THR	E	199	23.802	39.829	52.349	1.00	35.98	N
ATOM	2882	CA	THR	E	199	25.166	39.337	52.456	1.00	35.81	C
ATOM	2883	CB	THR	E	199	26.133	40.155	51.569	1.00	35.70	C
ATOM	2884	OG1	THR	E	199	25.709	40.055	50.206	1.00	35.18	O
ATOM	2885	CG2	THR	E	199	27.572	39.642	51.688	1.00	33.72	C
ATOM	2886	C	THR	E	199	25.595	39.381	53.927	1.00	36.36	C
ATOM	2887	O	THR	E	199	25.440	40.415	54.586	1.00	36.10	O
ATOM	2888	N	TYR	E	200	26.141	38.267	54.419	1.00	36.65	N
ATOM	2889	CA	TYR	E	200	26.420	38.101	55.851	1.00	37.33	C
ATOM	2890	CB	TYR	E	200	25.374	37.177	56.499	1.00	36.98	C
ATOM	2891	CG	TYR	E	200	23.993	37.750	56.311	1.00	37.22	C
ATOM	2892	CD1	TYR	E	200	23.149	37.294	55.291	1.00	37.37	C
ATOM	2893	CE1	TYR	E	200	21.895	37.855	55.097	1.00	37.03	C
ATOM	2894	CZ	TYR	E	200	21.486	38.902	55.907	1.00	37.88	C
ATOM	2895	OH	TYR	E	200	20.251	39.474	55.733	1.00	38.38	O
ATOM	2896	CE2	TYR	E	200	22.310	39.381	56.910	1.00	38.19	C
ATOM	2897	CD2	TYR	E	200	23.554	38.807	57.104	1.00	37.60	C
ATOM	2898	C	TYR	E	200	27.857	37.693	56.154	1.00	37.98	C
ATOM	2899	O	TYR	E	200	28.179	37.294	57.273	1.00	38.48	O
ATOM	2900	N	ALA	E	201	28.726	37.837	55.156	1.00	38.56	N
ATOM	2901	CA	ALA	E	201	30.155	37.589	55.321	1.00	38.98	C
ATOM	2902	CB	ALA	E	201	30.505	36.147	54.967	1.00	38.77	C
ATOM	2903	C	ALA	E	201	30.981	38.562	54.485	1.00	39.09	C
ATOM	2904	O	ALA	E	201	30.503	39.090	53.461	1.00	39.35	O
ATOM	2905	N	ASN	E	202	32.216	38.794	54.931	1.00	38.93	N
ATOM	2906	CA	ASN	E	202	33.185	39.618	54.210	1.00	39.20	C
ATOM	2907	CB	ASN	E	202	33.655	38.920	52.920	1.00	39.62	C
ATOM	2908	CG	ASN	E	202	34.006	37.452	53.141	1.00	42.06	C
ATOM	2909	OD1	ASN	E	202	33.411	36.554	52.523	1.00	44.77	O
ATOM	2910	ND2	ASN	E	202	34.949	37.199	54.044	1.00	42.34	N
ATOM	2911	C	ASN	E	202	32.603	40.988	53.890	1.00	38.37	C
ATOM	2912	O	ASN	E	202	32.671	41.445	52.752	1.00	38.15	O
ATOM	2913	N	ILE	E	203	32.012	41.625	54.893	1.00	37.61	N
ATOM	2914	CA	ILE	E	203	31.397	42.927	54.695	1.00	37.59	C
ATOM	2915	CB	ILE	E	203	30.390	43.283	55.814	1.00	37.59	C
ATOM	2916	CG1	ILE	E	203	29.319	42.186	55.934	1.00	38.42	C
ATOM	2917	CD1	ILE	E	203	28.553	41.878	54.627	1.00	39.07	C
ATOM	2918	CG2	ILE	E	203	29.763	44.636	55.555	1.00	36.29	C
ATOM	2919	C	ILE	E	203	32.493	43.963	54.583	1.00	37.46	C
ATOM	2920	O	ILE	E	203	33.316	44.107	55.492	1.00	36.69	O
ATOM	2921	N	ALA	E	204	32.521	44.648	53.442	1.00	37.30	N
ATOM	2922	CA	ALA	E	204	33.490	45.708	53.228	1.00	37.68	C
ATOM	2923	CB	ALA	E	204	33.650	45.993	51.729	1.00	37.26	C
ATOM	2924	C	ALA	E	204	33.045	46.954	54.001	1.00	37.92	C
ATOM	2925	O	ALA	E	204	31.959	47.507	53.751	1.00	38.21	O
ATOM	2926	N	MET	E	205	33.875	47.376	54.952	1.00	37.96	N
ATOM	2927	CA	MET	E	205	33.582	48.520	55.817	1.00	38.60	C
ATOM	2928	CB	MET	E	205	33.140	48.066	57.210	1.00	38.29	C
ATOM	2929	CG	MET	E	205	32.004	47.059	57.255	1.00	39.91	C
ATOM	2930	SD	MET	E	205	31.705	46.461	58.932	1.00	41.10	S
ATOM	2931	CE	MET	E	205	33.081	45.344	59.176	1.00	41.95	C
ATOM	2932	C	MET	E	205	34.820	49.399	55.990	1.00	38.57	C
ATOM	2933	O	MET	E	205	35.935	48.985	55.668	1.00	38.34	O
ATOM	2934	N	VAL	E	206	34.605	50.603	56.521	1.00	38.58	N
ATOM	2935	CA	VAL	E	206	35.678	51.543	56.832	1.00	38.89	C
ATOM	2936	CB	VAL	E	206	35.758	52.730	55.799	1.00	39.05	C
ATOM	2937	CG1	VAL	E	206	36.049	52.205	54.406	1.00	39.46	C
ATOM	2938	CG2	VAL	E	206	34.488	53.597	55.811	1.00	37.92	C
ATOM	2939	C	VAL	E	206	35.491	52.084	58.244	1.00	39.27	C
ATOM	2940	O	VAL	E	206	34.452	51.860	58.864	1.00	39.48	O
ATOM	2941	N	ARG	E	207	36.492	52.789	58.758	1.00	39.75	N
ATOM	2942	CA	ARG	E	207	36.332	53.508	60.020	1.00	40.62	C
ATOM	2943	CB	ARG	E	207	37.513	53.220	60.960	1.00	41.17	C
ATOM	2944	CG	ARG	E	207	37.791	51.718	61.064	1.00	43.58	C
ATOM	2945	CD	ARG	E	207	38.131	51.244	62.457	1.00	48.60	C
ATOM	2946	NE	ARG	E	207	37.644	52.143	63.500	1.00	51.61	N

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ATOM	2947	CZ	ARG	E	207	38.378	52.548	64.532	1.00	52.82	C
ATOM	2948	NH1	ARG	E	207	39.620	52.107	64.680	1.00	53.06	N
ATOM	2949	NH2	ARG	E	207	37.860	53.378	65.431	1.00	54.65	N
ATOM	2950	C	ARG	E	207	36.130	55.009	59.799	1.00	40.94	C
ATOM	2951	O	ARG	E	207	36.224	55.510	58.673	1.00	40.27	O
ATOM	2952	N	THR	E	208	35.831	55.705	60.891	1.00	41.25	N
ATOM	2953	CA	THR	E	208	35.636	57.154	60.918	1.00	42.09	C
ATOM	2954	CB	THR	E	208	35.454	57.592	62.398	1.00	41.93	C
ATOM	2955	OG1	THR	E	208	34.173	57.137	62.856	1.00	44.45	O
ATOM	2956	CG2	THR	E	208	35.552	59.094	62.569	1.00	43.60	C
ATOM	2957	C	THR	E	208	36.791	57.929	60.256	1.00	41.65	C
ATOM	2958	O	THR	E	208	36.578	58.869	59.474	1.00	41.59	O
ATOM	2959	N	THR	E	209	38.006	57.481	60.560	1.00	41.63	N
ATOM	2960	CA	THR	E	209	39.250	58.160	60.220	1.00	41.19	C
ATOM	2961	CB	THR	E	209	40.253	57.981	61.381	1.00	41.44	C
ATOM	2962	OG1	THR	E	209	40.385	56.584	61.674	1.00	42.56	O
ATOM	2963	CG2	THR	E	209	39.758	58.688	62.644	1.00	41.11	C
ATOM	2964	C	THR	E	209	39.875	57.639	58.913	1.00	40.87	C
ATOM	2965	O	THR	E	209	40.909	58.162	58.467	1.00	40.77	O
ATOM	2966	N	THR	E	210	39.248	56.623	58.304	1.00	40.06	N
ATOM	2967	CA	THR	E	210	39.716	56.041	57.041	1.00	39.45	C
ATOM	2968	CB	THR	E	210	38.816	54.856	56.571	1.00	39.63	C
ATOM	2969	OG1	THR	E	210	38.773	53.827	57.575	1.00	39.98	O
ATOM	2970	CG2	THR	E	210	39.350	54.249	55.274	1.00	39.56	C
ATOM	2971	C	THR	E	210	39.779	57.097	55.923	1.00	38.88	C
ATOM	2972	O	THR	E	210	38.763	57.713	55.601	1.00	39.10	O
ATOM	2973	N	PRO	E	211	40.975	57.311	55.335	1.00	38.19	N
ATOM	2974	CA	PRO	E	211	41.086	58.254	54.217	1.00	37.85	C
ATOM	2975	CB	PRO	E	211	42.564	58.185	53.834	1.00	37.80	C
ATOM	2976	CG	PRO	E	211	43.259	57.644	55.052	1.00	38.29	C
ATOM	2977	CD	PRO	E	211	42.276	56.714	55.693	1.00	37.59	C
ATOM	2978	C	PRO	E	211	40.214	57.870	53.020	1.00	37.69	C
ATOM	2979	O	PRO	E	211	39.984	56.681	52.775	1.00	37.80	O
ATOM	2980	N	VAL	E	212	39.729	58.882	52.302	1.00	37.47	N
ATOM	2981	CA	VAL	E	212	38.912	58.692	51.102	1.00	37.16	C
ATOM	2982	CB	VAL	E	212	38.548	60.056	50.442	1.00	37.40	C
ATOM	2983	CG1	VAL	E	212	37.987	59.860	49.019	1.00	37.52	C
ATOM	2984	CG2	VAL	E	212	37.560	60.813	51.315	1.00	36.94	C
ATOM	2985	C	VAL	E	212	39.581	57.756	50.084	1.00	36.74	C
ATOM	2986	O	VAL	E	212	38.923	56.869	49.541	1.00	36.06	O
ATOM	2987	N	TYR	E	213	40.884	57.945	49.849	1.00	36.53	N
ATOM	2988	CA	TYR	E	213	41.606	57.131	48.866	1.00	36.72	C
ATOM	2989	CB	TYR	E	213	43.034	57.655	48.598	1.00	37.16	C
ATOM	2990	CG	TYR	E	213	44.037	57.385	49.697	1.00	38.66	C
ATOM	2991	CD1	TYR	E	213	44.334	58.360	50.655	1.00	40.38	C
ATOM	2992	CE1	TYR	E	213	45.253	58.113	51.672	1.00	40.66	C
ATOM	2993	CZ	TYR	E	213	45.881	56.880	51.727	1.00	40.13	C
ATOM	2994	OH	TYR	E	213	46.790	56.619	52.715	1.00	40.71	O
ATOM	2995	CE2	TYR	E	213	45.612	55.904	50.784	1.00	40.49	C
ATOM	2996	CD2	TYR	E	213	44.695	56.156	49.778	1.00	39.45	C
ATOM	2997	C	TYR	E	213	41.611	55.647	49.239	1.00	36.34	C
ATOM	2998	O	TYR	E	213	41.599	54.792	48.357	1.00	36.39	O
ATOM	2999	N	VAL	E	214	41.612	55.350	50.541	1.00	35.96	N
ATOM	3000	CA	VAL	E	214	41.503	53.962	51.018	1.00	35.41	C
ATOM	3001	CB	VAL	E	214	41.856	53.810	52.533	1.00	35.64	C
ATOM	3002	CG1	VAL	E	214	41.701	52.360	52.988	1.00	35.39	C
ATOM	3003	CG2	VAL	E	214	43.294	54.285	52.819	1.00	35.60	C
ATOM	3004	C	VAL	E	214	40.112	53.394	50.709	1.00	35.25	C
ATOM	3005	O	VAL	E	214	39.988	52.275	50.181	1.00	34.69	O
ATOM	3006	N	ALA	E	215	39.071	54.172	51.014	1.00	34.82	N
ATOM	3007	CA	ALA	E	215	37.696	53.793	50.664	1.00	34.45	C
ATOM	3008	CB	ALA	E	215	36.698	54.862	51.106	1.00	33.92	C
ATOM	3009	C	ALA	E	215	37.554	53.503	49.167	1.00	34.24	C
ATOM	3010	O	ALA	E	215	36.936	52.516	48.788	1.00	33.80	O
ATOM	3011	N	LEU	E	216	38.154	54.354	48.333	1.00	34.28	N
ATOM	3012	CA	LEU	E	216	38.106	54.190	46.890	1.00	34.73	C
ATOM	3013	CB	LEU	E	216	38.821	55.344	46.164	1.00	35.32	C

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ATOM	3014	CG	LEU	E	216	38.264	56.771	46.253	1.00	36.53	C
ATOM	3015	CD1	LEU	E	216	38.945	57.649	45.216	1.00	37.65	C
ATOM	3016	CD2	LEU	E	216	36.764	56.824	46.079	1.00	39.11	C
ATOM	3017	C	LEU	E	216	38.701	52.860	46.453	1.00	35.10	C
ATOM	3018	O	LEU	E	216	38.108	52.166	45.644	1.00	35.83	O
ATOM	3019	N	GLY	E	217	39.874	52.512	46.978	1.00	35.42	N
ATOM	3020	CA	GLY	E	217	40.485	51.208	46.704	1.00	35.67	C
ATOM	3021	C	GLY	E	217	39.601	50.040	47.131	1.00	36.00	C
ATOM	3022	O	GLY	E	217	39.539	49.003	46.452	1.00	35.77	O
ATOM	3023	N	ILE	E	218	38.919	50.210	48.260	1.00	35.84	N
ATOM	3024	CA	ILE	E	218	37.965	49.223	48.732	1.00	36.26	C
ATOM	3025	CB	ILE	E	218	37.490	49.527	50.177	1.00	36.50	C
ATOM	3026	CG1	ILE	E	218	38.671	49.344	51.156	1.00	37.22	C
ATOM	3027	CD1	ILE	E	218	38.459	49.975	52.540	1.00	36.15	C
ATOM	3028	CG2	ILE	E	218	36.307	48.617	50.568	1.00	35.94	C
ATOM	3029	C	ILE	E	218	36.807	49.079	47.729	1.00	36.04	C
ATOM	3030	O	ILE	E	218	36.482	47.953	47.327	1.00	36.03	O
ATOM	3031	N	PHE	E	219	36.233	50.203	47.284	1.00	35.71	N
ATOM	3032	CA	PHE	E	219	35.205	50.168	46.228	1.00	35.49	C
ATOM	3033	CB	PHE	E	219	34.765	51.569	45.806	1.00	35.10	C
ATOM	3034	CG	PHE	E	219	33.783	52.232	46.745	1.00	34.99	C
ATOM	3035	CD1	PHE	E	219	33.997	53.552	47.168	1.00	34.37	C
ATOM	3036	CE1	PHE	E	219	33.091	54.196	48.024	1.00	34.81	C
ATOM	3037	CZ	PHE	E	219	31.949	53.505	48.469	1.00	33.84	C
ATOM	3038	CE2	PHE	E	219	31.724	52.183	48.037	1.00	34.65	C
ATOM	3039	CD2	PHE	E	219	32.642	51.562	47.181	1.00	34.24	C
ATOM	3040	C	PHE	E	219	35.688	49.435	44.981	1.00	36.05	C
ATOM	3041	O	PHE	E	219	34.946	48.650	44.385	1.00	35.61	O
ATOM	3042	N	VAL	E	220	36.923	49.730	44.573	1.00	36.40	N
ATOM	3043	CA	VAL	E	220	37.496	49.158	43.363	1.00	37.40	C
ATOM	3044	CB	VAL	E	220	38.814	49.876	42.931	1.00	37.05	C
ATOM	3045	CG1	VAL	E	220	39.573	49.061	41.855	1.00	37.88	C
ATOM	3046	CG2	VAL	E	220	38.503	51.274	42.412	1.00	36.59	C
ATOM	3047	C	VAL	E	220	37.691	47.645	43.487	1.00	38.09	C
ATOM	3048	O	VAL	E	220	37.342	46.898	42.568	1.00	38.80	O
ATOM	3049	N	GLN	E	221	38.230	47.185	44.614	1.00	38.57	N
ATOM	3050	CA	GLN	E	221	38.438	45.751	44.786	1.00	39.37	C
ATOM	3051	CB	GLN	E	221	39.409	45.467	45.921	1.00	39.55	C
ATOM	3052	CG	GLN	E	221	39.759	44.000	46.003	1.00	40.41	C
ATOM	3053	CD	GLN	E	221	41.028	43.745	46.750	1.00	43.01	C
ATOM	3054	OE1	GLN	E	221	41.523	44.615	47.473	1.00	43.71	O
ATOM	3055	NE2	GLN	E	221	41.580	42.540	46.585	1.00	42.63	N
ATOM	3056	C	GLN	E	221	37.155	44.924	44.994	1.00	39.68	C
ATOM	3057	O	GLN	E	221	37.032	43.819	44.466	1.00	39.47	O
ATOM	3058	N	HIS	E	222	36.218	45.456	45.770	1.00	40.29	N
ATOM	3059	CA	HIS	E	222	35.056	44.671	46.187	1.00	40.80	C
ATOM	3060	CB	HIS	E	222	34.783	44.883	47.680	1.00	41.50	C
ATOM	3061	CG	HIS	E	222	35.940	44.512	48.540	1.00	43.84	C
ATOM	3062	ND1	HIS	E	222	36.270	43.203	48.812	1.00	47.56	N
ATOM	3063	CE1	HIS	E	222	37.351	43.173	49.572	1.00	48.28	C
ATOM	3064	NE2	HIS	E	222	37.738	44.417	49.793	1.00	48.70	N
ATOM	3065	CD2	HIS	E	222	36.878	45.273	49.149	1.00	45.80	C
ATOM	3066	C	HIS	E	222	33.788	44.855	45.355	1.00	39.94	C
ATOM	3067	O	HIS	E	222	32.868	44.046	45.466	1.00	39.61	O
ATOM	3068	N	ARG	E	223	33.740	45.893	44.523	1.00	39.27	N
ATOM	3069	CA	ARG	E	223	32.607	46.092	43.602	1.00	39.77	C
ATOM	3070	CB	ARG	E	223	32.623	45.053	42.471	1.00	39.89	C
ATOM	3071	CG	ARG	E	223	33.853	45.149	41.563	1.00	42.38	C
ATOM	3072	CD	ARG	E	223	33.716	44.205	40.377	1.00	45.75	C
ATOM	3073	NE	ARG	E	223	34.987	43.991	39.677	1.00	52.18	N
ATOM	3074	CZ	ARG	E	223	35.098	43.453	38.460	1.00	53.91	C
ATOM	3075	NH1	ARG	E	223	34.013	43.081	37.787	1.00	54.81	N
ATOM	3076	NH2	ARG	E	223	36.299	43.292	37.910	1.00	54.83	N
ATOM	3077	C	ARG	E	223	31.261	46.090	44.348	1.00	38.83	C
ATOM	3078	O	ARG	E	223	30.348	45.306	44.066	1.00	37.98	O
ATOM	3079	N	VAL	E	224	31.176	47.008	45.294	1.00	38.03	N
ATOM	3080	CA	VAL	E	224	30.109	47.090	46.270	1.00	38.25	C

Figure 1

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ATOM	3081	CB	VAL	E	224	30.721	46.570	47.586	1.00	38.55	C
ATOM	3082	CG1	VAL	E	224	30.707	47.589	48.708	1.00	38.81	C
ATOM	3083	CG2	VAL	E	224	30.202	45.170	47.923	1.00	37.20	C
ATOM	3084	C	VAL	E	224	29.627	48.560	46.303	1.00	37.70	C
ATOM	3085	O	VAL	E	224	30.441	49.457	46.124	1.00	37.98	O
ATOM	3086	N	SER	E	225	28.326	48.812	46.489	1.00	37.42	N
ATOM	3087	CA	SER	E	225	27.789	50.170	46.261	1.00	37.21	C
ATOM	3088	CB	SER	E	225	26.327	50.140	45.781	1.00	37.20	C
ATOM	3089	OG	SER	E	225	25.440	49.830	46.858	1.00	40.76	O
ATOM	3090	C	SER	E	225	27.939	51.137	47.440	1.00	36.56	C
ATOM	3091	O	SER	E	225	27.815	52.343	47.265	1.00	35.83	O
ATOM	3092	N	ALA	E	226	28.170	50.610	48.641	1.00	35.63	N
ATOM	3093	CA	ALA	E	226	28.377	51.460	49.809	1.00	35.29	C
ATOM	3094	CB	ALA	E	226	27.044	51.956	50.370	1.00	34.80	C
ATOM	3095	C	ALA	E	226	29.148	50.722	50.889	1.00	35.49	C
ATOM	3096	O	ALA	E	226	29.125	49.490	50.956	1.00	35.18	O
ATOM	3097	N	LEU	E	227	29.816	51.503	51.734	1.00	35.37	N
ATOM	3098	CA	LEU	E	227	30.625	50.987	52.836	1.00	34.81	C
ATOM	3099	CB	LEU	E	227	32.096	51.414	52.655	1.00	34.58	C
ATOM	3100	CG	LEU	E	227	32.733	51.129	51.283	1.00	35.39	C
ATOM	3101	CD1	LEU	E	227	34.100	51.830	51.133	1.00	36.38	C
ATOM	3102	CD2	LEU	E	227	32.858	49.638	51.025	1.00	34.34	C
ATOM	3103	C	LEU	E	227	30.090	51.507	54.170	1.00	34.72	C
ATOM	3104	O	LEU	E	227	30.036	52.724	54.395	1.00	34.25	O
ATOM	3105	N	PRO	E	228	29.686	50.592	55.066	1.00	34.61	N
ATOM	3106	CA	PRO	E	228	29.388	51.067	56.420	1.00	35.00	C
ATOM	3107	CB	PRO	E	228	28.936	49.798	57.149	1.00	34.73	C
ATOM	3108	CG	PRO	E	228	28.463	48.889	56.054	1.00	34.73	C
ATOM	3109	CD	PRO	E	228	29.412	49.156	54.917	1.00	34.71	C
ATOM	3110	C	PRO	E	228	30.618	51.676	57.110	1.00	35.49	C
ATOM	3111	O	PRO	E	228	31.739	51.194	56.939	1.00	34.99	O
ATOM	3112	N	VAL	E	229	30.383	52.741	57.865	1.00	35.74	N
ATOM	3113	CA	VAL	E	229	31.415	53.404	58.658	1.00	36.54	C
ATOM	3114	CB	VAL	E	229	31.338	54.942	58.513	1.00	36.82	C
ATOM	3115	CG1	VAL	E	229	32.455	55.644	59.315	1.00	37.10	C
ATOM	3116	CG2	VAL	E	229	31.403	55.347	57.036	1.00	35.42	C
ATOM	3117	C	VAL	E	229	31.201	52.974	60.105	1.00	37.35	C
ATOM	3118	O	VAL	E	229	30.128	53.189	60.681	1.00	37.15	O
ATOM	3119	N	VAL	E	230	32.218	52.347	60.682	1.00	37.88	N
ATOM	3120	CA	VAL	E	230	32.086	51.758	61.998	1.00	38.88	C
ATOM	3121	CB	VAL	E	230	32.225	50.219	61.953	1.00	38.93	C
ATOM	3122	CG1	VAL	E	230	31.156	49.609	61.020	1.00	38.20	C
ATOM	3123	CG2	VAL	E	230	33.630	49.805	61.518	1.00	38.53	C
ATOM	3124	C	VAL	E	230	33.062	52.356	63.010	1.00	40.07	C
ATOM	3125	O	VAL	E	230	34.115	52.885	62.644	1.00	40.08	O
ATOM	3126	N	ASP	E	231	32.682	52.292	64.282	1.00	41.49	N
ATOM	3127	CA	ASP	E	231	33.550	52.732	65.367	1.00	43.03	C
ATOM	3128	CB	ASP	E	231	32.724	53.272	66.543	1.00	42.84	C
ATOM	3129	CG	ASP	E	231	31.840	52.212	67.203	1.00	43.83	C
ATOM	3130	OD1	ASP	E	231	30.931	52.620	67.966	1.00	44.72	O
ATOM	3131	OD2	ASP	E	231	32.044	50.991	66.983	1.00	42.75	O
ATOM	3132	C	ASP	E	231	34.481	51.592	65.788	1.00	43.91	C
ATOM	3133	O	ASP	E	231	34.457	50.506	65.194	1.00	44.06	O
ATOM	3134	N	GLU	E	232	35.292	51.835	66.812	1.00	45.03	N
ATOM	3135	CA	GLU	E	232	36.264	50.839	67.276	1.00	46.23	C
ATOM	3136	CB	GLU	E	232	37.101	51.396	68.439	1.00	46.54	C
ATOM	3137	CG	GLU	E	232	36.286	51.890	69.630	1.00	48.79	C
ATOM	3138	CD	GLU	E	232	36.949	53.055	70.349	1.00	52.59	C
ATOM	3139	OE1	GLU	E	232	37.607	53.878	69.665	1.00	53.76	O
ATOM	3140	OE2	GLU	E	232	36.807	53.151	71.593	1.00	53.00	O
ATOM	3141	C	GLU	E	232	35.614	49.501	67.657	1.00	46.19	C
ATOM	3142	O	GLU	E	232	36.257	48.449	67.591	1.00	46.60	O
ATOM	3143	N	LYS	E	233	34.340	49.552	68.041	1.00	45.90	N
ATOM	3144	CA	LYS	E	233	33.621	48.361	68.483	1.00	45.32	C
ATOM	3145	CB	LYS	E	233	32.733	48.692	69.685	1.00	45.59	C
ATOM	3146	CG	LYS	E	233	33.531	49.052	70.938	1.00	46.22	C
ATOM	3147	CD	LYS	E	233	32.654	49.636	72.036	1.00	47.88	C

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ATOM	3148	CE	LYS E 233	33.510	50.230	73.155	1.00	48.31	C
ATOM	3149	NZ	LYS E 233	32.687	50.748	74.289	1.00	49.23	N
ATOM	3150	C	LYS E 233	32.823	47.708	67.348	1.00	44.78	C
ATOM	3151	O	LYS E 233	32.053	46.777	67.576	1.00	44.65	O
ATOM	3152	N	GLY E 234	33.031	48.193	66.125	1.00	44.06	N
ATOM	3153	CA	GLY E 234	32.388	47.617	64.947	1.00	43.43	C
ATOM	3154	C	GLY E 234	30.917	47.979	64.820	1.00	42.81	C
ATOM	3155	O	GLY E 234	30.186	47.350	64.048	1.00	42.65	O
ATOM	3156	N	ARG E 235	30.487	48.984	65.576	1.00	42.05	N
ATOM	3157	CA	ARG E 235	29.134	49.514	65.456	1.00	41.64	C
ATOM	3158	CB	ARG E 235	28.675	50.127	66.782	1.00	41.80	C
ATOM	3159	CG	ARG E 235	28.578	49.133	67.929	1.00	42.85	C
ATOM	3160	CD	ARG E 235	28.238	49.830	69.235	1.00	43.69	C
ATOM	3161	NE	ARG E 235	29.329	50.682	69.700	1.00	46.04	N
ATOM	3162	CZ	ARG E 235	29.304	51.385	70.829	1.00	47.10	C
ATOM	3163	NH1	ARG E 235	28.239	51.343	71.619	1.00	47.32	N
ATOM	3164	NH2	ARG E 235	30.346	52.133	71.168	1.00	47.17	N
ATOM	3165	C	ARG E 235	29.052	50.555	64.344	1.00	40.78	C
ATOM	3166	O	ARG E 235	29.915	51.425	64.232	1.00	40.07	O
ATOM	3167	N	VAL E 236	28.007	50.460	63.526	1.00	40.03	N
ATOM	3168	CA	VAL E 236	27.822	51.381	62.409	1.00	39.67	C
ATOM	3169	CB	VAL E 236	26.775	50.852	61.407	1.00	39.54	C
ATOM	3170	CG1	VAL E 236	25.383	50.881	62.021	1.00	39.54	C
ATOM	3171	CG2	VAL E 236	26.816	51.662	60.117	1.00	38.83	C
ATOM	3172	C	VAL E 236	27.409	52.767	62.897	1.00	39.42	C
ATOM	3173	O	VAL E 236	26.457	52.909	63.662	1.00	39.72	O
ATOM	3174	N	VAL E 237	28.136	53.784	62.450	1.00	38.99	N
ATOM	3175	CA	VAL E 237	27.853	55.160	62.842	1.00	38.72	C
ATOM	3176	CB	VAL E 237	29.025	55.781	63.634	1.00	38.87	C
ATOM	3177	CG1	VAL E 237	29.105	55.175	65.029	1.00	39.18	C
ATOM	3178	CG2	VAL E 237	30.338	55.591	62.883	1.00	38.61	C
ATOM	3179	C	VAL E 237	27.545	56.030	61.627	1.00	38.54	C
ATOM	3180	O	VAL E 237	26.952	57.100	61.754	1.00	38.65	O
ATOM	3181	N	ASP E 238	27.951	55.562	60.451	1.00	38.22	N
ATOM	3182	CA	ASP E 238	27.700	56.286	59.212	1.00	38.17	C
ATOM	3183	CB	ASP E 238	28.725	57.410	59.028	1.00	38.49	C
ATOM	3184	CG	ASP E 238	28.111	58.671	58.452	1.00	39.79	C
ATOM	3185	OD1	ASP E 238	27.104	58.566	57.722	1.00	40.58	O
ATOM	3186	OD2	ASP E 238	28.633	59.773	58.732	1.00	44.41	O
ATOM	3187	C	ASP E 238	27.728	55.344	58.013	1.00	38.18	C
ATOM	3188	O	ASP E 238	27.919	54.135	58.164	1.00	37.82	O
ATOM	3189	N	ILE E 239	27.536	55.905	56.825	1.00	37.72	N
ATOM	3190	CA	ILE E 239	27.543	55.116	55.589	1.00	37.81	C
ATOM	3191	CB	ILE E 239	26.091	54.698	55.190	1.00	37.55	C
ATOM	3192	CG1	ILE E 239	26.065	53.810	53.941	1.00	38.14	C
ATOM	3193	CD1	ILE E 239	25.952	52.320	54.277	1.00	38.52	C
ATOM	3194	CG2	ILE E 239	25.181	55.904	55.047	1.00	37.42	C
ATOM	3195	C	ILE E 239	28.205	55.965	54.500	1.00	37.79	C
ATOM	3196	O	ILE E 239	27.846	57.126	54.324	1.00	37.31	O
ATOM	3197	N	TYR E 240	29.186	55.393	53.802	1.00	37.40	N
ATOM	3198	CA	TYR E 240	29.821	56.075	52.678	1.00	37.76	C
ATOM	3199	CB	TYR E 240	31.342	56.098	52.853	1.00	38.05	C
ATOM	3200	CG	TYR E 240	32.099	57.028	51.915	1.00	38.71	C
ATOM	3201	CD1	TYR E 240	33.077	56.530	51.053	1.00	39.18	C
ATOM	3202	CE1	TYR E 240	33.785	57.376	50.201	1.00	39.94	C
ATOM	3203	CZ	TYR E 240	33.522	58.734	50.213	1.00	40.35	C
ATOM	3204	OH	TYR E 240	34.208	59.572	49.377	1.00	40.07	O
ATOM	3205	CE2	TYR E 240	32.553	59.254	51.060	1.00	41.10	C
ATOM	3206	CD2	TYR E 240	31.847	58.395	51.904	1.00	39.11	C
ATOM	3207	C	TYR E 240	29.431	55.363	51.387	1.00	38.36	C
ATOM	3208	O	TYR E 240	29.933	54.266	51.084	1.00	38.60	O
ATOM	3209	N	SER E 241	28.488	55.958	50.666	1.00	38.12	N
ATOM	3210	CA	SER E 241	28.033	55.397	49.405	1.00	38.68	C
ATOM	3211	CB	SER E 241	26.588	55.825	49.127	1.00	38.55	C
ATOM	3212	OG	SER E 241	26.163	55.372	47.846	1.00	39.80	O
ATOM	3213	C	SER E 241	28.939	55.901	48.283	1.00	38.76	C
ATOM	3214	O	SER E 241	29.581	56.946	48.415	1.00	38.27	O

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ATOM	3215	N	LYS	E	242	28.988	55.148	47.190	1.00 39.19	N
ATOM	3216	CA	LYS	E	242	29.591	55.623	45.951	1.00 39.46	C
ATOM	3217	CB	LYS	E	242	29.368	54.620	44.827	1.00 39.38	C
ATOM	3218	CG	LYS	E	242	30.212	53.370	44.927	1.00 37.53	C
ATOM	3219	CD	LYS	E	242	30.009	52.477	43.723	1.00 35.51	C
ATOM	3220	CE	LYS	E	242	31.149	51.461	43.629	1.00 35.06	C
ATOM	3221	NZ	LYS	E	242	30.934	50.485	42.525	1.00 33.11	N
ATOM	3222	C	LYS	E	242	28.986	56.968	45.544	1.00 40.31	C
ATOM	3223	O	LYS	E	242	29.686	57.843	45.029	1.00 40.63	O
ATOM	3224	N	PHE	E	243	27.685	57.127	45.770	1.00 40.90	N
ATOM	3225	CA	PHE	E	243	27.028	58.395	45.486	1.00 41.64	C
ATOM	3226	CB	PHE	E	243	25.532	58.342	45.789	1.00 41.89	C
ATOM	3227	CG	PHE	E	243	24.841	59.667	45.576	1.00 42.83	C
ATOM	3228	CD1	PHE	E	243	24.748	60.218	44.295	1.00 44.46	C
ATOM	3229	CE1	PHE	E	243	24.131	61.463	44.084	1.00 43.97	C
ATOM	3230	CZ	PHE	E	243	23.619	62.169	45.178	1.00 43.98	C
ATOM	3231	CE2	PHE	E	243	23.728	61.634	46.462	1.00 44.11	C
ATOM	3232	CD2	PHE	E	243	24.348	60.394	46.656	1.00 43.09	C
ATOM	3233	C	PHE	E	243	27.664	59.575	46.231	1.00 41.58	C
ATOM	3234	O	PHE	E	243	27.671	60.692	45.726	1.00 41.92	O
ATOM	3235	N	ASP	E	244	28.185	59.329	47.430	1.00 41.45	N
ATOM	3236	CA	ASP	E	244	28.834	60.383	48.213	1.00 41.73	C
ATOM	3237	CB	ASP	E	244	29.012	59.949	49.670	1.00 41.35	C
ATOM	3238	CG	ASP	E	244	27.680	59.625	50.354	1.00 41.48	C
ATOM	3239	OD1	ASP	E	244	26.726	60.440	50.243	1.00 40.87	O
ATOM	3240	OD2	ASP	E	244	27.599	58.558	51.019	1.00 39.15	O
ATOM	3241	C	ASP	E	244	30.179	60.802	47.602	1.00 41.91	C
ATOM	3242	O	ASP	E	244	30.722	61.858	47.938	1.00 41.54	O
ATOM	3243	N	VAL	E	245	30.691	59.965	46.699	1.00 42.18	N
ATOM	3244	CA	VAL	E	245	31.979	60.186	46.061	1.00 42.78	C
ATOM	3245	CB	VAL	E	245	32.624	58.850	45.567	1.00 42.79	C
ATOM	3246	CG1	VAL	E	245	33.942	59.101	44.893	1.00 42.92	C
ATOM	3247	CG2	VAL	E	245	32.816	57.880	46.733	1.00 42.72	C
ATOM	3248	C	VAL	E	245	31.943	61.246	44.939	1.00 43.23	C
ATOM	3249	O	VAL	E	245	32.860	62.057	44.864	1.00 42.51	O
ATOM	3250	N	ILE	E	246	30.915	61.259	44.082	1.00 44.41	N
ATOM	3251	CA	ILE	E	246	30.906	62.262	42.987	1.00 45.87	C
ATOM	3252	CB	ILE	E	246	29.778	62.123	41.918	1.00 46.12	C
ATOM	3253	CG1	ILE	E	246	28.548	61.430	42.482	1.00 46.70	C
ATOM	3254	CD1	ILE	E	246	27.573	62.402	43.095	1.00 46.74	C
ATOM	3255	CG2	ILE	E	246	30.337	61.593	40.583	1.00 46.94	C
ATOM	3256	C	ILE	E	246	30.891	63.703	43.446	1.00 46.03	C
ATOM	3257	O	ILE	E	246	31.165	64.592	42.653	1.00 45.99	O
ATOM	3258	N	ASN	E	247	30.555	63.933	44.710	1.00 46.99	N
ATOM	3259	CA	ASN	E	247	30.761	65.240	45.320	1.00 48.09	C
ATOM	3260	CB	ASN	E	247	30.539	65.166	46.832	1.00 48.11	C
ATOM	3261	CG	ASN	E	247	30.755	66.496	47.510	1.00 49.74	C
ATOM	3262	OD1	ASN	E	247	31.846	66.778	48.020	1.00 51.26	O
ATOM	3263	ND2	ASN	E	247	29.728	67.344	47.493	1.00 50.09	N
ATOM	3264	C	ASN	E	247	32.174	65.762	45.007	1.00 48.45	C
ATOM	3265	O	ASN	E	247	32.349	66.938	44.711	1.00 48.15	O
ATOM	3266	N	LEU	E	248	33.160	64.861	45.044	1.00 49.03	N
ATOM	3267	CA	LEU	E	248	34.560	65.189	44.756	1.00 49.96	C
ATOM	3268	CB	LEU	E	248	35.452	63.947	44.912	1.00 49.78	C
ATOM	3269	CG	LEU	E	248	35.956	63.403	46.267	1.00 50.27	C
ATOM	3270	CD1	LEU	E	248	35.181	63.883	47.488	1.00 51.18	C
ATOM	3271	CD2	LEU	E	248	36.002	61.877	46.249	1.00 49.49	C
ATOM	3272	C	LEU	E	248	34.765	65.802	43.370	1.00 50.62	C
ATOM	3273	O	LEU	E	248	35.688	66.590	43.173	1.00 50.68	O
ATOM	3274	N	ALA	E	249	33.910	65.443	42.414	1.00 51.71	N
ATOM	3275	CA	ALA	E	249	34.009	65.983	41.052	1.00 53.03	C
ATOM	3276	CB	ALA	E	249	33.148	65.179	40.076	1.00 52.70	C
ATOM	3277	C	ALA	E	249	33.689	67.484	40.969	1.00 54.08	C
ATOM	3278	O	ALA	E	249	34.085	68.153	40.005	1.00 54.05	O
ATOM	3279	N	ALA	E	250	32.999	68.004	41.987	1.00 55.58	N
ATOM	3280	CA	ALA	E	250	32.678	69.435	42.073	1.00 57.25	C
ATOM	3281	CB	ALA	E	250	31.567	69.671	43.088	1.00 57.28	C

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ATOM	3282	C	ALA	E	250	33.900	70.310	42.396	1.00	58.33	C
ATOM	3283	O	ALA	E	250	33.974	71.461	41.953	1.00	58.55	O
ATOM	3284	N	GLU	E	251	34.844	69.760	43.163	1.00	59.78	N
ATOM	3285	CA	GLU	E	251	36.097	70.453	43.501	1.00	61.18	C
ATOM	3286	CB	GLU	E	251	36.811	69.759	44.683	1.00	61.13	C
ATOM	3287	CG	GLU	E	251	37.709	68.562	44.303	1.00	62.21	C
ATOM	3288	CD	GLU	E	251	38.144	67.684	45.487	1.00	62.94	C
ATOM	3289	OE1	GLU	E	251	38.682	68.219	46.486	1.00	64.24	O
ATOM	3290	OE2	GLU	E	251	37.972	66.445	45.401	1.00	62.92	O
ATOM	3291	C	GLU	E	251	37.006	70.538	42.269	1.00	61.71	C
ATOM	3292	O	GLU	E	251	37.023	69.627	41.438	1.00	61.93	O
ATOM	3293	N	LYS	E	252	37.747	71.634	42.139	1.00	62.55	N
ATOM	3294	CA	LYS	E	252	38.710	71.772	41.038	1.00	63.28	C
ATOM	3295	CB	LYS	E	252	38.956	73.247	40.701	1.00	63.40	C
ATOM	3296	CG	LYS	E	252	38.198	73.755	39.471	1.00	64.14	C
ATOM	3297	CD	LYS	E	252	38.736	73.163	38.161	1.00	64.92	C
ATOM	3298	CE	LYS	E	252	40.048	73.811	37.729	1.00	65.71	C
ATOM	3299	NZ	LYS	E	252	40.524	73.285	36.419	1.00	66.05	N
ATOM	3300	C	LYS	E	252	40.043	71.072	41.325	1.00	63.58	C
ATOM	3301	O	LYS	E	252	40.811	70.779	40.403	1.00	63.71	O
ATOM	3302	N	THR	E	253	40.293	70.790	42.602	1.00	63.80	N
ATOM	3303	CA	THR	E	253	41.612	70.360	43.073	1.00	64.01	C
ATOM	3304	CB	THR	E	253	41.910	70.894	44.516	1.00	64.14	C
ATOM	3305	OG1	THR	E	253	43.081	70.259	45.046	1.00	64.42	O
ATOM	3306	CG2	THR	E	253	40.725	70.658	45.466	1.00	64.05	C
ATOM	3307	C	THR	E	253	41.885	68.851	42.970	1.00	64.03	C
ATOM	3308	O	THR	E	253	42.978	68.450	42.556	1.00	64.17	O
ATOM	3309	N	TYR	E	254	40.897	68.031	43.343	1.00	63.74	N
ATOM	3310	CA	TYR	E	254	41.036	66.565	43.432	1.00	63.60	C
ATOM	3311	CB	TYR	E	254	41.329	65.929	42.064	1.00	63.88	C
ATOM	3312	CG	TYR	E	254	40.123	65.698	41.181	1.00	64.31	C
ATOM	3313	CD1	TYR	E	254	40.164	66.028	39.830	1.00	65.01	C
ATOM	3314	CE1	TYR	E	254	39.070	65.819	39.006	1.00	65.00	C
ATOM	3315	CZ	TYR	E	254	37.918	65.277	39.527	1.00	64.44	C
ATOM	3316	OH	TYR	E	254	36.847	65.079	38.696	1.00	64.39	O
ATOM	3317	CE2	TYR	E	254	37.841	64.941	40.868	1.00	64.98	C
ATOM	3318	CD2	TYR	E	254	38.945	65.150	41.689	1.00	64.85	C
ATOM	3319	C	TYR	E	254	42.084	66.082	44.441	1.00	63.09	C
ATOM	3320	O	TYR	E	254	42.196	64.882	44.697	1.00	63.29	O
ATOM	3321	N	ASN	E	255	42.844	67.014	45.009	1.00	62.31	N
ATOM	3322	CA	ASN	E	255	43.959	66.675	45.891	1.00	61.43	C
ATOM	3323	CB	ASN	E	255	45.004	67.803	45.894	1.00	61.43	C
ATOM	3324	CG	ASN	E	255	45.447	68.207	44.485	1.00	61.68	C
ATOM	3325	OD1	ASN	E	255	45.642	69.394	44.202	1.00	61.96	O
ATOM	3326	ND2	ASN	E	255	45.606	67.224	43.600	1.00	61.43	N
ATOM	3327	C	ASN	E	255	43.543	66.323	47.324	1.00	60.63	C
ATOM	3328	O	ASN	E	255	44.356	65.813	48.100	1.00	61.00	O
ATOM	3329	N	ASN	E	256	42.288	66.589	47.672	1.00	59.28	N
ATOM	3330	CA	ASN	E	256	41.797	66.324	49.024	1.00	58.17	C
ATOM	3331	CB	ASN	E	256	40.762	67.380	49.433	1.00	58.43	C
ATOM	3332	CG	ASN	E	256	41.395	68.635	50.019	1.00	59.33	C
ATOM	3333	OD1	ASN	E	256	41.052	69.048	51.132	1.00	60.07	O
ATOM	3334	ND2	ASN	E	256	42.317	69.250	49.275	1.00	59.61	N
ATOM	3335	C	ASN	E	256	41.215	64.916	49.197	1.00	57.01	C
ATOM	3336	O	ASN	E	256	40.103	64.756	49.707	1.00	56.94	O
ATOM	3337	N	LEU	E	257	41.969	63.902	48.764	1.00	55.53	N
ATOM	3338	CA	LEU	E	257	41.567	62.494	48.911	1.00	53.84	C
ATOM	3339	CB	LEU	E	257	41.893	61.693	47.651	1.00	53.83	C
ATOM	3340	CG	LEU	E	257	41.258	62.130	46.328	1.00	53.78	C
ATOM	3341	CD1	LEU	E	257	41.670	61.181	45.219	1.00	53.99	C
ATOM	3342	CD2	LEU	E	257	39.736	62.208	46.426	1.00	53.57	C
ATOM	3343	C	LEU	E	257	42.240	61.866	50.121	1.00	52.85	C
ATOM	3344	O	LEU	E	257	42.151	60.657	50.352	1.00	52.50	O
ATOM	3345	N	ASP	E	258	42.912	62.706	50.896	1.00	51.62	N
ATOM	3346	CA	ASP	E	258	43.593	62.264	52.096	1.00	50.68	C
ATOM	3347	CB	ASP	E	258	44.985	62.897	52.182	1.00	51.09	C
ATOM	3348	CG	ASP	E	258	45.879	62.488	51.017	1.00	52.05	C

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ATOM	3349	OD1	ASP	E	258	46.140	61.272	50.866	1.00	52.90	O
ATOM	3350	OD2	ASP	E	258	46.309	63.380	50.247	1.00	52.48	O
ATOM	3351	C	ASP	E	258	42.756	62.551	53.337	1.00	49.58	C
ATOM	3352	O	ASP	E	258	43.071	62.062	54.424	1.00	49.50	O
ATOM	3353	N	VAL	E	259	41.679	63.320	53.166	1.00	48.29	N
ATOM	3354	CA	VAL	E	259	40.723	63.563	54.252	1.00	47.27	C
ATOM	3355	CB	VAL	E	259	39.669	64.660	53.910	1.00	47.31	C
ATOM	3356	CG1	VAL	E	259	40.346	65.993	53.591	1.00	46.75	C
ATOM	3357	CG2	VAL	E	259	38.743	64.223	52.775	1.00	46.31	C
ATOM	3358	C	VAL	E	259	40.007	62.275	54.641	1.00	46.87	C
ATOM	3359	O	VAL	E	259	39.892	61.348	53.834	1.00	46.67	O
ATOM	3360	N	SER	E	260	39.537	62.219	55.884	1.00	46.29	N
ATOM	3361	CA	SER	E	260	38.771	61.078	56.364	1.00	45.84	C
ATOM	3362	CB	SER	E	260	38.590	61.139	57.884	1.00	45.92	C
ATOM	3363	OG	SER	E	260	37.667	62.147	58.259	1.00	45.49	O
ATOM	3364	C	SER	E	260	37.408	60.998	55.677	1.00	45.79	C
ATOM	3365	O	SER	E	260	36.884	61.996	55.163	1.00	45.54	O
ATOM	3366	N	VAL	E	261	36.849	59.797	55.665	1.00	45.57	N
ATOM	3367	CA	VAL	E	261	35.493	59.582	55.179	1.00	45.91	C
ATOM	3368	CB	VAL	E	261	35.128	58.080	55.211	1.00	45.55	C
ATOM	3369	CG1	VAL	E	261	33.634	57.883	55.332	1.00	46.30	C
ATOM	3370	CG2	VAL	E	261	35.648	57.404	53.962	1.00	45.32	C
ATOM	3371	C	VAL	E	261	34.473	60.446	55.944	1.00	45.93	C
ATOM	3372	O	VAL	E	261	33.542	60.989	55.347	1.00	45.83	O
ATOM	3373	N	THR	E	262	34.681	60.590	57.250	1.00	46.35	N
ATOM	3374	CA	THR	E	262	33.825	61.427	58.094	1.00	47.03	C
ATOM	3375	CB	THR	E	262	34.250	61.327	59.573	1.00	46.96	C
ATOM	3376	OG1	THR	E	262	34.134	59.965	59.994	1.00	47.94	O
ATOM	3377	CG2	THR	E	262	33.395	62.216	60.475	1.00	46.59	C
ATOM	3378	C	THR	E	262	33.845	62.882	57.621	1.00	47.44	C
ATOM	3379	O	THR	E	262	32.790	63.503	57.485	1.00	47.55	O
ATOM	3380	N	LYS	E	263	35.042	63.403	57.359	1.00	47.91	N
ATOM	3381	CA	LYS	E	263	35.214	64.753	56.832	1.00	48.59	C
ATOM	3382	CB	LYS	E	263	36.703	65.128	56.792	1.00	48.72	C
ATOM	3383	CG	LYS	E	263	36.976	66.618	56.668	1.00	49.97	C
ATOM	3384	CD	LYS	E	263	38.373	66.984	57.185	1.00	52.10	C
ATOM	3385	CE	LYS	E	263	38.815	68.353	56.673	1.00	52.97	C
ATOM	3386	NZ	LYS	E	263	40.253	68.661	56.954	1.00	53.98	N
ATOM	3387	C	LYS	E	263	34.574	64.906	55.450	1.00	48.76	C
ATOM	3388	O	LYS	E	263	33.945	65.927	55.162	1.00	48.54	O
ATOM	3389	N	ALA	E	264	34.735	63.890	54.608	1.00	49.40	N
ATOM	3390	CA	ALA	E	264	34.168	63.908	53.263	1.00	50.22	C
ATOM	3391	CB	ALA	E	264	34.591	62.665	52.493	1.00	50.02	C
ATOM	3392	C	ALA	E	264	32.645	64.018	53.301	1.00	50.90	C
ATOM	3393	O	ALA	E	264	32.032	64.574	52.390	1.00	50.76	O
ATOM	3394	N	LEU	E	265	32.044	63.488	54.361	1.00	51.84	N
ATOM	3395	CA	LEU	E	265	30.596	63.318	54.419	1.00	53.27	C
ATOM	3396	CB	LEU	E	265	30.236	62.067	55.225	1.00	52.70	C
ATOM	3397	CG	LEU	E	265	30.347	60.734	54.479	1.00	51.73	C
ATOM	3398	CD1	LEU	E	265	30.276	59.565	55.448	1.00	50.61	C
ATOM	3399	CD2	LEU	E	265	29.265	60.621	53.417	1.00	49.77	C
ATOM	3400	C	LEU	E	265	29.898	64.545	55.006	1.00	54.84	C
ATOM	3401	O	LEU	E	265	28.672	64.587	55.093	1.00	55.03	O
ATOM	3402	N	GLN	E	266	30.685	65.538	55.408	1.00	56.55	N
ATOM	3403	CA	GLN	E	266	30.148	66.856	55.731	1.00	58.61	C
ATOM	3404	CB	GLN	E	266	31.256	67.774	56.250	1.00	58.41	C
ATOM	3405	CG	GLN	E	266	31.857	67.339	57.576	1.00	59.10	C
ATOM	3406	CD	GLN	E	266	32.943	68.283	58.064	1.00	60.05	C
ATOM	3407	OE1	GLN	E	266	33.624	68.004	59.051	1.00	60.70	O
ATOM	3408	NE2	GLN	E	266	33.108	69.407	57.373	1.00	60.41	N
ATOM	3409	C	GLN	E	266	29.478	67.481	54.513	1.00	59.79	C
ATOM	3410	O	GLN	E	266	28.503	68.222	54.638	1.00	59.75	O
ATOM	3411	N	HIS	E	267	30.008	67.172	53.334	1.00	61.72	N
ATOM	3412	CA	HIS	E	267	29.429	67.635	52.078	1.00	63.56	C
ATOM	3413	CB	HIS	E	267	30.407	67.414	50.922	1.00	63.70	C
ATOM	3414	CG	HIS	E	267	31.284	68.595	50.639	1.00	64.68	C
ATOM	3415	ND1	HIS	E	267	32.317	68.971	51.471	1.00	65.54	N

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ATOM	3416	CE1	HIS	E	267	32.912	70.040	50.973	1.00	66.07	C
ATOM	3417	NE2	HIS	E	267	32.303	70.371	49.849	1.00	66.04	N
ATOM	3418	CD2	HIS	E	267	31.281	69.483	49.617	1.00	65.37	C
ATOM	3419	C	HIS	E	267	28.103	66.941	51.779	1.00	64.58	C
ATOM	3420	O	HIS	E	267	27.374	67.347	50.873	1.00	64.82	O
ATOM	3421	N	ARG	E	268	27.800	65.894	52.544	1.00	65.67	N
ATOM	3422	CA	ARG	E	268	26.509	65.219	52.445	1.00	66.52	C
ATOM	3423	CB	ARG	E	268	26.489	63.951	53.306	1.00	66.39	C
ATOM	3424	CG	ARG	E	268	25.094	63.403	53.574	1.00	66.11	C
ATOM	3425	CD	ARG	E	268	25.090	61.884	53.638	1.00	65.24	C
ATOM	3426	NE	ARG	E	268	25.737	61.388	54.849	1.00	63.48	N
ATOM	3427	CZ	ARG	E	268	26.022	60.111	55.075	1.00	62.12	C
ATOM	3428	NH1	ARG	E	268	25.720	59.189	54.172	1.00	61.43	N
ATOM	3429	NH2	ARG	E	268	26.612	59.755	56.206	1.00	62.23	N
ATOM	3430	C	ARG	E	268	25.372	66.152	52.845	1.00	67.31	C
ATOM	3431	O	ARG	E	268	24.737	65.969	53.886	1.00	67.69	O
ATOM	3432	N	SER	E	269	25.127	67.158	52.009	1.00	68.13	N
ATOM	3433	CA	SER	E	269	23.848	67.858	52.002	1.00	68.87	C
ATOM	3434	CB	SER	E	269	23.699	68.695	50.728	1.00	68.92	C
ATOM	3435	OG	SER	E	269	22.424	69.313	50.670	1.00	68.88	O
ATOM	3436	C	SER	E	269	22.684	66.881	52.126	1.00	69.30	C
ATOM	3437	O	SER	E	269	22.295	66.231	51.154	1.00	69.54	O
ATOM	3438	N	HIS	E	270	22.156	66.765	53.340	1.00	69.59	N
ATOM	3439	CA	HIS	E	270	20.739	67.007	53.594	1.00	69.90	C
ATOM	3440	CB	HIS	E	270	19.893	65.796	53.185	1.00	70.22	C
ATOM	3441	CG	HIS	E	270	19.379	65.865	51.780	1.00	71.57	C
ATOM	3442	ND1	HIS	E	270	19.039	67.059	51.169	1.00	72.87	N
ATOM	3443	CE1	HIS	E	270	18.621	66.815	49.940	1.00	73.14	C
ATOM	3444	NE2	HIS	E	270	18.677	65.506	49.731	1.00	73.30	N
ATOM	3445	CD2	HIS	E	270	19.148	64.890	50.867	1.00	72.57	C
ATOM	3446	C	HIS	E	270	20.527	67.332	55.067	1.00	69.53	C
ATOM	3447	O	HIS	E	270	20.958	68.380	55.553	1.00	69.60	O
ATOM	3448	N	TYR	E	271	19.860	66.427	55.773	1.00	69.11	N
ATOM	3449	CA	TYR	E	271	20.296	66.030	57.103	1.00	68.46	C
ATOM	3450	CB	TYR	E	271	19.428	66.682	58.182	1.00	68.87	C
ATOM	3451	CG	TYR	E	271	20.090	66.746	59.542	1.00	69.58	C
ATOM	3452	CD1	TYR	E	271	21.115	67.651	59.797	1.00	69.84	C
ATOM	3453	CE1	TYR	E	271	21.726	67.710	61.038	1.00	70.09	C
ATOM	3454	CZ	TYR	E	271	21.313	66.857	62.043	1.00	70.22	C
ATOM	3455	OH	TYR	E	271	21.916	66.912	63.279	1.00	70.25	O
ATOM	3456	CE2	TYR	E	271	20.299	65.949	61.815	1.00	70.38	C
ATOM	3457	CD2	TYR	E	271	19.694	65.898	60.570	1.00	70.27	C
ATOM	3458	C	TYR	E	271	20.269	64.513	57.235	1.00	67.61	C
ATOM	3459	O	TYR	E	271	19.914	63.801	56.294	1.00	67.71	O
ATOM	3460	N	PHE	E	272	20.654	64.024	58.407	1.00	66.36	N
ATOM	3461	CA	PHE	E	272	20.487	62.619	58.745	1.00	64.82	C
ATOM	3462	CB	PHE	E	272	21.657	62.150	59.614	1.00	65.15	C
ATOM	3463	CG	PHE	E	272	22.549	61.141	58.942	1.00	65.57	C
ATOM	3464	CD1	PHE	E	272	23.535	60.482	59.661	1.00	65.47	C
ATOM	3465	CE1	PHE	E	272	24.355	59.550	59.052	1.00	65.72	C
ATOM	3466	CZ	PHE	E	272	24.193	59.263	57.709	1.00	65.68	C
ATOM	3467	CE2	PHE	E	272	23.214	59.912	56.978	1.00	65.82	C
ATOM	3468	CD2	PHE	E	272	22.397	60.843	57.596	1.00	65.89	C
ATOM	3469	C	PHE	E	272	19.166	62.378	59.472	1.00	63.59	C
ATOM	3470	O	PHE	E	272	18.432	63.317	59.789	1.00	63.81	O
ATOM	3471	N	GLU	E	273	18.863	61.107	59.712	1.00	61.73	N
ATOM	3472	CA	GLU	E	273	18.941	60.555	61.058	1.00	59.84	C
ATOM	3473	CB	GLU	E	273	17.691	59.737	61.388	1.00	60.35	C
ATOM	3474	CG	GLU	E	273	16.575	60.544	62.038	1.00	61.04	C
ATOM	3475	CD	GLU	E	273	16.718	60.633	63.548	1.00	62.73	C
ATOM	3476	OE1	GLU	E	273	16.555	59.594	64.226	1.00	63.15	O
ATOM	3477	OE2	GLU	E	273	16.990	61.741	64.058	1.00	62.77	O
ATOM	3478	C	GLU	E	273	20.192	59.691	61.159	1.00	58.00	C
ATOM	3479	O	GLU	E	273	21.179	59.939	60.470	1.00	57.86	O
ATOM	3480	N	GLY	E	274	20.147	58.673	62.009	1.00	55.66	N
ATOM	3481	CA	GLY	E	274	21.132	57.606	61.944	1.00	52.27	C
ATOM	3482	C	GLY	E	274	21.325	57.078	60.533	1.00	49.82	C

Figure 1 Table 1a - 53

ATOM	3483	O	GLY	E	274	20.706	57.558	59.582	1.00 49.29	O
ATOM	3484	N	VAL	E	275	22.188	56.081	60.398	1.00 47.64	N
ATOM	3485	CA	VAL	E	275	22.150	55.203	59.240	1.00 45.38	C
ATOM	3486	CB	VAL	E	275	23.435	54.356	59.123	1.00 45.58	C
ATOM	3487	CG1	VAL	E	275	24.427	54.738	60.210	1.00 44.30	C
ATOM	3488	CG2	VAL	E	275	23.109	52.872	59.183	1.00 45.69	C
ATOM	3489	C	VAL	E	275	20.925	54.295	59.298	1.00 44.16	C
ATOM	3490	O	VAL	E	275	20.484	53.898	60.379	1.00 43.67	O
ATOM	3491	N	LEU	E	276	20.375	53.978	58.130	1.00 42.17	N
ATOM	3492	CA	LEU	E	276	19.144	53.202	58.046	1.00 40.92	C
ATOM	3493	CB	LEU	E	276	18.394	53.525	56.752	1.00 40.74	C
ATOM	3494	CG	LEU	E	276	17.749	54.911	56.686	1.00 42.67	C
ATOM	3495	CD1	LEU	E	276	17.566	55.353	55.244	1.00 43.60	C
ATOM	3496	CD2	LEU	E	276	16.420	54.924	57.430	1.00 44.42	C
ATOM	3497	C	LEU	E	276	19.432	51.710	58.135	1.00 39.84	C
ATOM	3498	O	LEU	E	276	20.101	51.143	57.269	1.00 39.05	O
ATOM	3499	N	LYS	E	277	18.922	51.078	59.188	1.00 38.87	N
ATOM	3500	CA	LYS	E	277	19.321	49.725	59.537	1.00 38.23	C
ATOM	3501	CB	LYS	E	277	19.950	49.717	60.927	1.00 38.14	C
ATOM	3502	CG	LYS	E	277	21.286	50.435	61.030	1.00 39.64	C
ATOM	3503	CD	LYS	E	277	21.630	50.755	62.482	1.00 41.08	C
ATOM	3504	CE	LYS	E	277	20.690	51.824	63.059	1.00 41.74	C
ATOM	3505	NZ	LYS	E	277	21.182	52.334	64.362	1.00 43.07	N
ATOM	3506	C	LYS	E	277	18.131	48.778	59.553	1.00 38.11	C
ATOM	3507	O	LYS	E	277	16.972	49.204	59.399	1.00 37.92	O
ATOM	3508	N	CYS	E	278	18.436	47.494	59.745	1.00 36.81	N
ATOM	3509	CA	CYS	E	278	17.435	46.489	60.001	1.00 36.59	C
ATOM	3510	CB	CYS	E	278	16.847	45.952	58.692	1.00 35.92	C
ATOM	3511	SG	CYS	E	278	17.977	44.992	57.729	1.00 38.44	S
ATOM	3512	C	CYS	E	278	18.020	45.342	60.830	1.00 35.93	C
ATOM	3513	O	CYS	E	278	19.234	45.214	60.978	1.00 35.72	O
ATOM	3514	N	TYR	E	279	17.137	44.512	61.362	1.00 35.85	N
ATOM	3515	CA	TYR	E	279	17.551	43.293	62.020	1.00 35.55	C
ATOM	3516	CB	TYR	E	279	16.796	43.118	63.329	1.00 36.00	C
ATOM	3517	CG	TYR	E	279	16.847	44.336	64.221	1.00 36.42	C
ATOM	3518	CD1	TYR	E	279	15.732	45.165	64.357	1.00 36.47	C
ATOM	3519	CE1	TYR	E	279	15.758	46.273	65.192	1.00 37.43	C
ATOM	3520	CZ	TYR	E	279	16.911	46.569	65.890	1.00 37.98	C
ATOM	3521	OH	TYR	E	279	16.925	47.669	66.713	1.00 39.97	O
ATOM	3522	CE2	TYR	E	279	18.037	45.773	65.769	1.00 37.84	C
ATOM	3523	CD2	TYR	E	279	18.000	44.661	64.926	1.00 37.30	C
ATOM	3524	C	TYR	E	279	17.306	42.108	61.102	1.00 35.32	C
ATOM	3525	O	TYR	E	279	16.447	42.165	60.219	1.00 34.78	O
ATOM	3526	N	LEU	E	280	18.077	41.048	61.329	1.00 35.34	N
ATOM	3527	CA	LEU	E	280	17.988	39.777	60.597	1.00 35.97	C
ATOM	3528	CB	LEU	E	280	18.954	38.759	61.221	1.00 36.58	C
ATOM	3529	CG	LEU	E	280	20.356	38.547	60.646	1.00 38.90	C
ATOM	3530	CD1	LEU	E	280	21.055	37.529	61.527	1.00 40.92	C
ATOM	3531	CD2	LEU	E	280	20.259	38.027	59.231	1.00 40.69	C
ATOM	3532	C	LEU	E	280	16.607	39.163	60.664	1.00 35.40	C
ATOM	3533	O	LEU	E	280	16.219	38.387	59.790	1.00 35.70	O
ATOM	3534	N	HIS	E	281	15.873	39.493	61.721	1.00 34.35	N
ATOM	3535	CA	HIS	E	281	14.626	38.815	61.991	1.00 33.85	C
ATOM	3536	CB	HIS	E	281	14.558	38.421	63.464	1.00 33.79	C
ATOM	3537	CG	HIS	E	281	15.693	37.547	63.885	1.00 34.70	C
ATOM	3538	ND1	HIS	E	281	15.812	36.239	63.467	1.00 35.23	N
ATOM	3539	CE1	HIS	E	281	16.916	35.720	63.973	1.00 35.02	C
ATOM	3540	NE2	HIS	E	281	17.514	36.644	64.706	1.00 35.50	N
ATOM	3541	CD2	HIS	E	281	16.773	37.799	64.660	1.00 34.02	C
ATOM	3542	C	HIS	E	281	13.403	39.615	61.573	1.00 33.50	C
ATOM	3543	O	HIS	E	281	12.285	39.232	61.886	1.00 33.12	O
ATOM	3544	N	GLU	E	282	13.613	40.719	60.868	1.00 33.41	N
ATOM	3545	CA	GLU	E	282	12.479	41.468	60.315	1.00 33.90	C
ATOM	3546	CB	GLU	E	282	12.868	42.921	60.029	1.00 33.39	C
ATOM	3547	CG	GLU	E	282	13.411	43.631	61.248	1.00 34.08	C
ATOM	3548	CD	GLU	E	282	13.368	45.142	61.108	1.00 35.66	C
ATOM	3549	OE1	GLU	E	282	12.271	45.726	61.201	1.00 34.34	O

Figure 1 Table 1a - 54

ATOM	3550	OE2	GLU	E	282	14.443	45.734	60.938	1.00	36.60	O
ATOM	3551	C	GLU	E	282	11.951	40.772	59.056	1.00	34.10	C
ATOM	3552	O	GLU	E	282	12.704	40.082	58.360	1.00	34.27	O
ATOM	3553	N	THR	E	283	10.658	40.944	58.781	1.00	34.02	N
ATOM	3554	CA	THR	E	283	10.021	40.338	57.609	1.00	34.46	C
ATOM	3555	CB	THR	E	283	8.487	40.414	57.697	1.00	34.41	C
ATOM	3556	OG1	THR	E	283	8.084	41.783	57.753	1.00	35.51	O
ATOM	3557	CG2	THR	E	283	7.970	39.677	58.951	1.00	33.83	C
ATOM	3558	C	THR	E	283	10.475	41.025	56.322	1.00	34.96	C
ATOM	3559	O	THR	E	283	10.912	42.186	56.345	1.00	34.37	O
ATOM	3560	N	LEU	E	284	10.372	40.305	55.206	1.00	34.90	N
ATOM	3561	CA	LEU	E	284	10.695	40.868	53.912	1.00	35.88	C
ATOM	3562	CB	LEU	E	284	10.465	39.831	52.805	1.00	36.28	C
ATOM	3563	CG	LEU	E	284	11.431	39.759	51.605	1.00	39.01	C
ATOM	3564	CD1	LEU	E	284	10.764	39.127	50.342	1.00	39.08	C
ATOM	3565	CD2	LEU	E	284	12.169	41.066	51.276	1.00	34.80	C
ATOM	3566	C	LEU	E	284	9.818	42.093	53.660	1.00	35.07	C
ATOM	3567	O	LEU	E	284	10.300	43.110	53.145	1.00	35.19	O
ATOM	3568	N	GLU	E	285	8.537	41.988	54.015	1.00	34.65	N
ATOM	3569	CA	GLU	E	285	7.601	43.114	53.890	1.00	35.52	C
ATOM	3570	CB	GLU	E	285	6.203	42.718	54.397	1.00	35.52	C
ATOM	3571	CG	GLU	E	285	5.152	43.813	54.206	1.00	36.68	C
ATOM	3572	CD	GLU	E	285	3.739	43.336	54.454	1.00	38.38	C
ATOM	3573	OE1	GLU	E	285	3.550	42.336	55.177	1.00	41.70	O
ATOM	3574	OE2	GLU	E	285	2.800	43.956	53.916	1.00	42.44	O
ATOM	3575	C	GLU	E	285	8.088	44.378	54.603	1.00	34.76	C
ATOM	3576	O	GLU	E	285	8.141	45.453	54.003	1.00	35.22	O
ATOM	3577	N	ALA	E	286	8.460	44.240	55.872	1.00	34.62	N
ATOM	3578	CA	ALA	E	286	8.952	45.367	56.661	1.00	34.01	C
ATOM	3579	CB	ALA	E	286	9.290	44.923	58.081	1.00	33.92	C
ATOM	3580	C	ALA	E	286	10.176	46.010	55.992	1.00	33.93	C
ATOM	3581	O	ALA	E	286	10.281	47.238	55.914	1.00	33.36	O
ATOM	3582	N	ILE	E	287	11.076	45.166	55.495	1.00	33.20	N
ATOM	3583	CA	ILE	E	287	12.302	45.629	54.856	1.00	34.05	C
ATOM	3584	CB	ILE	E	287	13.354	44.495	54.730	1.00	34.07	C
ATOM	3585	CG1	ILE	E	287	14.038	44.274	56.084	1.00	35.95	C
ATOM	3586	CD1	ILE	E	287	13.727	42.986	56.666	1.00	41.26	C
ATOM	3587	CG2	ILE	E	287	14.419	44.839	53.734	1.00	33.97	C
ATOM	3588	C	ILE	E	287	12.040	46.316	53.511	1.00	33.60	C
ATOM	3589	O	ILE	E	287	12.603	47.362	53.246	1.00	33.59	O
ATOM	3590	N	ILE	E	288	11.200	45.716	52.672	1.00	33.46	N
ATOM	3591	CA	ILE	E	288	10.798	46.363	51.428	1.00	33.26	C
ATOM	3592	CB	ILE	E	288	9.822	45.500	50.586	1.00	32.82	C
ATOM	3593	CG1	ILE	E	288	10.549	44.292	49.962	1.00	34.87	C
ATOM	3594	CD1	ILE	E	288	9.601	43.182	49.429	1.00	32.95	C
ATOM	3595	CG2	ILE	E	288	9.143	46.376	49.498	1.00	34.31	C
ATOM	3596	C	ILE	E	288	10.170	47.735	51.740	1.00	32.96	C
ATOM	3597	O	ILE	E	288	10.531	48.749	51.121	1.00	33.11	O
ATOM	3598	N	ASN	E	289	9.244	47.773	52.698	1.00	32.76	N
ATOM	3599	CA	ASN	E	289	8.587	49.038	53.047	1.00	33.25	C
ATOM	3600	CB	ASN	E	289	7.477	48.858	54.106	1.00	33.36	C
ATOM	3601	CG	ASN	E	289	6.312	48.033	53.595	1.00	34.13	C
ATOM	3602	OD1	ASN	E	289	6.213	47.758	52.408	1.00	36.54	O
ATOM	3603	ND2	ASN	E	289	5.426	47.630	54.492	1.00	36.50	N
ATOM	3604	C	ASN	E	289	9.585	50.099	53.482	1.00	33.14	C
ATOM	3605	O	ASN	E	289	9.510	51.244	53.013	1.00	33.72	O
ATOM	3606	N	ARG	E	290	10.525	49.720	54.349	1.00	33.01	N
ATOM	3607	CA	ARG	E	290	11.531	50.671	54.862	1.00	34.17	C
ATOM	3608	CB	ARG	E	290	12.421	50.021	55.943	1.00	33.77	C
ATOM	3609	CG	ARG	E	290	13.381	51.001	56.647	1.00	35.82	C
ATOM	3610	CD	ARG	E	290	14.006	50.393	57.936	1.00	35.52	C
ATOM	3611	NE	ARG	E	290	12.975	49.770	58.764	1.00	34.64	N
ATOM	3612	CZ	ARG	E	290	13.136	48.632	59.436	1.00	35.47	C
ATOM	3613	NH1	ARG	E	290	14.301	47.989	59.417	1.00	34.75	N
ATOM	3614	NH2	ARG	E	290	12.120	48.131	60.126	1.00	35.08	N
ATOM	3615	C	ARG	E	290	12.399	51.217	53.727	1.00	33.79	C
ATOM	3616	O	ARG	E	290	12.645	52.408	53.642	1.00	33.33	O

Figure 1

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ATOM	3617	N	LEU	E	291	12.846	50.318	52.856	1.00	33.64	N
ATOM	3618	CA	LEU	E	291	13.703	50.672	51.726	1.00	33.81	C
ATOM	3619	CB	LEU	E	291	14.089	49.365	51.043	1.00	34.19	C
ATOM	3620	CG	LEU	E	291	15.514	48.869	50.855	1.00	36.49	C
ATOM	3621	CD1	LEU	E	291	16.623	49.648	51.557	1.00	37.66	C
ATOM	3622	CD2	LEU	E	291	15.523	47.424	51.215	1.00	35.99	C
ATOM	3623	C	LEU	E	291	13.020	51.616	50.721	1.00	33.04	C
ATOM	3624	O	LEU	E	291	13.631	52.575	50.234	1.00	32.76	O
ATOM	3625	N	VAL	E	292	11.758	51.342	50.403	1.00	32.85	N
ATOM	3626	CA	VAL	E	292	11.000	52.163	49.453	1.00	32.58	C
ATOM	3627	CB	VAL	E	292	9.676	51.477	48.999	1.00	32.53	C
ATOM	3628	CG1	VAL	E	292	8.775	52.439	48.213	1.00	30.96	C
ATOM	3629	CG2	VAL	E	292	9.960	50.230	48.165	1.00	31.38	C
ATOM	3630	C	VAL	E	292	10.729	53.570	50.020	1.00	33.34	C
ATOM	3631	O	VAL	E	292	10.889	54.555	49.311	1.00	33.00	O
ATOM	3632	N	GLU	E	293	10.337	53.659	51.290	1.00	34.82	N
ATOM	3633	CA	GLU	E	293	10.108	54.964	51.933	1.00	36.53	C
ATOM	3634	CB	GLU	E	293	9.560	54.818	53.349	1.00	37.83	C
ATOM	3635	CG	GLU	E	293	8.290	54.012	53.442	1.00	43.71	C
ATOM	3636	CD	GLU	E	293	7.521	54.271	54.721	1.00	51.26	C
ATOM	3637	OE1	GLU	E	293	7.676	55.379	55.294	1.00	54.27	O
ATOM	3638	OE2	GLU	E	293	6.757	53.365	55.146	1.00	54.11	O
ATOM	3639	C	GLU	E	293	11.392	55.763	51.994	1.00	36.37	C
ATOM	3640	O	GLU	E	293	11.396	56.935	51.658	1.00	36.00	O
ATOM	3641	N	ALA	E	294	12.488	55.116	52.391	1.00	36.06	N
ATOM	3642	CA	ALA	E	294	13.770	55.818	52.535	1.00	36.26	C
ATOM	3643	CB	ALA	E	294	14.716	55.010	53.399	1.00	36.37	C
ATOM	3644	C	ALA	E	294	14.468	56.224	51.219	1.00	36.28	C
ATOM	3645	O	ALA	E	294	15.312	57.123	51.228	1.00	35.46	O
ATOM	3646	N	GLU	E	295	14.129	55.544	50.115	1.00	36.18	N
ATOM	3647	CA	GLU	E	295	14.717	55.800	48.785	1.00	36.62	C
ATOM	3648	CB	GLU	E	295	14.314	57.183	48.249	1.00	36.96	C
ATOM	3649	CG	GLU	E	295	12.820	57.428	48.287	1.00	39.09	C
ATOM	3650	CD	GLU	E	295	12.432	58.699	47.567	1.00	44.21	C
ATOM	3651	OE1	GLU	E	295	11.923	59.628	48.231	1.00	45.60	O
ATOM	3652	OE2	GLU	E	295	12.663	58.777	46.341	1.00	46.58	O
ATOM	3653	C	GLU	E	295	16.234	55.597	48.778	1.00	36.19	C
ATOM	3654	O	GLU	E	295	17.005	56.352	48.205	1.00	37.14	O
ATOM	3655	N	VAL	E	296	16.637	54.519	49.407	1.00	36.11	N
ATOM	3656	CA	VAL	E	296	18.019	54.231	49.685	1.00	35.71	C
ATOM	3657	CB	VAL	E	296	18.188	54.389	51.253	1.00	36.66	C
ATOM	3658	CG1	VAL	E	296	18.502	53.113	51.976	1.00	36.20	C
ATOM	3659	CG2	VAL	E	296	19.055	55.573	51.632	1.00	36.01	C
ATOM	3660	C	VAL	E	296	18.250	52.841	49.059	1.00	34.68	C
ATOM	3661	O	VAL	E	296	17.297	52.065	48.922	1.00	33.19	O
ATOM	3662	N	HIS	E	297	19.485	52.550	48.636	1.00	34.30	N
ATOM	3663	CA	HIS	E	297	19.794	51.303	47.905	1.00	33.39	C
ATOM	3664	CB	HIS	E	297	20.948	51.550	46.905	1.00	33.97	C
ATOM	3665	CG	HIS	E	297	21.309	50.358	46.062	1.00	34.84	C
ATOM	3666	ND1	HIS	E	297	20.628	50.018	44.909	1.00	34.33	N
ATOM	3667	CE1	HIS	E	297	21.161	48.930	44.386	1.00	34.93	C
ATOM	3668	NE2	HIS	E	297	22.176	48.558	45.147	1.00	36.12	N
ATOM	3669	CD2	HIS	E	297	22.297	49.439	46.196	1.00	35.54	C
ATOM	3670	C	HIS	E	297	20.041	50.071	48.811	1.00	32.98	C
ATOM	3671	O	HIS	E	297	19.880	48.932	48.369	1.00	32.78	O
ATOM	3672	N	ARG	E	298	20.431	50.294	50.063	1.00	32.80	N
ATOM	3673	CA	ARG	E	298	20.591	49.196	51.043	1.00	32.33	C
ATOM	3674	CB	ARG	E	298	21.992	48.539	50.970	1.00	32.72	C
ATOM	3675	CG	ARG	E	298	23.081	49.114	51.927	1.00	32.19	C
ATOM	3676	CD	ARG	E	298	23.473	50.569	51.586	1.00	33.33	C
ATOM	3677	NE	ARG	E	298	23.903	50.711	50.188	1.00	33.40	N
ATOM	3678	CZ	ARG	E	298	23.707	51.798	49.442	1.00	32.59	C
ATOM	3679	NH1	ARG	E	298	23.066	52.847	49.939	1.00	31.90	N
ATOM	3680	NH2	ARG	E	298	24.146	51.834	48.195	1.00	31.64	N
ATOM	3681	C	ARG	E	298	20.310	49.641	52.478	1.00	32.86	C
ATOM	3682	O	ARG	E	298	20.339	50.852	52.791	1.00	32.50	O
ATOM	3683	N	LEU	E	299	20.042	48.646	53.330	1.00	33.13	N

Figure 1 Table 1a - 56

ATOM	3684	CA	LEU	E	299	20.020	48.809	54.776	1.00 33.32	C
ATOM	3685	CB	LEU	E	299	18.719	48.242	55.375	1.00 33.34	C
ATOM	3686	CG	LEU	E	299	17.386	48.774	54.838	1.00 33.78	C
ATOM	3687	CD1	LEU	E	299	16.199	48.022	55.477	1.00 34.30	C
ATOM	3688	CD2	LEU	E	299	17.242	50.292	55.041	1.00 34.74	C
ATOM	3689	C	LEU	E	299	21.204	48.048	55.342	1.00 33.61	C
ATOM	3690	O	LEU	E	299	21.633	47.042	54.771	1.00 33.00	O
ATOM	3691	N	VAL	E	300	21.754	48.536	56.447	1.00 33.27	N
ATOM	3692	CA	VAL	E	300	22.805	47.792	57.128	1.00 34.17	C
ATOM	3693	CB	VAL	E	300	23.809	48.724	57.864	1.00 33.86	C
ATOM	3694	CG1	VAL	E	300	24.907	47.897	58.523	1.00 34.00	C
ATOM	3695	CG2	VAL	E	300	24.404	49.762	56.901	1.00 33.86	C
ATOM	3696	C	VAL	E	300	22.131	46.877	58.144	1.00 34.34	C
ATOM	3697	O	VAL	E	300	21.364	47.344	58.981	1.00 34.93	O
ATOM	3698	N	VAL	E	301	22.425	45.584	58.060	1.00 34.91	N
ATOM	3699	CA	VAL	E	301	21.927	44.588	59.012	1.00 35.05	C
ATOM	3700	CB	VAL	E	301	21.877	43.165	58.417	1.00 34.89	C
ATOM	3701	CG1	VAL	E	301	21.091	42.216	59.328	1.00 34.39	C
ATOM	3702	CG2	VAL	E	301	21.263	43.190	57.020	1.00 34.04	C
ATOM	3703	C	VAL	E	301	22.823	44.600	60.238	1.00 36.19	C
ATOM	3704	O	VAL	E	301	24.058	44.483	60.162	1.00 35.76	O
ATOM	3705	N	VAL	E	302	22.165	44.719	61.380	1.00 37.01	N
ATOM	3706	CA	VAL	E	302	22.811	45.048	62.619	1.00 38.13	C
ATOM	3707	CB	VAL	E	302	22.573	46.569	62.857	1.00 38.28	C
ATOM	3708	CG1	VAL	E	302	21.993	46.891	64.200	1.00 38.83	C
ATOM	3709	CG2	VAL	E	302	23.823	47.390	62.497	1.00 37.54	C
ATOM	3710	C	VAL	E	302	22.233	44.116	63.691	1.00 39.04	C
ATOM	3711	O	VAL	E	302	21.108	43.634	63.559	1.00 38.95	O
ATOM	3712	N	ASP	E	303	23.011	43.823	64.725	1.00 40.25	N
ATOM	3713	CA	ASP	E	303	22.461	43.109	65.864	1.00 41.58	C
ATOM	3714	CB	ASP	E	303	23.512	42.202	66.529	1.00 41.52	C
ATOM	3715	CG	ASP	E	303	24.591	42.979	67.302	1.00 41.60	C
ATOM	3716	OD1	ASP	E	303	24.591	44.227	67.346	1.00 41.06	O
ATOM	3717	OD2	ASP	E	303	25.457	42.303	67.880	1.00 42.68	O
ATOM	3718	C	ASP	E	303	21.834	44.090	66.860	1.00 42.64	C
ATOM	3719	O	ASP	E	303	21.739	45.297	66.586	1.00 42.45	O
ATOM	3720	N	GLU	E	304	21.423	43.553	68.004	1.00 43.60	N
ATOM	3721	CA	GLU	E	304	20.850	44.315	69.111	1.00 45.27	C
ATOM	3722	CB	GLU	E	304	20.712	43.401	70.341	1.00 45.32	C
ATOM	3723	CG	GLU	E	304	19.553	42.409	70.293	1.00 48.69	C
ATOM	3724	CD	GLU	E	304	19.827	41.119	69.500	1.00 52.28	C
ATOM	3725	OE1	GLU	E	304	20.708	41.103	68.601	1.00 52.77	O
ATOM	3726	OE2	GLU	E	304	19.120	40.114	69.772	1.00 52.67	O
ATOM	3727	C	GLU	E	304	21.675	45.545	69.509	1.00 45.23	C
ATOM	3728	O	GLU	E	304	21.123	46.529	70.012	1.00 45.75	O
ATOM	3729	N	HIS	E	305	22.990	45.474	69.297	1.00 45.05	N
ATOM	3730	CA	HIS	E	305	23.919	46.492	69.796	1.00 44.70	C
ATOM	3731	CB	HIS	E	305	25.057	45.818	70.563	1.00 45.01	C
ATOM	3732	CG	HIS	E	305	24.589	44.918	71.668	1.00 46.16	C
ATOM	3733	ND1	HIS	E	305	24.028	45.399	72.832	1.00 46.88	N
ATOM	3734	CE1	HIS	E	305	23.712	44.382	73.616	1.00 48.07	C
ATOM	3735	NE2	HIS	E	305	24.046	43.261	73.002	1.00 47.70	N
ATOM	3736	CD2	HIS	E	305	24.597	43.569	71.781	1.00 47.18	C
ATOM	3737	C	HIS	E	305	24.489	47.424	68.714	1.00 44.25	C
ATOM	3738	O	HIS	E	305	25.427	48.182	68.977	1.00 43.86	O
ATOM	3739	N	ASP	E	306	23.920	47.362	67.514	1.00 43.49	N
ATOM	3740	CA	ASP	E	306	24.342	48.229	66.414	1.00 43.28	C
ATOM	3741	CB	ASP	E	306	24.524	49.670	66.896	1.00 43.74	C
ATOM	3742	CG	ASP	E	306	23.282	50.514	66.693	1.00 45.86	C
ATOM	3743	OD1	ASP	E	306	22.237	49.957	66.290	1.00 47.38	O
ATOM	3744	OD2	ASP	E	306	23.352	51.739	66.940	1.00 48.89	O
ATOM	3745	C	ASP	E	306	25.629	47.729	65.763	1.00 42.21	C
ATOM	3746	O	ASP	E	306	26.213	48.412	64.920	1.00 41.88	O
ATOM	3747	N	VAL	E	307	26.066	46.537	66.159	1.00 41.15	N
ATOM	3748	CA	VAL	E	307	27.151	45.853	65.464	1.00 40.53	C
ATOM	3749	CB	VAL	E	307	27.751	44.723	66.324	1.00 40.49	C
ATOM	3750	CG1	VAL	E	307	28.792	43.942	65.530	1.00 40.09	C

Figure 1 Table 1a - 57

ATOM	3751	CG2	VAL	E	307	28.359	45.291	67.600	1.00	41.05	C
ATOM	3752	C	VAL	E	307	26.667	45.279	64.134	1.00	39.81	C
ATOM	3753	O	VAL	E	307	25.683	44.542	64.088	1.00	39.07	O
ATOM	3754	N	VAL	E	308	27.363	45.626	63.056	1.00	39.40	N
ATOM	3755	CA	VAL	E	308	26.915	45.273	61.712	1.00	39.21	C
ATOM	3756	CB	VAL	E	308	27.606	46.134	60.630	1.00	39.68	C
ATOM	3757	CG1	VAL	E	308	28.762	46.916	61.225	1.00	40.51	C
ATOM	3758	CG2	VAL	E	308	28.072	45.270	59.470	1.00	38.76	C
ATOM	3759	C	VAL	E	308	27.134	43.793	61.414	1.00	38.89	C
ATOM	3760	O	VAL	E	308	28.236	43.267	61.581	1.00	38.37	O
ATOM	3761	N	LYS	E	309	26.072	43.126	60.973	1.00	38.83	N
ATOM	3762	CA	LYS	E	309	26.115	41.692	60.711	1.00	38.26	C
ATOM	3763	CB	LYS	E	309	24.923	40.994	61.369	1.00	38.90	C
ATOM	3764	CG	LYS	E	309	24.739	41.323	62.844	1.00	40.46	C
ATOM	3765	CD	LYS	E	309	25.411	40.288	63.734	1.00	45.54	C
ATOM	3766	CE	LYS	E	309	26.839	40.684	64.067	1.00	46.35	C
ATOM	3767	NZ	LYS	E	309	27.229	40.231	65.431	1.00	47.07	N
ATOM	3768	C	LYS	E	309	26.119	41.407	59.214	1.00	37.86	C
ATOM	3769	O	LYS	E	309	26.553	40.342	58.778	1.00	38.68	O
ATOM	3770	N	GLY	E	310	25.631	42.364	58.431	1.00	36.65	N
ATOM	3771	CA	GLY	E	310	25.542	42.200	56.994	1.00	35.50	C
ATOM	3772	C	GLY	E	310	24.906	43.377	56.294	1.00	35.22	C
ATOM	3773	O	GLY	E	310	24.754	44.465	56.870	1.00	34.50	O
ATOM	3774	N	ILE	E	311	24.552	43.158	55.035	1.00	34.94	N
ATOM	3775	CA	ILE	E	311	23.860	44.165	54.233	1.00	34.82	C
ATOM	3776	CB	ILE	E	311	24.823	44.877	53.213	1.00	35.61	C
ATOM	3777	CG1	ILE	E	311	25.464	46.103	53.871	1.00	36.82	C
ATOM	3778	CD1	ILE	E	311	26.873	45.919	54.148	1.00	41.28	C
ATOM	3779	CG2	ILE	E	311	24.065	45.394	51.962	1.00	34.24	C
ATOM	3780	C	ILE	E	311	22.677	43.547	53.505	1.00	34.47	C
ATOM	3781	O	ILE	E	311	22.763	42.416	53.016	1.00	33.94	O
ATOM	3782	N	VAL	E	312	21.583	44.301	53.421	1.00	33.60	N
ATOM	3783	CA	VAL	E	312	20.489	43.914	52.535	1.00	33.73	C
ATOM	3784	CB	VAL	E	312	19.172	43.472	53.285	1.00	34.32	C
ATOM	3785	CG1	VAL	E	312	18.608	44.617	54.137	1.00	33.55	C
ATOM	3786	CG2	VAL	E	312	18.112	42.962	52.276	1.00	34.48	C
ATOM	3787	C	VAL	E	312	20.254	45.023	51.513	1.00	33.43	C
ATOM	3788	O	VAL	E	312	19.777	46.124	51.834	1.00	33.12	O
ATOM	3789	N	SER	E	313	20.617	44.702	50.277	1.00	32.54	N
ATOM	3790	CA	SER	E	313	20.597	45.637	49.172	1.00	32.91	C
ATOM	3791	CB	SER	E	313	21.857	45.415	48.343	1.00	32.21	C
ATOM	3792	OG	SER	E	313	21.811	46.186	47.171	1.00	35.68	O
ATOM	3793	C	SER	E	313	19.373	45.408	48.296	1.00	32.63	C
ATOM	3794	O	SER	E	313	18.780	44.328	48.327	1.00	31.55	O
ATOM	3795	N	LEU	E	314	19.026	46.418	47.490	1.00	32.49	N
ATOM	3796	CA	LEU	E	314	17.983	46.274	46.467	1.00	33.04	C
ATOM	3797	CB	LEU	E	314	17.742	47.596	45.713	1.00	32.55	C
ATOM	3798	CG	LEU	E	314	17.197	48.788	46.494	1.00	33.49	C
ATOM	3799	CD1	LEU	E	314	16.996	49.993	45.540	1.00	29.84	C
ATOM	3800	CD2	LEU	E	314	15.903	48.431	47.181	1.00	33.17	C
ATOM	3801	C	LEU	E	314	18.323	45.191	45.454	1.00	33.13	C
ATOM	3802	O	LEU	E	314	17.420	44.551	44.891	1.00	32.93	O
ATOM	3803	N	SER	E	315	19.620	45.014	45.206	1.00	32.98	N
ATOM	3804	CA	SER	E	315	20.112	43.906	44.402	1.00	33.76	C
ATOM	3805	CB	SER	E	315	21.640	43.977	44.300	1.00	33.74	C
ATOM	3806	OG	SER	E	315	22.036	45.187	43.661	1.00	33.76	O
ATOM	3807	C	SER	E	315	19.685	42.551	45.003	1.00	34.35	C
ATOM	3808	O	SER	E	315	19.268	41.640	44.273	1.00	34.45	O
ATOM	3809	N	ASP	E	316	19.780	42.431	46.324	1.00	34.21	N
ATOM	3810	CA	ASP	E	316	19.400	41.193	47.013	1.00	35.09	C
ATOM	3811	CB	ASP	E	316	19.804	41.243	48.482	1.00	35.00	C
ATOM	3812	CG	ASP	E	316	21.295	41.313	48.670	1.00	35.05	C
ATOM	3813	OD1	ASP	E	316	21.994	40.459	48.089	1.00	37.64	O
ATOM	3814	OD2	ASP	E	316	21.766	42.209	49.404	1.00	32.77	O
ATOM	3815	C	ASP	E	316	17.901	40.962	46.903	1.00	35.24	C
ATOM	3816	O	ASP	E	316	17.458	39.868	46.567	1.00	35.12	O
ATOM	3817	N	ILE	E	317	17.131	42.012	47.186	1.00	35.42	N

Figure 1 Table 1a - 58

ATOM	3818	CA	ILE	E	317	15.679	41.932	47.180	1.00 35.59	C
ATOM	3819	CB	ILE	E	317	15.053	43.229	47.759	1.00 36.26	C
ATOM	3820	CG1	ILE	E	317	15.287	43.245	49.278	1.00 38.12	C
ATOM	3821	CD1	ILE	E	317	15.280	44.612	49.838	1.00 43.23	C
ATOM	3822	CG2	ILE	E	317	13.553	43.310	47.470	1.00 34.52	C
ATOM	3823	C	ILE	E	317	15.105	41.563	45.812	1.00 35.38	C
ATOM	3824	O	ILE	E	317	14.270	40.658	45.709	1.00 35.05	O
ATOM	3825	N	LEU	E	318	15.557	42.260	44.774	1.00 34.93	N
ATOM	3826	CA	LEU	E	318	15.078	42.022	43.420	1.00 35.41	C
ATOM	3827	CB	LEU	E	318	15.537	43.134	42.476	1.00 35.10	C
ATOM	3828	CG	LEU	E	318	14.504	44.203	42.098	1.00 36.06	C
ATOM	3829	CD1	LEU	E	318	13.516	44.557	43.207	1.00 36.05	C
ATOM	3830	CD2	LEU	E	318	15.184	45.460	41.507	1.00 35.48	C
ATOM	3831	C	LEU	E	318	15.504	40.651	42.893	1.00 35.71	C
ATOM	3832	O	LEU	E	318	14.744	39.995	42.177	1.00 35.08	O
ATOM	3833	N	GLN	E	319	16.704	40.216	43.258	1.00 36.30	N
ATOM	3834	CA	GLN	E	319	17.110	38.863	42.925	1.00 38.20	C
ATOM	3835	CB	GLN	E	319	18.552	38.593	43.336	1.00 38.63	C
ATOM	3836	CG	GLN	E	319	19.053	37.220	42.865	1.00 42.83	C
ATOM	3837	CD	GLN	E	319	20.535	37.044	43.099	1.00 48.34	C
ATOM	3838	OE1	GLN	E	319	21.019	37.211	44.224	1.00 51.10	O
ATOM	3839	NE2	GLN	E	319	21.272	36.711	42.037	1.00 50.19	N
ATOM	3840	C	GLN	E	319	16.154	37.842	43.559	1.00 38.32	C
ATOM	3841	O	GLN	E	319	15.756	36.882	42.915	1.00 38.70	O
ATOM	3842	N	ALA	E	320	15.763	38.074	44.803	1.00 39.02	N
ATOM	3843	CA	ALA	E	320	14.817	37.181	45.492	1.00 40.01	C
ATOM	3844	CB	ALA	E	320	14.737	37.532	46.964	1.00 39.78	C
ATOM	3845	C	ALA	E	320	13.418	37.212	44.855	1.00 40.55	C
ATOM	3846	O	ALA	E	320	12.827	36.160	44.609	1.00 40.28	O
ATOM	3847	N	LEU	E	321	12.921	38.413	44.548	1.00 41.08	N
ATOM	3848	CA	LEU	E	321	11.576	38.579	43.998	1.00 41.78	C
ATOM	3849	CB	LEU	E	321	11.170	40.054	43.976	1.00 41.16	C
ATOM	3850	CG	LEU	E	321	10.937	40.745	45.325	1.00 40.13	C
ATOM	3851	CD1	LEU	E	321	10.436	42.148	45.090	1.00 38.00	C
ATOM	3852	CD2	LEU	E	321	9.962	39.963	46.239	1.00 38.21	C
ATOM	3853	C	LEU	E	321	11.433	37.961	42.609	1.00 43.34	C
ATOM	3854	O	LEU	E	321	10.330	37.616	42.183	1.00 43.27	O
ATOM	3855	N	VAL	E	322	12.555	37.806	41.924	1.00 45.41	N
ATOM	3856	CA	VAL	E	322	12.564	37.319	40.562	1.00 47.85	C
ATOM	3857	CB	VAL	E	322	13.667	38.045	39.735	1.00 47.78	C
ATOM	3858	CG1	VAL	E	322	14.901	37.176	39.532	1.00 46.91	C
ATOM	3859	CG2	VAL	E	322	13.109	38.554	38.413	1.00 47.32	C
ATOM	3860	C	VAL	E	322	12.678	35.786	40.510	1.00 49.87	C
ATOM	3861	O	VAL	E	322	12.305	35.171	39.516	1.00 49.99	O
ATOM	3862	N	LEU	E	323	13.180	35.191	41.591	1.00 52.41	N
ATOM	3863	CA	LEU	E	323	13.326	33.732	41.731	1.00 55.31	C
ATOM	3864	CB	LEU	E	323	14.696	33.398	42.331	1.00 55.17	C
ATOM	3865	CG	LEU	E	323	15.921	33.767	41.493	1.00 56.24	C
ATOM	3866	CD1	LEU	E	323	17.186	33.780	42.333	1.00 56.89	C
ATOM	3867	CD2	LEU	E	323	16.060	32.836	40.299	1.00 56.90	C
ATOM	3868	C	LEU	E	323	12.243	33.177	42.651	1.00 56.93	C
ATOM	3869	O	LEU	E	323	12.164	31.976	42.892	1.00 57.59	O
ATOM	3870	N	THR	E	324	11.369	34.080	43.082	1.00 59.08	N
ATOM	3871	CA	THR	E	324	10.597	33.992	44.301	1.00 60.99	C
ATOM	3872	CB	THR	E	324	9.156	33.443	44.201	1.00 61.12	C
ATOM	3873	OG1	THR	E	324	9.002	32.283	45.045	1.00 62.05	O
ATOM	3874	CG2	THR	E	324	8.803	33.073	42.749	1.00 61.43	C
ATOM	3875	C	THR	E	324	11.280	34.153	45.659	1.00 62.08	C
ATOM	3876	O	THR	E	324	12.400	33.645	45.857	1.00 62.18	O
ATOM	3877	N	GLY	E	325	10.636	34.882	46.573	1.00 63.19	N
ATOM	3878	CA	GLY	E	325	11.210	35.167	47.894	1.00 64.27	C
ATOM	3879	C	GLY	E	325	11.966	33.981	48.457	1.00 64.97	C
ATOM	3880	O	GLY	E	325	11.393	32.899	48.620	1.00 65.30	O
ATOM	3881	N	GLY	E	326	13.260	34.179	48.720	1.00 65.54	N
ATOM	3882	CA	GLY	E	326	14.136	33.116	49.230	1.00 66.00	C
ATOM	3883	C	GLY	E	326	15.496	33.059	48.547	1.00 66.47	C
ATOM	3884	O	GLY	E	326	15.837	33.920	47.724	1.00 66.71	O

Figure 1 Table 1a - 59

ATOM	3885	O3P	AMP	P	1	21.936	55.865	46.260	1.00	37.78	O
ATOM	3886	P	AMP	P	1	22.521	55.272	47.529	1.00	38.95	P
ATOM	3887	O1P	AMP	P	1	23.794	54.491	47.419	1.00	37.12	O
ATOM	3888	O2P	AMP	P	1	21.474	54.621	48.398	1.00	39.70	O
ATOM	3889	O5*	AMP	P	1	22.970	56.607	48.349	1.00	37.81	O
ATOM	3890	C5*	AMP	P	1	22.132	57.764	48.354	1.00	36.43	C
ATOM	3891	C4*	AMP	P	1	22.392	58.669	49.560	1.00	36.77	C
ATOM	3892	C3*	AMP	P	1	23.872	58.796	49.896	1.00	37.48	C
ATOM	3893	O3*	AMP	P	1	24.105	60.118	50.401	1.00	37.43	O
ATOM	3894	C2*	AMP	P	1	24.073	57.791	51.015	1.00	36.59	C
ATOM	3895	O2*	AMP	P	1	25.139	58.159	51.895	1.00	37.03	O
ATOM	3896	C1*	AMP	P	1	22.718	57.755	51.715	1.00	34.68	C
ATOM	3897	O4*	AMP	P	1	21.750	58.130	50.728	1.00	36.50	O
ATOM	3898	N9	AMP	P	1	22.447	56.385	52.219	1.00	34.71	N
ATOM	3899	C4	AMP	P	1	22.116	56.097	53.485	1.00	33.44	C
ATOM	3900	C5	AMP	P	1	21.953	54.631	53.532	1.00	33.48	C
ATOM	3901	N7	AMP	P	1	22.185	54.171	52.281	1.00	33.61	N
ATOM	3902	C8	AMP	P	1	22.477	55.245	51.503	1.00	32.98	C
ATOM	3903	N3	AMP	P	1	21.947	56.836	54.612	1.00	32.14	N
ATOM	3904	C2	AMP	P	1	21.622	56.240	55.772	1.00	33.25	C
ATOM	3905	N1	AMP	P	1	21.450	54.909	55.873	1.00	33.81	N
ATOM	3906	C6	AMP	P	1	21.591	54.046	54.835	1.00	33.56	C
ATOM	3907	N6	AMP	P	1	21.416	52.696	54.990	1.00	32.36	N
ATOM	3908	O3P	AMP	P	2	28.101	50.171	39.315	1.00	43.90	O
ATOM	3909	P	AMP	P	2	27.383	50.322	37.997	1.00	37.35	P
ATOM	3910	O1P	AMP	P	2	26.922	51.715	37.758	1.00	40.95	O
ATOM	3911	O2P	AMP	P	2	26.387	49.243	37.731	1.00	41.98	O
ATOM	3912	O5*	AMP	P	2	28.447	50.039	36.834	1.00	39.90	O
ATOM	3913	C5*	AMP	P	2	29.365	48.945	36.836	1.00	36.71	C
ATOM	3914	C4*	AMP	P	2	30.203	48.990	35.549	1.00	35.16	C
ATOM	3915	C3*	AMP	P	2	30.718	50.379	35.189	1.00	33.88	C
ATOM	3916	O3*	AMP	P	2	32.031	50.258	34.623	1.00	33.48	O
ATOM	3917	C2*	AMP	P	2	29.730	50.879	34.142	1.00	32.35	C
ATOM	3918	O2*	AMP	P	2	30.316	51.785	33.198	1.00	32.58	O
ATOM	3919	C1*	AMP	P	2	29.241	49.609	33.457	1.00	31.37	C
ATOM	3920	O4*	AMP	P	2	29.403	48.574	34.428	1.00	34.55	O
ATOM	3921	N9	AMP	P	2	27.797	49.663	33.096	1.00	31.42	N
ATOM	3922	C4	AMP	P	2	27.267	49.180	31.977	1.00	30.14	C
ATOM	3923	C5	AMP	P	2	25.822	49.448	32.067	1.00	30.00	C
ATOM	3924	N7	AMP	P	2	25.609	50.064	33.246	1.00	30.83	N
ATOM	3925	C8	AMP	P	2	26.806	50.185	33.854	1.00	29.76	C
ATOM	3926	N3	AMP	P	2	27.767	48.560	30.878	1.00	29.73	N
ATOM	3927	C2	AMP	P	2	26.956	48.187	29.880	1.00	30.23	C
ATOM	3928	N1	AMP	P	2	25.628	48.400	29.903	1.00	30.46	N
ATOM	3929	C6	AMP	P	2	24.995	49.006	30.929	1.00	29.30	C
ATOM	3930	N6	AMP	P	2	23.657	49.208	30.897	1.00	28.98	N
ATOM	3931	O3P	AMP	P	3	24.136	46.419	44.492	1.00	36.39	O
ATOM	3932	P	AMP	P	3	24.960	46.455	45.761	1.00	34.94	P
ATOM	3933	O1P	AMP	P	3	24.354	47.232	46.916	1.00	33.02	O
ATOM	3934	O2P	AMP	P	3	26.422	46.741	45.566	1.00	33.68	O
ATOM	3935	O5*	AMP	P	3	24.966	44.935	46.280	1.00	34.27	O
ATOM	3936	C5*	AMP	P	3	25.475	43.853	45.477	1.00	32.44	C
ATOM	3937	C4*	AMP	P	3	25.759	42.656	46.382	1.00	32.81	C
ATOM	3938	C3*	AMP	P	3	24.584	42.332	47.277	1.00	32.11	C
ATOM	3939	O3*	AMP	P	3	24.596	40.932	47.491	1.00	30.17	O
ATOM	3940	C2*	AMP	P	3	24.885	43.037	48.594	1.00	30.80	C
ATOM	3941	O2*	AMP	P	3	24.298	42.336	49.686	1.00	29.17	O
ATOM	3942	C1*	AMP	P	3	26.393	42.971	48.630	1.00	31.54	C
ATOM	3943	O4*	AMP	P	3	26.831	42.990	47.274	1.00	32.64	O
ATOM	3944	N9	AMP	P	3	26.997	44.127	49.308	1.00	31.90	N
ATOM	3945	C4	AMP	P	3	28.039	44.044	50.115	1.00	32.54	C
ATOM	3946	C5	AMP	P	3	28.297	45.428	50.549	1.00	32.63	C
ATOM	3947	N7	AMP	P	3	27.398	46.217	49.936	1.00	33.96	N
ATOM	3948	C8	AMP	P	3	26.622	45.419	49.185	1.00	32.90	C
ATOM	3949	N3	AMP	P	3	28.813	43.025	50.579	1.00	32.39	N
ATOM	3950	C2	AMP	P	3	29.820	43.310	51.432	1.00	33.02	C
ATOM	3951	N1	AMP	P	3	30.110	44.562	51.860	1.00	31.07	N

Figure 1 Table 1a - 60

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ATOM   3952  C6  AMP P   3      29.420  45.647  51.471  1.00 32.46      C
ATOM   3953  N6  AMP P   3      29.718  46.896  51.902  1.00 32.04      N
ATOM   3954  O   HOH W   1      13.183  71.127  22.913  1.00 27.90      O
ATOM   3955  O   HOH W   2      16.323  76.265  18.124  1.00 30.90      O
ATOM   3956  O   HOH W   3      15.106  64.081  23.854  1.00 31.50      O
ATOM   3957  O   HOH W   4       9.196  42.400  60.660  1.00 30.23      O
ATOM   3958  O   HOH W   5      16.946  58.514  33.507  1.00 33.74      O
ATOM   3959  O   HOH W   6      10.509  60.563  30.565  1.00 34.48      O
ATOM   3960  O   HOH W   7      55.767  63.401  35.489  1.00 21.77      O
ATOM   3961  O   HOH W   8      21.529  60.843  32.444  1.00 34.73      O
ATOM   3962  O   HOH W   9      14.891  52.196  47.877  1.00 33.22      O
ATOM   3963  O   HOH W  10      36.461  67.617  25.870  1.00 41.70      O
ATOM   3964  O   HOH W  11      18.964  59.197  22.606  1.00 29.20      O
ATOM   3965  O   HOH W  12      10.173  44.599  61.943  1.00 31.44      O
ATOM   3966  O   HOH W  13      -1.345  41.231  45.744  1.00 40.15      O
ATOM   3967  O   HOH W  14      20.250  50.373  40.413  1.00 30.22      O
ATOM   3968  O   HOH W  15      18.592  37.598  47.029  1.00 32.48      O
ATOM   3969  O   HOH W  16       6.194  51.313  24.726  1.00 46.73      O
ATOM   3970  O   HOH W  17      19.217  51.591  42.603  1.00 36.01      O
ATOM   3971  O   HOH W  18       8.831  48.940  57.454  1.00 35.53      O
ATOM   3972  O   HOH W  19      15.763  60.014  31.535  1.00 37.69      O
ATOM   3973  O   HOH W  20      28.420  64.136  18.754  1.00 36.87      O
ATOM   3974  O   HOH W  21      15.160  54.569  37.300  1.00 36.89      O
ATOM   3975  O   HOH W  22       9.705  83.211   7.685  1.00 35.79      O
ATOM   3976  O   HOH W  23       7.934  66.756  13.956  1.00 54.44      O
ATOM   3977  O   HOH W  24       8.497  36.556  44.055  1.00 39.42      O
ATOM   3978  O   HOH W  25      19.352  59.743  10.199  1.00 41.25      O
ATOM   3979  O   HOH W  26      15.990  65.354  13.107  1.00 44.02      O
ATOM   3980  O   HOH W  27      32.617  59.965  19.802  1.00 45.82      O
ATOM   3981  O   HOH W  28      20.014  41.245  63.596  1.00 35.34      O
ATOM   3982  O   HOH W  29      12.729  51.850  46.089  1.00 33.10      O
ATOM   3983  O   HOH W  30      25.755  48.601  49.677  1.00 40.66      O
ATOM   3984  O   HOH W  31      16.343  71.895  26.936  1.00 46.67      O
ATOM   3985  O   HOH W  32      33.469  49.328  42.274  1.00 36.48      O
ATOM   3986  O   HOH W  33      12.183  54.448  46.849  1.00 36.76      O
ATOM   3987  O   HOH W  34       8.682  64.897  20.010  1.00 39.26      O
ATOM   3988  O   HOH W  35      22.934  52.946  19.356  1.00 45.91      O
ATOM   3989  O   HOH W  36      23.422  44.496  40.060  1.00 42.60      O
ATOM   3990  O   HOH W  37      17.576  63.034  13.364  1.00 39.93      O
ATOM   3991  O   HOH W  38      28.369  51.579  13.345  1.00 51.05      O
ATOM   3992  O   HOH W  39      13.736  71.204  25.633  1.00 38.04      O
ATOM   3993  O   HOH W  40      11.452  66.202  29.895  1.00 36.00      O
ATOM   3994  O   HOH W  41      25.656  78.122  22.745  1.00 36.17      O
ATOM   3995  O   HOH W  42      33.070  61.969  49.136  1.00 52.24      O
ATOM   3996  O   HOH W  43      12.109  64.522  15.966  1.00 50.65      O
ATOM   3997  O   HOH W  44      12.690  75.584  12.908  1.00 39.71      O
ATOM   3998  O   HOH W  45      12.257  54.278  55.706  1.00 48.30      O
ATOM   3999  O   HOH W  46      24.806  61.949  13.005  1.00 43.43      O
ATOM   4000  O   HOH W  47      33.684  37.412  56.947  1.00 56.10      O
ATOM   4001  O   HOH W  48       9.360  48.764  60.037  1.00 42.52      O
ATOM   4002  O   HOH W  49       5.814  45.291  50.819  1.00 43.71      O
ATOM   4003  O   HOH W  50      46.936  59.264  35.520  1.00 53.24      O
ATOM   4004  O   HOH W  51      10.611  60.085  25.563  1.00 44.59      O
ATOM   4005  O   HOH W  52      14.810  61.632  22.596  1.00 30.67      O
ATOM   4006  O   HOH W  53      29.921  51.015  29.538  1.00 44.48      O
ATOM   4007  O   HOH W  54      23.004  55.889  63.022  1.00 53.70      O
ATOM   4008  O   HOH W  55      14.066  61.948  18.157  1.00 40.20      O
ATOM   4009  O   HOH W  56      14.059  68.436   1.781  1.00 52.79      O
ATOM   4010  O   HOH W  57      17.039  60.586  24.025  1.00 29.49      O
ATOM   4011  O   HOH W  58      -1.840  41.136  43.248  1.00 42.01      O
ATOM   4012  O   HOH W  59      47.466  61.113  38.242  1.00 53.03      O
ATOM   4013  O   HOH W  60      26.760  75.035  23.792  1.00 50.79      O
ATOM   4014  O   HOH W  61      20.314  53.425  19.700  1.00 46.16      O
ATOM   4015  O   HOH W  62       5.532  58.180  20.057  1.00 44.92      O
ATOM   4016  O   HOH W  63       7.838  80.702   8.619  1.00 36.92      O
ATOM   4017  O   HOH W  64       5.705  78.677   1.308  1.00 40.03      O
ATOM   4018  O   HOH W  65      21.150  43.087  40.659  1.00 48.29      O
```

Figure 1 Table 1a - 61

ATOM	4019	O	HOH	W	66	15.130	63.050	35.119	1.00	36.48	O
ATOM	4020	O	HOH	W	67	17.193	52.404	60.927	1.00	43.96	O
ATOM	4021	O	HOH	W	68	43.765	66.802	37.316	1.00	68.41	O
ATOM	4022	O	HOH	W	69	13.844	34.848	62.045	1.00	37.10	O
ATOM	4023	O	HOH	W	70	26.424	88.721	15.360	1.00	43.99	O
ATOM	4024	O	HOH	W	71	19.818	82.090	21.317	1.00	40.21	O
ATOM	4025	O	HOH	W	72	40.349	64.340	57.887	1.00	56.81	O
ATOM	4026	O	HOH	W	73	4.902	76.491	22.030	1.00	68.01	O
ATOM	4027	O	HOH	W	74	21.986	35.425	52.389	1.00	45.81	O
ATOM	4028	O	HOH	W	75	12.340	60.484	22.970	1.00	35.58	O
ATOM	4029	O	HOH	W	76	20.613	37.806	48.830	1.00	37.89	O
ATOM	4030	O	HOH	W	77	2.053	46.597	50.038	1.00	41.86	O
ATOM	4031	O	HOH	W	78	13.023	58.606	37.742	1.00	40.43	O
ATOM	4032	O	HOH	W	79	16.031	72.825	-3.233	1.00	38.34	O
ATOM	4033	O	HOH	W	80	4.041	40.321	56.688	1.00	58.09	O
ATOM	4034	O	HOH	W	81	35.916	54.519	63.816	1.00	66.10	O
ATOM	4035	O	HOH	W	82	28.859	74.708	27.420	1.00	49.11	O
ATOM	4036	O	HOH	W	83	26.445	75.744	20.917	1.00	47.05	O
ATOM	4037	O	HOH	W	84	32.949	64.740	49.449	1.00	55.46	O
ATOM	4038	O	HOH	W	85	17.457	56.850	36.317	1.00	37.84	O
ATOM	4039	O	HOH	W	86	32.504	53.517	30.155	1.00	42.53	O
ATOM	4040	O	HOH	W	87	28.530	48.898	42.970	1.00	42.95	O
ATOM	4041	O	HOH	W	88	-0.648	95.394	-20.551	1.00	44.97	O
ATOM	4042	O	HOH	W	89	2.979	46.312	47.492	1.00	43.57	O
ATOM	4043	O	HOH	W	90	31.233	69.671	32.615	1.00	42.41	O
ATOM	4044	O	HOH	W	91	9.313	56.644	48.410	1.00	48.04	O
ATOM	4045	O	HOH	W	92	7.015	51.781	51.723	1.00	44.93	O
ATOM	4046	O	HOH	W	93	23.855	53.922	63.600	1.00	53.55	O
ATOM	4047	O	HOH	W	94	2.919	46.409	53.659	1.00	38.89	O
ATOM	4048	O	HOH	W	95	2.392	80.795	25.822	1.00	65.12	O
ATOM	4049	O	HOH	W	96	27.817	46.408	43.471	1.00	35.82	O
ATOM	4050	O	HOH	W	97	40.352	46.585	49.144	1.00	53.62	O
ATOM	4051	O	HOH	W	98	42.106	50.587	49.995	1.00	45.82	O
ATOM	4052	O	HOH	W	99	2.632	55.132	32.113	1.00	38.79	O
ATOM	4053	O	HOH	W	100	20.787	59.347	37.268	1.00	42.66	O
ATOM	4054	O	HOH	W	101	35.331	54.763	68.142	1.00	74.06	O
ATOM	4055	O	HOH	W	102	3.133	60.056	31.154	1.00	43.32	O
ATOM	4056	O	HOH	W	103	29.069	70.782	33.550	1.00	48.16	O
ATOM	4057	O	HOH	W	104	24.350	39.878	44.893	1.00	51.35	O
ATOM	4058	O	HOH	W	105	13.626	63.030	10.670	1.00	44.97	O
ATOM	4059	O	HOH	W	106	29.692	40.881	48.756	1.00	42.29	O
ATOM	4060	O	HOH	W	107	20.544	93.678	9.726	1.00	47.45	O
ATOM	4061	O	HOH	W	108	12.567	56.169	44.979	1.00	41.04	O
ATOM	4062	O	HOH	W	109	9.781	58.532	43.102	1.00	46.77	O
ATOM	4063	O	HOH	W	110	-3.726	46.864	49.137	1.00	46.34	O
ATOM	4064	O	HOH	W	111	3.896	71.496	2.720	1.00	55.31	O
ATOM	4065	O	HOH	W	112	27.070	50.780	41.864	1.00	41.93	O
ATOM	4066	O	HOH	W	113	20.217	69.766	34.066	1.00	56.17	O
ATOM	4067	O	HOH	W	114	8.577	90.198	1.216	1.00	80.77	O
ATOM	4068	O	HOH	W	115	24.568	78.262	32.333	1.00	48.03	O
ATOM	4069	O	HOH	W	116	19.224	60.248	33.580	1.00	37.81	O
ATOM	4070	O	HOH	W	117	24.342	79.222	29.159	1.00	52.27	O
ATOM	4071	O	HOH	W	118	11.372	60.005	15.129	1.00	58.13	O
ATOM	4072	O	HOH	W	119	1.659	47.255	30.335	1.00	54.75	O
ATOM	4073	O	HOH	W	120	29.645	48.429	23.130	1.00	59.93	O
ATOM	4074	O	HOH	W	121	2.443	49.530	28.274	1.00	50.14	O
ATOM	4075	O	HOH	W	122	48.152	49.106	36.680	1.00	55.44	O
ATOM	4076	O	HOH	W	123	5.589	45.044	47.882	1.00	39.69	O
ATOM	4077	O	HOH	W	124	19.032	43.668	28.448	1.00	40.77	O
ATOM	4078	O	HOH	W	125	2.206	53.462	34.734	1.00	48.34	O
ATOM	4079	O	HOH	W	126	33.302	45.466	24.110	1.00	65.17	O
ATOM	4080	O	HOH	W	127	0.273	40.257	40.165	1.00	52.83	O
ATOM	4081	O	HOH	W	128	19.924	54.235	42.360	1.00	56.18	O
ATOM	4082	O	HOH	W	129	44.746	63.436	47.087	1.00	60.27	O
ATOM	4083	O	HOH	W	130	1.952	38.002	33.773	1.00	46.78	O
ATOM	4084	O	HOH	W	131	48.344	61.140	44.833	1.00	40.95	O
ATOM	4085	O	HOH	W	132	20.294	56.740	36.608	1.00	50.82	O

Figure 1 Table 1a - 62

ATOM	4086	O	HOH W 133	6.027	65.955	34.570	1.00	50.82	O
ATOM	4087	O	HOH W 134	32.195	40.808	57.516	1.00	54.12	O
ATOM	4088	O	HOH W 135	0.317	97.050	-29.586	1.00	68.72	O
ATOM	4089	O	HOH W 136	18.531	51.887	15.475	1.00	60.86	O
ATOM	4090	O	HOH W 137	29.963	82.445	7.350	1.00	45.60	O
ATOM	4091	O	HOH W 138	21.569	40.982	28.424	1.00	67.53	O
ATOM	4092	O	HOH W 139	-0.793	33.610	51.317	1.00	73.74	O
ATOM	4093	O	HOH W 140	31.463	41.217	41.012	1.00	77.54	O
ATOM	4094	O	HOH W 141	14.602	44.479	24.718	1.00	41.19	O
ATOM	4095	O	HOH W 142	11.197	59.264	28.209	1.00	42.60	O
ATOM	4096	O	HOH W 143	11.188	56.743	41.698	1.00	56.20	O
ATOM	4097	O	HOH W 144	1.787	29.101	47.559	1.00	72.34	O
ATOM	4098	O	HOH W 145	25.118	43.601	41.378	1.00	44.33	O
ATOM	4099	O	HOH W 146	12.481	61.011	9.201	1.00	72.55	O
ATOM	4100	O	HOH W 147	20.211	56.416	12.302	1.00	54.60	O
ATOM	4101	O	HOH W 148	22.679	33.754	54.506	1.00	69.85	O
ATOM	4102	O	HOH W 149	22.190	39.339	64.372	1.00	70.86	O
ATOM	4103	O	HOH W 150	2.939	41.535	48.363	1.00	48.73	O
ATOM	4104	O	HOH W 151	16.095	46.067	23.138	1.00	82.52	O
ATOM	4105	O	HOH W 152	10.663	46.102	21.241	1.00	47.05	O
ATOM	4106	O	HOH W 153	-2.850	61.716	29.155	1.00	58.07	O
ATOM	4107	O	HOH W 154	29.411	48.128	40.370	1.00	42.11	O
ATOM	4108	O	HOH W 155	41.055	51.729	39.306	1.00	46.66	O
ATOM	4109	O	HOH W 156	39.402	49.956	56.316	1.00	61.15	O
ATOM	4110	O	HOH W 157	10.869	51.668	59.130	1.00	48.89	O
ATOM	4111	O	HOH W 158	34.622	54.153	23.432	1.00	46.77	O
ATOM	4112	O	HOH W 159	-3.186	36.748	51.333	1.00	45.79	O
ATOM	4113	O	HOH W 160	22.636	63.612	2.611	1.00	53.30	O
ATOM	4114	O	HOH W 161	4.861	50.411	20.818	1.00	44.80	O
ATOM	4115	O	HOH W 162	18.158	65.826	38.378	1.00	75.95	O
ATOM	4116	O	HOH W 163	30.024	39.611	59.288	1.00	56.45	O
ATOM	4117	O	HOH W 164	15.411	58.618	45.171	1.00	66.13	O
ATOM	4118	O	HOH W 165	7.558	75.836	16.341	1.00	77.99	O
ATOM	4119	O	HOH W 166	25.156	63.400	4.976	1.00	61.67	O
ATOM	4120	O	HOH W 167	8.923	77.701	11.409	1.00	53.25	O
ATOM	4121	O	HOH W 168	19.883	93.893	7.021	1.00	55.27	O
ATOM	4122	O	HOH W 169	29.409	45.030	33.197	1.00	64.22	O
ATOM	4123	O	HOH W 170	5.757	80.583	29.226	1.00	71.30	O
ATOM	4124	O	HOH W 171	29.807	42.286	44.237	1.00	63.51	O
ATOM	4125	O	HOH W 172	18.672	50.946	18.870	1.00	58.23	O
ATOM	4126	O	HOH W 173	20.915	51.174	12.328	1.00	62.01	O
ATOM	4127	O	HOH W 174	36.345	70.038	57.826	1.00	76.85	O
ATOM	4128	O	HOH W 175	33.495	52.659	20.741	1.00	55.60	O
ATOM	4129	O	HOH W 176	54.517	62.487	43.164	1.00	44.92	O
ATOM	4130	O	HOH W 177	25.376	65.213	42.219	1.00	62.69	O
ATOM	4131	O	HOH W 178	26.320	94.953	15.874	1.00	57.91	O
ATOM	4132	O	HOH W 179	14.883	49.568	67.120	1.00	56.30	O
ATOM	4133	O	HOH W 180	17.765	56.299	13.648	1.00	69.61	O
ATOM	4134	O	HOH W 181	27.107	63.336	49.722	1.00	54.64	O
ATOM	4135	O	HOH W 182	32.657	63.746	17.952	1.00	52.46	O
ATOM	4136	O	HOH W 183	-2.261	49.407	44.391	1.00	55.29	O
ATOM	4137	O	HOH W 184	35.652	77.708	24.544	1.00	65.70	O
ATOM	4138	O	HOH W 185	26.225	35.941	52.925	1.00	43.81	O
ATOM	4139	O	HOH W 186	18.476	69.810	-2.326	1.00	46.88	O
ATOM	4140	O	HOH W 187	21.386	34.417	56.720	1.00	59.39	O
ATOM	4141	O	HOH W 188	16.660	49.424	63.177	1.00	67.01	O
ATOM	4142	O	HOH W 189	29.416	73.399	15.816	1.00	52.36	O
ATOM	4143	O	HOH W 190	36.663	46.227	54.862	1.00	61.06	O
ATOM	4144	O	HOH W 191	1.063	41.178	46.874	1.00	55.90	O
ATOM	4145	O	HOH W 192	41.794	54.822	60.226	1.00	63.73	O
ATOM	4146	O	HOH W 193	14.631	41.810	26.543	1.00	59.10	O
ATOM	4147	O	HOH W 194	30.423	63.396	58.744	1.00	63.21	O
ATOM	4148	O	HOH W 195	16.661	48.526	22.797	1.00	64.38	O
ATOM	4149	O	HOH W 196	11.273	36.669	63.175	1.00	50.47	O
ATOM	4150	O	HOH W 197	8.268	91.836	7.272	1.00	64.37	O
ATOM	4151	O	HOH W 198	16.725	39.765	30.472	1.00	48.45	O
ATOM	4152	O	HOH W 199	8.797	38.385	30.587	1.00	45.74	O

Figure 1 Table 1a - 63

ATOM	4153	O	HOH W 200	55.118	59.568	46.066	1.00	52.67	O
ATOM	4154	O	HOH W 201	41.876	48.559	45.033	1.00	50.43	O
ATOM	4155	O	HOH W 202	31.456	86.237	17.283	1.00	60.66	O
ATOM	4156	O	HOH W 203	32.885	41.349	49.780	1.00	60.79	O
ATOM	4157	O	HOH W 204	24.429	37.500	38.536	1.00	56.37	O
ATOM	4158	O	HOH W 205	1.327	48.088	54.550	1.00	67.49	O
ATOM	4159	O	HOH W 206	31.257	59.222	60.483	1.00	68.35	O
ATOM	4160	O	HOH W 207	28.798	66.228	14.536	1.00	53.94	O
ATOM	4161	O	HOH W 208	24.641	51.653	6.100	1.00	59.20	O
ATOM	4162	O	HOH W 209	17.742	49.147	20.375	1.00	49.83	O
ATOM	4163	O	HOH W 210	5.685	91.292	-15.982	1.00	56.41	O
ATOM	4164	O	HOH W 211	16.198	55.728	40.933	1.00	52.78	O
ATOM	4165	O	HOH W 212	21.853	40.934	42.112	1.00	49.96	O
ATOM	4166	O	HOH W 213	25.053	66.499	56.547	1.00	83.65	O
ATOM	4167	O	HOH W 214	48.823	54.896	48.661	1.00	55.41	O
ATOM	4168	O	HOH W 215	22.762	68.871	-1.690	1.00	62.27	O
ATOM	4169	O	HOH W 216	25.875	55.594	42.517	1.00	66.98	O
ATOM	4170	O	HOH W 217	-5.436	61.080	25.597	1.00	65.30	O
ATOM	4171	O	HOH W 218	12.356	86.424	24.128	1.00	59.72	O
ATOM	4172	O	HOH W 219	22.510	53.475	44.139	1.00	58.89	O
ATOM	4173	O	HOH W 220	44.929	51.703	40.161	1.00	59.29	O
ATOM	4174	O	HOH W 221	11.889	58.737	21.071	1.00	46.37	O
ATOM	4175	O	HOH W 222	2.377	36.742	54.223	1.00	50.93	O
ATOM	4176	O	HOH W 223	37.907	66.431	23.997	1.00	52.38	O
ATOM	4177	O	HOH W 224	-0.318	35.084	46.733	1.00	63.02	O
ATOM	4178	O	HOH W 225	35.210	54.687	17.445	1.00	57.64	O
ATOM	4179	O	HOH W 226	21.035	49.707	70.041	1.00	75.18	O
ATOM	4180	O	HOH W 227	19.012	54.823	0.855	1.00	77.70	O
ATOM	4181	O	HOH W 228	27.196	72.138	32.147	1.00	50.32	O
ATOM	4182	O	HOH W 229	36.546	45.028	31.439	1.00	86.36	O
ATOM	4183	O	HOH W 230	21.767	75.014	38.655	1.00	77.73	O
ATOM	4184	O	HOH W 231	11.281	61.906	18.648	1.00	64.20	O
ATOM	4185	O	HOH W 232	13.085	67.024	34.336	1.00	74.90	O
ATOM	4186	O	HOH W 233	27.855	51.751	74.679	1.00	67.16	O
ATOM	4187	O	HOH W 234	10.281	32.452	34.068	1.00	56.54	O
ATOM	4188	O	HOH W 235	6.591	29.675	38.806	1.00	73.00	O
ATOM	4189	O	HOH W 236	39.651	73.045	28.459	1.00	66.62	O
ATOM	4190	O	HOH W 237	16.451	69.224	37.053	1.00	74.23	O
ATOM	4191	O	HOH W 238	9.626	39.240	61.780	1.00	54.32	O
ATOM	4192	O	HOH W 239	29.512	44.676	36.627	1.00	57.77	O
ATOM	4193	O	HOH W 240	3.040	44.352	51.325	1.00	54.23	O
ATOM	4194	O	HOH W 241	31.791	48.763	15.080	1.00	96.21	O
ATOM	4195	O	HOH W 242	4.609	93.915	6.541	1.00	63.18	O
ATOM	4196	O	HOH W 243	31.181	78.092	14.598	1.00	50.66	O
ATOM	4197	O	HOH W 244	28.813	44.898	29.950	1.00	78.95	O
ATOM	4198	O	HOH W 245	40.418	42.694	50.644	1.00	66.51	O
ATOM	4199	O	HOH W 246	23.693	52.314	42.465	1.00	61.89	O
ATOM	4200	O	HOH W 247	30.714	81.231	24.854	1.00	52.52	O
ATOM	4201	O	HOH W 248	1.709	26.668	53.914	1.00	70.93	O
ATOM	4202	O	HOH W 249	7.267	71.708	18.353	1.00	58.07	O
ATOM	4203	O	HOH W 250	24.095	78.135	38.801	1.00	80.65	O
ATOM	4204	O	HOH W 251	31.142	41.795	59.722	1.00	65.65	O
ATOM	4205	O	HOH W 252	19.564	57.043	41.120	1.00	81.01	O
ATOM	4206	O	HOH W 253	46.447	63.136	44.226	1.00	57.83	O
ATOM	4207	O	HOH W 254	30.384	49.338	27.329	1.00	56.81	O
ATOM	4208	O	HOH W 255	33.751	47.674	25.074	1.00	78.98	O
ATOM	4209	O	HOH W 256	25.824	53.009	66.652	1.00	59.78	O
ATOM	4210	O	HOH W 257	4.959	62.792	13.938	1.00	82.01	O
ATOM	4211	O	HOH W 258	10.238	76.014	12.516	1.00	57.55	O
ATOM	4212	O	HOH W 259	12.264	98.518	-2.208	1.00	89.66	O
ATOM	4213	O	HOH W 260	49.228	57.400	50.168	1.00	58.87	O
ATOM	4214	O	HOH W 261	42.057	54.823	22.767	1.00	68.76	O
ATOM	4215	O	HOH W 262	28.362	75.116	-1.124	1.00	64.78	O
ATOM	4216	O	HOH W 263	49.735	63.460	29.660	1.00	61.13	O
ATOM	4217	O	HOH W 264	27.673	39.705	34.201	1.00	68.87	O
ATOM	4218	O	HOH W 265	15.551	30.213	59.769	1.00	75.13	O
ATOM	4219	O	HOH W 266	24.408	43.709	25.342	1.00	61.92	O

Figure 1 Table 1a - 64

ATOM	4220	O	HOH W 267	15.264	93.943	-1.744	1.00	67.58	O
ATOM	4221	O	HOH W 268	4.196	65.423	19.389	1.00	62.87	O
ATOM	4222	O	HOH W 269	8.669	87.807	7.454	1.00	63.23	O
ATOM	4223	O	HOH W 270	25.502	53.653	45.451	1.00	58.94	O
ATOM	4224	O	HOH W 271	27.857	77.822	29.856	1.00	57.03	O
ATOM	4225	O	HOH W 272	35.641	72.414	37.242	1.00	83.10	O
ATOM	4226	O	HOH W 273	18.918	58.929	56.977	1.00	60.97	O
ATOM	4227	O	HOH W 274	23.798	70.129	55.847	1.00	86.67	O
ATOM	4228	O	HOH W 275	20.220	36.787	65.685	1.00	53.39	O
ATOM	4229	O	HOH W 276	44.847	52.590	48.898	1.00	70.60	O
ATOM	4230	O	HOH W 277	36.013	48.723	63.926	1.00	72.22	O
ATOM	4231	O	HOH W 278	51.516	64.637	42.667	1.00	65.12	O
ATOM	4232	O	HOH W 279	21.721	59.409	44.876	1.00	84.43	O
ATOM	4233	O	HOH W 280	8.705	51.763	19.879	1.00	59.07	O
ATOM	4234	O	HOH W 281	31.610	75.283	4.359	1.00	85.88	O
ATOM	4235	O	HOH W 282	10.025	35.753	30.454	1.00	68.39	O
ATOM	4236	O	HOH W 283	31.357	53.077	74.259	1.00	74.42	O
ATOM	4237	O	HOH W 284	7.571	94.982	-10.064	1.00	63.46	O
ATOM	4238	O	HOH W 285	19.118	36.970	35.955	1.00	64.50	O
ATOM	4239	O	HOH W 286	40.176	49.470	38.326	1.00	63.99	O
ATOM	4240	O	HOH W 287	33.988	69.667	46.778	1.00	74.73	O
ATOM	4241	O	HOH W 288	8.430	91.072	11.669	1.00	73.53	O
ATOM	4242	O	HOH W 289	16.773	41.783	28.005	1.00	58.44	O
ATOM	4243	O	HOH W 290	11.096	29.811	56.908	1.00	72.51	O
ATOM	4244	O	HOH W 291	9.769	31.034	50.986	1.00	60.36	O
ATOM	4245	O	HOH W 292	37.467	53.187	23.541	1.00	55.50	O
ATOM	4246	O	HOH W 293	25.890	92.763	4.112	1.00	66.22	O
ATOM	4247	O	HOH W 294	35.846	57.039	17.604	1.00	59.77	O
ATOM	4248	O	HOH W 295	9.547	55.492	17.945	1.00	54.13	O
ATOM	4249	O	HOH W 296	44.715	49.866	46.409	1.00	58.32	O
ATOM	4250	O	HOH W 297	11.572	60.400	43.941	1.00	64.49	O
ATOM	4251	O	HOH W 298	43.335	44.340	49.492	1.00	47.46	O
ATOM	4252	O	HOH W 299	36.058	42.290	53.279	1.00	76.30	O
ATOM	4253	O	HOH W 300	17.854	59.120	49.563	1.00	59.08	O
ATOM	4254	O	HOH W 301	24.470	80.329	-0.868	1.00	53.00	O
ATOM	4255	O	HOH W 302	12.794	56.804	55.810	1.00	59.07	O
ATOM	4256	O	HOH W 303	16.849	53.192	13.904	1.00	72.58	O
ATOM	4257	O	HOH W 304	36.642	70.303	25.627	1.00	70.75	O
ATOM	4258	O	HOH W 305	24.369	77.773	-1.889	1.00	59.28	O
ATOM	4259	O	HOH W 306	13.638	96.432	19.967	1.00	70.54	O
ATOM	4260	O	HOH W 307	46.403	65.066	33.697	1.00	77.41	O
ATOM	4261	O	HOH W 308	3.887	78.466	25.274	1.00	83.64	O
ATOM	4262	O	HOH W 309	19.814	82.275	0.751	1.00	55.87	O
ATOM	4263	O	HOH W 310	6.711	54.462	50.684	1.00	67.49	O
ATOM	4264	O	HOH W 311	14.143	60.919	36.408	1.00	59.87	O
ATOM	4265	O	HOH W 312	3.547	58.934	12.129	1.00	70.32	O
ATOM	4266	O	HOH W 313	8.246	51.486	56.693	1.00	63.88	O
ATOM	4267	O	HOH W 314	7.223	54.293	17.700	1.00	73.80	O
ATOM	4268	O	HOH W 315	1.901	43.772	48.191	1.00	51.22	O
ATOM	4269	O	HOH W 316	19.972	35.440	33.015	1.00	79.59	O
ATOM	4270	O	HOH W 317	1.142	50.663	35.550	1.00	57.22	O
ATOM	4271	O	HOH W 318	59.599	60.561	38.534	1.00	43.19	O
ATOM	4272	O	HOH W 319	43.593	67.210	39.900	1.00	66.59	O
ATOM	4273	O	HOH W 320	48.877	54.820	35.318	1.00	54.03	O
ATOM	4274	O	HOH W 321	34.830	48.976	39.983	1.00	46.72	O
ATOM	4275	O	HOH W 322	35.030	79.269	28.189	1.00	73.16	O
ATOM	4276	O	HOH W 323	10.156	53.331	57.236	1.00	64.34	O
ATOM	4277	O	HOH W 324	10.565	43.812	22.634	1.00	68.81	O
ATOM	4278	O	HOH W 325	14.133	64.566	37.033	1.00	67.15	O
ATOM	4279	O	HOH W 326	22.107	33.778	44.053	1.00	71.21	O
ATOM	4280	O	HOH W 327	27.102	77.323	-2.851	1.00	58.59	O
ATOM	4281	O	HOH W 328	19.556	98.330	2.794	1.00	49.62	O
ATOM	4282	O	HOH W 329	16.741	57.422	59.751	1.00	83.41	O
ATOM	4283	O	HOH W 330	-0.079	60.433	22.613	1.00	64.42	O
ATOM	4284	O	HOH W 331	-0.225	35.978	53.982	1.00	62.85	O
ATOM	4285	O	HOH W 332	15.329	35.870	35.906	1.00	53.85	O
ATOM	4286	O	HOH W 333	2.059	83.495	26.841	1.00	74.42	O

Figure 1

Table 1a - 65

ATOM	4287	O	HOH W 334	25.206	64.330	10.492	1.00	58.48	O
ATOM	4288	O	HOH W 335	33.253	43.244	65.390	1.00	76.31	O
ATOM	4289	O	HOH W 336	17.773	35.856	37.967	1.00	84.72	O
ATOM	4290	O	HOH W 337	12.924	67.551	3.664	1.00	58.04	O
ATOM	4291	O	HOH W 338	41.411	44.437	21.933	1.00	78.46	O
ATOM	4292	O	HOH W 339	20.960	63.077	0.879	1.00	60.04	O
ATOM	4293	O	HOH W 340	29.768	63.846	50.516	1.00	77.40	O
ATOM	4294	O	HOH W 341	15.143	56.651	7.578	1.00	60.63	O
ATOM	4295	O	HOH W 342	32.158	57.582	10.544	1.00	64.93	O
ATOM	4296	O	HOH W 343	20.237	39.017	25.364	1.00	88.47	O
ATOM	4297	O	HOH W 344	1.837	52.649	30.655	1.00	49.04	O
ATOM	4298	O	HOH W 345	34.276	55.601	21.263	1.00	61.14	O
ATOM	4299	O	HOH W 346	18.181	55.470	62.197	1.00	73.06	O
ATOM	4300	O	HOH W 347	0.559	57.983	22.754	1.00	60.98	O
ATOM	4301	O	HOH W 348	10.302	40.976	27.440	1.00	45.33	O
ATOM	4302	O	HOH W 349	19.899	85.060	1.035	1.00	52.98	O
ATOM	4303	O	HOH W 350	1.000	33.290	41.856	1.00	61.20	O
ATOM	4304	O	HOH W 351	46.545	60.101	53.879	1.00	77.43	O
ATOM	4305	O	HOH W 352	32.355	47.476	38.587	1.00	71.34	O
ATOM	4306	O	HOH W 353	35.802	73.163	46.243	1.00	85.52	O
ATOM	4307	O	HOH W 354	26.371	54.126	73.847	1.00	72.29	O
ATOM	4308	O	HOH W 355	30.065	69.596	14.149	1.00	54.96	O
ATOM	4309	O	HOH W 356	27.795	62.254	4.791	1.00	77.85	O
ATOM	4310	O	HOH W 357	20.874	93.625	2.885	1.00	79.72	O
ATOM	4311	O	HOH W 358	17.997	70.641	31.815	1.00	65.74	O
ATOM	4312	O	HOH W 359	27.457	42.587	69.481	1.00	57.71	O
ATOM	4313	O	HOH W 360	29.611	41.007	35.236	1.00	71.73	O
ATOM	4314	O	HOH W 361	29.917	36.472	62.920	1.00	119.78	O
ATOM	4315	O	HOH W 362	5.671	33.439	36.357	1.00	59.89	O
ATOM	4316	O	HOH W 363	5.582	37.677	60.387	1.00	48.59	O
ATOM	4317	O	HOH W 364	2.178	45.681	56.170	1.00	62.35	O
ATOM	4318	O	HOH W 365	46.973	70.495	31.216	1.00	64.79	O
ATOM	4319	O	HOH W 366	22.549	75.679	-5.188	1.00	55.21	O
ATOM	4320	O	HOH W 367	22.110	39.657	44.203	1.00	70.19	O
ATOM	4321	O	HOH W 368	-0.799	91.477	-24.182	1.00	77.90	O
ATOM	4322	O	HOH W 369	3.050	64.097	8.269	1.00	86.57	O
ATOM	4323	O	HOH W 370	35.571	65.538	19.343	1.00	62.08	O
ATOM	4324	O	HOH W 371	6.792	80.217	13.024	1.00	69.37	O
ATOM	4325	O	HOH W 372	21.734	30.530	57.308	1.00	65.32	O
ATOM	4326	O	HOH W 373	37.968	77.934	26.678	1.00	70.86	O
ATOM	4327	O	HOH W 374	15.906	62.165	56.982	1.00	83.59	O
ATOM	4328	O	HOH W 375	36.468	45.621	58.033	1.00	74.29	O
ATOM	4329	O	HOH W 376	34.824	73.376	39.774	1.00	87.52	O
ATOM	4330	O	HOH W 377	30.506	36.806	59.147	1.00	63.09	O
ATOM	4331	O	HOH W 378	34.323	79.723	25.588	1.00	77.29	O
ATOM	4332	O	HOH W 379	-0.054	48.846	32.370	1.00	75.99	O
ATOM	4333	O	HOH W 380	-0.959	33.638	43.998	1.00	68.47	O
ATOM	4334	O	HOH W 381	2.009	85.529	8.648	1.00	67.44	O
ATOM	4335	O	HOH W 382	33.551	69.252	54.489	1.00	81.49	O
ATOM	4336	O	HOH W 383	16.798	88.211	3.257	1.00	66.58	O
ATOM	4337	O	HOH W 384	-0.840	38.502	34.363	1.00	63.66	O
ATOM	4338	O	HOH W 385	36.519	48.157	59.398	1.00	62.56	O
ATOM	4339	O	HOH W 386	35.387	66.369	37.364	1.00	59.14	O
ATOM	4340	O	HOH W 387	4.889	82.738	6.527	1.00	68.72	O
ATOM	4341	O	HOH W 388	17.032	85.619	2.170	1.00	55.91	O
ATOM	4342	O	HOH W 389	8.369	74.223	12.711	1.00	71.93	O
ATOM	4343	O	HOH W 390	-1.383	88.260	-23.107	1.00	70.36	O
ATOM	4344	O	HOH W 391	36.276	67.463	17.513	1.00	68.10	O
ATOM	4345	O	HOH W 392	10.431	56.402	15.171	1.00	66.64	O
ATOM	4346	O	HOH W 393	16.664	82.088	1.571	1.00	72.00	O
ATOM	4347	O	HOH W 394	50.722	62.498	44.703	1.00	46.36	O
ATOM	4348	O	HOH W 395	10.064	66.459	-4.087	1.00	72.56	O
ATOM	4349	O	HOH W 396	2.787	57.950	19.592	1.00	68.30	O
ATOM	4350	O	HOH W 397	26.725	81.879	-0.742	1.00	62.46	O
ATOM	4351	O	HOH W 398	16.499	97.109	19.759	1.00	78.87	O
ATOM	4352	O	HOH W 399	1.510	90.072	-23.714	1.00	65.33	O
ATOM	4353	O	HOH W 400	23.769	73.635	37.658	1.00	75.85	O

Figure 1 Table 1a - 66

ATOM	4354	O	HOH W 401	35.300	48.076	35.593	1.00	76.69	O
ATOM	4355	O	HOH W 402	29.794	41.182	46.294	1.00	81.33	O
ATOM	4356	O	HOH W 403	28.210	45.908	39.824	1.00	61.11	O
ATOM	4357	O	HOH W 404	32.854	51.327	31.197	1.00	63.72	O
ATOM	4358	O	HOH W 405	30.449	43.425	40.094	1.00	65.35	O
ATOM	4359	O	HOH W 406	29.165	64.095	12.476	1.00	73.91	O
ATOM	4360	O	HOH W 407	3.897	27.852	49.569	1.00	79.31	O
ATOM	4361	O	HOH W 408	32.820	66.199	18.933	1.00	60.64	O
ATOM	4362	O	HOH W 409	41.371	53.103	58.445	1.00	66.10	O
ATOM	4363	O	HOH W 410	35.346	56.341	65.864	1.00	73.46	O
ATOM	4364	O	HOH W 411	25.175	63.197	40.815	1.00	67.53	O
ATOM	4365	O	HOH W 412	26.792	65.019	45.238	1.00	67.73	O
ATOM	4366	O	HOH W 413	37.400	69.430	19.851	1.00	86.80	O
ATOM	4367	O	HOH W 414	31.168	55.612	6.866	1.00	74.79	O
ATOM	4368	O	HOH W 415	33.525	41.201	45.497	1.00	69.08	O
ATOM	4369	O	HOH W 416	23.814	64.701	49.441	1.00	72.80	O
ATOM	4370	O	HOH W 417	5.169	74.464	8.995	1.00	57.73	O
ATOM	4371	O	HOH W 418	2.688	61.224	16.650	1.00	75.84	O
ATOM	4372	O	HOH W 419	16.247	59.577	35.877	1.00	65.07	O
ATOM	4373	O	HOH W 420	6.841	60.427	18.847	1.00	68.04	O
ATOM	4374	O	HOH W 421	32.623	79.291	8.726	1.00	58.41	O
ATOM	4375	O	HOH W 422	15.896	92.838	8.988	1.00	65.32	O
ATOM	4376	O	HOH W 423	-0.771	42.447	36.985	1.00	65.97	O
ATOM	4377	O	HOH W 424	31.549	47.074	17.018	1.00	87.48	O
ATOM	4378	O	HOH W 425	17.434	58.858	53.352	1.00	70.84	O
ATOM	4379	O	HOH W 426	25.617	53.340	39.251	1.00	44.22	O
ATOM	4380	O	HOH W 427	26.316	55.831	39.286	1.00	47.41	O
ATOM	4381	O	HOH W 428	40.051	42.646	33.532	1.00	81.03	O

Table 1b

ATOM	1	N	SER A 393	24.326	73.990	34.321	1.00	53.14	N
ATOM	2	CA	SER A 393	23.333	74.032	33.209	1.00	52.89	C
ATOM	3	C	SER A 393	22.131	74.895	33.600	1.00	52.65	C
ATOM	4	O	SER A 393	20.987	74.422	33.620	1.00	53.07	O
ATOM	5	CB	SER A 393	22.893	72.617	32.828	1.00	52.63	C
ATOM	6	OG	SER A 393	22.054	72.075	33.825	1.00	52.80	O
ATOM	7	N	MET A 394	22.404	76.160	33.921	1.00	52.03	N
ATOM	8	CA	MET A 394	21.364	77.088	34.350	1.00	50.90	C
ATOM	9	C	MET A 394	20.584	77.707	33.184	1.00	49.33	C
ATOM	10	O	MET A 394	19.378	77.485	33.077	1.00	49.38	O
ATOM	11	CB	MET A 394	21.938	78.157	35.289	1.00	51.53	C
ATOM	12	CG	MET A 394	21.716	77.860	36.762	1.00	53.85	C
ATOM	13	SD	MET A 394	20.472	78.919	37.551	1.00	58.93	S
ATOM	14	CE	MET A 394	21.498	79.998	38.555	1.00	57.27	C
ATOM	15	N	ALA A 395	21.266	78.452	32.310	1.00	47.47	N
ATOM	16	CA	ALA A 395	20.591	79.256	31.268	1.00	45.53	C
ATOM	17	C	ALA A 395	20.628	78.670	29.845	1.00	44.17	C
ATOM	18	O	ALA A 395	21.659	78.699	29.165	1.00	44.14	O
ATOM	19	CB	ALA A 395	21.116	80.691	31.273	1.00	45.39	C
ATOM	20	N	TRP A 396	19.479	78.170	29.403	1.00	42.38	N
ATOM	21	CA	TRP A 396	19.332	77.547	28.091	1.00	40.72	C
ATOM	22	C	TRP A 396	18.858	78.560	27.055	1.00	40.39	C
ATOM	23	O	TRP A 396	17.887	79.278	27.281	1.00	40.57	O
ATOM	24	CB	TRP A 396	18.342	76.388	28.173	1.00	40.06	C
ATOM	25	CG	TRP A 396	18.838	75.239	29.028	1.00	39.13	C
ATOM	26	CD1	TRP A 396	18.468	74.947	30.307	1.00	38.58	C
ATOM	27	CD2	TRP A 396	19.799	74.243	28.648	1.00	38.01	C
ATOM	28	NE1	TRP A 396	19.138	73.823	30.752	1.00	38.39	N
ATOM	29	CE2	TRP A 396	19.958	73.370	29.751	1.00	38.27	C
ATOM	30	CE3	TRP A 396	20.536	73.997	27.477	1.00	37.70	C
ATOM	31	CZ2	TRP A 396	20.832	72.275	29.722	1.00	37.70	C
ATOM	32	CZ3	TRP A 396	21.406	72.908	27.449	1.00	37.64	C
ATOM	33	CH2	TRP A 396	21.541	72.059	28.566	1.00	37.90	C
ATOM	34	N	HIS A 397	19.549	78.613	25.923	1.00	39.50	N
ATOM	35	CA	HIS A 397	19.204	79.548	24.859	1.00	39.28	C
ATOM	36	C	HIS A 397	18.622	78.799	23.675	1.00	38.90	C
ATOM	37	O	HIS A 397	19.145	77.761	23.282	1.00	38.65	O
ATOM	38	CB	HIS A 397	20.438	80.348	24.447	1.00	39.14	C
ATOM	39	CG	HIS A 397	21.049	81.112	25.578	1.00	40.16	C
ATOM	40	ND1	HIS A 397	22.129	80.642	26.297	1.00	41.64	N
ATOM	41	CD2	HIS A 397	20.701	82.289	26.148	1.00	40.55	C
ATOM	42	CE1	HIS A 397	22.431	81.507	27.250	1.00	41.42	C
ATOM	43	NE2	HIS A 397	21.578	82.514	27.182	1.00	41.81	N
ATOM	44	N	LEU A 398	17.528	79.323	23.125	1.00	38.33	N
ATOM	45	CA	LEU A 398	16.930	78.755	21.927	1.00	37.94	C
ATOM	46	C	LEU A 398	17.815	79.080	20.723	1.00	38.20	C
ATOM	47	O	LEU A 398	18.057	80.265	20.406	1.00	37.26	O
ATOM	48	CB	LEU A 398	15.514	79.302	21.728	1.00	38.46	C
ATOM	49	CG	LEU A 398	14.708	78.823	20.511	1.00	38.52	C
ATOM	50	CD1	LEU A 398	14.168	77.415	20.710	1.00	38.10	C
ATOM	51	CD2	LEU A 398	13.564	79.797	20.220	1.00	36.92	C
ATOM	52	N	GLY A 399	18.303	78.025	20.066	1.00	37.80	N
ATOM	53	CA	GLY A 399	19.200	78.150	18.915	1.00	37.53	C
ATOM	54	C	GLY A 399	20.352	79.105	19.162	1.00	37.76	C
ATOM	55	O	GLY A 399	20.899	79.163	20.269	1.00	37.58	O
ATOM	56	N	ILE A 400	20.712	79.868	18.128	1.00	37.64	N
ATOM	57	CA	ILE A 400	21.853	80.777	18.183	1.00	38.03	C
ATOM	58	C	ILE A 400	21.446	82.138	17.625	1.00	38.00	C
ATOM	59	O	ILE A 400	20.581	82.216	16.763	1.00	37.63	O
ATOM	60	CB	ILE A 400	23.081	80.217	17.406	1.00	38.33	C
ATOM	61	CG1	ILE A 400	22.728	79.943	15.936	1.00	38.16	C
ATOM	62	CG2	ILE A 400	23.633	78.922	18.097	1.00	38.51	C
ATOM	63	CD1	ILE A 400	23.944	79.827	15.017	1.00	39.08	C
ATOM	64	N	ARG A 401	22.059	83.197	18.140	1.00	37.93	N

Figure 1 Table 1b - 2

ATOM	65	CA	ARG A 401	21.733	84.560	17.733	1.00	38.78	C
ATOM	66	C	ARG A 401	22.846	85.186	16.903	1.00	37.96	C
ATOM	67	O	ARG A 401	24.015	84.802	17.007	1.00	37.75	O
ATOM	68	CB	ARG A 401	21.399	85.441	18.946	1.00	38.59	C
ATOM	69	CG	ARG A 401	20.106	85.024	19.656	1.00	40.90	C
ATOM	70	CD	ARG A 401	19.780	85.892	20.870	1.00	42.08	C
ATOM	71	NE	ARG A 401	20.756	85.791	21.963	1.00	50.20	N
ATOM	72	CZ	ARG A 401	20.722	84.881	22.944	1.00	52.93	C
ATOM	73	NH1	ARG A 401	19.768	83.948	22.993	1.00	54.21	N
ATOM	74	NH2	ARG A 401	21.656	84.898	23.889	1.00	53.91	N
ATOM	75	N	SER A 402	22.465	86.153	16.074	1.00	37.64	N
ATOM	76	CA	SER A 402	23.390	86.814	15.171	1.00	37.56	C
ATOM	77	C	SER A 402	22.955	88.260	14.938	1.00	38.06	C
ATOM	78	O	SER A 402	21.757	88.575	14.934	1.00	37.79	O
ATOM	79	CB	SER A 402	23.432	86.069	13.834	1.00	37.60	C
ATOM	80	OG	SER A 402	24.417	86.601	12.967	1.00	36.69	O
ATOM	81	N	GLN A 403	23.931	89.140	14.754	1.00	37.97	N
ATOM	82	CA	GLN A 403	23.627	90.493	14.323	1.00	38.80	C
ATOM	83	C	GLN A 403	24.048	90.697	12.864	1.00	38.82	C
ATOM	84	O	GLN A 403	24.121	91.823	12.386	1.00	38.88	O
ATOM	85	CB	GLN A 403	24.241	91.527	15.285	1.00	38.63	C
ATOM	86	CG	GLN A 403	23.864	91.240	16.752	1.00	39.21	C
ATOM	87	CD	GLN A 403	24.247	92.346	17.721	1.00	39.60	C
ATOM	88	OE1	GLN A 403	25.356	92.882	17.681	1.00	41.16	O
ATOM	89	NE2	GLN A 403	23.326	92.680	18.614	1.00	40.10	N
ATOM	90	N	SER A 404	24.303	89.589	12.163	1.00	38.75	N
ATOM	91	CA	SER A 404	24.576	89.609	10.722	1.00	38.87	C
ATOM	92	C	SER A 404	23.293	89.910	9.946	1.00	38.84	C
ATOM	93	O	SER A 404	22.199	89.723	10.470	1.00	38.66	O
ATOM	94	CB	SER A 404	25.158	88.267	10.266	1.00	38.65	C
ATOM	95	OG	SER A 404	26.326	87.932	11.000	1.00	39.16	O
ATOM	96	N	ARG A 405	23.424	90.389	8.710	1.00	38.84	N
ATOM	97	CA	ARG A 405	22.252	90.671	7.884	1.00	39.66	C
ATOM	98	C	ARG A 405	21.530	89.346	7.611	1.00	40.04	C
ATOM	99	O	ARG A 405	22.192	88.343	7.337	1.00	40.13	O
ATOM	100	CB	ARG A 405	22.652	91.357	6.569	1.00	39.68	C
ATOM	101	CG	ARG A 405	23.071	92.837	6.697	1.00	39.94	C
ATOM	102	CD	ARG A 405	23.242	93.469	5.305	1.00	40.65	C
ATOM	103	NE	ARG A 405	22.974	94.909	5.284	1.00	44.35	N
ATOM	104	CZ	ARG A 405	23.504	95.776	4.414	1.00	45.08	C
ATOM	105	NH1	ARG A 405	24.357	95.362	3.482	1.00	45.93	N
ATOM	106	NH2	ARG A 405	23.189	97.069	4.475	1.00	44.50	N
ATOM	107	N	PRO A 406	20.184	89.325	7.722	1.00	40.31	N
ATOM	108	CA	PRO A 406	19.429	88.075	7.538	1.00	40.98	C
ATOM	109	C	PRO A 406	19.681	87.445	6.175	1.00	41.30	C
ATOM	110	O	PRO A 406	19.744	86.223	6.068	1.00	41.79	O
ATOM	111	CB	PRO A 406	17.969	88.521	7.649	1.00	41.09	C
ATOM	112	CG	PRO A 406	18.016	89.774	8.417	1.00	40.53	C
ATOM	113	CD	PRO A 406	19.290	90.453	8.033	1.00	40.41	C
ATOM	114	N	ASN A 407	19.835	88.287	5.151	1.00	41.68	N
ATOM	115	CA	ASN A 407	20.198	87.830	3.812	1.00	42.05	C
ATOM	116	C	ASN A 407	21.516	87.044	3.812	1.00	41.34	C
ATOM	117	O	ASN A 407	21.638	86.015	3.143	1.00	40.84	O
ATOM	118	CB	ASN A 407	20.234	89.006	2.802	1.00	42.58	C
ATOM	119	CG	ASN A 407	20.522	90.377	3.463	1.00	45.05	C
ATOM	120	OD1	ASN A 407	20.052	90.670	4.569	1.00	47.45	O
ATOM	121	ND2	ASN A 407	21.265	91.232	2.754	1.00	46.68	N
ATOM	122	N	ASP A 408	22.490	87.532	4.578	1.00	40.63	N
ATOM	123	CA	ASP A 408	23.776	86.851	4.718	1.00	40.22	C
ATOM	124	C	ASP A 408	23.661	85.569	5.553	1.00	40.01	C
ATOM	125	O	ASP A 408	24.348	84.577	5.282	1.00	39.61	O
ATOM	126	CB	ASP A 408	24.816	87.800	5.311	1.00	40.10	C
ATOM	127	CG	ASP A 408	25.075	89.007	4.422	1.00	40.60	C
ATOM	128	OD1	ASP A 408	24.633	88.999	3.247	1.00	39.26	O
ATOM	129	OD2	ASP A 408	25.720	89.965	4.901	1.00	40.94	O
ATOM	130	N	ILE A 409	22.785	85.586	6.553	1.00	39.78	N
ATOM	131	CA	ILE A 409	22.567	84.390	7.375	1.00	39.88	C

Figure 1 Table 1b - 3

ATOM	132	C	ILE	A	409	22.010	83.249	6.518	1.00	40.33	C
ATOM	133	O	ILE	A	409	22.553	82.151	6.525	1.00	40.19	O
ATOM	134	CB	ILE	A	409	21.674	84.665	8.605	1.00	39.63	C
ATOM	135	CG1	ILE	A	409	22.293	85.774	9.474	1.00	38.96	C
ATOM	136	CG2	ILE	A	409	21.481	83.388	9.431	1.00	39.28	C
ATOM	137	CD1	ILE	A	409	21.420	86.235	10.608	1.00	38.63	C
ATOM	138	N	MET	A	410	20.958	83.529	5.755	1.00	40.85	N
ATOM	139	CA	MET	A	410	20.331	82.512	4.919	1.00	41.58	C
ATOM	140	C	MET	A	410	21.259	82.030	3.813	1.00	41.97	C
ATOM	141	O	MET	A	410	21.400	80.828	3.616	1.00	42.38	O
ATOM	142	CB	MET	A	410	19.001	82.998	4.347	1.00	41.57	C
ATOM	143	CG	MET	A	410	17.998	83.438	5.399	1.00	42.88	C
ATOM	144	SD	MET	A	410	17.479	82.146	6.542	1.00	45.74	S
ATOM	145	CE	MET	A	410	18.737	82.150	7.807	1.00	47.94	C
ATOM	146	N	ALA	A	411	21.899	82.965	3.109	1.00	42.20	N
ATOM	147	CA	ALA	A	411	22.888	82.621	2.087	1.00	42.41	C
ATOM	148	C	ALA	A	411	23.922	81.639	2.630	1.00	42.50	C
ATOM	149	O	ALA	A	411	24.159	80.598	2.028	1.00	42.57	O
ATOM	150	CB	ALA	A	411	23.575	83.874	1.545	1.00	42.48	C
ATOM	151	N	GLU	A	412	24.513	81.968	3.775	1.00	42.36	N
ATOM	152	CA	GLU	A	412	25.536	81.120	4.389	1.00	42.58	C
ATOM	153	C	GLU	A	412	25.040	79.750	4.863	1.00	42.44	C
ATOM	154	O	GLU	A	412	25.754	78.761	4.697	1.00	41.88	O
ATOM	155	CB	GLU	A	412	26.271	81.853	5.515	1.00	42.44	C
ATOM	156	CG	GLU	A	412	27.268	82.889	5.001	1.00	43.56	C
ATOM	157	CD	GLU	A	412	28.425	82.254	4.255	1.00	43.80	C
ATOM	158	OE1	GLU	A	412	29.298	81.638	4.906	1.00	44.57	O
ATOM	159	OE2	GLU	A	412	28.460	82.374	3.018	1.00	44.23	O
ATOM	160	N	VAL	A	413	23.838	79.686	5.439	1.00	42.91	N
ATOM	161	CA	VAL	A	413	23.301	78.382	5.859	1.00	43.55	C
ATOM	162	C	VAL	A	413	23.010	77.493	4.642	1.00	43.93	C
ATOM	163	O	VAL	A	413	23.305	76.297	4.674	1.00	43.70	O
ATOM	164	CB	VAL	A	413	22.091	78.435	6.867	1.00	43.62	C
ATOM	165	CG1	VAL	A	413	22.335	79.420	7.997	1.00	43.77	C
ATOM	166	CG2	VAL	A	413	20.785	78.724	6.187	1.00	45.85	C
ATOM	167	N	CYS	A	414	22.480	78.086	3.563	1.00	43.98	N
ATOM	168	CA	CYS	A	414	22.286	77.351	2.310	1.00	44.50	C
ATOM	169	C	CYS	A	414	23.602	76.867	1.707	1.00	44.42	C
ATOM	170	O	CYS	A	414	23.660	75.759	1.175	1.00	44.06	O
ATOM	171	CB	CYS	A	414	21.504	78.181	1.296	1.00	44.57	C
ATOM	172	SG	CYS	A	414	19.778	78.310	1.737	1.00	46.97	S
ATOM	173	N	ARG	A	415	24.646	77.697	1.796	1.00	44.50	N
ATOM	174	CA	ARG	A	415	25.995	77.305	1.376	1.00	44.82	C
ATOM	175	C	ARG	A	415	26.516	76.111	2.188	1.00	44.64	C
ATOM	176	O	ARG	A	415	27.071	75.172	1.615	1.00	44.70	O
ATOM	177	CB	ARG	A	415	26.983	78.474	1.473	1.00	44.85	C
ATOM	178	CG	ARG	A	415	28.385	78.150	0.929	1.00	45.28	C
ATOM	179	CD	ARG	A	415	29.474	79.135	1.395	1.00	46.01	C
ATOM	180	NE	ARG	A	415	29.489	79.357	2.846	1.00	48.25	N
ATOM	181	CZ	ARG	A	415	29.845	78.455	3.765	1.00	49.62	C
ATOM	182	NH1	ARG	A	415	30.226	77.226	3.418	1.00	49.30	N
ATOM	183	NH2	ARG	A	415	29.812	78.785	5.049	1.00	49.58	N
ATOM	184	N	ALA	A	416	26.345	76.164	3.510	1.00	44.29	N
ATOM	185	CA	ALA	A	416	26.770	75.073	4.400	1.00	44.42	C
ATOM	186	C	ALA	A	416	26.001	73.784	4.148	1.00	44.27	C
ATOM	187	O	ALA	A	416	26.590	72.702	4.161	1.00	44.35	O
ATOM	188	CB	ALA	A	416	26.646	75.477	5.858	1.00	44.03	C
ATOM	189	N	ILE	A	417	24.694	73.908	3.922	1.00	44.29	N
ATOM	190	CA	ILE	A	417	23.841	72.755	3.631	1.00	44.74	C
ATOM	191	C	ILE	A	417	24.339	72.039	2.374	1.00	44.87	C
ATOM	192	O	ILE	A	417	24.515	70.814	2.375	1.00	44.36	O
ATOM	193	CB	ILE	A	417	22.346	73.159	3.482	1.00	44.92	C
ATOM	194	CG1	ILE	A	417	21.749	73.496	4.851	1.00	44.27	C
ATOM	195	CG2	ILE	A	417	21.539	72.032	2.809	1.00	45.39	C
ATOM	196	CD1	ILE	A	417	20.472	74.318	4.795	1.00	45.08	C
ATOM	197	N	LYS	A	418	24.589	72.824	1.322	1.00	44.80	N
ATOM	198	CA	LYS	A	418	25.129	72.321	0.064	1.00	45.13	C

Figure 1 Table 1b - 4

ATOM	199	C	LYS	A	418	26.519	71.700	0.252	1.00	45.49	C
ATOM	200	O	LYS	A	418	26.824	70.661	-0.333	1.00	45.50	O
ATOM	201	CB	LYS	A	418	25.180	73.450	-0.973	1.00	45.07	C
ATOM	202	CG	LYS	A	418	25.203	72.968	-2.409	1.00	45.62	C
ATOM	203	CD	LYS	A	418	25.719	74.033	-3.354	1.00	46.52	C
ATOM	204	CE	LYS	A	418	26.009	73.437	-4.721	1.00	47.21	C
ATOM	205	NZ	LYS	A	418	26.719	74.403	-5.609	1.00	47.96	N
ATOM	206	N	GLN	A	419	27.348	72.339	1.076	1.00	45.91	N
ATOM	207	CA	GLN	A	419	28.704	71.868	1.366	1.00	46.47	C
ATOM	208	C	GLN	A	419	28.714	70.527	2.109	1.00	46.48	C
ATOM	209	O	GLN	A	419	29.624	69.719	1.928	1.00	46.66	O
ATOM	210	CB	GLN	A	419	29.445	72.911	2.206	1.00	46.77	C
ATOM	211	CG	GLN	A	419	30.965	72.836	2.126	1.00	48.48	C
ATOM	212	CD	GLN	A	419	31.546	73.716	1.030	1.00	50.64	C
ATOM	213	OE1	GLN	A	419	30.982	74.761	0.677	1.00	51.97	O
ATOM	214	NE2	GLN	A	419	32.689	73.304	0.492	1.00	51.70	N
ATOM	215	N	LEU	A	420	27.700	70.304	2.944	1.00	46.35	N
ATOM	216	CA	LEU	A	420	27.581	69.086	3.748	1.00	46.27	C
ATOM	217	C	LEU	A	420	26.825	67.964	3.032	1.00	46.38	C
ATOM	218	O	LEU	A	420	26.642	66.874	3.589	1.00	46.57	O
ATOM	219	CB	LEU	A	420	26.891	69.411	5.077	1.00	46.11	C
ATOM	220	CG	LEU	A	420	27.724	69.940	6.253	1.00	46.71	C
ATOM	221	CD1	LEU	A	420	28.900	70.794	5.789	1.00	47.25	C
ATOM	222	CD2	LEU	A	420	26.844	70.711	7.228	1.00	45.39	C
ATOM	223	N	ASP	A	421	26.388	68.244	1.807	1.00	46.53	N
ATOM	224	CA	ASP	A	421	25.599	67.316	0.985	1.00	46.99	C
ATOM	225	C	ASP	A	421	24.246	66.952	1.595	1.00	46.87	C
ATOM	226	O	ASP	A	421	23.739	65.838	1.403	1.00	46.81	O
ATOM	227	CB	ASP	A	421	26.400	66.057	0.632	1.00	47.03	C
ATOM	228	CG	ASP	A	421	27.567	66.355	-0.263	1.00	48.54	C
ATOM	229	OD1	ASP	A	421	27.348	66.937	-1.352	1.00	50.02	O
ATOM	230	OD2	ASP	A	421	28.706	66.001	0.120	1.00	50.30	O
ATOM	231	N	TYR	A	422	23.667	67.887	2.340	1.00	46.74	N
ATOM	232	CA	TYR	A	422	22.294	67.728	2.781	1.00	46.70	C
ATOM	233	C	TYR	A	422	21.396	68.177	1.633	1.00	46.27	C
ATOM	234	O	TYR	A	422	21.806	68.983	0.794	1.00	46.23	O
ATOM	235	CB	TYR	A	422	22.001	68.553	4.044	1.00	46.97	C
ATOM	236	CG	TYR	A	422	22.830	68.224	5.278	1.00	47.81	C
ATOM	237	CD1	TYR	A	422	22.667	68.963	6.455	1.00	48.49	C
ATOM	238	CD2	TYR	A	422	23.785	67.203	5.272	1.00	47.84	C
ATOM	239	CE1	TYR	A	422	23.417	68.684	7.596	1.00	49.18	C
ATOM	240	CE2	TYR	A	422	24.546	66.922	6.407	1.00	49.00	C
ATOM	241	CZ	TYR	A	422	24.354	67.669	7.563	1.00	49.55	C
ATOM	242	OH	TYR	A	422	25.096	67.398	8.691	1.00	50.86	O
ATOM	243	N	GLU	A	423	20.187	67.636	1.572	1.00	45.72	N
ATOM	244	CA	GLU	A	423	19.182	68.188	0.684	1.00	45.39	C
ATOM	245	C	GLU	A	423	18.344	69.204	1.469	1.00	44.60	C
ATOM	246	O	GLU	A	423	18.281	69.151	2.705	1.00	44.13	O
ATOM	247	CB	GLU	A	423	18.349	67.089	-0.004	1.00	46.08	C
ATOM	248	CG	GLU	A	423	17.613	66.144	0.920	1.00	48.27	C
ATOM	249	CD	GLU	A	423	17.645	64.680	0.460	1.00	50.79	C
ATOM	250	OE1	GLU	A	423	17.360	64.399	-0.725	1.00	50.71	O
ATOM	251	OE2	GLU	A	423	17.947	63.800	1.305	1.00	52.81	O
ATOM	252	N	TRP	A	424	17.758	70.162	0.757	1.00	43.28	N
ATOM	253	CA	TRP	A	424	16.913	71.176	1.384	1.00	42.60	C
ATOM	254	C	TRP	A	424	15.863	71.707	0.428	1.00	41.40	C
ATOM	255	O	TRP	A	424	16.000	71.596	-0.793	1.00	40.68	O
ATOM	256	CB	TRP	A	424	17.744	72.343	1.956	1.00	43.09	C
ATOM	257	CG	TRP	A	424	18.211	73.342	0.927	1.00	44.09	C
ATOM	258	CD1	TRP	A	424	17.716	74.609	0.720	1.00	44.83	C
ATOM	259	CD2	TRP	A	424	19.266	73.164	-0.028	1.00	44.90	C
ATOM	260	NE1	TRP	A	424	18.396	75.222	-0.309	1.00	44.88	N
ATOM	261	CE2	TRP	A	424	19.353	74.361	-0.784	1.00	45.58	C
ATOM	262	CE3	TRP	A	424	20.143	72.107	-0.324	1.00	45.33	C
ATOM	263	CZ2	TRP	A	424	20.288	74.532	-1.811	1.00	45.29	C
ATOM	264	CZ3	TRP	A	424	21.074	72.279	-1.342	1.00	45.02	C
ATOM	265	CH2	TRP	A	424	21.134	73.484	-2.078	1.00	45.24	C

Figure 1 Table 1b - 5

ATOM	266	N	LYS A 425	14.808	72.264	1.010	1.00	40.11	N
ATOM	267	CA	LYS A 425	13.804	73.007	0.273	1.00	39.34	C
ATOM	268	C	LYS A 425	13.538	74.317	1.009	1.00	38.53	C
ATOM	269	O	LYS A 425	13.525	74.352	2.237	1.00	37.95	O
ATOM	270	CB	LYS A 425	12.521	72.199	0.138	1.00	39.42	C
ATOM	271	CG	LYS A 425	12.629	71.109	-0.930	1.00	41.11	C
ATOM	272	CD	LYS A 425	11.498	70.117	-0.868	1.00	42.93	C
ATOM	273	CE	LYS A 425	11.850	68.878	-1.689	1.00	43.01	C
ATOM	274	NZ	LYS A 425	10.747	67.897	-1.653	1.00	47.51	N
ATOM	275	N	VAL A 426	13.316	75.373	0.239	1.00	37.62	N
ATOM	276	CA	VAL A 426	12.997	76.695	0.770	1.00	37.40	C
ATOM	277	C	VAL A 426	11.483	76.841	0.852	1.00	37.15	C
ATOM	278	O	VAL A 426	10.801	76.932	-0.173	1.00	36.83	O
ATOM	279	CB	VAL A 426	13.593	77.805	-0.139	1.00	37.15	C
ATOM	280	CG1	VAL A 426	13.324	79.204	0.429	1.00	37.55	C
ATOM	281	CG2	VAL A 426	15.092	77.580	-0.313	1.00	37.21	C
ATOM	282	N	VAL A 427	10.957	76.849	2.074	1.00	36.86	N
ATOM	283	CA	VAL A 427	9.521	77.055	2.266	1.00	36.61	C
ATOM	284	C	VAL A 427	9.195	78.549	2.144	1.00	36.34	C
ATOM	285	O	VAL A 427	8.306	78.919	1.385	1.00	36.31	O
ATOM	286	CB	VAL A 427	9.014	76.507	3.638	1.00	36.67	C
ATOM	287	CG1	VAL A 427	7.498	76.656	3.730	1.00	36.27	C
ATOM	288	CG2	VAL A 427	9.415	75.030	3.846	1.00	36.69	C
ATOM	289	N	ASN A 428	9.914	79.363	2.929	1.00	36.57	N
ATOM	290	CA	ASN A 428	9.869	80.836	2.982	1.00	36.93	C
ATOM	291	C	ASN A 428	11.299	81.289	2.828	1.00	36.84	C
ATOM	292	O	ASN A 428	12.209	80.494	3.102	1.00	36.67	O
ATOM	293	CB	ASN A 428	9.512	81.328	4.406	1.00	37.75	C
ATOM	294	CG	ASN A 428	8.095	81.092	4.757	1.00	39.55	C
ATOM	295	OD1	ASN A 428	7.203	81.254	3.925	1.00	46.05	O
ATOM	296	ND2	ASN A 428	7.857	80.711	5.988	1.00	40.67	N
ATOM	297	N	PRO A 429	11.518	82.586	2.499	1.00	36.25	N
ATOM	298	CA	PRO A 429	12.876	83.134	2.579	1.00	36.42	C
ATOM	299	C	PRO A 429	13.599	82.886	3.916	1.00	36.49	C
ATOM	300	O	PRO A 429	14.830	82.880	3.948	1.00	36.53	O
ATOM	301	CB	PRO A 429	12.659	84.639	2.348	1.00	36.20	C
ATOM	302	CG	PRO A 429	11.459	84.676	1.430	1.00	36.16	C
ATOM	303	CD	PRO A 429	10.556	83.595	2.006	1.00	36.09	C
ATOM	304	N	TYR A 430	12.853	82.664	4.995	1.00	36.38	N
ATOM	305	CA	TYR A 430	13.473	82.449	6.298	1.00	37.34	C
ATOM	306	C	TYR A 430	13.151	81.099	6.921	1.00	36.80	C
ATOM	307	O	TYR A 430	13.274	80.937	8.129	1.00	36.49	O
ATOM	308	CB	TYR A 430	13.099	83.580	7.274	1.00	37.54	C
ATOM	309	CG	TYR A 430	13.337	84.963	6.728	1.00	39.58	C
ATOM	310	CD1	TYR A 430	12.263	85.794	6.405	1.00	41.33	C
ATOM	311	CD2	TYR A 430	14.631	85.447	6.526	1.00	40.75	C
ATOM	312	CE1	TYR A 430	12.470	87.080	5.900	1.00	41.44	C
ATOM	313	CE2	TYR A 430	14.850	86.738	6.014	1.00	41.37	C
ATOM	314	CZ	TYR A 430	13.767	87.543	5.708	1.00	41.18	C
ATOM	315	OH	TYR A 430	13.971	88.819	5.216	1.00	41.17	O
ATOM	316	N	TYR A 431	12.759	80.135	6.090	1.00	37.36	N
ATOM	317	CA	TYR A 431	12.268	78.840	6.567	1.00	37.44	C
ATOM	318	C	TYR A 431	12.690	77.722	5.606	1.00	37.69	C
ATOM	319	O	TYR A 431	12.212	77.652	4.473	1.00	37.20	O
ATOM	320	CB	TYR A 431	10.746	78.910	6.745	1.00	37.90	C
ATOM	321	CG	TYR A 431	10.046	77.660	7.253	1.00	39.68	C
ATOM	322	CD1	TYR A 431	10.723	76.674	7.974	1.00	41.72	C
ATOM	323	CD2	TYR A 431	8.682	77.495	7.038	1.00	40.29	C
ATOM	324	CE1	TYR A 431	10.051	75.532	8.439	1.00	42.14	C
ATOM	325	CE2	TYR A 431	8.010	76.385	7.491	1.00	40.92	C
ATOM	326	CZ	TYR A 431	8.691	75.405	8.184	1.00	41.65	C
ATOM	327	OH	TYR A 431	7.985	74.311	8.623	1.00	42.24	O
ATOM	328	N	LEU A 432	13.603	76.877	6.073	1.00	37.57	N
ATOM	329	CA	LEU A 432	14.119	75.762	5.288	1.00	38.54	C
ATOM	330	C	LEU A 432	13.780	74.435	5.941	1.00	39.23	C
ATOM	331	O	LEU A 432	13.766	74.324	7.166	1.00	39.03	O
ATOM	332	CB	LEU A 432	15.636	75.847	5.164	1.00	38.24	C

Figure 1 Table 1b - 6

ATOM	333	CG	LEU	A	432	16.248	77.178	4.722	1.00	37.95	C
ATOM	334	CD1	LEU	A	432	17.734	77.029	4.727	1.00	38.98	C
ATOM	335	CD2	LEU	A	432	15.755	77.610	3.349	1.00	37.00	C
ATOM	336	N	ARG	A	433	13.517	73.437	5.106	1.00	40.08	N
ATOM	337	CA	ARG	A	433	13.356	72.064	5.551	1.00	41.44	C
ATOM	338	C	ARG	A	433	14.550	71.312	4.993	1.00	41.76	C
ATOM	339	O	ARG	A	433	14.827	71.405	3.794	1.00	42.28	O
ATOM	340	CB	ARG	A	433	12.023	71.515	5.038	1.00	41.40	C
ATOM	341	CG	ARG	A	433	10.939	71.540	6.109	1.00	44.22	C
ATOM	342	CD	ARG	A	433	9.681	72.309	5.734	1.00	47.25	C
ATOM	343	NE	ARG	A	433	8.665	71.518	5.049	1.00	50.79	N
ATOM	344	CZ	ARG	A	433	7.372	71.852	4.962	1.00	52.71	C
ATOM	345	NH1	ARG	A	433	6.913	72.961	5.531	1.00	52.64	N
ATOM	346	NH2	ARG	A	433	6.525	71.068	4.296	1.00	53.14	N
ATOM	347	N	VAL	A	434	15.305	70.635	5.855	1.00	42.17	N
ATOM	348	CA	VAL	A	434	16.519	69.951	5.400	1.00	43.03	C
ATOM	349	C	VAL	A	434	16.494	68.454	5.706	1.00	43.30	C
ATOM	350	O	VAL	A	434	15.853	68.009	6.660	1.00	43.13	O
ATOM	351	CB	VAL	A	434	17.861	70.642	5.868	1.00	43.23	C
ATOM	352	CG1	VAL	A	434	17.639	72.098	6.295	1.00	43.56	C
ATOM	353	CG2	VAL	A	434	18.549	69.868	6.966	1.00	44.98	C
ATOM	354	N	ARG	A	435	17.184	67.692	4.866	1.00	43.59	N
ATOM	355	CA	ARG	A	435	17.217	66.246	4.967	1.00	44.04	C
ATOM	356	C	ARG	A	435	18.637	65.765	4.676	1.00	44.06	C
ATOM	357	O	ARG	A	435	19.310	66.272	3.770	1.00	43.58	O
ATOM	358	CB	ARG	A	435	16.208	65.642	3.990	1.00	44.14	C
ATOM	359	CG	ARG	A	435	16.003	64.148	4.091	1.00	46.47	C
ATOM	360	CD	ARG	A	435	14.866	63.743	3.166	1.00	48.51	C
ATOM	361	NE	ARG	A	435	14.763	62.300	3.016	1.00	51.05	N
ATOM	362	CZ	ARG	A	435	14.948	61.642	1.873	1.00	52.24	C
ATOM	363	NH1	ARG	A	435	15.253	62.290	0.752	1.00	51.86	N
ATOM	364	NH2	ARG	A	435	14.824	60.321	1.855	1.00	53.06	N
ATOM	365	N	ARG	A	436	19.072	64.787	5.461	1.00	44.00	N
ATOM	366	CA	ARG	A	436	20.428	64.273	5.437	1.00	44.61	C
ATOM	367	C	ARG	A	436	20.357	62.744	5.493	1.00	44.33	C
ATOM	368	O	ARG	A	436	19.593	62.188	6.285	1.00	44.04	O
ATOM	369	CB	ARG	A	436	21.186	64.812	6.669	1.00	45.18	C
ATOM	370	CG	ARG	A	436	22.579	64.232	6.906	1.00	47.80	C
ATOM	371	CD	ARG	A	436	22.556	63.015	7.804	1.00	51.78	C
ATOM	372	NE	ARG	A	436	22.923	63.331	9.182	1.00	54.91	N
ATOM	373	CZ	ARG	A	436	22.536	62.626	10.245	1.00	55.57	C
ATOM	374	NH1	ARG	A	436	21.737	61.574	10.096	1.00	55.73	N
ATOM	375	NH2	ARG	A	436	22.933	62.990	11.459	1.00	55.98	N
ATOM	376	N	LYS	A	437	21.141	62.073	4.651	1.00	43.96	N
ATOM	377	CA	LYS	A	437	21.330	60.628	4.769	1.00	43.77	C
ATOM	378	C	LYS	A	437	22.550	60.360	5.649	1.00	43.57	C
ATOM	379	O	LYS	A	437	23.650	60.848	5.374	1.00	43.54	O
ATOM	380	CB	LYS	A	437	21.500	59.979	3.391	1.00	43.88	C
ATOM	381	CG	LYS	A	437	21.509	58.451	3.405	1.00	43.71	C
ATOM	382	CD	LYS	A	437	21.699	57.899	2.006	1.00	44.16	C
ATOM	383	CE	LYS	A	437	21.723	56.376	1.991	1.00	44.11	C
ATOM	384	NZ	LYS	A	437	21.867	55.848	0.597	1.00	44.98	N
ATOM	385	N	ASN	A	438	22.352	59.615	6.726	1.00	43.49	N
ATOM	386	CA	ASN	A	438	23.465	59.232	7.582	1.00	43.91	C
ATOM	387	C	ASN	A	438	24.435	58.310	6.830	1.00	44.35	C
ATOM	388	O	ASN	A	438	24.028	57.258	6.346	1.00	44.37	O
ATOM	389	CB	ASN	A	438	22.959	58.563	8.861	1.00	43.68	C
ATOM	390	CG	ASN	A	438	24.049	58.394	9.897	1.00	43.19	C
ATOM	391	OD1	ASN	A	438	25.092	57.803	9.629	1.00	42.43	O
ATOM	392	ND2	ASN	A	438	23.808	58.907	11.091	1.00	42.39	N
ATOM	393	N	PRO	A	439	25.714	58.721	6.707	1.00	44.97	N
ATOM	394	CA	PRO	A	439	26.714	57.924	5.981	1.00	45.42	C
ATOM	395	C	PRO	A	439	26.965	56.533	6.573	1.00	45.76	C
ATOM	396	O	PRO	A	439	27.171	55.578	5.821	1.00	45.98	O
ATOM	397	CB	PRO	A	439	27.987	58.782	6.066	1.00	45.57	C
ATOM	398	CG	PRO	A	439	27.752	59.724	7.210	1.00	45.42	C
ATOM	399	CD	PRO	A	439	26.282	59.983	7.219	1.00	45.02	C

Figure 1 Table 1b - 7

ATOM	400	N	VAL	A	440	26.940	56.426	7.900	1.00	46.02	N
ATOM	401	CA	VAL	A	440	27.239	55.170	8.589	1.00	46.35	C
ATOM	402	C	VAL	A	440	26.018	54.247	8.597	1.00	46.59	C
ATOM	403	O	VAL	A	440	26.109	53.072	8.227	1.00	46.64	O
ATOM	404	CB	VAL	A	440	27.735	55.416	10.049	1.00	46.27	C
ATOM	405	CG1	VAL	A	440	28.059	54.101	10.747	1.00	46.17	C
ATOM	406	CG2	VAL	A	440	28.955	56.338	10.061	1.00	46.22	C
ATOM	407	N	THR	A	441	24.881	54.808	8.995	1.00	46.74	N
ATOM	408	CA	THR	A	441	23.648	54.068	9.243	1.00	47.23	C
ATOM	409	C	THR	A	441	22.761	53.911	8.001	1.00	46.62	C
ATOM	410	O	THR	A	441	21.957	52.979	7.926	1.00	46.32	O
ATOM	411	CB	THR	A	441	22.836	54.760	10.374	1.00	47.63	C
ATOM	412	OG1	THR	A	441	23.682	54.944	11.521	1.00	49.57	O
ATOM	413	CG2	THR	A	441	21.648	53.901	10.791	1.00	49.01	C
ATOM	414	N	SER	A	442	22.912	54.832	7.046	1.00	46.25	N
ATOM	415	CA	SER	A	442	22.093	54.898	5.823	1.00	46.05	C
ATOM	416	C	SER	A	442	20.659	55.401	6.047	1.00	46.19	C
ATOM	417	O	SER	A	442	19.839	55.352	5.130	1.00	46.53	O
ATOM	418	CB	SER	A	442	22.096	53.568	5.041	1.00	46.12	C
ATOM	419	OG	SER	A	442	23.413	53.168	4.695	1.00	45.28	O
ATOM	420	N	THR	A	443	20.354	55.891	7.248	1.00	45.93	N
ATOM	421	CA	THR	A	443	19.015	56.429	7.519	1.00	45.71	C
ATOM	422	C	THR	A	443	18.893	57.908	7.155	1.00	45.73	C
ATOM	423	O	THR	A	443	19.891	58.605	6.981	1.00	45.53	O
ATOM	424	CB	THR	A	443	18.583	56.248	8.991	1.00	45.86	C
ATOM	425	OG1	THR	A	443	19.508	56.924	9.853	1.00	45.17	O
ATOM	426	CG2	THR	A	443	18.490	54.758	9.362	1.00	45.39	C
ATOM	427	N	PHE	A	444	17.652	58.367	7.036	1.00	45.58	N
ATOM	428	CA	PHE	A	444	17.368	59.749	6.738	1.00	45.96	C
ATOM	429	C	PHE	A	444	16.823	60.442	7.973	1.00	45.93	C
ATOM	430	O	PHE	A	444	16.004	59.874	8.715	1.00	45.76	O
ATOM	431	CB	PHE	A	444	16.381	59.878	5.575	1.00	46.13	C
ATOM	432	CG	PHE	A	444	16.988	59.605	4.229	1.00	46.80	C
ATOM	433	CD1	PHE	A	444	16.914	58.336	3.663	1.00	46.84	C
ATOM	434	CD2	PHE	A	444	17.635	60.620	3.523	1.00	47.51	C
ATOM	435	CE1	PHE	A	444	17.472	58.075	2.399	1.00	48.13	C
ATOM	436	CE2	PHE	A	444	18.193	60.378	2.261	1.00	48.01	C
ATOM	437	CZ	PHE	A	444	18.116	59.095	1.699	1.00	47.97	C
ATOM	438	N	SER	A	445	17.315	61.659	8.187	1.00	45.13	N
ATOM	439	CA	SER	A	445	16.838	62.546	9.233	1.00	45.36	C
ATOM	440	C	SER	A	445	16.470	63.921	8.656	1.00	45.14	C
ATOM	441	O	SER	A	445	17.107	64.408	7.722	1.00	44.63	O
ATOM	442	CB	SER	A	445	17.892	62.692	10.323	1.00	44.93	C
ATOM	443	OG	SER	A	445	17.906	61.540	11.139	1.00	47.61	O
ATOM	444	N	LYS	A	446	15.431	64.521	9.227	1.00	44.99	N
ATOM	445	CA	LYS	A	446	14.887	65.779	8.752	1.00	45.10	C
ATOM	446	C	LYS	A	446	14.823	66.796	9.893	1.00	44.74	C
ATOM	447	O	LYS	A	446	14.564	66.444	11.046	1.00	43.91	O
ATOM	448	CB	LYS	A	446	13.484	65.571	8.188	1.00	45.17	C
ATOM	449	CG	LYS	A	446	13.383	64.609	7.008	1.00	46.07	C
ATOM	450	CD	LYS	A	446	11.929	64.368	6.623	1.00	46.72	C
ATOM	451	CE	LYS	A	446	11.148	63.665	7.745	1.00	49.16	C
ATOM	452	NZ	LYS	A	446	9.727	63.379	7.379	1.00	50.49	N
ATOM	453	N	MET	A	447	15.062	68.058	9.556	1.00	44.63	N
ATOM	454	CA	MET	A	447	14.876	69.161	10.498	1.00	44.85	C
ATOM	455	C	MET	A	447	14.425	70.432	9.765	1.00	44.10	C
ATOM	456	O	MET	A	447	14.487	70.492	8.532	1.00	43.30	O
ATOM	457	CB	MET	A	447	16.145	69.398	11.322	1.00	44.69	C
ATOM	458	CG	MET	A	447	17.390	69.770	10.526	1.00	45.76	C
ATOM	459	SD	MET	A	447	18.719	70.264	11.642	1.00	49.16	S
ATOM	460	CE	MET	A	447	20.057	70.567	10.506	1.00	47.72	C
ATOM	461	N	SER	A	448	13.929	71.404	10.535	1.00	43.13	N
ATOM	462	CA	SER	A	448	13.543	72.717	10.031	1.00	43.41	C
ATOM	463	C	SER	A	448	14.482	73.769	10.584	1.00	42.72	C
ATOM	464	O	SER	A	448	14.933	73.666	11.732	1.00	42.38	O
ATOM	465	CB	SER	A	448	12.134	73.081	10.484	1.00	43.12	C
ATOM	466	OG	SER	A	448	11.177	72.333	9.776	1.00	46.86	O

Figure 1 Table 1b - 8

ATOM	467	N	LEU A 449	14.769	74.772	9.759	1.00	42.21	N
ATOM	468	CA	LEU A 449	15.479	75.972	10.189	1.00	41.63	C
ATOM	469	C	LEU A 449	14.578	77.174	9.973	1.00	41.16	C
ATOM	470	O	LEU A 449	14.003	77.326	8.895	1.00	41.08	O
ATOM	471	CB	LEU A 449	16.773	76.148	9.404	1.00	41.67	C
ATOM	472	CG	LEU A 449	18.005	75.446	9.969	1.00	44.23	C
ATOM	473	CD1	LEU A 449	18.113	74.033	9.431	1.00	46.14	C
ATOM	474	CD2	LEU A 449	19.258	76.226	9.628	1.00	46.70	C
ATOM	475	N	GLN A 450	14.460	78.020	10.998	1.00	39.88	N
ATOM	476	CA	GLN A 450	13.641	79.214	10.923	1.00	39.52	C
ATOM	477	C	GLN A 450	14.375	80.419	11.519	1.00	39.40	C
ATOM	478	O	GLN A 450	14.757	80.404	12.692	1.00	38.80	O
ATOM	479	CB	GLN A 450	12.295	79.006	11.628	1.00	39.80	C
ATOM	480	CG	GLN A 450	11.459	80.294	11.791	1.00	38.09	C
ATOM	481	CD	GLN A 450	10.780	80.749	10.504	1.00	38.34	C
ATOM	482	OE1	GLN A 450	9.949	80.028	9.948	1.00	38.13	O
ATOM	483	NE2	GLN A 450	11.111	81.977	10.038	1.00	37.73	N
ATOM	484	N	LEU A 451	14.576	81.445	10.694	1.00	38.87	N
ATOM	485	CA	LEU A 451	15.125	82.717	11.164	1.00	38.82	C
ATOM	486	C	LEU A 451	14.032	83.627	11.720	1.00	39.18	C
ATOM	487	O	LEU A 451	13.004	83.848	11.073	1.00	39.40	O
ATOM	488	CB	LEU A 451	15.922	83.437	10.060	1.00	38.84	C
ATOM	489	CG	LEU A 451	16.826	84.616	10.493	1.00	38.96	C
ATOM	490	CD1	LEU A 451	17.933	84.132	11.431	1.00	39.48	C
ATOM	491	CD2	LEU A 451	17.452	85.318	9.303	1.00	38.05	C
ATOM	492	N	TYR A 452	14.292	84.158	12.917	1.00	39.36	N
ATOM	493	CA	TYR A 452	13.416	85.082	13.625	1.00	39.74	C
ATOM	494	C	TYR A 452	14.145	86.398	13.902	1.00	39.82	C
ATOM	495	O	TYR A 452	15.372	86.428	13.977	1.00	39.43	O
ATOM	496	CB	TYR A 452	13.020	84.507	14.984	1.00	40.22	C
ATOM	497	CG	TYR A 452	12.030	83.377	14.948	1.00	40.92	C
ATOM	498	CD1	TYR A 452	12.425	82.073	15.258	1.00	41.28	C
ATOM	499	CD2	TYR A 452	10.694	83.605	14.618	1.00	41.20	C
ATOM	500	CE1	TYR A 452	11.508	81.023	15.235	1.00	41.52	C
ATOM	501	CE2	TYR A 452	9.774	82.563	14.583	1.00	42.02	C
ATOM	502	CZ	TYR A 452	10.185	81.281	14.895	1.00	41.66	C
ATOM	503	OH	TYR A 452	9.277	80.252	14.866	1.00	43.37	O
ATOM	504	N	GLN A 453	13.385	87.476	14.064	1.00	40.01	N
ATOM	505	CA	GLN A 453	13.950	88.753	14.514	1.00	40.66	C
ATOM	506	C	GLN A 453	13.629	88.906	15.992	1.00	40.45	C
ATOM	507	O	GLN A 453	12.473	88.747	16.386	1.00	40.48	O
ATOM	508	CB	GLN A 453	13.392	89.934	13.707	1.00	40.32	C
ATOM	509	CG	GLN A 453	14.068	91.282	14.042	1.00	41.88	C
ATOM	510	CD	GLN A 453	13.610	92.443	13.165	1.00	41.10	C
ATOM	511	OE1	GLN A 453	13.166	92.256	12.042	1.00	42.55	O
ATOM	512	NE2	GLN A 453	13.731	93.649	13.684	1.00	43.44	N
ATOM	513	N	VAL A 454	14.647	89.186	16.806	1.00	40.84	N
ATOM	514	CA	VAL A 454	14.444	89.344	18.253	1.00	41.30	C
ATOM	515	C	VAL A 454	14.629	90.767	18.796	1.00	41.79	C
ATOM	516	O	VAL A 454	14.031	91.100	19.811	1.00	41.80	O
ATOM	517	CB	VAL A 454	15.267	88.334	19.110	1.00	41.46	C
ATOM	518	CG1	VAL A 454	14.731	86.914	18.937	1.00	41.06	C
ATOM	519	CG2	VAL A 454	16.755	88.411	18.798	1.00	41.49	C
ATOM	520	N	ASP A 455	15.467	91.569	18.135	1.00	42.11	N
ATOM	521	CA	ASP A 455	15.645	93.005	18.431	1.00	43.50	C
ATOM	522	C	ASP A 455	15.420	93.761	17.141	1.00	43.56	C
ATOM	523	O	ASP A 455	14.784	93.257	16.225	1.00	44.37	O
ATOM	524	CB	ASP A 455	17.073	93.319	18.903	1.00	43.12	C
ATOM	525	CG	ASP A 455	17.264	93.121	20.375	1.00	44.73	C
ATOM	526	OD1	ASP A 455	16.682	92.176	20.954	1.00	47.86	O
ATOM	527	OD2	ASP A 455	18.031	93.906	20.967	1.00	47.32	O
ATOM	528	N	SER A 456	15.966	94.968	17.067	1.00	43.91	N
ATOM	529	CA	SER A 456	16.095	95.676	15.803	1.00	44.00	C
ATOM	530	C	SER A 456	17.478	95.420	15.188	1.00	43.86	C
ATOM	531	O	SER A 456	17.712	95.720	14.017	1.00	44.36	O
ATOM	532	CB	SER A 456	15.866	97.169	16.020	1.00	43.92	C
ATOM	533	OG	SER A 456	16.326	97.544	17.308	1.00	44.97	O

Figure 1 Table 1b - 9

ATOM	534	N	ARG A 457	18.389	94.871	15.990	1.00	43.56	N
ATOM	535	CA	ARG A 457	19.741	94.520	15.533	1.00	43.32	C
ATOM	536	C	ARG A 457	19.999	92.995	15.509	1.00	42.40	C
ATOM	537	O	ARG A 457	21.039	92.543	15.016	1.00	42.58	O
ATOM	538	CB	ARG A 457	20.794	95.193	16.423	1.00	43.26	C
ATOM	539	CG	ARG A 457	20.353	96.518	17.050	1.00	44.14	C
ATOM	540	CD	ARG A 457	21.520	97.343	17.632	1.00	45.21	C
ATOM	541	NE	ARG A 457	22.555	97.609	16.632	1.00	47.48	N
ATOM	542	CZ	ARG A 457	23.751	97.026	16.615	1.00	48.20	C
ATOM	543	NH1	ARG A 457	24.096	96.155	17.558	1.00	48.31	N
ATOM	544	NH2	ARG A 457	24.615	97.325	15.657	1.00	49.41	N
ATOM	545	N	THR A 458	19.067	92.204	16.037	1.00	41.02	N
ATOM	546	CA	THR A 458	19.399	90.830	16.406	1.00	39.51	C
ATOM	547	C	THR A 458	18.442	89.782	15.825	1.00	38.60	C
ATOM	548	O	THR A 458	17.216	89.936	15.866	1.00	37.69	O
ATOM	549	CB	THR A 458	19.528	90.663	17.951	1.00	39.38	C
ATOM	550	OG1	THR A 458	20.301	91.739	18.500	1.00	40.32	O
ATOM	551	CG2	THR A 458	20.204	89.339	18.314	1.00	39.56	C
ATOM	552	N	TYR A 459	19.034	88.716	15.293	1.00	37.90	N
ATOM	553	CA	TYR A 459	18.285	87.601	14.715	1.00	37.44	C
ATOM	554	C	TYR A 459	18.640	86.305	15.429	1.00	37.38	C
ATOM	555	O	TYR A 459	19.713	86.186	16.019	1.00	36.91	O
ATOM	556	CB	TYR A 459	18.524	87.507	13.200	1.00	37.68	C
ATOM	557	CG	TYR A 459	18.318	88.857	12.542	1.00	38.00	C
ATOM	558	CD1	TYR A 459	19.390	89.722	12.338	1.00	37.67	C
ATOM	559	CD2	TYR A 459	17.040	89.297	12.216	1.00	37.99	C
ATOM	560	CE1	TYR A 459	19.196	90.990	11.782	1.00	38.72	C
ATOM	561	CE2	TYR A 459	16.831	90.539	11.660	1.00	38.53	C
ATOM	562	CZ	TYR A 459	17.913	91.387	11.448	1.00	38.60	C
ATOM	563	OH	TYR A 459	17.698	92.615	10.894	1.00	38.26	O
ATOM	564	N	LEU A 460	17.710	85.358	15.377	1.00	36.95	N
ATOM	565	CA	LEU A 460	17.838	84.084	16.055	1.00	36.97	C
ATOM	566	C	LEU A 460	17.498	82.965	15.070	1.00	36.85	C
ATOM	567	O	LEU A 460	16.429	82.963	14.445	1.00	36.84	O
ATOM	568	CB	LEU A 460	16.961	84.084	17.321	1.00	37.05	C
ATOM	569	CG	LEU A 460	16.282	82.942	18.112	1.00	37.10	C
ATOM	570	CD1	LEU A 460	16.507	81.524	17.616	1.00	37.53	C
ATOM	571	CD2	LEU A 460	16.578	83.061	19.600	1.00	35.36	C
ATOM	572	N	LEU A 461	18.444	82.047	14.902	1.00	36.86	N
ATOM	573	CA	LEU A 461	18.236	80.879	14.061	1.00	36.96	C
ATOM	574	C	LEU A 461	17.739	79.744	14.954	1.00	37.10	C
ATOM	575	O	LEU A 461	18.418	79.333	15.897	1.00	36.97	O
ATOM	576	CB	LEU A 461	19.520	80.504	13.309	1.00	36.74	C
ATOM	577	CG	LEU A 461	19.463	79.351	12.283	1.00	38.08	C
ATOM	578	CD1	LEU A 461	18.542	79.684	11.092	1.00	38.07	C
ATOM	579	CD2	LEU A 461	20.867	79.060	11.788	1.00	37.86	C
ATOM	580	N	ASP A 462	16.524	79.290	14.675	1.00	37.27	N
ATOM	581	CA	ASP A 462	15.872	78.251	15.438	1.00	38.51	C
ATOM	582	C	ASP A 462	15.908	76.923	14.652	1.00	38.39	C
ATOM	583	O	ASP A 462	15.632	76.909	13.455	1.00	38.15	O
ATOM	584	CB	ASP A 462	14.431	78.679	15.738	1.00	38.77	C
ATOM	585	CG	ASP A 462	13.605	77.571	16.354	1.00	41.36	C
ATOM	586	OD1	ASP A 462	14.074	76.911	17.302	1.00	43.88	O
ATOM	587	OD2	ASP A 462	12.476	77.347	15.877	1.00	45.94	O
ATOM	588	N	PHE A 463	16.257	75.828	15.337	1.00	38.64	N
ATOM	589	CA	PHE A 463	16.350	74.477	14.738	1.00	38.94	C
ATOM	590	C	PHE A 463	15.326	73.569	15.399	1.00	39.41	C
ATOM	591	O	PHE A 463	15.229	73.542	16.625	1.00	38.72	O
ATOM	592	CB	PHE A 463	17.718	73.833	14.992	1.00	39.21	C
ATOM	593	CG	PHE A 463	18.893	74.649	14.550	1.00	39.75	C
ATOM	594	CD1	PHE A 463	19.310	75.768	15.285	1.00	40.04	C
ATOM	595	CD2	PHE A 463	19.630	74.265	13.441	1.00	40.48	C
ATOM	596	CE1	PHE A 463	20.414	76.517	14.886	1.00	40.48	C
ATOM	597	CE2	PHE A 463	20.737	75.020	13.025	1.00	41.53	C
ATOM	598	CZ	PHE A 463	21.128	76.139	13.756	1.00	40.70	C
ATOM	599	N	ARG A 464	14.579	72.817	14.595	1.00	39.47	N
ATOM	600	CA	ARG A 464	13.557	71.935	15.121	1.00	40.60	C

Figure 1 Table 1b - 10

ATOM	601	C	ARG	A	464	13.630	70.588	14.402	1.00	40.78	C
ATOM	602	O	ARG	A	464	13.667	70.546	13.176	1.00	40.29	O
ATOM	603	CB	ARG	A	464	12.179	72.554	14.927	1.00	40.88	C
ATOM	604	CG	ARG	A	464	11.078	71.843	15.688	1.00	43.16	C
ATOM	605	CD	ARG	A	464	9.704	72.249	15.174	1.00	47.29	C
ATOM	606	NE	ARG	A	464	8.630	71.519	15.848	1.00	51.54	N
ATOM	607	CZ	ARG	A	464	8.243	70.279	15.544	1.00	53.18	C
ATOM	608	NH1	ARG	A	464	8.844	69.593	14.575	1.00	54.11	N
ATOM	609	NH2	ARG	A	464	7.253	69.718	16.223	1.00	53.95	N
ATOM	610	N	SER	A	465	13.660	69.492	15.156	1.00	41.03	N
ATOM	611	CA	SER	A	465	13.698	68.182	14.526	1.00	41.75	C
ATOM	612	C	SER	A	465	12.305	67.812	14.041	1.00	42.45	C
ATOM	613	O	SER	A	465	11.297	68.236	14.613	1.00	41.86	O
ATOM	614	CB	SER	A	465	14.248	67.101	15.476	1.00	41.74	C
ATOM	615	OG	SER	A	465	13.361	66.869	16.547	1.00	41.77	O
ATOM	616	N	ILE	A	466	12.268	67.020	12.977	1.00	43.71	N
ATOM	617	CA	ILE	A	466	11.021	66.576	12.391	1.00	45.54	C
ATOM	618	C	ILE	A	466	10.918	65.073	12.572	1.00	47.39	C
ATOM	619	O	ILE	A	466	11.794	64.327	12.125	1.00	47.27	O
ATOM	620	CB	ILE	A	466	10.938	66.946	10.900	1.00	45.10	C
ATOM	621	CG1	ILE	A	466	10.841	68.466	10.749	1.00	45.11	C
ATOM	622	CG2	ILE	A	466	9.748	66.221	10.221	1.00	44.80	C
ATOM	623	CD1	ILE	A	466	11.143	68.957	9.358	1.00	47.16	C
ATOM	624	N	ASP	A	467	9.844	64.651	13.236	1.00	50.09	N
ATOM	625	CA	ASP	A	467	9.628	63.256	13.588	1.00	52.83	C
ATOM	626	C	ASP	A	467	9.400	62.409	12.350	1.00	54.41	C
ATOM	627	O	ASP	A	467	8.783	62.861	11.383	1.00	54.71	O
ATOM	628	CB	ASP	A	467	8.433	63.118	14.545	1.00	53.04	C
ATOM	629	CG	ASP	A	467	8.622	63.902	15.849	1.00	54.61	C
ATOM	630	OD1	ASP	A	467	9.729	63.856	16.428	1.00	56.04	O
ATOM	631	OD2	ASP	A	467	7.656	64.556	16.302	1.00	56.36	O
ATOM	632	N	ASP	A	468	9.906	61.179	12.400	1.00	56.65	N
ATOM	633	CA	ASP	A	468	9.706	60.184	11.346	1.00	58.54	C
ATOM	634	C	ASP	A	468	8.232	59.957	11.019	1.00	59.46	C
ATOM	635	O	ASP	A	468	7.443	59.583	11.895	1.00	59.68	O
ATOM	636	CB	ASP	A	468	10.331	58.851	11.757	1.00	58.75	C
ATOM	637	CG	ASP	A	468	11.812	58.768	11.437	1.00	59.89	C
ATOM	638	OD1	ASP	A	468	12.291	57.630	11.210	1.00	62.01	O
ATOM	639	OD2	ASP	A	468	12.496	59.815	11.415	1.00	59.91	O
ATOM	640	N	GLU	A	469	7.881	60.198	9.755	1.00	60.59	N
ATOM	641	CA	GLU	A	469	6.558	59.888	9.191	1.00	61.57	C
ATOM	642	C	GLU	A	469	5.540	61.002	9.435	1.00	61.87	C
ATOM	643	O	GLU	A	469	4.549	61.116	8.706	1.00	62.34	O
ATOM	644	CB	GLU	A	469	6.033	58.553	9.726	1.00	61.56	C
ATOM	645	CG	GLU	A	469	5.641	57.560	8.653	1.00	62.97	C
ATOM	646	CD	GLU	A	469	5.952	56.130	9.062	1.00	64.34	C
ATOM	647	OE1	GLU	A	469	6.989	55.922	9.735	1.00	65.23	O
ATOM	648	OE2	GLU	A	469	5.169	55.218	8.710	1.00	64.39	O
ATOM	649	N	VAL	A	524	20.919	41.662	24.791	1.00	49.46	N
ATOM	650	CA	VAL	A	524	20.279	42.662	23.936	1.00	49.35	C
ATOM	651	C	VAL	A	524	21.108	43.953	23.870	1.00	49.42	C
ATOM	652	O	VAL	A	524	21.304	44.638	24.886	1.00	49.38	O
ATOM	653	CB	VAL	A	524	18.817	42.947	24.382	1.00	49.42	C
ATOM	654	CG1	VAL	A	524	18.243	44.150	23.644	1.00	49.13	C
ATOM	655	CG2	VAL	A	524	17.940	41.715	24.160	1.00	48.89	C
ATOM	656	N	ALA	A	525	21.582	44.267	22.662	1.00	49.25	N
ATOM	657	CA	ALA	A	525	22.497	45.386	22.425	1.00	49.17	C
ATOM	658	C	ALA	A	525	22.027	46.256	21.253	1.00	48.94	C
ATOM	659	O	ALA	A	525	21.615	45.726	20.220	1.00	49.21	O
ATOM	660	CB	ALA	A	525	23.915	44.866	22.176	1.00	49.10	C
ATOM	661	N	PRO	A	526	22.105	47.593	21.403	1.00	48.64	N
ATOM	662	CA	PRO	A	526	21.520	48.543	20.446	1.00	48.24	C
ATOM	663	C	PRO	A	526	22.123	48.479	19.052	1.00	47.90	C
ATOM	664	O	PRO	A	526	23.301	48.150	18.889	1.00	47.98	O
ATOM	665	CB	PRO	A	526	21.844	49.912	21.056	1.00	48.06	C
ATOM	666	CG	PRO	A	526	22.153	49.655	22.448	1.00	48.37	C
ATOM	667	CD	PRO	A	526	22.781	48.300	22.506	1.00	48.82	C

Figure 1 Table 1b - 11

ATOM	668	N	ARG A 527	21.298	48.795	18.061	1.00	47.47	N
ATOM	669	CA	ARG A 527	21.760	49.018	16.704	1.00	47.10	C
ATOM	670	C	ARG A 527	22.298	50.446	16.601	1.00	46.17	C
ATOM	671	O	ARG A 527	21.957	51.294	17.430	1.00	45.98	O
ATOM	672	CB	ARG A 527	20.604	48.819	15.722	1.00	47.17	C
ATOM	673	CG	ARG A 527	20.389	47.370	15.254	1.00	48.24	C
ATOM	674	CD	ARG A 527	19.025	47.177	14.558	1.00	48.78	C
ATOM	675	NE	ARG A 527	18.443	48.432	14.054	1.00	52.00	N
ATOM	676	CZ	ARG A 527	17.447	49.089	14.646	1.00	52.64	C
ATOM	677	NH1	ARG A 527	16.911	48.628	15.771	1.00	54.80	N
ATOM	678	NH2	ARG A 527	16.989	50.213	14.117	1.00	54.96	N
ATOM	679	N	PRO A 528	23.171	50.711	15.606	1.00	45.40	N
ATOM	680	CA	PRO A 528	23.554	52.096	15.296	1.00	44.47	C
ATOM	681	C	PRO A 528	22.338	53.019	15.074	1.00	43.68	C
ATOM	682	O	PRO A 528	21.337	52.602	14.475	1.00	44.01	O
ATOM	683	CB	PRO A 528	24.377	51.954	14.009	1.00	44.18	C
ATOM	684	CG	PRO A 528	24.936	50.557	14.066	1.00	45.32	C
ATOM	685	CD	PRO A 528	23.885	49.729	14.759	1.00	45.27	C
ATOM	686	N	GLY A 529	22.426	54.245	15.584	1.00	42.24	N
ATOM	687	CA	GLY A 529	21.398	55.250	15.376	1.00	40.96	C
ATOM	688	C	GLY A 529	20.706	55.809	16.611	1.00	39.69	C
ATOM	689	O	GLY A 529	20.434	55.092	17.561	1.00	39.51	O
ATOM	690	N	SER A 530	20.431	57.107	16.574	1.00	38.49	N
ATOM	691	CA	SER A 530	19.510	57.759	17.508	1.00	37.66	C
ATOM	692	C	SER A 530	19.033	59.031	16.846	1.00	37.06	C
ATOM	693	O	SER A 530	19.828	59.940	16.610	1.00	36.69	O
ATOM	694	CB	SER A 530	20.174	58.097	18.850	1.00	37.35	C
ATOM	695	OG	SER A 530	19.357	58.978	19.612	1.00	37.34	O
ATOM	696	N	HIS A 531	17.742	59.087	16.547	1.00	36.66	N
ATOM	697	CA	HIS A 531	17.154	60.241	15.902	1.00	37.25	C
ATOM	698	C	HIS A 531	17.484	61.535	16.665	1.00	36.51	C
ATOM	699	O	HIS A 531	17.827	62.540	16.055	1.00	36.03	O
ATOM	700	CB	HIS A 531	15.640	60.060	15.759	1.00	38.00	C
ATOM	701	CG	HIS A 531	15.000	61.069	14.856	1.00	41.28	C
ATOM	702	ND1	HIS A 531	14.473	62.256	15.317	1.00	44.19	N
ATOM	703	CD2	HIS A 531	14.818	61.074	13.511	1.00	44.36	C
ATOM	704	CE1	HIS A 531	13.988	62.947	14.300	1.00	44.05	C
ATOM	705	NE2	HIS A 531	14.188	62.256	13.193	1.00	44.81	N
ATOM	706	N	THR A 532	17.404	61.489	17.995	1.00	35.84	N
ATOM	707	CA	THR A 532	17.676	62.669	18.822	1.00	35.40	C
ATOM	708	C	THR A 532	19.140	63.082	18.781	1.00	35.17	C
ATOM	709	O	THR A 532	19.445	64.261	18.603	1.00	35.23	O
ATOM	710	CB	THR A 532	17.209	62.502	20.277	1.00	35.18	C
ATOM	711	OG1	THR A 532	15.779	62.456	20.305	1.00	36.11	O
ATOM	712	CG2	THR A 532	17.670	63.691	21.139	1.00	36.47	C
ATOM	713	N	ILE A 533	20.053	62.129	18.933	1.00	34.70	N
ATOM	714	CA	ILE A 533	21.469	62.494	18.941	1.00	34.50	C
ATOM	715	C	ILE A 533	21.923	62.983	17.556	1.00	34.99	C
ATOM	716	O	ILE A 533	22.716	63.936	17.443	1.00	34.44	O
ATOM	717	CB	ILE A 533	22.364	61.352	19.445	1.00	33.62	C
ATOM	718	CG1	ILE A 533	21.974	60.948	20.882	1.00	33.44	C
ATOM	719	CG2	ILE A 533	23.839	61.743	19.334	1.00	33.63	C
ATOM	720	CD1	ILE A 533	22.037	62.070	21.950	1.00	31.13	C
ATOM	721	N	GLU A 534	21.414	62.323	16.517	1.00	34.97	N
ATOM	722	CA	GLU A 534	21.668	62.730	15.139	1.00	36.18	C
ATOM	723	C	GLU A 534	21.150	64.129	14.798	1.00	36.24	C
ATOM	724	O	GLU A 534	21.770	64.832	14.011	1.00	36.73	O
ATOM	725	CB	GLU A 534	21.084	61.707	14.172	1.00	35.92	C
ATOM	726	CG	GLU A 534	21.854	60.415	14.183	1.00	38.20	C
ATOM	727	CD	GLU A 534	21.190	59.355	13.369	1.00	38.79	C
ATOM	728	OE1	GLU A 534	20.982	59.582	12.161	1.00	41.61	O
ATOM	729	OE2	GLU A 534	20.883	58.297	13.940	1.00	40.73	O
ATOM	730	N	PHE A 535	20.012	64.520	15.375	1.00	36.54	N
ATOM	731	CA	PHE A 535	19.504	65.895	15.220	1.00	36.37	C
ATOM	732	C	PHE A 535	20.525	66.890	15.787	1.00	36.85	C
ATOM	733	O	PHE A 535	20.853	67.905	15.139	1.00	36.44	O
ATOM	734	CB	PHE A 535	18.109	66.040	15.863	1.00	35.91	C

Figure 1 Table 1b - 12

ATOM	735	CG	PHE	A	535	17.690	67.472	16.141	1.00	36.19	C
ATOM	736	CD1	PHE	A	535	17.443	68.377	15.089	1.00	35.76	C
ATOM	737	CD2	PHE	A	535	17.535	67.913	17.448	1.00	34.94	C
ATOM	738	CE1	PHE	A	535	17.051	69.697	15.351	1.00	34.44	C
ATOM	739	CE2	PHE	A	535	17.154	69.239	17.725	1.00	35.70	C
ATOM	740	CZ	PHE	A	535	16.901	70.129	16.665	1.00	34.28	C
ATOM	741	N	PHE	A	536	21.061	66.575	16.968	1.00	36.94	N
ATOM	742	CA	PHE	A	536	22.099	67.403	17.594	1.00	37.15	C
ATOM	743	C	PHE	A	536	23.337	67.542	16.699	1.00	37.56	C
ATOM	744	O	PHE	A	536	23.883	68.647	16.535	1.00	37.14	O
ATOM	745	CB	PHE	A	536	22.515	66.848	18.967	1.00	36.58	C
ATOM	746	CG	PHE	A	536	21.449	66.962	20.035	1.00	36.41	C
ATOM	747	CD1	PHE	A	536	21.388	66.036	21.066	1.00	34.39	C
ATOM	748	CD2	PHE	A	536	20.498	67.977	19.998	1.00	36.38	C
ATOM	749	CE1	PHE	A	536	20.409	66.125	22.063	1.00	35.52	C
ATOM	750	CE2	PHE	A	536	19.512	68.074	20.981	1.00	35.61	C
ATOM	751	CZ	PHE	A	536	19.469	67.148	22.023	1.00	34.57	C
ATOM	752	N	GLU	A	537	23.777	66.419	16.137	1.00	37.93	N
ATOM	753	CA	GLU	A	537	24.963	66.399	15.291	1.00	38.70	C
ATOM	754	C	GLU	A	537	24.737	67.173	14.006	1.00	39.43	C
ATOM	755	O	GLU	A	537	25.628	67.901	13.579	1.00	39.65	O
ATOM	756	CB	GLU	A	537	25.422	64.970	14.998	1.00	38.77	C
ATOM	757	CG	GLU	A	537	25.981	64.261	16.247	1.00	38.77	C
ATOM	758	CD	GLU	A	537	26.711	62.980	15.931	1.00	40.34	C
ATOM	759	OE1	GLU	A	537	26.343	62.301	14.943	1.00	41.39	O
ATOM	760	OE2	GLU	A	537	27.650	62.640	16.687	1.00	40.75	O
ATOM	761	N	MET	A	538	23.557	67.006	13.402	1.00	39.93	N
ATOM	762	CA	MET	A	538	23.162	67.781	12.222	1.00	41.74	C
ATOM	763	C	MET	A	538	23.250	69.284	12.497	1.00	41.04	C
ATOM	764	O	MET	A	538	23.823	70.032	11.699	1.00	41.04	O
ATOM	765	CB	MET	A	538	21.739	67.449	11.794	1.00	41.04	C
ATOM	766	CG	MET	A	538	21.611	66.292	10.825	1.00	44.43	C
ATOM	767	SD	MET	A	538	20.044	66.407	9.931	1.00	46.29	S
ATOM	768	CE	MET	A	538	18.970	65.700	11.181	1.00	46.24	C
ATOM	769	N	CYS	A	539	22.654	69.711	13.612	1.00	40.73	N
ATOM	770	CA	CYS	A	539	22.703	71.112	14.047	1.00	40.83	C
ATOM	771	C	CYS	A	539	24.123	71.602	14.252	1.00	40.76	C
ATOM	772	O	CYS	A	539	24.504	72.653	13.729	1.00	40.72	O
ATOM	773	CB	CYS	A	539	21.910	71.316	15.334	1.00	40.59	C
ATOM	774	SG	CYS	A	539	20.142	71.073	15.162	1.00	42.87	S
ATOM	775	N	ALA	A	540	24.909	70.844	15.010	1.00	40.64	N
ATOM	776	CA	ALA	A	540	26.278	71.231	15.292	1.00	41.09	C
ATOM	777	C	ALA	A	540	27.101	71.322	14.006	1.00	41.49	C
ATOM	778	O	ALA	A	540	27.936	72.213	13.872	1.00	41.18	O
ATOM	779	CB	ALA	A	540	26.924	70.273	16.286	1.00	41.04	C
ATOM	780	N	ASN	A	541	26.862	70.397	13.076	1.00	41.72	N
ATOM	781	CA	ASN	A	541	27.565	70.376	11.804	1.00	42.43	C
ATOM	782	C	ASN	A	541	27.197	71.589	10.952	1.00	42.57	C
ATOM	783	O	ASN	A	541	28.070	72.237	10.370	1.00	42.00	O
ATOM	784	CB	ASN	A	541	27.276	69.083	11.029	1.00	42.71	C
ATOM	785	CG	ASN	A	541	27.918	67.854	11.663	1.00	44.49	C
ATOM	786	OD1	ASN	A	541	28.798	67.961	12.524	1.00	46.10	O
ATOM	787	ND2	ASN	A	541	27.478	66.671	11.232	1.00	45.50	N
ATOM	788	N	LEU	A	542	25.905	71.897	10.889	1.00	42.75	N
ATOM	789	CA	LEU	A	542	25.464	73.062	10.139	1.00	43.55	C
ATOM	790	C	LEU	A	542	26.022	74.358	10.711	1.00	43.46	C
ATOM	791	O	LEU	A	542	26.522	75.180	9.959	1.00	42.99	O
ATOM	792	CB	LEU	A	542	23.945	73.107	10.020	1.00	43.99	C
ATOM	793	CG	LEU	A	542	23.476	72.426	8.737	1.00	45.66	C
ATOM	794	CD1	LEU	A	542	21.986	72.241	8.769	1.00	48.00	C
ATOM	795	CD2	LEU	A	542	23.888	73.271	7.521	1.00	46.25	C
ATOM	796	N	ILE	A	543	25.962	74.509	12.034	1.00	43.57	N
ATOM	797	CA	ILE	A	543	26.510	75.671	12.727	1.00	43.98	C
ATOM	798	C	ILE	A	543	28.013	75.846	12.458	1.00	44.54	C
ATOM	799	O	ILE	A	543	28.462	76.921	12.041	1.00	44.39	O
ATOM	800	CB	ILE	A	543	26.205	75.623	14.248	1.00	43.93	C
ATOM	801	CG1	ILE	A	543	24.705	75.859	14.490	1.00	43.77	C

Figure 1 Table 1b - 13

ATOM	802	CG2	ILE A 543	27.045	76.664	15.011	1.00	43.65	C
ATOM	803	CD1	ILE A 543	24.225	75.515	15.911	1.00	43.39	C
ATOM	804	N	LYS A 544	28.784	74.783	12.679	1.00	44.97	N
ATOM	805	CA	LYS A 544	30.229	74.821	12.466	1.00	45.42	C
ATOM	806	C	LYS A 544	30.597	75.331	11.067	1.00	45.63	C
ATOM	807	O	LYS A 544	31.538	76.117	10.904	1.00	45.26	O
ATOM	808	CB	LYS A 544	30.845	73.437	12.709	1.00	45.36	C
ATOM	809	CG	LYS A 544	32.323	73.348	12.384	1.00	46.15	C
ATOM	810	CD	LYS A 544	32.969	72.086	12.929	1.00	48.67	C
ATOM	811	CE	LYS A 544	34.494	72.167	12.783	1.00	49.92	C
ATOM	812	NZ	LYS A 544	35.209	71.071	13.510	1.00	51.36	N
ATOM	813	N	ASN A 545	29.740	74.977	10.065	1.00	45.82	N
ATOM	814	CA	ASN A 545	30.066	75.179	8.657	1.00	46.42	C
ATOM	815	CB	ASN A 545	29.686	73.936	7.852	1.00	46.49	C
ATOM	816	CG	ASN A 545	30.779	72.896	7.858	1.00	47.03	C
ATOM	817	OD1	ASN A 545	31.733	72.986	7.090	1.00	48.68	O
ATOM	818	ND2	ASN A 545	30.649	71.899	8.727	1.00	46.62	N
ATOM	819	C	ASN A 545	29.519	76.441	7.985	1.00	46.51	C
ATOM	820	O	ASN A 545	29.913	76.762	6.869	1.00	46.61	O
ATOM	821	N	SER A 546	28.628	77.157	8.662	1.00	46.69	N
ATOM	822	CA	SER A 546	27.962	78.306	8.057	1.00	47.33	C
ATOM	823	CB	SER A 546	26.455	78.102	8.139	1.00	46.98	C
ATOM	824	OG	SER A 546	26.051	77.958	9.488	1.00	46.93	O
ATOM	825	C	SER A 546	28.308	79.628	8.748	1.00	47.81	C
ATOM	826	O	SER A 546	27.857	80.695	8.337	1.00	47.72	O
ATOM	827	N	CYS A 547	29.151	79.545	9.767	1.00	48.43	N
ATOM	828	CA	CYS A 547	28.946	80.334	10.952	1.00	48.77	C
ATOM	829	CB	CYS A 547	27.883	79.567	11.730	1.00	49.14	C
ATOM	830	SG	CYS A 547	27.190	80.291	13.127	1.00	50.01	S
ATOM	831	C	CYS A 547	30.226	80.398	11.763	1.00	49.19	C
ATOM	832	O	CYS A 547	30.985	79.426	11.809	1.00	49.17	O
ATOM	833	N	THR A 548	30.462	81.537	12.411	1.00	49.53	N
ATOM	834	CA	THR A 548	31.647	81.721	13.250	1.00	49.87	C
ATOM	835	CB	THR A 548	32.796	82.387	12.437	1.00	49.96	C
ATOM	836	OG1	THR A 548	33.703	81.375	11.988	1.00	50.19	O
ATOM	837	CG2	THR A 548	33.557	83.410	13.241	1.00	50.04	C
ATOM	838	C	THR A 548	31.310	82.462	14.549	1.00	50.03	C
ATOM	839	O	THR A 548	30.463	83.345	14.559	1.00	49.66	O
ATOM	840	N	VAL A 549	31.950	82.067	15.645	1.00	50.72	N
ATOM	841	CA	VAL A 549	31.734	82.707	16.947	1.00	51.50	C
ATOM	842	CB	VAL A 549	32.379	81.887	18.095	1.00	51.53	C
ATOM	843	CG1	VAL A 549	32.112	82.528	19.458	1.00	51.42	C
ATOM	844	CG2	VAL A 549	31.869	80.454	18.079	1.00	51.81	C
ATOM	845	C	VAL A 549	32.295	84.134	16.953	1.00	52.00	C
ATOM	846	O	VAL A 549	33.356	84.390	16.383	1.00	52.03	O
ATOM	847	N	ASN A 550	31.564	85.053	17.579	1.00	52.69	N
ATOM	848	CA	ASN A 550	32.048	86.415	17.816	1.00	53.55	C
ATOM	849	CB	ASN A 550	30.922	87.431	17.633	1.00	53.71	C
ATOM	850	CG	ASN A 550	30.569	87.651	16.181	1.00	54.26	C
ATOM	851	OD1	ASN A 550	31.416	88.045	15.376	1.00	55.52	O
ATOM	852	ND2	ASN A 550	29.308	87.419	15.841	1.00	53.84	N
ATOM	853	C	ASN A 550	32.657	86.573	19.208	1.00	53.76	C
ATOM	854	O	ASN A 550	32.069	86.138	20.202	1.00	54.26	O
TER	855		ASN A 550						
ATOM	856	N	GLY B 190	-0.551	94.442	-28.859	1.00	46.65	N
ATOM	857	CA	GLY B 190	0.192	93.570	-27.899	1.00	46.39	C
ATOM	858	C	GLY B 190	1.003	94.370	-26.894	1.00	46.25	C
ATOM	859	O	GLY B 190	2.229	94.479	-27.016	1.00	46.62	O
ATOM	860	N	GLN B 191	0.316	94.915	-25.893	1.00	45.63	N
ATOM	861	CA	GLN B 191	0.926	95.806	-24.905	1.00	44.75	C
ATOM	862	C	GLN B 191	1.860	95.062	-23.954	1.00	44.54	C
ATOM	863	O	GLN B 191	1.624	93.897	-23.618	1.00	44.79	O
ATOM	864	CB	GLN B 191	-0.171	96.538	-24.120	1.00	44.60	C
ATOM	865	CG	GLN B 191	0.303	97.675	-23.217	1.00	43.84	C
ATOM	866	CD	GLN B 191	-0.808	98.210	-22.319	1.00	44.08	C
ATOM	867	OE1	GLN B 191	-1.650	97.452	-21.834	1.00	43.56	O
ATOM	868	NE2	GLN B 191	-0.812	99.519	-22.093	1.00	41.81	N

Figure 1 Table 1b - 14

ATOM	869	N	GLU	B	192	2.925	95.743	-23.532	1.00	44.17	N
ATOM	870	CA	GLU	B	192	3.807	95.245	-22.477	1.00	43.96	C
ATOM	871	C	GLU	B	192	3.006	95.031	-21.191	1.00	43.97	C
ATOM	872	O	GLU	B	192	2.077	95.790	-20.895	1.00	43.54	O
ATOM	873	CB	GLU	B	192	4.977	96.215	-22.239	1.00	43.98	C
ATOM	874	CG	GLU	B	192	4.635	97.535	-21.493	1.00	43.38	C
ATOM	875	CD	GLU	B	192	3.879	98.571	-22.331	1.00	42.99	C
ATOM	876	OE1	GLU	B	192	3.949	98.546	-23.581	1.00	42.73	O
ATOM	877	OE2	GLU	B	192	3.206	99.430	-21.725	1.00	41.59	O
ATOM	878	N	MET	B	193	3.358	93.992	-20.443	1.00	43.99	N
ATOM	879	CA	MET	B	193	2.669	93.674	-19.194	1.00	44.37	C
ATOM	880	C	MET	B	193	3.484	94.065	-17.970	1.00	43.71	C
ATOM	881	O	MET	B	193	4.716	94.003	-17.983	1.00	43.82	O
ATOM	882	CB	MET	B	193	2.273	92.196	-19.140	1.00	44.55	C
ATOM	883	CG	MET	B	193	1.124	91.856	-20.094	1.00	45.52	C
ATOM	884	SD	MET	B	193	0.004	90.598	-19.447	1.00	46.44	S
ATOM	885	CE	MET	B	193	-1.259	90.653	-20.713	1.00	44.96	C
ATOM	886	N	TYR	B	194	2.779	94.457	-16.914	1.00	42.89	N
ATOM	887	CA	TYR	B	194	3.401	95.012	-15.723	1.00	42.30	C
ATOM	888	C	TYR	B	194	3.336	94.064	-14.536	1.00	42.47	C
ATOM	889	O	TYR	B	194	2.367	93.323	-14.367	1.00	42.53	O
ATOM	890	CB	TYR	B	194	2.760	96.368	-15.380	1.00	41.84	C
ATOM	891	CG	TYR	B	194	3.011	97.410	-16.446	1.00	41.20	C
ATOM	892	CD1	TYR	B	194	2.305	97.386	-17.652	1.00	40.42	C
ATOM	893	CD2	TYR	B	194	3.967	98.411	-16.261	1.00	41.22	C
ATOM	894	CE1	TYR	B	194	2.536	98.328	-18.643	1.00	40.30	C
ATOM	895	CE2	TYR	B	194	4.206	99.369	-17.250	1.00	40.78	C
ATOM	896	CZ	TYR	B	194	3.487	99.315	-18.438	1.00	40.59	C
ATOM	897	OH	TYR	B	194	3.710	100.248	-19.424	1.00	41.38	O
ATOM	898	N	ALA	B	195	4.384	94.094	-13.723	1.00	42.48	N
ATOM	899	CA	ALA	B	195	4.476	93.243	-12.555	1.00	42.86	C
ATOM	900	C	ALA	B	195	4.382	94.064	-11.275	1.00	43.15	C
ATOM	901	O	ALA	B	195	5.088	95.056	-11.105	1.00	42.31	O
ATOM	902	CB	ALA	B	195	5.762	92.446	-12.580	1.00	42.67	C
ATOM	903	N	PHE	B	196	3.508	93.618	-10.379	1.00	44.00	N
ATOM	904	CA	PHE	B	196	3.301	94.250	-9.089	1.00	45.34	C
ATOM	905	C	PHE	B	196	3.874	93.328	-8.019	1.00	47.52	C
ATOM	906	O	PHE	B	196	3.373	92.218	-7.802	1.00	47.09	O
ATOM	907	CB	PHE	B	196	1.812	94.498	-8.854	1.00	43.94	C
ATOM	908	CG	PHE	B	196	1.205	95.502	-9.800	1.00	42.41	C
ATOM	909	CD1	PHE	B	196	0.876	95.146	-11.108	1.00	39.67	C
ATOM	910	CD2	PHE	B	196	0.954	96.807	-9.380	1.00	40.00	C
ATOM	911	CE1	PHE	B	196	0.310	96.081	-11.987	1.00	39.88	C
ATOM	912	CE2	PHE	B	196	0.386	97.745	-10.257	1.00	38.86	C
ATOM	913	CZ	PHE	B	196	0.068	97.378	-11.556	1.00	39.31	C
ATOM	914	N	ARG	B	197	4.937	93.795	-7.371	1.00	50.60	N
ATOM	915	CA	ARG	B	197	5.673	92.988	-6.401	1.00	53.95	C
ATOM	916	C	ARG	B	197	5.478	93.526	-5.000	1.00	56.02	C
ATOM	917	O	ARG	B	197	6.039	94.571	-4.649	1.00	56.01	O
ATOM	918	CB	ARG	B	197	7.168	92.979	-6.727	1.00	54.04	C
ATOM	919	CG	ARG	B	197	7.530	92.168	-7.942	1.00	55.44	C
ATOM	920	CD	ARG	B	197	8.927	92.513	-8.460	1.00	57.95	C
ATOM	921	NE	ARG	B	197	9.190	91.985	-9.806	1.00	59.99	N
ATOM	922	CZ	ARG	B	197	8.687	90.850	-10.297	1.00	60.39	C
ATOM	923	NH1	ARG	B	197	7.883	90.092	-9.557	1.00	60.03	N
ATOM	924	NH2	ARG	B	197	8.996	90.462	-11.532	1.00	60.25	N
ATOM	925	N	SER	B	198	4.689	92.795	-4.210	1.00	58.82	N
ATOM	926	CA	SER	B	198	4.476	93.083	-2.786	1.00	61.59	C
ATOM	927	C	SER	B	198	5.796	93.393	-2.085	1.00	63.29	C
ATOM	928	O	SER	B	198	5.832	94.146	-1.105	1.00	63.80	O
ATOM	929	CB	SER	B	198	3.797	91.891	-2.103	1.00	61.68	C
ATOM	930	OG	SER	B	198	4.512	90.690	-2.347	1.00	62.14	O
ATOM	931	N	GLU	B	199	6.866	92.789	-2.608	1.00	65.35	N
ATOM	932	CA	GLU	B	199	8.256	93.082	-2.250	1.00	67.21	C
ATOM	933	C	GLU	B	199	8.575	92.680	-0.815	1.00	67.94	C
ATOM	934	O	GLU	B	199	9.445	91.829	-0.571	1.00	68.39	O
ATOM	935	CB	GLU	B	199	8.589	94.565	-2.497	1.00	67.12	C

Figure 1 Table 1b - 15

ATOM	936	CG	GLU	B	199	10.021	94.827	-2.959	1.00	68.02	C
ATOM	937	CD	GLU	B	199	10.387	96.307	-2.948	1.00	68.57	C
ATOM	938	OE1	GLU	B	199	9.505	97.158	-3.216	1.00	69.55	O
ATOM	939	OE2	GLU	B	199	11.566	96.622	-2.667	1.00	70.18	O
ATOM	940	N	GLU	B	200	7.844	93.274	0.125	1.00	68.80	N
ATOM	941	CA	GLU	B	200	8.149	93.146	1.538	1.00	69.32	C
ATOM	942	C	GLU	B	200	7.000	92.568	2.377	1.00	69.28	C
ATOM	943	O	GLU	B	200	6.378	93.265	3.190	1.00	69.53	O
ATOM	944	CB	GLU	B	200	8.638	94.498	2.080	1.00	69.76	C
ATOM	945	CG	GLU	B	200	10.162	94.678	1.997	1.00	71.21	C
ATOM	946	CD	GLU	B	200	10.696	94.910	0.596	1.00	72.81	C
ATOM	947	OE1	GLU	B	200	10.483	96.017	0.056	1.00	73.84	O
ATOM	948	OE2	GLU	B	200	11.358	93.995	0.054	1.00	72.98	O
ATOM	949	N	ARG	B	201	6.713	91.290	2.128	1.00	68.99	N
ATOM	950	CA	ARG	B	201	6.008	90.424	3.069	1.00	68.72	C
ATOM	951	C	ARG	B	201	7.086	89.779	3.932	1.00	67.91	C
ATOM	952	O	ARG	B	201	6.859	89.411	5.092	1.00	67.76	O
ATOM	953	CB	ARG	B	201	5.282	89.299	2.331	1.00	68.89	C
ATOM	954	CG	ARG	B	201	4.131	89.706	1.411	1.00	69.55	C
ATOM	955	CD	ARG	B	201	3.500	88.453	0.770	1.00	69.71	C
ATOM	956	NE	ARG	B	201	3.456	87.318	1.702	1.00	71.17	N
ATOM	957	CZ	ARG	B	201	2.502	87.115	2.612	1.00	71.71	C
ATOM	958	NH1	ARG	B	201	1.485	87.964	2.723	1.00	71.95	N
ATOM	959	NH2	ARG	B	201	2.564	86.058	3.416	1.00	71.97	N
ATOM	960	N	PHE	B	202	8.256	89.622	3.317	1.00	66.89	N
ATOM	961	CA	PHE	B	202	9.426	89.029	3.937	1.00	65.84	C
ATOM	962	C	PHE	B	202	10.565	90.046	3.886	1.00	65.46	C
ATOM	963	O	PHE	B	202	11.690	89.721	3.483	1.00	65.30	O
ATOM	964	CB	PHE	B	202	9.812	87.731	3.213	1.00	65.53	C
ATOM	965	CG	PHE	B	202	8.768	86.649	3.301	1.00	64.69	C
ATOM	966	CD1	PHE	B	202	7.887	86.428	2.247	1.00	63.75	C
ATOM	967	CD2	PHE	B	202	8.668	85.849	4.437	1.00	64.04	C
ATOM	968	CE1	PHE	B	202	6.919	85.427	2.323	1.00	63.50	C
ATOM	969	CE2	PHE	B	202	7.700	84.841	4.524	1.00	63.96	C
ATOM	970	CZ	PHE	B	202	6.825	84.631	3.465	1.00	63.99	C
ATOM	971	N	LYS	B	203	10.244	91.287	4.266	1.00	64.83	N
ATOM	972	CA	LYS	B	203	11.236	92.342	4.453	1.00	64.27	C
ATOM	973	C	LYS	B	203	12.254	91.860	5.473	1.00	63.64	C
ATOM	974	O	LYS	B	203	13.449	91.753	5.187	1.00	63.75	O
ATOM	975	CB	LYS	B	203	10.557	93.620	4.969	1.00	64.41	C
ATOM	976	CG	LYS	B	203	11.506	94.790	5.232	1.00	64.50	C
ATOM	977	CD	LYS	B	203	10.793	95.962	5.908	1.00	64.75	C
ATOM	978	CE	LYS	B	203	10.090	96.874	4.904	1.00	64.58	C
ATOM	979	NZ	LYS	B	203	9.492	98.060	5.585	1.00	65.44	N
ATOM	980	N	SER	B	204	11.747	91.555	6.662	1.00	62.73	N
ATOM	981	CA	SER	B	204	12.557	91.070	7.758	1.00	62.01	C
ATOM	982	C	SER	B	204	12.016	89.721	8.233	1.00	61.43	C
ATOM	983	O	SER	B	204	10.833	89.426	8.028	1.00	61.13	O
ATOM	984	CB	SER	B	204	12.518	92.082	8.898	1.00	62.00	C
ATOM	985	OG	SER	B	204	11.186	92.286	9.331	1.00	62.09	O
ATOM	986	N	PRO	B	205	12.880	88.892	8.859	1.00	60.91	N
ATOM	987	CA	PRO	B	205	12.408	87.677	9.505	1.00	60.75	C
ATOM	988	C	PRO	B	205	11.239	87.957	10.445	1.00	60.99	C
ATOM	989	O	PRO	B	205	11.172	89.039	11.034	1.00	60.94	O
ATOM	990	CB	PRO	B	205	13.627	87.218	10.305	1.00	60.57	C
ATOM	991	CG	PRO	B	205	14.773	87.725	9.556	1.00	60.33	C
ATOM	992	CD	PRO	B	205	14.344	89.029	8.967	1.00	60.78	C
ATOM	993	N	PRO	B	206	10.322	86.987	10.596	1.00	61.41	N
ATOM	994	CA	PRO	B	206	9.190	87.188	11.491	1.00	61.96	C
ATOM	995	C	PRO	B	206	9.650	87.505	12.906	1.00	62.85	C
ATOM	996	O	PRO	B	206	10.721	87.060	13.326	1.00	62.64	O
ATOM	997	CB	PRO	B	206	8.480	85.827	11.473	1.00	61.71	C
ATOM	998	CG	PRO	B	206	9.481	84.869	10.940	1.00	61.24	C
ATOM	999	CD	PRO	B	206	10.290	85.649	9.976	1.00	61.19	C
ATOM	1000	N	ILE	B	207	8.847	88.277	13.631	1.00	64.06	N
ATOM	1001	CA	ILE	B	207	9.116	88.518	15.044	1.00	65.46	C
ATOM	1002	C	ILE	B	207	8.919	87.203	15.775	1.00	66.14	C

Figure 1 Table 1b - 16

ATOM	1003	O	ILE	B	207	8.180	86.333	15.306	1.00	66.15	O
ATOM	1004	CB	ILE	B	207	8.247	89.658	15.649	1.00	65.34	C
ATOM	1005	CG1	ILE	B	207	6.749	89.315	15.620	1.00	65.89	C
ATOM	1006	CG2	ILE	B	207	8.527	90.971	14.935	1.00	65.67	C
ATOM	1007	CD1	ILE	B	207	6.215	88.682	16.906	1.00	65.72	C
ATOM	1008	N	LEU	B	208	9.580	87.059	16.916	1.00	67.36	N
ATOM	1009	CA	LEU	B	208	9.696	85.753	17.553	1.00	68.25	C
ATOM	1010	C	LEU	B	208	8.370	85.055	17.921	1.00	69.15	C
ATOM	1011	O	LEU	B	208	7.904	84.213	17.155	1.00	69.35	O
ATOM	1012	CB	LEU	B	208	10.687	85.791	18.733	1.00	68.35	C
ATOM	1013	CG	LEU	B	208	11.023	84.484	19.465	1.00	67.78	C
ATOM	1014	CD1	LEU	B	208	11.597	83.430	18.532	1.00	67.53	C
ATOM	1015	CD2	LEU	B	208	11.987	84.764	20.591	1.00	68.10	C
ATOM	1016	N	PRO	B	209	7.741	85.438	19.052	1.00	70.00	N
ATOM	1017	CA	PRO	B	209	6.926	84.475	19.811	1.00	70.71	C
ATOM	1018	C	PRO	B	209	5.667	83.857	19.162	1.00	71.33	C
ATOM	1019	O	PRO	B	209	4.623	84.518	19.079	1.00	71.53	O
ATOM	1020	CB	PRO	B	209	6.554	85.252	21.089	1.00	70.74	C
ATOM	1021	CG	PRO	B	209	6.627	86.676	20.703	1.00	70.35	C
ATOM	1022	CD	PRO	B	209	7.723	86.778	19.676	1.00	70.11	C
ATOM	1023	N	PRO	B	210	5.782	82.592	18.700	1.00	71.72	N
ATOM	1024	CA	PRO	B	210	4.678	81.644	18.782	1.00	72.07	C
ATOM	1025	C	PRO	B	210	4.943	80.912	20.100	1.00	72.37	C
ATOM	1026	O	PRO	B	210	5.341	79.738	20.111	1.00	72.42	O
ATOM	1027	CB	PRO	B	210	4.904	80.732	17.570	1.00	72.09	C
ATOM	1028	CG	PRO	B	210	6.342	80.975	17.125	1.00	72.06	C
ATOM	1029	CD	PRO	B	210	6.955	81.977	18.057	1.00	71.75	C
ATOM	1030	N	HIS	B	211	4.702	81.635	21.193	1.00	72.53	N
ATOM	1031	CA	HIS	B	211	5.542	81.583	22.398	1.00	72.76	C
ATOM	1032	C	HIS	B	211	6.783	80.703	22.499	1.00	72.53	C
ATOM	1033	O	HIS	B	211	6.854	79.764	23.303	1.00	72.53	O
ATOM	1034	CB	HIS	B	211	4.778	81.712	23.710	1.00	73.00	C
ATOM	1035	CG	HIS	B	211	5.180	82.924	24.490	1.00	74.04	C
ATOM	1036	ND1	HIS	B	211	5.866	82.848	25.684	1.00	75.05	N
ATOM	1037	CD2	HIS	B	211	5.050	84.245	24.215	1.00	74.90	C
ATOM	1038	CE1	HIS	B	211	6.109	84.069	26.128	1.00	75.36	C
ATOM	1039	NE2	HIS	B	211	5.625	84.936	25.255	1.00	75.50	N
ATOM	1040	N	LEU	B	212	7.763	81.043	21.668	1.00	72.22	N
ATOM	1041	CA	LEU	B	212	9.096	80.489	21.762	1.00	71.73	C
ATOM	1042	C	LEU	B	212	9.923	81.394	22.656	1.00	71.38	C
ATOM	1043	O	LEU	B	212	10.172	82.553	22.321	1.00	71.43	O
ATOM	1044	CB	LEU	B	212	9.730	80.385	20.375	1.00	71.83	C
ATOM	1045	CG	LEU	B	212	9.452	79.116	19.573	1.00	71.38	C
ATOM	1046	CD1	LEU	B	212	9.869	79.320	18.128	1.00	71.42	C
ATOM	1047	CD2	LEU	B	212	10.167	77.913	20.189	1.00	70.73	C
ATOM	1048	N	LEU	B	213	10.326	80.866	23.806	1.00	70.99	N
ATOM	1049	CA	LEU	B	213	11.149	81.625	24.739	1.00	70.52	C
ATOM	1050	C	LEU	B	213	12.622	81.543	24.353	1.00	70.07	C
ATOM	1051	O	LEU	B	213	13.171	80.447	24.173	1.00	70.14	O
ATOM	1052	CB	LEU	B	213	10.929	81.144	26.178	1.00	70.68	C
ATOM	1053	CG	LEU	B	213	9.596	81.499	26.849	1.00	70.76	C
ATOM	1054	CD1	LEU	B	213	9.372	80.632	28.082	1.00	71.27	C
ATOM	1055	CD2	LEU	B	213	9.521	82.983	27.206	1.00	71.10	C
ATOM	1056	N	GLN	B	214	13.240	82.716	24.213	1.00	69.40	N
ATOM	1057	CA	GLN	B	214	14.667	82.844	23.916	1.00	68.89	C
ATOM	1058	C	GLN	B	214	15.536	82.135	24.941	1.00	68.43	C
ATOM	1059	O	GLN	B	214	16.583	81.590	24.602	1.00	68.03	O
ATOM	1060	CB	GLN	B	214	15.071	84.317	23.913	1.00	68.89	C
ATOM	1061	CG	GLN	B	214	14.937	85.025	22.592	1.00	69.13	C
ATOM	1062	CD	GLN	B	214	15.620	86.371	22.606	1.00	68.94	C
ATOM	1063	OE1	GLN	B	214	16.842	86.456	22.716	1.00	69.00	O
ATOM	1064	NE2	GLN	B	214	14.834	87.434	22.500	1.00	69.50	N
ATOM	1065	N	VAL	B	215	15.102	82.186	26.199	1.00	68.21	N
ATOM	1066	CA	VAL	B	215	15.882	81.703	27.328	1.00	68.25	C
ATOM	1067	C	VAL	B	215	15.004	80.862	28.253	1.00	68.41	C
ATOM	1068	O	VAL	B	215	13.894	81.260	28.604	1.00	68.29	O
ATOM	1069	CB	VAL	B	215	16.516	82.880	28.140	1.00	68.21	C

Figure 1 Table 1b - 17

ATOM	1070	CG1	VAL	B	215	17.406	82.357	29.262	1.00	68.00	C
ATOM	1071	CG2	VAL	B	215	17.314	83.817	27.235	1.00	68.11	C
ATOM	1072	N	ILE	B	216	15.505	79.689	28.625	1.00	68.76	N
ATOM	1073	CA	ILE	B	216	14.897	78.886	29.681	1.00	69.29	C
ATOM	1074	C	ILE	B	216	15.887	78.829	30.836	1.00	69.80	C
ATOM	1075	O	ILE	B	216	17.031	78.406	30.658	1.00	69.59	O
ATOM	1076	CB	ILE	B	216	14.543	77.445	29.208	1.00	69.18	C
ATOM	1077	CG1	ILE	B	216	13.701	77.463	27.918	1.00	69.09	C
ATOM	1078	CG2	ILE	B	216	13.861	76.651	30.329	1.00	68.97	C
ATOM	1079	CD1	ILE	B	216	12.358	78.184	28.008	1.00	68.79	C
ATOM	1080	N	LEU	B	217	15.448	79.273	32.010	1.00	70.71	N
ATOM	1081	CA	LEU	B	217	16.289	79.256	33.204	1.00	71.77	C
ATOM	1082	C	LEU	B	217	15.957	78.075	34.111	1.00	72.40	C
ATOM	1083	O	LEU	B	217	14.882	78.024	34.712	1.00	72.50	O
ATOM	1084	CB	LEU	B	217	16.173	80.580	33.965	1.00	71.71	C
ATOM	1085	CG	LEU	B	217	16.926	81.772	33.369	1.00	72.03	C
ATOM	1086	CD1	LEU	B	217	16.281	83.097	33.773	1.00	72.15	C
ATOM	1087	CD2	LEU	B	217	18.403	81.738	33.762	1.00	72.27	C
ATOM	1088	N	ASN	B	218	16.887	77.124	34.192	1.00	73.33	N
ATOM	1089	CA	ASN	B	218	16.720	75.925	35.015	1.00	74.30	C
ATOM	1090	C	ASN	B	218	17.701	75.857	36.186	1.00	74.83	C
ATOM	1091	O	ASN	B	218	18.897	75.620	36.001	1.00	74.92	O
ATOM	1092	CB	ASN	B	218	16.827	74.654	34.158	1.00	74.33	C
ATOM	1093	CG	ASN	B	218	15.639	74.471	33.220	1.00	74.90	C
ATOM	1094	OD1	ASN	B	218	14.647	75.197	33.299	1.00	75.61	O
ATOM	1095	ND2	ASN	B	218	15.738	73.491	32.329	1.00	75.41	N
ATOM	1096	N	LYS	B	219	17.183	76.071	37.391	1.00	75.59	N
ATOM	1097	CA	LYS	B	219	17.979	75.951	38.610	1.00	76.34	C
ATOM	1098	C	LYS	B	219	17.580	74.695	39.385	1.00	76.88	C
ATOM	1099	O	LYS	B	219	16.391	74.437	39.591	1.00	77.01	O
ATOM	1100	CB	LYS	B	219	17.820	77.205	39.485	1.00	76.28	C
ATOM	1101	CG	LYS	B	219	18.504	77.153	40.861	1.00	76.43	C
ATOM	1102	CD	LYS	B	219	20.030	77.195	40.767	1.00	76.57	C
ATOM	1103	CE	LYS	B	219	20.674	77.567	42.102	1.00	76.65	C
ATOM	1104	NZ	LYS	B	219	20.576	76.485	43.128	1.00	76.62	N
ATOM	1105	N	ASP	B	220	18.577	73.911	39.790	1.00	77.47	N
ATOM	1106	CA	ASP	B	220	18.367	72.836	40.750	1.00	78.07	C
ATOM	1107	C	ASP	B	220	18.154	73.508	42.107	1.00	78.42	C
ATOM	1108	O	ASP	B	220	19.115	73.798	42.828	1.00	78.50	O
ATOM	1109	CB	ASP	B	220	19.565	71.876	40.778	1.00	78.12	C
ATOM	1110	CG	ASP	B	220	19.744	71.106	39.469	1.00	78.41	C
ATOM	1111	OD1	ASP	B	220	20.027	69.887	39.531	1.00	78.26	O
ATOM	1112	OD2	ASP	B	220	19.610	71.713	38.381	1.00	78.61	O
ATOM	1113	N	THR	B	221	16.885	73.768	42.429	1.00	78.80	N
ATOM	1114	CA	THR	B	221	16.494	74.572	43.596	1.00	79.17	C
ATOM	1115	C	THR	B	221	17.109	74.078	44.912	1.00	79.38	C
ATOM	1116	O	THR	B	221	17.564	74.884	45.730	1.00	79.46	O
ATOM	1117	CB	THR	B	221	14.947	74.682	43.725	1.00	79.20	C
ATOM	1118	OG1	THR	B	221	14.381	75.060	42.463	1.00	79.25	O
ATOM	1119	CG2	THR	B	221	14.553	75.720	44.780	1.00	79.27	C
ATOM	1120	N	ASN	B	222	17.121	72.759	45.103	1.00	79.57	N
ATOM	1121	CA	ASN	B	222	17.747	72.152	46.277	1.00	79.73	C
ATOM	1122	C	ASN	B	222	19.198	71.747	46.010	1.00	79.77	C
ATOM	1123	O	ASN	B	222	19.607	71.582	44.857	1.00	79.81	O
ATOM	1124	CB	ASN	B	222	16.930	70.951	46.776	1.00	79.78	C
ATOM	1125	CG	ASN	B	222	17.077	69.722	45.886	1.00	80.03	C
ATOM	1126	OD1	ASN	B	222	16.941	69.796	44.661	1.00	80.35	O
ATOM	1127	ND2	ASN	B	222	17.348	68.579	46.507	1.00	80.07	N
ATOM	1128	N	PRO	B	233	3.177	72.092	31.646	1.00	68.13	N
ATOM	1129	CA	PRO	B	233	4.507	72.609	31.319	1.00	67.95	C
ATOM	1130	C	PRO	B	233	4.440	73.686	30.235	1.00	67.65	C
ATOM	1131	O	PRO	B	233	3.371	74.261	30.000	1.00	67.84	O
ATOM	1132	CB	PRO	B	233	5.249	71.368	30.800	1.00	68.03	C
ATOM	1133	CG	PRO	B	233	4.528	70.209	31.407	1.00	68.19	C
ATOM	1134	CD	PRO	B	233	3.091	70.629	31.483	1.00	68.24	C
ATOM	1135	N	ASN	B	234	5.578	73.966	29.599	1.00	67.14	N
ATOM	1136	CA	ASN	B	234	5.616	74.825	28.415	1.00	66.49	C

Figure 1 Table 1b - 18

ATOM	1137	C	ASN	B	234	5.125	74.036	27.206	1.00	65.65	C
ATOM	1138	O	ASN	B	234	5.691	72.989	26.864	1.00	65.69	O
ATOM	1139	CB	ASN	B	234	7.032	75.357	28.165	1.00	66.86	C
ATOM	1140	CG	ASN	B	234	7.401	76.527	29.073	1.00	67.31	C
ATOM	1141	OD1	ASN	B	234	7.812	77.588	28.595	1.00	68.28	O
ATOM	1142	ND2	ASN	B	234	7.270	76.335	30.383	1.00	67.58	N
ATOM	1143	N	HIS	B	235	4.077	74.552	26.565	1.00	64.45	N
ATOM	1144	CA	HIS	B	235	3.310	73.807	25.554	1.00	63.08	C
ATOM	1145	C	HIS	B	235	4.144	73.036	24.509	1.00	61.58	C
ATOM	1146	O	HIS	B	235	4.242	71.803	24.580	1.00	61.46	O
ATOM	1147	CB	HIS	B	235	2.247	74.704	24.890	1.00	63.38	C
ATOM	1148	CG	HIS	B	235	1.201	75.209	25.840	1.00	64.22	C
ATOM	1149	ND1	HIS	B	235	0.623	74.413	26.808	1.00	65.05	N
ATOM	1150	CD2	HIS	B	235	0.617	76.426	25.958	1.00	64.79	C
ATOM	1151	CE1	HIS	B	235	-0.262	75.121	27.489	1.00	65.24	C
ATOM	1152	NE2	HIS	B	235	-0.287	76.345	26.992	1.00	65.28	N
ATOM	1153	N	VAL	B	236	4.740	73.757	23.556	1.00	59.54	N
ATOM	1154	CA	VAL	B	236	5.504	73.108	22.484	1.00	57.41	C
ATOM	1155	C	VAL	B	236	6.808	73.839	22.069	1.00	55.57	C
ATOM	1156	O	VAL	B	236	6.940	74.384	20.957	1.00	55.24	O
ATOM	1157	CB	VAL	B	236	4.591	72.707	21.271	1.00	57.84	C
ATOM	1158	CG1	VAL	B	236	4.248	73.913	20.371	1.00	57.83	C
ATOM	1159	CG2	VAL	B	236	5.219	71.574	20.470	1.00	58.07	C
ATOM	1160	N	MET	B	237	7.758	73.846	23.002	1.00	52.68	N
ATOM	1161	CA	MET	B	237	9.166	74.011	22.671	1.00	50.01	C
ATOM	1162	C	MET	B	237	9.732	72.634	22.324	1.00	46.79	C
ATOM	1163	O	MET	B	237	10.950	72.453	22.226	1.00	45.43	O
ATOM	1164	CB	MET	B	237	9.942	74.654	23.823	1.00	50.10	C
ATOM	1165	CG	MET	B	237	9.338	74.476	25.206	1.00	51.37	C
ATOM	1166	SD	MET	B	237	9.774	75.869	26.300	1.00	53.87	S
ATOM	1167	CE	MET	B	237	8.950	77.239	25.484	1.00	54.01	C
ATOM	1168	N	LEU	B	238	8.819	71.675	22.147	1.00	43.81	N
ATOM	1169	CA	LEU	B	238	9.154	70.309	21.756	1.00	41.29	C
ATOM	1170	C	LEU	B	238	9.930	70.285	20.458	1.00	39.47	C
ATOM	1171	O	LEU	B	238	9.581	70.989	19.509	1.00	38.40	O
ATOM	1172	CB	LEU	B	238	7.894	69.452	21.592	1.00	41.35	C
ATOM	1173	CG	LEU	B	238	7.241	68.855	22.836	1.00	41.59	C
ATOM	1174	CD1	LEU	B	238	6.065	67.952	22.433	1.00	41.48	C
ATOM	1175	CD2	LEU	B	238	8.255	68.090	23.674	1.00	40.65	C
ATOM	1176	N	ASN	B	239	10.992	69.484	20.445	1.00	37.61	N
ATOM	1177	CA	ASN	B	239	11.801	69.233	19.253	1.00	36.53	C
ATOM	1178	C	ASN	B	239	12.728	70.393	18.861	1.00	35.89	C
ATOM	1179	O	ASN	B	239	13.457	70.275	17.885	1.00	35.67	O
ATOM	1180	CB	ASN	B	239	10.920	68.874	18.051	1.00	36.35	C
ATOM	1181	CG	ASN	B	239	10.313	67.481	18.134	1.00	37.78	C
ATOM	1182	OD1	ASN	B	239	10.179	66.890	19.209	1.00	37.10	O
ATOM	1183	ND2	ASN	B	239	9.928	66.951	16.972	1.00	38.37	N
ATOM	1184	N	HIS	B	240	12.695	71.493	19.614	1.00	34.71	N
ATOM	1185	CA	HIS	B	240	13.535	72.662	19.330	1.00	34.88	C
ATOM	1186	C	HIS	B	240	14.885	72.530	20.000	1.00	34.45	C
ATOM	1187	O	HIS	B	240	14.982	71.982	21.102	1.00	33.52	O
ATOM	1188	CB	HIS	B	240	12.867	73.961	19.802	1.00	34.80	C
ATOM	1189	CG	HIS	B	240	11.711	74.395	18.952	1.00	36.23	C
ATOM	1190	ND1	HIS	B	240	11.833	75.338	17.953	1.00	37.72	N
ATOM	1191	CD2	HIS	B	240	10.410	74.018	18.956	1.00	37.04	C
ATOM	1192	CE1	HIS	B	240	10.659	75.515	17.372	1.00	38.50	C
ATOM	1193	NE2	HIS	B	240	9.778	74.730	17.966	1.00	38.99	N
ATOM	1194	N	LEU	B	241	15.922	73.035	19.331	1.00	34.34	N
ATOM	1195	CA	LEU	B	241	17.273	73.028	19.885	1.00	34.29	C
ATOM	1196	C	LEU	B	241	17.493	74.161	20.882	1.00	34.26	C
ATOM	1197	O	LEU	B	241	17.232	75.356	20.590	1.00	33.28	O
ATOM	1198	CB	LEU	B	241	18.345	73.118	18.790	1.00	34.84	C
ATOM	1199	CG	LEU	B	241	19.822	73.047	19.222	1.00	34.58	C
ATOM	1200	CD1	LEU	B	241	20.231	71.589	19.589	1.00	35.10	C
ATOM	1201	CD2	LEU	B	241	20.697	73.584	18.123	1.00	35.49	C
ATOM	1202	N	TYR	B	242	18.002	73.762	22.045	1.00	33.57	N
ATOM	1203	CA	TYR	B	242	18.494	74.683	23.054	1.00	34.05	C

Figure 1 Table 1b - 19

ATOM	1204	C	TYR	B	242	19.966	74.391	23.290	1.00	34.24	C
ATOM	1205	O	TYR	B	242	20.435	73.290	22.998	1.00	34.42	O
ATOM	1206	CB	TYR	B	242	17.703	74.535	24.357	1.00	34.04	C
ATOM	1207	CG	TYR	B	242	16.325	75.120	24.271	1.00	33.86	C
ATOM	1208	CD1	TYR	B	242	15.260	74.374	23.768	1.00	34.33	C
ATOM	1209	CD2	TYR	B	242	16.082	76.431	24.679	1.00	34.76	C
ATOM	1210	CE1	TYR	B	242	13.988	74.919	23.676	1.00	34.26	C
ATOM	1211	CE2	TYR	B	242	14.818	76.988	24.588	1.00	34.19	C
ATOM	1212	CZ	TYR	B	242	13.778	76.223	24.088	1.00	34.76	C
ATOM	1213	OH	TYR	B	242	12.525	76.777	24.000	1.00	36.36	O
ATOM	1214	N	ALA	B	243	20.692	75.379	23.811	1.00	34.20	N
ATOM	1215	CA	ALA	B	243	22.105	75.211	24.120	1.00	34.24	C
ATOM	1216	C	ALA	B	243	22.529	76.116	25.255	1.00	34.53	C
ATOM	1217	O	ALA	B	243	21.928	77.170	25.481	1.00	34.12	O
ATOM	1218	CB	ALA	B	243	22.965	75.484	22.886	1.00	34.32	C
ATOM	1219	N	LEU	B	244	23.562	75.692	25.974	1.00	34.93	N
ATOM	1220	CA	LEU	B	244	24.233	76.561	26.932	1.00	35.39	C
ATOM	1221	C	LEU	B	244	25.291	77.363	26.195	1.00	35.72	C
ATOM	1222	O	LEU	B	244	25.698	76.989	25.096	1.00	35.32	O
ATOM	1223	CB	LEU	B	244	24.893	75.739	28.044	1.00	35.01	C
ATOM	1224	CG	LEU	B	244	24.006	74.858	28.925	1.00	35.86	C
ATOM	1225	CD1	LEU	B	244	24.870	73.997	29.848	1.00	35.44	C
ATOM	1226	CD2	LEU	B	244	23.008	75.696	29.733	1.00	36.64	C
ATOM	1227	N	SER	B	245	25.732	78.463	26.799	1.00	36.79	N
ATOM	1228	CA	SER	B	245	26.912	79.171	26.325	1.00	37.83	C
ATOM	1229	C	SER	B	245	28.066	78.182	26.237	1.00	38.36	C
ATOM	1230	O	SER	B	245	28.219	77.328	27.111	1.00	38.55	O
ATOM	1231	CB	SER	B	245	27.296	80.294	27.292	1.00	37.97	C
ATOM	1232	OG	SER	B	245	26.393	81.382	27.216	1.00	39.17	O
ATOM	1233	N	ILE	B	246	28.875	78.286	25.189	1.00	38.89	N
ATOM	1234	CA	ILE	B	246	30.064	77.447	25.089	1.00	39.60	C
ATOM	1235	C	ILE	B	246	31.045	77.782	26.219	1.00	40.29	C
ATOM	1236	O	ILE	B	246	31.397	78.947	26.421	1.00	40.21	O
ATOM	1237	CB	ILE	B	246	30.729	77.563	23.700	1.00	39.50	C
ATOM	1238	CG1	ILE	B	246	29.883	76.825	22.657	1.00	39.49	C
ATOM	1239	CG2	ILE	B	246	32.161	77.020	23.724	1.00	38.85	C
ATOM	1240	CD1	ILE	B	246	30.214	77.210	21.228	1.00	40.37	C
ATOM	1241	N	LYS	B	247	31.445	76.750	26.959	1.00	41.34	N
ATOM	1242	CA	LYS	B	247	32.412	76.860	28.058	1.00	42.73	C
ATOM	1243	C	LYS	B	247	33.532	75.839	27.900	1.00	43.16	C
ATOM	1244	O	LYS	B	247	33.265	74.658	27.684	1.00	43.18	O
ATOM	1245	CB	LYS	B	247	31.730	76.644	29.417	1.00	42.78	C
ATOM	1246	CG	LYS	B	247	31.653	77.887	30.295	1.00	44.00	C
ATOM	1247	CD	LYS	B	247	31.482	77.507	31.761	1.00	44.80	C
ATOM	1248	CE	LYS	B	247	31.728	78.698	32.680	1.00	46.35	C
ATOM	1249	NZ	LYS	B	247	32.056	78.266	34.077	1.00	46.41	N
ATOM	1250	N	ASP	B	248	34.778	76.306	27.995	1.00	43.88	N
ATOM	1251	CA	ASP	B	248	35.972	75.444	27.951	1.00	44.37	C
ATOM	1252	C	ASP	B	248	35.973	74.441	26.791	1.00	44.19	C
ATOM	1253	O	ASP	B	248	36.307	73.268	26.983	1.00	44.49	O
ATOM	1254	CB	ASP	B	248	36.156	74.698	29.282	1.00	44.55	C
ATOM	1255	CG	ASP	B	248	36.737	75.576	30.388	1.00	45.89	C
ATOM	1256	OD1	ASP	B	248	37.548	76.489	30.100	1.00	46.91	O
ATOM	1257	OD2	ASP	B	248	36.390	75.327	31.565	1.00	47.50	O
ATOM	1258	N	SER	B	249	35.589	74.912	25.605	1.00	43.77	N
ATOM	1259	CA	SER	B	249	35.575	74.111	24.368	1.00	43.73	C
ATOM	1260	C	SER	B	249	34.547	72.957	24.342	1.00	43.45	C
ATOM	1261	O	SER	B	249	34.721	71.974	23.611	1.00	43.16	O
ATOM	1262	CB	SER	B	249	36.989	73.610	24.018	1.00	43.84	C
ATOM	1263	OG	SER	B	249	37.896	74.689	23.830	1.00	44.76	O
ATOM	1264	N	VAL	B	250	33.478	73.084	25.127	1.00	43.02	N
ATOM	1265	CA	VAL	B	250	32.379	72.114	25.085	1.00	42.73	C
ATOM	1266	C	VAL	B	250	31.005	72.748	24.806	1.00	42.58	C
ATOM	1267	O	VAL	B	250	30.573	73.684	25.489	1.00	42.27	O
ATOM	1268	CB	VAL	B	250	32.377	71.110	26.322	1.00	42.83	C
ATOM	1269	CG1	VAL	B	250	32.977	71.734	27.583	1.00	42.78	C
ATOM	1270	CG2	VAL	B	250	30.985	70.534	26.599	1.00	42.25	C

Figure 1 Table 1b - 20

ATOM	1271	N	MET	B	251	30.367	72.242	23.751	1.00	42.37	N
ATOM	1272	CA	MET	B	251	28.973	72.502	23.446	1.00	43.30	C
ATOM	1273	C	MET	B	251	28.075	71.646	24.327	1.00	41.75	C
ATOM	1274	O	MET	B	251	28.379	70.475	24.588	1.00	41.33	O
ATOM	1275	CB	MET	B	251	28.663	72.083	22.017	1.00	43.06	C
ATOM	1276	CG	MET	B	251	29.106	73.002	20.933	1.00	46.38	C
ATOM	1277	SD	MET	B	251	28.568	72.218	19.402	1.00	48.98	S
ATOM	1278	CE	MET	B	251	29.756	70.870	19.279	1.00	48.35	C
ATOM	1279	N	VAL	B	252	26.961	72.227	24.765	1.00	40.56	N
ATOM	1280	CA	VAL	B	252	25.902	71.455	25.399	1.00	39.38	C
ATOM	1281	C	VAL	B	252	24.621	71.758	24.652	1.00	38.66	C
ATOM	1282	O	VAL	B	252	24.092	72.876	24.722	1.00	38.55	O
ATOM	1283	CB	VAL	B	252	25.733	71.748	26.903	1.00	39.41	C
ATOM	1284	CG1	VAL	B	252	24.769	70.742	27.526	1.00	38.77	C
ATOM	1285	CG2	VAL	B	252	27.074	71.699	27.625	1.00	39.76	C
ATOM	1286	N	LEU	B	253	24.163	70.764	23.902	1.00	37.50	N
ATOM	1287	CA	LEU	B	253	22.950	70.851	23.111	1.00	37.30	C
ATOM	1288	C	LEU	B	253	21.842	70.087	23.805	1.00	37.28	C
ATOM	1289	O	LEU	B	253	22.085	69.045	24.416	1.00	37.14	O
ATOM	1290	CB	LEU	B	253	23.187	70.271	21.714	1.00	37.02	C
ATOM	1291	CG	LEU	B	253	24.334	70.928	20.942	1.00	38.51	C
ATOM	1292	CD1	LEU	B	253	24.586	70.232	19.625	1.00	38.80	C
ATOM	1293	CD2	LEU	B	253	24.054	72.436	20.724	1.00	37.65	C
ATOM	1294	N	SER	B	254	20.625	70.606	23.710	1.00	37.08	N
ATOM	1295	CA	SER	B	254	19.498	70.002	24.399	1.00	36.84	C
ATOM	1296	C	SER	B	254	18.215	70.115	23.597	1.00	36.30	C
ATOM	1297	O	SER	B	254	18.029	71.066	22.816	1.00	35.79	O
ATOM	1298	CB	SER	B	254	19.313	70.664	25.766	1.00	37.24	C
ATOM	1299	OG	SER	B	254	18.485	69.873	26.588	1.00	39.39	O
ATOM	1300	N	ALA	B	255	17.330	69.140	23.787	1.00	35.10	N
ATOM	1301	CA	ALA	B	255	15.984	69.198	23.223	1.00	34.53	C
ATOM	1302	C	ALA	B	255	15.091	68.256	23.984	1.00	34.34	C
ATOM	1303	O	ALA	B	255	15.571	67.298	24.587	1.00	34.60	O
ATOM	1304	CB	ALA	B	255	15.982	68.857	21.717	1.00	34.44	C
ATOM	1305	N	THR	B	256	13.794	68.543	23.969	1.00	34.06	N
ATOM	1306	CA	THR	B	256	12.793	67.667	24.560	1.00	33.91	C
ATOM	1307	C	THR	B	256	11.991	66.987	23.450	1.00	33.63	C
ATOM	1308	O	THR	B	256	11.459	67.663	22.558	1.00	33.12	O
ATOM	1309	CB	THR	B	256	11.852	68.445	25.512	1.00	33.67	C
ATOM	1310	OG1	THR	B	256	12.638	69.124	26.500	1.00	34.38	O
ATOM	1311	CG2	THR	B	256	10.874	67.490	26.213	1.00	34.34	C
ATOM	1312	N	HIS	B	257	11.925	65.654	23.502	1.00	32.79	N
ATOM	1313	CA	HIS	B	257	11.164	64.864	22.528	1.00	32.90	C
ATOM	1314	C	HIS	B	257	10.172	63.945	23.236	1.00	32.60	C
ATOM	1315	O	HIS	B	257	10.346	63.604	24.399	1.00	31.64	O
ATOM	1316	CB	HIS	B	257	12.081	64.011	21.633	1.00	33.26	C
ATOM	1317	CG	HIS	B	257	12.981	64.806	20.742	1.00	34.93	C
ATOM	1318	ND1	HIS	B	257	14.234	65.227	21.136	1.00	36.97	N
ATOM	1319	CD2	HIS	B	257	12.810	65.264	19.477	1.00	36.76	C
ATOM	1320	CE1	HIS	B	257	14.794	65.912	20.153	1.00	37.26	C
ATOM	1321	NE2	HIS	B	257	13.952	65.947	19.134	1.00	36.65	N
ATOM	1322	N	ARG	B	258	9.148	63.541	22.497	1.00	32.22	N
ATOM	1323	CA	ARG	B	258	8.039	62.792	23.026	1.00	32.71	C
ATOM	1324	C	ARG	B	258	8.133	61.368	22.517	1.00	32.33	C
ATOM	1325	O	ARG	B	258	8.391	61.144	21.332	1.00	32.02	O
ATOM	1326	CB	ARG	B	258	6.744	63.407	22.515	1.00	33.55	C
ATOM	1327	CG	ARG	B	258	5.492	63.042	23.261	1.00	35.13	C
ATOM	1328	CD	ARG	B	258	4.268	63.353	22.402	1.00	40.01	C
ATOM	1329	NE	ARG	B	258	3.619	62.101	22.021	1.00	44.98	N
ATOM	1330	CZ	ARG	B	258	3.377	61.694	20.781	1.00	45.62	C
ATOM	1331	NH1	ARG	B	258	3.687	62.451	19.733	1.00	44.81	N
ATOM	1332	NH2	ARG	B	258	2.791	60.519	20.602	1.00	46.37	N
ATOM	1333	N	TYR	B	259	7.931	60.417	23.423	1.00	31.77	N
ATOM	1334	CA	TYR	B	259	7.701	59.028	23.055	1.00	31.24	C
ATOM	1335	C	TYR	B	259	6.392	58.624	23.711	1.00	31.63	C
ATOM	1336	O	TYR	B	259	6.290	58.579	24.947	1.00	30.98	O
ATOM	1337	CB	TYR	B	259	8.848	58.107	23.499	1.00	31.03	C

Figure 1 Table 1b - 21

ATOM	1338	CG	TYR	B	259	8.583	56.634	23.199	1.00	30.67	C
ATOM	1339	CD1	TYR	B	259	8.843	56.101	21.932	1.00	31.38	C
ATOM	1340	CD2	TYR	B	259	8.049	55.789	24.168	1.00	30.29	C
ATOM	1341	CE1	TYR	B	259	8.590	54.747	21.648	1.00	30.48	C
ATOM	1342	CE2	TYR	B	259	7.786	54.435	23.893	1.00	30.22	C
ATOM	1343	CZ	TYR	B	259	8.063	53.927	22.628	1.00	30.40	C
ATOM	1344	OH	TYR	B	259	7.814	52.599	22.339	1.00	29.42	O
ATOM	1345	N	LYS	B	260	5.396	58.346	22.871	1.00	31.61	N
ATOM	1346	CA	LYS	B	260	4.026	58.132	23.318	1.00	32.08	C
ATOM	1347	C	LYS	B	260	3.612	59.271	24.250	1.00	32.21	C
ATOM	1348	O	LYS	B	260	3.465	60.406	23.802	1.00	32.49	O
ATOM	1349	CB	LYS	B	260	3.859	56.755	23.972	1.00	31.67	C
ATOM	1350	CG	LYS	B	260	4.163	55.598	23.047	1.00	32.15	C
ATOM	1351	CD	LYS	B	260	3.774	54.294	23.705	1.00	34.54	C
ATOM	1352	CE	LYS	B	260	4.005	53.104	22.796	1.00	35.29	C
ATOM	1353	NZ	LYS	B	260	3.706	51.844	23.532	1.00	37.70	N
ATOM	1354	N	LYS	B	261	3.463	58.991	25.541	1.00	32.33	N
ATOM	1355	CA	LYS	B	261	3.051	60.036	26.476	1.00	32.46	C
ATOM	1356	C	LYS	B	261	4.161	60.509	27.423	1.00	31.94	C
ATOM	1357	O	LYS	B	261	3.896	61.202	28.402	1.00	32.19	O
ATOM	1358	CB	LYS	B	261	1.794	59.607	27.231	1.00	32.53	C
ATOM	1359	CG	LYS	B	261	0.609	59.421	26.305	1.00	34.74	C
ATOM	1360	CD	LYS	B	261	-0.713	59.634	27.001	1.00	37.76	C
ATOM	1361	CE	LYS	B	261	-1.780	60.036	25.989	1.00	39.43	C
ATOM	1362	NZ	LYS	B	261	-3.050	60.411	26.658	1.00	40.93	N
ATOM	1363	N	LYS	B	262	5.401	60.144	27.112	1.00	31.35	N
ATOM	1364	CA	LYS	B	262	6.536	60.433	27.981	1.00	31.37	C
ATOM	1365	C	LYS	B	262	7.473	61.406	27.274	1.00	31.51	C
ATOM	1366	O	LYS	B	262	7.621	61.344	26.058	1.00	31.22	O
ATOM	1367	CB	LYS	B	262	7.305	59.149	28.334	1.00	31.22	C
ATOM	1368	CG	LYS	B	262	6.417	57.955	28.712	1.00	30.64	C
ATOM	1369	CD	LYS	B	262	6.183	57.847	30.203	1.00	28.97	C
ATOM	1370	CE	LYS	B	262	4.980	56.977	30.513	1.00	27.57	C
ATOM	1371	NZ	LYS	B	262	5.141	56.276	31.792	1.00	27.19	N
ATOM	1372	N	TYR	B	263	8.111	62.276	28.051	1.00	31.33	N
ATOM	1373	CA	TYR	B	263	8.966	63.320	27.511	1.00	32.16	C
ATOM	1374	C	TYR	B	263	10.347	63.193	28.087	1.00	31.72	C
ATOM	1375	O	TYR	B	263	10.512	63.058	29.306	1.00	31.52	O
ATOM	1376	CB	TYR	B	263	8.393	64.705	27.829	1.00	32.44	C
ATOM	1377	CG	TYR	B	263	7.002	64.904	27.278	1.00	34.02	C
ATOM	1378	CD1	TYR	B	263	5.875	64.498	28.000	1.00	34.05	C
ATOM	1379	CD2	TYR	B	263	6.811	65.473	26.022	1.00	33.52	C
ATOM	1380	CE1	TYR	B	263	4.594	64.665	27.481	1.00	35.18	C
ATOM	1381	CE2	TYR	B	263	5.542	65.650	25.503	1.00	34.34	C
ATOM	1382	CZ	TYR	B	263	4.439	65.248	26.230	1.00	34.83	C
ATOM	1383	OH	TYR	B	263	3.178	65.425	25.697	1.00	34.57	O
ATOM	1384	N	VAL	B	264	11.343	63.196	27.208	1.00	31.35	N
ATOM	1385	CA	VAL	B	264	12.716	63.216	27.673	1.00	31.13	C
ATOM	1386	C	VAL	B	264	13.438	64.429	27.107	1.00	30.87	C
ATOM	1387	O	VAL	B	264	13.333	64.727	25.923	1.00	30.94	O
ATOM	1388	CB	VAL	B	264	13.491	61.892	27.384	1.00	31.22	C
ATOM	1389	CG1	VAL	B	264	13.591	61.599	25.891	1.00	30.44	C
ATOM	1390	CG2	VAL	B	264	14.877	61.925	28.031	1.00	31.36	C
ATOM	1391	N	THR	B	265	14.140	65.120	27.995	1.00	31.03	N
ATOM	1392	CA	THR	B	265	15.012	66.236	27.660	1.00	31.23	C
ATOM	1393	C	THR	B	265	16.407	65.658	27.683	1.00	31.49	C
ATOM	1394	O	THR	B	265	16.925	65.258	28.741	1.00	32.34	O
ATOM	1395	CB	THR	B	265	14.881	67.347	28.702	1.00	31.08	C
ATOM	1396	OG1	THR	B	265	13.503	67.732	28.785	1.00	31.92	O
ATOM	1397	CG2	THR	B	265	15.760	68.567	28.347	1.00	32.17	C
ATOM	1398	N	THR	B	266	16.985	65.553	26.500	1.00	31.49	N
ATOM	1399	CA	THR	B	266	18.299	64.963	26.324	1.00	31.75	C
ATOM	1400	C	THR	B	266	19.324	66.081	26.218	1.00	32.04	C
ATOM	1401	O	THR	B	266	19.098	67.057	25.504	1.00	31.85	O
ATOM	1402	CB	THR	B	266	18.343	64.107	25.045	1.00	31.63	C
ATOM	1403	OG1	THR	B	266	17.221	63.212	25.031	1.00	32.63	O
ATOM	1404	CG2	THR	B	266	19.643	63.304	24.968	1.00	30.50	C

Figure 1 Table 1b - 22

ATOM	1405	N	LEU	B	267	20.436	65.934	26.927	1.00 31.98	N
ATOM	1406	CA	LEU	B	267	21.542	66.869	26.831	1.00 33.33	C
ATOM	1407	C	LEU	B	267	22.723	66.136	26.244	1.00 33.66	C
ATOM	1408	O	LEU	B	267	23.078	65.057	26.714	1.00 34.78	O
ATOM	1409	CB	LEU	B	267	21.935	67.398	28.215	1.00 33.28	C
ATOM	1410	CG	LEU	B	267	21.020	68.361	28.965	1.00 33.43	C
ATOM	1411	CD1	LEU	B	267	19.768	67.665	29.471	1.00 33.20	C
ATOM	1412	CD2	LEU	B	267	21.810	68.953	30.125	1.00 33.18	C
ATOM	1413	N	LEU	B	268	23.324	66.705	25.208	1.00 33.59	N
ATOM	1414	CA	LEU	B	268	24.547	66.148	24.661	1.00 33.72	C
ATOM	1415	C	LEU	B	268	25.726	67.053	24.950	1.00 34.38	C
ATOM	1416	O	LEU	B	268	25.731	68.234	24.551	1.00 34.67	O
ATOM	1417	CB	LEU	B	268	24.426	65.895	23.155	1.00 33.22	C
ATOM	1418	CG	LEU	B	268	25.673	65.342	22.453	1.00 32.78	C
ATOM	1419	CD1	LEU	B	268	26.014	63.924	22.917	1.00 32.42	C
ATOM	1420	CD2	LEU	B	268	25.493	65.391	20.940	1.00 33.23	C
ATOM	1421	N	TYR	B	269	26.712	66.484	25.649	1.00 35.01	N
ATOM	1422	CA	TYR	B	269	28.017	67.102	25.863	1.00 35.73	C
ATOM	1423	C	TYR	B	269	28.964	66.627	24.784	1.00 37.03	C
ATOM	1424	O	TYR	B	269	29.239	65.437	24.668	1.00 36.86	O
ATOM	1425	CB	TYR	B	269	28.576	66.758	27.251	1.00 34.95	C
ATOM	1426	CG	TYR	B	269	27.928	67.550	28.350	1.00 34.04	C
ATOM	1427	CD1	TYR	B	269	26.597	67.322	28.693	1.00 33.52	C
ATOM	1428	CD2	TYR	B	269	28.633	68.544	29.034	1.00 34.23	C
ATOM	1429	CE1	TYR	B	269	25.978	68.053	29.686	1.00 34.23	C
ATOM	1430	CE2	TYR	B	269	28.014	69.297	30.040	1.00 34.44	C
ATOM	1431	CZ	TYR	B	269	26.683	69.038	30.352	1.00 33.50	C
ATOM	1432	OH	TYR	B	269	26.042	69.747	31.327	1.00 34.42	O
ATOM	1433	N	LYS	B	270	29.474	67.581	24.018	1.00 38.66	N
ATOM	1434	CA	LYS	B	270	30.236	67.318	22.810	1.00 40.74	C
ATOM	1435	C	LYS	B	270	31.370	68.354	22.693	1.00 41.37	C
ATOM	1436	O	LYS	B	270	31.107	69.562	22.733	1.00 41.68	O
ATOM	1437	CB	LYS	B	270	29.281	67.443	21.614	1.00 40.89	C
ATOM	1438	CG	LYS	B	270	29.820	66.970	20.281	1.00 42.80	C
ATOM	1439	CD	LYS	B	270	28.962	67.488	19.112	1.00 42.21	C
ATOM	1440	CE	LYS	B	270	29.486	66.951	17.786	1.00 43.40	C
ATOM	1441	NZ	LYS	B	270	28.987	67.735	16.608	1.00 46.47	N
ATOM	1442	N	PRO	B	271	32.631	67.897	22.550	1.00 41.98	N
ATOM	1443	CA	PRO	B	271	33.710	68.849	22.255	1.00 42.76	C
ATOM	1444	C	PRO	B	271	33.503	69.505	20.890	1.00 43.45	C
ATOM	1445	O	PRO	B	271	32.883	68.905	20.010	1.00 43.53	O
ATOM	1446	CB	PRO	B	271	34.964	67.967	22.216	1.00 42.49	C
ATOM	1447	CG	PRO	B	271	34.582	66.706	22.908	1.00 42.58	C
ATOM	1448	CD	PRO	B	271	33.131	66.516	22.646	1.00 42.06	C
ATOM	1449	N	ILE	B	272	34.005	70.724	20.718	1.00 44.42	N
ATOM	1450	CA	ILE	B	272	33.924	71.396	19.414	1.00 45.57	C
ATOM	1451	C	ILE	B	272	35.205	71.167	18.605	1.00 45.71	C
ATOM	1452	O	ILE	B	272	35.388	71.739	17.516	1.00 46.62	O
ATOM	1453	CB	ILE	B	272	33.639	72.921	19.530	1.00 45.60	C
ATOM	1454	CG1	ILE	B	272	32.909	73.263	20.834	1.00 46.23	C
ATOM	1455	CG2	ILE	B	272	32.832	73.407	18.317	1.00 46.48	C
ATOM	1456	CD1	ILE	B	272	32.964	74.740	21.191	1.00 45.70	C
TER	1457		ILE	B	272					
ATOM	1458	N	SER	E	23	7.069	31.078	49.277	1.00 64.53	N
ATOM	1459	CA	SER	E	23	5.642	30.947	48.848	1.00 64.47	C
ATOM	1460	C	SER	E	23	5.445	31.239	47.371	1.00 64.18	C
ATOM	1461	O	SER	E	23	6.287	31.896	46.735	1.00 64.43	O
ATOM	1462	CB	SER	E	23	4.766	31.931	49.624	1.00 64.58	C
ATOM	1463	OG	SER	E	23	3.414	31.922	49.164	1.00 64.92	O
ATOM	1464	N	ASN	E	24	4.321	30.744	46.840	1.00 63.47	N
ATOM	1465	CA	ASN	E	24	3.718	31.303	45.629	1.00 62.60	C
ATOM	1466	C	ASN	E	24	4.534	31.063	44.362	1.00 61.78	C
ATOM	1467	O	ASN	E	24	5.768	30.936	44.422	1.00 61.92	O
ATOM	1468	CB	ASN	E	24	3.527	32.823	45.832	1.00 62.46	C
ATOM	1469	CG	ASN	E	24	2.338	33.396	45.070	1.00 62.84	C
ATOM	1470	OD1	ASN	E	24	2.215	34.620	44.940	1.00 62.37	O
ATOM	1471	ND2	ASN	E	24	1.451	32.527	44.579	1.00 62.54	N

Figure 1 Table 1b - 23

ATOM	1472	N	SER	E	25	3.851	30.987	43.218	1.00 60.50	N
ATOM	1473	CA	SER	E	25	4.490	31.360	41.962	1.00 58.90	C
ATOM	1474	C	SER	E	25	4.913	32.765	42.332	1.00 57.45	C
ATOM	1475	O	SER	E	25	5.742	32.941	43.227	1.00 57.95	O
ATOM	1476	CB	SER	E	25	3.491	31.365	40.802	1.00 59.15	C
ATOM	1477	OG	SER	E	25	3.998	32.095	39.693	1.00 59.76	O
ATOM	1478	N	SER	E	26	4.335	33.782	41.719	1.00 55.12	N
ATOM	1479	CA	SER	E	26	4.427	35.066	42.367	1.00 52.75	C
ATOM	1480	C	SER	E	26	3.481	36.083	41.807	1.00 51.11	C
ATOM	1481	O	SER	E	26	3.411	36.300	40.602	1.00 51.13	O
ATOM	1482	CB	SER	E	26	5.865	35.600	42.377	1.00 53.06	C
ATOM	1483	OG	SER	E	26	6.078	36.446	43.489	1.00 51.99	O
ATOM	1484	N	VAL	E	27	2.750	36.694	42.724	1.00 48.97	N
ATOM	1485	CA	VAL	E	27	2.121	37.970	42.503	1.00 47.57	C
ATOM	1486	C	VAL	E	27	3.167	38.928	41.869	1.00 46.29	C
ATOM	1487	O	VAL	E	27	2.842	39.687	40.957	1.00 46.19	O
ATOM	1488	CB	VAL	E	27	1.561	38.506	43.846	1.00 47.53	C
ATOM	1489	CG1	VAL	E	27	1.075	39.913	43.705	1.00 48.31	C
ATOM	1490	CG2	VAL	E	27	0.421	37.612	44.353	1.00 47.71	C
ATOM	1491	N	TYR	E	28	4.422	38.832	42.319	1.00 44.63	N
ATOM	1492	CA	TYR	E	28	5.534	39.642	41.795	1.00 43.59	C
ATOM	1493	C	TYR	E	28	5.999	39.259	40.389	1.00 43.03	C
ATOM	1494	O	TYR	E	28	6.129	40.117	39.523	1.00 42.34	O
ATOM	1495	CB	TYR	E	28	6.727	39.601	42.754	1.00 43.04	C
ATOM	1496	CG	TYR	E	28	6.471	40.347	44.036	1.00 42.81	C
ATOM	1497	CD1	TYR	E	28	6.034	39.678	45.180	1.00 41.64	C
ATOM	1498	CD2	TYR	E	28	6.650	41.731	44.103	1.00 42.05	C
ATOM	1499	CE1	TYR	E	28	5.790	40.363	46.360	1.00 41.96	C
ATOM	1500	CE2	TYR	E	28	6.407	42.427	45.282	1.00 42.13	C
ATOM	1501	CZ	TYR	E	28	5.976	41.739	46.402	1.00 42.35	C
ATOM	1502	OH	TYR	E	28	5.739	42.421	47.568	1.00 42.97	O
ATOM	1503	N	THR	E	29	6.262	37.971	40.182	1.00 42.46	N
ATOM	1504	CA	THR	E	29	6.737	37.450	38.898	1.00 42.35	C
ATOM	1505	C	THR	E	29	5.685	37.695	37.808	1.00 41.61	C
ATOM	1506	O	THR	E	29	6.012	38.124	36.699	1.00 41.65	O
ATOM	1507	CB	THR	E	29	7.093	35.942	39.020	1.00 42.96	C
ATOM	1508	OG1	THR	E	29	8.048	35.765	40.078	1.00 44.44	O
ATOM	1509	CG2	THR	E	29	7.702	35.418	37.746	1.00 43.96	C
ATOM	1510	N	THR	E	30	4.423	37.447	38.155	1.00 41.01	N
ATOM	1511	CA	THR	E	30	3.277	37.675	37.272	1.00 40.24	C
ATOM	1512	C	THR	E	30	3.178	39.144	36.866	1.00 39.79	C
ATOM	1513	O	THR	E	30	3.083	39.456	35.673	1.00 39.37	O
ATOM	1514	CB	THR	E	30	1.961	37.229	37.958	1.00 40.26	C
ATOM	1515	OG1	THR	E	30	1.999	35.815	38.178	1.00 40.34	O
ATOM	1516	CG2	THR	E	30	0.745	37.573	37.109	1.00 40.03	C
ATOM	1517	N	PHE	E	31	3.193	40.029	37.865	1.00 39.33	N
ATOM	1518	CA	PHE	E	31	3.187	41.481	37.646	1.00 38.87	C
ATOM	1519	C	PHE	E	31	4.305	41.940	36.710	1.00 38.64	C
ATOM	1520	O	PHE	E	31	4.071	42.747	35.808	1.00 38.49	O
ATOM	1521	CB	PHE	E	31	3.299	42.227	38.985	1.00 38.74	C
ATOM	1522	CG	PHE	E	31	3.151	43.723	38.860	1.00 38.72	C
ATOM	1523	CD1	PHE	E	31	4.257	44.529	38.585	1.00 38.48	C
ATOM	1524	CD2	PHE	E	31	1.906	44.324	39.015	1.00 38.86	C
ATOM	1525	CE1	PHE	E	31	4.122	45.917	38.457	1.00 38.83	C
ATOM	1526	CE2	PHE	E	31	1.763	45.714	38.905	1.00 39.96	C
ATOM	1527	CZ	PHE	E	31	2.870	46.508	38.612	1.00 38.33	C
ATOM	1528	N	MET	E	32	5.516	41.439	36.949	1.00 38.55	N
ATOM	1529	CA	MET	E	32	6.697	41.826	36.180	1.00 39.40	C
ATOM	1530	C	MET	E	32	6.619	41.390	34.721	1.00 39.15	C
ATOM	1531	O	MET	E	32	7.004	42.136	33.813	1.00 38.46	O
ATOM	1532	CB	MET	E	32	7.965	41.293	36.843	1.00 39.23	C
ATOM	1533	CG	MET	E	32	8.385	42.084	38.071	1.00 39.32	C
ATOM	1534	SD	MET	E	32	9.981	41.560	38.712	1.00 42.74	S
ATOM	1535	CE	MET	E	32	9.515	40.528	40.100	1.00 42.87	C
ATOM	1536	N	LYS	E	33	6.102	40.185	34.506	1.00 39.37	N
ATOM	1537	CA	LYS	E	33	5.888	39.643	33.166	1.00 39.79	C
ATOM	1538	C	LYS	E	33	4.744	40.344	32.421	1.00 40.20	C

Figure 1 Table 1b - 24

ATOM	1539	O	LYS	E	33	4.757	40.394	31.192	1.00	40.25	O
ATOM	1540	CB	LYS	E	33	5.658	38.119	33.226	1.00	39.83	C
ATOM	1541	CG	LYS	E	33	6.916	37.322	33.558	1.00	39.18	C
ATOM	1542	CD	LYS	E	33	6.617	35.839	33.696	1.00	40.35	C
ATOM	1543	CE	LYS	E	33	7.884	35.060	34.001	1.00	40.81	C
ATOM	1544	NZ	LYS	E	33	7.587	33.674	34.443	1.00	43.22	N
ATOM	1545	N	SER	E	34	3.773	40.894	33.152	1.00	40.64	N
ATOM	1546	CA	SER	E	34	2.616	41.551	32.520	1.00	41.70	C
ATOM	1547	C	SER	E	34	2.794	43.056	32.268	1.00	41.82	C
ATOM	1548	O	SER	E	34	1.950	43.689	31.627	1.00	42.61	O
ATOM	1549	CB	SER	E	34	1.330	41.284	33.311	1.00	41.87	C
ATOM	1550	OG	SER	E	34	1.315	42.002	34.535	1.00	43.51	O
ATOM	1551	N	HIS	E	35	3.892	43.627	32.757	1.00	41.74	N
ATOM	1552	CA	HIS	E	35	4.160	45.054	32.584	1.00	41.31	C
ATOM	1553	C	HIS	E	35	5.384	45.348	31.727	1.00	40.93	C
ATOM	1554	O	HIS	E	35	6.395	44.647	31.813	1.00	40.69	O
ATOM	1555	CB	HIS	E	35	4.266	45.745	33.944	1.00	41.64	C
ATOM	1556	CG	HIS	E	35	2.941	45.958	34.598	1.00	42.40	C
ATOM	1557	ND1	HIS	E	35	2.287	44.961	35.288	1.00	42.85	N
ATOM	1558	CD2	HIS	E	35	2.125	47.038	34.630	1.00	42.75	C
ATOM	1559	CE1	HIS	E	35	1.128	45.420	35.725	1.00	43.74	C
ATOM	1560	NE2	HIS	E	35	1.010	46.682	35.349	1.00	43.27	N
ATOM	1561	N	ARG	E	36	5.263	46.382	30.893	1.00	40.29	N
ATOM	1562	CA	ARG	E	36	6.343	46.847	30.021	1.00	40.38	C
ATOM	1563	C	ARG	E	36	7.228	47.858	30.736	1.00	39.35	C
ATOM	1564	O	ARG	E	36	6.762	48.611	31.591	1.00	38.99	O
ATOM	1565	CB	ARG	E	36	5.779	47.508	28.757	1.00	40.26	C
ATOM	1566	CG	ARG	E	36	4.899	46.606	27.923	1.00	42.30	C
ATOM	1567	CD	ARG	E	36	4.460	47.239	26.600	1.00	42.86	C
ATOM	1568	NE	ARG	E	36	3.500	46.361	25.920	1.00	49.23	N
ATOM	1569	CZ	ARG	E	36	3.817	45.270	25.217	1.00	50.71	C
ATOM	1570	NH1	ARG	E	36	5.086	44.905	25.066	1.00	51.20	N
ATOM	1571	NH2	ARG	E	36	2.858	44.534	24.656	1.00	51.27	N
ATOM	1572	N	CYS	E	37	8.504	47.886	30.367	1.00	38.87	N
ATOM	1573	CA	CYS	E	37	9.429	48.903	30.863	1.00	38.57	C
ATOM	1574	C	CYS	E	37	8.900	50.334	30.705	1.00	38.11	C
ATOM	1575	O	CYS	E	37	9.099	51.175	31.591	1.00	37.73	O
ATOM	1576	CB	CYS	E	37	10.781	48.738	30.191	1.00	38.41	C
ATOM	1577	SG	CYS	E	37	11.625	47.276	30.848	1.00	42.01	S
ATOM	1578	N	TYR	E	38	8.204	50.590	29.594	1.00	37.46	N
ATOM	1579	CA	TYR	E	38	7.541	51.875	29.355	1.00	37.17	C
ATOM	1580	C	TYR	E	38	6.736	52.373	30.567	1.00	36.95	C
ATOM	1581	O	TYR	E	38	6.737	53.572	30.870	1.00	37.37	O
ATOM	1582	CB	TYR	E	38	6.625	51.773	28.126	1.00	37.32	C
ATOM	1583	CG	TYR	E	38	5.778	53.006	27.886	1.00	37.10	C
ATOM	1584	CD1	TYR	E	38	4.446	53.052	28.296	1.00	36.73	C
ATOM	1585	CD2	TYR	E	38	6.322	54.132	27.277	1.00	36.88	C
ATOM	1586	CE1	TYR	E	38	3.671	54.184	28.088	1.00	37.19	C
ATOM	1587	CE2	TYR	E	38	5.556	55.270	27.056	1.00	38.45	C
ATOM	1588	CZ	TYR	E	38	4.237	55.295	27.466	1.00	37.61	C
ATOM	1589	OH	TYR	E	38	3.488	56.431	27.255	1.00	36.92	O
ATOM	1590	N	ASP	E	39	6.061	51.445	31.247	1.00	36.32	N
ATOM	1591	CA	ASP	E	39	5.154	51.753	32.354	1.00	35.92	C
ATOM	1592	C	ASP	E	39	5.831	52.430	33.537	1.00	35.09	C
ATOM	1593	O	ASP	E	39	5.172	53.117	34.305	1.00	35.20	O
ATOM	1594	CB	ASP	E	39	4.461	50.477	32.859	1.00	35.96	C
ATOM	1595	CG	ASP	E	39	3.480	49.895	31.855	1.00	38.00	C
ATOM	1596	OD1	ASP	E	39	3.125	50.585	30.875	1.00	39.14	O
ATOM	1597	OD2	ASP	E	39	3.047	48.740	32.056	1.00	38.96	O
ATOM	1598	N	LEU	E	40	7.127	52.204	33.710	1.00	34.60	N
ATOM	1599	CA	LEU	E	40	7.849	52.777	34.841	1.00	34.42	C
ATOM	1600	C	LEU	E	40	8.516	54.110	34.513	1.00	33.75	C
ATOM	1601	O	LEU	E	40	9.128	54.725	35.388	1.00	33.59	O
ATOM	1602	CB	LEU	E	40	8.945	51.834	35.361	1.00	34.29	C
ATOM	1603	CG	LEU	E	40	8.949	50.309	35.485	1.00	35.94	C
ATOM	1604	CD1	LEU	E	40	9.431	49.958	36.897	1.00	34.31	C
ATOM	1605	CD2	LEU	E	40	7.641	49.637	35.180	1.00	36.20	C

Figure 1 Table 1b - 25

ATOM	1606	N	ILE	E	41	8.443	54.540	33.258	1.00 33.59	N
ATOM	1607	CA	ILE	E	41	9.080	55.806	32.864	1.00 33.41	C
ATOM	1608	C	ILE	E	41	8.232	56.986	33.369	1.00 33.42	C
ATOM	1609	O	ILE	E	41	7.013	57.003	33.165	1.00 33.40	O
ATOM	1610	CB	ILE	E	41	9.277	55.888	31.325	1.00 33.36	C
ATOM	1611	CG1	ILE	E	41	10.100	54.687	30.825	1.00 33.45	C
ATOM	1612	CG2	ILE	E	41	9.930	57.248	30.897	1.00 32.51	C
ATOM	1613	CD1	ILE	E	41	10.195	54.601	29.302	1.00 34.21	C
ATOM	1614	N	PRO	E	42	8.867	57.982	34.025	1.00 33.42	N
ATOM	1615	CA	PRO	E	42	8.087	59.122	34.480	1.00 33.39	C
ATOM	1616	C	PRO	E	42	7.652	59.961	33.276	1.00 33.44	C
ATOM	1617	O	PRO	E	42	8.195	59.797	32.175	1.00 33.43	O
ATOM	1618	CB	PRO	E	42	9.069	59.898	35.367	1.00 33.46	C
ATOM	1619	CG	PRO	E	42	10.409	59.549	34.846	1.00 32.98	C
ATOM	1620	CD	PRO	E	42	10.296	58.120	34.361	1.00 33.64	C
ATOM	1621	N	THR	E	43	6.657	60.815	33.484	1.00 33.20	N
ATOM	1622	CA	THR	E	43	6.106	61.644	32.411	1.00 33.86	C
ATOM	1623	C	THR	E	43	7.185	62.553	31.832	1.00 34.04	C
ATOM	1624	O	THR	E	43	7.290	62.689	30.620	1.00 33.73	O
ATOM	1625	CB	THR	E	43	4.880	62.437	32.893	1.00 33.54	C
ATOM	1626	OG1	THR	E	43	3.828	61.511	33.191	1.00 33.79	O
ATOM	1627	CG2	THR	E	43	4.396	63.428	31.832	1.00 33.76	C
ATOM	1628	N	SER	E	44	8.008	63.126	32.706	1.00 34.98	N
ATOM	1629	CA	SER	E	44	9.123	63.964	32.278	1.00 36.65	C
ATOM	1630	C	SER	E	44	10.438	63.529	32.931	1.00 36.67	C
ATOM	1631	O	SER	E	44	10.475	63.185	34.112	1.00 36.69	O
ATOM	1632	CB	SER	E	44	8.809	65.436	32.564	1.00 36.60	C
ATOM	1633	OG	SER	E	44	9.882	66.248	32.127	1.00 41.86	O
ATOM	1634	N	SER	E	45	11.513	63.515	32.150	1.00 37.07	N
ATOM	1635	CA	SER	E	45	12.839	63.184	32.679	1.00 37.26	C
ATOM	1636	C	SER	E	45	13.920	63.848	31.853	1.00 37.10	C
ATOM	1637	O	SER	E	45	13.653	64.294	30.745	1.00 37.34	O
ATOM	1638	CB	SER	E	45	13.065	61.662	32.733	1.00 37.42	C
ATOM	1639	OG	SER	E	45	13.063	61.054	31.446	1.00 37.77	O
ATOM	1640	N	LYS	E	46	15.125	63.939	32.416	1.00 36.89	N
ATOM	1641	CA	LYS	E	46	16.294	64.349	31.668	1.00 36.67	C
ATOM	1642	C	LYS	E	46	17.308	63.226	31.499	1.00 35.87	C
ATOM	1643	O	LYS	E	46	17.382	62.272	32.294	1.00 35.82	O
ATOM	1644	CB	LYS	E	46	16.951	65.609	32.262	1.00 37.42	C
ATOM	1645	CG	LYS	E	46	17.684	65.420	33.570	1.00 40.47	C
ATOM	1646	CD	LYS	E	46	18.497	66.669	33.893	1.00 43.12	C
ATOM	1647	CE	LYS	E	46	18.522	66.910	35.385	1.00 46.22	C
ATOM	1648	NZ	LYS	E	46	18.773	68.356	35.681	1.00 46.93	N
ATOM	1649	N	LEU	E	47	18.102	63.362	30.455	1.00 34.79	N
ATOM	1650	CA	LEU	E	47	19.087	62.368	30.111	1.00 34.25	C
ATOM	1651	C	LEU	E	47	20.323	63.097	29.643	1.00 34.08	C
ATOM	1652	O	LEU	E	47	20.268	63.912	28.721	1.00 33.32	O
ATOM	1653	CB	LEU	E	47	18.551	61.458	28.997	1.00 33.95	C
ATOM	1654	CG	LEU	E	47	19.454	60.296	28.590	1.00 34.34	C
ATOM	1655	CD1	LEU	E	47	19.340	59.158	29.636	1.00 32.29	C
ATOM	1656	CD2	LEU	E	47	19.072	59.827	27.211	1.00 33.03	C
ATOM	1657	N	VAL	E	48	21.433	62.819	30.308	1.00 34.00	N
ATOM	1658	CA	VAL	E	48	22.704	63.388	29.927	1.00 34.41	C
ATOM	1659	C	VAL	E	48	23.448	62.337	29.098	1.00 34.44	C
ATOM	1660	O	VAL	E	48	23.596	61.202	29.535	1.00 33.92	O
ATOM	1661	CB	VAL	E	48	23.546	63.793	31.163	1.00 34.88	C
ATOM	1662	CG1	VAL	E	48	24.882	64.364	30.723	1.00 33.63	C
ATOM	1663	CG2	VAL	E	48	22.776	64.798	32.050	1.00 34.72	C
ATOM	1664	N	VAL	E	49	23.898	62.733	27.908	1.00 34.24	N
ATOM	1665	CA	VAL	E	49	24.667	61.857	27.025	1.00 34.56	C
ATOM	1666	C	VAL	E	49	26.033	62.474	26.740	1.00 34.90	C
ATOM	1667	O	VAL	E	49	26.134	63.666	26.405	1.00 35.18	O
ATOM	1668	CB	VAL	E	49	23.916	61.605	25.681	1.00 34.58	C
ATOM	1669	CG1	VAL	E	49	24.768	60.775	24.715	1.00 34.19	C
ATOM	1670	CG2	VAL	E	49	22.556	60.929	25.937	1.00 34.00	C
ATOM	1671	N	PHE	E	50	27.087	61.672	26.871	1.00 34.94	N
ATOM	1672	CA	PHE	E	50	28.415	62.139	26.510	1.00 35.61	C

Figure 1 Table 1b - 26

ATOM	1673	C	PHE	E	50	28.900	61.546	25.192	1.00	36.01	C
ATOM	1674	O	PHE	E	50	28.843	60.330	24.984	1.00	35.75	O
ATOM	1675	CB	PHE	E	50	29.449	61.838	27.601	1.00	35.60	C
ATOM	1676	CG	PHE	E	50	29.085	62.359	28.969	1.00	35.78	C
ATOM	1677	CD1	PHE	E	50	29.160	61.522	30.077	1.00	35.61	C
ATOM	1678	CD2	PHE	E	50	28.702	63.688	29.157	1.00	36.33	C
ATOM	1679	CE1	PHE	E	50	28.840	61.992	31.362	1.00	36.43	C
ATOM	1680	CE2	PHE	E	50	28.375	64.169	30.428	1.00	36.83	C
ATOM	1681	CZ	PHE	E	50	28.437	63.315	31.535	1.00	35.53	C
ATOM	1682	N	ASP	E	51	29.385	62.417	24.313	1.00	35.72	N
ATOM	1683	CA	ASP	E	51	30.202	61.984	23.201	1.00	36.38	C
ATOM	1684	C	ASP	E	51	31.497	61.404	23.785	1.00	36.72	C
ATOM	1685	O	ASP	E	51	32.066	61.967	24.728	1.00	36.67	O
ATOM	1686	CB	ASP	E	51	30.489	63.171	22.273	1.00	36.42	C
ATOM	1687	CG	ASP	E	51	31.162	62.753	20.986	1.00	37.38	C
ATOM	1688	OD1	ASP	E	51	30.494	62.788	19.929	1.00	39.87	O
ATOM	1689	OD2	ASP	E	51	32.351	62.374	21.026	1.00	37.43	O
ATOM	1690	N	THR	E	52	31.956	60.279	23.234	1.00	36.96	N
ATOM	1691	CA	THR	E	52	33.134	59.574	23.763	1.00	37.07	C
ATOM	1692	C	THR	E	52	34.471	60.321	23.605	1.00	37.54	C
ATOM	1693	O	THR	E	52	35.481	59.908	24.173	1.00	37.54	O
ATOM	1694	CB	THR	E	52	33.262	58.135	23.191	1.00	37.19	C
ATOM	1695	OG1	THR	E	52	33.244	58.174	21.760	1.00	37.22	O
ATOM	1696	CG2	THR	E	52	32.115	57.239	23.697	1.00	36.48	C
ATOM	1697	N	SER	E	53	34.469	61.417	22.846	1.00	37.54	N
ATOM	1698	CA	SER	E	53	35.650	62.263	22.704	1.00	37.89	C
ATOM	1699	C	SER	E	53	35.729	63.350	23.784	1.00	38.38	C
ATOM	1700	O	SER	E	53	36.715	64.080	23.855	1.00	38.50	O
ATOM	1701	CB	SER	E	53	35.710	62.888	21.304	1.00	37.89	C
ATOM	1702	OG	SER	E	53	34.563	63.679	21.059	1.00	37.24	O
ATOM	1703	N	LEU	E	54	34.703	63.447	24.627	1.00	38.99	N
ATOM	1704	CA	LEU	E	54	34.708	64.384	25.753	1.00	39.77	C
ATOM	1705	C	LEU	E	54	35.797	64.010	26.756	1.00	40.44	C
ATOM	1706	O	LEU	E	54	35.985	62.827	27.060	1.00	40.50	O
ATOM	1707	CB	LEU	E	54	33.365	64.335	26.481	1.00	39.67	C
ATOM	1708	CG	LEU	E	54	32.635	65.581	27.002	1.00	40.57	C
ATOM	1709	CD1	LEU	E	54	31.913	65.244	28.295	1.00	38.15	C
ATOM	1710	CD2	LEU	E	54	33.497	66.834	27.176	1.00	40.32	C
ATOM	1711	N	GLN	E	55	36.501	65.018	27.274	1.00	40.86	N
ATOM	1712	CA	GLN	E	55	37.425	64.805	28.383	1.00	41.72	C
ATOM	1713	C	GLN	E	55	36.690	64.253	29.606	1.00	41.37	C
ATOM	1714	O	GLN	E	55	35.612	64.726	29.971	1.00	41.06	O
ATOM	1715	CB	GLN	E	55	38.161	66.093	28.748	1.00	41.29	C
ATOM	1716	CG	GLN	E	55	39.314	66.430	27.814	1.00	43.37	C
ATOM	1717	CD	GLN	E	55	40.131	67.634	28.280	1.00	44.31	C
ATOM	1718	OE1	GLN	E	55	40.125	67.995	29.465	1.00	48.72	O
ATOM	1719	NE2	GLN	E	55	40.852	68.248	27.352	1.00	45.93	N
ATOM	1720	N	VAL	E	56	37.298	63.245	30.223	1.00	41.46	N
ATOM	1721	CA	VAL	E	56	36.755	62.562	31.385	1.00	41.68	C
ATOM	1722	C	VAL	E	56	36.424	63.503	32.554	1.00	41.41	C
ATOM	1723	O	VAL	E	56	35.359	63.403	33.159	1.00	41.15	O
ATOM	1724	CB	VAL	E	56	37.703	61.385	31.794	1.00	42.15	C
ATOM	1725	CG1	VAL	E	56	37.797	61.220	33.280	1.00	42.58	C
ATOM	1726	CG2	VAL	E	56	37.263	60.101	31.124	1.00	41.85	C
ATOM	1727	N	LYS	E	57	37.325	64.435	32.838	1.00	41.42	N
ATOM	1728	CA	LYS	E	57	37.119	65.424	33.893	1.00	41.43	C
ATOM	1729	C	LYS	E	57	35.876	66.285	33.658	1.00	40.66	C
ATOM	1730	O	LYS	E	57	35.155	66.616	34.602	1.00	40.49	O
ATOM	1731	CB	LYS	E	57	38.350	66.312	34.003	1.00	41.79	C
ATOM	1732	CG	LYS	E	57	38.698	66.739	35.414	1.00	44.65	C
ATOM	1733	CD	LYS	E	57	39.685	67.917	35.370	1.00	49.12	C
ATOM	1734	CE	LYS	E	57	40.499	68.046	36.656	1.00	50.50	C
ATOM	1735	NZ	LYS	E	57	41.476	69.174	36.519	1.00	53.14	N
ATOM	1736	N	LYS	E	58	35.629	66.645	32.399	1.00	39.81	N
ATOM	1737	CA	LYS	E	58	34.439	67.422	32.040	1.00	39.39	C
ATOM	1738	C	LYS	E	58	33.161	66.588	32.175	1.00	38.69	C
ATOM	1739	O	LYS	E	58	32.133	67.089	32.622	1.00	37.91	O

Figure 1 Table 1b - 27

ATOM	1740	CB	LYS	E	58	34.565	67.989	30.620	1.00	39.34	C
ATOM	1741	CG	LYS	E	58	35.730	68.961	30.437	1.00	40.46	C
ATOM	1742	CD	LYS	E	58	36.060	69.131	28.962	1.00	42.37	C
ATOM	1743	CE	LYS	E	58	37.378	69.869	28.746	1.00	43.61	C
ATOM	1744	NZ	LYS	E	58	37.129	71.237	28.237	1.00	44.76	N
ATOM	1745	N	ALA	E	59	33.243	65.320	31.779	1.00	38.22	N
ATOM	1746	CA	ALA	E	59	32.125	64.384	31.894	1.00	38.61	C
ATOM	1747	C	ALA	E	59	31.677	64.208	33.344	1.00	38.26	C
ATOM	1748	O	ALA	E	59	30.494	64.267	33.642	1.00	37.72	O
ATOM	1749	CB	ALA	E	59	32.484	63.027	31.271	1.00	38.55	C
ATOM	1750	N	PHE	E	60	32.627	64.035	34.253	1.00	38.62	N
ATOM	1751	CA	PHE	E	60	32.259	63.848	35.649	1.00	39.35	C
ATOM	1752	C	PHE	E	60	31.694	65.082	36.332	1.00	39.22	C
ATOM	1753	O	PHE	E	60	30.781	64.974	37.147	1.00	38.96	O
ATOM	1754	CB	PHE	E	60	33.403	63.220	36.431	1.00	40.27	C
ATOM	1755	CG	PHE	E	60	33.679	61.807	36.024	1.00	41.48	C
ATOM	1756	CD1	PHE	E	60	34.912	61.446	35.513	1.00	42.64	C
ATOM	1757	CD2	PHE	E	60	32.681	60.839	36.126	1.00	44.06	C
ATOM	1758	CE1	PHE	E	60	35.164	60.130	35.134	1.00	43.69	C
ATOM	1759	CE2	PHE	E	60	32.919	59.520	35.748	1.00	45.32	C
ATOM	1760	CZ	PHE	E	60	34.164	59.168	35.247	1.00	43.97	C
ATOM	1761	N	PHE	E	61	32.212	66.255	35.974	1.00	39.21	N
ATOM	1762	CA	PHE	E	61	31.654	67.506	36.470	1.00	39.09	C
ATOM	1763	C	PHE	E	61	30.228	67.710	35.962	1.00	38.22	C
ATOM	1764	O	PHE	E	61	29.364	68.222	36.683	1.00	37.73	O
ATOM	1765	CB	PHE	E	61	32.546	68.692	36.089	1.00	39.85	C
ATOM	1766	CG	PHE	E	61	32.126	69.990	36.718	1.00	41.28	C
ATOM	1767	CD1	PHE	E	61	32.037	70.113	38.101	1.00	43.15	C
ATOM	1768	CD2	PHE	E	61	31.821	71.093	35.928	1.00	42.98	C
ATOM	1769	CE1	PHE	E	61	31.644	71.321	38.686	1.00	44.49	C
ATOM	1770	CE2	PHE	E	61	31.435	72.307	36.507	1.00	44.21	C
ATOM	1771	CZ	PHE	E	61	31.347	72.417	37.890	1.00	42.84	C
ATOM	1772	N	ALA	E	62	29.985	67.288	34.724	1.00	37.62	N
ATOM	1773	CA	ALA	E	62	28.662	67.385	34.125	1.00	37.41	C
ATOM	1774	C	ALA	E	62	27.622	66.516	34.845	1.00	37.40	C
ATOM	1775	O	ALA	E	62	26.448	66.882	34.898	1.00	37.29	O
ATOM	1776	CB	ALA	E	62	28.725	67.035	32.661	1.00	37.51	C
ATOM	1777	N	LEU	E	63	28.051	65.375	35.395	1.00	37.62	N
ATOM	1778	CA	LEU	E	63	27.169	64.526	36.219	1.00	37.83	C
ATOM	1779	C	LEU	E	63	26.747	65.260	37.483	1.00	37.87	C
ATOM	1780	O	LEU	E	63	25.570	65.280	37.825	1.00	37.85	O
ATOM	1781	CB	LEU	E	63	27.846	63.200	36.603	1.00	37.65	C
ATOM	1782	CG	LEU	E	63	28.215	62.164	35.536	1.00	37.69	C
ATOM	1783	CD1	LEU	E	63	28.753	60.930	36.223	1.00	38.44	C
ATOM	1784	CD2	LEU	E	63	27.027	61.787	34.655	1.00	38.37	C
ATOM	1785	N	VAL	E	64	27.720	65.847	38.176	1.00	38.43	N
ATOM	1786	CA	VAL	E	64	27.448	66.677	39.354	1.00	39.30	C
ATOM	1787	C	VAL	E	64	26.523	67.830	38.997	1.00	39.27	C
ATOM	1788	O	VAL	E	64	25.481	68.009	39.630	1.00	39.90	O
ATOM	1789	CB	VAL	E	64	28.748	67.226	39.983	1.00	39.40	C
ATOM	1790	CG1	VAL	E	64	28.439	68.253	41.081	1.00	40.92	C
ATOM	1791	CG2	VAL	E	64	29.561	66.097	40.550	1.00	39.99	C
ATOM	1792	N	THR	E	65	26.897	68.585	37.963	1.00	39.28	N
ATOM	1793	CA	THR	E	65	26.148	69.767	37.518	1.00	39.31	C
ATOM	1794	C	THR	E	65	24.685	69.462	37.223	1.00	39.11	C
ATOM	1795	O	THR	E	65	23.794	70.242	37.557	1.00	39.22	O
ATOM	1796	CB	THR	E	65	26.807	70.387	36.266	1.00	39.22	C
ATOM	1797	OG1	THR	E	65	28.104	70.880	36.622	1.00	40.14	O
ATOM	1798	CG2	THR	E	65	25.984	71.540	35.715	1.00	40.57	C
ATOM	1799	N	ASN	E	66	24.443	68.320	36.595	1.00	38.89	N
ATOM	1800	CA	ASN	E	66	23.094	67.941	36.204	1.00	38.56	C
ATOM	1801	C	ASN	E	66	22.326	67.122	37.248	1.00	38.82	C
ATOM	1802	O	ASN	E	66	21.142	66.846	37.066	1.00	38.70	O
ATOM	1803	CB	ASN	E	66	23.147	67.235	34.853	1.00	38.28	C
ATOM	1804	CG	ASN	E	66	23.476	68.197	33.721	1.00	37.34	C
ATOM	1805	OD1	ASN	E	66	22.651	69.021	33.353	1.00	38.54	O
ATOM	1806	ND2	ASN	E	66	24.686	68.108	33.182	1.00	35.33	N

Figure 1 Table 1b - 28

ATOM	1807	N	GLY	E	67	22.998	66.758	38.338	1.00 39.19	N
ATOM	1808	CA	GLY	E	67	22.391	65.930	39.392	1.00 40.33	C
ATOM	1809	C	GLY	E	67	21.985	64.564	38.864	1.00 40.81	C
ATOM	1810	O	GLY	E	67	20.862	64.114	39.069	1.00 41.28	O
ATOM	1811	N	VAL	E	68	22.916	63.919	38.176	1.00 40.98	N
ATOM	1812	CA	VAL	E	68	22.665	62.668	37.478	1.00 41.30	C
ATOM	1813	C	VAL	E	68	23.792	61.692	37.852	1.00 40.99	C
ATOM	1814	O	VAL	E	68	24.927	62.117	38.085	1.00 41.02	O
ATOM	1815	CB	VAL	E	68	22.552	62.967	35.948	1.00 41.71	C
ATOM	1816	CG1	VAL	E	68	23.290	61.967	35.083	1.00 42.46	C
ATOM	1817	CG2	VAL	E	68	21.075	63.163	35.533	1.00 41.06	C
ATOM	1818	N	ARG	E	69	23.477	60.401	37.926	1.00 40.54	N
ATOM	1819	CA	ARG	E	69	24.446	59.392	38.370	1.00 40.24	C
ATOM	1820	C	ARG	E	69	24.994	58.512	37.252	1.00 39.50	C
ATOM	1821	O	ARG	E	69	25.866	57.676	37.493	1.00 38.99	O
ATOM	1822	CB	ARG	E	69	23.836	58.502	39.453	1.00 40.75	C
ATOM	1823	CG	ARG	E	69	23.179	59.277	40.574	1.00 43.64	C
ATOM	1824	CD	ARG	E	69	23.423	58.611	41.885	1.00 47.80	C
ATOM	1825	NE	ARG	E	69	22.346	57.711	42.275	1.00 52.21	N
ATOM	1826	CZ	ARG	E	69	22.467	56.777	43.218	1.00 53.83	C
ATOM	1827	NH1	ARG	E	69	23.614	56.614	43.856	1.00 53.55	N
ATOM	1828	NH2	ARG	E	69	21.438	55.998	43.519	1.00 56.35	N
ATOM	1829	N	ALA	E	70	24.480	58.696	36.039	1.00 38.40	N
ATOM	1830	CA	ALA	E	70	24.862	57.857	34.907	1.00 37.84	C
ATOM	1831	C	ALA	E	70	24.487	58.532	33.607	1.00 37.18	C
ATOM	1832	O	ALA	E	70	23.495	59.253	33.549	1.00 37.30	O
ATOM	1833	CB	ALA	E	70	24.193	56.500	34.993	1.00 37.23	C
ATOM	1834	N	ALA	E	71	25.278	58.268	32.571	1.00 36.76	N
ATOM	1835	CA	ALA	E	71	25.099	58.871	31.258	1.00 36.43	C
ATOM	1836	C	ALA	E	71	25.444	57.879	30.147	1.00 36.14	C
ATOM	1837	O	ALA	E	71	26.531	57.327	30.150	1.00 36.56	O
ATOM	1838	CB	ALA	E	71	25.980	60.102	31.149	1.00 36.26	C
ATOM	1839	N	PRO	E	72	24.523	57.649	29.189	1.00 36.42	N
ATOM	1840	CA	PRO	E	72	24.909	56.876	27.983	1.00 36.49	C
ATOM	1841	C	PRO	E	72	26.079	57.513	27.234	1.00 36.59	C
ATOM	1842	O	PRO	E	72	26.293	58.737	27.317	1.00 36.59	O
ATOM	1843	CB	PRO	E	72	23.655	56.915	27.088	1.00 36.13	C
ATOM	1844	CG	PRO	E	72	22.528	57.343	27.961	1.00 36.62	C
ATOM	1845	CD	PRO	E	72	23.112	58.086	29.151	1.00 36.45	C
ATOM	1846	N	LEU	E	73	26.822	56.679	26.508	1.00 36.45	N
ATOM	1847	CA	LEU	E	73	27.998	57.113	25.760	1.00 36.41	C
ATOM	1848	C	LEU	E	73	27.744	56.953	24.284	1.00 36.39	C
ATOM	1849	O	LEU	E	73	27.396	55.862	23.817	1.00 35.96	O
ATOM	1850	CB	LEU	E	73	29.257	56.332	26.185	1.00 36.43	C
ATOM	1851	CG	LEU	E	73	29.675	56.501	27.654	1.00 37.24	C
ATOM	1852	CD1	LEU	E	73	30.913	55.685	27.989	1.00 36.65	C
ATOM	1853	CD2	LEU	E	73	29.898	57.976	28.009	1.00 37.47	C
ATOM	1854	N	TRP	E	74	27.877	58.061	23.556	1.00 35.93	N
ATOM	1855	CA	TRP	E	74	27.667	58.066	22.121	1.00 36.18	C
ATOM	1856	C	TRP	E	74	29.021	58.097	21.411	1.00 36.57	C
ATOM	1857	O	TRP	E	74	29.844	58.996	21.642	1.00 36.72	O
ATOM	1858	CB	TRP	E	74	26.791	59.254	21.716	1.00 36.08	C
ATOM	1859	CG	TRP	E	74	26.569	59.428	20.223	1.00 35.87	C
ATOM	1860	CD1	TRP	E	74	27.264	60.255	19.383	1.00 34.99	C
ATOM	1861	CD2	TRP	E	74	25.569	58.789	19.417	1.00 34.91	C
ATOM	1862	NE1	TRP	E	74	26.770	60.160	18.107	1.00 35.54	N
ATOM	1863	CE2	TRP	E	74	25.723	59.275	18.098	1.00 35.27	C
ATOM	1864	CE3	TRP	E	74	24.551	57.863	19.684	1.00 35.32	C
ATOM	1865	CZ2	TRP	E	74	24.901	58.856	17.037	1.00 34.95	C
ATOM	1866	CZ3	TRP	E	74	23.730	57.442	18.628	1.00 35.53	C
ATOM	1867	CH2	TRP	E	74	23.916	57.941	17.318	1.00 35.32	C
ATOM	1868	N	ASP	E	75	29.259	57.086	20.579	1.00 36.72	N
ATOM	1869	CA	ASP	E	75	30.425	57.055	19.710	1.00 37.21	C
ATOM	1870	C	ASP	E	75	30.024	57.660	18.364	1.00 37.16	C
ATOM	1871	O	ASP	E	75	29.237	57.074	17.617	1.00 36.82	O
ATOM	1872	CB	ASP	E	75	30.920	55.617	19.541	1.00 37.28	C
ATOM	1873	CG	ASP	E	75	32.231	55.526	18.771	1.00 38.59	C

Figure 1 Table 1b - 29

ATOM	1874	OD1	ASP	E	75	33.056	54.650	19.107	1.00 39.81	O
ATOM	1875	OD2	ASP	E	75	32.445	56.318	17.830	1.00 39.44	O
ATOM	1876	N	SER	E	76	30.569	58.836	18.064	1.00 37.60	N
ATOM	1877	CA	SER	E	76	30.170	59.584	16.871	1.00 38.16	C
ATOM	1878	C	SER	E	76	30.584	58.902	15.557	1.00 38.37	C
ATOM	1879	O	SER	E	76	29.812	58.880	14.597	1.00 38.41	O
ATOM	1880	CB	SER	E	76	30.706	61.013	16.925	1.00 38.15	C
ATOM	1881	OG	SER	E	76	30.022	61.826	15.987	1.00 39.03	O
ATOM	1882	N	LYS	E	77	31.795	58.350	15.518	1.00 38.95	N
ATOM	1883	CA	LYS	E	77	32.270	57.619	14.332	1.00 39.42	C
ATOM	1884	C	LYS	E	77	31.373	56.431	13.998	1.00 39.09	C
ATOM	1885	O	LYS	E	77	31.012	56.227	12.839	1.00 39.23	O
ATOM	1886	CB	LYS	E	77	33.713	57.145	14.512	1.00 39.79	C
ATOM	1887	CG	LYS	E	77	34.731	58.267	14.529	1.00 42.04	C
ATOM	1888	CD	LYS	E	77	36.010	57.867	13.815	1.00 45.11	C
ATOM	1889	CE	LYS	E	77	37.210	58.653	14.340	1.00 46.72	C
ATOM	1890	NZ	LYS	E	77	37.635	58.149	15.690	1.00 47.24	N
ATOM	1891	N	LYS	E	78	31.010	55.663	15.023	1.00 38.69	N
ATOM	1892	CA	LYS	E	78	30.161	54.487	14.871	1.00 38.32	C
ATOM	1893	C	LYS	E	78	28.685	54.836	14.768	1.00 37.97	C
ATOM	1894	O	LYS	E	78	27.888	54.021	14.298	1.00 38.22	O
ATOM	1895	CB	LYS	E	78	30.371	53.529	16.046	1.00 38.63	C
ATOM	1896	CG	LYS	E	78	31.711	52.833	16.031	1.00 39.35	C
ATOM	1897	CD	LYS	E	78	31.923	52.044	17.304	1.00 42.05	C
ATOM	1898	CE	LYS	E	78	33.159	51.159	17.201	1.00 42.92	C
ATOM	1899	NZ	LYS	E	78	33.419	50.488	18.510	1.00 44.70	N
ATOM	1900	N	GLN	E	79	28.323	56.039	15.216	1.00 37.23	N
ATOM	1901	CA	GLN	E	79	26.929	56.495	15.224	1.00 36.35	C
ATOM	1902	C	GLN	E	79	26.044	55.587	16.087	1.00 36.04	C
ATOM	1903	O	GLN	E	79	24.951	55.199	15.681	1.00 35.32	O
ATOM	1904	CB	GLN	E	79	26.373	56.618	13.799	1.00 36.27	C
ATOM	1905	CG	GLN	E	79	26.959	57.779	12.995	1.00 35.77	C
ATOM	1906	CD	GLN	E	79	26.461	59.114	13.514	1.00 34.96	C
ATOM	1907	OE1	GLN	E	79	25.283	59.426	13.391	1.00 33.63	O
ATOM	1908	NE2	GLN	E	79	27.350	59.890	14.123	1.00 34.56	N
ATOM	1909	N	SER	E	80	26.536	55.250	17.277	1.00 35.94	N
ATOM	1910	CA	SER	E	80	25.757	54.473	18.229	1.00 36.22	C
ATOM	1911	C	SER	E	80	26.201	54.673	19.658	1.00 35.96	C
ATOM	1912	O	SER	E	80	27.322	55.105	19.933	1.00 36.23	O
ATOM	1913	CB	SER	E	80	25.789	52.977	17.899	1.00 36.06	C
ATOM	1914	OG	SER	E	80	27.108	52.499	17.916	1.00 37.91	O
ATOM	1915	N	PHE	E	81	25.281	54.371	20.560	1.00 35.90	N
ATOM	1916	CA	PHE	E	81	25.592	54.183	21.964	1.00 35.68	C
ATOM	1917	C	PHE	E	81	26.491	52.961	22.124	1.00 35.84	C
ATOM	1918	O	PHE	E	81	26.221	51.909	21.536	1.00 36.11	O
ATOM	1919	CB	PHE	E	81	24.302	53.995	22.756	1.00 35.26	C
ATOM	1920	CG	PHE	E	81	23.420	55.199	22.761	1.00 35.11	C
ATOM	1921	CD1	PHE	E	81	22.202	55.183	22.093	1.00 34.49	C
ATOM	1922	CD2	PHE	E	81	23.811	56.358	23.430	1.00 34.57	C
ATOM	1923	CE1	PHE	E	81	21.374	56.298	22.095	1.00 35.92	C
ATOM	1924	CE2	PHE	E	81	22.998	57.484	23.436	1.00 35.39	C
ATOM	1925	CZ	PHE	E	81	21.777	57.459	22.770	1.00 35.83	C
ATOM	1926	N	VAL	E	82	27.555	53.106	22.913	1.00 35.70	N
ATOM	1927	CA	VAL	E	82	28.532	52.032	23.102	1.00 35.98	C
ATOM	1928	C	VAL	E	82	28.705	51.586	24.562	1.00 36.04	C
ATOM	1929	O	VAL	E	82	29.427	50.628	24.838	1.00 36.02	O
ATOM	1930	CB	VAL	E	82	29.922	52.403	22.522	1.00 35.87	C
ATOM	1931	CG1	VAL	E	82	29.878	52.459	20.993	1.00 36.15	C
ATOM	1932	CG2	VAL	E	82	30.447	53.714	23.120	1.00 35.83	C
ATOM	1933	N	GLY	E	83	28.064	52.289	25.491	1.00 36.31	N
ATOM	1934	CA	GLY	E	83	28.250	52.005	26.912	1.00 36.26	C
ATOM	1935	C	GLY	E	83	27.684	53.083	27.809	1.00 36.51	C
ATOM	1936	O	GLY	E	83	26.922	53.948	27.353	1.00 36.06	O
ATOM	1937	N	MET	E	84	28.074	53.020	29.082	1.00 36.52	N
ATOM	1938	CA	MET	E	84	27.636	53.947	30.118	1.00 37.26	C
ATOM	1939	C	MET	E	84	28.833	54.539	30.849	1.00 37.26	C
ATOM	1940	O	MET	E	84	29.912	53.950	30.891	1.00 37.50	O

Figure 1 Table 1b - 30

ATOM	1941	CB	MET	E	84	26.736	53.236	31.135	1.00 37.94	C
ATOM	1942	CG	MET	E	84	25.427	52.698	30.564	1.00 39.66	C
ATOM	1943	SD	MET	E	84	24.186	53.978	30.309	1.00 42.44	S
ATOM	1944	CE	MET	E	84	23.530	53.430	28.771	1.00 43.79	C
ATOM	1945	N	LEU	E	85	28.649	55.725	31.407	1.00 37.41	N
ATOM	1946	CA	LEU	E	85	29.603	56.248	32.366	1.00 37.31	C
ATOM	1947	C	LEU	E	85	28.827	56.498	33.649	1.00 37.09	C
ATOM	1948	O	LEU	E	85	27.851	57.253	33.667	1.00 37.60	O
ATOM	1949	CB	LEU	E	85	30.281	57.521	31.845	1.00 37.48	C
ATOM	1950	CG	LEU	E	85	31.553	57.993	32.573	1.00 38.12	C
ATOM	1951	CD1	LEU	E	85	32.749	57.107	32.238	1.00 37.41	C
ATOM	1952	CD2	LEU	E	85	31.867	59.441	32.202	1.00 37.46	C
ATOM	1953	N	THR	E	86	29.243	55.831	34.715	1.00 36.60	N
ATOM	1954	CA	THR	E	86	28.527	55.886	35.985	1.00 35.75	C
ATOM	1955	C	THR	E	86	29.517	56.329	37.056	1.00 35.89	C
ATOM	1956	O	THR	E	86	30.695	56.555	36.755	1.00 35.52	O
ATOM	1957	CB	THR	E	86	27.904	54.517	36.356	1.00 35.89	C
ATOM	1958	OG1	THR	E	86	28.919	53.640	36.869	1.00 34.52	O
ATOM	1959	CG2	THR	E	86	27.191	53.876	35.151	1.00 33.77	C
ATOM	1960	N	ILE	E	87	29.040	56.453	38.292	1.00 35.85	N
ATOM	1961	CA	ILE	E	87	29.897	56.829	39.416	1.00 35.99	C
ATOM	1962	C	ILE	E	87	30.960	55.767	39.696	1.00 35.84	C
ATOM	1963	O	ILE	E	87	32.040	56.095	40.170	1.00 35.93	O
ATOM	1964	CB	ILE	E	87	29.096	57.112	40.719	1.00 36.07	C
ATOM	1965	CG1	ILE	E	87	27.972	58.137	40.496	1.00 37.05	C
ATOM	1966	CG2	ILE	E	87	30.038	57.540	41.860	1.00 35.74	C
ATOM	1967	CD1	ILE	E	87	28.290	59.240	39.514	1.00 40.64	C
ATOM	1968	N	THR	E	88	30.652	54.505	39.397	1.00 35.58	N
ATOM	1969	CA	THR	E	88	31.636	53.431	39.538	1.00 35.63	C
ATOM	1970	C	THR	E	88	32.886	53.732	38.707	1.00 36.03	C
ATOM	1971	O	THR	E	88	34.009	53.605	39.205	1.00 35.93	O
ATOM	1972	CB	THR	E	88	31.049	52.055	39.167	1.00 35.59	C
ATOM	1973	OG1	THR	E	88	30.058	51.693	40.135	1.00 34.38	O
ATOM	1974	CG2	THR	E	88	32.138	50.979	39.144	1.00 34.98	C
ATOM	1975	N	ASP	E	89	32.676	54.166	37.462	1.00 35.94	N
ATOM	1976	CA	ASP	E	89	33.765	54.565	36.571	1.00 36.57	C
ATOM	1977	C	ASP	E	89	34.567	55.748	37.103	1.00 36.82	C
ATOM	1978	O	ASP	E	89	35.784	55.787	36.947	1.00 36.88	O
ATOM	1979	CB	ASP	E	89	33.211	54.885	35.178	1.00 36.79	C
ATOM	1980	CG	ASP	E	89	32.458	53.712	34.582	1.00 36.38	C
ATOM	1981	OD1	ASP	E	89	31.252	53.842	34.307	1.00 36.91	O
ATOM	1982	OD2	ASP	E	89	33.068	52.642	34.422	1.00 37.09	O
ATOM	1983	N	PHE	E	90	33.883	56.705	37.733	1.00 37.22	N
ATOM	1984	CA	PHE	E	90	34.551	57.840	38.376	1.00 37.22	C
ATOM	1985	C	PHE	E	90	35.485	57.330	39.453	1.00 36.86	C
ATOM	1986	O	PHE	E	90	36.624	57.763	39.553	1.00 36.74	O
ATOM	1987	CB	PHE	E	90	33.528	58.803	38.987	1.00 37.55	C
ATOM	1988	CG	PHE	E	90	34.142	59.985	39.686	1.00 38.88	C
ATOM	1989	CD1	PHE	E	90	34.947	60.894	38.985	1.00 39.21	C
ATOM	1990	CD2	PHE	E	90	33.904	60.206	41.040	1.00 40.01	C
ATOM	1991	CE1	PHE	E	90	35.515	61.998	39.628	1.00 39.91	C
ATOM	1992	CE2	PHE	E	90	34.461	61.307	41.696	1.00 40.49	C
ATOM	1993	CZ	PHE	E	90	35.264	62.211	40.988	1.00 40.58	C
ATOM	1994	N	ILE	E	91	34.987	56.400	40.255	1.00 36.27	N
ATOM	1995	CA	ILE	E	91	35.783	55.823	41.326	1.00 36.61	C
ATOM	1996	C	ILE	E	91	37.004	55.048	40.804	1.00 36.68	C
ATOM	1997	O	ILE	E	91	38.097	55.180	41.361	1.00 37.03	O
ATOM	1998	CB	ILE	E	91	34.909	54.968	42.254	1.00 36.40	C
ATOM	1999	CG1	ILE	E	91	33.957	55.887	43.030	1.00 36.05	C
ATOM	2000	CG2	ILE	E	91	35.769	54.112	43.195	1.00 36.42	C
ATOM	2001	CD1	ILE	E	91	32.786	55.186	43.652	1.00 35.33	C
ATOM	2002	N	ASN	E	92	36.817	54.261	39.744	1.00 36.66	N
ATOM	2003	CA	ASN	E	92	37.932	53.552	39.099	1.00 37.28	C
ATOM	2004	C	ASN	E	92	39.001	54.529	38.606	1.00 37.44	C
ATOM	2005	O	ASN	E	92	40.201	54.293	38.792	1.00 36.82	O
ATOM	2006	CB	ASN	E	92	37.454	52.705	37.915	1.00 37.31	C
ATOM	2007	CG	ASN	E	92	36.462	51.631	38.311	1.00 39.21	C

Figure 1 Table 1b - 31

ATOM	2008	OD1	ASN	E	92	36.451	51.155	39.445	1.00	40.58	O
ATOM	2009	ND2	ASN	E	92	35.610	51.247	37.367	1.00	40.01	N
ATOM	2010	N	ILE	E	93	38.546	55.621	37.982	1.00	37.44	N
ATOM	2011	CA	ILE	E	93	39.435	56.665	37.460	1.00	38.19	C
ATOM	2012	C	ILE	E	93	40.151	57.457	38.560	1.00	38.23	C
ATOM	2013	O	ILE	E	93	41.363	57.669	38.476	1.00	38.23	O
ATOM	2014	CB	ILE	E	93	38.677	57.612	36.477	1.00	38.17	C
ATOM	2015	CG1	ILE	E	93	38.259	56.818	35.243	1.00	38.96	C
ATOM	2016	CG2	ILE	E	93	39.555	58.806	36.049	1.00	39.51	C
ATOM	2017	CD1	ILE	E	93	37.088	57.383	34.466	1.00	41.34	C
ATOM	2018	N	LEU	E	94	39.401	57.905	39.571	1.00	38.76	N
ATOM	2019	CA	LEU	E	94	39.977	58.619	40.717	1.00	39.45	C
ATOM	2020	C	LEU	E	94	41.033	57.790	41.438	1.00	39.49	C
ATOM	2021	O	LEU	E	94	42.074	58.306	41.837	1.00	39.60	O
ATOM	2022	CB	LEU	E	94	38.904	59.000	41.735	1.00	39.34	C
ATOM	2023	CG	LEU	E	94	38.293	60.397	41.783	1.00	41.47	C
ATOM	2024	CD1	LEU	E	94	37.664	60.588	43.155	1.00	42.03	C
ATOM	2025	CD2	LEU	E	94	39.308	61.512	41.500	1.00	42.57	C
ATOM	2026	N	HIS	E	95	40.747	56.509	41.625	1.00	39.86	N
ATOM	2027	CA	HIS	E	95	41.687	55.625	42.299	1.00	40.27	C
ATOM	2028	C	HIS	E	95	42.960	55.477	41.470	1.00	40.67	C
ATOM	2029	O	HIS	E	95	44.059	55.572	42.009	1.00	40.25	O
ATOM	2030	CB	HIS	E	95	41.058	54.265	42.594	1.00	39.94	C
ATOM	2031	CG	HIS	E	95	41.934	53.370	43.414	1.00	41.09	C
ATOM	2032	ND1	HIS	E	95	42.396	52.155	42.955	1.00	41.99	N
ATOM	2033	CD2	HIS	E	95	42.452	53.527	44.656	1.00	41.26	C
ATOM	2034	CE1	HIS	E	95	43.150	51.596	43.884	1.00	42.17	C
ATOM	2035	NE2	HIS	E	95	43.206	52.412	44.922	1.00	42.70	N
ATOM	2036	N	ARG	E	96	42.798	55.257	40.166	1.00	41.46	N
ATOM	2037	CA	ARG	E	96	43.926	55.201	39.237	1.00	43.18	C
ATOM	2038	C	ARG	E	96	44.747	56.486	39.240	1.00	43.04	C
ATOM	2039	O	ARG	E	96	45.972	56.439	39.246	1.00	43.70	O
ATOM	2040	CB	ARG	E	96	43.436	54.927	37.818	1.00	43.68	C
ATOM	2041	CG	ARG	E	96	43.611	53.495	37.368	1.00	47.73	C
ATOM	2042	CD	ARG	E	96	45.064	53.205	37.035	1.00	52.19	C
ATOM	2043	NE	ARG	E	96	45.262	51.794	36.730	1.00	56.27	N
ATOM	2044	CZ	ARG	E	96	45.212	51.272	35.506	1.00	58.30	C
ATOM	2045	NH1	ARG	E	96	44.970	52.045	34.455	1.00	58.81	N
ATOM	2046	NH2	ARG	E	96	45.407	49.968	35.337	1.00	59.63	N
ATOM	2047	N	TYR	E	97	44.052	57.620	39.237	1.00	42.84	N
ATOM	2048	CA	TYR	E	97	44.667	58.944	39.281	1.00	42.85	C
ATOM	2049	C	TYR	E	97	45.485	59.139	40.555	1.00	41.65	C
ATOM	2050	O	TYR	E	97	46.618	59.617	40.500	1.00	41.46	O
ATOM	2051	CB	TYR	E	97	43.585	60.035	39.137	1.00	44.05	C
ATOM	2052	CG	TYR	E	97	44.014	61.434	39.548	1.00	45.79	C
ATOM	2053	CD1	TYR	E	97	44.600	62.302	38.623	1.00	47.34	C
ATOM	2054	CD2	TYR	E	97	43.826	61.889	40.858	1.00	46.92	C
ATOM	2055	CE1	TYR	E	97	45.001	63.586	38.991	1.00	48.38	C
ATOM	2056	CE2	TYR	E	97	44.230	63.169	41.243	1.00	48.25	C
ATOM	2057	CZ	TYR	E	97	44.811	64.014	40.303	1.00	48.54	C
ATOM	2058	OH	TYR	E	97	45.209	65.291	40.668	1.00	49.43	O
ATOM	2059	N	TYR	E	98	44.908	58.771	41.696	1.00	40.39	N
ATOM	2060	CA	TYR	E	98	45.599	58.930	42.975	1.00	39.15	C
ATOM	2061	C	TYR	E	98	46.917	58.141	43.013	1.00	38.09	C
ATOM	2062	O	TYR	E	98	47.969	58.684	43.372	1.00	37.32	O
ATOM	2063	CB	TYR	E	98	44.686	58.556	44.154	1.00	39.30	C
ATOM	2064	CG	TYR	E	98	45.408	58.578	45.483	1.00	39.92	C
ATOM	2065	CD1	TYR	E	98	45.541	59.763	46.212	1.00	40.00	C
ATOM	2066	CD2	TYR	E	98	45.983	57.416	46.002	1.00	38.90	C
ATOM	2067	CE1	TYR	E	98	46.224	59.782	47.432	1.00	39.79	C
ATOM	2068	CE2	TYR	E	98	46.667	57.430	47.209	1.00	39.50	C
ATOM	2069	CZ	TYR	E	98	46.780	58.614	47.920	1.00	40.42	C
ATOM	2070	OH	TYR	E	98	47.455	58.620	49.126	1.00	42.24	O
ATOM	2071	N	LYS	E	99	46.854	56.869	42.623	1.00	37.00	N
ATOM	2072	CA	LYS	E	99	48.039	56.007	42.621	1.00	36.09	C
ATOM	2073	C	LYS	E	99	49.082	56.450	41.590	1.00	35.15	C
ATOM	2074	O	LYS	E	99	50.270	56.510	41.901	1.00	34.60	O

Figure 1

Table 1b - 32

ATOM	2075	CB	LYS	E	99	47.652	54.533	42.423	1.00	36.22	C
ATOM	2076	CG	LYS	E	99	46.779	53.945	43.547	1.00	36.13	C
ATOM	2077	CD	LYS	E	99	47.551	53.804	44.858	1.00	36.71	C
ATOM	2078	CE	LYS	E	99	46.834	52.878	45.854	1.00	37.70	C
ATOM	2079	NZ	LYS	E	99	47.599	52.808	47.135	1.00	37.53	N
ATOM	2080	N	SER	E	100	48.632	56.783	40.381	1.00	34.16	N
ATOM	2081	CA	SER	E	100	49.529	57.221	39.309	1.00	33.29	C
ATOM	2082	C	SER	E	100	50.282	58.516	39.662	1.00	32.68	C
ATOM	2083	O	SER	E	100	51.459	58.671	39.314	1.00	31.67	O
ATOM	2084	CB	SER	E	100	48.753	57.416	38.002	1.00	33.95	C
ATOM	2085	OG	SER	E	100	48.061	56.235	37.628	1.00	34.68	O
ATOM	2086	N	ALA	E	101	49.601	59.433	40.354	1.00	31.92	N
ATOM	2087	CA	ALA	E	101	50.206	60.698	40.795	1.00	31.50	C
ATOM	2088	C	ALA	E	101	51.400	60.468	41.725	1.00	31.28	C
ATOM	2089	O	ALA	E	101	52.399	61.192	41.648	1.00	30.97	O
ATOM	2090	CB	ALA	E	101	49.163	61.593	41.454	1.00	31.33	C
ATOM	2091	N	LEU	E	102	51.305	59.434	42.565	1.00	30.89	N
ATOM	2092	CA	LEU	E	102	52.379	59.051	43.490	1.00	30.90	C
ATOM	2093	C	LEU	E	102	53.633	58.577	42.755	1.00	30.76	C
ATOM	2094	O	LEU	E	102	54.728	58.490	43.326	1.00	30.41	O
ATOM	2095	CB	LEU	E	102	51.886	57.973	44.478	1.00	31.21	C
ATOM	2096	CG	LEU	E	102	50.814	58.391	45.497	1.00	32.10	C
ATOM	2097	CD1	LEU	E	102	50.299	57.190	46.294	1.00	31.92	C
ATOM	2098	CD2	LEU	E	102	51.358	59.459	46.447	1.00	34.11	C
ATOM	2099	N	VAL	E	103	53.463	58.327	41.463	1.00	30.88	N
ATOM	2100	CA	VAL	E	103	54.511	57.800	40.605	1.00	30.47	C
ATOM	2101	C	VAL	E	103	54.713	58.813	39.444	1.00	30.43	C
ATOM	2102	O	VAL	E	103	55.405	58.563	38.441	1.00	29.94	O
ATOM	2103	CB	VAL	E	103	54.120	56.326	40.241	1.00	31.08	C
ATOM	2104	CG1	VAL	E	103	53.570	56.173	38.842	1.00	31.08	C
ATOM	2105	CG2	VAL	E	103	55.249	55.364	40.553	1.00	31.13	C
ATOM	2106	N	GLN	E	104	54.128	59.995	39.643	1.00	30.35	N
ATOM	2107	CA	GLN	E	104	54.278	61.162	38.750	1.00	30.50	C
ATOM	2108	C	GLN	E	104	53.775	60.883	37.327	1.00	31.12	C
ATOM	2109	O	GLN	E	104	54.352	61.342	36.340	1.00	30.56	O
ATOM	2110	CB	GLN	E	104	55.723	61.710	38.753	1.00	30.12	C
ATOM	2111	CG	GLN	E	104	56.302	62.020	40.145	1.00	29.56	C
ATOM	2112	CD	GLN	E	104	56.787	60.764	40.894	1.00	29.63	C
ATOM	2113	OE1	GLN	E	104	57.497	59.931	40.340	1.00	29.24	O
ATOM	2114	NE2	GLN	E	104	56.408	60.644	42.155	1.00	28.71	N
ATOM	2115	N	ILE	E	105	52.700	60.106	37.247	1.00	32.51	N
ATOM	2116	CA	ILE	E	105	51.997	59.851	36.000	1.00	34.29	C
ATOM	2117	C	ILE	E	105	50.684	60.615	36.097	1.00	35.95	C
ATOM	2118	O	ILE	E	105	49.846	60.331	36.955	1.00	35.86	O
ATOM	2119	CB	ILE	E	105	51.789	58.328	35.739	1.00	34.43	C
ATOM	2120	CG1	ILE	E	105	53.136	57.668	35.395	1.00	33.88	C
ATOM	2121	CG2	ILE	E	105	50.761	58.089	34.615	1.00	33.99	C
ATOM	2122	CD1	ILE	E	105	53.117	56.153	35.367	1.00	34.13	C
ATOM	2123	N	TYR	E	106	50.543	61.623	35.241	1.00	38.08	N
ATOM	2124	CA	TYR	E	106	49.388	62.511	35.262	1.00	40.54	C
ATOM	2125	C	TYR	E	106	48.773	62.509	33.873	1.00	42.95	C
ATOM	2126	O	TYR	E	106	49.023	63.412	33.082	1.00	43.83	O
ATOM	2127	CB	TYR	E	106	49.809	63.937	35.645	1.00	39.59	C
ATOM	2128	CG	TYR	E	106	50.726	64.030	36.846	1.00	38.80	C
ATOM	2129	CD1	TYR	E	106	52.096	64.212	36.682	1.00	37.99	C
ATOM	2130	CD2	TYR	E	106	50.223	63.946	38.147	1.00	37.22	C
ATOM	2131	CE1	TYR	E	106	52.945	64.305	37.777	1.00	37.50	C
ATOM	2132	CE2	TYR	E	106	51.064	64.038	39.247	1.00	36.68	C
ATOM	2133	CZ	TYR	E	106	52.423	64.216	39.052	1.00	36.97	C
ATOM	2134	OH	TYR	E	106	53.267	64.309	40.127	1.00	37.54	O
ATOM	2135	N	GLU	E	107	48.003	61.471	33.565	1.00	45.96	N
ATOM	2136	CA	GLU	E	107	47.402	61.322	32.245	1.00	48.79	C
ATOM	2137	C	GLU	E	107	45.911	61.449	32.375	1.00	50.41	C
ATOM	2138	O	GLU	E	107	45.281	62.336	31.788	1.00	50.80	O
ATOM	2139	CB	GLU	E	107	47.641	59.915	31.688	1.00	48.86	C
ATOM	2140	CG	GLU	E	107	49.064	59.482	31.502	1.00	49.31	C
ATOM	2141	CD	GLU	E	107	49.168	58.006	31.153	1.00	49.53	C

Figure 1

Table 1b - 33

ATOM	2142	OE1	GLU	E	107	48.368	57.206	31.694	1.00	51.81	O
ATOM	2143	OE2	GLU	E	107	50.048	57.643	30.344	1.00	49.78	O
ATOM	2144	N	LEU	E	108	45.363	60.532	33.167	1.00	52.32	N
ATOM	2145	CA	LEU	E	108	43.947	60.216	33.157	1.00	53.91	C
ATOM	2146	C	LEU	E	108	43.037	61.424	33.092	1.00	54.79	C
ATOM	2147	O	LEU	E	108	41.995	61.375	32.440	1.00	55.36	O
ATOM	2148	CB	LEU	E	108	43.578	59.375	34.373	1.00	53.92	C
ATOM	2149	CG	LEU	E	108	44.116	57.953	34.477	1.00	54.89	C
ATOM	2150	CD1	LEU	E	108	43.819	57.496	35.861	1.00	54.72	C
ATOM	2151	CD2	LEU	E	108	43.498	57.004	33.452	1.00	56.18	C
ATOM	2152	N	GLU	E	109	43.411	62.509	33.760	1.00	55.59	N
ATOM	2153	CA	GLU	E	109	42.457	63.595	33.895	1.00	56.65	C
ATOM	2154	C	GLU	E	109	42.279	64.390	32.593	1.00	56.53	C
ATOM	2155	O	GLU	E	109	41.210	64.966	32.356	1.00	57.19	O
ATOM	2156	CB	GLU	E	109	42.761	64.453	35.126	1.00	57.14	C
ATOM	2157	CG	GLU	E	109	41.548	64.642	36.057	1.00	58.51	C
ATOM	2158	CD	GLU	E	109	40.973	63.337	36.635	1.00	60.55	C
ATOM	2159	OE1	GLU	E	109	40.644	63.316	37.845	1.00	61.11	O
ATOM	2160	OE2	GLU	E	109	40.830	62.338	35.891	1.00	61.33	O
ATOM	2161	N	GLU	E	110	43.302	64.361	31.737	1.00	56.28	N
ATOM	2162	CA	GLU	E	110	43.193	64.862	30.354	1.00	55.85	C
ATOM	2163	C	GLU	E	110	42.818	63.775	29.331	1.00	55.02	C
ATOM	2164	O	GLU	E	110	42.670	64.062	28.135	1.00	54.76	O
ATOM	2165	CB	GLU	E	110	44.470	65.599	29.936	1.00	56.18	C
ATOM	2166	CG	GLU	E	110	44.482	67.095	30.278	1.00	58.08	C
ATOM	2167	CD	GLU	E	110	43.733	67.421	31.568	1.00	60.35	C
ATOM	2168	OE1	GLU	E	110	42.486	67.546	31.514	1.00	61.91	O
ATOM	2169	OE2	GLU	E	110	44.388	67.554	32.629	1.00	60.70	O
ATOM	2170	N	HIS	E	111	42.676	62.537	29.814	1.00	53.93	N
ATOM	2171	CA	HIS	E	111	42.080	61.438	29.053	1.00	53.09	C
ATOM	2172	C	HIS	E	111	40.684	61.826	28.586	1.00	52.07	C
ATOM	2173	O	HIS	E	111	39.921	62.449	29.331	1.00	51.63	O
ATOM	2174	CB	HIS	E	111	41.923	60.194	29.945	1.00	53.55	C
ATOM	2175	CG	HIS	E	111	42.990	59.156	29.775	1.00	54.94	C
ATOM	2176	ND1	HIS	E	111	44.271	59.449	29.352	1.00	57.16	N
ATOM	2177	CD2	HIS	E	111	42.970	57.822	30.011	1.00	56.03	C
ATOM	2178	CE1	HIS	E	111	44.986	58.337	29.313	1.00	57.15	C
ATOM	2179	NE2	HIS	E	111	44.220	57.335	29.712	1.00	56.68	N
ATOM	2180	N	LYS	E	112	40.349	61.456	27.358	1.00	50.97	N
ATOM	2181	CA	LYS	E	112	38.957	61.471	26.949	1.00	50.31	C
ATOM	2182	C	LYS	E	112	38.321	60.122	27.307	1.00	49.74	C
ATOM	2183	O	LYS	E	112	39.032	59.148	27.600	1.00	49.33	O
ATOM	2184	CB	LYS	E	112	38.817	61.817	25.466	1.00	50.46	C
ATOM	2185	CG	LYS	E	112	39.360	60.784	24.500	1.00	50.60	C
ATOM	2186	CD	LYS	E	112	40.232	61.434	23.414	1.00	50.48	C
ATOM	2187	CE	LYS	E	112	39.565	62.623	22.742	1.00	50.43	C
ATOM	2188	NZ	LYS	E	112	40.487	63.278	21.760	1.00	50.54	N
ATOM	2189	N	ILE	E	113	36.992	60.083	27.305	1.00	49.02	N
ATOM	2190	CA	ILE	E	113	36.233	58.879	27.652	1.00	48.58	C
ATOM	2191	C	ILE	E	113	36.708	57.667	26.840	1.00	49.05	C
ATOM	2192	O	ILE	E	113	36.955	56.593	27.401	1.00	48.44	O
ATOM	2193	CB	ILE	E	113	34.703	59.117	27.507	1.00	48.18	C
ATOM	2194	CG1	ILE	E	113	34.220	60.099	28.583	1.00	46.59	C
ATOM	2195	CG2	ILE	E	113	33.936	57.802	27.566	1.00	47.30	C
ATOM	2196	CD1	ILE	E	113	32.810	60.591	28.399	1.00	43.47	C
ATOM	2197	N	GLU	E	114	36.845	57.869	25.528	1.00	49.72	N
ATOM	2198	CA	GLU	E	114	37.417	56.888	24.602	1.00	50.81	C
ATOM	2199	C	GLU	E	114	38.678	56.222	25.127	1.00	51.15	C
ATOM	2200	O	GLU	E	114	38.774	54.996	25.167	1.00	50.90	O
ATOM	2201	CB	GLU	E	114	37.793	57.573	23.293	1.00	50.86	C
ATOM	2202	CG	GLU	E	114	36.784	57.458	22.210	1.00	52.69	C
ATOM	2203	CD	GLU	E	114	37.391	57.722	20.851	1.00	54.91	C
ATOM	2204	OE1	GLU	E	114	38.201	58.673	20.728	1.00	55.85	O
ATOM	2205	OE2	GLU	E	114	37.062	56.969	19.910	1.00	55.53	O
ATOM	2206	N	THR	E	115	39.646	57.054	25.503	1.00	52.06	N
ATOM	2207	CA	THR	E	115	40.974	56.588	25.871	1.00	53.37	C
ATOM	2208	C	THR	E	115	40.981	55.857	27.208	1.00	54.00	C

Figure 1 Table 1b - 34

ATOM	2209	O	THR	E	115	41.741	54.904	27.380	1.00	54.03	O
ATOM	2210	CB	THR	E	115	42.014	57.732	25.873	1.00	53.20	C
ATOM	2211	OG1	THR	E	115	41.601	58.759	26.782	1.00	54.24	O
ATOM	2212	CG2	THR	E	115	42.146	58.323	24.485	1.00	53.43	C
ATOM	2213	N	TRP	E	116	40.139	56.284	28.148	1.00	55.09	N
ATOM	2214	CA	TRP	E	116	40.010	55.533	29.395	1.00	56.40	C
ATOM	2215	C	TRP	E	116	39.375	54.163	29.152	1.00	56.67	C
ATOM	2216	O	TRP	E	116	39.823	53.161	29.710	1.00	56.66	O
ATOM	2217	CB	TRP	E	116	39.248	56.297	30.486	1.00	57.11	C
ATOM	2218	CG	TRP	E	116	39.200	55.488	31.765	1.00	58.42	C
ATOM	2219	CD1	TRP	E	116	40.214	55.324	32.670	1.00	59.07	C
ATOM	2220	CD2	TRP	E	116	38.103	54.692	32.246	1.00	59.62	C
ATOM	2221	NE1	TRP	E	116	39.811	54.491	33.689	1.00	60.40	N
ATOM	2222	CE2	TRP	E	116	38.520	54.089	33.453	1.00	59.72	C
ATOM	2223	CE3	TRP	E	116	36.809	54.433	31.774	1.00	60.18	C
ATOM	2224	CZ2	TRP	E	116	37.685	53.249	34.204	1.00	60.40	C
ATOM	2225	CZ3	TRP	E	116	35.978	53.595	32.518	1.00	59.85	C
ATOM	2226	CH2	TRP	E	116	36.420	53.014	33.723	1.00	59.64	C
ATOM	2227	N	ARG	E	117	38.345	54.123	28.312	1.00	57.15	N
ATOM	2228	CA	ARG	E	117	37.667	52.872	27.996	1.00	57.84	C
ATOM	2229	C	ARG	E	117	38.589	51.865	27.304	1.00	58.78	C
ATOM	2230	O	ARG	E	117	38.562	50.675	27.620	1.00	58.66	O
ATOM	2231	CB	ARG	E	117	36.414	53.134	27.166	1.00	57.40	C
ATOM	2232	CG	ARG	E	117	35.270	53.715	27.981	1.00	56.47	C
ATOM	2233	CD	ARG	E	117	34.127	54.213	27.101	1.00	54.27	C
ATOM	2234	NE	ARG	E	117	33.671	53.226	26.121	1.00	52.53	N
ATOM	2235	CZ	ARG	E	117	32.888	52.185	26.392	1.00	51.77	C
ATOM	2236	NH1	ARG	E	117	32.458	51.956	27.631	1.00	51.20	N
ATOM	2237	NH2	ARG	E	117	32.540	51.361	25.413	1.00	51.43	N
ATOM	2238	N	GLU	E	118	39.412	52.355	26.379	1.00	60.05	N
ATOM	2239	CA	GLU	E	118	40.404	51.526	25.697	1.00	61.70	C
ATOM	2240	C	GLU	E	118	41.467	51.016	26.677	1.00	62.45	C
ATOM	2241	O	GLU	E	118	41.966	49.899	26.534	1.00	62.48	O
ATOM	2242	CB	GLU	E	118	41.056	52.313	24.558	1.00	61.76	C
ATOM	2243	CG	GLU	E	118	41.979	51.496	23.650	1.00	63.54	C
ATOM	2244	CD	GLU	E	118	41.232	50.713	22.575	1.00	65.67	C
ATOM	2245	OE1	GLU	E	118	40.461	51.336	21.805	1.00	66.17	O
ATOM	2246	OE2	GLU	E	118	41.430	49.477	22.492	1.00	65.96	O
ATOM	2247	N	VAL	E	119	41.794	51.844	27.670	1.00	63.70	N
ATOM	2248	CA	VAL	E	119	42.785	51.513	28.701	1.00	64.79	C
ATOM	2249	C	VAL	E	119	42.323	50.402	29.657	1.00	65.67	C
ATOM	2250	O	VAL	E	119	43.155	49.676	30.201	1.00	65.83	O
ATOM	2251	CB	VAL	E	119	43.269	52.796	29.460	1.00	64.74	C
ATOM	2252	CG1	VAL	E	119	43.666	52.506	30.909	1.00	64.75	C
ATOM	2253	CG2	VAL	E	119	44.422	53.456	28.704	1.00	64.57	C
ATOM	2254	N	TYR	E	120	41.013	50.253	29.849	1.00	66.85	N
ATOM	2255	CA	TYR	E	120	40.514	49.119	30.631	1.00	68.05	C
ATOM	2256	C	TYR	E	120	39.817	48.019	29.824	1.00	68.54	C
ATOM	2257	O	TYR	E	120	40.183	46.852	29.939	1.00	68.96	O
ATOM	2258	CB	TYR	E	120	39.650	49.552	31.820	1.00	68.45	C
ATOM	2259	CG	TYR	E	120	39.288	48.375	32.707	1.00	69.47	C
ATOM	2260	CD1	TYR	E	120	40.258	47.751	33.505	1.00	70.11	C
ATOM	2261	CD2	TYR	E	120	37.986	47.861	32.728	1.00	70.33	C
ATOM	2262	CE1	TYR	E	120	39.938	46.658	34.311	1.00	70.18	C
ATOM	2263	CE2	TYR	E	120	37.655	46.765	33.533	1.00	70.07	C
ATOM	2264	CZ	TYR	E	120	38.634	46.171	34.321	1.00	70.13	C
ATOM	2265	OH	TYR	E	120	38.310	45.091	35.118	1.00	69.88	O
ATOM	2266	N	LEU	E	121	38.818	48.371	29.022	1.00	69.04	N
ATOM	2267	CA	LEU	E	121	38.063	47.361	28.266	1.00	69.55	C
ATOM	2268	C	LEU	E	121	38.843	46.816	27.057	1.00	69.89	C
ATOM	2269	O	LEU	E	121	38.292	46.733	25.950	1.00	70.15	O
ATOM	2270	CB	LEU	E	121	36.714	47.934	27.795	1.00	69.53	C
ATOM	2271	CG	LEU	E	121	35.776	48.661	28.765	1.00	69.57	C
ATOM	2272	CD1	LEU	E	121	34.680	49.340	27.978	1.00	69.48	C
ATOM	2273	CD2	LEU	E	121	35.179	47.725	29.808	1.00	69.52	C
ATOM	2274	N	GLN	E	122	40.106	46.434	27.276	1.00	70.10	N
ATOM	2275	CA	GLN	E	122	41.027	46.047	26.189	1.00	70.24	C

Figure 1

Table 1b - 35

ATOM	2276	C	GLN	E	122	40.477	44.908	25.322	1.00	70.07	C
ATOM	2277	O	GLN	E	122	39.819	45.155	24.306	1.00	70.12	O
ATOM	2278	CB	GLN	E	122	42.420	45.673	26.727	1.00	70.41	C
ATOM	2279	CG	GLN	E	122	42.870	46.409	27.989	1.00	71.19	C
ATOM	2280	CD	GLN	E	122	42.686	45.587	29.264	1.00	72.21	C
ATOM	2281	OE1	GLN	E	122	43.396	45.792	30.251	1.00	72.63	O
ATOM	2282	NE2	GLN	E	122	41.729	44.658	29.249	1.00	72.43	N
ATOM	2283	N	ASP	E	123	40.766	43.670	25.721	1.00	69.82	N
ATOM	2284	CA	ASP	E	123	40.187	42.486	25.089	1.00	69.48	C
ATOM	2285	C	ASP	E	123	38.876	42.133	25.785	1.00	69.02	C
ATOM	2286	O	ASP	E	123	37.970	41.558	25.173	1.00	69.10	O
ATOM	2287	CB	ASP	E	123	41.150	41.296	25.165	1.00	69.65	C
ATOM	2288	CG	ASP	E	123	42.523	41.611	24.593	1.00	70.23	C
ATOM	2289	OD1	ASP	E	123	43.244	42.442	25.190	1.00	71.03	O
ATOM	2290	OD2	ASP	E	123	42.887	41.013	23.555	1.00	70.59	O
ATOM	2291	N	SER	E	124	38.796	42.495	27.067	1.00	68.30	N
ATOM	2292	CA	SER	E	124	37.638	42.232	27.923	1.00	67.39	C
ATOM	2293	C	SER	E	124	36.379	42.951	27.434	1.00	66.43	C
ATOM	2294	O	SER	E	124	36.124	44.103	27.799	1.00	66.51	O
ATOM	2295	CB	SER	E	124	37.956	42.628	29.372	1.00	67.58	C
ATOM	2296	OG	SER	E	124	38.308	44.000	29.464	1.00	67.94	O
ATOM	2297	N	PHE	E	125	35.603	42.252	26.605	1.00	65.20	N
ATOM	2298	CA	PHE	E	125	34.377	42.789	26.016	1.00	63.87	C
ATOM	2299	C	PHE	E	125	33.308	43.081	27.071	1.00	62.50	C
ATOM	2300	O	PHE	E	125	32.879	42.178	27.803	1.00	62.26	O
ATOM	2301	CB	PHE	E	125	33.790	41.811	24.984	1.00	64.33	C
ATOM	2302	CG	PHE	E	125	34.595	41.682	23.713	1.00	65.08	C
ATOM	2303	CD1	PHE	E	125	35.255	40.487	23.412	1.00	65.68	C
ATOM	2304	CD2	PHE	E	125	34.667	42.735	22.799	1.00	65.45	C
ATOM	2305	CE1	PHE	E	125	35.990	40.347	22.230	1.00	65.63	C
ATOM	2306	CE2	PHE	E	125	35.401	42.609	21.617	1.00	65.48	C
ATOM	2307	CZ	PHE	E	125	36.063	41.413	21.332	1.00	65.51	C
ATOM	2308	N	LYS	E	126	32.887	44.343	27.142	1.00	60.46	N
ATOM	2309	CA	LYS	E	126	31.704	44.727	27.915	1.00	58.52	C
ATOM	2310	C	LYS	E	126	30.804	45.611	27.051	1.00	56.62	C
ATOM	2311	O	LYS	E	126	30.898	46.837	27.109	1.00	56.95	O
ATOM	2312	CB	LYS	E	126	32.077	45.448	29.223	1.00	58.81	C
ATOM	2313	CG	LYS	E	126	32.964	44.655	30.188	1.00	59.56	C
ATOM	2314	CD	LYS	E	126	32.273	43.413	30.742	1.00	60.71	C
ATOM	2315	CE	LYS	E	126	33.242	42.579	31.556	1.00	61.27	C
ATOM	2316	NZ	LYS	E	126	32.762	41.178	31.697	1.00	62.35	N
ATOM	2317	N	PRO	E	127	29.935	44.989	26.230	1.00	54.50	N
ATOM	2318	CA	PRO	E	127	29.040	45.761	25.374	1.00	52.49	C
ATOM	2319	C	PRO	E	127	27.935	46.439	26.175	1.00	50.46	C
ATOM	2320	O	PRO	E	127	27.661	46.052	27.313	1.00	49.88	O
ATOM	2321	CB	PRO	E	127	28.431	44.696	24.461	1.00	52.56	C
ATOM	2322	CG	PRO	E	127	28.463	43.451	25.276	1.00	53.54	C
ATOM	2323	CD	PRO	E	127	29.738	43.535	26.063	1.00	54.35	C
ATOM	2324	N	LEU	E	128	27.308	47.440	25.568	1.00	48.32	N
ATOM	2325	CA	LEU	E	128	26.196	48.141	26.188	1.00	46.20	C
ATOM	2326	C	LEU	E	128	25.009	47.202	26.360	1.00	44.75	C
ATOM	2327	O	LEU	E	128	24.555	46.582	25.393	1.00	44.55	O
ATOM	2328	CB	LEU	E	128	25.775	49.347	25.347	1.00	45.88	C
ATOM	2329	CG	LEU	E	128	24.524	50.077	25.855	1.00	45.97	C
ATOM	2330	CD1	LEU	E	128	24.762	50.697	27.228	1.00	45.34	C
ATOM	2331	CD2	LEU	E	128	24.079	51.129	24.878	1.00	45.82	C
ATOM	2332	N	VAL	E	129	24.510	47.100	27.587	1.00	42.82	N
ATOM	2333	CA	VAL	E	129	23.279	46.359	27.801	1.00	41.35	C
ATOM	2334	C	VAL	E	129	22.098	47.324	27.972	1.00	40.38	C
ATOM	2335	O	VAL	E	129	22.152	48.297	28.737	1.00	40.07	O
ATOM	2336	CB	VAL	E	129	23.397	45.252	28.907	1.00	41.29	C
ATOM	2337	CG1	VAL	E	129	24.858	44.870	29.146	1.00	41.02	C
ATOM	2338	CG2	VAL	E	129	22.737	45.640	30.191	1.00	41.43	C
ATOM	2339	N	CYS	E	130	21.045	47.062	27.216	1.00	39.18	N
ATOM	2340	CA	CYS	E	130	19.892	47.943	27.184	1.00	38.57	C
ATOM	2341	C	CYS	E	130	18.634	47.108	27.098	1.00	38.13	C
ATOM	2342	O	CYS	E	130	18.705	45.861	27.001	1.00	37.72	O

Figure 1 Table 1b - 36

ATOM	2343	CB	CYS	E	130	19.987	48.897	25.989	1.00	38.24	C
ATOM	2344	SG	CYS	E	130	19.891	48.082	24.381	1.00	40.09	S
ATOM	2345	N	ILE	E	131	17.491	47.789	27.119	1.00	37.24	N
ATOM	2346	CA	ILE	E	131	16.200	47.123	27.020	1.00	36.97	C
ATOM	2347	C	ILE	E	131	15.184	47.981	26.272	1.00	37.08	C
ATOM	2348	O	ILE	E	131	15.199	49.207	26.375	1.00	36.83	O
ATOM	2349	CB	ILE	E	131	15.661	46.722	28.421	1.00	36.98	C
ATOM	2350	CG1	ILE	E	131	14.507	45.739	28.267	1.00	37.45	C
ATOM	2351	CG2	ILE	E	131	15.252	47.964	29.251	1.00	36.35	C
ATOM	2352	CD1	ILE	E	131	14.438	44.700	29.320	1.00	39.05	C
ATOM	2353	N	SER	E	132	14.305	47.322	25.526	1.00	36.73	N
ATOM	2354	CA	SER	E	132	13.221	47.987	24.826	1.00	36.91	C
ATOM	2355	C	SER	E	132	12.144	48.467	25.804	1.00	37.05	C
ATOM	2356	O	SER	E	132	11.876	47.789	26.801	1.00	36.53	O
ATOM	2357	CB	SER	E	132	12.600	47.027	23.812	1.00	36.83	C
ATOM	2358	OG	SER	E	132	11.508	47.641	23.154	1.00	38.56	O
ATOM	2359	N	PRO	E	133	11.512	49.636	25.521	1.00	36.91	N
ATOM	2360	CA	PRO	E	133	10.354	50.081	26.317	1.00	36.99	C
ATOM	2361	C	PRO	E	133	9.198	49.064	26.293	1.00	37.22	C
ATOM	2362	O	PRO	E	133	8.392	49.014	27.230	1.00	37.10	O
ATOM	2363	CB	PRO	E	133	9.932	51.395	25.632	1.00	36.90	C
ATOM	2364	CG	PRO	E	133	10.530	51.321	24.241	1.00	37.28	C
ATOM	2365	CD	PRO	E	133	11.829	50.587	24.437	1.00	37.19	C
ATOM	2366	N	ASN	E	134	9.137	48.256	25.235	1.00	37.17	N
ATOM	2367	CA	ASN	E	134	8.103	47.237	25.094	1.00	37.74	C
ATOM	2368	C	ASN	E	134	8.439	45.893	25.739	1.00	37.42	C
ATOM	2369	O	ASN	E	134	7.585	45.018	25.783	1.00	37.52	O
ATOM	2370	CB	ASN	E	134	7.744	47.022	23.620	1.00	37.98	C
ATOM	2371	CG	ASN	E	134	7.001	48.194	23.033	1.00	40.04	C
ATOM	2372	OD1	ASN	E	134	6.171	48.821	23.700	1.00	42.30	O
ATOM	2373	ND2	ASN	E	134	7.295	48.508	21.778	1.00	42.62	N
ATOM	2374	N	ALA	E	135	9.667	45.730	26.230	1.00	37.10	N
ATOM	2375	CA	ALA	E	135	10.058	44.494	26.908	1.00	37.08	C
ATOM	2376	C	ALA	E	135	9.541	44.484	28.340	1.00	36.92	C
ATOM	2377	O	ALA	E	135	9.283	45.545	28.921	1.00	36.91	O
ATOM	2378	CB	ALA	E	135	11.562	44.329	26.886	1.00	37.16	C
ATOM	2379	N	SER	E	136	9.413	43.290	28.915	1.00	36.40	N
ATOM	2380	CA	SER	E	136	8.822	43.138	30.237	1.00	35.88	C
ATOM	2381	C	SER	E	136	9.731	43.666	31.336	1.00	35.93	C
ATOM	2382	O	SER	E	136	10.958	43.707	31.189	1.00	35.49	O
ATOM	2383	CB	SER	E	136	8.473	41.672	30.518	1.00	35.95	C
ATOM	2384	OG	SER	E	136	9.655	40.902	30.638	1.00	35.45	O
ATOM	2385	N	LEU	E	137	9.104	44.069	32.439	1.00	35.99	N
ATOM	2386	CA	LEU	E	137	9.807	44.431	33.652	1.00	36.22	C
ATOM	2387	C	LEU	E	137	10.631	43.251	34.185	1.00	35.97	C
ATOM	2388	O	LEU	E	137	11.731	43.440	34.715	1.00	35.65	O
ATOM	2389	CB	LEU	E	137	8.796	44.929	34.690	1.00	36.15	C
ATOM	2390	CG	LEU	E	137	9.258	45.372	36.082	1.00	37.81	C
ATOM	2391	CD1	LEU	E	137	10.376	46.431	36.020	1.00	37.89	C
ATOM	2392	CD2	LEU	E	137	8.048	45.911	36.856	1.00	37.43	C
ATOM	2393	N	PHE	E	138	10.100	42.035	34.025	1.00	35.58	N
ATOM	2394	CA	PHE	E	138	10.805	40.807	34.412	1.00	35.75	C
ATOM	2395	C	PHE	E	138	12.128	40.691	33.661	1.00	35.94	C
ATOM	2396	O	PHE	E	138	13.149	40.330	34.249	1.00	36.11	O
ATOM	2397	CB	PHE	E	138	9.918	39.576	34.150	1.00	35.34	C
ATOM	2398	CG	PHE	E	138	10.477	38.282	34.689	1.00	35.91	C
ATOM	2399	CD1	PHE	E	138	10.244	37.899	36.009	1.00	35.84	C
ATOM	2400	CD2	PHE	E	138	11.216	37.426	33.862	1.00	36.56	C
ATOM	2401	CE1	PHE	E	138	10.750	36.680	36.507	1.00	37.12	C
ATOM	2402	CE2	PHE	E	138	11.727	36.209	34.349	1.00	37.06	C
ATOM	2403	CZ	PHE	E	138	11.491	35.835	35.671	1.00	35.77	C
ATOM	2404	N	ASP	E	139	12.109	41.012	32.366	1.00	36.44	N
ATOM	2405	CA	ASP	E	139	13.321	40.978	31.541	1.00	37.21	C
ATOM	2406	C	ASP	E	139	14.334	42.032	31.992	1.00	37.12	C
ATOM	2407	O	ASP	E	139	15.545	41.777	31.991	1.00	36.99	O
ATOM	2408	CB	ASP	E	139	12.991	41.160	30.054	1.00	37.53	C
ATOM	2409	CG	ASP	E	139	12.534	39.863	29.376	1.00	40.03	C

Figure 1 Table 1b - 37

ATOM	2410	OD1	ASP	E	139	12.461	38.798	30.037	1.00	42.32	O
ATOM	2411	OD2	ASP	E	139	12.254	39.912	28.159	1.00	42.25	O
ATOM	2412	N	ALA	E	140	13.829	43.208	32.375	1.00	36.79	N
ATOM	2413	CA	ALA	E	140	14.661	44.287	32.925	1.00	36.44	C
ATOM	2414	C	ALA	E	140	15.371	43.863	34.208	1.00	36.08	C
ATOM	2415	O	ALA	E	140	16.587	44.017	34.327	1.00	35.84	O
ATOM	2416	CB	ALA	E	140	13.824	45.552	33.162	1.00	35.77	C
ATOM	2417	N	VAL	E	141	14.610	43.323	35.159	1.00	36.20	N
ATOM	2418	CA	VAL	E	141	15.180	42.876	36.429	1.00	36.28	C
ATOM	2419	C	VAL	E	141	16.243	41.805	36.179	1.00	36.17	C
ATOM	2420	O	VAL	E	141	17.349	41.895	36.718	1.00	36.12	O
ATOM	2421	CB	VAL	E	141	14.095	42.376	37.435	1.00	36.58	C
ATOM	2422	CG1	VAL	E	141	14.735	41.782	38.694	1.00	36.43	C
ATOM	2423	CG2	VAL	E	141	13.179	43.503	37.826	1.00	36.69	C
ATOM	2424	N	SER	E	142	15.913	40.821	35.341	1.00	35.98	N
ATOM	2425	CA	SER	E	142	16.842	39.743	34.999	1.00	36.23	C
ATOM	2426	C	SER	E	142	18.135	40.259	34.368	1.00	36.13	C
ATOM	2427	O	SER	E	142	19.224	39.777	34.678	1.00	36.42	O
ATOM	2428	CB	SER	E	142	16.169	38.740	34.058	1.00	36.36	C
ATOM	2429	OG	SER	E	142	15.005	38.201	34.660	1.00	37.67	O
ATOM	2430	N	SER	E	143	18.004	41.226	33.472	1.00	35.88	N
ATOM	2431	CA	SER	E	143	19.156	41.872	32.858	1.00	36.15	C
ATOM	2432	C	SER	E	143	20.049	42.613	33.862	1.00	36.25	C
ATOM	2433	O	SER	E	143	21.276	42.544	33.762	1.00	36.64	O
ATOM	2434	CB	SER	E	143	18.698	42.824	31.757	1.00	35.79	C
ATOM	2435	OG	SER	E	143	19.814	43.399	31.129	1.00	36.76	O
ATOM	2436	N	LEU	E	144	19.448	43.331	34.814	1.00	36.28	N
ATOM	2437	CA	LEU	E	144	20.227	44.012	35.853	1.00	36.18	C
ATOM	2438	C	LEU	E	144	21.044	43.015	36.671	1.00	36.32	C
ATOM	2439	O	LEU	E	144	22.247	43.190	36.845	1.00	36.12	O
ATOM	2440	CB	LEU	E	144	19.331	44.848	36.776	1.00	36.27	C
ATOM	2441	CG	LEU	E	144	18.789	46.191	36.254	1.00	36.40	C
ATOM	2442	CD1	LEU	E	144	17.702	46.687	37.172	1.00	37.30	C
ATOM	2443	CD2	LEU	E	144	19.884	47.250	36.118	1.00	36.21	C
ATOM	2444	N	ILE	E	145	20.382	41.961	37.147	1.00	36.69	N
ATOM	2445	CA	ILE	E	145	21.035	40.896	37.933	1.00	37.41	C
ATOM	2446	C	ILE	E	145	22.134	40.182	37.139	1.00	37.36	C
ATOM	2447	O	ILE	E	145	23.293	40.152	37.564	1.00	37.42	O
ATOM	2448	CB	ILE	E	145	19.996	39.872	38.464	1.00	37.68	C
ATOM	2449	CG1	ILE	E	145	18.914	40.588	39.276	1.00	39.08	C
ATOM	2450	CG2	ILE	E	145	20.666	38.786	39.320	1.00	38.12	C
ATOM	2451	CD1	ILE	E	145	17.610	39.819	39.363	1.00	41.72	C
ATOM	2452	N	ARG	E	146	21.774	39.641	35.979	1.00	37.42	N
ATOM	2453	CA	ARG	E	146	22.690	38.830	35.172	1.00	37.86	C
ATOM	2454	C	ARG	E	146	23.955	39.590	34.758	1.00	37.38	C
ATOM	2455	O	ARG	E	146	25.051	39.031	34.743	1.00	36.66	O
ATOM	2456	CB	ARG	E	146	21.954	38.258	33.944	1.00	38.31	C
ATOM	2457	CG	ARG	E	146	22.854	37.826	32.781	1.00	39.31	C
ATOM	2458	CD	ARG	E	146	22.072	37.230	31.614	1.00	39.37	C
ATOM	2459	NE	ARG	E	146	21.396	38.245	30.811	1.00	43.06	N
ATOM	2460	CZ	ARG	E	146	20.092	38.500	30.861	1.00	42.92	C
ATOM	2461	NH1	ARG	E	146	19.302	37.808	31.673	1.00	43.20	N
ATOM	2462	NH2	ARG	E	146	19.579	39.442	30.086	1.00	43.27	N
ATOM	2463	N	ASN	E	147	23.800	40.871	34.440	1.00	37.06	N
ATOM	2464	CA	ASN	E	147	24.932	41.677	34.013	1.00	36.86	C
ATOM	2465	C	ASN	E	147	25.674	42.373	35.149	1.00	36.88	C
ATOM	2466	O	ASN	E	147	26.697	43.024	34.917	1.00	36.93	O
ATOM	2467	CB	ASN	E	147	24.489	42.653	32.919	1.00	36.94	C
ATOM	2468	CG	ASN	E	147	24.026	41.925	31.674	1.00	36.80	C
ATOM	2469	OD1	ASN	E	147	24.821	41.268	31.011	1.00	36.65	O
ATOM	2470	ND2	ASN	E	147	22.731	42.002	31.374	1.00	35.57	N
ATOM	2471	N	LYS	E	148	25.164	42.212	36.373	1.00	36.84	N
ATOM	2472	CA	LYS	E	148	25.764	42.804	37.576	1.00	36.46	C
ATOM	2473	C	LYS	E	148	25.924	44.327	37.410	1.00	36.26	C
ATOM	2474	O	LYS	E	148	27.001	44.902	37.560	1.00	35.56	O
ATOM	2475	CB	LYS	E	148	27.071	42.094	37.932	1.00	36.61	C
ATOM	2476	CG	LYS	E	148	26.830	40.698	38.470	1.00	37.41	C

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ATOM	2477	CD	LYS	E	148	28.126	39.946	38.716	1.00	41.01	C
ATOM	2478	CE	LYS	E	148	27.835	38.540	39.238	1.00	42.07	C
ATOM	2479	NZ	LYS	E	148	29.085	37.843	39.616	1.00	44.92	N
ATOM	2480	N	ILE	E	149	24.791	44.951	37.130	1.00	36.02	N
ATOM	2481	CA	ILE	E	149	24.735	46.321	36.696	1.00	36.71	C
ATOM	2482	C	ILE	E	149	23.631	47.066	37.476	1.00	36.50	C
ATOM	2483	O	ILE	E	149	22.716	46.427	38.009	1.00	36.23	O
ATOM	2484	CB	ILE	E	149	24.583	46.295	35.145	1.00	36.59	C
ATOM	2485	CG1	ILE	E	149	25.654	47.136	34.491	1.00	38.18	C
ATOM	2486	CG2	ILE	E	149	23.146	46.459	34.648	1.00	37.14	C
ATOM	2487	CD1	ILE	E	149	27.002	46.473	34.511	1.00	38.49	C
ATOM	2488	N	HIS	E	150	23.750	48.397	37.568	1.00	36.56	N
ATOM	2489	CA	HIS	E	150	22.807	49.253	38.318	1.00	36.04	C
ATOM	2490	C	HIS	E	150	22.034	50.268	37.455	1.00	36.20	C
ATOM	2491	O	HIS	E	150	21.177	50.996	37.968	1.00	36.04	O
ATOM	2492	CB	HIS	E	150	23.543	50.005	39.439	1.00	35.73	C
ATOM	2493	CG	HIS	E	150	24.132	49.108	40.484	1.00	35.02	C
ATOM	2494	ND1	HIS	E	150	25.407	48.596	40.390	1.00	34.99	N
ATOM	2495	CD2	HIS	E	150	23.617	48.629	41.641	1.00	34.62	C
ATOM	2496	CE1	HIS	E	150	25.652	47.835	41.443	1.00	35.49	C
ATOM	2497	NE2	HIS	E	150	24.585	47.847	42.223	1.00	35.31	N
ATOM	2498	N	ARG	E	151	22.342	50.312	36.161	1.00	36.20	N
ATOM	2499	CA	ARG	E	151	21.758	51.297	35.239	1.00	37.11	C
ATOM	2500	C	ARG	E	151	21.358	50.585	33.962	1.00	36.73	C
ATOM	2501	O	ARG	E	151	22.199	50.009	33.270	1.00	37.70	O
ATOM	2502	CB	ARG	E	151	22.756	52.423	34.921	1.00	36.41	C
ATOM	2503	CG	ARG	E	151	23.471	53.019	36.143	1.00	38.39	C
ATOM	2504	CD	ARG	E	151	22.612	54.061	36.867	1.00	40.54	C
ATOM	2505	NE	ARG	E	151	22.929	54.107	38.293	1.00	43.29	N
ATOM	2506	CZ	ARG	E	151	22.291	54.851	39.194	1.00	43.73	C
ATOM	2507	NH1	ARG	E	151	21.288	55.655	38.835	1.00	42.68	N
ATOM	2508	NH2	ARG	E	151	22.666	54.790	40.465	1.00	44.63	N
ATOM	2509	N	LEU	E	152	20.070	50.586	33.662	1.00	36.21	N
ATOM	2510	CA	LEU	E	152	19.610	49.909	32.467	1.00	35.88	C
ATOM	2511	C	LEU	E	152	18.886	50.899	31.564	1.00	35.47	C
ATOM	2512	O	LEU	E	152	17.733	51.241	31.821	1.00	35.86	O
ATOM	2513	CB	LEU	E	152	18.725	48.703	32.822	1.00	36.06	C
ATOM	2514	CG	LEU	E	152	18.228	47.834	31.670	1.00	35.83	C
ATOM	2515	CD1	LEU	E	152	19.375	47.120	30.957	1.00	37.26	C
ATOM	2516	CD2	LEU	E	152	17.247	46.829	32.211	1.00	36.43	C
ATOM	2517	N	PRO	E	153	19.566	51.361	30.498	1.00	35.13	N
ATOM	2518	CA	PRO	E	153	18.929	52.297	29.570	1.00	35.08	C
ATOM	2519	C	PRO	E	153	17.814	51.635	28.782	1.00	35.03	C
ATOM	2520	O	PRO	E	153	17.985	50.520	28.259	1.00	35.09	O
ATOM	2521	CB	PRO	E	153	20.071	52.705	28.636	1.00	35.33	C
ATOM	2522	CG	PRO	E	153	21.010	51.545	28.667	1.00	35.62	C
ATOM	2523	CD	PRO	E	153	20.941	51.032	30.093	1.00	34.70	C
ATOM	2524	N	VAL	E	154	16.671	52.308	28.740	1.00	34.73	N
ATOM	2525	CA	VAL	E	154	15.527	51.868	27.979	1.00	34.53	C
ATOM	2526	C	VAL	E	154	15.659	52.564	26.626	1.00	35.24	C
ATOM	2527	O	VAL	E	154	15.607	53.801	26.545	1.00	34.39	O
ATOM	2528	CB	VAL	E	154	14.209	52.246	28.683	1.00	34.91	C
ATOM	2529	CG1	VAL	E	154	13.008	51.862	27.841	1.00	34.59	C
ATOM	2530	CG2	VAL	E	154	14.122	51.596	30.074	1.00	33.71	C
ATOM	2531	N	ILE	E	155	15.867	51.769	25.572	1.00	34.86	N
ATOM	2532	CA	ILE	E	155	16.154	52.324	24.246	1.00	35.03	C
ATOM	2533	C	ILE	E	155	15.085	51.887	23.251	1.00	35.55	C
ATOM	2534	O	ILE	E	155	14.855	50.683	23.053	1.00	35.01	O
ATOM	2535	CB	ILE	E	155	17.582	51.942	23.746	1.00	35.31	C
ATOM	2536	CG1	ILE	E	155	18.650	52.402	24.755	1.00	34.43	C
ATOM	2537	CG2	ILE	E	155	17.838	52.484	22.324	1.00	34.78	C
ATOM	2538	CD1	ILE	E	155	20.098	52.207	24.291	1.00	34.94	C
ATOM	2539	N	ASP	E	156	14.413	52.877	22.662	1.00	35.60	N
ATOM	2540	CA	ASP	E	156	13.391	52.651	21.646	1.00	36.30	C
ATOM	2541	C	ASP	E	156	14.039	52.092	20.376	1.00	36.44	C
ATOM	2542	O	ASP	E	156	14.854	52.779	19.750	1.00	35.95	O
ATOM	2543	CB	ASP	E	156	12.662	53.970	21.347	1.00	36.84	C

Figure 1 Table 1b - 39

ATOM	2544	CG	ASP	E	156	11.649	53.851	20.217	1.00	37.80	C
ATOM	2545	OD1	ASP	E	156	11.117	52.754	19.986	1.00	40.06	O
ATOM	2546	OD2	ASP	E	156	11.371	54.871	19.564	1.00	39.49	O
ATOM	2547	N	PRO	E	157	13.684	50.840	19.991	1.00	36.71	N
ATOM	2548	CA	PRO	E	157	14.296	50.267	18.781	1.00	36.77	C
ATOM	2549	C	PRO	E	157	13.969	51.038	17.497	1.00	37.11	C
ATOM	2550	O	PRO	E	157	14.805	51.101	16.598	1.00	37.49	O
ATOM	2551	CB	PRO	E	157	13.749	48.830	18.734	1.00	36.68	C
ATOM	2552	CG	PRO	E	157	12.539	48.839	19.591	1.00	36.79	C
ATOM	2553	CD	PRO	E	157	12.747	49.899	20.636	1.00	36.53	C
ATOM	2554	N	GLU	E	158	12.782	51.636	17.416	1.00	37.36	N
ATOM	2555	CA	GLU	E	158	12.379	52.359	16.209	1.00	38.03	C
ATOM	2556	C	GLU	E	158	13.191	53.639	15.982	1.00	37.75	C
ATOM	2557	O	GLU	E	158	13.645	53.890	14.870	1.00	37.83	O
ATOM	2558	CB	GLU	E	158	10.877	52.660	16.224	1.00	38.70	C
ATOM	2559	CG	GLU	E	158	10.000	51.406	16.457	1.00	42.43	C
ATOM	2560	CD	GLU	E	158	8.715	51.409	15.644	1.00	46.94	C
ATOM	2561	OE1	GLU	E	158	8.415	52.432	14.977	1.00	50.13	O
ATOM	2562	OE2	GLU	E	158	8.004	50.377	15.661	1.00	49.17	O
ATOM	2563	N	SER	E	159	13.374	54.411	17.054	1.00	37.06	N
ATOM	2564	CA	SER	E	159	14.097	55.694	17.071	1.00	37.09	C
ATOM	2565	C	SER	E	159	15.588	55.540	17.285	1.00	35.90	C
ATOM	2566	O	SER	E	159	16.383	56.328	16.770	1.00	35.51	O
ATOM	2567	CB	SER	E	159	13.594	56.529	18.255	1.00	36.74	C
ATOM	2568	OG	SER	E	159	12.535	57.362	17.842	1.00	41.35	O
ATOM	2569	N	GLY	E	160	15.943	54.561	18.113	1.00	34.64	N
ATOM	2570	CA	GLY	E	160	17.291	54.424	18.625	1.00	33.86	C
ATOM	2571	C	GLY	E	160	17.522	55.340	19.815	1.00	33.63	C
ATOM	2572	O	GLY	E	160	18.636	55.402	20.332	1.00	34.65	O
ATOM	2573	N	ASN	E	161	16.472	56.048	20.241	1.00	32.56	N
ATOM	2574	CA	ASN	E	161	16.544	57.000	21.346	1.00	31.90	C
ATOM	2575	C	ASN	E	161	16.532	56.318	22.717	1.00	32.43	C
ATOM	2576	O	ASN	E	161	15.679	55.474	23.003	1.00	31.79	O
ATOM	2577	CB	ASN	E	161	15.372	58.002	21.287	1.00	31.72	C
ATOM	2578	CG	ASN	E	161	15.465	58.979	20.111	1.00	30.33	C
ATOM	2579	OD1	ASN	E	161	14.455	59.529	19.677	1.00	33.62	O
ATOM	2580	ND2	ASN	E	161	16.657	59.185	19.593	1.00	26.32	N
ATOM	2581	N	THR	E	162	17.470	56.705	23.571	1.00	32.48	N
ATOM	2582	CA	THR	E	162	17.401	56.331	24.967	1.00	32.84	C
ATOM	2583	C	THR	E	162	16.320	57.196	25.611	1.00	32.87	C
ATOM	2584	O	THR	E	162	16.314	58.417	25.456	1.00	32.27	O
ATOM	2585	CB	THR	E	162	18.751	56.526	25.651	1.00	33.08	C
ATOM	2586	OG1	THR	E	162	19.712	55.679	25.013	1.00	34.28	O
ATOM	2587	CG2	THR	E	162	18.671	56.161	27.122	1.00	33.00	C
ATOM	2588	N	LEU	E	163	15.387	56.554	26.306	1.00	32.83	N
ATOM	2589	CA	LEU	E	163	14.255	57.274	26.883	1.00	32.93	C
ATOM	2590	C	LEU	E	163	14.432	57.554	28.355	1.00	33.41	C
ATOM	2591	O	LEU	E	163	13.888	58.519	28.872	1.00	33.41	O
ATOM	2592	CB	LEU	E	163	12.967	56.471	26.689	1.00	32.58	C
ATOM	2593	CG	LEU	E	163	12.672	55.967	25.273	1.00	32.24	C
ATOM	2594	CD1	LEU	E	163	11.477	55.048	25.337	1.00	30.34	C
ATOM	2595	CD2	LEU	E	163	12.464	57.130	24.257	1.00	30.72	C
ATOM	2596	N	TYR	E	164	15.168	56.675	29.033	1.00	34.06	N
ATOM	2597	CA	TYR	E	164	15.155	56.630	30.479	1.00	34.35	C
ATOM	2598	C	TYR	E	164	16.185	55.627	30.938	1.00	34.08	C
ATOM	2599	O	TYR	E	164	16.499	54.687	30.203	1.00	34.15	O
ATOM	2600	CB	TYR	E	164	13.751	56.210	30.966	1.00	35.22	C
ATOM	2601	CG	TYR	E	164	13.579	56.277	32.468	1.00	36.08	C
ATOM	2602	CD1	TYR	E	164	13.718	57.493	33.152	1.00	35.89	C
ATOM	2603	CD2	TYR	E	164	13.290	55.124	33.199	1.00	36.10	C
ATOM	2604	CE1	TYR	E	164	13.576	57.550	34.539	1.00	37.56	C
ATOM	2605	CE2	TYR	E	164	13.135	55.160	34.568	1.00	35.82	C
ATOM	2606	CZ	TYR	E	164	13.283	56.368	35.235	1.00	37.14	C
ATOM	2607	OH	TYR	E	164	13.133	56.397	36.596	1.00	37.71	O
ATOM	2608	N	ILE	E	165	16.740	55.825	32.130	1.00	32.32	N
ATOM	2609	CA	ILE	E	165	17.660	54.866	32.729	1.00	31.89	C
ATOM	2610	CB	ILE	E	165	18.995	55.512	33.154	1.00	31.88	C

Figure 1 Table 1b - 40

ATOM	2611	CG1	ILE	E	165	19.705	56.160	31.959	1.00	31.84	C
ATOM	2612	CD1	ILE	E	165	20.760	57.139	32.388	1.00	33.35	C
ATOM	2613	CG2	ILE	E	165	19.928	54.473	33.830	1.00	32.02	C
ATOM	2614	C	ILE	E	165	16.978	54.203	33.930	1.00	32.57	C
ATOM	2615	O	ILE	E	165	16.715	54.844	34.956	1.00	32.14	O
ATOM	2616	N	LEU	E	166	16.722	52.909	33.793	1.00	34.33	N
ATOM	2617	CA	LEU	E	166	16.043	52.110	34.810	1.00	35.20	C
ATOM	2618	C	LEU	E	166	17.019	51.722	35.918	1.00	34.38	C
ATOM	2619	O	LEU	E	166	18.176	51.411	35.643	1.00	34.32	O
ATOM	2620	CB	LEU	E	166	15.467	50.869	34.126	1.00	35.43	C
ATOM	2621	CG	LEU	E	166	14.058	50.348	34.390	1.00	38.00	C
ATOM	2622	CD1	LEU	E	166	13.021	51.428	34.671	1.00	37.90	C
ATOM	2623	CD2	LEU	E	166	13.631	49.461	33.204	1.00	37.65	C
ATOM	2624	N	THR	E	167	16.558	51.783	37.171	1.00	34.28	N
ATOM	2625	CA	THR	E	167	17.380	51.454	38.348	1.00	33.80	C
ATOM	2626	C	THR	E	167	16.632	50.474	39.267	1.00	33.06	C
ATOM	2627	O	THR	E	167	15.416	50.371	39.172	1.00	32.59	O
ATOM	2628	CB	THR	E	167	17.693	52.713	39.192	1.00	33.45	C
ATOM	2629	OG1	THR	E	167	16.464	53.261	39.686	1.00	33.88	O
ATOM	2630	CG2	THR	E	167	18.462	53.784	38.373	1.00	34.98	C
ATOM	2631	N	HIS	E	168	17.355	49.803	40.177	1.00	32.87	N
ATOM	2632	CA	HIS	E	168	16.730	48.922	41.198	1.00	32.86	C
ATOM	2633	C	HIS	E	168	15.713	49.696	42.053	1.00	32.85	C
ATOM	2634	O	HIS	E	168	14.613	49.217	42.326	1.00	32.29	O
ATOM	2635	CB	HIS	E	168	17.784	48.326	42.143	1.00	32.46	C
ATOM	2636	CG	HIS	E	168	18.697	47.316	41.513	1.00	33.32	C
ATOM	2637	ND1	HIS	E	168	19.758	47.665	40.703	1.00	33.37	N
ATOM	2638	CD2	HIS	E	168	18.747	45.964	41.632	1.00	34.18	C
ATOM	2639	CE1	HIS	E	168	20.395	46.571	40.316	1.00	34.94	C
ATOM	2640	NE2	HIS	E	168	19.808	45.526	40.875	1.00	33.26	N
ATOM	2641	N	LYS	E	169	16.103	50.900	42.468	1.00	33.31	N
ATOM	2642	CA	LYS	E	169	15.278	51.762	43.309	1.00	34.51	C
ATOM	2643	C	LYS	E	169	13.908	52.046	42.688	1.00	33.90	C
ATOM	2644	O	LYS	E	169	12.873	51.874	43.336	1.00	34.35	O
ATOM	2645	CB	LYS	E	169	16.046	53.056	43.591	1.00	34.36	C
ATOM	2646	CG	LYS	E	169	15.636	53.841	44.840	1.00	37.66	C
ATOM	2647	CD	LYS	E	169	16.604	55.044	45.082	1.00	36.58	C
ATOM	2648	CE	LYS	E	169	18.048	54.534	45.246	1.00	40.84	C
ATOM	2649	NZ	LYS	E	169	19.017	55.432	45.950	1.00	42.16	N
ATOM	2650	N	ARG	E	170	13.911	52.460	41.429	1.00	33.79	N
ATOM	2651	CA	ARG	E	170	12.682	52.757	40.698	1.00	33.73	C
ATOM	2652	C	ARG	E	170	11.763	51.543	40.606	1.00	33.13	C
ATOM	2653	O	ARG	E	170	10.554	51.640	40.831	1.00	32.94	O
ATOM	2654	CB	ARG	E	170	13.007	53.238	39.280	1.00	33.19	C
ATOM	2655	CG	ARG	E	170	11.785	53.606	38.459	1.00	33.62	C
ATOM	2656	CD	ARG	E	170	11.180	54.938	38.919	1.00	34.32	C
ATOM	2657	NE	ARG	E	170	10.160	55.401	37.974	1.00	33.92	N
ATOM	2658	CZ	ARG	E	170	9.425	56.502	38.112	1.00	32.14	C
ATOM	2659	NH1	ARG	E	170	9.587	57.308	39.160	1.00	30.24	N
ATOM	2660	NH2	ARG	E	170	8.528	56.797	37.180	1.00	30.31	N
ATOM	2661	N	ILE	E	171	12.355	50.417	40.230	1.00	33.37	N
ATOM	2662	CA	ILE	E	171	11.635	49.164	40.085	1.00	33.19	C
ATOM	2663	C	ILE	E	171	10.973	48.743	41.403	1.00	33.17	C
ATOM	2664	O	ILE	E	171	9.785	48.451	41.417	1.00	33.63	O
ATOM	2665	CB	ILE	E	171	12.564	48.040	39.540	1.00	33.22	C
ATOM	2666	CG1	ILE	E	171	12.956	48.366	38.088	1.00	33.76	C
ATOM	2667	CG2	ILE	E	171	11.880	46.657	39.687	1.00	33.01	C
ATOM	2668	CD1	ILE	E	171	14.149	47.598	37.522	1.00	32.28	C
ATOM	2669	N	LEU	E	172	11.717	48.726	42.507	1.00	32.95	N
ATOM	2670	CA	LEU	E	172	11.099	48.292	43.771	1.00	32.77	C
ATOM	2671	C	LEU	E	172	9.971	49.228	44.182	1.00	32.62	C
ATOM	2672	O	LEU	E	172	8.931	48.768	44.666	1.00	31.46	O
ATOM	2673	CB	LEU	E	172	12.107	48.129	44.913	1.00	32.89	C
ATOM	2674	CG	LEU	E	172	11.523	47.411	46.149	1.00	32.87	C
ATOM	2675	CD1	LEU	E	172	11.161	45.945	45.854	1.00	33.95	C
ATOM	2676	CD2	LEU	E	172	12.435	47.507	47.375	1.00	32.57	C
ATOM	2677	N	LYS	E	173	10.161	50.536	43.964	1.00	32.93	N

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ATOM	2678	CA	LYS	E	173	9.092	51.499	44.286	1.00	33.35	C
ATOM	2679	C	LYS	E	173	7.822	51.204	43.476	1.00	33.27	C
ATOM	2680	O	LYS	E	173	6.713	51.149	44.021	1.00	32.63	O
ATOM	2681	CB	LYS	E	173	9.540	52.944	44.066	1.00	33.63	C
ATOM	2682	CG	LYS	E	173	8.511	53.969	44.550	1.00	35.40	C
ATOM	2683	CD	LYS	E	173	9.033	55.395	44.381	1.00	38.49	C
ATOM	2684	CE	LYS	E	173	8.120	56.400	45.086	1.00	40.18	C
ATOM	2685	NZ	LYS	E	173	8.892	57.621	45.497	1.00	40.93	N
ATOM	2686	N	PHE	E	174	7.997	51.010	42.174	1.00	33.72	N
ATOM	2687	CA	PHE	E	174	6.881	50.694	41.289	1.00	34.52	C
ATOM	2688	C	PHE	E	174	6.148	49.428	41.766	1.00	34.76	C
ATOM	2689	O	PHE	E	174	4.922	49.420	41.872	1.00	34.83	O
ATOM	2690	CB	PHE	E	174	7.399	50.535	39.866	1.00	34.55	C
ATOM	2691	CG	PHE	E	174	6.332	50.531	38.822	1.00	36.25	C
ATOM	2692	CD1	PHE	E	174	5.837	49.325	38.322	1.00	37.02	C
ATOM	2693	CD2	PHE	E	174	5.843	51.730	38.298	1.00	36.04	C
ATOM	2694	CE1	PHE	E	174	4.840	49.317	37.333	1.00	37.07	C
ATOM	2695	CE2	PHE	E	174	4.849	51.733	37.317	1.00	37.30	C
ATOM	2696	CZ	PHE	E	174	4.351	50.522	36.832	1.00	37.34	C
ATOM	2697	N	LEU	E	175	6.907	48.375	42.059	1.00	35.06	N
ATOM	2698	CA	LEU	E	175	6.336	47.110	42.566	1.00	35.52	C
ATOM	2699	C	LEU	E	175	5.511	47.321	43.829	1.00	35.91	C
ATOM	2700	O	LEU	E	175	4.363	46.892	43.898	1.00	36.10	O
ATOM	2701	CB	LEU	E	175	7.440	46.077	42.832	1.00	35.29	C
ATOM	2702	CG	LEU	E	175	8.191	45.513	41.619	1.00	35.76	C
ATOM	2703	CD1	LEU	E	175	9.356	44.627	42.031	1.00	34.17	C
ATOM	2704	CD2	LEU	E	175	7.264	44.785	40.658	1.00	36.09	C
ATOM	2705	N	LYS	E	176	6.098	48.004	44.812	1.00	36.51	N
ATOM	2706	CA	LYS	E	176	5.443	48.312	46.086	1.00	37.10	C
ATOM	2707	C	LYS	E	176	4.135	49.077	45.892	1.00	37.54	C
ATOM	2708	O	LYS	E	176	3.120	48.771	46.524	1.00	37.98	O
ATOM	2709	CB	LYS	E	176	6.409	49.095	46.999	1.00	36.99	C
ATOM	2710	CG	LYS	E	176	5.757	49.856	48.170	1.00	37.98	C
ATOM	2711	CD	LYS	E	176	5.279	48.928	49.280	1.00	39.73	C
ATOM	2712	CE	LYS	E	176	4.355	49.656	50.260	1.00	40.13	C
ATOM	2713	NZ	LYS	E	176	3.861	48.715	51.307	1.00	43.53	N
ATOM	2714	N	LEU	E	177	4.158	50.059	45.000	1.00	38.08	N
ATOM	2715	CA	LEU	E	177	3.006	50.912	44.774	1.00	38.39	C
ATOM	2716	C	LEU	E	177	1.856	50.240	44.054	1.00	38.29	C
ATOM	2717	O	LEU	E	177	0.701	50.453	44.412	1.00	38.19	O
ATOM	2718	CB	LEU	E	177	3.414	52.167	43.996	1.00	38.43	C
ATOM	2719	CG	LEU	E	177	4.089	53.248	44.835	1.00	39.44	C
ATOM	2720	CD1	LEU	E	177	4.648	54.339	43.946	1.00	38.87	C
ATOM	2721	CD2	LEU	E	177	3.084	53.813	45.831	1.00	41.57	C
ATOM	2722	N	PHE	E	178	2.165	49.460	43.026	1.00	38.63	N
ATOM	2723	CA	PHE	E	178	1.123	48.975	42.115	1.00	39.45	C
ATOM	2724	C	PHE	E	178	0.651	47.553	42.371	1.00	40.36	C
ATOM	2725	O	PHE	E	178	-0.267	47.069	41.704	1.00	40.93	O
ATOM	2726	CB	PHE	E	178	1.538	49.173	40.655	1.00	39.27	C
ATOM	2727	CG	PHE	E	178	1.434	50.601	40.200	1.00	38.96	C
ATOM	2728	CD1	PHE	E	178	2.543	51.441	40.241	1.00	38.64	C
ATOM	2729	CD2	PHE	E	178	0.214	51.118	39.772	1.00	38.41	C
ATOM	2730	CE1	PHE	E	178	2.448	52.770	39.845	1.00	37.15	C
ATOM	2731	CE2	PHE	E	178	0.109	52.444	39.368	1.00	38.45	C
ATOM	2732	CZ	PHE	E	178	1.230	53.272	39.405	1.00	37.40	C
ATOM	2733	N	ILE	E	179	1.256	46.890	43.348	1.00	40.98	N
ATOM	2734	CA	ILE	E	179	0.789	45.569	43.722	1.00	41.76	C
ATOM	2735	C	ILE	E	179	-0.041	45.636	44.997	1.00	42.27	C
ATOM	2736	O	ILE	E	179	0.410	46.140	46.023	1.00	42.03	O
ATOM	2737	CB	ILE	E	179	1.938	44.556	43.862	1.00	41.68	C
ATOM	2738	CG1	ILE	E	179	2.691	44.434	42.534	1.00	41.89	C
ATOM	2739	CG2	ILE	E	179	1.383	43.204	44.284	1.00	42.26	C
ATOM	2740	CD1	ILE	E	179	3.888	43.501	42.567	1.00	42.27	C
ATOM	2741	N	THR	E	180	-1.266	45.132	44.900	1.00	43.33	N
ATOM	2742	CA	THR	E	180	-2.161	45.001	46.037	1.00	44.97	C
ATOM	2743	C	THR	E	180	-1.477	44.284	47.192	1.00	45.47	C
ATOM	2744	O	THR	E	180	-0.602	43.440	46.980	1.00	45.72	O

Figure 1 Table 1b - 42

ATOM	2745	CB	THR	E	180	-3.408	44.197	45.670	1.00 44.67	C
ATOM	2746	OG1	THR	E	180	-3.687	44.351	44.275	1.00 47.07	O
ATOM	2747	CG2	THR	E	180	-4.557	44.721	46.434	1.00 45.88	C
ATOM	2748	N	GLU	E	181	-1.877	44.621	48.412	1.00 46.26	N
ATOM	2749	CA	GLU	E	181	-1.282	44.005	49.582	1.00 47.04	C
ATOM	2750	C	GLU	E	181	-1.761	42.564	49.781	1.00 47.30	C
ATOM	2751	O	GLU	E	181	-0.941	41.681	50.029	1.00 47.23	O
ATOM	2752	CB	GLU	E	181	-1.546	44.847	50.837	1.00 47.05	C
ATOM	2753	CG	GLU	E	181	-0.892	44.288	52.107	1.00 47.62	C
ATOM	2754	CD	GLU	E	181	-1.318	45.002	53.383	1.00 48.12	C
ATOM	2755	OE1	GLU	E	181	-0.920	44.539	54.475	1.00 48.73	O
ATOM	2756	OE2	GLU	E	181	-2.047	46.016	53.301	1.00 49.58	O
ATOM	2757	N	PHE	E	182	-3.066	42.319	49.638	1.00 47.64	N
ATOM	2758	CA	PHE	E	182	-3.664	41.138	50.282	1.00 48.36	C
ATOM	2759	C	PHE	E	182	-4.102	39.887	49.512	1.00 48.35	C
ATOM	2760	O	PHE	E	182	-4.774	39.016	50.088	1.00 48.89	O
ATOM	2761	CB	PHE	E	182	-4.701	41.538	51.334	1.00 48.59	C
ATOM	2762	CG	PHE	E	182	-4.128	41.628	52.709	1.00 49.25	C
ATOM	2763	CD1	PHE	E	182	-3.521	40.511	53.291	1.00 49.50	C
ATOM	2764	CD2	PHE	E	182	-4.170	42.822	53.418	1.00 49.64	C
ATOM	2765	CE1	PHE	E	182	-2.975	40.581	54.560	1.00 49.83	C
ATOM	2766	CE2	PHE	E	182	-3.630	42.902	54.697	1.00 50.54	C
ATOM	2767	CZ	PHE	E	182	-3.029	41.781	55.269	1.00 50.56	C
ATOM	2768	N	PRO	E	183	-3.767	39.790	48.215	1.00 47.95	N
ATOM	2769	CA	PRO	E	183	-3.270	38.470	47.828	1.00 47.24	C
ATOM	2770	C	PRO	E	183	-1.763	38.482	48.149	1.00 46.40	C
ATOM	2771	O	PRO	E	183	-0.949	38.921	47.330	1.00 45.73	O
ATOM	2772	CB	PRO	E	183	-3.555	38.405	46.317	1.00 47.53	C
ATOM	2773	CG	PRO	E	183	-4.276	39.711	45.975	1.00 47.80	C
ATOM	2774	CD	PRO	E	183	-3.923	40.682	47.060	1.00 47.75	C
ATOM	2775	N	LYS	E	184	-1.414	38.054	49.362	1.00 45.25	N
ATOM	2776	CA	LYS	E	184	-0.048	38.210	49.872	1.00 44.51	C
ATOM	2777	C	LYS	E	184	0.710	36.883	49.959	1.00 43.74	C
ATOM	2778	O	LYS	E	184	0.246	35.937	50.603	1.00 43.68	O
ATOM	2779	CB	LYS	E	184	-0.048	38.911	51.237	1.00 44.39	C
ATOM	2780	CG	LYS	E	184	1.348	39.236	51.775	1.00 44.65	C
ATOM	2781	CD	LYS	E	184	1.308	39.867	53.170	1.00 44.54	C
ATOM	2782	CE	LYS	E	184	0.773	41.294	53.136	1.00 43.77	C
ATOM	2783	NZ	LYS	E	184	0.588	41.862	54.500	1.00 43.44	N
ATOM	2784	N	PRO	E	185	1.887	36.817	49.314	1.00 42.90	N
ATOM	2785	CA	PRO	E	185	2.714	35.624	49.393	1.00 42.36	C
ATOM	2786	C	PRO	E	185	3.141	35.331	50.831	1.00 41.83	C
ATOM	2787	O	PRO	E	185	3.457	36.258	51.590	1.00 41.36	O
ATOM	2788	CB	PRO	E	185	3.934	35.990	48.540	1.00 42.36	C
ATOM	2789	CG	PRO	E	185	3.472	37.081	47.649	1.00 42.49	C
ATOM	2790	CD	PRO	E	185	2.508	37.855	48.475	1.00 42.66	C
ATOM	2791	N	GLU	E	186	3.125	34.050	51.189	1.00 40.94	N
ATOM	2792	CA	GLU	E	186	3.584	33.571	52.494	1.00 40.90	C
ATOM	2793	C	GLU	E	186	4.989	34.096	52.817	1.00 39.74	C
ATOM	2794	O	GLU	E	186	5.260	34.473	53.963	1.00 39.21	O
ATOM	2795	CB	GLU	E	186	3.541	32.024	52.559	1.00 40.84	C
ATOM	2796	CG	GLU	E	186	2.120	31.408	52.522	1.00 42.00	C
ATOM	2797	CD	GLU	E	186	2.070	29.966	51.968	1.00 43.86	C
ATOM	2798	OE1	GLU	E	186	2.323	29.776	50.750	1.00 47.32	O
ATOM	2799	OE2	GLU	E	186	1.745	29.023	52.739	1.00 45.40	O
ATOM	2800	N	PHE	E	187	5.861	34.156	51.806	1.00 38.90	N
ATOM	2801	CA	PHE	E	187	7.256	34.576	52.015	1.00 38.55	C
ATOM	2802	C	PHE	E	187	7.430	36.022	52.511	1.00 38.12	C
ATOM	2803	O	PHE	E	187	8.455	36.354	53.109	1.00 37.83	O
ATOM	2804	CB	PHE	E	187	8.151	34.271	50.794	1.00 38.65	C
ATOM	2805	CG	PHE	E	187	7.877	35.123	49.570	1.00 39.40	C
ATOM	2806	CD1	PHE	E	187	8.249	36.469	49.528	1.00 39.63	C
ATOM	2807	CD2	PHE	E	187	7.309	34.554	48.435	1.00 39.47	C
ATOM	2808	CE1	PHE	E	187	8.013	37.242	48.390	1.00 40.37	C
ATOM	2809	CE2	PHE	E	187	7.075	35.308	47.296	1.00 40.14	C
ATOM	2810	CZ	PHE	E	187	7.424	36.658	47.270	1.00 40.68	C
ATOM	2811	N	MET	E	188	6.424	36.863	52.278	1.00 37.58	N

Figure 1 Table 1b - 43

ATOM	2812	CA	MET	E	188	6.466	38.262	52.726	1.00	37.75	C
ATOM	2813	C	MET	E	188	6.502	38.381	54.253	1.00	37.23	C
ATOM	2814	O	MET	E	188	7.058	39.335	54.785	1.00	36.69	O
ATOM	2815	CB	MET	E	188	5.281	39.056	52.156	1.00	37.72	C
ATOM	2816	CG	MET	E	188	5.367	39.305	50.653	1.00	38.77	C
ATOM	2817	SD	MET	E	188	6.751	40.351	50.175	1.00	42.66	S
ATOM	2818	CE	MET	E	188	6.154	41.944	50.743	1.00	43.40	C
ATOM	2819	N	SER	E	189	5.905	37.403	54.935	1.00	36.85	N
ATOM	2820	CA	SER	E	189	5.888	37.344	56.404	1.00	37.43	C
ATOM	2821	C	SER	E	189	7.048	36.536	57.011	1.00	37.36	C
ATOM	2822	O	SER	E	189	7.069	36.267	58.216	1.00	37.27	O
ATOM	2823	CB	SER	E	189	4.548	36.777	56.883	1.00	37.65	C
ATOM	2824	OG	SER	E	189	3.483	37.553	56.343	1.00	39.90	O
ATOM	2825	N	LYS	E	190	7.993	36.131	56.166	1.00	37.13	N
ATOM	2826	CA	LYS	E	190	9.195	35.436	56.615	1.00	36.57	C
ATOM	2827	C	LYS	E	190	10.362	36.411	56.728	1.00	36.32	C
ATOM	2828	O	LYS	E	190	10.439	37.389	55.985	1.00	35.59	O
ATOM	2829	CB	LYS	E	190	9.537	34.309	55.643	1.00	36.70	C
ATOM	2830	CG	LYS	E	190	8.566	33.138	55.731	1.00	38.12	C
ATOM	2831	CD	LYS	E	190	8.913	32.073	54.729	1.00	41.72	C
ATOM	2832	CE	LYS	E	190	8.013	30.847	54.908	1.00	44.22	C
ATOM	2833	NZ	LYS	E	190	8.302	29.855	53.842	1.00	46.07	N
ATOM	2834	N	SER	E	191	11.277	36.129	57.648	1.00	36.45	N
ATOM	2835	CA	SER	E	191	12.395	37.028	57.919	1.00	36.42	C
ATOM	2836	C	SER	E	191	13.532	36.913	56.899	1.00	36.56	C
ATOM	2837	O	SER	E	191	13.605	35.945	56.138	1.00	35.85	O
ATOM	2838	CB	SER	E	191	12.925	36.782	59.328	1.00	36.35	C
ATOM	2839	OG	SER	E	191	13.532	35.506	59.426	1.00	36.95	O
ATOM	2840	N	LEU	E	192	14.417	37.911	56.898	1.00	37.24	N
ATOM	2841	CA	LEU	E	192	15.653	37.881	56.104	1.00	37.92	C
ATOM	2842	C	LEU	E	192	16.471	36.644	56.444	1.00	38.52	C
ATOM	2843	O	LEU	E	192	17.062	36.018	55.569	1.00	38.54	O
ATOM	2844	CB	LEU	E	192	16.501	39.115	56.385	1.00	37.62	C
ATOM	2845	CG	LEU	E	192	15.996	40.461	55.857	1.00	39.00	C
ATOM	2846	CD1	LEU	E	192	17.012	41.554	56.166	1.00	40.14	C
ATOM	2847	CD2	LEU	E	192	15.692	40.408	54.351	1.00	39.07	C
ATOM	2848	N	GLU	E	193	16.523	36.341	57.735	1.00	38.78	N
ATOM	2849	CA	GLU	E	193	17.153	35.141	58.261	1.00	39.80	C
ATOM	2850	C	GLU	E	193	16.661	33.864	57.556	1.00	39.56	C
ATOM	2851	O	GLU	E	193	17.449	33.120	56.980	1.00	39.49	O
ATOM	2852	CB	GLU	E	193	16.894	35.072	59.771	1.00	39.77	C
ATOM	2853	CG	GLU	E	193	17.312	33.770	60.450	1.00	43.50	C
ATOM	2854	CD	GLU	E	193	18.795	33.702	60.694	1.00	47.04	C
ATOM	2855	OE1	GLU	E	193	19.577	34.139	59.819	1.00	50.20	O
ATOM	2856	OE2	GLU	E	193	19.184	33.207	61.765	1.00	49.83	O
ATOM	2857	N	GLU	E	194	15.357	33.628	57.582	1.00	39.66	N
ATOM	2858	CA	GLU	E	194	14.832	32.399	57.015	1.00	40.13	C
ATOM	2859	C	GLU	E	194	14.828	32.380	55.492	1.00	39.46	C
ATOM	2860	O	GLU	E	194	14.999	31.321	54.884	1.00	38.78	O
ATOM	2861	CB	GLU	E	194	13.467	32.030	57.596	1.00	40.49	C
ATOM	2862	CG	GLU	E	194	12.445	33.132	57.643	1.00	42.28	C
ATOM	2863	CD	GLU	E	194	11.286	32.815	58.592	1.00	43.42	C
ATOM	2864	OE1	GLU	E	194	10.998	31.605	58.804	1.00	47.18	O
ATOM	2865	OE2	GLU	E	194	10.665	33.772	59.123	1.00	44.71	O
ATOM	2866	N	LEU	E	195	14.664	33.549	54.872	1.00	38.35	N
ATOM	2867	CA	LEU	E	195	14.706	33.628	53.422	1.00	38.20	C
ATOM	2868	C	LEU	E	195	16.127	33.603	52.877	1.00	37.88	C
ATOM	2869	O	LEU	E	195	16.331	33.346	51.697	1.00	37.77	O
ATOM	2870	CB	LEU	E	195	13.954	34.864	52.911	1.00	38.06	C
ATOM	2871	CG	LEU	E	195	12.447	34.860	53.183	1.00	38.81	C
ATOM	2872	CD1	LEU	E	195	11.830	36.196	52.814	1.00	39.66	C
ATOM	2873	CD2	LEU	E	195	11.726	33.706	52.462	1.00	39.09	C
ATOM	2874	N	GLN	E	196	17.096	33.865	53.749	1.00	37.89	N
ATOM	2875	CA	GLN	E	196	18.504	34.041	53.377	1.00	38.83	C
ATOM	2876	C	GLN	E	196	18.698	35.103	52.283	1.00	38.61	C
ATOM	2877	O	GLN	E	196	19.280	34.863	51.216	1.00	38.74	O
ATOM	2878	CB	GLN	E	196	19.176	32.692	53.072	1.00	38.30	C

Figure 1 Table 1b - 44

ATOM	2879	CG	GLN	E	196	19.014	31.710	54.253	1.00	39.98	C
ATOM	2880	CD	GLN	E	196	19.700	30.376	54.050	1.00	40.61	C
ATOM	2881	OE1	GLN	E	196	20.115	30.041	52.939	1.00	43.09	O
ATOM	2882	NE2	GLN	E	196	19.813	29.596	55.128	1.00	42.37	N
ATOM	2883	N	ILE	E	197	18.174	36.288	52.565	1.00	38.95	N
ATOM	2884	CA	ILE	E	197	18.323	37.426	51.668	1.00	38.73	C
ATOM	2885	C	ILE	E	197	19.318	38.385	52.309	1.00	38.96	C
ATOM	2886	O	ILE	E	197	19.134	38.811	53.460	1.00	39.43	O
ATOM	2887	CB	ILE	E	197	16.964	38.117	51.390	1.00	38.85	C
ATOM	2888	CG1	ILE	E	197	15.985	37.130	50.739	1.00	39.06	C
ATOM	2889	CG2	ILE	E	197	17.146	39.361	50.504	1.00	38.30	C
ATOM	2890	CD1	ILE	E	197	14.558	37.675	50.573	1.00	38.18	C
ATOM	2891	N	GLY	E	198	20.382	38.692	51.571	1.00	38.55	N
ATOM	2892	CA	GLY	E	198	21.404	39.637	52.021	1.00	37.75	C
ATOM	2893	C	GLY	E	198	22.792	39.030	51.957	1.00	37.20	C
ATOM	2894	O	GLY	E	198	22.953	37.880	51.552	1.00	36.98	O
ATOM	2895	N	THR	E	199	23.796	39.811	52.341	1.00	36.43	N
ATOM	2896	CA	THR	E	199	25.165	39.331	52.446	1.00	36.10	C
ATOM	2897	C	THR	E	199	25.589	39.376	53.916	1.00	36.66	C
ATOM	2898	O	THR	E	199	25.417	40.407	54.581	1.00	36.37	O
ATOM	2899	CB	THR	E	199	26.125	40.160	51.568	1.00	36.02	C
ATOM	2900	OG1	THR	E	199	25.703	40.073	50.204	1.00	35.68	O
ATOM	2901	CG2	THR	E	199	27.563	39.659	51.682	1.00	34.35	C
ATOM	2902	N	TYR	E	200	26.144	38.264	54.406	1.00	36.66	N
ATOM	2903	CA	TYR	E	200	26.429	38.098	55.837	1.00	37.10	C
ATOM	2904	C	TYR	E	200	27.863	37.685	56.142	1.00	37.47	C
ATOM	2905	O	TYR	E	200	28.175	37.278	57.259	1.00	37.76	O
ATOM	2906	CB	TYR	E	200	25.387	37.178	56.496	1.00	36.77	C
ATOM	2907	CG	TYR	E	200	24.005	37.749	56.312	1.00	36.88	C
ATOM	2908	CD1	TYR	E	200	23.167	37.302	55.285	1.00	37.14	C
ATOM	2909	CD2	TYR	E	200	23.559	38.789	57.121	1.00	37.13	C
ATOM	2910	CE1	TYR	E	200	21.912	37.859	55.097	1.00	36.71	C
ATOM	2911	CE2	TYR	E	200	22.314	39.357	56.932	1.00	37.83	C
ATOM	2912	CZ	TYR	E	200	21.495	38.891	55.921	1.00	37.68	C
ATOM	2913	OH	TYR	E	200	20.255	39.465	55.750	1.00	37.64	O
ATOM	2914	N	ALA	E	201	28.737	37.837	55.148	1.00	37.87	N
ATOM	2915	CA	ALA	E	201	30.168	37.590	55.318	1.00	38.22	C
ATOM	2916	C	ALA	E	201	31.001	38.556	54.481	1.00	38.27	C
ATOM	2917	O	ALA	E	201	30.531	39.065	53.449	1.00	38.56	O
ATOM	2918	CB	ALA	E	201	30.519	36.146	54.968	1.00	38.06	C
ATOM	2919	N	ASN	E	202	32.233	38.797	54.933	1.00	38.12	N
ATOM	2920	CA	ASN	E	202	33.196	39.633	54.215	1.00	38.49	C
ATOM	2921	C	ASN	E	202	32.601	41.001	53.893	1.00	37.80	C
ATOM	2922	O	ASN	E	202	32.656	41.455	52.752	1.00	37.62	O
ATOM	2923	CB	ASN	E	202	33.679	38.946	52.924	1.00	38.77	C
ATOM	2924	CG	ASN	E	202	34.043	37.481	53.137	1.00	40.97	C
ATOM	2925	OD1	ASN	E	202	33.421	36.579	52.555	1.00	43.16	O
ATOM	2926	ND2	ASN	E	202	35.034	37.237	53.988	1.00	41.24	N
ATOM	2927	N	ILE	E	203	32.005	41.633	54.897	1.00	37.25	N
ATOM	2928	CA	ILE	E	203	31.403	42.945	54.706	1.00	37.50	C
ATOM	2929	C	ILE	E	203	32.513	43.975	54.583	1.00	37.40	C
ATOM	2930	O	ILE	E	203	33.351	44.105	55.478	1.00	36.74	O
ATOM	2931	CB	ILE	E	203	30.408	43.302	55.836	1.00	37.53	C
ATOM	2932	CG1	ILE	E	203	29.340	42.200	55.978	1.00	38.14	C
ATOM	2933	CG2	ILE	E	203	29.775	44.659	55.586	1.00	36.69	C
ATOM	2934	CD1	ILE	E	203	28.553	41.875	54.691	1.00	38.76	C
ATOM	2935	N	ALA	E	204	32.542	44.663	53.445	1.00	37.56	N
ATOM	2936	CA	ALA	E	204	33.520	45.717	53.231	1.00	38.05	C
ATOM	2937	C	ALA	E	204	33.079	46.958	54.012	1.00	38.37	C
ATOM	2938	O	ALA	E	204	31.998	47.507	53.769	1.00	38.96	O
ATOM	2939	CB	ALA	E	204	33.674	46.014	51.734	1.00	37.68	C
ATOM	2940	N	MET	E	205	33.905	47.372	54.970	1.00	38.61	N
ATOM	2941	CA	MET	E	205	33.603	48.514	55.835	1.00	39.11	C
ATOM	2942	C	MET	E	205	34.830	49.411	55.985	1.00	38.92	C
ATOM	2943	O	MET	E	205	35.949	49.008	55.656	1.00	38.88	O
ATOM	2944	CB	MET	E	205	33.175	48.056	57.232	1.00	38.85	C
ATOM	2945	CG	MET	E	205	32.007	47.089	57.286	1.00	40.18	C

Figure 1 Table 1b - 45

ATOM	2946	SD	MET	E	205	31.711	46.491	58.961	1.00	40.80	S
ATOM	2947	CE	MET	E	205	33.041	45.309	59.170	1.00	41.44	C
ATOM	2948	N	VAL	E	206	34.601	50.620	56.498	1.00	38.83	N
ATOM	2949	CA	VAL	E	206	35.668	51.568	56.821	1.00	38.83	C
ATOM	2950	C	VAL	E	206	35.490	52.083	58.243	1.00	39.04	C
ATOM	2951	O	VAL	E	206	34.461	51.845	58.869	1.00	39.24	O
ATOM	2952	CB	VAL	E	206	35.715	52.784	55.821	1.00	38.92	C
ATOM	2953	CG1	VAL	E	206	36.087	52.323	54.429	1.00	39.17	C
ATOM	2954	CG2	VAL	E	206	34.396	53.561	55.802	1.00	37.97	C
ATOM	2955	N	ARG	E	207	36.488	52.794	58.754	1.00	39.51	N
ATOM	2956	CA	ARG	E	207	36.332	53.500	60.021	1.00	40.23	C
ATOM	2957	C	ARG	E	207	36.135	55.004	59.810	1.00	40.49	C
ATOM	2958	O	ARG	E	207	36.235	55.509	58.686	1.00	39.84	O
ATOM	2959	CB	ARG	E	207	37.523	53.211	60.941	1.00	40.74	C
ATOM	2960	CG	ARG	E	207	37.724	51.709	61.170	1.00	42.78	C
ATOM	2961	CD	ARG	E	207	38.448	51.420	62.456	1.00	47.22	C
ATOM	2962	NE	ARG	E	207	37.918	52.219	63.557	1.00	49.87	N
ATOM	2963	CZ	ARG	E	207	38.567	52.452	64.691	1.00	50.98	C
ATOM	2964	NH1	ARG	E	207	39.774	51.935	64.888	1.00	51.71	N
ATOM	2965	NH2	ARG	E	207	38.007	53.205	65.628	1.00	52.64	N
ATOM	2966	N	THR	E	208	35.839	55.697	60.906	1.00	40.74	N
ATOM	2967	CA	THR	E	208	35.649	57.151	60.939	1.00	41.48	C
ATOM	2968	C	THR	E	208	36.800	57.932	60.277	1.00	41.07	C
ATOM	2969	O	THR	E	208	36.580	58.871	59.500	1.00	41.15	O
ATOM	2970	CB	THR	E	208	35.461	57.592	62.419	1.00	41.32	C
ATOM	2971	OG1	THR	E	208	34.173	57.153	62.871	1.00	43.22	O
ATOM	2972	CG2	THR	E	208	35.570	59.096	62.588	1.00	42.78	C
ATOM	2973	N	THR	E	209	38.019	57.492	60.574	1.00	41.04	N
ATOM	2974	CA	THR	E	209	39.253	58.179	60.224	1.00	40.61	C
ATOM	2975	C	THR	E	209	39.878	57.655	58.920	1.00	40.34	C
ATOM	2976	O	THR	E	209	40.916	58.166	58.477	1.00	40.19	O
ATOM	2977	CB	THR	E	209	40.263	58.016	61.376	1.00	40.83	C
ATOM	2978	OG1	THR	E	209	40.419	56.620	61.664	1.00	41.78	O
ATOM	2979	CG2	THR	E	209	39.760	58.709	62.641	1.00	40.49	C
ATOM	2980	N	THR	E	210	39.243	56.650	58.308	1.00	39.74	N
ATOM	2981	CA	THR	E	210	39.722	56.058	57.056	1.00	39.26	C
ATOM	2982	C	THR	E	210	39.787	57.108	55.934	1.00	38.72	C
ATOM	2983	O	THR	E	210	38.773	57.731	55.613	1.00	38.78	O
ATOM	2984	CB	THR	E	210	38.826	54.867	56.596	1.00	39.46	C
ATOM	2985	OG1	THR	E	210	38.803	53.842	57.604	1.00	40.08	O
ATOM	2986	CG2	THR	E	210	39.349	54.262	55.292	1.00	39.40	C
ATOM	2987	N	PRO	E	211	40.981	57.307	55.339	1.00	38.09	N
ATOM	2988	CA	PRO	E	211	41.108	58.241	54.216	1.00	37.89	C
ATOM	2989	C	PRO	E	211	40.221	57.868	53.027	1.00	37.87	C
ATOM	2990	O	PRO	E	211	39.961	56.681	52.788	1.00	37.86	O
ATOM	2991	CB	PRO	E	211	42.581	58.130	53.827	1.00	37.86	C
ATOM	2992	CG	PRO	E	211	43.266	57.589	55.039	1.00	38.16	C
ATOM	2993	CD	PRO	E	211	42.271	56.690	55.696	1.00	37.57	C
ATOM	2994	N	VAL	E	212	39.755	58.887	52.304	1.00	37.67	N
ATOM	2995	CA	VAL	E	212	38.923	58.704	51.115	1.00	37.33	C
ATOM	2996	C	VAL	E	212	39.579	57.767	50.091	1.00	37.08	C
ATOM	2997	O	VAL	E	212	38.911	56.892	49.541	1.00	36.55	O
ATOM	2998	CB	VAL	E	212	38.562	60.070	50.461	1.00	37.59	C
ATOM	2999	CG1	VAL	E	212	38.027	59.885	49.025	1.00	37.64	C
ATOM	3000	CG2	VAL	E	212	37.549	60.809	51.323	1.00	36.99	C
ATOM	3001	N	TYR	E	213	40.881	57.947	49.857	1.00	36.94	N
ATOM	3002	CA	TYR	E	213	41.600	57.138	48.872	1.00	37.28	C
ATOM	3003	C	TYR	E	213	41.611	55.650	49.239	1.00	36.90	C
ATOM	3004	O	TYR	E	213	41.607	54.799	48.351	1.00	36.94	O
ATOM	3005	CB	TYR	E	213	43.024	57.666	48.612	1.00	37.72	C
ATOM	3006	CG	TYR	E	213	44.030	57.393	49.707	1.00	39.11	C
ATOM	3007	CD1	TYR	E	213	44.325	58.363	50.667	1.00	40.50	C
ATOM	3008	CD2	TYR	E	213	44.701	56.169	49.776	1.00	39.93	C
ATOM	3009	CE1	TYR	E	213	45.252	58.117	51.676	1.00	40.79	C
ATOM	3010	CE2	TYR	E	213	45.625	55.915	50.776	1.00	40.33	C
ATOM	3011	CZ	TYR	E	213	45.889	56.888	51.722	1.00	40.10	C
ATOM	3012	OH	TYR	E	213	46.805	56.632	52.708	1.00	40.38	O

Figure 1 Table 1b - 46

ATOM	3013	N	VAL	E	214	41.614	55.351	50.540	1.00	36.52	N
ATOM	3014	CA	VAL	E	214	41.511	53.966	51.021	1.00	35.95	C
ATOM	3015	C	VAL	E	214	40.126	53.392	50.704	1.00	35.79	C
ATOM	3016	O	VAL	E	214	40.015	52.273	50.178	1.00	35.46	O
ATOM	3017	CB	VAL	E	214	41.847	53.829	52.541	1.00	36.16	C
ATOM	3018	CG1	VAL	E	214	41.708	52.380	53.007	1.00	35.91	C
ATOM	3019	CG2	VAL	E	214	43.268	54.328	52.837	1.00	35.80	C
ATOM	3020	N	ALA	E	215	39.079	54.165	51.002	1.00	35.25	N
ATOM	3021	CA	ALA	E	215	37.708	53.782	50.651	1.00	34.87	C
ATOM	3022	C	ALA	E	215	37.547	53.500	49.156	1.00	34.82	C
ATOM	3023	O	ALA	E	215	36.900	52.525	48.781	1.00	34.56	O
ATOM	3024	CB	ALA	E	215	36.710	54.832	51.108	1.00	34.39	C
ATOM	3025	N	LEU	E	216	38.151	54.344	48.317	1.00	34.74	N
ATOM	3026	CA	LEU	E	216	38.102	54.180	46.873	1.00	35.17	C
ATOM	3027	C	LEU	E	216	38.705	52.852	46.440	1.00	35.52	C
ATOM	3028	O	LEU	E	216	38.124	52.155	45.622	1.00	36.23	O
ATOM	3029	CB	LEU	E	216	38.820	55.335	46.146	1.00	35.59	C
ATOM	3030	CG	LEU	E	216	38.290	56.771	46.258	1.00	36.50	C
ATOM	3031	CD1	LEU	E	216	38.957	57.648	45.211	1.00	37.67	C
ATOM	3032	CD2	LEU	E	216	36.788	56.841	46.116	1.00	38.50	C
ATOM	3033	N	GLY	E	217	39.873	52.512	46.978	1.00	35.87	N
ATOM	3034	CA	GLY	E	217	40.502	51.216	46.712	1.00	36.22	C
ATOM	3035	C	GLY	E	217	39.626	50.043	47.134	1.00	36.65	C
ATOM	3036	O	GLY	E	217	39.589	49.005	46.462	1.00	36.68	O
ATOM	3037	N	ILE	E	218	38.922	50.217	48.249	1.00	36.58	N
ATOM	3038	CA	ILE	E	218	37.964	49.232	48.724	1.00	36.83	C
ATOM	3039	C	ILE	E	218	36.797	49.081	47.733	1.00	36.81	C
ATOM	3040	O	ILE	E	218	36.458	47.949	47.352	1.00	36.72	O
ATOM	3041	CB	ILE	E	218	37.494	49.539	50.171	1.00	36.90	C
ATOM	3042	CG1	ILE	E	218	38.673	49.355	51.148	1.00	37.30	C
ATOM	3043	CG2	ILE	E	218	36.306	48.642	50.564	1.00	36.70	C
ATOM	3044	CD1	ILE	E	218	38.459	49.971	52.541	1.00	36.43	C
ATOM	3045	N	PHE	E	219	36.222	50.203	47.286	1.00	36.41	N
ATOM	3046	CA	PHE	E	219	35.191	50.164	46.236	1.00	36.43	C
ATOM	3047	C	PHE	E	219	35.673	49.435	44.989	1.00	36.86	C
ATOM	3048	O	PHE	E	219	34.924	48.666	44.385	1.00	36.70	O
ATOM	3049	CB	PHE	E	219	34.743	51.563	45.801	1.00	35.90	C
ATOM	3050	CG	PHE	E	219	33.778	52.239	46.741	1.00	35.78	C
ATOM	3051	CD1	PHE	E	219	34.010	53.558	47.153	1.00	35.30	C
ATOM	3052	CD2	PHE	E	219	32.628	51.587	47.186	1.00	35.35	C
ATOM	3053	CE1	PHE	E	219	33.117	54.218	48.011	1.00	34.76	C
ATOM	3054	CE2	PHE	E	219	31.727	52.225	48.043	1.00	35.71	C
ATOM	3055	CZ	PHE	E	219	31.971	53.548	48.465	1.00	34.48	C
ATOM	3056	N	VAL	E	220	36.911	49.724	44.585	1.00	37.21	N
ATOM	3057	CA	VAL	E	220	37.481	49.167	43.366	1.00	38.10	C
ATOM	3058	C	VAL	E	220	37.675	47.649	43.469	1.00	38.74	C
ATOM	3059	O	VAL	E	220	37.345	46.915	42.532	1.00	39.25	O
ATOM	3060	CB	VAL	E	220	38.798	49.890	42.946	1.00	37.81	C
ATOM	3061	CG1	VAL	E	220	39.564	49.084	41.876	1.00	38.45	C
ATOM	3062	CG2	VAL	E	220	38.489	51.288	42.422	1.00	37.54	C
ATOM	3063	N	GLN	E	221	38.191	47.176	44.601	1.00	39.19	N
ATOM	3064	CA	GLN	E	221	38.412	45.741	44.764	1.00	39.91	C
ATOM	3065	C	GLN	E	221	37.136	44.910	44.974	1.00	40.03	C
ATOM	3066	O	GLN	E	221	37.010	43.811	44.430	1.00	39.77	O
ATOM	3067	CB	GLN	E	221	39.398	45.456	45.891	1.00	40.08	C
ATOM	3068	CG	GLN	E	221	39.733	43.979	45.987	1.00	41.11	C
ATOM	3069	CD	GLN	E	221	40.980	43.711	46.769	1.00	43.42	C
ATOM	3070	OE1	GLN	E	221	41.433	44.558	47.542	1.00	44.30	O
ATOM	3071	NE2	GLN	E	221	41.557	42.521	46.577	1.00	43.43	N
ATOM	3072	N	HIS	E	222	36.203	45.436	45.760	1.00	40.46	N
ATOM	3073	CA	HIS	E	222	35.045	44.654	46.186	1.00	40.84	C
ATOM	3074	C	HIS	E	222	33.778	44.835	45.354	1.00	40.19	C
ATOM	3075	O	HIS	E	222	32.850	44.037	45.475	1.00	39.88	O
ATOM	3076	CB	HIS	E	222	34.772	44.886	47.673	1.00	41.50	C
ATOM	3077	CG	HIS	E	222	35.930	44.531	48.541	1.00	43.57	C
ATOM	3078	ND1	HIS	E	222	36.289	43.226	48.799	1.00	46.90	N
ATOM	3079	CD2	HIS	E	222	36.838	45.306	49.179	1.00	45.48	C

Figure 1 Table 1b - 47

ATOM	3080	CE1	HIS	E	222	37.359	43.212	49.575	1.00 47.63	C
ATOM	3081	NE2	HIS	E	222	37.710	44.461	49.823	1.00 48.04	N
ATOM	3082	N	ARG	E	223	33.740	45.868	44.515	1.00 39.68	N
ATOM	3083	CA	ARG	E	223	32.605	46.088	43.601	1.00 39.81	C
ATOM	3084	C	ARG	E	223	31.259	46.090	44.340	1.00 39.06	C
ATOM	3085	O	ARG	E	223	30.339	45.314	44.045	1.00 38.29	O
ATOM	3086	CB	ARG	E	223	32.612	45.070	42.457	1.00 40.19	C
ATOM	3087	CG	ARG	E	223	33.871	45.119	41.602	1.00 42.96	C
ATOM	3088	CD	ARG	E	223	33.729	44.207	40.395	1.00 47.90	C
ATOM	3089	NE	ARG	E	223	35.010	43.963	39.731	1.00 52.44	N
ATOM	3090	CZ	ARG	E	223	35.143	43.552	38.469	1.00 54.15	C
ATOM	3091	NH1	ARG	E	223	34.069	43.348	37.709	1.00 54.98	N
ATOM	3092	NH2	ARG	E	223	36.354	43.351	37.961	1.00 54.78	N
ATOM	3093	N	VAL	E	224	31.178	47.009	45.288	1.00 38.18	N
ATOM	3094	CA	VAL	E	224	30.116	47.097	46.266	1.00 38.23	C
ATOM	3095	C	VAL	E	224	29.646	48.573	46.299	1.00 37.82	C
ATOM	3096	O	VAL	E	224	30.466	49.466	46.118	1.00 38.06	O
ATOM	3097	CB	VAL	E	224	30.718	46.581	47.587	1.00 38.42	C
ATOM	3098	CG1	VAL	E	224	30.643	47.581	48.716	1.00 38.62	C
ATOM	3099	CG2	VAL	E	224	30.213	45.168	47.911	1.00 37.61	C
ATOM	3100	N	SER	E	225	28.348	48.827	46.491	1.00 37.47	N
ATOM	3101	CA	SER	E	225	27.798	50.179	46.263	1.00 37.58	C
ATOM	3102	C	SER	E	225	27.926	51.153	47.442	1.00 37.11	C
ATOM	3103	O	SER	E	225	27.793	52.362	47.259	1.00 36.30	O
ATOM	3104	CB	SER	E	225	26.347	50.132	45.759	1.00 37.36	C
ATOM	3105	OG	SER	E	225	25.436	49.843	46.816	1.00 40.55	O
ATOM	3106	N	ALA	E	226	28.159	50.628	48.646	1.00 36.35	N
ATOM	3107	CA	ALA	E	226	28.365	51.467	49.825	1.00 36.19	C
ATOM	3108	C	ALA	E	226	29.158	50.738	50.899	1.00 36.53	C
ATOM	3109	O	ALA	E	226	29.149	49.502	50.967	1.00 36.30	O
ATOM	3110	CB	ALA	E	226	27.035	51.940	50.395	1.00 35.83	C
ATOM	3111	N	LEU	E	227	29.834	51.525	51.735	1.00 36.37	N
ATOM	3112	CA	LEU	E	227	30.639	51.015	52.838	1.00 35.92	C
ATOM	3113	C	LEU	E	227	30.103	51.530	54.170	1.00 35.91	C
ATOM	3114	O	LEU	E	227	30.036	52.749	54.388	1.00 35.62	O
ATOM	3115	CB	LEU	E	227	32.110	51.431	52.665	1.00 35.69	C
ATOM	3116	CG	LEU	E	227	32.750	51.149	51.295	1.00 36.67	C
ATOM	3117	CD1	LEU	E	227	34.131	51.808	51.166	1.00 36.69	C
ATOM	3118	CD2	LEU	E	227	32.833	49.655	51.011	1.00 35.90	C
ATOM	3119	N	PRO	E	228	29.700	50.612	55.069	1.00 35.75	N
ATOM	3120	CA	PRO	E	228	29.403	51.072	56.427	1.00 36.04	C
ATOM	3121	C	PRO	E	228	30.630	51.685	57.107	1.00 36.32	C
ATOM	3122	O	PRO	E	228	31.753	51.205	56.929	1.00 36.02	O
ATOM	3123	CB	PRO	E	228	28.963	49.793	57.152	1.00 35.88	C
ATOM	3124	CG	PRO	E	228	28.488	48.887	56.052	1.00 35.89	C
ATOM	3125	CD	PRO	E	228	29.427	49.175	54.906	1.00 35.88	C
ATOM	3126	N	VAL	E	229	30.395	52.754	57.858	1.00 36.40	N
ATOM	3127	CA	VAL	E	229	31.429	53.409	58.652	1.00 36.89	C
ATOM	3128	C	VAL	E	229	31.216	52.968	60.099	1.00 37.42	C
ATOM	3129	O	VAL	E	229	30.141	53.165	60.672	1.00 37.13	O
ATOM	3130	CB	VAL	E	229	31.352	54.950	58.515	1.00 37.12	C
ATOM	3131	CG1	VAL	E	229	32.486	55.643	59.284	1.00 37.15	C
ATOM	3132	CG2	VAL	E	229	31.382	55.356	57.042	1.00 35.90	C
ATOM	3133	N	VAL	E	230	32.235	52.347	60.677	1.00 37.91	N
ATOM	3134	CA	VAL	E	230	32.098	51.754	61.992	1.00 38.86	C
ATOM	3135	C	VAL	E	230	33.065	52.351	63.010	1.00 39.77	C
ATOM	3136	O	VAL	E	230	34.115	52.892	62.648	1.00 39.81	O
ATOM	3137	CB	VAL	E	230	32.248	50.212	61.941	1.00 38.95	C
ATOM	3138	CG1	VAL	E	230	31.207	49.603	60.990	1.00 38.41	C
ATOM	3139	CG2	VAL	E	230	33.662	49.810	61.525	1.00 38.84	C
ATOM	3140	N	ASP	E	231	32.685	52.275	64.281	1.00 40.91	N
ATOM	3141	CA	ASP	E	231	33.559	52.696	65.368	1.00 42.19	C
ATOM	3142	C	ASP	E	231	34.493	51.552	65.770	1.00 42.96	C
ATOM	3143	O	ASP	E	231	34.468	50.477	65.158	1.00 43.10	O
ATOM	3144	CB	ASP	E	231	32.745	53.226	66.559	1.00 42.03	C
ATOM	3145	CG	ASP	E	231	31.867	52.161	67.218	1.00 42.77	C
ATOM	3146	OD1	ASP	E	231	30.971	52.563	67.996	1.00 43.29	O

Figure 1 Table 1b - 48

ATOM	3147	OD2	ASP	E	231	32.061	50.943	66.982	1.00	42.48	O
ATOM	3148	N	GLU	E	232	35.307	51.783	66.795	1.00	43.89	N
ATOM	3149	CA	GLU	E	232	36.280	50.787	67.255	1.00	44.84	C
ATOM	3150	C	GLU	E	232	35.631	49.456	67.652	1.00	44.84	C
ATOM	3151	O	GLU	E	232	36.280	48.406	67.616	1.00	45.25	O
ATOM	3152	CB	GLU	E	232	37.126	51.349	68.408	1.00	45.09	C
ATOM	3153	CG	GLU	E	232	36.315	51.927	69.563	1.00	46.81	C
ATOM	3154	CD	GLU	E	232	36.987	53.127	70.206	1.00	49.68	C
ATOM	3155	OE1	GLU	E	232	37.635	53.911	69.470	1.00	50.36	O
ATOM	3156	OE2	GLU	E	232	36.862	53.291	71.445	1.00	49.94	O
ATOM	3157	N	LYS	E	233	34.352	49.509	68.016	1.00	44.57	N
ATOM	3158	CA	LYS	E	233	33.626	48.328	68.476	1.00	44.01	C
ATOM	3159	C	LYS	E	233	32.825	47.670	67.349	1.00	43.53	C
ATOM	3160	O	LYS	E	233	32.049	46.745	67.587	1.00	43.52	O
ATOM	3161	CB	LYS	E	233	32.732	48.687	69.664	1.00	44.17	C
ATOM	3162	CG	LYS	E	233	33.518	49.141	70.890	1.00	44.66	C
ATOM	3163	CD	LYS	E	233	32.616	49.645	72.001	1.00	45.79	C
ATOM	3164	CE	LYS	E	233	33.447	50.229	73.143	1.00	46.17	C
ATOM	3165	NZ	LYS	E	233	32.605	50.680	74.289	1.00	47.04	N
ATOM	3166	N	GLY	E	234	33.032	48.146	66.123	1.00	42.82	N
ATOM	3167	CA	GLY	E	234	32.388	47.568	64.948	1.00	42.20	C
ATOM	3168	C	GLY	E	234	30.921	47.941	64.814	1.00	41.63	C
ATOM	3169	O	GLY	E	234	30.186	47.311	64.048	1.00	41.55	O
ATOM	3170	N	ARG	E	235	30.499	48.958	65.568	1.00	40.84	N
ATOM	3171	CA	ARG	E	235	29.135	49.476	65.494	1.00	40.26	C
ATOM	3172	C	ARG	E	235	29.040	50.529	64.394	1.00	39.62	C
ATOM	3173	O	ARG	E	235	29.914	51.390	64.278	1.00	39.01	O
ATOM	3174	CB	ARG	E	235	28.703	50.087	66.830	1.00	40.46	C
ATOM	3175	CG	ARG	E	235	28.556	49.089	67.965	1.00	41.32	C
ATOM	3176	CD	ARG	E	235	28.238	49.792	69.271	1.00	42.78	C
ATOM	3177	NE	ARG	E	235	29.299	50.715	69.667	1.00	44.02	N
ATOM	3178	CZ	ARG	E	235	29.358	51.346	70.838	1.00	44.78	C
ATOM	3179	NH1	ARG	E	235	28.412	51.166	71.752	1.00	44.66	N
ATOM	3180	NH2	ARG	E	235	30.372	52.163	71.096	1.00	44.67	N
ATOM	3181	N	VAL	E	236	27.973	50.459	63.602	1.00	39.02	N
ATOM	3182	CA	VAL	E	236	27.793	51.372	62.476	1.00	38.82	C
ATOM	3183	C	VAL	E	236	27.406	52.778	62.952	1.00	38.70	C
ATOM	3184	O	VAL	E	236	26.501	52.945	63.764	1.00	38.91	O
ATOM	3185	CB	VAL	E	236	26.796	50.803	61.421	1.00	38.58	C
ATOM	3186	CG1	VAL	E	236	25.368	50.787	61.950	1.00	38.48	C
ATOM	3187	CG2	VAL	E	236	26.903	51.569	60.099	1.00	38.05	C
ATOM	3188	N	VAL	E	237	28.123	53.777	62.454	1.00	38.63	N
ATOM	3189	CA	VAL	E	237	27.875	55.172	62.831	1.00	38.59	C
ATOM	3190	C	VAL	E	237	27.540	56.029	61.610	1.00	38.59	C
ATOM	3191	O	VAL	E	237	26.912	57.076	61.734	1.00	38.58	O
ATOM	3192	CB	VAL	E	237	29.061	55.790	63.638	1.00	38.50	C
ATOM	3193	CG1	VAL	E	237	29.124	55.189	65.044	1.00	38.97	C
ATOM	3194	CG2	VAL	E	237	30.396	55.608	62.908	1.00	38.46	C
ATOM	3195	N	ASP	E	238	27.956	55.575	60.430	1.00	38.56	N
ATOM	3196	CA	ASP	E	238	27.694	56.306	59.200	1.00	38.70	C
ATOM	3197	C	ASP	E	238	27.708	55.349	58.010	1.00	38.90	C
ATOM	3198	O	ASP	E	238	27.871	54.127	58.168	1.00	38.53	O
ATOM	3199	CB	ASP	E	238	28.726	57.438	59.012	1.00	38.91	C
ATOM	3200	CG	ASP	E	238	28.113	58.708	58.438	1.00	39.81	C
ATOM	3201	OD1	ASP	E	238	27.131	58.617	57.674	1.00	39.86	O
ATOM	3202	OD2	ASP	E	238	28.611	59.816	58.753	1.00	43.88	O
ATOM	3203	N	ILE	E	239	27.533	55.910	56.818	1.00	38.66	N
ATOM	3204	CA	ILE	E	239	27.542	55.123	55.583	1.00	38.80	C
ATOM	3205	C	ILE	E	239	28.199	55.971	54.487	1.00	38.74	C
ATOM	3206	O	ILE	E	239	27.824	57.125	54.294	1.00	38.42	O
ATOM	3207	CB	ILE	E	239	26.092	54.681	55.193	1.00	38.58	C
ATOM	3208	CG1	ILE	E	239	26.076	53.795	53.943	1.00	39.13	C
ATOM	3209	CG2	ILE	E	239	25.170	55.878	55.040	1.00	38.48	C
ATOM	3210	CD1	ILE	E	239	25.932	52.306	54.266	1.00	39.58	C
ATOM	3211	N	TYR	E	240	29.197	55.408	53.809	1.00	38.40	N
ATOM	3212	CA	TYR	E	240	29.839	56.076	52.680	1.00	38.60	C
ATOM	3213	C	TYR	E	240	29.442	55.372	51.385	1.00	39.16	C

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ATOM	3214	O	TYR	E	240	29.955	54.286	51.061	1.00	39.46	O
ATOM	3215	CB	TYR	E	240	31.361	56.082	52.855	1.00	38.73	C
ATOM	3216	CG	TYR	E	240	32.118	57.015	51.922	1.00	39.35	C
ATOM	3217	CD1	TYR	E	240	33.108	56.525	51.072	1.00	39.49	C
ATOM	3218	CD2	TYR	E	240	31.849	58.382	51.900	1.00	39.38	C
ATOM	3219	CE1	TYR	E	240	33.814	57.374	50.221	1.00	40.18	C
ATOM	3220	CE2	TYR	E	240	32.550	59.243	51.053	1.00	40.95	C
ATOM	3221	CZ	TYR	E	240	33.532	58.730	50.220	1.00	40.24	C
ATOM	3222	OH	TYR	E	240	34.215	59.571	49.381	1.00	39.90	O
ATOM	3223	N	SER	E	241	28.485	55.959	50.679	1.00	38.82	N
ATOM	3224	CA	SER	E	241	28.032	55.405	49.415	1.00	39.27	C
ATOM	3225	C	SER	E	241	28.930	55.896	48.281	1.00	39.60	C
ATOM	3226	O	SER	E	241	29.602	56.930	48.406	1.00	39.24	O
ATOM	3227	CB	SER	E	241	26.582	55.812	49.144	1.00	39.15	C
ATOM	3228	OG	SER	E	241	26.173	55.392	47.849	1.00	40.20	O
ATOM	3229	N	LYS	E	242	28.946	55.143	47.184	1.00	39.92	N
ATOM	3230	CA	LYS	E	242	29.570	55.596	45.948	1.00	40.16	C
ATOM	3231	C	LYS	E	242	28.991	56.953	45.539	1.00	40.78	C
ATOM	3232	O	LYS	E	242	29.710	57.821	45.040	1.00	41.00	O
ATOM	3233	CB	LYS	E	242	29.335	54.589	44.827	1.00	40.05	C
ATOM	3234	CG	LYS	E	242	30.166	53.325	44.929	1.00	38.71	C
ATOM	3235	CD	LYS	E	242	29.991	52.446	43.705	1.00	36.91	C
ATOM	3236	CE	LYS	E	242	31.151	51.458	43.589	1.00	36.88	C
ATOM	3237	NZ	LYS	E	242	30.934	50.470	42.495	1.00	35.52	N
ATOM	3238	N	PHE	E	243	27.691	57.127	45.753	1.00	41.28	N
ATOM	3239	CA	PHE	E	243	27.038	58.397	45.475	1.00	41.92	C
ATOM	3240	C	PHE	E	243	27.672	59.582	46.216	1.00	41.89	C
ATOM	3241	O	PHE	E	243	27.679	60.697	45.700	1.00	42.11	O
ATOM	3242	CB	PHE	E	243	25.540	58.338	45.775	1.00	42.09	C
ATOM	3243	CG	PHE	E	243	24.841	59.660	45.569	1.00	42.84	C
ATOM	3244	CD1	PHE	E	243	24.749	60.223	44.296	1.00	44.06	C
ATOM	3245	CD2	PHE	E	243	24.322	60.365	46.651	1.00	43.07	C
ATOM	3246	CE1	PHE	E	243	24.118	61.459	44.095	1.00	43.92	C
ATOM	3247	CE2	PHE	E	243	23.689	61.599	46.467	1.00	44.02	C
ATOM	3248	CZ	PHE	E	243	23.587	62.145	45.188	1.00	43.65	C
ATOM	3249	N	ASP	E	244	28.198	59.342	47.415	1.00	41.68	N
ATOM	3250	CA	ASP	E	244	28.841	60.402	48.197	1.00	41.74	C
ATOM	3251	C	ASP	E	244	30.184	60.820	47.594	1.00	41.93	C
ATOM	3252	O	ASP	E	244	30.737	61.864	47.952	1.00	41.38	O
ATOM	3253	CB	ASP	E	244	29.020	59.978	49.655	1.00	41.33	C
ATOM	3254	CG	ASP	E	244	27.698	59.655	50.341	1.00	41.50	C
ATOM	3255	OD1	ASP	E	244	26.753	60.482	50.255	1.00	40.44	O
ATOM	3256	OD2	ASP	E	244	27.611	58.575	50.982	1.00	39.50	O
ATOM	3257	N	VAL	E	245	30.688	59.994	46.677	1.00	42.25	N
ATOM	3258	CA	VAL	E	245	31.980	60.206	46.046	1.00	42.68	C
ATOM	3259	C	VAL	E	245	31.955	61.253	44.913	1.00	43.18	C
ATOM	3260	O	VAL	E	245	32.896	62.038	44.806	1.00	42.42	O
ATOM	3261	CB	VAL	E	245	32.620	58.866	45.569	1.00	42.74	C
ATOM	3262	CG1	VAL	E	245	33.963	59.103	44.937	1.00	42.60	C
ATOM	3263	CG2	VAL	E	245	32.769	57.894	46.741	1.00	42.54	C
ATOM	3264	N	ILE	E	246	30.909	61.286	44.079	1.00	44.17	N
ATOM	3265	CA	ILE	E	246	30.894	62.293	42.989	1.00	45.53	C
ATOM	3266	C	ILE	E	246	30.896	63.735	43.460	1.00	45.74	C
ATOM	3267	O	ILE	E	246	31.185	64.627	42.673	1.00	45.89	O
ATOM	3268	CB	ILE	E	246	29.757	62.154	41.932	1.00	45.67	C
ATOM	3269	CG1	ILE	E	246	28.540	61.442	42.502	1.00	46.07	C
ATOM	3270	CG2	ILE	E	246	30.303	61.610	40.603	1.00	46.32	C
ATOM	3271	CD1	ILE	E	246	27.557	62.395	43.131	1.00	45.87	C
ATOM	3272	N	ASN	E	247	30.565	63.960	44.728	1.00	46.62	N
ATOM	3273	CA	ASN	E	247	30.782	65.260	45.352	1.00	47.63	C
ATOM	3274	C	ASN	E	247	32.197	65.773	45.041	1.00	47.99	C
ATOM	3275	O	ASN	E	247	32.385	66.954	44.761	1.00	47.61	O
ATOM	3276	CB	ASN	E	247	30.562	65.170	46.865	1.00	47.65	C
ATOM	3277	CG	ASN	E	247	30.823	66.482	47.568	1.00	49.13	C
ATOM	3278	OD1	ASN	E	247	31.935	66.738	48.040	1.00	50.60	O
ATOM	3279	ND2	ASN	E	247	29.804	67.339	47.621	1.00	49.61	N
ATOM	3280	N	LEU	E	248	33.172	64.861	45.061	1.00	48.51	N

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ATOM	3281	CA	LEU	E	248	34.574	65.179	44.768	1.00	49.41	C
ATOM	3282	C	LEU	E	248	34.781	65.789	43.379	1.00	50.01	C
ATOM	3283	O	LEU	E	248	35.711	66.565	43.178	1.00	50.03	O
ATOM	3284	CB	LEU	E	248	35.458	63.932	44.933	1.00	49.25	C
ATOM	3285	CG	LEU	E	248	35.953	63.398	46.295	1.00	49.64	C
ATOM	3286	CD1	LEU	E	248	35.142	63.851	47.502	1.00	50.26	C
ATOM	3287	CD2	LEU	E	248	36.031	61.878	46.272	1.00	49.19	C
ATOM	3288	N	ALA	E	249	33.919	65.439	42.426	1.00	51.02	N
ATOM	3289	CA	ALA	E	249	34.024	65.969	41.061	1.00	52.19	C
ATOM	3290	C	ALA	E	249	33.701	67.467	40.974	1.00	53.13	C
ATOM	3291	O	ALA	E	249	34.087	68.135	40.006	1.00	53.18	O
ATOM	3292	CB	ALA	E	249	33.160	65.165	40.090	1.00	51.94	C
ATOM	3293	N	ALA	E	250	33.013	67.986	41.993	1.00	54.41	N
ATOM	3294	CA	ALA	E	250	32.682	69.413	42.078	1.00	55.82	C
ATOM	3295	C	ALA	E	250	33.901	70.292	42.390	1.00	56.71	C
ATOM	3296	O	ALA	E	250	33.955	71.450	41.968	1.00	56.93	O
ATOM	3297	CB	ALA	E	250	31.578	69.642	43.101	1.00	55.83	C
ATOM	3298	N	GLU	E	251	34.868	69.738	43.126	1.00	57.94	N
ATOM	3299	CA	GLU	E	251	36.113	70.447	43.454	1.00	59.12	C
ATOM	3300	C	GLU	E	251	37.031	70.524	42.227	1.00	59.51	C
ATOM	3301	O	GLU	E	251	37.068	69.597	41.413	1.00	59.70	O
ATOM	3302	CB	GLU	E	251	36.831	69.785	44.652	1.00	59.04	C
ATOM	3303	CG	GLU	E	251	37.680	68.544	44.312	1.00	59.84	C
ATOM	3304	CD	GLU	E	251	38.145	67.740	45.533	1.00	60.18	C
ATOM	3305	OE1	GLU	E	251	38.666	68.341	46.501	1.00	61.56	O
ATOM	3306	OE2	GLU	E	251	38.011	66.494	45.507	1.00	60.30	O
ATOM	3307	N	LYS	E	252	37.755	71.630	42.087	1.00	60.16	N
ATOM	3308	CA	LYS	E	252	38.709	71.786	40.984	1.00	60.69	C
ATOM	3309	C	LYS	E	252	40.059	71.109	41.248	1.00	60.95	C
ATOM	3310	O	LYS	E	252	40.856	70.925	40.323	1.00	61.08	O
ATOM	3311	CB	LYS	E	252	38.925	73.267	40.651	1.00	60.81	C
ATOM	3312	CG	LYS	E	252	38.147	73.766	39.430	1.00	61.22	C
ATOM	3313	CD	LYS	E	252	38.738	73.260	38.108	1.00	61.69	C
ATOM	3314	CE	LYS	E	252	39.989	74.033	37.703	1.00	62.33	C
ATOM	3315	NZ	LYS	E	252	40.453	73.671	36.333	1.00	62.42	N
ATOM	3316	N	THR	E	253	40.297	70.722	42.501	1.00	61.10	N
ATOM	3317	CA	THR	E	253	41.632	70.318	42.953	1.00	61.26	C
ATOM	3318	C	THR	E	253	41.914	68.808	42.940	1.00	61.28	C
ATOM	3319	O	THR	E	253	43.024	68.394	42.590	1.00	61.44	O
ATOM	3320	CB	THR	E	253	41.981	70.937	44.347	1.00	61.36	C
ATOM	3321	OG1	THR	E	253	43.249	70.445	44.799	1.00	61.54	O
ATOM	3322	CG2	THR	E	253	40.905	70.625	45.394	1.00	61.26	C
ATOM	3323	N	TYR	E	254	40.917	68.005	43.320	1.00	61.01	N
ATOM	3324	CA	TYR	E	254	41.058	66.545	43.493	1.00	60.86	C
ATOM	3325	C	TYR	E	254	42.087	66.113	44.545	1.00	60.39	C
ATOM	3326	O	TYR	E	254	42.143	64.939	44.912	1.00	60.55	O
ATOM	3327	CB	TYR	E	254	41.359	65.834	42.162	1.00	61.11	C
ATOM	3328	CG	TYR	E	254	40.163	65.622	41.259	1.00	61.38	C
ATOM	3329	CD1	TYR	E	254	40.221	65.977	39.914	1.00	61.99	C
ATOM	3330	CD2	TYR	E	254	38.978	65.071	41.743	1.00	61.83	C
ATOM	3331	CE1	TYR	E	254	39.135	65.786	39.074	1.00	61.92	C
ATOM	3332	CE2	TYR	E	254	37.882	64.878	40.906	1.00	61.95	C
ATOM	3333	CZ	TYR	E	254	37.974	65.238	39.571	1.00	61.45	C
ATOM	3334	OH	TYR	E	254	36.910	65.055	38.726	1.00	61.26	O
ATOM	3335	N	ASN	E	255	42.889	67.060	45.026	1.00	59.70	N
ATOM	3336	CA	ASN	E	255	43.986	66.766	45.951	1.00	58.89	C
ATOM	3337	C	ASN	E	255	43.543	66.444	47.385	1.00	58.15	C
ATOM	3338	O	ASN	E	255	44.360	66.028	48.212	1.00	58.45	O
ATOM	3339	CB	ASN	E	255	45.009	67.914	45.950	1.00	58.87	C
ATOM	3340	CG	ASN	E	255	45.545	68.237	44.553	1.00	59.12	C
ATOM	3341	OD1	ASN	E	255	45.856	69.393	44.249	1.00	59.43	O
ATOM	3342	ND2	ASN	E	255	45.658	67.218	43.702	1.00	58.87	N
ATOM	3343	N	ASN	E	256	42.258	66.631	47.676	1.00	56.94	N
ATOM	3344	CA	ASN	E	256	41.724	66.365	49.010	1.00	55.96	C
ATOM	3345	C	ASN	E	256	41.177	64.940	49.176	1.00	54.93	C
ATOM	3346	O	ASN	E	256	40.058	64.751	49.663	1.00	54.94	O
ATOM	3347	CB	ASN	E	256	40.642	67.393	49.366	1.00	56.12	C

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ATOM	3348	CG	ASN	E	256	41.215	68.680	49.942	1.00	56.90	C
ATOM	3349	OD1	ASN	E	256	40.964	69.014	51.104	1.00	57.55	O
ATOM	3350	ND2	ASN	E	256	41.984	69.411	49.133	1.00	56.95	N
ATOM	3351	N	LEU	E	257	41.966	63.944	48.765	1.00	53.66	N
ATOM	3352	CA	LEU	E	257	41.586	62.526	48.908	1.00	52.14	C
ATOM	3353	C	LEU	E	257	42.259	61.895	50.120	1.00	51.23	C
ATOM	3354	O	LEU	E	257	42.150	60.688	50.355	1.00	50.96	O
ATOM	3355	CB	LEU	E	257	41.934	61.728	47.650	1.00	52.14	C
ATOM	3356	CG	LEU	E	257	41.280	62.110	46.322	1.00	52.13	C
ATOM	3357	CD1	LEU	E	257	41.806	61.217	45.214	1.00	52.44	C
ATOM	3358	CD2	LEU	E	257	39.760	62.042	46.388	1.00	52.13	C
ATOM	3359	N	ASP	E	258	42.957	62.724	50.885	1.00	50.10	N
ATOM	3360	CA	ASP	E	258	43.628	62.272	52.090	1.00	49.20	C
ATOM	3361	C	ASP	E	258	42.780	62.556	53.324	1.00	48.23	C
ATOM	3362	O	ASP	E	258	43.099	62.086	54.419	1.00	48.17	O
ATOM	3363	CB	ASP	E	258	45.017	62.908	52.199	1.00	49.55	C
ATOM	3364	CG	ASP	E	258	45.918	62.538	51.029	1.00	50.29	C
ATOM	3365	OD1	ASP	E	258	46.158	61.328	50.819	1.00	50.77	O
ATOM	3366	OD2	ASP	E	258	46.382	63.456	50.314	1.00	50.87	O
ATOM	3367	N	VAL	E	259	41.691	63.307	53.139	1.00	47.05	N
ATOM	3368	CA	VAL	E	259	40.739	63.570	54.221	1.00	46.05	C
ATOM	3369	C	VAL	E	259	40.013	62.291	54.622	1.00	45.60	C
ATOM	3370	O	VAL	E	259	39.898	61.356	53.825	1.00	45.49	O
ATOM	3371	CB	VAL	E	259	39.695	64.676	53.869	1.00	46.08	C
ATOM	3372	CG1	VAL	E	259	40.384	66.000	53.524	1.00	45.67	C
ATOM	3373	CG2	VAL	E	259	38.751	64.233	52.750	1.00	45.33	C
ATOM	3374	N	SER	E	260	39.531	62.255	55.861	1.00	44.99	N
ATOM	3375	CA	SER	E	260	38.770	61.114	56.351	1.00	44.50	C
ATOM	3376	C	SER	E	260	37.409	61.020	55.666	1.00	44.43	C
ATOM	3377	O	SER	E	260	36.876	62.013	55.152	1.00	44.15	O
ATOM	3378	CB	SER	E	260	38.592	61.186	57.871	1.00	44.57	C
ATOM	3379	OG	SER	E	260	37.629	62.160	58.238	1.00	44.01	O
ATOM	3380	N	VAL	E	261	36.858	59.813	55.658	1.00	44.14	N
ATOM	3381	CA	VAL	E	261	35.503	59.584	55.178	1.00	44.39	C
ATOM	3382	C	VAL	E	261	34.480	60.436	55.949	1.00	44.36	C
ATOM	3383	O	VAL	E	261	33.538	60.968	55.359	1.00	44.31	O
ATOM	3384	CB	VAL	E	261	35.157	58.074	55.215	1.00	44.10	C
ATOM	3385	CG1	VAL	E	261	33.668	57.852	55.351	1.00	44.57	C
ATOM	3386	CG2	VAL	E	261	35.686	57.401	53.962	1.00	44.10	C
ATOM	3387	N	THR	E	262	34.696	60.581	57.254	1.00	44.74	N
ATOM	3388	CA	THR	E	262	33.841	61.409	58.107	1.00	45.29	C
ATOM	3389	C	THR	E	262	33.853	62.872	57.655	1.00	45.54	C
ATOM	3390	O	THR	E	262	32.795	63.491	57.532	1.00	45.64	O
ATOM	3391	CB	THR	E	262	34.255	61.281	59.589	1.00	45.22	C
ATOM	3392	OG1	THR	E	262	34.112	59.914	59.991	1.00	46.20	O
ATOM	3393	CG2	THR	E	262	33.401	62.168	60.499	1.00	45.01	C
ATOM	3394	N	LYS	E	263	35.048	63.403	57.397	1.00	45.86	N
ATOM	3395	CA	LYS	E	263	35.210	64.759	56.872	1.00	46.45	C
ATOM	3396	C	LYS	E	263	34.568	64.906	55.490	1.00	46.63	C
ATOM	3397	O	LYS	E	263	33.931	65.920	55.202	1.00	46.38	O
ATOM	3398	CB	LYS	E	263	36.696	65.152	56.840	1.00	46.52	C
ATOM	3399	CG	LYS	E	263	36.959	66.627	56.561	1.00	47.42	C
ATOM	3400	CD	LYS	E	263	38.320	67.085	57.105	1.00	48.95	C
ATOM	3401	CE	LYS	E	263	38.807	68.349	56.394	1.00	49.52	C
ATOM	3402	NZ	LYS	E	263	40.151	68.819	56.852	1.00	50.29	N
ATOM	3403	N	ALA	E	264	34.724	63.881	54.650	1.00	47.19	N
ATOM	3404	CA	ALA	E	264	34.139	63.871	53.308	1.00	47.89	C
ATOM	3405	C	ALA	E	264	32.610	63.937	53.323	1.00	48.50	C
ATOM	3406	O	ALA	E	264	32.000	64.510	52.418	1.00	48.38	O
ATOM	3407	CB	ALA	E	264	34.608	62.650	52.530	1.00	47.75	C
ATOM	3408	N	LEU	E	265	32.002	63.359	54.356	1.00	49.43	N
ATOM	3409	CA	LEU	E	265	30.542	63.291	54.466	1.00	50.73	C
ATOM	3410	C	LEU	E	265	29.883	64.547	55.062	1.00	52.13	C
ATOM	3411	O	LEU	E	265	28.658	64.614	55.169	1.00	52.31	O
ATOM	3412	CB	LEU	E	265	30.119	62.034	55.235	1.00	50.23	C
ATOM	3413	CG	LEU	E	265	30.292	60.709	54.480	1.00	49.39	C
ATOM	3414	CD1	LEU	E	265	30.259	59.528	55.428	1.00	48.12	C

Figure 1 Table 1b - 52

ATOM	3415	CD2	LEU	E	265	29.245	60.555	53.388	1.00	47.64	C
ATOM	3416	N	GLN	E	266	30.692	65.533	55.449	1.00	53.69	N
ATOM	3417	CA	GLN	E	266	30.172	66.850	55.828	1.00	55.56	C
ATOM	3418	C	GLN	E	266	29.485	67.482	54.619	1.00	56.64	C
ATOM	3419	O	GLN	E	266	28.510	68.223	54.755	1.00	56.61	O
ATOM	3420	CB	GLN	E	266	31.298	67.759	56.322	1.00	55.33	C
ATOM	3421	CG	GLN	E	266	31.947	67.319	57.627	1.00	55.83	C
ATOM	3422	CD	GLN	E	266	33.078	68.244	58.081	1.00	56.28	C
ATOM	3423	OE1	GLN	E	266	33.828	67.909	59.002	1.00	56.96	O
ATOM	3424	NE2	GLN	E	266	33.203	69.410	57.439	1.00	56.68	N
ATOM	3425	N	HIS	E	267	30.005	67.157	53.437	1.00	58.40	N
ATOM	3426	CA	HIS	E	267	29.459	67.616	52.160	1.00	60.07	C
ATOM	3427	C	HIS	E	267	28.116	66.994	51.778	1.00	60.95	C
ATOM	3428	O	HIS	E	267	27.433	67.516	50.890	1.00	61.06	O
ATOM	3429	CB	HIS	E	267	30.476	67.391	51.035	1.00	60.22	C
ATOM	3430	CG	HIS	E	267	31.295	68.603	50.711	1.00	61.04	C
ATOM	3431	ND1	HIS	E	267	32.310	69.056	51.526	1.00	61.89	N
ATOM	3432	CD2	HIS	E	267	31.247	69.456	49.660	1.00	61.63	C
ATOM	3433	CE1	HIS	E	267	32.851	70.137	50.993	1.00	62.32	C
ATOM	3434	NE2	HIS	E	267	32.226	70.399	49.858	1.00	62.37	N
ATOM	3435	N	ARG	E	268	27.747	65.885	52.432	1.00	61.97	N
ATOM	3436	CA	ARG	E	268	26.460	65.217	52.179	1.00	62.79	C
ATOM	3437	C	ARG	E	268	25.299	66.159	52.479	1.00	63.56	C
ATOM	3438	O	ARG	E	268	24.812	66.234	53.612	1.00	63.88	O
ATOM	3439	CB	ARG	E	268	26.328	63.895	52.959	1.00	62.68	C
ATOM	3440	CG	ARG	E	268	24.995	63.151	52.730	1.00	62.47	C
ATOM	3441	CD	ARG	E	268	25.052	61.676	53.158	1.00	62.45	C
ATOM	3442	NE	ARG	E	268	25.576	61.517	54.510	1.00	60.81	N
ATOM	3443	CZ	ARG	E	268	25.969	60.368	55.044	1.00	59.69	C
ATOM	3444	NH1	ARG	E	268	25.904	59.238	54.356	1.00	58.26	N
ATOM	3445	NH2	ARG	E	268	26.433	60.361	56.283	1.00	59.88	N
ATOM	3446	N	SER	E	269	24.886	66.889	51.444	1.00	64.41	N
ATOM	3447	CA	SER	E	269	23.818	67.871	51.551	1.00	65.05	C
ATOM	3448	C	SER	E	269	22.493	67.178	51.832	1.00	65.49	C
ATOM	3449	O	SER	E	269	22.208	66.113	51.274	1.00	65.69	O
ATOM	3450	CB	SER	E	269	23.725	68.718	50.279	1.00	65.08	C
ATOM	3451	OG	SER	E	269	22.732	69.720	50.410	1.00	64.95	O
ATOM	3452	N	HIS	E	270	21.724	67.808	52.722	1.00	65.87	N
ATOM	3453	CA	HIS	E	270	20.417	67.368	53.239	1.00	66.18	C
ATOM	3454	C	HIS	E	270	20.496	67.510	54.757	1.00	65.89	C
ATOM	3455	O	HIS	E	270	21.079	68.471	55.278	1.00	66.02	O
ATOM	3456	CB	HIS	E	270	20.053	65.920	52.852	1.00	66.39	C
ATOM	3457	CG	HIS	E	270	19.367	65.797	51.524	1.00	67.64	C
ATOM	3458	ND1	HIS	E	270	18.475	66.738	51.052	1.00	68.80	N
ATOM	3459	CD2	HIS	E	270	19.434	64.833	50.573	1.00	68.60	C
ATOM	3460	CE1	HIS	E	270	18.032	66.365	49.863	1.00	69.07	C
ATOM	3461	NE2	HIS	E	270	18.597	65.212	49.550	1.00	69.25	N
ATOM	3462	N	TYR	E	271	19.888	66.566	55.461	1.00	65.39	N
ATOM	3463	CA	TYR	E	271	20.270	66.296	56.835	1.00	64.80	C
ATOM	3464	C	TYR	E	271	20.327	64.792	57.050	1.00	64.00	C
ATOM	3465	O	TYR	E	271	19.848	64.008	56.220	1.00	64.05	O
ATOM	3466	CB	TYR	E	271	19.359	66.992	57.855	1.00	65.17	C
ATOM	3467	CG	TYR	E	271	19.962	67.009	59.248	1.00	65.77	C
ATOM	3468	CD1	TYR	E	271	21.126	67.737	59.517	1.00	66.12	C
ATOM	3469	CD2	TYR	E	271	19.386	66.278	60.290	1.00	66.33	C
ATOM	3470	CE1	TYR	E	271	21.695	67.745	60.789	1.00	66.23	C
ATOM	3471	CE2	TYR	E	271	19.948	66.280	61.567	1.00	66.48	C
ATOM	3472	CZ	TYR	E	271	21.101	67.017	61.808	1.00	66.17	C
ATOM	3473	OH	TYR	E	271	21.657	67.025	63.066	1.00	66.01	O
ATOM	3474	N	PHE	E	272	20.939	64.396	58.156	1.00	62.83	N
ATOM	3475	CA	PHE	E	272	21.166	62.998	58.444	1.00	61.42	C
ATOM	3476	C	PHE	E	272	20.482	62.632	59.755	1.00	60.37	C
ATOM	3477	O	PHE	E	272	20.814	63.181	60.814	1.00	60.62	O
ATOM	3478	CB	PHE	E	272	22.681	62.747	58.524	1.00	61.60	C
ATOM	3479	CG	PHE	E	272	23.088	61.319	58.263	1.00	61.46	C
ATOM	3480	CD1	PHE	E	272	23.809	60.606	59.221	1.00	61.18	C
ATOM	3481	CD2	PHE	E	272	22.765	60.691	57.058	1.00	61.51	C

Figure 1 Table 1b - 53

ATOM	3482	CE1	PHE	E	272	24.191	59.285	58.991	1.00 61.43	C
ATOM	3483	CE2	PHE	E	272	23.144	59.370	56.816	1.00 61.42	C
ATOM	3484	CZ	PHE	E	272	23.859	58.666	57.787	1.00 61.24	C
ATOM	3485	N	GLU	E	273	19.497	61.739	59.681	1.00 58.68	N
ATOM	3486	CA	GLU	E	273	19.119	60.962	60.856	1.00 57.15	C
ATOM	3487	C	GLU	E	273	20.220	59.918	60.974	1.00 55.52	C
ATOM	3488	O	GLU	E	273	21.298	60.098	60.412	1.00 55.52	O
ATOM	3489	CB	GLU	E	273	17.738	60.317	60.699	1.00 57.52	C
ATOM	3490	CG	GLU	E	273	16.623	61.012	61.495	1.00 58.78	C
ATOM	3491	CD	GLU	E	273	16.691	60.743	63.003	1.00 60.44	C
ATOM	3492	OE1	GLU	E	273	16.567	59.566	63.414	1.00 61.12	O
ATOM	3493	OE2	GLU	E	273	16.853	61.712	63.781	1.00 60.85	O
ATOM	3494	N	GLY	E	274	19.983	58.826	61.683	1.00 53.50	N
ATOM	3495	CA	GLY	E	274	21.006	57.787	61.736	1.00 50.60	C
ATOM	3496	C	GLY	E	274	21.217	57.087	60.399	1.00 48.41	C
ATOM	3497	O	GLY	E	274	20.629	57.449	59.372	1.00 47.94	O
ATOM	3498	N	VAL	E	275	22.066	56.075	60.403	1.00 46.41	N
ATOM	3499	CA	VAL	E	275	22.079	55.168	59.274	1.00 44.35	C
ATOM	3500	C	VAL	E	275	20.815	54.307	59.333	1.00 43.27	C
ATOM	3501	O	VAL	E	275	20.325	53.966	60.418	1.00 42.87	O
ATOM	3502	CB	VAL	E	275	23.438	54.405	59.092	1.00 44.50	C
ATOM	3503	CG1	VAL	E	275	24.350	54.561	60.298	1.00 43.78	C
ATOM	3504	CG2	VAL	E	275	23.239	52.940	58.670	1.00 43.64	C
ATOM	3505	N	LEU	E	276	20.257	54.021	58.163	1.00 41.60	N
ATOM	3506	CA	LEU	E	276	19.059	53.210	58.064	1.00 40.38	C
ATOM	3507	C	LEU	E	276	19.443	51.742	58.156	1.00 39.53	C
ATOM	3508	O	LEU	E	276	20.216	51.224	57.339	1.00 38.83	O
ATOM	3509	CB	LEU	E	276	18.275	53.535	56.788	1.00 40.13	C
ATOM	3510	CG	LEU	E	276	17.685	54.957	56.804	1.00 41.68	C
ATOM	3511	CD1	LEU	E	276	17.623	55.548	55.415	1.00 42.01	C
ATOM	3512	CD2	LEU	E	276	16.309	54.994	57.486	1.00 42.54	C
ATOM	3513	N	LYS	E	277	18.904	51.087	59.180	1.00 38.80	N
ATOM	3514	CA	LYS	E	277	19.312	49.740	59.537	1.00 38.10	C
ATOM	3515	C	LYS	E	277	18.129	48.788	59.561	1.00 37.93	C
ATOM	3516	O	LYS	E	277	16.969	49.207	59.425	1.00 37.51	O
ATOM	3517	CB	LYS	E	277	19.948	49.745	60.925	1.00 38.07	C
ATOM	3518	CG	LYS	E	277	21.304	50.424	61.009	1.00 39.24	C
ATOM	3519	CD	LYS	E	277	21.651	50.763	62.456	1.00 41.03	C
ATOM	3520	CE	LYS	E	277	20.716	51.838	63.024	1.00 41.56	C
ATOM	3521	NZ	LYS	E	277	21.129	52.263	64.382	1.00 42.45	N
ATOM	3522	N	CYS	E	278	18.443	47.505	59.740	1.00 36.88	N
ATOM	3523	CA	CYS	E	278	17.444	46.494	60.001	1.00 36.77	C
ATOM	3524	C	CYS	E	278	18.033	45.348	60.829	1.00 36.17	C
ATOM	3525	O	CYS	E	278	19.248	45.213	60.964	1.00 35.81	O
ATOM	3526	CB	CYS	E	278	16.847	45.958	58.696	1.00 36.26	C
ATOM	3527	SG	CYS	E	278	17.972	44.995	57.727	1.00 38.49	S
ATOM	3528	N	TYR	E	279	17.149	44.534	61.382	1.00 36.25	N
ATOM	3529	CA	TYR	E	279	17.553	43.306	62.044	1.00 36.19	C
ATOM	3530	C	TYR	E	279	17.315	42.120	61.123	1.00 36.06	C
ATOM	3531	O	TYR	E	279	16.449	42.171	60.249	1.00 35.58	O
ATOM	3532	CB	TYR	E	279	16.781	43.129	63.342	1.00 36.61	C
ATOM	3533	CG	TYR	E	279	16.834	44.341	64.237	1.00 36.94	C
ATOM	3534	CD1	TYR	E	279	15.718	45.164	64.389	1.00 36.91	C
ATOM	3535	CD2	TYR	E	279	17.997	44.671	64.921	1.00 37.68	C
ATOM	3536	CE1	TYR	E	279	15.756	46.275	65.222	1.00 37.90	C
ATOM	3537	CE2	TYR	E	279	18.046	45.781	65.757	1.00 38.08	C
ATOM	3538	CZ	TYR	E	279	16.924	46.574	65.898	1.00 38.12	C
ATOM	3539	OH	TYR	E	279	16.963	47.674	66.721	1.00 39.79	O
ATOM	3540	N	LEU	E	280	18.102	41.066	61.338	1.00 36.23	N
ATOM	3541	CA	LEU	E	280	18.006	39.793	60.613	1.00 36.53	C
ATOM	3542	C	LEU	E	280	16.622	39.175	60.680	1.00 35.89	C
ATOM	3543	O	LEU	E	280	16.240	38.395	59.807	1.00 36.04	O
ATOM	3544	CB	LEU	E	280	18.978	38.774	61.227	1.00 37.21	C
ATOM	3545	CG	LEU	E	280	20.391	38.574	60.676	1.00 38.83	C
ATOM	3546	CD1	LEU	E	280	21.098	37.571	61.570	1.00 40.80	C
ATOM	3547	CD2	LEU	E	280	20.325	38.051	59.265	1.00 40.28	C
ATOM	3548	N	HIS	E	281	15.880	39.503	61.732	1.00 34.77	N

Figure 1 Table 1b - 54

ATOM	3549	CA	HIS	E	281	14.632	38.817	61.991	1.00	34.28	C
ATOM	3550	C	HIS	E	281	13.403	39.607	61.573	1.00	33.89	C
ATOM	3551	O	HIS	E	281	12.286	39.210	61.873	1.00	33.43	O
ATOM	3552	CB	HIS	E	281	14.554	38.395	63.460	1.00	34.26	C
ATOM	3553	CG	HIS	E	281	15.698	37.534	63.884	1.00	34.98	C
ATOM	3554	ND1	HIS	E	281	15.824	36.221	63.487	1.00	35.55	N
ATOM	3555	CD2	HIS	E	281	16.780	37.803	64.651	1.00	34.64	C
ATOM	3556	CE1	HIS	E	281	16.934	35.716	63.994	1.00	35.08	C
ATOM	3557	NE2	HIS	E	281	17.531	36.655	64.707	1.00	35.70	N
ATOM	3558	N	GLU	E	282	13.609	40.716	60.870	1.00	33.67	N
ATOM	3559	CA	GLU	E	282	12.476	41.467	60.326	1.00	33.97	C
ATOM	3560	C	GLU	E	282	11.951	40.776	59.066	1.00	34.22	C
ATOM	3561	O	GLU	E	282	12.708	40.090	58.367	1.00	34.47	O
ATOM	3562	CB	GLU	E	282	12.867	42.924	60.043	1.00	33.42	C
ATOM	3563	CG	GLU	E	282	13.419	43.631	61.264	1.00	33.51	C
ATOM	3564	CD	GLU	E	282	13.384	45.144	61.126	1.00	34.87	C
ATOM	3565	OE1	GLU	E	282	12.292	45.732	61.230	1.00	33.83	O
ATOM	3566	OE2	GLU	E	282	14.457	45.732	60.939	1.00	35.24	O
ATOM	3567	N	THR	E	283	10.660	40.950	58.789	1.00	34.28	N
ATOM	3568	CA	THR	E	283	10.024	40.339	57.621	1.00	34.99	C
ATOM	3569	C	THR	E	283	10.471	41.018	56.330	1.00	35.56	C
ATOM	3570	O	THR	E	283	10.904	42.181	56.348	1.00	35.14	O
ATOM	3571	CB	THR	E	283	8.491	40.414	57.700	1.00	34.96	C
ATOM	3572	OG1	THR	E	283	8.081	41.786	57.747	1.00	36.34	O
ATOM	3573	CG2	THR	E	283	7.969	39.676	58.938	1.00	34.39	C
ATOM	3574	N	LEU	E	284	10.363	40.293	55.217	1.00	35.59	N
ATOM	3575	CA	LEU	E	284	10.687	40.845	53.915	1.00	36.48	C
ATOM	3576	C	LEU	E	284	9.821	42.076	53.665	1.00	36.00	C
ATOM	3577	O	LEU	E	284	10.308	43.083	53.148	1.00	36.16	O
ATOM	3578	CB	LEU	E	284	10.449	39.810	52.806	1.00	36.78	C
ATOM	3579	CG	LEU	E	284	11.421	39.737	51.608	1.00	39.06	C
ATOM	3580	CD1	LEU	E	284	10.771	39.076	50.352	1.00	38.39	C
ATOM	3581	CD2	LEU	E	284	12.110	41.059	51.259	1.00	34.72	C
ATOM	3582	N	GLU	E	285	8.544	41.983	54.031	1.00	35.78	N
ATOM	3583	CA	GLU	E	285	7.609	43.103	53.902	1.00	36.45	C
ATOM	3584	C	GLU	E	285	8.094	44.372	54.610	1.00	36.12	C
ATOM	3585	O	GLU	E	285	8.142	45.446	54.004	1.00	36.39	O
ATOM	3586	CB	GLU	E	285	6.221	42.702	54.417	1.00	36.58	C
ATOM	3587	CG	GLU	E	285	5.171	43.793	54.249	1.00	38.04	C
ATOM	3588	CD	GLU	E	285	3.760	43.298	54.452	1.00	40.73	C
ATOM	3589	OE1	GLU	E	285	3.557	42.306	55.182	1.00	43.34	O
ATOM	3590	OE2	GLU	E	285	2.836	43.897	53.871	1.00	43.11	O
ATOM	3591	N	ALA	E	286	8.464	44.237	55.883	1.00	35.92	N
ATOM	3592	CA	ALA	E	286	8.960	45.358	56.673	1.00	35.49	C
ATOM	3593	C	ALA	E	286	10.182	46.002	56.011	1.00	35.37	C
ATOM	3594	O	ALA	E	286	10.293	47.232	55.954	1.00	34.80	O
ATOM	3595	CB	ALA	E	286	9.293	44.909	58.094	1.00	35.49	C
ATOM	3596	N	ILE	E	287	11.078	45.165	55.495	1.00	34.65	N
ATOM	3597	CA	ILE	E	287	12.307	45.633	54.863	1.00	35.20	C
ATOM	3598	C	ILE	E	287	12.054	46.318	53.515	1.00	34.78	C
ATOM	3599	O	ILE	E	287	12.644	47.354	53.240	1.00	34.56	O
ATOM	3600	CB	ILE	E	287	13.371	44.504	54.744	1.00	35.44	C
ATOM	3601	CG1	ILE	E	287	14.069	44.302	56.093	1.00	36.98	C
ATOM	3602	CG2	ILE	E	287	14.429	44.836	53.724	1.00	34.99	C
ATOM	3603	CD1	ILE	E	287	13.743	43.027	56.710	1.00	42.33	C
ATOM	3604	N	ILE	E	288	11.194	45.731	52.684	1.00	34.46	N
ATOM	3605	CA	ILE	E	288	10.800	46.367	51.432	1.00	34.35	C
ATOM	3606	C	ILE	E	288	10.165	47.737	51.733	1.00	34.00	C
ATOM	3607	O	ILE	E	288	10.517	48.742	51.102	1.00	33.99	O
ATOM	3608	CB	ILE	E	288	9.824	45.497	50.591	1.00	34.04	C
ATOM	3609	CG1	ILE	E	288	10.547	44.283	49.976	1.00	35.70	C
ATOM	3610	CG2	ILE	E	288	9.135	46.361	49.496	1.00	35.13	C
ATOM	3611	CD1	ILE	E	288	9.594	43.177	49.448	1.00	33.98	C
ATOM	3612	N	ASN	E	289	9.241	47.773	52.692	1.00	33.84	N
ATOM	3613	CA	ASN	E	289	8.579	49.032	53.057	1.00	34.24	C
ATOM	3614	C	ASN	E	289	9.584	50.092	53.491	1.00	34.21	C
ATOM	3615	O	ASN	E	289	9.525	51.234	53.007	1.00	34.93	O

Figure 1 Table 1b - 55

ATOM	3616	CB	ASN	E	289	7.478	48.836	54.119	1.00	34.23	C
ATOM	3617	CG	ASN	E	289	6.301	48.028	53.600	1.00	34.71	C
ATOM	3618	OD1	ASN	E	289	6.195	47.770	52.407	1.00	36.63	O
ATOM	3619	ND2	ASN	E	289	5.413	47.620	54.494	1.00	35.75	N
ATOM	3620	N	ARG	E	290	10.515	49.712	54.366	1.00	34.10	N
ATOM	3621	CA	ARG	E	290	11.551	50.634	54.860	1.00	34.99	C
ATOM	3622	C	ARG	E	290	12.420	51.189	53.725	1.00	34.75	C
ATOM	3623	O	ARG	E	290	12.639	52.391	53.639	1.00	33.92	O
ATOM	3624	CB	ARG	E	290	12.434	49.967	55.933	1.00	34.74	C
ATOM	3625	CG	ARG	E	290	13.401	50.938	56.632	1.00	36.42	C
ATOM	3626	CD	ARG	E	290	13.997	50.354	57.936	1.00	35.78	C
ATOM	3627	NE	ARG	E	290	12.957	49.744	58.756	1.00	35.34	N
ATOM	3628	CZ	ARG	E	290	13.119	48.628	59.464	1.00	35.88	C
ATOM	3629	NH1	ARG	E	290	14.295	48.008	59.490	1.00	35.03	N
ATOM	3630	NH2	ARG	E	290	12.098	48.132	60.146	1.00	35.72	N
ATOM	3631	N	LEU	E	291	12.896	50.298	52.856	1.00	34.37	N
ATOM	3632	CA	LEU	E	291	13.719	50.676	51.701	1.00	34.52	C
ATOM	3633	C	LEU	E	291	13.027	51.628	50.716	1.00	33.84	C
ATOM	3634	O	LEU	E	291	13.640	52.586	50.235	1.00	33.32	O
ATOM	3635	CB	LEU	E	291	14.136	49.403	50.968	1.00	35.12	C
ATOM	3636	CG	LEU	E	291	15.560	48.854	50.904	1.00	37.12	C
ATOM	3637	CD1	LEU	E	291	16.656	49.660	51.592	1.00	38.11	C
ATOM	3638	CD2	LEU	E	291	15.536	47.432	51.346	1.00	38.21	C
ATOM	3639	N	VAL	E	292	11.762	51.353	50.405	1.00	33.67	N
ATOM	3640	CA	VAL	E	292	10.998	52.170	49.459	1.00	33.52	C
ATOM	3641	C	VAL	E	292	10.725	53.574	50.035	1.00	34.44	C
ATOM	3642	O	VAL	E	292	10.881	54.563	49.328	1.00	34.17	O
ATOM	3643	CB	VAL	E	292	9.672	51.483	49.007	1.00	33.43	C
ATOM	3644	CG1	VAL	E	292	8.794	52.433	48.189	1.00	32.00	C
ATOM	3645	CG2	VAL	E	292	9.954	50.220	48.191	1.00	31.85	C
ATOM	3646	N	GLU	E	293	10.329	53.651	51.306	1.00	35.57	N
ATOM	3647	CA	GLU	E	293	10.093	54.946	51.964	1.00	37.11	C
ATOM	3648	C	GLU	E	293	11.377	55.753	52.008	1.00	36.90	C
ATOM	3649	O	GLU	E	293	11.376	56.918	51.646	1.00	36.65	O
ATOM	3650	CB	GLU	E	293	9.524	54.786	53.380	1.00	38.14	C
ATOM	3651	CG	GLU	E	293	8.267	53.928	53.445	1.00	42.80	C
ATOM	3652	CD	GLU	E	293	7.369	54.234	54.637	1.00	48.61	C
ATOM	3653	OE1	GLU	E	293	7.196	55.427	54.977	1.00	50.86	O
ATOM	3654	OE2	GLU	E	293	6.811	53.269	55.217	1.00	51.53	O
ATOM	3655	N	ALA	E	294	12.480	55.115	52.396	1.00	36.50	N
ATOM	3656	CA	ALA	E	294	13.761	55.820	52.530	1.00	36.55	C
ATOM	3657	C	ALA	E	294	14.465	56.221	51.216	1.00	36.43	C
ATOM	3658	O	ALA	E	294	15.323	57.105	51.232	1.00	35.60	O
ATOM	3659	CB	ALA	E	294	14.709	55.026	53.406	1.00	36.62	C
ATOM	3660	N	GLU	E	295	14.123	55.553	50.107	1.00	36.26	N
ATOM	3661	CA	GLU	E	295	14.717	55.813	48.777	1.00	36.63	C
ATOM	3662	C	GLU	E	295	16.231	55.583	48.760	1.00	36.26	C
ATOM	3663	O	GLU	E	295	17.011	56.314	48.161	1.00	36.93	O
ATOM	3664	CB	GLU	E	295	14.334	57.209	48.256	1.00	36.86	C
ATOM	3665	CG	GLU	E	295	12.839	57.465	48.271	1.00	38.63	C
ATOM	3666	CD	GLU	E	295	12.462	58.741	47.545	1.00	42.96	C
ATOM	3667	OE1	GLU	E	295	11.990	59.684	48.211	1.00	44.01	O
ATOM	3668	OE2	GLU	E	295	12.661	58.807	46.312	1.00	44.84	O
ATOM	3669	N	VAL	E	296	16.621	54.508	49.407	1.00	36.16	N
ATOM	3670	CA	VAL	E	296	17.999	54.213	49.696	1.00	35.70	C
ATOM	3671	C	VAL	E	296	18.244	52.825	49.071	1.00	34.93	C
ATOM	3672	O	VAL	E	296	17.300	52.044	48.927	1.00	33.72	O
ATOM	3673	CB	VAL	E	296	18.171	54.371	51.262	1.00	36.58	C
ATOM	3674	CG1	VAL	E	296	18.494	53.091	51.980	1.00	35.83	C
ATOM	3675	CG2	VAL	E	296	19.066	55.540	51.632	1.00	36.27	C
ATOM	3676	N	HIS	E	297	19.479	52.548	48.643	1.00	34.49	N
ATOM	3677	CA	HIS	E	297	19.793	51.305	47.912	1.00	33.80	C
ATOM	3678	C	HIS	E	297	20.028	50.072	48.818	1.00	33.47	C
ATOM	3679	O	HIS	E	297	19.852	48.944	48.373	1.00	33.31	O
ATOM	3680	CB	HIS	E	297	20.964	51.542	46.934	1.00	34.19	C
ATOM	3681	CG	HIS	E	297	21.299	50.361	46.067	1.00	34.99	C
ATOM	3682	ND1	HIS	E	297	20.598	50.046	44.922	1.00	34.54	N

Figure 1 Table 1b - 56

ATOM	3683	CD2	HIS	E	297	22.274	49.425	46.177	1.00	36.40	C
ATOM	3684	CE1	HIS	E	297	21.112	48.961	44.372	1.00	35.87	C
ATOM	3685	NE2	HIS	E	297	22.129	48.562	45.115	1.00	36.72	N
ATOM	3686	N	ARG	E	298	20.428	50.289	50.070	1.00	33.41	N
ATOM	3687	CA	ARG	E	298	20.589	49.190	51.055	1.00	33.18	C
ATOM	3688	C	ARG	E	298	20.304	49.636	52.489	1.00	33.84	C
ATOM	3689	O	ARG	E	298	20.329	50.851	52.803	1.00	33.39	O
ATOM	3690	CB	ARG	E	298	21.992	48.542	50.981	1.00	33.41	C
ATOM	3691	CG	ARG	E	298	23.086	49.113	51.929	1.00	32.61	C
ATOM	3692	CD	ARG	E	298	23.477	50.575	51.587	1.00	33.22	C
ATOM	3693	NE	ARG	E	298	23.887	50.729	50.188	1.00	33.02	N
ATOM	3694	CZ	ARG	E	298	23.685	51.822	49.449	1.00	32.53	C
ATOM	3695	NH1	ARG	E	298	23.056	52.873	49.955	1.00	31.28	N
ATOM	3696	NH2	ARG	E	298	24.105	51.858	48.197	1.00	30.82	N
ATOM	3697	N	LEU	E	299	20.027	48.642	53.340	1.00	34.05	N
ATOM	3698	CA	LEU	E	299	20.016	48.807	54.788	1.00	34.19	C
ATOM	3699	C	LEU	E	299	21.203	48.046	55.352	1.00	34.44	C
ATOM	3700	O	LEU	E	299	21.642	47.046	54.773	1.00	33.82	O
ATOM	3701	CB	LEU	E	299	18.717	48.253	55.396	1.00	34.19	C
ATOM	3702	CG	LEU	E	299	17.381	48.777	54.869	1.00	34.58	C
ATOM	3703	CD1	LEU	E	299	16.209	47.985	55.459	1.00	34.92	C
ATOM	3704	CD2	LEU	E	299	17.203	50.292	55.130	1.00	35.49	C
ATOM	3705	N	VAL	E	300	21.748	48.533	56.460	1.00	34.05	N
ATOM	3706	CA	VAL	E	300	22.800	47.802	57.145	1.00	34.63	C
ATOM	3707	C	VAL	E	300	22.124	46.877	58.155	1.00	34.73	C
ATOM	3708	O	VAL	E	300	21.340	47.330	58.988	1.00	35.08	O
ATOM	3709	CB	VAL	E	300	23.802	48.737	57.876	1.00	34.61	C
ATOM	3710	CG1	VAL	E	300	24.907	47.918	58.534	1.00	34.19	C
ATOM	3711	CG2	VAL	E	300	24.400	49.769	56.905	1.00	34.34	C
ATOM	3712	N	VAL	E	301	22.425	45.589	58.061	1.00	35.11	N
ATOM	3713	CA	VAL	E	301	21.926	44.594	59.012	1.00	35.07	C
ATOM	3714	C	VAL	E	301	22.814	44.611	60.242	1.00	35.93	C
ATOM	3715	O	VAL	E	301	24.044	44.498	60.167	1.00	35.79	O
ATOM	3716	CB	VAL	E	301	21.868	43.171	58.415	1.00	34.95	C
ATOM	3717	CG1	VAL	E	301	21.086	42.227	59.338	1.00	34.33	C
ATOM	3718	CG2	VAL	E	301	21.243	43.200	57.024	1.00	33.91	C
ATOM	3719	N	VAL	E	302	22.156	44.732	61.382	1.00	36.78	N
ATOM	3720	CA	VAL	E	302	22.801	45.054	62.626	1.00	37.65	C
ATOM	3721	C	VAL	E	302	22.228	44.127	63.704	1.00	38.56	C
ATOM	3722	O	VAL	E	302	21.095	43.660	63.584	1.00	38.43	O
ATOM	3723	CB	VAL	E	302	22.572	46.575	62.880	1.00	37.79	C
ATOM	3724	CG1	VAL	E	302	22.032	46.884	64.244	1.00	37.85	C
ATOM	3725	CG2	VAL	E	302	23.821	47.392	62.504	1.00	37.05	C
ATOM	3726	N	ASP	E	303	23.016	43.827	64.729	1.00	39.78	N
ATOM	3727	CA	ASP	E	303	22.482	43.105	65.875	1.00	41.21	C
ATOM	3728	C	ASP	E	303	21.846	44.067	66.885	1.00	42.21	C
ATOM	3729	O	ASP	E	303	21.713	45.274	66.623	1.00	42.24	O
ATOM	3730	CB	ASP	E	303	23.547	42.207	66.529	1.00	41.09	C
ATOM	3731	CG	ASP	E	303	24.614	42.990	67.306	1.00	41.54	C
ATOM	3732	OD1	ASP	E	303	24.592	44.238	67.352	1.00	41.36	O
ATOM	3733	OD2	ASP	E	303	25.493	42.327	67.884	1.00	42.34	O
ATOM	3734	N	GLU	E	304	21.466	43.511	68.030	1.00	43.11	N
ATOM	3735	CA	GLU	E	304	20.907	44.239	69.164	1.00	44.53	C
ATOM	3736	C	GLU	E	304	21.709	45.487	69.578	1.00	44.44	C
ATOM	3737	O	GLU	E	304	21.143	46.429	70.141	1.00	44.80	O
ATOM	3738	CB	GLU	E	304	20.801	43.288	70.369	1.00	44.59	C
ATOM	3739	CG	GLU	E	304	19.625	42.295	70.341	1.00	47.56	C
ATOM	3740	CD	GLU	E	304	19.839	41.035	69.475	1.00	50.46	C
ATOM	3741	OE1	GLU	E	304	20.698	41.035	68.557	1.00	50.78	O
ATOM	3742	OE2	GLU	E	304	19.112	40.036	69.713	1.00	50.98	O
ATOM	3743	N	HIS	E	305	23.017	45.480	69.311	1.00	44.28	N
ATOM	3744	CA	HIS	E	305	23.926	46.524	69.803	1.00	44.00	C
ATOM	3745	C	HIS	E	305	24.514	47.441	68.715	1.00	43.59	C
ATOM	3746	O	HIS	E	305	25.475	48.171	68.971	1.00	43.29	O
ATOM	3747	CB	HIS	E	305	25.062	45.887	70.607	1.00	44.25	C
ATOM	3748	CG	HIS	E	305	24.594	44.967	71.695	1.00	45.37	C
ATOM	3749	ND1	HIS	E	305	24.019	45.423	72.862	1.00	45.97	N

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ATOM	3750	CD2	HIS	E	305	24.622	43.616	71.793	1.00	46.22	C
ATOM	3751	CE1	HIS	E	305	23.710	44.392	73.630	1.00	46.82	C
ATOM	3752	NE2	HIS	E	305	24.065	43.285	73.004	1.00	46.45	N
ATOM	3753	N	ASP	E	306	23.933	47.409	67.517	1.00	42.93	N
ATOM	3754	CA	ASP	E	306	24.416	48.200	66.359	1.00	42.72	C
ATOM	3755	C	ASP	E	306	25.679	47.654	65.686	1.00	41.70	C
ATOM	3756	O	ASP	E	306	26.212	48.285	64.766	1.00	41.27	O
ATOM	3757	CB	ASP	E	306	24.604	49.685	66.701	1.00	43.10	C
ATOM	3758	CG	ASP	E	306	23.316	50.475	66.620	1.00	45.09	C
ATOM	3759	OD1	ASP	E	306	22.266	49.897	66.249	1.00	46.74	O
ATOM	3760	OD2	ASP	E	306	23.361	51.689	66.936	1.00	47.82	O
ATOM	3761	N	VAL	E	307	26.154	46.493	66.135	1.00	40.72	N
ATOM	3762	CA	VAL	E	307	27.267	45.820	65.459	1.00	40.11	C
ATOM	3763	C	VAL	E	307	26.781	45.321	64.094	1.00	39.47	C
ATOM	3764	O	VAL	E	307	25.758	44.635	64.014	1.00	38.97	O
ATOM	3765	CB	VAL	E	307	27.829	44.641	66.300	1.00	40.02	C
ATOM	3766	CG1	VAL	E	307	28.913	43.876	65.529	1.00	39.72	C
ATOM	3767	CG2	VAL	E	307	28.374	45.143	67.638	1.00	40.49	C
ATOM	3768	N	VAL	E	308	27.492	45.679	63.023	1.00	39.00	N
ATOM	3769	CA	VAL	E	308	27.078	45.233	61.685	1.00	38.71	C
ATOM	3770	C	VAL	E	308	27.264	43.724	61.445	1.00	38.48	C
ATOM	3771	O	VAL	E	308	28.321	43.151	61.715	1.00	37.97	O
ATOM	3772	CB	VAL	E	308	27.586	46.145	60.492	1.00	39.02	C
ATOM	3773	CG1	VAL	E	308	28.641	47.152	60.924	1.00	39.52	C
ATOM	3774	CG2	VAL	E	308	28.017	45.329	59.273	1.00	38.02	C
ATOM	3775	N	LYS	E	309	26.192	43.106	60.953	1.00	38.51	N
ATOM	3776	CA	LYS	E	309	26.125	41.667	60.705	1.00	38.11	C
ATOM	3777	C	LYS	E	309	26.074	41.387	59.211	1.00	37.82	C
ATOM	3778	O	LYS	E	309	26.453	40.308	58.768	1.00	38.45	O
ATOM	3779	CB	LYS	E	309	24.867	41.081	61.351	1.00	38.55	C
ATOM	3780	CG	LYS	E	309	24.716	41.318	62.858	1.00	39.69	C
ATOM	3781	CD	LYS	E	309	25.515	40.318	63.691	1.00	43.84	C
ATOM	3782	CE	LYS	E	309	26.858	40.880	64.122	1.00	44.51	C
ATOM	3783	NZ	LYS	E	309	27.394	40.148	65.302	1.00	44.70	N
ATOM	3784	N	GLY	E	310	25.579	42.351	58.437	1.00	36.78	N
ATOM	3785	CA	GLY	E	310	25.489	42.197	56.996	1.00	35.87	C
ATOM	3786	C	GLY	E	310	24.884	43.386	56.280	1.00	35.72	C
ATOM	3787	O	GLY	E	310	24.753	44.479	56.848	1.00	35.28	O
ATOM	3788	N	ILE	E	311	24.531	43.167	55.019	1.00	35.51	N
ATOM	3789	CA	ILE	E	311	23.862	44.174	54.195	1.00	35.33	C
ATOM	3790	C	ILE	E	311	22.679	43.559	53.466	1.00	35.03	C
ATOM	3791	O	ILE	E	311	22.768	42.433	52.956	1.00	34.64	O
ATOM	3792	CB	ILE	E	311	24.846	44.859	53.177	1.00	35.79	C
ATOM	3793	CG1	ILE	E	311	25.554	46.032	53.851	1.00	36.63	C
ATOM	3794	CG2	ILE	E	311	24.106	45.439	51.942	1.00	35.04	C
ATOM	3795	CD1	ILE	E	311	26.952	45.748	54.144	1.00	40.36	C
ATOM	3796	N	VAL	E	312	21.571	44.293	53.420	1.00	34.12	N
ATOM	3797	CA	VAL	E	312	20.475	43.908	52.538	1.00	34.00	C
ATOM	3798	C	VAL	E	312	20.247	45.021	51.517	1.00	34.04	C
ATOM	3799	O	VAL	E	312	19.781	46.123	51.844	1.00	33.37	O
ATOM	3800	CB	VAL	E	312	19.165	43.477	53.282	1.00	34.37	C
ATOM	3801	CG1	VAL	E	312	18.625	44.605	54.165	1.00	34.07	C
ATOM	3802	CG2	VAL	E	312	18.098	43.011	52.272	1.00	34.20	C
ATOM	3803	N	SER	E	313	20.607	44.701	50.281	1.00	33.30	N
ATOM	3804	CA	SER	E	313	20.594	45.641	49.187	1.00	33.93	C
ATOM	3805	C	SER	E	313	19.378	45.403	48.308	1.00	33.64	C
ATOM	3806	O	SER	E	313	18.788	44.318	48.339	1.00	32.69	O
ATOM	3807	CB	SER	E	313	21.873	45.453	48.382	1.00	33.33	C
ATOM	3808	OG	SER	E	313	21.799	46.157	47.169	1.00	36.64	O
ATOM	3809	N	LEU	E	314	19.020	46.416	47.510	1.00	33.28	N
ATOM	3810	CA	LEU	E	314	17.979	46.271	46.493	1.00	33.33	C
ATOM	3811	C	LEU	E	314	18.331	45.194	45.471	1.00	33.15	C
ATOM	3812	O	LEU	E	314	17.436	44.561	44.897	1.00	33.07	O
ATOM	3813	CB	LEU	E	314	17.723	47.594	45.748	1.00	32.95	C
ATOM	3814	CG	LEU	E	314	17.174	48.790	46.521	1.00	33.41	C
ATOM	3815	CD1	LEU	E	314	17.027	49.996	45.568	1.00	30.31	C
ATOM	3816	CD2	LEU	E	314	15.854	48.466	47.170	1.00	32.71	C

Figure 1 Table 1b - 58

ATOM	3817	N	SER	E	315	19.625	45.016	45.226	1.00	32.88	N
ATOM	3818	CA	SER	E	315	20.108	43.917	44.402	1.00	33.79	C
ATOM	3819	C	SER	E	315	19.679	42.557	44.996	1.00	34.28	C
ATOM	3820	O	SER	E	315	19.260	41.648	44.266	1.00	34.32	O
ATOM	3821	CB	SER	E	315	21.634	43.982	44.285	1.00	33.69	C
ATOM	3822	OG	SER	E	315	22.043	45.180	43.632	1.00	34.25	O
ATOM	3823	N	ASP	E	316	19.768	42.441	46.318	1.00	34.40	N
ATOM	3824	CA	ASP	E	316	19.401	41.206	47.018	1.00	35.37	C
ATOM	3825	C	ASP	E	316	17.905	40.965	46.907	1.00	35.62	C
ATOM	3826	O	ASP	E	316	17.473	39.867	46.563	1.00	35.57	O
ATOM	3827	CB	ASP	E	316	19.799	41.288	48.488	1.00	35.12	C
ATOM	3828	CG	ASP	E	316	21.288	41.349	48.679	1.00	35.39	C
ATOM	3829	OD1	ASP	E	316	21.985	40.514	48.069	1.00	37.01	O
ATOM	3830	OD2	ASP	E	316	21.763	42.222	49.442	1.00	33.03	O
ATOM	3831	N	ILE	E	317	17.128	42.011	47.191	1.00	35.75	N
ATOM	3832	CA	ILE	E	317	15.676	41.931	47.188	1.00	35.76	C
ATOM	3833	C	ILE	E	317	15.102	41.565	45.819	1.00	35.57	C
ATOM	3834	O	ILE	E	317	14.252	40.677	45.720	1.00	35.07	O
ATOM	3835	CB	ILE	E	317	15.049	43.235	47.756	1.00	36.33	C
ATOM	3836	CG1	ILE	E	317	15.270	43.265	49.274	1.00	38.07	C
ATOM	3837	CG2	ILE	E	317	13.552	43.320	47.456	1.00	34.62	C
ATOM	3838	CD1	ILE	E	317	15.211	44.632	49.835	1.00	42.85	C
ATOM	3839	N	LEU	E	318	15.567	42.250	44.777	1.00	35.32	N
ATOM	3840	CA	LEU	E	318	15.080	42.019	43.422	1.00	35.67	C
ATOM	3841	C	LEU	E	318	15.501	40.648	42.892	1.00	36.08	C
ATOM	3842	O	LEU	E	318	14.739	39.996	42.179	1.00	35.39	O
ATOM	3843	CB	LEU	E	318	15.539	43.130	42.473	1.00	35.43	C
ATOM	3844	CG	LEU	E	318	14.514	44.209	42.089	1.00	35.86	C
ATOM	3845	CD1	LEU	E	318	13.544	44.580	43.208	1.00	35.06	C
ATOM	3846	CD2	LEU	E	318	15.207	45.457	41.499	1.00	35.46	C
ATOM	3847	N	GLN	E	319	16.706	40.213	43.241	1.00	36.79	N
ATOM	3848	CA	GLN	E	319	17.105	38.860	42.901	1.00	38.55	C
ATOM	3849	C	GLN	E	319	16.150	37.842	43.547	1.00	38.68	C
ATOM	3850	O	GLN	E	319	15.723	36.900	42.899	1.00	39.22	O
ATOM	3851	CB	GLN	E	319	18.555	38.585	43.284	1.00	38.90	C
ATOM	3852	CG	GLN	E	319	19.037	37.196	42.818	1.00	42.52	C
ATOM	3853	CD	GLN	E	319	20.518	37.003	43.032	1.00	47.18	C
ATOM	3854	OE1	GLN	E	319	21.020	37.169	44.149	1.00	50.12	O
ATOM	3855	NE2	GLN	E	319	21.232	36.652	41.963	1.00	48.61	N
ATOM	3856	N	ALA	E	320	15.791	38.060	44.803	1.00	39.29	N
ATOM	3857	CA	ALA	E	320	14.833	37.184	45.494	1.00	40.19	C
ATOM	3858	C	ALA	E	320	13.432	37.218	44.863	1.00	40.62	C
ATOM	3859	O	ALA	E	320	12.827	36.165	44.642	1.00	40.18	O
ATOM	3860	CB	ALA	E	320	14.762	37.539	46.969	1.00	40.08	C
ATOM	3861	N	LEU	E	321	12.938	38.418	44.543	1.00	41.02	N
ATOM	3862	CA	LEU	E	321	11.590	38.572	44.000	1.00	41.67	C
ATOM	3863	C	LEU	E	321	11.459	37.966	42.604	1.00	42.87	C
ATOM	3864	O	LEU	E	321	10.360	37.627	42.163	1.00	42.73	O
ATOM	3865	CB	LEU	E	321	11.160	40.043	43.991	1.00	41.42	C
ATOM	3866	CG	LEU	E	321	10.919	40.733	45.341	1.00	40.97	C
ATOM	3867	CD1	LEU	E	321	10.445	42.152	45.111	1.00	39.67	C
ATOM	3868	CD2	LEU	E	321	9.921	39.966	46.233	1.00	39.44	C
ATOM	3869	N	VAL	E	322	12.587	37.823	41.922	1.00	44.58	N
ATOM	3870	CA	VAL	E	322	12.593	37.339	40.556	1.00	46.75	C
ATOM	3871	C	VAL	E	322	12.663	35.803	40.529	1.00	48.57	C
ATOM	3872	O	VAL	E	322	12.300	35.179	39.535	1.00	48.65	O
ATOM	3873	CB	VAL	E	322	13.717	38.035	39.727	1.00	46.65	C
ATOM	3874	CG1	VAL	E	322	14.950	37.148	39.568	1.00	45.99	C
ATOM	3875	CG2	VAL	E	322	13.185	38.509	38.376	1.00	46.25	C
ATOM	3876	N	LEU	E	323	13.119	35.216	41.637	1.00	50.80	N
ATOM	3877	CA	LEU	E	323	13.165	33.759	41.823	1.00	53.39	C
ATOM	3878	C	LEU	E	323	12.096	33.325	42.825	1.00	54.80	C
ATOM	3879	O	LEU	E	323	12.096	32.187	43.279	1.00	55.42	O
ATOM	3880	CB	LEU	E	323	14.546	33.326	42.339	1.00	53.14	C
ATOM	3881	CG	LEU	E	323	15.789	33.765	41.556	1.00	54.15	C
ATOM	3882	CD1	LEU	E	323	17.032	33.730	42.436	1.00	54.59	C
ATOM	3883	CD2	LEU	E	323	15.987	32.934	40.294	1.00	54.51	C

Figure 1 Table 1b - 59

ATOM	3884	N	THR	E	324	11.174	34.239	43.133	1.00	56.91	N
ATOM	3885	CA	THR	E	324	10.239	34.147	44.274	1.00	58.45	C
ATOM	3886	C	THR	E	324	10.991	34.176	45.622	1.00	59.47	C
ATOM	3887	O	THR	E	324	12.037	33.530	45.778	1.00	59.58	O
ATOM	3888	CB	THR	E	324	9.228	32.965	44.166	1.00	58.77	C
ATOM	3889	OG1	THR	E	324	9.824	31.752	44.651	1.00	58.97	O
ATOM	3890	CG2	THR	E	324	8.764	32.774	42.710	1.00	59.10	C
ATOM	3891	N	GLY	E	325	10.477	34.970	46.565	1.00	60.49	N
ATOM	3892	CA	GLY	E	325	11.131	35.203	47.866	1.00	61.43	C
ATOM	3893	C	GLY	E	325	11.933	34.029	48.399	1.00	62.08	C
ATOM	3894	O	GLY	E	325	11.394	32.929	48.576	1.00	62.33	O
ATOM	3895	N	GLY	E	326	13.226	34.266	48.638	1.00	62.57	N
ATOM	3896	CA	GLY	E	326	14.154	33.220	49.094	1.00	62.97	C
ATOM	3897	C	GLY	E	326	15.577	33.403	48.582	1.00	63.34	C
ATOM	3898	O	GLY	E	326	15.814	34.037	47.543	1.00	63.44	O
TER	3899		GLY	E	326						
HETATM	3900	P	AMP	E	1327	22.506	55.282	47.542	1.00	39.41	P
HETATM	3901	O1P	AMP	E	1327	21.920	55.832	46.255	1.00	38.55	O
HETATM	3902	O2P	AMP	E	1327	23.791	54.512	47.437	1.00	37.92	O
HETATM	3903	O3P	AMP	E	1327	21.469	54.647	48.427	1.00	40.23	O
HETATM	3904	O5'	AMP	E	1327	22.953	56.627	48.343	1.00	38.64	O
HETATM	3905	C5'	AMP	E	1327	22.102	57.775	48.385	1.00	36.81	C
HETATM	3906	C4'	AMP	E	1327	22.394	58.677	49.589	1.00	36.83	C
HETATM	3907	O4'	AMP	E	1327	21.763	58.142	50.762	1.00	36.37	O
HETATM	3908	C3'	AMP	E	1327	23.877	58.804	49.916	1.00	36.85	C
HETATM	3909	O3'	AMP	E	1327	24.122	60.127	50.408	1.00	36.91	O
HETATM	3910	C2'	AMP	E	1327	24.087	57.805	51.038	1.00	35.53	C
HETATM	3911	O2'	AMP	E	1327	25.151	58.153	51.932	1.00	35.66	O
HETATM	3912	C1'	AMP	E	1327	22.741	57.767	51.736	1.00	34.74	C
HETATM	3913	N9	AMP	E	1327	22.473	56.396	52.230	1.00	35.20	N
HETATM	3914	C8	AMP	E	1327	22.520	55.258	51.510	1.00	34.02	C
HETATM	3915	N7	AMP	E	1327	22.224	54.181	52.283	1.00	34.64	N
HETATM	3916	C5	AMP	E	1327	21.976	54.637	53.528	1.00	34.61	C
HETATM	3917	C6	AMP	E	1327	21.602	54.050	54.828	1.00	34.74	C
HETATM	3918	N6	AMP	E	1327	21.429	52.702	54.977	1.00	33.92	N
HETATM	3919	N1	AMP	E	1327	21.442	54.911	55.864	1.00	34.79	N
HETATM	3920	C2	AMP	E	1327	21.608	56.242	55.765	1.00	34.26	C
HETATM	3921	N3	AMP	E	1327	21.945	56.840	54.612	1.00	33.34	N
HETATM	3922	C4	AMP	E	1327	22.132	56.106	53.485	1.00	34.38	C
HETATM	3923	P	AMP	E	1328	27.377	50.307	37.980	1.00	39.09	P
HETATM	3924	O1P	AMP	E	1328	28.064	50.132	39.311	1.00	44.50	O
HETATM	3925	O2P	AMP	E	1328	26.947	51.717	37.739	1.00	42.28	O
HETATM	3926	O3P	AMP	E	1328	26.324	49.288	37.676	1.00	42.98	O
HETATM	3927	O5'	AMP	E	1328	28.470	50.020	36.846	1.00	40.06	O
HETATM	3928	C5'	AMP	E	1328	29.414	48.952	36.870	1.00	36.68	C
HETATM	3929	C4'	AMP	E	1328	30.223	48.993	35.566	1.00	34.46	C
HETATM	3930	O4'	AMP	E	1328	29.397	48.572	34.467	1.00	33.63	O
HETATM	3931	C3'	AMP	E	1328	30.717	50.385	35.196	1.00	33.24	C
HETATM	3932	O3'	AMP	E	1328	32.034	50.274	34.640	1.00	33.14	O
HETATM	3933	C2'	AMP	E	1328	29.732	50.867	34.140	1.00	31.79	C
HETATM	3934	O2'	AMP	E	1328	30.326	51.756	33.188	1.00	32.07	O
HETATM	3935	C1'	AMP	E	1328	29.250	49.586	33.471	1.00	29.88	C
HETATM	3936	N9	AMP	E	1328	27.811	49.636	33.102	1.00	29.34	N
HETATM	3937	C8	AMP	E	1328	26.815	50.146	33.860	1.00	28.27	C
HETATM	3938	N7	AMP	E	1328	25.618	50.028	33.250	1.00	28.46	N
HETATM	3939	C5	AMP	E	1328	25.839	49.428	32.064	1.00	27.79	C
HETATM	3940	C6	AMP	E	1328	25.013	48.997	30.927	1.00	27.22	C
HETATM	3941	N6	AMP	E	1328	23.676	49.199	30.912	1.00	27.64	N
HETATM	3942	N1	AMP	E	1328	25.640	48.405	29.893	1.00	28.78	N
HETATM	3943	C2	AMP	E	1328	26.969	48.196	29.865	1.00	28.44	C
HETATM	3944	N3	AMP	E	1328	27.777	48.558	30.869	1.00	27.84	N
HETATM	3945	C4	AMP	E	1328	27.282	49.166	31.973	1.00	28.03	C
HETATM	3946	P	AMP	E	1329	24.991	46.480	45.770	1.00	35.39	P
HETATM	3947	O1P	AMP	E	1329	24.137	46.427	44.527	1.00	36.26	O
HETATM	3948	O2P	AMP	E	1329	24.392	47.233	46.942	1.00	34.49	O
HETATM	3949	O3P	AMP	E	1329	26.452	46.767	45.555	1.00	33.94	O
HETATM	3950	O5'	AMP	E	1329	25.003	44.948	46.286	1.00	35.49	O

Figure 1 Table 1b - 60

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HETATM 3951  C5' AMP E1329      25.499  43.856  45.487  1.00 33.68           C
HETATM 3952  C4' AMP E1329      25.773  42.652  46.393  1.00 33.62           C
HETATM 3953  O4' AMP E1329      26.846  42.965  47.288  1.00 33.47           O
HETATM 3954  C3' AMP E1329      24.591  42.325  47.280  1.00 33.15           C
HETATM 3955  O3' AMP E1329      24.572  40.922  47.484  1.00 31.79           O
HETATM 3956  C2' AMP E1329      24.893  43.023  48.599  1.00 32.08           C
HETATM 3957  O2' AMP E1329      24.283  42.358  49.705  1.00 31.02           O
HETATM 3958  C1' AMP E1329      26.402  42.949  48.642  1.00 33.23           C
HETATM 3959  N9  AMP E1329      26.999  44.111  49.312  1.00 34.00           N
HETATM 3960  C8  AMP E1329      26.616  45.401  49.165  1.00 34.79           C
HETATM 3961  N7  AMP E1329      27.380  46.215  49.911  1.00 35.49           N
HETATM 3962  C5  AMP E1329      28.281  45.445  50.540  1.00 34.76           C
HETATM 3963  C6  AMP E1329      29.395  45.683  51.474  1.00 34.85           C
HETATM 3964  N6  AMP E1329      29.683  46.939  51.890  1.00 34.29           N
HETATM 3965  N1  AMP E1329      30.094  44.606  51.892  1.00 33.45           N
HETATM 3966  C2  AMP E1329      29.810  43.351  51.477  1.00 34.81           C
HETATM 3967  N3  AMP E1329      28.813  43.053  50.623  1.00 34.46           N
HETATM 3968  C4  AMP E1329      28.032  44.050  50.133  1.00 34.62           C
HETATM 3969  O   HOH A2001      17.753  49.212  20.345  1.00 49.34           O
HETATM 3970  O   HOH A2002      22.773  90.901  22.907  1.00 68.04           O
HETATM 3971  O   HOH A2003      25.685  89.095  23.629  1.00 54.17           O
HETATM 3972  O   HOH A2004      27.059  93.980   8.107  1.00 59.23           O
HETATM 3973  O   HOH A2005      17.083  85.557   2.155  1.00 53.42           O
HETATM 3974  O   HOH A2006      26.662  81.795  -0.972  1.00 52.89           O
HETATM 3975  O   HOH A2007      27.198  77.245  -2.776  1.00 57.07           O
HETATM 3976  O   HOH A2008      27.814  62.346   4.446  1.00 70.13           O
HETATM 3977  O   HOH A2009      10.240  76.009  12.454  1.00 57.50           O
HETATM 3978  O   HOH A2010      13.639  96.429  19.891  1.00 63.59           O
HETATM 3979  O   HOH A2011      24.554  78.314  32.340  1.00 47.55           O
HETATM 3980  O   HOH A2012      24.316  79.149  29.126  1.00 50.50           O
HETATM 3981  O   HOH A2013      18.075  70.636  31.822  1.00 63.77           O
HETATM 3982  O   HOH A2014      19.864  82.066  21.360  1.00 40.25           O
HETATM 3983  O   HOH A2015      23.442  87.642  24.175  1.00 75.54           O
HETATM 3984  O   HOH A2016      26.408  88.721  15.394  1.00 41.81           O
HETATM 3985  O   HOH A2017      25.628  93.361  10.261  1.00 65.42           O
HETATM 3986  O   HOH A2018      26.309  94.824  15.719  1.00 56.37           O
HETATM 3987  O   HOH A2019      26.288  93.320  20.799  1.00 64.43           O
HETATM 3988  O   HOH A2020      19.977  85.037   1.034  1.00 48.68           O
HETATM 3989  O   HOH A2021      20.586  93.793   3.289  1.00 84.25           O
HETATM 3990  O   HOH A2022      25.890  92.454   3.908  1.00 69.71           O
HETATM 3991  O   HOH A2023      26.768  90.272   7.472  1.00 62.59           O
HETATM 3992  O   HOH A2024      24.424  80.390  -0.875  1.00 52.58           O
HETATM 3993  O   HOH A2025      19.758  82.292   0.792  1.00 54.03           O
HETATM 3994  O   HOH A2026      29.960  82.468   7.390  1.00 43.49           O
HETATM 3995  O   HOH A2027      24.205  77.687  -1.837  1.00 60.23           O
HETATM 3996  O   HOH A2028      28.358  75.073  -1.182  1.00 67.31           O
HETATM 3997  O   HOH A2029      22.641  75.532  -5.413  1.00 55.71           O
HETATM 3998  O   HOH A2030      22.700  63.573   2.591  1.00 54.45           O
HETATM 3999  O   HOH A2031      23.103  69.075  -1.505  1.00 57.23           O
HETATM 4000  O   HOH A2032      20.863  63.141   0.932  1.00 57.82           O
HETATM 4001  O   HOH A2033      16.042  72.857  -3.199  1.00 39.32           O
HETATM 4002  O   HOH A2034      18.481  69.831  -2.309  1.00 46.46           O
HETATM 4003  O   HOH A2035      14.095  68.365   1.739  1.00 50.21           O
HETATM 4004  O   HOH A2036      10.093  66.542  -4.025  1.00 73.44           O
HETATM 4005  O   HOH A2037       7.582  70.086  -1.418  1.00 69.30           O
HETATM 4006  O   HOH A2038       5.650  78.688   1.283  1.00 40.51           O
HETATM 4007  O   HOH A2039      16.430  82.415   1.795  1.00 73.03           O
HETATM 4008  O   HOH A2040      16.821  88.204   3.294  1.00 62.69           O
HETATM 4009  O   HOH A2041       5.188  74.472   8.985  1.00 56.02           O
HETATM 4010  O   HOH A2042      25.190  64.326  10.454  1.00 57.05           O
HETATM 4011  O   HOH A2043      25.227  63.363   5.008  1.00 58.40           O
HETATM 4012  O   HOH A2044      18.822  54.957   0.939  1.00 77.53           O
HETATM 4013  O   HOH A2045      31.172  55.361   6.997  1.00 71.57           O
HETATM 4014  O   HOH A2046      24.572  51.582   6.160  1.00 54.23           O
HETATM 4015  O   HOH A2047      20.210  56.419  12.284  1.00 53.42           O
HETATM 4016  O   HOH A2048      15.138  56.703   7.570  1.00 57.86           O
HETATM 4017  O   HOH A2049      19.377  59.738  10.213  1.00 38.57           O
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Figure 1 Table 1b - 61

HETATM	4018	O	HOH A2050	17.492	62.981	13.383	1.00 39.45	O
HETATM	4019	O	HOH A2051	13.683	63.097	10.651	1.00 45.79	O
HETATM	4020	O	HOH A2052	15.992	65.323	13.117	1.00 44.42	O
HETATM	4021	O	HOH A2053	12.652	75.564	12.916	1.00 38.40	O
HETATM	4022	O	HOH A2054	7.827	80.700	8.608	1.00 37.04	O
HETATM	4023	O	HOH A2055	8.974	77.740	11.396	1.00 54.81	O
HETATM	4024	O	HOH A2056	9.725	83.217	7.681	1.00 34.77	O
HETATM	4025	O	HOH A2057	6.913	80.604	13.094	1.00 75.77	O
HETATM	4026	O	HOH A2058	16.944	97.202	19.757	1.00 73.64	O
HETATM	4027	O	HOH A2059	20.531	93.719	9.757	1.00 47.98	O
HETATM	4028	O	HOH A2060	15.781	92.994	9.093	1.00 63.18	O
HETATM	4029	O	HOH A2061	16.264	76.228	18.141	1.00 30.11	O
HETATM	4030	O	HOH A2062	12.147	64.531	15.991	1.00 57.96	O
HETATM	4031	O	HOH A2063	11.340	62.006	18.533	1.00 63.40	O
HETATM	4032	O	HOH A2064	7.943	66.708	13.961	1.00 53.95	O
HETATM	4033	O	HOH A2065	5.070	62.995	13.899	1.00 78.74	O
HETATM	4034	O	HOH A2066	11.359	60.044	15.204	1.00 56.02	O
HETATM	4035	O	HOH A2067	12.552	60.996	9.068	1.00 75.41	O
HETATM	4036	O	HOH A2068	3.603	58.972	12.046	1.00 70.57	O
HETATM	4037	O	HOH A2069	3.265	64.073	8.414	1.00 85.06	O
HETATM	4038	O	HOH A2070	20.009	39.155	25.412	1.00 84.95	O
HETATM	4039	O	HOH A2071	18.683	51.875	15.471	1.00 57.39	O
HETATM	4040	O	HOH A2072	18.718	51.030	18.765	1.00 61.65	O
HETATM	4041	O	HOH A2073	22.909	52.967	19.343	1.00 45.98	O
HETATM	4042	O	HOH A2074	16.672	52.830	14.085	1.00 76.71	O
HETATM	4043	O	HOH A2075	20.886	51.099	12.378	1.00 62.45	O
HETATM	4044	O	HOH A2076	20.334	53.407	19.666	1.00 47.47	O
HETATM	4045	O	HOH A2077	8.542	74.012	12.528	1.00 69.91	O
HETATM	4046	O	HOH A2078	14.779	61.632	22.597	1.00 32.39	O
HETATM	4047	O	HOH A2079	24.817	61.954	13.045	1.00 42.85	O
HETATM	4048	O	HOH A2080	28.452	64.139	18.778	1.00 38.07	O
HETATM	4049	O	HOH A2081	29.378	73.484	15.841	1.00 49.22	O
HETATM	4050	O	HOH A2082	30.078	69.534	14.137	1.00 53.46	O
HETATM	4051	O	HOH A2083	29.375	64.143	12.420	1.00 69.81	O
HETATM	4052	O	HOH A2084	32.668	79.251	8.583	1.00 55.32	O
HETATM	4053	O	HOH A2085	35.791	74.685	9.903	1.00 68.12	O
HETATM	4054	O	HOH A2086	31.131	78.095	14.568	1.00 47.93	O
HETATM	4055	O	HOH B2001	0.244	96.990	-29.610	1.00 67.37	O
HETATM	4056	O	HOH B2002	-0.655	95.367	-20.577	1.00 42.29	O
HETATM	4057	O	HOH B2003	1.407	100.977	-22.758	1.00 35.31	O
HETATM	4058	O	HOH B2004	5.502	91.342	-15.985	1.00 53.66	O
HETATM	4059	O	HOH B2005	7.571	94.970	-10.185	1.00 59.52	O
HETATM	4060	O	HOH B2006	8.522	89.913	0.775	1.00 75.12	O
HETATM	4061	O	HOH B2007	12.623	99.110	-2.374	1.00 87.27	O
HETATM	4062	O	HOH B2008	15.319	94.090	-1.646	1.00 60.93	O
HETATM	4063	O	HOH B2009	4.432	93.727	6.668	1.00 58.67	O
HETATM	4064	O	HOH B2010	8.531	91.915	7.277	1.00 56.81	O
HETATM	4065	O	HOH B2011	8.501	87.762	7.460	1.00 53.23	O
HETATM	4066	O	HOH B2012	8.630	91.199	11.564	1.00 73.48	O
HETATM	4067	O	HOH B2013	3.818	78.762	25.094	1.00 75.56	O
HETATM	4068	O	HOH B2014	2.272	80.836	25.911	1.00 60.88	O
HETATM	4069	O	HOH B2015	2.010	83.506	26.842	1.00 68.44	O
HETATM	4070	O	HOH B2016	12.361	86.380	24.226	1.00 60.57	O
HETATM	4071	O	HOH B2017	5.937	80.636	29.719	1.00 71.07	O
HETATM	4072	O	HOH B2018	4.915	76.523	22.070	1.00 65.12	O
HETATM	4073	O	HOH B2019	7.298	71.594	18.266	1.00 58.06	O
HETATM	4074	O	HOH B2020	8.690	64.872	19.981	1.00 38.90	O
HETATM	4075	O	HOH B2021	7.575	76.013	16.450	1.00 79.63	O
HETATM	4076	O	HOH B2022	13.196	71.098	22.917	1.00 29.13	O
HETATM	4077	O	HOH B2023	26.763	75.057	23.823	1.00 47.79	O
HETATM	4078	O	HOH B2024	28.837	74.736	27.488	1.00 46.70	O
HETATM	4079	O	HOH B2025	27.908	77.769	29.818	1.00 56.74	O
HETATM	4080	O	HOH B2026	30.726	81.185	24.831	1.00 52.58	O
HETATM	4081	O	HOH B2027	34.143	79.941	25.713	1.00 68.94	O
HETATM	4082	O	HOH B2028	37.957	78.002	26.808	1.00 67.11	O
HETATM	4083	O	HOH B2029	34.946	79.368	28.309	1.00 66.82	O
HETATM	4084	O	HOH B2030	35.497	77.858	24.694	1.00 65.78	O

Figure 1 Table 1b - 62

HETATM	4085	O	HOH B2031	16.311	71.818	26.902	1.00 43.97	O
HETATM	4086	O	HOH B2032	13.747	71.211	25.664	1.00 38.78	O
HETATM	4087	O	HOH B2033	2.820	61.288	16.985	1.00 75.24	O
HETATM	4088	O	HOH B2034	4.364	65.297	19.367	1.00 60.06	O
HETATM	4089	O	HOH B2035	6.648	60.495	18.823	1.00 69.35	O
HETATM	4090	O	HOH B2036	-0.094	60.531	22.579	1.00 65.84	O
HETATM	4091	O	HOH B2037	2.829	57.943	19.667	1.00 63.32	O
HETATM	4092	O	HOH B2038	5.598	58.128	20.046	1.00 43.58	O
HETATM	4093	O	HOH B2039	-5.360	61.185	25.464	1.00 69.81	O
HETATM	4094	O	HOH B2040	10.592	60.033	25.573	1.00 46.67	O
HETATM	4095	O	HOH B2041	2.611	55.162	32.163	1.00 39.32	O
HETATM	4096	O	HOH B2042	15.091	64.072	23.884	1.00 32.27	O
HETATM	4097	O	HOH B2043	27.227	72.176	32.127	1.00 50.44	O
HETATM	4098	O	HOH B2044	28.823	66.202	14.496	1.00 58.01	O
HETATM	4099	O	HOH B2045	32.846	66.117	18.836	1.00 59.94	O
HETATM	4100	O	HOH B2046	37.539	69.676	20.153	1.00 88.37	O
HETATM	4101	O	HOH B2047	14.669	97.838	0.422	1.00 72.92	O
HETATM	4102	O	HOH B2048	26.475	75.733	20.950	1.00 49.21	O
HETATM	4103	O	HOH B2049	0.537	58.088	22.744	1.00 60.29	O
HETATM	4104	O	HOH B2050	12.342	60.467	22.972	1.00 35.25	O
HETATM	4105	O	HOH E2001	9.637	31.086	51.041	1.00 59.38	O
HETATM	4106	O	HOH E2002	0.855	33.379	41.823	1.00 56.61	O
HETATM	4107	O	HOH E2003	-0.271	34.926	46.740	1.00 63.23	O
HETATM	4108	O	HOH E2004	-0.892	33.810	43.934	1.00 68.80	O
HETATM	4109	O	HOH E2005	1.893	29.351	47.681	1.00 73.27	O
HETATM	4110	O	HOH E2006	6.373	30.036	38.950	1.00 69.49	O
HETATM	4111	O	HOH E2007	8.459	36.529	44.065	1.00 38.47	O
HETATM	4112	O	HOH E2008	0.170	40.507	40.433	1.00 47.64	O
HETATM	4113	O	HOH E2009	5.631	45.058	47.910	1.00 36.15	O
HETATM	4114	O	HOH E2010	2.991	41.526	48.286	1.00 45.07	O
HETATM	4115	O	HOH E2011	2.038	38.050	33.777	1.00 44.78	O
HETATM	4116	O	HOH E2012	10.488	32.449	33.985	1.00 52.34	O
HETATM	4117	O	HOH E2013	5.496	33.568	36.382	1.00 58.66	O
HETATM	4118	O	HOH E2014	-0.814	42.540	36.913	1.00 68.41	O
HETATM	4119	O	HOH E2015	-0.411	49.020	36.611	1.00 57.22	O
HETATM	4120	O	HOH E2016	2.164	53.549	34.831	1.00 46.48	O
HETATM	4121	O	HOH E2017	1.792	52.607	30.665	1.00 47.83	O
HETATM	4122	O	HOH E2018	2.475	49.488	28.234	1.00 51.60	O
HETATM	4123	O	HOH E2019	-0.276	49.255	32.432	1.00 64.97	O
HETATM	4124	O	HOH E2020	1.743	47.251	30.292	1.00 52.92	O
HETATM	4125	O	HOH E2021	3.172	60.029	31.171	1.00 44.58	O
HETATM	4126	O	HOH E2022	11.494	66.214	29.938	1.00 35.31	O
HETATM	4127	O	HOH E2023	13.079	66.938	34.274	1.00 71.73	O
HETATM	4128	O	HOH E2024	10.491	60.587	30.573	1.00 35.46	O
HETATM	4129	O	HOH E2025	15.713	60.072	31.519	1.00 38.77	O
HETATM	4130	O	HOH E2026	15.147	63.043	35.114	1.00 37.41	O
HETATM	4131	O	HOH E2027	19.227	60.214	33.573	1.00 39.36	O
HETATM	4132	O	HOH E2028	16.538	69.325	36.920	1.00 74.54	O
HETATM	4133	O	HOH E2029	32.712	63.682	17.886	1.00 50.53	O
HETATM	4134	O	HOH E2030	32.669	59.961	19.802	1.00 43.95	O
HETATM	4135	O	HOH E2031	38.001	66.392	23.989	1.00 53.90	O
HETATM	4136	O	HOH E2032	35.509	65.558	19.325	1.00 55.49	O
HETATM	4137	O	HOH E2033	36.515	67.627	25.875	1.00 42.01	O
HETATM	4138	O	HOH E2034	43.718	66.845	37.301	1.00 69.72	O
HETATM	4139	O	HOH E2035	39.645	73.143	28.537	1.00 64.27	O
HETATM	4140	O	HOH E2036	31.230	69.650	32.595	1.00 42.03	O
HETATM	4141	O	HOH E2037	36.598	70.309	25.514	1.00 71.50	O
HETATM	4142	O	HOH E2038	29.068	70.800	33.554	1.00 49.38	O
HETATM	4143	O	HOH E2039	23.660	73.483	37.611	1.00 71.68	O
HETATM	4144	O	HOH E2040	20.286	69.856	34.048	1.00 56.80	O
HETATM	4145	O	HOH E2041	18.148	66.099	38.670	1.00 74.74	O
HETATM	4146	O	HOH E2042	25.291	63.349	40.872	1.00 61.56	O
HETATM	4147	O	HOH E2043	20.813	59.325	37.185	1.00 42.59	O
HETATM	4148	O	HOH E2044	26.012	55.496	42.541	1.00 65.41	O
HETATM	4149	O	HOH E2045	22.348	53.605	44.127	1.00 59.56	O
HETATM	4150	O	HOH E2046	26.378	55.763	39.272	1.00 45.08	O
HETATM	4151	O	HOH E2047	21.734	59.251	44.870	1.00 81.86	O

Figure 1 Table 1b - 63

HETATM	4152	O	HOH E2048	19.877	54.218	42.342	1.00 53.32	O
HETATM	4153	O	HOH E2049	19.630	57.009	41.195	1.00 76.54	O
HETATM	4154	O	HOH E2050	21.543	60.894	32.471	1.00 37.25	O
HETATM	4155	O	HOH E2051	33.484	52.600	20.667	1.00 57.10	O
HETATM	4156	O	HOH E2052	34.280	55.612	21.257	1.00 60.46	O
HETATM	4157	O	HOH E2053	35.174	54.604	17.443	1.00 58.62	O
HETATM	4158	O	HOH E2054	32.863	57.608	10.292	1.00 65.64	O
HETATM	4159	O	HOH E2055	33.200	52.819	12.665	1.00 61.89	O
HETATM	4160	O	HOH E2056	28.435	51.545	13.320	1.00 50.02	O
HETATM	4161	O	HOH E2057	31.696	47.558	16.690	1.00 76.69	O
HETATM	4162	O	HOH E2058	29.587	48.344	23.066	1.00 58.44	O
HETATM	4163	O	HOH E2059	29.892	51.030	29.555	1.00 44.98	O
HETATM	4164	O	HOH E2060	32.476	53.527	30.180	1.00 43.01	O
HETATM	4165	O	HOH E2061	41.074	51.695	39.337	1.00 47.00	O
HETATM	4166	O	HOH E2062	34.784	49.003	40.000	1.00 44.44	O
HETATM	4167	O	HOH E2063	35.551	48.096	35.500	1.00 69.65	O
HETATM	4168	O	HOH E2064	44.708	49.922	46.441	1.00 54.92	O
HETATM	4169	O	HOH E2065	44.901	51.828	40.252	1.00 57.71	O
HETATM	4170	O	HOH E2066	43.581	67.149	39.908	1.00 66.93	O
HETATM	4171	O	HOH E2067	47.509	61.161	38.329	1.00 51.50	O
HETATM	4172	O	HOH E2068	48.351	61.156	44.852	1.00 41.72	O
HETATM	4173	O	HOH E2069	49.356	57.477	50.181	1.00 60.93	O
HETATM	4174	O	HOH E2070	48.822	54.828	48.667	1.00 59.16	O
HETATM	4175	O	HOH E2071	48.782	54.840	35.332	1.00 54.41	O
HETATM	4176	O	HOH E2072	55.122	59.299	46.082	1.00 49.62	O
HETATM	4177	O	HOH E2073	55.749	63.411	35.484	1.00 22.24	O
HETATM	4178	O	HOH E2074	54.537	62.476	43.194	1.00 46.22	O
HETATM	4179	O	HOH E2075	59.648	60.536	38.587	1.00 42.34	O
HETATM	4180	O	HOH E2076	49.654	63.432	29.587	1.00 56.19	O
HETATM	4181	O	HOH E2077	51.550	64.593	42.698	1.00 62.71	O
HETATM	4182	O	HOH E2078	46.237	64.992	33.739	1.00 72.65	O
HETATM	4183	O	HOH E2079	46.897	59.276	35.562	1.00 51.09	O
HETATM	4184	O	HOH E2080	47.026	70.547	31.274	1.00 58.68	O
HETATM	4185	O	HOH E2081	45.726	61.671	29.155	1.00 58.60	O
HETATM	4186	O	HOH E2082	37.467	53.176	23.563	1.00 54.93	O
HETATM	4187	O	HOH E2083	35.890	57.021	17.555	1.00 58.54	O
HETATM	4188	O	HOH E2084	42.153	54.865	22.877	1.00 72.38	O
HETATM	4189	O	HOH E2085	34.650	54.170	23.463	1.00 47.21	O
HETATM	4190	O	HOH E2086	40.596	42.976	33.146	1.00 88.85	O
HETATM	4191	O	HOH E2087	41.243	44.169	22.130	1.00 83.81	O
HETATM	4192	O	HOH E2088	36.259	44.875	31.324	1.00 85.94	O
HETATM	4193	O	HOH E2089	33.744	47.635	25.215	1.00 75.44	O
HETATM	4194	O	HOH E2090	30.386	49.339	27.378	1.00 55.30	O
HETATM	4195	O	HOH E2091	33.203	45.398	24.097	1.00 62.79	O
HETATM	4196	O	HOH E2092	28.797	44.594	29.699	1.00 80.62	O
HETATM	4197	O	HOH E2093	24.446	43.695	25.336	1.00 61.25	O
HETATM	4198	O	HOH E2094	19.098	43.657	28.492	1.00 38.59	O
HETATM	4199	O	HOH E2095	15.896	46.068	23.037	1.00 84.84	O
HETATM	4200	O	HOH E2096	14.606	44.452	24.768	1.00 38.95	O
HETATM	4201	O	HOH E2097	10.604	46.145	21.227	1.00 48.67	O
HETATM	4202	O	HOH E2098	6.165	51.290	24.751	1.00 47.94	O
HETATM	4203	O	HOH E2099	4.926	50.443	20.820	1.00 43.06	O
HETATM	4204	O	HOH E2100	8.821	38.354	30.606	1.00 43.51	O
HETATM	4205	O	HOH E2101	14.617	41.761	26.507	1.00 57.03	O
HETATM	4206	O	HOH E2102	10.279	40.997	27.425	1.00 41.10	O
HETATM	4207	O	HOH E2103	15.354	35.872	35.922	1.00 49.94	O
HETATM	4208	O	HOH E2104	19.177	37.008	35.901	1.00 58.48	O
HETATM	4209	O	HOH E2105	24.348	37.611	38.547	1.00 50.70	O
HETATM	4210	O	HOH E2106	27.689	39.760	34.129	1.00 67.91	O
HETATM	4211	O	HOH E2107	21.602	40.931	28.478	1.00 64.93	O
HETATM	4212	O	HOH E2108	19.868	35.474	33.088	1.00 76.69	O
HETATM	4213	O	HOH E2109	16.797	39.685	30.473	1.00 48.03	O
HETATM	4214	O	HOH E2110	29.657	40.971	35.425	1.00 66.73	O
HETATM	4215	O	HOH E2111	28.197	46.008	39.753	1.00 60.77	O
HETATM	4216	O	HOH E2112	29.484	44.636	36.606	1.00 59.94	O
HETATM	4217	O	HOH E2113	23.442	44.455	40.007	1.00 42.75	O
HETATM	4218	O	HOH E2114	20.242	50.371	40.426	1.00 30.72	O

Figure 1

Table 1b - 64

HETATM	4219	O	HOH E2115	23.649	52.356	42.531	1.00	61.46	O
HETATM	4220	O	HOH E2116	20.297	56.753	36.626	1.00	52.11	O
HETATM	4221	O	HOH E2117	16.543	48.486	22.680	1.00	62.64	O
HETATM	4222	O	HOH E2118	8.655	51.798	19.885	1.00	56.60	O
HETATM	4223	O	HOH E2119	9.511	55.458	17.961	1.00	56.06	O
HETATM	4224	O	HOH E2120	7.224	54.263	17.701	1.00	76.98	O
HETATM	4225	O	HOH E2121	17.858	56.449	13.827	1.00	66.85	O
HETATM	4226	O	HOH E2122	11.837	58.740	21.059	1.00	47.93	O
HETATM	4227	O	HOH E2123	13.994	61.877	18.169	1.00	39.12	O
HETATM	4228	O	HOH E2124	17.027	60.593	24.010	1.00	30.84	O
HETATM	4229	O	HOH E2125	18.972	59.213	22.649	1.00	30.40	O
HETATM	4230	O	HOH E2126	11.124	59.303	28.241	1.00	46.52	O
HETATM	4231	O	HOH E2127	13.044	58.593	37.750	1.00	40.46	O
HETATM	4232	O	HOH E2128	15.173	54.579	37.316	1.00	36.41	O
HETATM	4233	O	HOH E2129	16.934	58.483	33.527	1.00	35.39	O
HETATM	4234	O	HOH E2130	17.436	56.830	36.318	1.00	39.38	O
HETATM	4235	O	HOH E2131	16.151	55.763	40.908	1.00	54.81	O
HETATM	4236	O	HOH E2132	21.055	43.063	40.696	1.00	46.68	O
HETATM	4237	O	HOH E2133	12.732	51.821	46.116	1.00	31.82	O
HETATM	4238	O	HOH E2134	11.201	56.784	41.691	1.00	59.96	O
HETATM	4239	O	HOH E2135	9.774	58.478	43.085	1.00	46.71	O
HETATM	4240	O	HOH E2136	2.107	46.674	50.054	1.00	40.74	O
HETATM	4241	O	HOH E2137	2.978	46.377	47.492	1.00	40.30	O
HETATM	4242	O	HOH E2138	-2.276	49.292	44.443	1.00	56.66	O
HETATM	4243	O	HOH E2139	1.861	43.777	48.183	1.00	49.64	O
HETATM	4244	O	HOH E2140	-1.294	41.229	45.741	1.00	37.25	O
HETATM	4245	O	HOH E2141	1.072	41.178	46.903	1.00	51.23	O
HETATM	4246	O	HOH E2142	-3.758	46.910	49.125	1.00	46.01	O
HETATM	4247	O	HOH E2143	-0.816	33.586	51.265	1.00	70.50	O
HETATM	4248	O	HOH E2144	-0.097	36.280	54.199	1.00	62.42	O
HETATM	4249	O	HOH E2145	-3.220	36.730	51.342	1.00	46.32	O
HETATM	4250	O	HOH E2146	3.990	27.885	49.723	1.00	76.95	O
HETATM	4251	O	HOH E2147	1.822	26.606	53.826	1.00	64.65	O
HETATM	4252	O	HOH E2148	2.349	36.708	54.267	1.00	48.13	O
HETATM	4253	O	HOH E2149	5.626	37.634	60.358	1.00	45.30	O
HETATM	4254	O	HOH E2150	22.081	39.300	64.355	1.00	71.84	O
HETATM	4255	O	HOH E2151	13.828	34.816	62.074	1.00	37.39	O
HETATM	4256	O	HOH E2152	11.012	29.939	56.925	1.00	67.43	O
HETATM	4257	O	HOH E2153	15.591	29.938	59.623	1.00	64.35	O
HETATM	4258	O	HOH E2154	20.583	37.818	48.797	1.00	38.40	O
HETATM	4259	O	HOH E2155	21.961	35.411	52.432	1.00	45.47	O
HETATM	4260	O	HOH E2156	30.588	36.815	59.242	1.00	61.93	O
HETATM	4261	O	HOH E2157	26.275	35.967	52.924	1.00	42.33	O
HETATM	4262	O	HOH E2158	28.591	34.241	57.696	1.00	55.95	O
HETATM	4263	O	HOH E2159	30.056	39.554	59.160	1.00	59.58	O
HETATM	4264	O	HOH E2160	36.070	42.344	53.431	1.00	77.61	O
HETATM	4265	O	HOH E2161	32.901	41.279	49.681	1.00	60.92	O
HETATM	4266	O	HOH E2162	33.775	37.465	56.872	1.00	54.40	O
HETATM	4267	O	HOH E2163	32.136	40.901	57.579	1.00	53.69	O
HETATM	4268	O	HOH E2164	36.864	46.316	54.632	1.00	59.13	O
HETATM	4269	O	HOH E2165	39.221	49.882	56.410	1.00	60.27	O
HETATM	4270	O	HOH E2166	35.458	56.279	65.789	1.00	73.23	O
HETATM	4271	O	HOH E2167	41.818	54.838	60.212	1.00	64.77	O
HETATM	4272	O	HOH E2168	41.391	53.121	58.371	1.00	63.34	O
HETATM	4273	O	HOH E2169	44.194	52.434	48.479	1.00	63.48	O
HETATM	4274	O	HOH E2170	42.156	50.668	50.032	1.00	45.79	O
HETATM	4275	O	HOH E2171	41.946	48.590	45.100	1.00	53.42	O
HETATM	4276	O	HOH E2172	33.459	49.335	42.244	1.00	38.70	O
HETATM	4277	O	HOH E2173	43.278	44.269	49.490	1.00	47.03	O
HETATM	4278	O	HOH E2174	40.320	46.569	49.167	1.00	51.78	O
HETATM	4279	O	HOH E2175	33.561	41.165	45.571	1.00	67.08	O
HETATM	4280	O	HOH E2176	40.410	42.502	50.522	1.00	69.41	O
HETATM	4281	O	HOH E2177	29.787	42.219	44.276	1.00	57.76	O
HETATM	4282	O	HOH E2178	36.014	54.499	63.856	1.00	64.32	O
HETATM	4283	O	HOH E2179	36.219	48.855	63.842	1.00	71.83	O
HETATM	4284	O	HOH E2180	35.366	54.801	68.032	1.00	75.90	O
HETATM	4285	O	HOH E2181	31.402	53.098	74.293	1.00	69.45	O

Figure 1 Table 1b - 65

HETATM	4286	O	HOH E2182	33.138	43.272	65.239	1.00	76.68	O
HETATM	4287	O	HOH E2183	27.862	51.664	74.764	1.00	68.40	O
HETATM	4288	O	HOH E2184	23.870	53.803	63.518	1.00	57.86	O
HETATM	4289	O	HOH E2185	26.617	65.043	45.254	1.00	65.14	O
HETATM	4290	O	HOH E2186	24.179	78.084	38.917	1.00	80.28	O
HETATM	4291	O	HOH E2187	28.596	48.924	42.984	1.00	43.13	O
HETATM	4292	O	HOH E2188	33.078	61.971	49.193	1.00	48.86	O
HETATM	4293	O	HOH E2189	27.114	63.295	49.687	1.00	51.33	O
HETATM	4294	O	HOH E2190	32.895	64.764	49.472	1.00	51.08	O
HETATM	4295	O	HOH E2191	31.695	41.422	41.067	1.00	74.17	O
HETATM	4296	O	HOH E2192	34.783	73.474	39.971	1.00	82.34	O
HETATM	4297	O	HOH E2193	33.974	69.859	46.656	1.00	72.27	O
HETATM	4298	O	HOH E2194	35.408	66.388	37.433	1.00	49.90	O
HETATM	4299	O	HOH E2195	44.771	63.531	47.092	1.00	58.49	O
HETATM	4300	O	HOH E2196	36.665	48.207	59.426	1.00	60.82	O
HETATM	4301	O	HOH E2197	46.680	60.178	53.772	1.00	77.78	O
HETATM	4302	O	HOH E2198	40.282	64.408	57.773	1.00	50.69	O
HETATM	4303	O	HOH E2199	31.378	59.203	60.382	1.00	67.35	O
HETATM	4304	O	HOH E2200	30.464	63.353	58.834	1.00	57.42	O
HETATM	4305	O	HOH E2201	30.084	63.721	50.629	1.00	74.52	O
HETATM	4306	O	HOH E2202	33.480	69.705	54.654	1.00	87.86	O
HETATM	4307	O	HOH E2203	36.337	69.842	57.828	1.00	82.02	O
HETATM	4308	O	HOH E2204	25.303	66.641	56.541	1.00	76.84	O
HETATM	4309	O	HOH E2205	23.994	64.679	49.536	1.00	67.21	O
HETATM	4310	O	HOH E2206	24.018	70.182	55.415	1.00	74.88	O
HETATM	4311	O	HOH E2207	16.006	62.013	57.059	1.00	73.55	O
HETATM	4312	O	HOH E2208	18.929	58.875	57.027	1.00	60.95	O
HETATM	4313	O	HOH E2209	18.377	55.316	62.398	1.00	69.74	O
HETATM	4314	O	HOH E2210	22.912	55.918	63.045	1.00	55.20	O
HETATM	4315	O	HOH E2211	17.246	52.380	60.955	1.00	43.03	O
HETATM	4316	O	HOH E2212	14.790	49.549	67.090	1.00	54.41	O
HETATM	4317	O	HOH E2213	20.171	36.660	65.678	1.00	52.26	O
HETATM	4318	O	HOH E2214	9.660	39.265	61.782	1.00	53.31	O
HETATM	4319	O	HOH E2215	11.267	36.678	63.168	1.00	52.90	O
HETATM	4320	O	HOH E2216	10.191	44.605	61.911	1.00	31.98	O
HETATM	4321	O	HOH E2217	9.200	42.383	60.636	1.00	30.94	O
HETATM	4322	O	HOH E2218	2.059	45.716	56.032	1.00	62.53	O
HETATM	4323	O	HOH E2219	3.142	44.513	51.332	1.00	52.42	O
HETATM	4324	O	HOH E2220	2.908	46.392	53.609	1.00	36.74	O
HETATM	4325	O	HOH E2221	4.078	40.304	56.706	1.00	55.23	O
HETATM	4326	O	HOH E2222	8.822	48.929	57.493	1.00	35.47	O
HETATM	4327	O	HOH E2223	5.809	45.217	50.754	1.00	41.41	O
HETATM	4328	O	HOH E2224	6.995	51.674	51.709	1.00	46.80	O
HETATM	4329	O	HOH E2225	12.219	54.266	55.691	1.00	48.01	O
HETATM	4330	O	HOH E2226	9.398	48.811	60.036	1.00	44.09	O
HETATM	4331	O	HOH E2227	10.744	51.604	59.075	1.00	48.88	O
HETATM	4332	O	HOH E2228	9.256	56.571	48.427	1.00	48.54	O
HETATM	4333	O	HOH E2229	12.189	54.430	46.840	1.00	35.85	O
HETATM	4334	O	HOH E2230	8.202	51.454	56.713	1.00	62.85	O
HETATM	4335	O	HOH E2231	17.203	58.784	53.431	1.00	63.10	O
HETATM	4336	O	HOH E2232	17.863	59.237	49.550	1.00	61.13	O
HETATM	4337	O	HOH E2233	11.583	60.504	43.957	1.00	61.07	O
HETATM	4338	O	HOH E2234	15.361	58.656	45.179	1.00	66.01	O
HETATM	4339	O	HOH E2235	12.566	56.122	44.962	1.00	37.66	O
HETATM	4340	O	HOH E2236	14.927	52.194	47.881	1.00	36.07	O
HETATM	4341	O	HOH E2237	19.217	51.578	42.587	1.00	38.32	O
HETATM	4342	O	HOH E2238	25.776	48.622	49.644	1.00	39.48	O
HETATM	4343	O	HOH E2239	20.028	41.241	63.628	1.00	35.31	O
HETATM	4344	O	HOH E2240	27.476	42.530	69.490	1.00	60.29	O
HETATM	4345	O	HOH E2241	19.456	36.665	71.091	1.00	63.53	O
HETATM	4346	O	HOH E2242	21.314	49.819	70.094	1.00	72.70	O
HETATM	4347	O	HOH E2243	25.757	53.031	66.671	1.00	56.82	O
HETATM	4348	O	HOH E2244	20.313	47.944	67.313	1.00	52.87	O
HETATM	4349	O	HOH E2245	21.905	40.907	42.084	1.00	46.57	O
HETATM	4350	O	HOH E2246	32.468	47.540	38.563	1.00	67.77	O
HETATM	4351	O	HOH E2247	18.620	37.601	47.049	1.00	29.89	O
HETATM	4352	O	HOH E2248	22.113	39.599	44.147	1.00	68.92	O

Figure 1 Table 1b - 66

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HETATM 4353  O   HOH E2249      -0.718  38.386  34.222  1.00 62.08           O
HETATM 4354  O   HOH E2250       1.147  50.711  35.605  1.00 60.99           O
HETATM 4355  O   HOH E2251      14.165  60.960  36.390  1.00 57.75           O
HETATM 4356  O   HOH E2252      14.034  64.537  36.995  1.00 73.40           O
HETATM 4357  O   HOH E2253      36.291  67.373  17.449  1.00 69.48           O
HETATM 4358  O   HOH E2254      21.891  75.150  38.680  1.00 74.50           O
HETATM 4359  O   HOH E2255      25.375  65.330  42.328  1.00 60.24           O
HETATM 4360  O   HOH E2256      40.160  49.407  38.271  1.00 61.66           O
HETATM 4361  O   HOH E2257      50.669  62.527  44.751  1.00 46.42           O
HETATM 4362  O   HOH E2258      54.593  65.922  34.579  1.00 53.30           O
HETATM 4363  O   HOH E2259      16.734  41.736  28.009  1.00 55.01           O
HETATM 4364  O   HOH E2260      10.455  43.879  22.619  1.00 62.92           O
HETATM 4365  O   HOH E2261      10.012  35.701  30.526  1.00 74.68           O
HETATM 4366  O   HOH E2262      17.646  36.020  37.701  1.00 79.05           O
HETATM 4367  O   HOH E2263      29.487  45.031  33.266  1.00 64.55           O
HETATM 4368  O   HOH E2264      30.400  43.433  40.130  1.00 63.56           O
HETATM 4369  O   HOH E2265      25.170  43.601  41.384  1.00 45.07           O
HETATM 4370  O   HOH E2266      10.485  56.144  15.014  1.00 63.46           O
HETATM 4371  O   HOH E2267      16.290  59.617  35.951  1.00 62.28           O
HETATM 4372  O   HOH E2268      -1.826  41.082  43.232  1.00 40.05           O
HETATM 4373  O   HOH E2269      -2.003  25.806  55.938  1.00 65.09           O
HETATM 4374  O   HOH E2270      28.985  38.614  61.826  1.00 51.17           O
HETATM 4375  O   HOH E2271      31.180  41.753  59.870  1.00 65.57           O
HETATM 4376  O   HOH E2272      36.558  45.759  57.951  1.00 79.55           O
HETATM 4377  O   HOH E2273      26.337  54.171  74.097  1.00 74.86           O
HETATM 4378  O   HOH E2274      35.650  72.471  37.114  1.00 82.48           O
HETATM 4379  O   HOH E2275      35.712  73.138  45.975  1.00 80.78           O
HETATM 4380  O   HOH E2276      46.405  63.103  44.212  1.00 56.70           O
HETATM 4381  O   HOH E2277      16.908  57.033  60.333  1.00 87.05           O
HETATM 4382  O   HOH E2278      11.399  51.777  68.307  1.00 55.47           O
HETATM 4383  O   HOH E2279       1.248  48.123  54.497  1.00 68.17           O
HETATM 4384  O   HOH E2280      10.164  53.370  57.168  1.00 57.48           O
HETATM 4385  O   HOH E2281      12.713  56.854  55.827  1.00 56.87           O
HETATM 4386  O   HOH E2282       6.647  54.330  50.647  1.00 69.31           O
HETATM 4387  O   HOH E2283      25.494  53.584  45.418  1.00 60.52           O
HETATM 4388  O   HOH E2284      25.649  53.279  39.234  1.00 43.89           O
HETATM 4389  O   HOH E2285      33.042  51.331  31.222  1.00 65.83           O
HETATM 4390  O   HOH E2286      29.417  48.127  40.409  1.00 41.76           O
HETATM 4391  O   HOH E2287      27.065  50.701  41.824  1.00 41.27           O
HETATM 4392  O   HOH E2288      29.763  41.094  46.369  1.00 81.20           O
HETATM 4393  O   HOH E2289      29.796  40.874  48.818  1.00 42.46           O
HETATM 4394  O   HOH E2290      24.392  39.855  44.878  1.00 51.44           O
HETATM 4395  O   HOH E2291      27.876  46.368  43.491  1.00 35.60           O
END
```

Figure 2 - Table 2a

ATOM	1	N	SER	A	393	23.331	-12.608	29.185	1.00	64.91	N
ATOM	2	CA	SER	A	393	22.856	-13.254	30.442	1.00	64.87	C
ATOM	3	CB	SER	A	393	22.394	-12.186	31.431	1.00	65.00	C
ATOM	4	OG	SER	A	393	21.282	-11.476	30.912	1.00	65.73	O
ATOM	5	C	SER	A	393	21.736	-14.278	30.170	1.00	64.66	C
ATOM	6	O	SER	A	393	20.551	-13.922	30.059	1.00	64.69	O
ATOM	7	N	MET	A	394	22.128	-15.552	30.090	1.00	64.16	N
ATOM	8	CA	MET	A	394	21.257	-16.623	29.594	1.00	63.37	C
ATOM	9	CB	MET	A	394	22.072	-17.572	28.704	1.00	63.73	C
ATOM	10	CG	MET	A	394	21.516	-17.808	27.295	1.00	64.77	C
ATOM	11	SD	MET	A	394	21.114	-19.547	26.929	1.00	66.97	S
ATOM	12	CE	MET	A	394	21.789	-19.729	25.270	1.00	66.12	C
ATOM	13	C	MET	A	394	20.505	-17.374	30.716	1.00	62.24	C
ATOM	14	O	MET	A	394	19.306	-17.163	30.908	1.00	61.94	O
ATOM	15	N	ALA	A	395	21.197	-18.233	31.461	1.00	61.15	N
ATOM	16	CA	ALA	A	395	20.517	-19.078	32.452	1.00	59.74	C
ATOM	17	CB	ALA	A	395	21.134	-20.456	32.480	1.00	59.77	C
ATOM	18	C	ALA	A	395	20.506	-18.466	33.847	1.00	58.87	C
ATOM	19	O	ALA	A	395	21.568	-18.282	34.438	1.00	59.10	O
ATOM	20	N	TRP	A	396	19.305	-18.167	34.362	1.00	57.51	N
ATOM	21	CA	TRP	A	396	19.121	-17.617	35.723	1.00	56.19	C
ATOM	22	CB	TRP	A	396	18.121	-16.464	35.711	1.00	55.50	C
ATOM	23	CG	TRP	A	396	18.606	-15.307	34.942	1.00	54.70	C
ATOM	24	CD1	TRP	A	396	18.291	-14.987	33.644	1.00	52.45	C
ATOM	25	NE1	TRP	A	396	18.963	-13.856	33.266	1.00	52.04	N
ATOM	26	CE2	TRP	A	396	19.728	-13.414	34.314	1.00	52.93	C
ATOM	27	CD2	TRP	A	396	19.534	-14.312	35.388	1.00	53.52	C
ATOM	28	CE3	TRP	A	396	20.216	-14.088	36.591	1.00	52.80	C
ATOM	29	CZ3	TRP	A	396	21.065	-12.994	36.685	1.00	52.12	C
ATOM	30	CH2	TRP	A	396	21.241	-12.113	35.602	1.00	52.52	C
ATOM	31	CZ2	TRP	A	396	20.579	-12.303	34.411	1.00	52.98	C
ATOM	32	C	TRP	A	396	18.657	-18.657	36.745	1.00	55.92	C
ATOM	33	O	TRP	A	396	17.677	-19.363	36.526	1.00	55.91	O
ATOM	34	N	HIS	A	397	19.344	-18.738	37.875	1.00	55.47	N
ATOM	35	CA	HIS	A	397	18.951	-19.699	38.905	1.00	55.42	C
ATOM	36	CB	HIS	A	397	20.134	-20.591	39.290	1.00	55.39	C
ATOM	37	CG	HIS	A	397	20.797	-21.229	38.114	1.00	56.27	C
ATOM	38	ND1	HIS	A	397	21.680	-20.549	37.301	1.00	57.69	N
ATOM	39	CE1	HIS	A	397	22.082	-21.347	36.326	1.00	57.94	C
ATOM	40	NE2	HIS	A	397	21.490	-22.517	36.479	1.00	58.33	N
ATOM	41	CD2	HIS	A	397	20.673	-22.468	37.583	1.00	57.68	C
ATOM	42	C	HIS	A	397	18.373	-18.985	40.119	1.00	54.91	C
ATOM	43	O	HIS	A	397	18.920	-17.978	40.564	1.00	54.73	O
ATOM	44	N	LEU	A	398	17.248	-19.489	40.623	1.00	54.66	N
ATOM	45	CA	LEU	A	398	16.645	-18.951	41.840	1.00	54.65	C
ATOM	46	CB	LEU	A	398	15.221	-19.476	42.042	1.00	54.38	C
ATOM	47	CG	LEU	A	398	14.515	-18.973	43.317	1.00	55.03	C
ATOM	48	CD1	LEU	A	398	14.202	-17.474	43.233	1.00	52.73	C
ATOM	49	CD2	LEU	A	398	13.247	-19.770	43.597	1.00	54.20	C
ATOM	50	C	LEU	A	398	17.516	-19.316	43.034	1.00	54.73	C
ATOM	51	O	LEU	A	398	17.793	-20.484	43.254	1.00	54.77	O
ATOM	52	N	GLY	A	399	17.965	-18.303	43.774	1.00	55.13	N
ATOM	53	CA	GLY	A	399	18.794	-18.491	44.958	1.00	55.49	C
ATOM	54	C	GLY	A	399	20.053	-19.278	44.657	1.00	56.43	C
ATOM	55	O	GLY	A	399	20.632	-19.140	43.581	1.00	57.15	O
ATOM	56	N	ILE	A	400	20.472	-20.101	45.619	1.00	56.67	N
ATOM	57	CA	ILE	A	400	21.600	-21.013	45.466	1.00	56.72	C
ATOM	58	CB	ILE	A	400	22.862	-20.550	46.265	1.00	56.83	C
ATOM	59	CG1	ILE	A	400	22.616	-20.606	47.772	1.00	56.75	C
ATOM	60	CD1	ILE	A	400	23.779	-20.099	48.612	1.00	57.76	C
ATOM	61	CG2	ILE	A	400	23.304	-19.135	45.837	1.00	57.15	C
ATOM	62	C	ILE	A	400	21.165	-22.400	45.937	1.00	56.82	C
ATOM	63	O	ILE	A	400	20.219	-22.533	46.714	1.00	57.36	O
ATOM	64	N	ARG	A	401	21.855	-23.420	45.448	1.00	56.46	N

Figure 2 Table 2a - 2

ATOM	65	CA	ARG	A	401	21.533	-24.784	45.750	1.00	56.52	C
ATOM	66	CB	ARG	A	401	21.312	-25.570	44.452	1.00	56.99	C
ATOM	67	CG	ARG	A	401	20.052	-25.182	43.696	1.00	58.46	C
ATOM	68	CD	ARG	A	401	19.786	-26.085	42.508	1.00	58.98	C
ATOM	69	NE	ARG	A	401	21.004	-26.455	41.789	1.00	62.60	N
ATOM	70	CZ	ARG	A	401	21.594	-25.724	40.840	1.00	64.47	C
ATOM	71	NH1	ARG	A	401	21.098	-24.540	40.466	1.00	65.82	N
ATOM	72	NH2	ARG	A	401	22.698	-26.181	40.263	1.00	64.43	N
ATOM	73	C	ARG	A	401	22.671	-25.413	46.544	1.00	56.19	C
ATOM	74	O	ARG	A	401	23.826	-24.972	46.454	1.00	56.11	O
ATOM	75	N	SER	A	402	22.335	-26.453	47.305	1.00	55.34	N
ATOM	76	CA	SER	A	402	23.290	-27.141	48.154	1.00	54.96	C
ATOM	77	CB	SER	A	402	23.483	-26.366	49.455	1.00	54.81	C
ATOM	78	OG	SER	A	402	24.505	-26.942	50.245	1.00	55.02	O
ATOM	79	C	SER	A	402	22.823	-28.566	48.466	1.00	54.73	C
ATOM	80	O	SER	A	402	21.629	-28.833	48.589	1.00	54.66	O
ATOM	81	N	GLN	A	403	23.776	-29.478	48.579	1.00	54.44	N
ATOM	82	CA	GLN	A	403	23.474	-30.843	48.977	1.00	54.47	C
ATOM	83	CB	GLN	A	403	24.003	-31.845	47.942	1.00	54.39	C
ATOM	84	CG	GLN	A	403	23.276	-31.722	46.602	1.00	54.82	C
ATOM	85	CD	GLN	A	403	23.921	-32.506	45.472	1.00	54.97	C
ATOM	86	OE1	GLN	A	403	24.773	-33.366	45.694	1.00	54.59	O
ATOM	87	NE2	GLN	A	403	23.509	-32.205	44.244	1.00	55.93	N
ATOM	88	C	GLN	A	403	24.004	-31.124	50.380	1.00	54.27	C
ATOM	89	O	GLN	A	403	24.189	-32.277	50.766	1.00	54.35	O
ATOM	90	N	SER	A	404	24.231	-30.057	51.144	1.00	54.13	N
ATOM	91	CA	SER	A	404	24.535	-30.188	52.568	1.00	54.12	C
ATOM	92	CB	SER	A	404	25.156	-28.904	53.112	1.00	54.13	C
ATOM	93	OG	SER	A	404	26.213	-28.470	52.273	1.00	54.44	O
ATOM	94	C	SER	A	404	23.269	-30.546	53.338	1.00	53.94	C
ATOM	95	O	SER	A	404	22.158	-30.372	52.845	1.00	53.50	O
ATOM	96	N	ARG	A	405	23.436	-31.079	54.536	1.00	54.68	N
ATOM	97	CA	ARG	A	405	22.284	-31.359	55.390	1.00	55.60	C
ATOM	98	CB	ARG	A	405	22.728	-32.002	56.707	1.00	55.47	C
ATOM	99	CG	ARG	A	405	23.008	-33.480	56.633	1.00	57.01	C
ATOM	100	CD	ARG	A	405	23.658	-33.964	57.928	1.00	60.64	C
ATOM	101	NE	ARG	A	405	25.126	-33.913	57.859	1.00	65.29	N
ATOM	102	CZ	ARG	A	405	25.942	-33.709	58.899	1.00	66.70	C
ATOM	103	NH1	ARG	A	405	25.458	-33.510	60.120	1.00	68.25	N
ATOM	104	NH2	ARG	A	405	27.258	-33.692	58.721	1.00	67.07	N
ATOM	105	C	ARG	A	405	21.502	-30.059	55.658	1.00	55.41	C
ATOM	106	O	ARG	A	405	22.105	-29.029	55.970	1.00	55.07	O
ATOM	107	N	PRO	A	406	20.162	-30.104	55.521	1.00	55.67	N
ATOM	108	CA	PRO	A	406	19.313	-28.940	55.799	1.00	56.11	C
ATOM	109	CB	PRO	A	406	17.903	-29.534	55.849	1.00	55.92	C
ATOM	110	CG	PRO	A	406	17.970	-30.746	55.017	1.00	55.95	C
ATOM	111	CD	PRO	A	406	19.373	-31.273	55.094	1.00	55.95	C
ATOM	112	C	PRO	A	406	19.649	-28.278	57.136	1.00	56.41	C
ATOM	113	O	PRO	A	406	19.773	-27.060	57.206	1.00	56.05	O
ATOM	114	N	ASN	A	407	19.807	-29.092	58.175	1.00	57.05	N
ATOM	115	CA	ASN	A	407	20.125	-28.599	59.512	1.00	57.68	C
ATOM	116	CB	ASN	A	407	20.030	-29.716	60.558	1.00	57.94	C
ATOM	117	CG	ASN	A	407	20.424	-31.099	60.001	1.00	59.95	C
ATOM	118	OD1	ASN	A	407	20.141	-31.424	58.837	1.00	62.23	O
ATOM	119	ND2	ASN	A	407	21.064	-31.921	60.839	1.00	59.83	N
ATOM	120	C	ASN	A	407	21.487	-27.913	59.540	1.00	57.64	C
ATOM	121	O	ASN	A	407	21.674	-26.930	60.266	1.00	57.89	O
ATOM	122	N	ASP	A	408	22.423	-28.419	58.734	1.00	57.21	N
ATOM	123	CA	ASP	A	408	23.727	-27.773	58.563	1.00	56.92	C
ATOM	124	CB	ASP	A	408	24.678	-28.648	57.738	1.00	56.83	C
ATOM	125	CG	ASP	A	408	25.051	-29.943	58.436	1.00	57.76	C
ATOM	126	OD1	ASP	A	408	24.645	-30.154	59.603	1.00	59.04	O
ATOM	127	OD2	ASP	A	408	25.762	-30.762	57.810	1.00	58.54	O
ATOM	128	C	ASP	A	408	23.571	-26.405	57.889	1.00	56.33	C
ATOM	129	O	ASP	A	408	24.136	-25.414	58.347	1.00	56.15	O
ATOM	130	N	ILE	A	409	22.800	-26.367	56.803	1.00	55.88	N
ATOM	131	CA	ILE	A	409	22.593	-25.140	56.035	1.00	55.08	C

Figure 2 Table 2a - 3

ATOM	132	CB	ILE	A	409	21.638	-25.362	54.841	1.00	55.13	C
ATOM	133	CG1	ILE	A	409	22.183	-26.448	53.902	1.00	53.29	C
ATOM	134	CD1	ILE	A	409	21.176	-26.952	52.891	1.00	51.28	C
ATOM	135	CG2	ILE	A	409	21.409	-24.061	54.090	1.00	54.31	C
ATOM	136	C	ILE	A	409	22.045	-24.037	56.924	1.00	55.33	C
ATOM	137	O	ILE	A	409	22.641	-22.961	57.009	1.00	55.24	O
ATOM	138	N	MET	A	410	20.932	-24.325	57.605	1.00	55.42	N
ATOM	139	CA	MET	A	410	20.273	-23.371	58.495	1.00	55.93	C
ATOM	140	CB	MET	A	410	18.960	-23.941	59.031	1.00	56.00	C
ATOM	141	CG	MET	A	410	17.911	-24.192	57.984	1.00	57.12	C
ATOM	142	SD	MET	A	410	17.365	-22.702	57.127	1.00	59.71	S
ATOM	143	CE	MET	A	410	18.412	-22.697	55.696	1.00	61.04	C
ATOM	144	C	MET	A	410	21.147	-22.930	59.666	1.00	56.10	C
ATOM	145	O	MET	A	410	21.118	-21.765	60.057	1.00	56.16	O
ATOM	146	N	ALA	A	411	21.905	-23.865	60.230	1.00	56.21	N
ATOM	147	CA	ALA	A	411	22.814	-23.536	61.321	1.00	56.34	C
ATOM	148	CB	ALA	A	411	23.399	-24.799	61.959	1.00	55.75	C
ATOM	149	C	ALA	A	411	23.915	-22.619	60.805	1.00	56.58	C
ATOM	150	O	ALA	A	411	24.262	-21.640	61.458	1.00	56.95	O
ATOM	151	N	GLU	A	412	24.447	-22.919	59.625	1.00	56.73	N
ATOM	152	CA	GLU	A	412	25.519	-22.110	59.075	1.00	57.31	C
ATOM	153	CB	GLU	A	412	26.251	-22.843	57.950	1.00	57.36	C
ATOM	154	CG	GLU	A	412	27.325	-23.786	58.442	1.00	57.91	C
ATOM	155	CD	GLU	A	412	28.437	-23.097	59.238	1.00	59.52	C
ATOM	156	OE1	GLU	A	412	29.137	-22.231	58.670	1.00	59.94	O
ATOM	157	OE2	GLU	A	412	28.634	-23.451	60.425	1.00	60.50	O
ATOM	158	C	GLU	A	412	25.081	-20.705	58.635	1.00	57.62	C
ATOM	159	O	GLU	A	412	25.851	-19.749	58.777	1.00	57.51	O
ATOM	160	N	VAL	A	413	23.857	-20.563	58.127	1.00	58.04	N
ATOM	161	CA	VAL	A	413	23.394	-19.215	57.769	1.00	58.86	C
ATOM	162	CB	VAL	A	413	22.139	-19.160	56.810	1.00	58.97	C
ATOM	163	CG1	VAL	A	413	22.231	-20.220	55.696	1.00	58.87	C
ATOM	164	CG2	VAL	A	413	20.836	-19.286	57.581	1.00	60.16	C
ATOM	165	C	VAL	A	413	23.205	-18.365	59.026	1.00	58.91	C
ATOM	166	O	VAL	A	413	23.451	-17.153	58.999	1.00	59.05	O
ATOM	167	N	CYS	A	414	22.806	-19.024	60.114	1.00	58.69	N
ATOM	168	CA	CYS	A	414	22.589	-18.383	61.412	1.00	59.16	C
ATOM	169	CB	CYS	A	414	21.897	-19.353	62.375	1.00	59.05	C
ATOM	170	SG	CYS	A	414	20.125	-19.370	62.140	1.00	60.01	S
ATOM	171	C	CYS	A	414	23.883	-17.886	62.039	1.00	59.20	C
ATOM	172	O	CYS	A	414	23.933	-16.762	62.550	1.00	58.94	O
ATOM	173	N	ARG	A	415	24.916	-18.731	62.010	1.00	59.18	N
ATOM	174	CA	ARG	A	415	26.250	-18.317	62.414	1.00	59.28	C
ATOM	175	CB	ARG	A	415	27.253	-19.468	62.313	1.00	59.35	C
ATOM	176	CG	ARG	A	415	28.602	-19.183	62.985	1.00	59.35	C
ATOM	177	CD	ARG	A	415	29.686	-20.186	62.577	1.00	59.14	C
ATOM	178	NE	ARG	A	415	29.805	-20.301	61.123	1.00	60.06	N
ATOM	179	CZ	ARG	A	415	30.227	-19.324	60.318	1.00	60.71	C
ATOM	180	NH1	ARG	A	415	30.573	-18.142	60.818	1.00	61.23	N
ATOM	181	NH2	ARG	A	415	30.285	-19.522	59.006	1.00	60.25	N
ATOM	182	C	ARG	A	415	26.708	-17.123	61.578	1.00	59.26	C
ATOM	183	O	ARG	A	415	27.205	-16.150	62.131	1.00	59.62	O
ATOM	184	N	ALA	A	416	26.523	-17.190	60.259	1.00	59.17	N
ATOM	185	CA	ALA	A	416	26.870	-16.065	59.364	1.00	59.38	C
ATOM	186	CB	ALA	A	416	26.618	-16.426	57.913	1.00	59.01	C
ATOM	187	C	ALA	A	416	26.161	-14.757	59.707	1.00	59.33	C
ATOM	188	O	ALA	A	416	26.798	-13.704	59.749	1.00	59.59	O
ATOM	189	N	ILE	A	417	24.853	-14.825	59.945	1.00	59.34	N
ATOM	190	CA	ILE	A	417	24.072	-13.643	60.349	1.00	59.71	C
ATOM	191	CB	ILE	A	417	22.566	-13.989	60.586	1.00	59.59	C
ATOM	192	CG1	ILE	A	417	21.852	-14.294	59.267	1.00	58.13	C
ATOM	193	CD1	ILE	A	417	20.660	-15.235	59.434	1.00	56.16	C
ATOM	194	CG2	ILE	A	417	21.834	-12.841	61.294	1.00	59.88	C
ATOM	195	C	ILE	A	417	24.667	-12.976	61.601	1.00	60.09	C
ATOM	196	O	ILE	A	417	24.899	-11.765	61.611	1.00	60.18	O
ATOM	197	N	LYS	A	418	24.925	-13.782	62.632	1.00	60.44	N
ATOM	198	CA	LYS	A	418	25.468	-13.303	63.897	1.00	61.05	C

Figure 2 Table 2a - 4

ATOM	199	CB	LYS	A	418	25.495	-14.434	64.931	1.00	61.03	C
ATOM	200	CG	LYS	A	418	25.492	-13.946	66.366	1.00	61.24	C
ATOM	201	CD	LYS	A	418	25.909	-15.026	67.342	1.00	62.16	C
ATOM	202	CE	LYS	A	418	26.205	-14.417	68.714	1.00	63.38	C
ATOM	203	NZ	LYS	A	418	26.724	-15.408	69.716	1.00	63.97	N
ATOM	204	C	LYS	A	418	26.863	-12.705	63.708	1.00	61.53	C
ATOM	205	O	LYS	A	418	27.164	-11.622	64.217	1.00	61.65	O
ATOM	206	N	GLN	A	419	27.703	-13.411	62.960	1.00	62.11	N
ATOM	207	CA	GLN	A	419	29.030	-12.926	62.613	1.00	62.69	C
ATOM	208	CB	GLN	A	419	29.688	-13.887	61.616	1.00	62.89	C
ATOM	209	CG	GLN	A	419	31.210	-13.930	61.676	1.00	64.11	C
ATOM	210	CD	GLN	A	419	31.731	-14.582	62.946	1.00	66.03	C
ATOM	211	OE1	GLN	A	419	31.093	-15.479	63.517	1.00	67.35	O
ATOM	212	NE2	GLN	A	419	32.900	-14.139	63.396	1.00	66.71	N
ATOM	213	C	GLN	A	419	28.941	-11.518	62.020	1.00	62.86	C
ATOM	214	O	GLN	A	419	29.608	-10.597	62.492	1.00	63.24	O
ATOM	215	N	LEU	A	420	28.085	-11.360	61.009	1.00	62.79	N
ATOM	216	CA	LEU	A	420	27.902	-10.102	60.280	1.00	62.44	C
ATOM	217	CB	LEU	A	420	27.106	-10.379	59.003	1.00	62.62	C
ATOM	218	CG	LEU	A	420	27.785	-10.542	57.637	1.00	62.94	C
ATOM	219	CD1	LEU	A	420	29.219	-11.059	57.720	1.00	63.22	C
ATOM	220	CD2	LEU	A	420	26.928	-11.448	56.766	1.00	62.46	C
ATOM	221	C	LEU	A	420	27.196	-8.997	61.060	1.00	62.33	C
ATOM	222	O	LEU	A	420	27.058	-7.877	60.552	1.00	62.51	O
ATOM	223	N	ASP	A	421	26.737	-9.303	62.275	1.00	62.20	N
ATOM	224	CA	ASP	A	421	26.005	-8.336	63.115	1.00	61.98	C
ATOM	225	CB	ASP	A	421	26.824	-7.059	63.337	1.00	62.18	C
ATOM	226	CG	ASP	A	421	27.605	-7.091	64.620	1.00	63.87	C
ATOM	227	OD1	ASP	A	421	27.108	-7.681	65.612	1.00	64.86	O
ATOM	228	OD2	ASP	A	421	28.718	-6.518	64.640	1.00	66.04	O
ATOM	229	C	ASP	A	421	24.625	-7.968	62.572	1.00	61.41	C
ATOM	230	O	ASP	A	421	24.106	-6.873	62.846	1.00	61.08	O
ATOM	231	N	TYR	A	422	24.049	-8.868	61.777	1.00	60.65	N
ATOM	232	CA	TYR	A	422	22.676	-8.706	61.324	1.00	59.91	C
ATOM	233	CB	TYR	A	422	22.408	-9.495	60.038	1.00	60.20	C
ATOM	234	CG	TYR	A	422	23.179	-9.053	58.808	1.00	60.24	C
ATOM	235	CD1	TYR	A	422	23.021	-9.722	57.603	1.00	60.74	C
ATOM	236	CE1	TYR	A	422	23.725	-9.328	56.457	1.00	61.64	C
ATOM	237	CZ	TYR	A	422	24.598	-8.254	56.520	1.00	61.48	C
ATOM	238	OH	TYR	A	422	25.288	-7.880	55.392	1.00	62.26	O
ATOM	239	CE2	TYR	A	422	24.781	-7.567	57.710	1.00	61.03	C
ATOM	240	CD2	TYR	A	422	24.072	-7.974	58.850	1.00	61.60	C
ATOM	241	C	TYR	A	422	21.766	-9.186	62.449	1.00	59.15	C
ATOM	242	O	TYR	A	422	22.209	-9.911	63.340	1.00	59.28	O
ATOM	243	N	GLU	A	423	20.510	-8.757	62.447	1.00	58.13	N
ATOM	244	CA	GLU	A	423	19.573	-9.287	63.426	1.00	57.25	C
ATOM	245	CB	GLU	A	423	18.939	-8.193	64.287	1.00	57.34	C
ATOM	246	CG	GLU	A	423	18.057	-7.200	63.576	1.00	57.64	C
ATOM	247	CD	GLU	A	423	17.940	-5.876	64.357	1.00	59.77	C
ATOM	248	OE1	GLU	A	423	17.928	-5.916	65.608	1.00	57.51	O
ATOM	249	OE2	GLU	A	423	17.866	-4.795	63.712	1.00	60.42	O
ATOM	250	C	GLU	A	423	18.550	-10.167	62.731	1.00	56.53	C
ATOM	251	O	GLU	A	423	18.247	-9.973	61.548	1.00	56.23	O
ATOM	252	N	TRP	A	424	18.062	-11.167	63.454	1.00	55.36	N
ATOM	253	CA	TRP	A	424	17.186	-12.154	62.857	1.00	54.60	C
ATOM	254	CB	TRP	A	424	18.001	-13.299	62.221	1.00	55.14	C
ATOM	255	CG	TRP	A	424	18.557	-14.312	63.203	1.00	55.92	C
ATOM	256	CD1	TRP	A	424	18.152	-15.606	63.353	1.00	56.10	C
ATOM	257	NE1	TRP	A	424	18.889	-16.225	64.343	1.00	56.72	N
ATOM	258	CE2	TRP	A	424	19.790	-15.329	64.855	1.00	57.37	C
ATOM	259	CD2	TRP	A	424	19.609	-14.106	64.165	1.00	56.19	C
ATOM	260	CE3	TRP	A	424	20.421	-13.012	64.502	1.00	55.47	C
ATOM	261	CZ3	TRP	A	424	21.367	-13.164	65.504	1.00	56.18	C
ATOM	262	CH2	TRP	A	424	21.522	-14.392	66.179	1.00	57.43	C
ATOM	263	CZ2	TRP	A	424	20.748	-15.487	65.867	1.00	57.96	C
ATOM	264	C	TRP	A	424	16.117	-12.698	63.795	1.00	53.55	C
ATOM	265	O	TRP	A	424	16.199	-12.581	65.014	1.00	52.91	O

Figure 2 Table 2a - 5

ATOM	266	N	LYS	A	425	15.107	-13.290	63.174	1.00	52.81	N
ATOM	267	CA	LYS	A	425	14.053	-14.004	63.845	1.00	52.15	C
ATOM	268	CB	LYS	A	425	12.776	-13.183	63.813	1.00	52.02	C
ATOM	269	CG	LYS	A	425	12.685	-12.252	64.975	1.00	52.47	C
ATOM	270	CD	LYS	A	425	11.633	-11.208	64.793	1.00	53.95	C
ATOM	271	CE	LYS	A	425	11.823	-10.143	65.861	1.00	55.20	C
ATOM	272	NZ	LYS	A	425	11.394	-8.823	65.372	1.00	57.75	N
ATOM	273	C	LYS	A	425	13.844	-15.317	63.127	1.00	51.60	C
ATOM	274	O	LYS	A	425	13.881	-15.378	61.902	1.00	52.12	O
ATOM	275	N	VAL	A	426	13.621	-16.367	63.901	1.00	51.40	N
ATOM	276	CA	VAL	A	426	13.343	-17.688	63.372	1.00	50.48	C
ATOM	277	CB	VAL	A	426	14.029	-18.789	64.234	1.00	50.52	C
ATOM	278	CG1	VAL	A	426	13.725	-20.209	63.689	1.00	48.46	C
ATOM	279	CG2	VAL	A	426	15.544	-18.526	64.304	1.00	48.63	C
ATOM	280	C	VAL	A	426	11.832	-17.869	63.325	1.00	50.80	C
ATOM	281	O	VAL	A	426	11.184	-18.082	64.347	1.00	51.07	O
ATOM	282	N	VAL	A	427	11.275	-17.741	62.129	1.00	51.07	N
ATOM	283	CA	VAL	A	427	9.849	-18.003	61.906	1.00	50.99	C
ATOM	284	CB	VAL	A	427	9.365	-17.392	60.548	1.00	50.90	C
ATOM	285	CG1	VAL	A	427	7.844	-17.416	60.441	1.00	50.28	C
ATOM	286	CG2	VAL	A	427	9.870	-15.956	60.394	1.00	50.13	C
ATOM	287	C	VAL	A	427	9.585	-19.521	61.983	1.00	50.86	C
ATOM	288	O	VAL	A	427	8.868	-19.962	62.872	1.00	50.81	O
ATOM	289	N	ASN	A	428	10.193	-20.272	61.052	1.00	50.90	N
ATOM	290	CA	ASN	A	428	10.222	-21.744	60.948	1.00	51.69	C
ATOM	291	CB	ASN	A	428	9.836	-22.191	59.519	1.00	52.41	C
ATOM	292	CG	ASN	A	428	8.416	-21.904	59.196	1.00	54.24	C
ATOM	293	OD1	ASN	A	428	7.529	-22.145	60.023	1.00	59.28	O
ATOM	294	ND2	ASN	A	428	8.171	-21.372	58.016	1.00	53.12	N
ATOM	295	C	ASN	A	428	11.648	-22.227	61.076	1.00	51.43	C
ATOM	296	O	ASN	A	428	12.576	-21.446	60.852	1.00	51.55	O
ATOM	297	N	PRO	A	429	11.842	-23.535	61.341	1.00	50.89	N
ATOM	298	CA	PRO	A	429	13.174	-24.098	61.108	1.00	50.57	C
ATOM	299	CB	PRO	A	429	12.952	-25.601	61.301	1.00	50.30	C
ATOM	300	CG	PRO	A	429	11.839	-25.678	62.267	1.00	49.35	C
ATOM	301	CD	PRO	A	429	10.918	-24.548	61.887	1.00	50.69	C
ATOM	302	C	PRO	A	429	13.750	-23.817	59.713	1.00	50.57	C
ATOM	303	O	PRO	A	429	14.964	-23.919	59.529	1.00	50.96	O
ATOM	304	N	TYR	A	430	12.917	-23.460	58.738	1.00	50.33	N
ATOM	305	CA	TYR	A	430	13.451	-23.170	57.399	1.00	50.18	C
ATOM	306	CB	TYR	A	430	12.989	-24.217	56.377	1.00	49.70	C
ATOM	307	CG	TYR	A	430	13.275	-25.611	56.826	1.00	48.38	C
ATOM	308	CD1	TYR	A	430	12.233	-26.476	57.131	1.00	48.22	C
ATOM	309	CE1	TYR	A	430	12.485	-27.756	57.578	1.00	48.32	C
ATOM	310	CZ	TYR	A	430	13.787	-28.168	57.736	1.00	47.63	C
ATOM	311	OH	TYR	A	430	14.018	-29.430	58.175	1.00	48.36	O
ATOM	312	CE2	TYR	A	430	14.847	-27.319	57.455	1.00	47.92	C
ATOM	313	CD2	TYR	A	430	14.585	-26.047	57.007	1.00	46.29	C
ATOM	314	C	TYR	A	430	13.143	-21.780	56.881	1.00	50.68	C
ATOM	315	O	TYR	A	430	13.300	-21.517	55.695	1.00	50.82	O
ATOM	316	N	TYR	A	431	12.713	-20.892	57.771	1.00	51.41	N
ATOM	317	CA	TYR	A	431	12.292	-19.567	57.372	1.00	51.90	C
ATOM	318	CB	TYR	A	431	10.769	-19.533	57.184	1.00	51.99	C
ATOM	319	CG	TYR	A	431	10.176	-18.201	56.793	1.00	53.41	C
ATOM	320	CD1	TYR	A	431	10.907	-17.258	56.058	1.00	54.10	C
ATOM	321	CE1	TYR	A	431	10.350	-16.048	55.695	1.00	53.63	C
ATOM	322	CZ	TYR	A	431	9.047	-15.759	56.061	1.00	55.06	C
ATOM	323	OH	TYR	A	431	8.483	-14.546	55.726	1.00	56.02	O
ATOM	324	CE2	TYR	A	431	8.300	-16.671	56.770	1.00	54.14	C
ATOM	325	CD2	TYR	A	431	8.866	-17.891	57.128	1.00	54.02	C
ATOM	326	C	TYR	A	431	12.804	-18.531	58.372	1.00	52.39	C
ATOM	327	O	TYR	A	431	12.495	-18.568	59.574	1.00	51.92	O
ATOM	328	N	LEU	A	432	13.614	-17.618	57.844	1.00	53.01	N
ATOM	329	CA	LEU	A	432	14.258	-16.592	58.632	1.00	53.56	C
ATOM	330	CB	LEU	A	432	15.773	-16.747	58.583	1.00	53.49	C
ATOM	331	CG	LEU	A	432	16.451	-18.053	58.984	1.00	53.00	C
ATOM	332	CD1	LEU	A	432	17.942	-17.801	58.931	1.00	52.17	C

Figure 2 Table 2a - 6

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ATOM    333  CD2 LEU A 432      16.025 -18.548  60.371  1.00 51.39           C
ATOM    334  C   LEU A 432      13.932 -15.237  58.089  1.00 54.19           C
ATOM    335  O   LEU A 432      13.999 -15.006  56.886  1.00 53.88           O
ATOM    336  N   ARG A 433      13.574 -14.347  59.003  1.00 55.63           N
ATOM    337  CA  ARG A 433      13.472 -12.920  58.740  1.00 56.34           C
ATOM    338  CB  ARG A 433      12.244 -12.357  59.460  1.00 57.05           C
ATOM    339  CG  ARG A 433      11.165 -11.789  58.529  1.00 60.59           C
ATOM    340  CD  ARG A 433       9.991 -12.731  58.276  1.00 63.42           C
ATOM    341  NE  ARG A 433       8.810 -12.376  59.078  1.00 65.06           N
ATOM    342  CZ  ARG A 433       7.564 -12.809  58.833  1.00 66.09           C
ATOM    343  NH1 ARG A 433       7.315 -13.609  57.789  1.00 65.32           N
ATOM    344  NH2 ARG A 433       6.560 -12.451  59.632  1.00 64.39           N
ATOM    345  C   ARG A 433      14.758 -12.271  59.268  1.00 56.08           C
ATOM    346  O   ARG A 433      15.178 -12.571  60.385  1.00 55.76           O
ATOM    347  N   VAL A 434      15.406 -11.427  58.459  1.00 56.24           N
ATOM    348  CA  VAL A 434      16.634 -10.726  58.883  1.00 56.14           C
ATOM    349  CB  VAL A 434      17.963 -11.399  58.367  1.00 56.16           C
ATOM    350  CG1 VAL A 434      17.717 -12.814  57.857  1.00 56.36           C
ATOM    351  CG2 VAL A 434      18.636 -10.588  57.312  1.00 56.15           C
ATOM    352  C   VAL A 434      16.615  -9.215  58.601  1.00 56.53           C
ATOM    353  O   VAL A 434      15.990  -8.759  57.646  1.00 56.15           O
ATOM    354  N   ARG A 435      17.303  -8.463  59.462  1.00 56.87           N
ATOM    355  CA  ARG A 435      17.352  -7.017  59.433  1.00 57.46           C
ATOM    356  CB  ARG A 435      16.410  -6.468  60.497  1.00 57.84           C
ATOM    357  CG  ARG A 435      16.163  -4.968  60.461  1.00 58.33           C
ATOM    358  CD  ARG A 435      15.069  -4.628  61.453  1.00 60.62           C
ATOM    359  NE  ARG A 435      14.963  -3.192  61.716  1.00 62.87           N
ATOM    360  CZ  ARG A 435      15.338  -2.611  62.854  1.00 63.62           C
ATOM    361  NH1 ARG A 435      15.851  -3.327  63.849  1.00 64.36           N
ATOM    362  NH2 ARG A 435      15.195  -1.308  63.001  1.00 64.12           N
ATOM    363  C   ARG A 435      18.784  -6.519  59.674  1.00 57.96           C
ATOM    364  O   ARG A 435      19.527  -7.077  60.487  1.00 58.31           O
ATOM    365  N   ARG A 436      19.158  -5.454  58.975  1.00 58.11           N
ATOM    366  CA  ARG A 436      20.531  -5.002  58.936  1.00 58.34           C
ATOM    367  CB  ARG A 436      21.113  -5.375  57.573  1.00 58.39           C
ATOM    368  CG  ARG A 436      22.610  -5.266  57.460  1.00 59.57           C
ATOM    369  CD  ARG A 436      23.078  -3.884  57.032  1.00 60.60           C
ATOM    370  NE  ARG A 436      23.204  -3.758  55.582  1.00 62.38           N
ATOM    371  CZ  ARG A 436      22.396  -3.038  54.804  1.00 62.52           C
ATOM    372  NH1 ARG A 436      21.362  -2.372  55.323  1.00 61.53           N
ATOM    373  NH2 ARG A 436      22.627  -2.985  53.499  1.00 61.49           N
ATOM    374  C   ARG A 436      20.535  -3.497  59.091  1.00 58.56           C
ATOM    375  O   ARG A 436      19.721  -2.826  58.462  1.00 58.89           O
ATOM    376  N   LYS A 437      21.431  -2.960  59.921  1.00 58.83           N
ATOM    377  CA  LYS A 437      21.627  -1.507  59.971  1.00 59.00           C
ATOM    378  CB  LYS A 437      21.848  -0.987  61.391  1.00 58.95           C
ATOM    379  CG  LYS A 437      21.898   0.548  61.465  1.00 59.20           C
ATOM    380  CD  LYS A 437      22.307   1.076  62.839  1.00 58.77           C
ATOM    381  CE  LYS A 437      22.265   2.601  62.863  1.00 59.37           C
ATOM    382  NZ  LYS A 437      22.766   3.169  64.144  1.00 59.35           N
ATOM    383  C   LYS A 437      22.814  -1.147  59.099  1.00 59.36           C
ATOM    384  O   LYS A 437      23.889  -1.726  59.256  1.00 59.58           O
ATOM    385  N   ASN A 438      22.603  -0.203  58.178  1.00 59.45           N
ATOM    386  CA  ASN A 438      23.617   0.207  57.216  1.00 59.58           C
ATOM    387  CB  ASN A 438      22.957   0.949  56.051  1.00 59.63           C
ATOM    388  CG  ASN A 438      23.906   1.193  54.897  1.00 59.62           C
ATOM    389  OD1 ASN A 438      24.769   2.070  54.956  1.00 59.24           O
ATOM    390  ND2 ASN A 438      23.744   0.417  53.828  1.00 60.07           N
ATOM    391  C   ASN A 438      24.715   1.063  57.866  1.00 60.00           C
ATOM    392  O   ASN A 438      24.470   2.215  58.249  1.00 59.87           O
ATOM    393  N   PRO A 439      25.936   0.501  57.980  1.00 60.34           N
ATOM    394  CA  PRO A 439      27.013   1.164  58.725  1.00 60.43           C
ATOM    395  CB  PRO A 439      28.176   0.158  58.661  1.00 60.44           C
ATOM    396  CG  PRO A 439      27.847  -0.775  57.553  1.00 60.63           C
ATOM    397  CD  PRO A 439      26.358  -0.801  57.423  1.00 60.37           C
ATOM    398  C   PRO A 439      27.425   2.525  58.163  1.00 60.50           C
ATOM    399  O   PRO A 439      28.077   3.303  58.868  1.00 60.72           O
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Figure 2 Table 2a - 7

ATOM	400	N	VAL	A	440	27.040	2.820	56.923	1.00	60.46	N
ATOM	401	CA	VAL	A	440	27.340	4.121	56.311	1.00	60.30	C
ATOM	402	CB	VAL	A	440	27.817	3.982	54.827	1.00	60.16	C
ATOM	403	CG1	VAL	A	440	28.037	5.345	54.192	1.00	59.87	C
ATOM	404	CG2	VAL	A	440	29.098	3.153	54.740	1.00	59.81	C
ATOM	405	C	VAL	A	440	26.143	5.076	56.401	1.00	60.39	C
ATOM	406	O	VAL	A	440	26.276	6.209	56.863	1.00	60.34	O
ATOM	407	N	THR	A	441	24.979	4.598	55.976	1.00	60.65	N
ATOM	408	CA	THR	A	441	23.794	5.441	55.798	1.00	60.95	C
ATOM	409	CB	THR	A	441	22.933	4.939	54.619	1.00	61.13	C
ATOM	410	OG1	THR	A	441	23.767	4.302	53.645	1.00	62.07	O
ATOM	411	CG2	THR	A	441	22.191	6.095	53.970	1.00	61.24	C
ATOM	412	C	THR	A	441	22.898	5.488	57.030	1.00	60.80	C
ATOM	413	O	THR	A	441	22.071	6.396	57.159	1.00	60.55	O
ATOM	414	N	SER	A	442	23.045	4.497	57.913	1.00	60.52	N
ATOM	415	CA	SER	A	442	22.207	4.368	59.106	1.00	60.45	C
ATOM	416	CB	SER	A	442	22.229	5.656	59.951	1.00	60.49	C
ATOM	417	OG	SER	A	442	23.546	6.039	60.305	1.00	60.50	O
ATOM	418	C	SER	A	442	20.762	3.984	58.772	1.00	60.34	C
ATOM	419	O	SER	A	442	19.858	4.208	59.580	1.00	60.71	O
ATOM	420	N	THR	A	443	20.537	3.421	57.586	1.00	59.92	N
ATOM	421	CA	THR	A	443	19.214	2.911	57.227	1.00	59.44	C
ATOM	422	CB	THR	A	443	18.867	3.132	55.744	1.00	59.48	C
ATOM	423	OG1	THR	A	443	19.927	2.635	54.918	1.00	59.89	O
ATOM	424	CG2	THR	A	443	18.634	4.614	55.450	1.00	59.40	C
ATOM	425	C	THR	A	443	19.128	1.425	57.529	1.00	59.33	C
ATOM	426	O	THR	A	443	20.146	0.754	57.744	1.00	59.09	O
ATOM	427	N	PHE	A	444	17.903	0.916	57.537	1.00	58.97	N
ATOM	428	CA	PHE	A	444	17.657	-0.475	57.841	1.00	58.35	C
ATOM	429	CB	PHE	A	444	16.706	-0.596	59.021	1.00	58.20	C
ATOM	430	CG	PHE	A	444	17.365	-0.374	60.340	1.00	58.60	C
ATOM	431	CD1	PHE	A	444	17.353	0.892	60.935	1.00	58.29	C
ATOM	432	CE1	PHE	A	444	17.976	1.113	62.168	1.00	58.13	C
ATOM	433	CZ	PHE	A	444	18.617	0.056	62.818	1.00	58.69	C
ATOM	434	CE2	PHE	A	444	18.635	-1.227	62.226	1.00	58.42	C
ATOM	435	CD2	PHE	A	444	18.017	-1.427	60.992	1.00	58.53	C
ATOM	436	C	PHE	A	444	17.094	-1.210	56.651	1.00	58.41	C
ATOM	437	O	PHE	A	444	16.234	-0.680	55.949	1.00	57.99	O
ATOM	438	N	SER	A	445	17.591	-2.432	56.440	1.00	58.42	N
ATOM	439	CA	SER	A	445	17.119	-3.314	55.377	1.00	58.81	C
ATOM	440	CB	SER	A	445	18.153	-3.434	54.265	1.00	58.79	C
ATOM	441	OG	SER	A	445	17.928	-2.446	53.272	1.00	61.00	O
ATOM	442	C	SER	A	445	16.724	-4.698	55.885	1.00	58.99	C
ATOM	443	O	SER	A	445	17.399	-5.297	56.740	1.00	58.79	O
ATOM	444	N	LYS	A	446	15.621	-5.193	55.339	1.00	58.83	N
ATOM	445	CA	LYS	A	446	15.040	-6.449	55.743	1.00	58.74	C
ATOM	446	CB	LYS	A	446	13.642	-6.235	56.321	1.00	58.94	C
ATOM	447	CG	LYS	A	446	13.623	-5.623	57.706	1.00	61.25	C
ATOM	448	CD	LYS	A	446	12.298	-5.860	58.433	1.00	64.15	C
ATOM	449	CE	LYS	A	446	11.225	-4.881	57.967	1.00	67.22	C
ATOM	450	NZ	LYS	A	446	10.080	-4.795	58.936	1.00	69.19	N
ATOM	451	C	LYS	A	446	14.967	-7.391	54.551	1.00	58.52	C
ATOM	452	O	LYS	A	446	14.720	-6.962	53.414	1.00	57.87	O
ATOM	453	N	MET	A	447	15.201	-8.674	54.826	1.00	58.28	N
ATOM	454	CA	MET	A	447	15.014	-9.736	53.847	1.00	58.33	C
ATOM	455	CB	MET	A	447	16.245	-9.894	52.959	1.00	58.20	C
ATOM	456	CG	MET	A	447	17.493	-10.366	53.676	1.00	59.77	C
ATOM	457	SD	MET	A	447	18.664	-11.039	52.487	1.00	63.52	S
ATOM	458	CE	MET	A	447	20.124	-11.217	53.486	1.00	62.84	C
ATOM	459	C	MET	A	447	14.657	-11.058	54.519	1.00	57.66	C
ATOM	460	O	MET	A	447	14.777	-11.204	55.728	1.00	56.79	O
ATOM	461	N	SER	A	448	14.230	-12.008	53.697	1.00	57.51	N
ATOM	462	CA	SER	A	448	13.751	-13.299	54.125	1.00	57.01	C
ATOM	463	CB	SER	A	448	12.342	-13.488	53.600	1.00	56.79	C
ATOM	464	OG	SER	A	448	11.407	-13.309	54.630	1.00	58.23	O
ATOM	465	C	SER	A	448	14.603	-14.410	53.546	1.00	57.20	C
ATOM	466	O	SER	A	448	14.903	-14.393	52.360	1.00	57.13	O

Figure 2 Table 2a - 8

ATOM	467	N	LEU	A	449	14.958	-15.386	54.375	1.00	57.11	N
ATOM	468	CA	LEU	A	449	15.551	-16.619	53.891	1.00	57.19	C
ATOM	469	CB	LEU	A	449	16.846	-16.913	54.634	1.00	57.79	C
ATOM	470	CG	LEU	A	449	18.049	-16.083	54.196	1.00	60.12	C
ATOM	471	CD1	LEU	A	449	18.131	-14.843	55.035	1.00	61.60	C
ATOM	472	CD2	LEU	A	449	19.312	-16.899	54.360	1.00	62.22	C
ATOM	473	C	LEU	A	449	14.593	-17.798	54.035	1.00	56.78	C
ATOM	474	O	LEU	A	449	14.033	-18.022	55.113	1.00	57.04	O
ATOM	475	N	GLN	A	450	14.410	-18.543	52.942	1.00	55.91	N
ATOM	476	CA	GLN	A	450	13.573	-19.735	52.924	1.00	55.12	C
ATOM	477	CB	GLN	A	450	12.245	-19.479	52.204	1.00	55.08	C
ATOM	478	CG	GLN	A	450	11.385	-20.730	51.995	1.00	55.06	C
ATOM	479	CD	GLN	A	450	10.739	-21.227	53.281	1.00	56.01	C
ATOM	480	OE1	GLN	A	450	9.807	-20.608	53.803	1.00	57.29	O
ATOM	481	NE2	GLN	A	450	11.244	-22.333	53.811	1.00	55.25	N
ATOM	482	C	GLN	A	450	14.314	-20.874	52.233	1.00	55.20	C
ATOM	483	O	GLN	A	450	14.840	-20.707	51.112	1.00	54.60	O
ATOM	484	N	LEU	A	451	14.353	-22.027	52.908	1.00	54.51	N
ATOM	485	CA	LEU	A	451	14.952	-23.218	52.341	1.00	54.03	C
ATOM	486	CB	LEU	A	451	15.838	-23.932	53.356	1.00	54.04	C
ATOM	487	CG	LEU	A	451	16.776	-25.032	52.833	1.00	53.09	C
ATOM	488	CD1	LEU	A	451	17.999	-24.437	52.157	1.00	53.04	C
ATOM	489	CD2	LEU	A	451	17.208	-25.954	53.938	1.00	50.96	C
ATOM	490	C	LEU	A	451	13.877	-24.145	51.801	1.00	54.31	C
ATOM	491	O	LEU	A	451	12.857	-24.402	52.452	1.00	54.10	O
ATOM	492	N	TYR	A	452	14.120	-24.635	50.595	1.00	54.75	N
ATOM	493	CA	TYR	A	452	13.217	-25.549	49.925	1.00	55.47	C
ATOM	494	CB	TYR	A	452	12.732	-24.947	48.605	1.00	55.60	C
ATOM	495	CG	TYR	A	452	11.797	-23.772	48.731	1.00	55.29	C
ATOM	496	CD1	TYR	A	452	12.222	-22.487	48.419	1.00	53.82	C
ATOM	497	CE1	TYR	A	452	11.350	-21.407	48.514	1.00	54.61	C
ATOM	498	CZ	TYR	A	452	10.039	-21.618	48.949	1.00	55.32	C
ATOM	499	OH	TYR	A	452	9.156	-20.566	49.064	1.00	55.59	O
ATOM	500	CE2	TYR	A	452	9.600	-22.889	49.261	1.00	54.55	C
ATOM	501	CD2	TYR	A	452	10.471	-23.953	49.150	1.00	55.36	C
ATOM	502	C	TYR	A	452	13.979	-26.813	49.601	1.00	56.04	C
ATOM	503	O	TYR	A	452	15.196	-26.777	49.411	1.00	56.40	O
ATOM	504	N	GLN	A	453	13.261	-27.928	49.531	1.00	56.58	N
ATOM	505	CA	GLN	A	453	13.808	-29.159	48.960	1.00	56.90	C
ATOM	506	CB	GLN	A	453	13.200	-30.381	49.645	1.00	56.84	C
ATOM	507	CG	GLN	A	453	13.570	-31.698	49.008	1.00	56.76	C
ATOM	508	CD	GLN	A	453	13.642	-32.863	49.981	1.00	56.72	C
ATOM	509	OE1	GLN	A	453	13.456	-32.712	51.194	1.00	58.49	O
ATOM	510	NE2	GLN	A	453	13.926	-34.039	49.448	1.00	56.86	N
ATOM	511	C	GLN	A	453	13.496	-29.167	47.474	1.00	57.11	C
ATOM	512	O	GLN	A	453	12.356	-28.926	47.078	1.00	57.48	O
ATOM	513	N	VAL	A	454	14.507	-29.411	46.647	1.00	57.35	N
ATOM	514	CA	VAL	A	454	14.291	-29.492	45.196	1.00	57.37	C
ATOM	515	CB	VAL	A	454	15.031	-28.370	44.363	1.00	57.39	C
ATOM	516	CG1	VAL	A	454	14.356	-27.034	44.564	1.00	57.45	C
ATOM	517	CG2	VAL	A	454	16.513	-28.274	44.711	1.00	57.46	C
ATOM	518	C	VAL	A	454	14.565	-30.887	44.650	1.00	57.37	C
ATOM	519	O	VAL	A	454	14.033	-31.240	43.606	1.00	57.41	O
ATOM	520	N	ASP	A	455	15.377	-31.665	45.370	1.00	57.65	N
ATOM	521	CA	ASP	A	455	15.640	-33.087	45.074	1.00	57.67	C
ATOM	522	CB	ASP	A	455	17.055	-33.281	44.548	1.00	57.68	C
ATOM	523	CG	ASP	A	455	17.124	-33.314	43.063	1.00	59.15	C
ATOM	524	OD1	ASP	A	455	16.236	-32.740	42.407	1.00	61.34	O
ATOM	525	OD2	ASP	A	455	18.086	-33.914	42.538	1.00	62.40	O
ATOM	526	C	ASP	A	455	15.576	-33.880	46.352	1.00	57.49	C
ATOM	527	O	ASP	A	455	15.478	-33.305	47.425	1.00	57.43	O
ATOM	528	N	SER	A	456	15.689	-35.203	46.241	1.00	57.39	N
ATOM	529	CA	SER	A	456	15.928	-36.040	47.418	1.00	57.31	C
ATOM	530	CB	SER	A	456	15.907	-37.533	47.050	1.00	57.24	C
ATOM	531	OG	SER	A	456	16.750	-37.834	45.945	1.00	56.21	O
ATOM	532	C	SER	A	456	17.255	-35.651	48.091	1.00	57.42	C
ATOM	533	O	SER	A	456	17.394	-35.734	49.312	1.00	57.06	O

Figure 2 Table 2a - 9

ATOM	534	N	ARG	A	457	18.206	-35.190	47.278	1.00	57.68	N
ATOM	535	CA	ARG	A	457	19.567	-34.890	47.728	1.00	58.08	C
ATOM	536	CB	ARG	A	457	20.600	-35.511	46.773	1.00	58.04	C
ATOM	537	CG	ARG	A	457	20.261	-36.913	46.270	1.00	59.75	C
ATOM	538	CD	ARG	A	457	21.259	-37.396	45.207	1.00	61.90	C
ATOM	539	NE	ARG	A	457	22.330	-38.230	45.770	1.00	63.40	N
ATOM	540	CZ	ARG	A	457	23.453	-37.761	46.314	1.00	64.23	C
ATOM	541	NH1	ARG	A	457	23.682	-36.451	46.396	1.00	65.10	N
ATOM	542	NH2	ARG	A	457	24.355	-38.606	46.781	1.00	64.97	N
ATOM	543	C	ARG	A	457	19.833	-33.389	47.829	1.00	57.79	C
ATOM	544	O	ARG	A	457	20.739	-32.973	48.552	1.00	57.84	O
ATOM	545	N	THR	A	458	19.050	-32.590	47.104	1.00	57.58	N
ATOM	546	CA	THR	A	458	19.362	-31.170	46.895	1.00	57.70	C
ATOM	547	CB	THR	A	458	19.456	-30.830	45.386	1.00	57.52	C
ATOM	548	OG1	THR	A	458	19.925	-31.969	44.659	1.00	59.00	O
ATOM	549	CG2	THR	A	458	20.388	-29.665	45.141	1.00	57.57	C
ATOM	550	C	THR	A	458	18.365	-30.206	47.545	1.00	57.51	C
ATOM	551	O	THR	A	458	17.152	-30.436	47.527	1.00	57.31	O
ATOM	552	N	TYR	A	459	18.902	-29.113	48.091	1.00	57.55	N
ATOM	553	CA	TYR	A	459	18.104	-28.023	48.673	1.00	57.53	C
ATOM	554	CB	TYR	A	459	18.306	-27.952	50.189	1.00	57.48	C
ATOM	555	CG	TYR	A	459	18.156	-29.315	50.810	1.00	58.34	C
ATOM	556	CD1	TYR	A	459	19.277	-30.098	51.089	1.00	58.71	C
ATOM	557	CE1	TYR	A	459	19.147	-31.365	51.619	1.00	60.03	C
ATOM	558	CZ	TYR	A	459	17.883	-31.870	51.862	1.00	59.90	C
ATOM	559	OH	TYR	A	459	17.745	-33.122	52.390	1.00	59.16	O
ATOM	560	CE2	TYR	A	459	16.755	-31.119	51.577	1.00	59.69	C
ATOM	561	CD2	TYR	A	459	16.896	-29.854	51.046	1.00	58.21	C
ATOM	562	C	TYR	A	459	18.426	-26.695	48.000	1.00	57.31	C
ATOM	563	O	TYR	A	459	19.408	-26.595	47.259	1.00	57.12	O
ATOM	564	N	LEU	A	460	17.582	-25.695	48.255	1.00	56.87	N
ATOM	565	CA	LEU	A	460	17.655	-24.409	47.588	1.00	56.42	C
ATOM	566	CB	LEU	A	460	16.707	-24.413	46.388	1.00	56.43	C
ATOM	567	CG	LEU	A	460	16.265	-23.213	45.519	1.00	56.40	C
ATOM	568	CD1	LEU	A	460	16.804	-21.845	45.922	1.00	55.50	C
ATOM	569	CD2	LEU	A	460	16.550	-23.525	44.054	1.00	54.60	C
ATOM	570	C	LEU	A	460	17.361	-23.260	48.564	1.00	56.81	C
ATOM	571	O	LEU	A	460	16.241	-23.121	49.090	1.00	56.78	O
ATOM	572	N	LEU	A	461	18.383	-22.450	48.824	1.00	56.44	N
ATOM	573	CA	LEU	A	461	18.212	-21.316	49.706	1.00	56.44	C
ATOM	574	CB	LEU	A	461	19.501	-21.000	50.471	1.00	56.14	C
ATOM	575	CG	LEU	A	461	19.420	-19.841	51.476	1.00	56.10	C
ATOM	576	CD1	LEU	A	461	18.246	-19.989	52.464	1.00	55.15	C
ATOM	577	CD2	LEU	A	461	20.747	-19.689	52.225	1.00	55.90	C
ATOM	578	C	LEU	A	461	17.734	-20.126	48.879	1.00	56.64	C
ATOM	579	O	LEU	A	461	18.346	-19.767	47.881	1.00	56.66	O
ATOM	580	N	ASP	A	462	16.632	-19.530	49.319	1.00	56.72	N
ATOM	581	CA	ASP	A	462	15.920	-18.515	48.578	1.00	56.35	C
ATOM	582	CB	ASP	A	462	14.489	-18.996	48.340	1.00	56.12	C
ATOM	583	CG	ASP	A	462	13.628	-17.967	47.669	1.00	57.54	C
ATOM	584	OD1	ASP	A	462	14.044	-17.381	46.655	1.00	60.43	O
ATOM	585	OD2	ASP	A	462	12.512	-17.735	48.158	1.00	60.22	O
ATOM	586	C	ASP	A	462	15.944	-17.239	49.397	1.00	56.62	C
ATOM	587	O	ASP	A	462	15.786	-17.269	50.625	1.00	56.70	O
ATOM	588	N	PHE	A	463	16.148	-16.113	48.721	1.00	56.68	N
ATOM	589	CA	PHE	A	463	16.185	-14.817	49.384	1.00	55.72	C
ATOM	590	CB	PHE	A	463	17.561	-14.170	49.221	1.00	55.66	C
ATOM	591	CG	PHE	A	463	18.708	-15.087	49.538	1.00	54.34	C
ATOM	592	CD1	PHE	A	463	18.924	-16.234	48.794	1.00	54.80	C
ATOM	593	CE1	PHE	A	463	19.983	-17.082	49.085	1.00	53.61	C
ATOM	594	CZ	PHE	A	463	20.838	-16.782	50.123	1.00	53.25	C
ATOM	595	CE2	PHE	A	463	20.635	-15.635	50.869	1.00	54.58	C
ATOM	596	CD2	PHE	A	463	19.577	-14.794	50.574	1.00	54.30	C
ATOM	597	C	PHE	A	463	15.109	-13.894	48.826	1.00	56.22	C
ATOM	598	O	PHE	A	463	14.946	-13.783	47.612	1.00	55.84	O
ATOM	599	N	ARG	A	464	14.380	-13.229	49.717	1.00	56.67	N
ATOM	600	CA	ARG	A	464	13.401	-12.232	49.315	1.00	57.44	C

Figure 2 Table 2a - 10

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ATOM    601  CB  ARG A 464      11.984 -12.740  49.580  1.00 57.60           C
ATOM    602  CG  ARG A 464      10.926 -12.116  48.689  1.00 59.96           C
ATOM    603  CD  ARG A 464       9.525 -12.370  49.222  1.00 64.21           C
ATOM    604  NE  ARG A 464       8.566 -11.404  48.689  1.00 69.64           N
ATOM    605  CZ  ARG A 464       7.748 -11.643  47.667  1.00 71.45           C
ATOM    606  NH1 ARG A 464       7.761 -12.827  47.065  1.00 73.34           N
ATOM    607  NH2 ARG A 464       6.914 -10.701  47.249  1.00 71.51           N
ATOM    608  C   ARG A 464      13.634 -10.917  50.052  1.00 57.84           C
ATOM    609  O   ARG A 464      13.672 -10.881  51.285  1.00 58.42           O
ATOM    610  N   SER A 465      13.791  -9.838  49.292  1.00 57.65           N
ATOM    611  CA  SER A 465      13.800  -8.502  49.867  1.00 58.06           C
ATOM    612  CB  SER A 465      14.303  -7.479  48.843  1.00 57.90           C
ATOM    613  OG  SER A 465      13.313  -7.197  47.870  1.00 58.31           O
ATOM    614  C   SER A 465      12.409  -8.116  50.358  1.00 58.41           C
ATOM    615  O   SER A 465      11.403  -8.477  49.747  1.00 57.75           O
ATOM    616  N   ILE A 466      12.361  -7.379  51.463  1.00 59.70           N
ATOM    617  CA  ILE A 466      11.095  -7.017  52.086  1.00 61.63           C
ATOM    618  CB  ILE A 466      11.008  -7.537  53.535  1.00 61.46           C
ATOM    619  CG1 ILE A 466      11.096  -9.067  53.557  1.00 61.35           C
ATOM    620  CD1 ILE A 466      11.298  -9.656  54.939  1.00 61.65           C
ATOM    621  CG2 ILE A 466       9.720  -7.069  54.194  1.00 61.21           C
ATOM    622  C   ILE A 466      10.893  -5.506  52.071  1.00 63.39           C
ATOM    623  O   ILE A 466      11.731  -4.750  52.563  1.00 63.64           O
ATOM    624  N   ASP A 467       9.773  -5.071  51.501  1.00 65.88           N
ATOM    625  CA  ASP A 467       9.571  -3.664  51.170  1.00 68.01           C
ATOM    626  CB  ASP A 467       8.454  -3.515  50.136  1.00 68.21           C
ATOM    627  CG  ASP A 467       8.889  -3.934  48.744  1.00 69.81           C
ATOM    628  OD1 ASP A 467      10.108  -3.905  48.465  1.00 71.22           O
ATOM    629  OD2 ASP A 467       8.014  -4.291  47.928  1.00 71.59           O
ATOM    630  C   ASP A 467       9.252  -2.833  52.407  1.00 69.51           C
ATOM    631  O   ASP A 467       8.757  -3.355  53.405  1.00 69.50           O
ATOM    632  N   ASP A 468       9.538  -1.536  52.331  1.00 71.76           N
ATOM    633  CA  ASP A 468       9.256  -0.616  53.430  1.00 73.68           C
ATOM    634  CB  ASP A 468      10.119   0.644  53.313  1.00 73.91           C
ATOM    635  CG  ASP A 468      11.605   0.341  53.351  1.00 74.91           C
ATOM    636  OD1 ASP A 468      12.399   1.295  53.497  1.00 76.49           O
ATOM    637  OD2 ASP A 468      11.981  -0.845  53.232  1.00 75.06           O
ATOM    638  C   ASP A 468       7.782  -0.228  53.466  1.00 74.63           C
ATOM    639  O   ASP A 468       7.102  -0.236  52.437  1.00 74.91           O
ATOM    640  N   GLU A 469       7.298   0.113  54.658  1.00 75.51           N
ATOM    641  CA  GLU A 469       5.965   0.692  54.822  1.00 76.35           C
ATOM    642  CB  GLU A 469       5.779   1.899  53.896  1.00 76.32           C
ATOM    643  CG  GLU A 469       4.788   1.670  52.762  1.00 76.94           C
ATOM    644  CD  GLU A 469       3.903   2.878  52.506  1.00 77.91           C
ATOM    645  OE1 GLU A 469       2.692   2.691  52.261  1.00 77.60           O
ATOM    646  OE2 GLU A 469       4.416   4.017  52.552  1.00 78.21           O
ATOM    647  C   GLU A 469       4.871  -0.344  54.575  1.00 76.71           C
ATOM    648  O   GLU A 469       5.140  -1.547  54.516  1.00 77.21           O
ATOM    649  N   VAL A 524      21.360  18.013  40.487  1.00 67.89           N
ATOM    650  CA  VAL A 524      20.706  16.917  41.207  1.00 67.83           C
ATOM    651  CB  VAL A 524      19.305  16.590  40.611  1.00 67.87           C
ATOM    652  CG1 VAL A 524      18.573  15.547  41.465  1.00 67.65           C
ATOM    653  CG2 VAL A 524      18.463  17.865  40.475  1.00 67.60           C
ATOM    654  C   VAL A 524      21.588  15.655  41.263  1.00 67.76           C
ATOM    655  O   VAL A 524      21.739  14.941  40.260  1.00 67.62           O
ATOM    656  N   ALA A 525      22.156  15.401  42.446  1.00 67.61           N
ATOM    657  CA  ALA A 525      23.041  14.252  42.696  1.00 67.64           C
ATOM    658  CB  ALA A 525      24.419  14.732  43.166  1.00 67.62           C
ATOM    659  C   ALA A 525      22.436  13.254  43.705  1.00 67.39           C
ATOM    660  O   ALA A 525      21.907  13.663  44.738  1.00 67.63           O
ATOM    661  N   PRO A 526      22.526  11.943  43.416  1.00 67.11           N
ATOM    662  CA  PRO A 526      21.796  10.919  44.201  1.00 66.97           C
ATOM    663  CB  PRO A 526      22.038   9.625  43.416  1.00 66.80           C
ATOM    664  CG  PRO A 526      23.311   9.862  42.691  1.00 67.42           C
ATOM    665  CD  PRO A 526      23.331  11.336  42.340  1.00 67.12           C
ATOM    666  C   PRO A 526      22.266  10.750  45.652  1.00 66.56           C
ATOM    667  O   PRO A 526      21.477  10.953  46.581  1.00 66.67           O
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Figure 2 Table 2a - 11

ATOM	668	N	ARG	A	527	23.529	10.363	45.832	1.00	65.98	N
ATOM	669	CA	ARG	A	527	24.131	10.208	47.166	1.00	65.39	C
ATOM	670	CB	ARG	A	527	24.310	11.602	47.823	1.00	66.02	C
ATOM	671	CG	ARG	A	527	25.703	11.882	48.453	1.00	67.72	C
ATOM	672	CD	ARG	A	527	26.874	11.362	47.602	1.00	70.43	C
ATOM	673	NE	ARG	A	527	27.901	10.690	48.413	1.00	71.74	N
ATOM	674	CZ	ARG	A	527	29.081	11.216	48.748	1.00	72.00	C
ATOM	675	NH1	ARG	A	527	29.420	12.439	48.344	1.00	71.58	N
ATOM	676	NH2	ARG	A	527	29.934	10.507	49.485	1.00	71.62	N
ATOM	677	C	ARG	A	527	23.357	9.146	48.012	1.00	63.92	C
ATOM	678	O	ARG	A	527	22.383	8.574	47.522	1.00	63.84	O
ATOM	679	N	PRO	A	528	23.759	8.900	49.277	1.00	62.73	N
ATOM	680	CA	PRO	A	528	23.695	7.519	49.833	1.00	61.30	C
ATOM	681	CB	PRO	A	528	24.146	7.704	51.291	1.00	61.20	C
ATOM	682	CG	PRO	A	528	24.899	8.987	51.310	1.00	62.22	C
ATOM	683	CD	PRO	A	528	24.218	9.864	50.298	1.00	62.60	C
ATOM	684	C	PRO	A	528	22.370	6.715	49.774	1.00	59.99	C
ATOM	685	O	PRO	A	528	21.293	7.235	50.074	1.00	60.09	O
ATOM	686	N	GLY	A	529	22.480	5.441	49.402	1.00	58.26	N
ATOM	687	CA	GLY	A	529	21.361	4.515	49.491	1.00	56.48	C
ATOM	688	C	GLY	A	529	20.813	3.928	48.198	1.00	55.30	C
ATOM	689	O	GLY	A	529	20.685	4.618	47.192	1.00	54.95	O
ATOM	690	N	SER	A	530	20.492	2.637	48.237	1.00	54.44	N
ATOM	691	CA	SER	A	530	19.643	1.990	47.232	1.00	53.51	C
ATOM	692	CB	SER	A	530	20.360	1.762	45.901	1.00	53.77	C
ATOM	693	OG	SER	A	530	19.660	0.812	45.103	1.00	52.94	O
ATOM	694	C	SER	A	530	19.188	0.675	47.788	1.00	52.95	C
ATOM	695	O	SER	A	530	19.989	-0.244	47.967	1.00	52.73	O
ATOM	696	N	HIS	A	531	17.893	0.592	48.061	1.00	52.47	N
ATOM	697	CA	HIS	A	531	17.311	-0.584	48.678	1.00	52.20	C
ATOM	698	CB	HIS	A	531	15.802	-0.399	48.817	1.00	52.91	C
ATOM	699	CG	HIS	A	531	15.146	-1.411	49.700	1.00	55.59	C
ATOM	700	ND1	HIS	A	531	14.648	-2.605	49.221	1.00	57.51	N
ATOM	701	CE1	HIS	A	531	14.130	-3.298	50.221	1.00	58.85	C
ATOM	702	NE2	HIS	A	531	14.275	-2.595	51.334	1.00	59.76	N
ATOM	703	CD2	HIS	A	531	14.905	-1.410	51.036	1.00	58.00	C
ATOM	704	C	HIS	A	531	17.647	-1.839	47.889	1.00	51.51	C
ATOM	705	O	HIS	A	531	18.095	-2.827	48.468	1.00	52.23	O
ATOM	706	N	THR	A	532	17.469	-1.792	46.568	1.00	50.62	N
ATOM	707	CA	THR	A	532	17.740	-2.943	45.694	1.00	49.51	C
ATOM	708	CB	THR	A	532	17.295	-2.681	44.244	1.00	49.27	C
ATOM	709	OG1	THR	A	532	15.884	-2.463	44.210	1.00	47.85	O
ATOM	710	CG2	THR	A	532	17.612	-3.868	43.358	1.00	48.72	C
ATOM	711	C	THR	A	532	19.200	-3.392	45.696	1.00	49.59	C
ATOM	712	O	THR	A	532	19.474	-4.586	45.785	1.00	49.88	O
ATOM	713	N	ILE	A	533	20.138	-2.451	45.577	1.00	49.58	N
ATOM	714	CA	ILE	A	533	21.562	-2.805	45.614	1.00	49.23	C
ATOM	715	CB	ILE	A	533	22.471	-1.666	45.108	1.00	48.98	C
ATOM	716	CG1	ILE	A	533	21.977	-1.099	43.763	1.00	47.92	C
ATOM	717	CD1	ILE	A	533	21.885	-2.100	42.601	1.00	45.27	C
ATOM	718	CG2	ILE	A	533	23.918	-2.154	45.016	1.00	48.63	C
ATOM	719	C	ILE	A	533	22.015	-3.281	47.004	1.00	49.52	C
ATOM	720	O	ILE	A	533	22.834	-4.207	47.132	1.00	49.91	O
ATOM	721	N	GLU	A	534	21.462	-2.679	48.047	1.00	49.62	N
ATOM	722	CA	GLU	A	534	21.800	-3.096	49.413	1.00	49.95	C
ATOM	723	CB	GLU	A	534	21.288	-2.081	50.438	1.00	49.76	C
ATOM	724	CG	GLU	A	534	22.015	-0.734	50.354	1.00	50.00	C
ATOM	725	CD	GLU	A	534	21.417	0.305	51.275	1.00	50.91	C
ATOM	726	OE1	GLU	A	534	21.132	-0.030	52.453	1.00	54.98	O
ATOM	727	OE2	GLU	A	534	21.233	1.447	50.833	1.00	47.85	O
ATOM	728	C	GLU	A	534	21.301	-4.496	49.729	1.00	49.83	C
ATOM	729	O	GLU	A	534	21.926	-5.224	50.505	1.00	50.43	O
ATOM	730	N	PHE	A	535	20.172	-4.859	49.131	1.00	50.04	N
ATOM	731	CA	PHE	A	535	19.647	-6.215	49.210	1.00	50.18	C
ATOM	732	CB	PHE	A	535	18.260	-6.296	48.549	1.00	49.77	C
ATOM	733	CG	PHE	A	535	17.786	-7.700	48.283	1.00	50.27	C
ATOM	734	CD1	PHE	A	535	17.558	-8.602	49.337	1.00	50.59	C

Figure 2 Table 2a - 12

ATOM	735	CE1	PHE	A	535	17.111	-9.903	49.092	1.00	49.03	C
ATOM	736	CZ	PHE	A	535	16.900	-10.337	47.780	1.00	49.28	C
ATOM	737	CE2	PHE	A	535	17.136	-9.472	46.716	1.00	49.08	C
ATOM	738	CD2	PHE	A	535	17.576	-8.143	46.972	1.00	50.80	C
ATOM	739	C	PHE	A	535	20.630	-7.200	48.568	1.00	50.73	C
ATOM	740	O	PHE	A	535	20.895	-8.271	49.136	1.00	50.32	O
ATOM	741	N	PHE	A	536	21.168	-6.846	47.395	1.00	50.98	N
ATOM	742	CA	PHE	A	536	22.131	-7.740	46.726	1.00	51.38	C
ATOM	743	CB	PHE	A	536	22.567	-7.228	45.336	1.00	50.68	C
ATOM	744	CG	PHE	A	536	21.472	-7.220	44.299	1.00	49.32	C
ATOM	745	CD1	PHE	A	536	21.435	-6.227	43.325	1.00	47.58	C
ATOM	746	CE1	PHE	A	536	20.432	-6.198	42.360	1.00	46.98	C
ATOM	747	CZ	PHE	A	536	19.445	-7.156	42.368	1.00	47.75	C
ATOM	748	CE2	PHE	A	536	19.463	-8.152	43.344	1.00	48.22	C
ATOM	749	CD2	PHE	A	536	20.479	-8.185	44.295	1.00	47.79	C
ATOM	750	C	PHE	A	536	23.364	-7.947	47.597	1.00	52.08	C
ATOM	751	O	PHE	A	536	23.882	-9.066	47.686	1.00	51.76	O
ATOM	752	N	GLU	A	537	23.828	-6.868	48.234	1.00	52.94	N
ATOM	753	CA	GLU	A	537	25.023	-6.927	49.081	1.00	53.87	C
ATOM	754	CB	GLU	A	537	25.555	-5.533	49.398	1.00	53.71	C
ATOM	755	CG	GLU	A	537	26.055	-4.830	48.145	1.00	54.63	C
ATOM	756	CD	GLU	A	537	26.718	-3.501	48.413	1.00	54.79	C
ATOM	757	OE1	GLU	A	537	26.396	-2.873	49.440	1.00	55.52	O
ATOM	758	OE2	GLU	A	537	27.557	-3.085	47.581	1.00	54.50	O
ATOM	759	C	GLU	A	537	24.827	-7.752	50.346	1.00	54.70	C
ATOM	760	O	GLU	A	537	25.709	-8.527	50.715	1.00	55.04	O
ATOM	761	N	MET	A	538	23.678	-7.602	50.996	1.00	55.39	N
ATOM	762	CA	MET	A	538	23.330	-8.476	52.107	1.00	56.83	C
ATOM	763	CB	MET	A	538	21.940	-8.168	52.644	1.00	57.05	C
ATOM	764	CG	MET	A	538	21.837	-6.900	53.442	1.00	59.65	C
ATOM	765	SD	MET	A	538	20.287	-6.893	54.357	1.00	64.14	S
ATOM	766	CE	MET	A	538	19.126	-6.596	53.015	1.00	63.14	C
ATOM	767	C	MET	A	538	23.376	-9.938	51.699	1.00	56.73	C
ATOM	768	O	MET	A	538	23.976	-10.772	52.404	1.00	57.19	O
ATOM	769	N	CYS	A	539	22.736	-10.250	50.575	1.00	56.30	N
ATOM	770	CA	CYS	A	539	22.742	-11.610	50.050	1.00	56.24	C
ATOM	771	CB	CYS	A	539	21.963	-11.686	48.749	1.00	55.59	C
ATOM	772	SG	CYS	A	539	20.224	-11.488	48.989	1.00	57.13	S
ATOM	773	C	CYS	A	539	24.157	-12.094	49.807	1.00	56.19	C
ATOM	774	O	CYS	A	539	24.534	-13.172	50.250	1.00	56.32	O
ATOM	775	N	ALA	A	540	24.924	-11.285	49.085	1.00	56.21	N
ATOM	776	CA	ALA	A	540	26.283	-11.623	48.738	1.00	56.33	C
ATOM	777	CB	ALA	A	540	26.928	-10.504	47.932	1.00	55.55	C
ATOM	778	C	ALA	A	540	27.071	-11.897	50.007	1.00	56.51	C
ATOM	779	O	ALA	A	540	27.792	-12.890	50.079	1.00	56.51	O
ATOM	780	N	ASN	A	541	26.917	-11.016	50.998	1.00	56.83	N
ATOM	781	CA	ASN	A	541	27.613	-11.152	52.279	1.00	57.34	C
ATOM	782	CB	ASN	A	541	27.328	-9.960	53.188	1.00	57.62	C
ATOM	783	CG	ASN	A	541	28.047	-8.709	52.741	1.00	58.61	C
ATOM	784	OD1	ASN	A	541	29.203	-8.765	52.309	1.00	59.70	O
ATOM	785	ND2	ASN	A	541	27.369	-7.567	52.841	1.00	58.15	N
ATOM	786	C	ASN	A	541	27.248	-12.434	52.996	1.00	56.98	C
ATOM	787	O	ASN	A	541	28.120	-13.173	53.416	1.00	56.66	O
ATOM	788	N	LEU	A	542	25.948	-12.681	53.112	1.00	57.03	N
ATOM	789	CA	LEU	A	542	25.429	-13.879	53.731	1.00	57.02	C
ATOM	790	CB	LEU	A	542	23.912	-13.868	53.730	1.00	56.97	C
ATOM	791	CG	LEU	A	542	23.265	-13.517	55.061	1.00	58.16	C
ATOM	792	CD1	LEU	A	542	21.820	-13.240	54.828	1.00	58.91	C
ATOM	793	CD2	LEU	A	542	23.403	-14.692	56.044	1.00	60.32	C
ATOM	794	C	LEU	A	542	25.933	-15.146	53.064	1.00	57.24	C
ATOM	795	O	LEU	A	542	26.245	-16.107	53.755	1.00	57.36	O
ATOM	796	N	ILE	A	543	26.026	-15.148	51.739	1.00	56.83	N
ATOM	797	CA	ILE	A	543	26.531	-16.316	51.014	1.00	56.56	C
ATOM	798	CB	ILE	A	543	26.194	-16.241	49.509	1.00	56.29	C
ATOM	799	CG1	ILE	A	543	24.673	-16.326	49.323	1.00	56.02	C
ATOM	800	CD1	ILE	A	543	24.168	-15.792	48.004	1.00	55.63	C
ATOM	801	CG2	ILE	A	543	26.886	-17.352	48.733	1.00	55.63	C

Figure 2 Table 2a - 13

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ATOM    802  C   ILE A 543      28.032 -16.538  51.266  1.00 56.99      C
ATOM    803  O   ILE A 543      28.452 -17.642  51.647  1.00 57.15      O
ATOM    804  N   LYS A 544      28.829 -15.489  51.077  1.00 57.17      N
ATOM    805  CA  LYS A 544      30.275 -15.552  51.267  1.00 57.51      C
ATOM    806  CB  LYS A 544      30.885 -14.171  51.026  1.00 57.31      C
ATOM    807  CG  LYS A 544      32.380 -14.091  51.299  1.00 58.17      C
ATOM    808  CD  LYS A 544      32.962 -12.744  50.903  1.00 58.85      C
ATOM    809  CE  LYS A 544      34.408 -12.630  51.364  1.00 59.12      C
ATOM    810  NZ  LYS A 544      35.173 -11.668  50.523  1.00 59.93      N
ATOM    811  C   LYS A 544      30.651 -16.051  52.666  1.00 57.83      C
ATOM    812  O   LYS A 544      31.612 -16.820  52.838  1.00 57.87      O
ATOM    813  N   ILE A 545      29.870 -15.622  53.653  1.00 57.98      N
ATOM    814  CA  ILE A 545      30.209 -15.800  55.059  1.00 58.23      C
ATOM    815  CB  ILE A 545      29.825 -14.513  55.864  1.00 58.29      C
ATOM    816  CG1 ILE A 545      30.753 -13.346  55.480  1.00 58.32      C
ATOM    817  CD1 ILE A 545      32.185 -13.487  56.004  1.00 59.14      C
ATOM    818  CG2 ILE A 545      29.909 -14.721  57.353  1.00 59.39      C
ATOM    819  C   ILE A 545      29.657 -17.115  55.647  1.00 58.26      C
ATOM    820  O   ILE A 545      29.765 -17.371  56.848  1.00 58.17      O
ATOM    821  N   LEU A 546      29.122 -17.977  54.781  1.00 58.49      N
ATOM    822  CA  LEU A 546      28.648 -19.284  55.220  1.00 58.67      C
ATOM    823  CB  LEU A 546      27.245 -19.135  55.796  1.00 58.87      C
ATOM    824  CG  LEU A 546      25.962 -19.096  54.978  1.00 58.87      C
ATOM    825  CD1 LEU A 546      25.144 -18.052  55.623  1.00 61.27      C
ATOM    826  CD2 LEU A 546      26.121 -18.753  53.523  1.00 58.95      C
ATOM    827  C   LEU A 546      28.674 -20.422  54.193  1.00 58.63      C
ATOM    828  O   LEU A 546      28.415 -21.564  54.534  1.00 58.80      O
ATOM    829  N   ALA A 547      28.961 -20.116  52.941  1.00 58.80      N
ATOM    830  CA  ALA A 547      28.764 -21.096  51.887  1.00 58.83      C
ATOM    831  CB  ALA A 547      27.703 -20.594  50.867  1.00 58.04      C
ATOM    832  C   ALA A 547      30.089 -21.416  51.203  1.00 58.82      C
ATOM    833  O   ALA A 547      30.960 -20.548  51.071  1.00 58.84      O
ATOM    834  N   GLN A 548      30.223 -22.672  50.777  1.00 58.73      N
ATOM    835  CA  GLN A 548      31.386 -23.159  50.038  1.00 58.52      C
ATOM    836  CB  GLN A 548      31.272 -22.805  48.550  1.00 58.48      C
ATOM    837  CG  GLN A 548      32.476 -23.233  47.727  1.00 59.40      C
ATOM    838  CD  GLN A 548      32.105 -23.753  46.354  1.00 60.51      C
ATOM    839  OE1 GLN A 548      32.299 -24.942  46.064  1.00 59.79      O
ATOM    840  NE2 GLN A 548      31.569 -22.867  45.494  1.00 60.38      N
ATOM    841  C   GLN A 548      32.694 -22.637  50.625  1.00 58.40      C
ATOM    842  O   GLN A 548      33.568 -23.408  51.015  1.00 58.23      O
ATOM    843  N   GLY B 190      -0.472 -36.106  92.790  1.00 61.29      N
ATOM    844  CA  GLY B 190      -0.502 -35.260  91.600  1.00 61.22      C
ATOM    845  C   GLY B 190       0.376 -35.794  90.486  1.00 61.24      C
ATOM    846  O   GLY B 190       1.603 -35.718  90.562  1.00 61.37      O
ATOM    847  N   GLN B 191      -0.256 -36.331  89.446  1.00 61.08      N
ATOM    848  CA  GLN B 191       0.455 -37.081  88.414  1.00 60.89      C
ATOM    849  CB  GLN B 191      -0.537 -37.713  87.431  1.00 60.84      C
ATOM    850  CG  GLN B 191       0.091 -38.716  86.473  1.00 60.79      C
ATOM    851  CD  GLN B 191      -0.931 -39.638  85.836  1.00 61.28      C
ATOM    852  OE1 GLN B 191      -2.082 -39.252  85.619  1.00 62.19      O
ATOM    853  NE2 GLN B 191      -0.513 -40.866  85.532  1.00 60.83      N
ATOM    854  C   GLN B 191       1.451 -36.205  87.661  1.00 60.60      C
ATOM    855  O   GLN B 191       1.272 -34.991  87.561  1.00 60.83      O
ATOM    856  N   GLU B 192       2.501 -36.829  87.134  1.00 60.16      N
ATOM    857  CA  GLU B 192       3.323 -36.208  86.104  1.00 59.90      C
ATOM    858  CB  GLU B 192       4.519 -37.100  85.756  1.00 59.88      C
ATOM    859  CG  GLU B 192       4.182 -38.287  84.863  1.00 60.19      C
ATOM    860  CD  GLU B 192       3.708 -39.498  85.646  1.00 61.17      C
ATOM    861  OE1 GLU B 192       4.252 -39.754  86.743  1.00 61.69      O
ATOM    862  OE2 GLU B 192       2.791 -40.197  85.164  1.00 61.41      O
ATOM    863  C   GLU B 192       2.498 -35.915  84.854  1.00 59.75      C
ATOM    864  O   GLU B 192       1.459 -36.534  84.626  1.00 59.69      O
ATOM    865  N   MET B 193       2.966 -34.966  84.050  1.00 59.46      N
ATOM    866  CA  MET B 193       2.291 -34.621  82.807  1.00 59.36      C
ATOM    867  CB  MET B 193       1.895 -33.144  82.799  1.00 59.26      C
ATOM    868  CG  MET B 193       0.797 -32.802  83.788  1.00 59.11      C
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Figure 2 Table 2a - 14

ATOM	869	SD	MET	B	193	-0.241	-31.442	83.229	1.00	59.40	S
ATOM	870	CE	MET	B	193	-1.384	-31.315	84.603	1.00	58.93	C
ATOM	871	C	MET	B	193	3.158	-34.947	81.598	1.00	59.40	C
ATOM	872	O	MET	B	193	4.385	-34.982	81.692	1.00	59.25	O
ATOM	873	N	TYR	B	194	2.509	-35.186	80.463	1.00	59.63	N
ATOM	874	CA	TYR	B	194	3.181	-35.755	79.301	1.00	59.91	C
ATOM	875	CB	TYR	B	194	2.534	-37.084	78.909	1.00	59.59	C
ATOM	876	CG	TYR	B	194	2.759	-38.188	79.917	1.00	58.81	C
ATOM	877	CD1	TYR	B	194	2.003	-38.257	81.081	1.00	58.38	C
ATOM	878	CE1	TYR	B	194	2.207	-39.263	82.007	1.00	57.70	C
ATOM	879	CZ	TYR	B	194	3.176	-40.217	81.773	1.00	57.22	C
ATOM	880	OH	TYR	B	194	3.383	-41.219	82.690	1.00	55.66	O
ATOM	881	CE2	TYR	B	194	3.940	-40.170	80.626	1.00	57.51	C
ATOM	882	CD2	TYR	B	194	3.729	-39.159	79.707	1.00	58.33	C
ATOM	883	C	TYR	B	194	3.171	-34.789	78.119	1.00	60.44	C
ATOM	884	O	TYR	B	194	2.220	-34.032	77.931	1.00	60.34	O
ATOM	885	N	ALA	B	195	4.240	-34.819	77.330	1.00	61.22	N
ATOM	886	CA	ALA	B	195	4.380	-33.918	76.195	1.00	62.16	C
ATOM	887	CB	ALA	B	195	5.699	-33.160	76.275	1.00	61.93	C
ATOM	888	C	ALA	B	195	4.277	-34.675	74.876	1.00	62.89	C
ATOM	889	O	ALA	B	195	5.130	-35.501	74.554	1.00	62.78	O
ATOM	890	N	PHE	B	196	3.224	-34.386	74.120	1.00	64.23	N
ATOM	891	CA	PHE	B	196	3.131	-34.828	72.736	1.00	65.51	C
ATOM	892	CB	PHE	B	196	1.692	-35.213	72.390	1.00	65.07	C
ATOM	893	CG	PHE	B	196	1.113	-36.263	73.294	1.00	63.46	C
ATOM	894	CD1	PHE	B	196	0.391	-35.904	74.420	1.00	61.83	C
ATOM	895	CE1	PHE	B	196	-0.140	-36.864	75.254	1.00	61.95	C
ATOM	896	CZ	PHE	B	196	0.047	-38.203	74.971	1.00	62.25	C
ATOM	897	CE2	PHE	B	196	0.765	-38.573	73.851	1.00	61.91	C
ATOM	898	CD2	PHE	B	196	1.294	-37.607	73.021	1.00	62.18	C
ATOM	899	C	PHE	B	196	3.637	-33.747	71.790	1.00	67.42	C
ATOM	900	O	PHE	B	196	3.219	-32.589	71.869	1.00	67.63	O
ATOM	901	N	ARG	B	197	4.545	-34.135	70.899	1.00	69.75	N
ATOM	902	CA	ARG	B	197	5.479	-33.190	70.300	1.00	72.03	C
ATOM	903	CB	ARG	B	197	6.863	-33.313	70.944	1.00	71.89	C
ATOM	904	CG	ARG	B	197	7.138	-32.254	72.001	1.00	72.62	C
ATOM	905	CD	ARG	B	197	8.627	-32.068	72.232	1.00	73.11	C
ATOM	906	NE	ARG	B	197	9.066	-32.686	73.481	1.00	74.67	N
ATOM	907	CZ	ARG	B	197	9.001	-32.096	74.672	1.00	75.06	C
ATOM	908	NH1	ARG	B	197	8.512	-30.867	74.782	1.00	75.20	N
ATOM	909	NH2	ARG	B	197	9.426	-32.734	75.754	1.00	74.73	N
ATOM	910	C	ARG	B	197	5.566	-33.389	68.793	1.00	73.62	C
ATOM	911	O	ARG	B	197	5.627	-34.517	68.300	1.00	73.47	O
ATOM	912	N	SER	B	198	5.589	-32.275	68.072	1.00	75.85	N
ATOM	913	CA	SER	B	198	4.639	-32.045	66.993	1.00	77.82	C
ATOM	914	CB	SER	B	198	4.593	-30.550	66.644	1.00	77.89	C
ATOM	915	OG	SER	B	198	4.028	-30.343	65.358	1.00	78.53	O
ATOM	916	C	SER	B	198	4.962	-32.847	65.731	1.00	79.12	C
ATOM	917	O	SER	B	198	4.061	-33.392	65.092	1.00	79.62	O
ATOM	918	N	GLU	B	199	6.246	-32.930	65.387	1.00	80.52	N
ATOM	919	CA	GLU	B	199	6.744	-34.051	64.625	1.00	81.67	C
ATOM	920	CB	GLU	B	199	8.015	-34.645	65.206	1.00	81.84	C
ATOM	921	CG	GLU	B	199	8.990	-33.596	65.743	1.00	81.97	C
ATOM	922	CD	GLU	B	199	10.168	-34.224	66.463	1.00	82.58	C
ATOM	923	OE1	GLU	B	199	10.757	-33.550	67.335	1.00	82.21	O
ATOM	924	OE2	GLU	B	199	10.505	-35.392	66.160	1.00	83.60	O
ATOM	925	C	GLU	B	199	6.898	-33.626	63.180	1.00	82.45	C
ATOM	926	O	GLU	B	199	5.960	-33.096	62.579	1.00	82.75	O
ATOM	927	N	GLU	B	200	8.078	-33.858	62.616	1.00	83.15	N
ATOM	928	CA	GLU	B	200	8.391	-33.373	61.279	1.00	83.78	C
ATOM	929	CB	GLU	B	200	7.890	-34.353	60.213	1.00	84.00	C
ATOM	930	CG	GLU	B	200	8.329	-34.012	58.794	1.00	85.38	C
ATOM	931	CD	GLU	B	200	7.346	-34.500	57.745	1.00	87.38	C
ATOM	932	OE1	GLU	B	200	6.124	-34.435	57.997	1.00	88.33	O
ATOM	933	OE2	GLU	B	200	7.795	-34.946	56.666	1.00	88.17	O
ATOM	934	C	GLU	B	200	7.782	-31.992	61.053	1.00	83.78	C
ATOM	935	O	GLU	B	200	8.403	-30.973	61.369	1.00	83.76	O

Figure 2 Table 2a - 15

ATOM	936	N	ARG	B	201	6.557	-31.968	60.527	1.00	83.67	N
ATOM	937	CA	ARG	B	201	6.165	-30.979	59.523	1.00	83.57	C
ATOM	938	CB	ARG	B	201	5.106	-30.023	60.081	1.00	84.03	C
ATOM	939	CG	ARG	B	201	4.440	-29.156	59.018	1.00	85.18	C
ATOM	940	CD	ARG	B	201	2.924	-29.158	59.168	1.00	87.64	C
ATOM	941	NE	ARG	B	201	2.247	-28.894	57.900	1.00	88.78	N
ATOM	942	CZ	ARG	B	201	1.257	-29.637	57.409	1.00	88.90	C
ATOM	943	NH1	ARG	B	201	0.818	-30.696	58.080	1.00	88.67	N
ATOM	944	NH2	ARG	B	201	0.704	-29.318	56.246	1.00	88.98	N
ATOM	945	C	ARG	B	201	7.369	-30.195	59.009	1.00	82.77	C
ATOM	946	O	ARG	B	201	7.523	-29.997	57.804	1.00	83.03	O
ATOM	947	N	PHE	B	202	8.217	-29.755	59.932	1.00	81.69	N
ATOM	948	CA	PHE	B	202	9.436	-29.068	59.585	1.00	80.64	C
ATOM	949	CB	PHE	B	202	9.598	-27.838	60.457	1.00	80.50	C
ATOM	950	CG	PHE	B	202	8.454	-26.911	60.366	1.00	80.02	C
ATOM	951	CD1	PHE	B	202	7.528	-26.850	61.364	1.00	79.78	C
ATOM	952	CE1	PHE	B	202	6.462	-26.012	61.258	1.00	80.27	C
ATOM	953	CZ	PHE	B	202	6.308	-25.230	60.147	1.00	79.94	C
ATOM	954	CE2	PHE	B	202	7.213	-25.293	59.147	1.00	79.32	C
ATOM	955	CD2	PHE	B	202	8.279	-26.127	59.250	1.00	79.47	C
ATOM	956	C	PHE	B	202	10.546	-30.027	59.822	1.00	79.80	C
ATOM	957	O	PHE	B	202	11.541	-29.708	60.444	1.00	79.88	O
ATOM	958	N	GLY	B	203	10.336	-31.229	59.329	1.00	78.73	N
ATOM	959	CA	GLY	B	203	11.352	-32.269	59.365	1.00	77.35	C
ATOM	960	C	GLY	B	203	12.054	-32.427	58.031	1.00	76.40	C
ATOM	961	O	GLY	B	203	13.232	-32.783	57.976	1.00	76.50	O
ATOM	962	N	ALA	B	204	11.325	-32.164	56.951	1.00	75.06	N
ATOM	963	CA	ALA	B	204	11.940	-31.772	55.689	1.00	73.74	C
ATOM	964	CB	ALA	B	204	11.568	-32.757	54.587	1.00	73.48	C
ATOM	965	C	ALA	B	204	11.523	-30.353	55.309	1.00	72.86	C
ATOM	966	O	ALA	B	204	10.359	-29.982	55.462	1.00	72.72	O
ATOM	967	N	PRO	B	205	12.479	-29.560	54.822	1.00	71.92	N
ATOM	968	CA	PRO	B	205	12.159	-28.308	54.128	1.00	71.35	C
ATOM	969	CB	PRO	B	205	13.465	-27.967	53.407	1.00	71.37	C
ATOM	970	CG	PRO	B	205	14.523	-28.604	54.234	1.00	71.49	C
ATOM	971	CD	PRO	B	205	13.918	-29.869	54.771	1.00	71.66	C
ATOM	972	C	PRO	B	205	11.032	-28.484	53.117	1.00	70.95	C
ATOM	973	O	PRO	B	205	10.994	-29.489	52.410	1.00	70.76	O
ATOM	974	N	PRO	B	206	10.124	-27.511	53.050	1.00	70.95	N
ATOM	975	CA	PRO	B	206	9.087	-27.497	52.012	1.00	71.23	C
ATOM	976	CB	PRO	B	206	8.454	-26.113	52.173	1.00	71.03	C
ATOM	977	CG	PRO	B	206	9.530	-25.276	52.769	1.00	70.61	C
ATOM	978	CD	PRO	B	206	10.295	-26.190	53.680	1.00	70.74	C
ATOM	979	C	PRO	B	206	9.676	-27.645	50.614	1.00	71.65	C
ATOM	980	O	PRO	B	206	10.848	-27.333	50.402	1.00	71.48	O
ATOM	981	N	ILE	B	207	8.869	-28.124	49.671	1.00	72.53	N
ATOM	982	CA	ILE	B	207	9.299	-28.215	48.282	1.00	68.70	C
ATOM	983	CB	ILE	B	207	8.699	-29.445	47.572	1.00	68.66	C
ATOM	984	CG1	ILE	B	207	7.214	-29.594	47.915	1.00	69.35	C
ATOM	985	CD1	ILE	B	207	6.285	-29.268	46.760	1.00	69.94	C
ATOM	986	CG2	ILE	B	207	9.473	-30.706	47.940	1.00	68.67	C
ATOM	987	C	ILE	B	207	8.930	-26.953	47.514	1.00	69.60	C
ATOM	988	O	ILE	B	207	7.912	-26.317	47.798	1.00	69.69	O
ATOM	989	N	LEU	B	208	9.765	-26.596	46.542	1.00	70.93	N
ATOM	990	CA	LEU	B	208	9.525	-25.413	45.724	1.00	72.02	C
ATOM	991	CB	LEU	B	208	10.496	-25.367	44.540	1.00	72.04	C
ATOM	992	CG	LEU	B	208	10.973	-23.986	44.082	1.00	71.68	C
ATOM	993	CD1	LEU	B	208	11.573	-23.211	45.241	1.00	71.45	C
ATOM	994	CD2	LEU	B	208	11.980	-24.119	42.951	1.00	71.56	C
ATOM	995	C	LEU	B	208	8.078	-25.354	45.234	1.00	73.03	C
ATOM	996	O	LEU	B	208	7.180	-24.972	45.986	1.00	73.29	O
ATOM	997	N	PRO	B	209	7.855	-25.752	43.982	1.00	74.00	N
ATOM	998	CA	PRO	B	209	7.013	-24.970	43.069	1.00	74.76	C
ATOM	999	CB	PRO	B	209	6.842	-25.907	41.869	1.00	74.73	C
ATOM	1000	CG	PRO	B	209	8.069	-26.746	41.881	1.00	74.30	C
ATOM	1001	CD	PRO	B	209	8.386	-26.966	43.335	1.00	74.08	C
ATOM	1002	C	PRO	B	209	5.652	-24.618	43.666	1.00	75.49	C

Figure 2 Table 2a - 16

ATOM	1003	O	PRO	B	209	4.713	-25.411	43.566	1.00	75.50	O
ATOM	1004	N	PRO	B	210	5.552	-23.437	44.282	1.00	75.96	N
ATOM	1005	CA	PRO	B	210	4.281	-22.707	44.306	1.00	76.33	C
ATOM	1006	CB	PRO	B	210	4.600	-21.481	45.170	1.00	76.39	C
ATOM	1007	CG	PRO	B	210	5.715	-21.928	46.054	1.00	76.04	C
ATOM	1008	CD	PRO	B	210	6.543	-22.853	45.207	1.00	75.88	C
ATOM	1009	C	PRO	B	210	3.871	-22.277	42.898	1.00	76.57	C
ATOM	1010	O	PRO	B	210	3.087	-22.969	42.247	1.00	76.62	O
ATOM	1011	N	HIS	B	211	4.401	-21.147	42.440	1.00	76.75	N
ATOM	1012	CA	HIS	B	211	4.499	-20.866	41.010	1.00	76.97	C
ATOM	1013	CB	HIS	B	211	3.434	-19.848	40.591	1.00	80.86	C
ATOM	1014	CG	HIS	B	211	2.600	-20.289	39.427	1.00	81.13	C
ATOM	1015	ND1	HIS	B	211	1.224	-20.372	39.488	1.00	81.12	N
ATOM	1016	CE1	HIS	B	211	0.760	-20.787	38.322	1.00	81.39	C
ATOM	1017	NE2	HIS	B	211	1.785	-20.978	37.507	1.00	81.27	N
ATOM	1018	CD2	HIS	B	211	2.948	-20.674	38.174	1.00	81.35	C
ATOM	1019	C	HIS	B	211	5.896	-20.341	40.671	1.00	76.85	C
ATOM	1020	O	HIS	B	211	6.065	-19.540	39.748	1.00	76.95	O
ATOM	1021	N	LEU	B	212	6.891	-20.807	41.421	1.00	80.86	N
ATOM	1022	CA	LEU	B	212	8.129	-20.062	41.613	1.00	80.60	C
ATOM	1023	CB	LEU	B	212	8.468	-19.973	43.103	1.00	80.80	C
ATOM	1024	CG	LEU	B	212	8.647	-18.572	43.692	1.00	81.03	C
ATOM	1025	CD1	LEU	B	212	8.924	-18.659	45.185	1.00	81.10	C
ATOM	1026	CD2	LEU	B	212	9.758	-17.812	42.976	1.00	80.65	C
ATOM	1027	C	LEU	B	212	9.282	-20.710	40.855	1.00	80.30	C
ATOM	1028	O	LEU	B	212	9.784	-21.764	41.251	1.00	80.03	O
ATOM	1029	N	LEU	B	213	9.699	-20.075	39.764	1.00	80.03	N
ATOM	1030	CA	LEU	B	213	10.507	-20.746	38.751	1.00	79.73	C
ATOM	1031	CB	LEU	B	213	10.517	-19.945	37.445	1.00	79.73	C
ATOM	1032	CG	LEU	B	213	9.188	-19.846	36.692	1.00	79.50	C
ATOM	1033	CD1	LEU	B	213	9.299	-18.875	35.525	1.00	79.46	C
ATOM	1034	CD2	LEU	B	213	8.734	-21.216	36.215	1.00	79.53	C
ATOM	1035	C	LEU	B	213	11.934	-20.982	39.240	1.00	79.30	C
ATOM	1036	O	LEU	B	213	12.606	-20.055	39.692	1.00	79.24	O
ATOM	1037	N	GLN	B	214	12.384	-22.229	39.144	1.00	78.65	N
ATOM	1038	CA	GLN	B	214	13.710	-22.616	39.608	1.00	78.13	C
ATOM	1039	CB	GLN	B	214	13.813	-24.140	39.690	1.00	78.16	C
ATOM	1040	CG	GLN	B	214	15.084	-24.648	40.350	1.00	78.20	C
ATOM	1041	CD	GLN	B	214	15.036	-26.135	40.633	1.00	77.95	C
ATOM	1042	OE1	GLN	B	214	16.059	-26.818	40.586	1.00	78.75	O
ATOM	1043	NE2	GLN	B	214	13.846	-26.645	40.926	1.00	77.67	N
ATOM	1044	C	GLN	B	214	14.798	-22.068	38.692	1.00	77.92	C
ATOM	1045	O	GLN	B	214	15.818	-21.560	39.158	1.00	77.51	O
ATOM	1046	N	VAL	B	215	14.573	-22.182	37.386	1.00	78.01	N
ATOM	1047	CA	VAL	B	215	15.466	-21.593	36.397	1.00	78.08	C
ATOM	1048	CB	VAL	B	215	16.158	-22.672	35.541	1.00	78.10	C
ATOM	1049	CG1	VAL	B	215	17.321	-23.291	36.303	1.00	77.55	C
ATOM	1050	CG2	VAL	B	215	15.160	-23.739	35.115	1.00	78.08	C
ATOM	1051	C	VAL	B	215	14.720	-20.624	35.484	1.00	78.26	C
ATOM	1052	O	VAL	B	215	13.541	-20.821	35.186	1.00	78.04	O
ATOM	1053	N	ILE	B	216	15.412	-19.575	35.051	1.00	78.81	N
ATOM	1054	CA	ILE	B	216	14.907	-18.699	34.000	1.00	79.36	C
ATOM	1055	CB	ILE	B	216	14.731	-17.249	34.503	1.00	79.20	C
ATOM	1056	CG1	ILE	B	216	13.952	-17.225	35.821	1.00	78.68	C
ATOM	1057	CD1	ILE	B	216	12.499	-17.618	35.687	1.00	78.07	C
ATOM	1058	CG2	ILE	B	216	14.037	-16.396	33.448	1.00	78.72	C
ATOM	1059	C	ILE	B	216	15.854	-18.697	32.808	1.00	80.11	C
ATOM	1060	O	ILE	B	216	16.986	-18.220	32.905	1.00	79.95	O
ATOM	1061	N	LEU	B	217	15.387	-19.238	31.686	1.00	81.27	N
ATOM	1062	CA	LEU	B	217	16.141	-19.196	30.433	1.00	82.47	C
ATOM	1063	CB	LEU	B	217	15.757	-20.375	29.523	1.00	82.55	C
ATOM	1064	CG	LEU	B	217	16.522	-21.712	29.449	1.00	82.91	C
ATOM	1065	CD1	LEU	B	217	17.645	-21.675	28.410	1.00	82.40	C
ATOM	1066	CD2	LEU	B	217	17.040	-22.192	30.815	1.00	83.54	C
ATOM	1067	C	LEU	B	217	15.854	-17.883	29.718	1.00	83.17	C
ATOM	1068	O	LEU	B	217	14.721	-17.633	29.304	1.00	83.12	O
ATOM	1069	N	ASN	B	218	16.878	-17.039	29.597	1.00	84.36	N

Figure 2 Table 2a - 17

ATOM	1070	CA	ASN	B	218	16.784	-15.800	28.818	1.00	85.47	C
ATOM	1071	CB	ASN	B	218	16.920	-14.562	29.716	1.00	85.23	C
ATOM	1072	CG	ASN	B	218	15.678	-14.315	30.569	1.00	85.28	C
ATOM	1073	OD1	ASN	B	218	14.617	-14.892	30.328	1.00	85.07	O
ATOM	1074	ND2	ASN	B	218	15.808	-13.448	31.567	1.00	84.94	N
ATOM	1075	C	ASN	B	218	17.782	-15.772	27.659	1.00	86.41	C
ATOM	1076	O	ASN	B	218	18.665	-14.911	27.597	1.00	86.64	O
ATOM	1077	N	LYS	B	219	17.632	-16.743	26.757	1.00	87.57	N
ATOM	1078	CA	LYS	B	219	18.384	-16.801	25.504	1.00	88.81	C
ATOM	1079	CB	LYS	B	219	18.319	-18.223	24.908	1.00	88.78	C
ATOM	1080	CG	LYS	B	219	18.405	-18.357	23.376	1.00	89.06	C
ATOM	1081	CD	LYS	B	219	19.819	-18.258	22.819	1.00	89.11	C
ATOM	1082	CE	LYS	B	219	19.845	-18.693	21.360	1.00	88.82	C
ATOM	1083	NZ	LYS	B	219	21.178	-18.488	20.741	1.00	88.76	N
ATOM	1084	C	LYS	B	219	17.854	-15.729	24.547	1.00	89.68	C
ATOM	1085	O	LYS	B	219	18.527	-14.720	24.322	1.00	89.73	O
ATOM	1086	N	ASP	B	220	16.650	-15.955	24.008	1.00	90.76	N
ATOM	1087	CA	ASP	B	220	15.920	-14.999	23.146	1.00	91.77	C
ATOM	1088	CB	ASP	B	220	15.520	-13.730	23.933	1.00	91.82	C
ATOM	1089	CG	ASP	B	220	14.836	-14.041	25.267	1.00	92.39	C
ATOM	1090	OD1	ASP	B	220	13.927	-14.901	25.303	1.00	93.04	O
ATOM	1091	OD2	ASP	B	220	15.206	-13.409	26.284	1.00	92.64	O
ATOM	1092	C	ASP	B	220	16.621	-14.598	21.834	1.00	92.34	C
ATOM	1093	O	ASP	B	220	15.953	-14.161	20.890	1.00	92.44	O
ATOM	1094	N	THR	B	221	17.944	-14.792	21.776	1.00	93.05	N
ATOM	1095	CA	THR	B	221	18.870	-14.093	20.852	1.00	93.68	C
ATOM	1096	CB	THR	B	221	18.317	-13.943	19.385	1.00	93.69	C
ATOM	1097	OG1	THR	B	221	17.791	-15.198	18.934	1.00	93.84	O
ATOM	1098	CG2	THR	B	221	19.410	-13.482	18.409	1.00	93.53	C
ATOM	1099	C	THR	B	221	19.255	-12.738	21.488	1.00	94.08	C
ATOM	1100	O	THR	B	221	19.364	-11.710	20.802	1.00	94.20	O
ATOM	1101	N	ASN	B	222	19.466	-12.764	22.810	1.00	94.45	N
ATOM	1102	CA	ASN	B	222	19.714	-11.564	23.625	1.00	94.78	C
ATOM	1103	CB	ASN	B	222	19.546	-11.894	25.118	1.00	94.81	C
ATOM	1104	CG	ASN	B	222	19.401	-10.650	25.987	1.00	95.28	C
ATOM	1105	OD1	ASN	B	222	18.581	-9.769	25.712	1.00	95.64	O
ATOM	1106	ND2	ASN	B	222	20.192	-10.587	27.057	1.00	95.36	N
ATOM	1107	C	ASN	B	222	21.087	-10.933	23.373	1.00	94.84	C
ATOM	1108	O	ASN	B	222	21.254	-9.713	23.478	1.00	94.86	O
ATOM	1109	N	PRO	B	233	5.051	-10.657	31.915	1.00	80.05	N
ATOM	1110	CA	PRO	B	233	4.371	-11.890	32.335	1.00	79.87	C
ATOM	1111	CB	PRO	B	233	5.101	-12.986	31.543	1.00	80.00	C
ATOM	1112	CG	PRO	B	233	5.664	-12.280	30.340	1.00	80.08	C
ATOM	1113	CD	PRO	B	233	6.025	-10.896	30.828	1.00	80.13	C
ATOM	1114	C	PRO	B	233	4.504	-12.120	33.840	1.00	79.63	C
ATOM	1115	O	PRO	B	233	4.541	-11.153	34.605	1.00	79.81	O
ATOM	1116	N	ASN	B	234	4.580	-13.387	34.247	1.00	79.25	N
ATOM	1117	CA	ASN	B	234	4.689	-13.787	35.663	1.00	78.66	C
ATOM	1118	CB	ASN	B	234	4.763	-15.328	35.782	1.00	79.10	C
ATOM	1119	CG	ASN	B	234	5.894	-15.948	34.960	1.00	79.75	C
ATOM	1120	OD1	ASN	B	234	6.922	-16.358	35.513	1.00	80.81	O
ATOM	1121	ND2	ASN	B	234	5.695	-16.044	33.642	1.00	79.31	N
ATOM	1122	C	ASN	B	234	5.821	-13.122	36.480	1.00	77.93	C
ATOM	1123	O	ASN	B	234	6.852	-12.766	35.900	1.00	77.86	O
ATOM	1124	N	HIS	B	235	5.655	-12.918	37.802	1.00	76.81	N
ATOM	1125	CA	HIS	B	235	4.430	-13.154	38.593	1.00	75.61	C
ATOM	1126	CB	HIS	B	235	3.942	-14.611	38.469	1.00	76.05	C
ATOM	1127	CG	HIS	B	235	2.449	-14.752	38.369	1.00	77.32	C
ATOM	1128	ND1	HIS	B	235	1.722	-14.262	37.302	1.00	78.10	N
ATOM	1129	CE1	HIS	B	235	0.442	-14.538	37.479	1.00	78.53	C
ATOM	1130	NE2	HIS	B	235	0.310	-15.196	38.618	1.00	78.71	N
ATOM	1131	CD2	HIS	B	235	1.550	-15.348	39.193	1.00	77.98	C
ATOM	1132	C	HIS	B	235	4.695	-12.817	40.073	1.00	74.31	C
ATOM	1133	O	HIS	B	235	4.571	-11.656	40.494	1.00	74.36	O
ATOM	1134	N	VAL	B	236	5.063	-13.847	40.843	1.00	72.24	N
ATOM	1135	CA	VAL	B	236	5.340	-13.753	42.282	1.00	69.88	C
ATOM	1136	CB	VAL	B	236	4.454	-14.767	43.084	1.00	70.25	C

Figure 2 Table 2a - 18

ATOM	1137	CG1	VAL	B	236	4.811	-16.224	42.728	1.00	70.42	C
ATOM	1138	CG2	VAL	B	236	4.521	-14.523	44.607	1.00	70.26	C
ATOM	1139	C	VAL	B	236	6.833	-14.010	42.553	1.00	68.13	C
ATOM	1140	O	VAL	B	236	7.240	-14.283	43.697	1.00	68.19	O
ATOM	1141	N	MET	B	237	7.642	-13.946	41.489	1.00	65.39	N
ATOM	1142	CA	MET	B	237	9.092	-14.056	41.621	1.00	62.42	C
ATOM	1143	CB	MET	B	237	9.745	-14.729	40.404	1.00	62.48	C
ATOM	1144	CG	MET	B	237	9.179	-14.366	39.038	1.00	63.43	C
ATOM	1145	SD	MET	B	237	9.337	-15.755	37.839	1.00	65.69	S
ATOM	1146	CE	MET	B	237	8.210	-16.936	38.589	1.00	65.80	C
ATOM	1147	C	MET	B	237	9.678	-12.683	41.927	1.00	59.98	C
ATOM	1148	O	MET	B	237	10.899	-12.519	42.012	1.00	59.41	O
ATOM	1149	N	LEU	B	238	8.784	-11.709	42.110	1.00	57.08	N
ATOM	1150	CA	LEU	B	238	9.155	-10.374	42.545	1.00	54.75	C
ATOM	1151	CB	LEU	B	238	7.924	-9.498	42.756	1.00	54.68	C
ATOM	1152	CG	LEU	B	238	7.219	-8.889	41.552	1.00	56.05	C
ATOM	1153	CD1	LEU	B	238	5.975	-8.169	42.043	1.00	57.05	C
ATOM	1154	CD2	LEU	B	238	8.121	-7.955	40.711	1.00	55.72	C
ATOM	1155	C	LEU	B	238	9.917	-10.438	43.844	1.00	52.96	C
ATOM	1156	O	LEU	B	238	9.558	-11.201	44.734	1.00	52.40	O
ATOM	1157	N	ASN	B	239	10.962	-9.624	43.932	1.00	51.23	N
ATOM	1158	CA	ASN	B	239	11.788	-9.478	45.132	1.00	50.49	C
ATOM	1159	CB	ASN	B	239	10.949	-9.085	46.378	1.00	50.35	C
ATOM	1160	CG	ASN	B	239	10.277	-7.721	46.243	1.00	49.77	C
ATOM	1161	OD1	ASN	B	239	10.078	-7.218	45.146	1.00	51.71	O
ATOM	1162	ND2	ASN	B	239	9.914	-7.129	47.364	1.00	50.47	N
ATOM	1163	C	ASN	B	239	12.699	-10.664	45.442	1.00	49.66	C
ATOM	1164	O	ASN	B	239	13.414	-10.647	46.428	1.00	49.80	O
ATOM	1165	N	HIS	B	240	12.672	-11.684	44.596	1.00	49.04	N
ATOM	1166	CA	HIS	B	240	13.493	-12.865	44.789	1.00	48.47	C
ATOM	1167	CB	HIS	B	240	12.766	-14.121	44.306	1.00	47.90	C
ATOM	1168	CG	HIS	B	240	11.699	-14.568	45.244	1.00	46.76	C
ATOM	1169	ND1	HIS	B	240	11.928	-15.483	46.249	1.00	45.98	N
ATOM	1170	CE1	HIS	B	240	10.819	-15.657	46.944	1.00	46.04	C
ATOM	1171	NE2	HIS	B	240	9.880	-14.885	46.431	1.00	46.87	N
ATOM	1172	CD2	HIS	B	240	10.410	-14.183	45.374	1.00	46.75	C
ATOM	1173	C	HIS	B	240	14.829	-12.736	44.106	1.00	48.66	C
ATOM	1174	O	HIS	B	240	14.926	-12.177	43.000	1.00	49.09	O
ATOM	1175	N	LEU	B	241	15.858	-13.262	44.764	1.00	48.40	N
ATOM	1176	CA	LEU	B	241	17.211	-13.227	44.227	1.00	48.31	C
ATOM	1177	CB	LEU	B	241	18.261	-13.327	45.352	1.00	48.23	C
ATOM	1178	CG	LEU	B	241	19.754	-13.192	45.014	1.00	48.15	C
ATOM	1179	CD1	LEU	B	241	20.110	-11.750	44.608	1.00	46.77	C
ATOM	1180	CD2	LEU	B	241	20.632	-13.678	46.162	1.00	46.68	C
ATOM	1181	C	LEU	B	241	17.425	-14.307	43.161	1.00	48.30	C
ATOM	1182	O	LEU	B	241	17.099	-15.490	43.354	1.00	47.93	O
ATOM	1183	N	TYR	B	242	17.951	-13.862	42.023	1.00	48.25	N
ATOM	1184	CA	TYR	B	242	18.401	-14.754	40.959	1.00	48.30	C
ATOM	1185	CB	TYR	B	242	17.582	-14.529	39.687	1.00	48.54	C
ATOM	1186	CG	TYR	B	242	16.193	-15.118	39.775	1.00	48.95	C
ATOM	1187	CD1	TYR	B	242	15.147	-14.418	40.395	1.00	48.43	C
ATOM	1188	CE1	TYR	B	242	13.878	-14.962	40.481	1.00	48.06	C
ATOM	1189	CZ	TYR	B	242	13.651	-16.218	39.953	1.00	50.37	C
ATOM	1190	OH	TYR	B	242	12.403	-16.790	40.036	1.00	53.28	O
ATOM	1191	CE2	TYR	B	242	14.672	-16.937	39.354	1.00	49.53	C
ATOM	1192	CD2	TYR	B	242	15.931	-16.386	39.269	1.00	48.76	C
ATOM	1193	C	TYR	B	242	19.871	-14.492	40.699	1.00	48.18	C
ATOM	1194	O	TYR	B	242	20.373	-13.387	40.949	1.00	48.23	O
ATOM	1195	N	ALA	B	243	20.562	-15.513	40.213	1.00	48.03	N
ATOM	1196	CA	ALA	B	243	21.981	-15.408	39.915	1.00	47.96	C
ATOM	1197	CB	ALA	B	243	22.806	-15.788	41.135	1.00	47.18	C
ATOM	1198	C	ALA	B	243	22.392	-16.236	38.693	1.00	48.28	C
ATOM	1199	O	ALA	B	243	21.771	-17.263	38.381	1.00	47.97	O
ATOM	1200	N	LEU	B	244	23.420	-15.749	37.993	1.00	48.97	N
ATOM	1201	CA	LEU	B	244	24.139	-16.529	36.987	1.00	49.63	C
ATOM	1202	CB	LEU	B	244	24.760	-15.630	35.908	1.00	49.53	C
ATOM	1203	CG	LEU	B	244	23.944	-14.663	35.054	1.00	49.44	C

Figure 2 Table 2a - 19

ATOM	1204	CD1	LEU	B	244	24.864	-13.934	34.063	1.00	48.89	C
ATOM	1205	CD2	LEU	B	244	22.820	-15.384	34.327	1.00	48.64	C
ATOM	1206	C	LEU	B	244	25.273	-17.241	37.691	1.00	50.35	C
ATOM	1207	O	LEU	B	244	25.765	-16.766	38.719	1.00	50.02	O
ATOM	1208	N	SER	B	245	25.696	-18.371	37.126	1.00	51.61	N
ATOM	1209	CA	SER	B	245	26.870	-19.099	37.606	1.00	52.83	C
ATOM	1210	CB	SER	B	245	27.230	-20.229	36.637	1.00	53.03	C
ATOM	1211	OG	SER	B	245	26.080	-20.960	36.248	1.00	54.74	O
ATOM	1212	C	SER	B	245	28.055	-18.149	37.709	1.00	53.18	C
ATOM	1213	O	SER	B	245	28.253	-17.299	36.825	1.00	53.36	O
ATOM	1214	N	ILE	B	246	28.830	-18.285	38.783	1.00	53.56	N
ATOM	1215	CA	ILE	B	246	30.064	-17.527	38.928	1.00	53.96	C
ATOM	1216	CB	ILE	B	246	30.707	-17.711	40.318	1.00	53.76	C
ATOM	1217	CG1	ILE	B	246	29.779	-17.148	41.403	1.00	54.05	C
ATOM	1218	CD1	ILE	B	246	30.137	-17.550	42.821	1.00	53.66	C
ATOM	1219	CG2	ILE	B	246	32.084	-17.045	40.366	1.00	53.12	C
ATOM	1220	C	ILE	B	246	31.028	-17.921	37.810	1.00	54.67	C
ATOM	1221	O	ILE	B	246	31.338	-19.095	37.622	1.00	54.80	O
ATOM	1222	N	LYS	B	247	31.459	-16.926	37.045	1.00	55.47	N
ATOM	1223	CA	LYS	B	247	32.400	-17.140	35.966	1.00	56.36	C
ATOM	1224	CB	LYS	B	247	31.692	-17.040	34.608	1.00	56.64	C
ATOM	1225	CG	LYS	B	247	31.139	-18.360	34.069	1.00	57.60	C
ATOM	1226	CD	LYS	B	247	30.889	-18.256	32.560	1.00	58.60	C
ATOM	1227	CE	LYS	B	247	30.589	-19.618	31.939	1.00	59.34	C
ATOM	1228	NZ	LYS	B	247	30.679	-19.583	30.442	1.00	59.22	N
ATOM	1229	C	LYS	B	247	33.502	-16.100	36.052	1.00	56.66	C
ATOM	1230	O	LYS	B	247	33.220	-14.899	36.042	1.00	56.56	O
ATOM	1231	N	ASP	B	248	34.749	-16.569	36.146	1.00	56.98	N
ATOM	1232	CA	ASP	B	248	35.933	-15.695	36.089	1.00	57.29	C
ATOM	1233	CB	ASP	B	248	36.051	-15.043	34.697	1.00	57.35	C
ATOM	1234	CG	ASP	B	248	37.480	-14.665	34.333	1.00	57.62	C
ATOM	1235	OD1	ASP	B	248	38.437	-15.309	34.820	1.00	58.49	O
ATOM	1236	OD2	ASP	B	248	37.643	-13.717	33.539	1.00	57.85	O
ATOM	1237	C	ASP	B	248	35.914	-14.641	37.214	1.00	57.36	C
ATOM	1238	O	ASP	B	248	36.121	-13.434	36.978	1.00	57.31	O
ATOM	1239	N	SER	B	249	35.643	-15.130	38.426	1.00	57.21	N
ATOM	1240	CA	SER	B	249	35.642	-14.341	39.670	1.00	57.38	C
ATOM	1241	CB	SER	B	249	37.038	-13.768	39.968	1.00	57.41	C
ATOM	1242	OG	SER	B	249	37.973	-14.790	40.280	1.00	58.28	O
ATOM	1243	C	SER	B	249	34.572	-13.244	39.786	1.00	57.23	C
ATOM	1244	O	SER	B	249	34.687	-12.368	40.647	1.00	57.35	O
ATOM	1245	N	VAL	B	250	33.533	-13.300	38.950	1.00	57.04	N
ATOM	1246	CA	VAL	B	250	32.453	-12.295	38.989	1.00	56.59	C
ATOM	1247	CB	VAL	B	250	32.443	-11.372	37.707	1.00	56.87	C
ATOM	1248	CG1	VAL	B	250	32.554	-12.174	36.421	1.00	57.31	C
ATOM	1249	CG2	VAL	B	250	31.212	-10.439	37.659	1.00	56.92	C
ATOM	1250	C	VAL	B	250	31.064	-12.870	39.336	1.00	56.10	C
ATOM	1251	O	VAL	B	250	30.630	-13.888	38.777	1.00	55.52	O
ATOM	1252	N	MET	B	251	30.404	-12.197	40.286	1.00	55.71	N
ATOM	1253	CA	MET	B	251	29.032	-12.485	40.720	1.00	55.74	C
ATOM	1254	CB	MET	B	251	28.849	-12.126	42.192	1.00	55.86	C
ATOM	1255	CG	MET	B	251	29.202	-13.192	43.189	1.00	58.44	C
ATOM	1256	SD	MET	B	251	28.263	-12.895	44.703	1.00	63.16	S
ATOM	1257	CE	MET	B	251	28.865	-14.204	45.781	1.00	60.97	C
ATOM	1258	C	MET	B	251	28.025	-11.649	39.944	1.00	54.74	C
ATOM	1259	O	MET	B	251	28.179	-10.424	39.830	1.00	55.07	O
ATOM	1260	N	VAL	B	252	26.979	-12.291	39.437	1.00	53.42	N
ATOM	1261	CA	VAL	B	252	25.876	-11.547	38.835	1.00	51.69	C
ATOM	1262	CB	VAL	B	252	25.738	-11.779	37.313	1.00	51.83	C
ATOM	1263	CG1	VAL	B	252	24.786	-10.736	36.713	1.00	51.19	C
ATOM	1264	CG2	VAL	B	252	27.104	-11.723	36.629	1.00	50.73	C
ATOM	1265	C	VAL	B	252	24.569	-11.846	39.563	1.00	50.88	C
ATOM	1266	O	VAL	B	252	23.991	-12.930	39.439	1.00	50.10	O
ATOM	1267	N	LEU	B	253	24.133	-10.854	40.328	1.00	50.17	N
ATOM	1268	CA	LEU	B	253	22.928	-10.931	41.130	1.00	49.88	C
ATOM	1269	CB	LEU	B	253	23.200	-10.407	42.540	1.00	49.54	C
ATOM	1270	CG	LEU	B	253	24.286	-11.182	43.309	1.00	49.01	C

Figure 2 Table 2a - 20

ATOM	1271	CD1	LEU	B	253	24.481	-10.580	44.695	1.00	48.28	C
ATOM	1272	CD2	LEU	B	253	23.986	-12.696	43.380	1.00	45.18	C
ATOM	1273	C	LEU	B	253	21.818	-10.135	40.484	1.00	50.14	C
ATOM	1274	O	LEU	B	253	22.061	-9.098	39.874	1.00	50.84	O
ATOM	1275	N	SER	B	254	20.594	-10.628	40.616	1.00	50.08	N
ATOM	1276	CA	SER	B	254	19.462	-10.068	39.913	1.00	49.74	C
ATOM	1277	CB	SER	B	254	19.384	-10.675	38.513	1.00	49.91	C
ATOM	1278	OG	SER	B	254	18.074	-10.595	37.978	1.00	51.92	O
ATOM	1279	C	SER	B	254	18.163	-10.296	40.666	1.00	48.92	C
ATOM	1280	O	SER	B	254	18.015	-11.294	41.369	1.00	49.16	O
ATOM	1281	N	ALA	B	255	17.237	-9.352	40.511	1.00	48.17	N
ATOM	1282	CA	ALA	B	255	15.902	-9.414	41.106	1.00	47.29	C
ATOM	1283	CB	ALA	B	255	15.957	-9.066	42.585	1.00	46.75	C
ATOM	1284	C	ALA	B	255	14.996	-8.440	40.367	1.00	46.95	C
ATOM	1285	O	ALA	B	255	15.476	-7.465	39.786	1.00	46.53	O
ATOM	1286	N	THR	B	256	13.693	-8.704	40.387	1.00	46.74	N
ATOM	1287	CA	THR	B	256	12.722	-7.763	39.850	1.00	46.64	C
ATOM	1288	CB	THR	B	256	11.752	-8.449	38.877	1.00	46.85	C
ATOM	1289	OG1	THR	B	256	12.496	-9.154	37.870	1.00	46.36	O
ATOM	1290	CG2	THR	B	256	10.861	-7.412	38.194	1.00	46.55	C
ATOM	1291	C	THR	B	256	11.956	-7.100	40.992	1.00	47.03	C
ATOM	1292	O	THR	B	256	11.450	-7.779	41.897	1.00	47.43	O
ATOM	1293	N	HIS	B	257	11.894	-5.772	40.962	1.00	46.92	N
ATOM	1294	CA	HIS	B	257	11.166	-5.004	41.962	1.00	47.07	C
ATOM	1295	CB	HIS	B	257	12.113	-4.145	42.809	1.00	47.33	C
ATOM	1296	CG	HIS	B	257	12.969	-4.946	43.742	1.00	50.37	C
ATOM	1297	ND1	HIS	B	257	14.145	-5.553	43.340	1.00	51.70	N
ATOM	1298	CE1	HIS	B	257	14.672	-6.199	44.367	1.00	52.54	C
ATOM	1299	NE2	HIS	B	257	13.875	-6.045	45.413	1.00	51.47	N
ATOM	1300	CD2	HIS	B	257	12.802	-5.270	45.050	1.00	50.38	C
ATOM	1301	C	HIS	B	257	10.144	-4.134	41.275	1.00	46.58	C
ATOM	1302	O	HIS	B	257	10.191	-3.961	40.065	1.00	46.75	O
ATOM	1303	N	ARG	B	258	9.244	-3.564	42.071	1.00	46.15	N
ATOM	1304	CA	ARG	B	258	8.102	-2.815	41.587	1.00	45.29	C
ATOM	1305	CB	ARG	B	258	6.842	-3.543	42.029	1.00	45.82	C
ATOM	1306	CG	ARG	B	258	5.530	-2.998	41.529	1.00	46.56	C
ATOM	1307	CD	ARG	B	258	4.411	-3.731	42.268	1.00	49.89	C
ATOM	1308	NE	ARG	B	258	3.321	-2.829	42.628	1.00	52.78	N
ATOM	1309	CZ	ARG	B	258	3.215	-2.185	43.787	1.00	53.01	C
ATOM	1310	NH1	ARG	B	258	4.127	-2.340	44.733	1.00	53.33	N
ATOM	1311	NH2	ARG	B	258	2.182	-1.387	43.996	1.00	53.70	N
ATOM	1312	C	ARG	B	258	8.110	-1.409	42.168	1.00	44.52	C
ATOM	1313	O	ARG	B	258	8.283	-1.223	43.373	1.00	44.02	O
ATOM	1314	N	TYR	B	259	7.952	-0.427	41.287	1.00	43.42	N
ATOM	1315	CA	TYR	B	259	7.696	0.941	41.678	1.00	42.51	C
ATOM	1316	CB	TYR	B	259	8.818	1.892	41.217	1.00	41.83	C
ATOM	1317	CG	TYR	B	259	8.589	3.345	41.611	1.00	40.41	C
ATOM	1318	CD1	TYR	B	259	8.845	3.789	42.913	1.00	38.61	C
ATOM	1319	CE1	TYR	B	259	8.634	5.110	43.279	1.00	37.78	C
ATOM	1320	CZ	TYR	B	259	8.150	6.019	42.345	1.00	38.12	C
ATOM	1321	OH	TYR	B	259	7.927	7.333	42.719	1.00	36.59	O
ATOM	1322	CE2	TYR	B	259	7.881	5.604	41.055	1.00	37.69	C
ATOM	1323	CD2	TYR	B	259	8.102	4.269	40.694	1.00	39.08	C
ATOM	1324	C	TYR	B	259	6.357	1.317	41.061	1.00	42.66	C
ATOM	1325	O	TYR	B	259	6.210	1.368	39.831	1.00	42.58	O
ATOM	1326	N	LYS	B	260	5.381	1.570	41.924	1.00	42.58	N
ATOM	1327	CA	LYS	B	260	4.009	1.779	41.494	1.00	42.68	C
ATOM	1328	CB	LYS	B	260	3.828	3.186	40.951	1.00	42.64	C
ATOM	1329	CG	LYS	B	260	4.013	4.249	42.003	1.00	43.31	C
ATOM	1330	CD	LYS	B	260	4.062	5.609	41.367	1.00	45.27	C
ATOM	1331	CE	LYS	B	260	4.332	6.671	42.405	1.00	46.73	C
ATOM	1332	NZ	LYS	B	260	4.627	7.952	41.701	1.00	48.73	N
ATOM	1333	C	LYS	B	260	3.590	0.702	40.490	1.00	42.64	C
ATOM	1334	O	LYS	B	260	3.378	-0.440	40.885	1.00	42.39	O
ATOM	1335	N	LYS	B	261	3.508	1.052	39.204	1.00	42.69	N
ATOM	1336	CA	LYS	B	261	3.077	0.103	38.157	1.00	42.67	C
ATOM	1337	CB	LYS	B	261	1.985	0.720	37.280	1.00	42.51	C

Figure 2 Table 2a - 21

ATOM	1338	CG	LYS	B	261	0.738	1.159	38.015	1.00	43.58	C
ATOM	1339	CD	LYS	B	261	-0.113	-0.028	38.437	1.00	46.28	C
ATOM	1340	CE	LYS	B	261	-1.334	0.436	39.208	1.00	47.93	C
ATOM	1341	NZ	LYS	B	261	-1.954	1.613	38.523	1.00	49.43	N
ATOM	1342	C	LYS	B	261	4.218	-0.384	37.258	1.00	42.53	C
ATOM	1343	O	LYS	B	261	3.981	-1.090	36.265	1.00	42.26	O
ATOM	1344	N	LYS	B	262	5.445	-0.001	37.596	1.00	42.11	N
ATOM	1345	CA	LYS	B	262	6.584	-0.291	36.742	1.00	42.14	C
ATOM	1346	CB	LYS	B	262	7.430	0.956	36.473	1.00	41.78	C
ATOM	1347	CG	LYS	B	262	6.665	2.209	36.055	1.00	41.16	C
ATOM	1348	CD	LYS	B	262	5.934	2.087	34.738	1.00	39.69	C
ATOM	1349	CE	LYS	B	262	5.307	3.418	34.373	1.00	38.02	C
ATOM	1350	NZ	LYS	B	262	4.734	3.405	33.025	1.00	36.97	N
ATOM	1351	C	LYS	B	262	7.440	-1.349	37.404	1.00	42.20	C
ATOM	1352	O	LYS	B	262	7.576	-1.358	38.619	1.00	42.18	O
ATOM	1353	N	TYR	B	263	8.023	-2.220	36.584	1.00	42.08	N
ATOM	1354	CA	TYR	B	263	8.871	-3.297	37.055	1.00	42.29	C
ATOM	1355	CB	TYR	B	263	8.255	-4.660	36.703	1.00	42.83	C
ATOM	1356	CG	TYR	B	263	6.861	-4.854	37.266	1.00	43.62	C
ATOM	1357	CD1	TYR	B	263	5.745	-4.329	36.602	1.00	43.38	C
ATOM	1358	CE1	TYR	B	263	4.463	-4.488	37.118	1.00	44.00	C
ATOM	1359	CZ	TYR	B	263	4.288	-5.180	38.305	1.00	45.21	C
ATOM	1360	OH	TYR	B	263	3.016	-5.325	38.796	1.00	47.39	O
ATOM	1361	CE2	TYR	B	263	5.376	-5.716	38.991	1.00	43.58	C
ATOM	1362	CD2	TYR	B	263	6.659	-5.546	38.470	1.00	42.97	C
ATOM	1363	C	TYR	B	263	10.235	-3.169	36.428	1.00	41.89	C
ATOM	1364	O	TYR	B	263	10.366	-2.932	35.233	1.00	42.05	O
ATOM	1365	N	VAL	B	264	11.260	-3.310	37.245	1.00	41.90	N
ATOM	1366	CA	VAL	B	264	12.622	-3.288	36.741	1.00	41.40	C
ATOM	1367	CB	VAL	B	264	13.335	-1.926	37.025	1.00	41.02	C
ATOM	1368	CG1	VAL	B	264	13.554	-1.694	38.503	1.00	38.48	C
ATOM	1369	CG2	VAL	B	264	14.646	-1.843	36.280	1.00	41.58	C
ATOM	1370	C	VAL	B	264	13.402	-4.488	37.294	1.00	41.79	C
ATOM	1371	O	VAL	B	264	13.361	-4.785	38.489	1.00	41.23	O
ATOM	1372	N	THR	B	265	14.062	-5.186	36.385	1.00	42.53	N
ATOM	1373	CA	THR	B	265	14.970	-6.264	36.707	1.00	43.69	C
ATOM	1374	CB	THR	B	265	14.931	-7.322	35.590	1.00	43.84	C
ATOM	1375	OG1	THR	B	265	13.618	-7.885	35.534	1.00	44.94	O
ATOM	1376	CG2	THR	B	265	15.937	-8.438	35.835	1.00	44.51	C
ATOM	1377	C	THR	B	265	16.350	-5.645	36.774	1.00	44.03	C
ATOM	1378	O	THR	B	265	16.874	-5.172	35.759	1.00	44.50	O
ATOM	1379	N	THR	B	266	16.927	-5.641	37.969	1.00	44.33	N
ATOM	1380	CA	THR	B	266	18.240	-5.051	38.212	1.00	44.54	C
ATOM	1381	CB	THR	B	266	18.241	-4.258	39.539	1.00	44.68	C
ATOM	1382	OG1	THR	B	266	17.169	-3.297	39.534	1.00	44.19	O
ATOM	1383	CG2	THR	B	266	19.568	-3.533	39.735	1.00	44.97	C
ATOM	1384	C	THR	B	266	19.324	-6.126	38.271	1.00	44.68	C
ATOM	1385	O	THR	B	266	19.149	-7.144	38.953	1.00	45.05	O
ATOM	1386	N	LEU	B	267	20.434	-5.897	37.567	1.00	44.49	N
ATOM	1387	CA	LEU	B	267	21.569	-6.817	37.583	1.00	44.88	C
ATOM	1388	CB	LEU	B	267	21.936	-7.282	36.165	1.00	44.58	C
ATOM	1389	CG	LEU	B	267	21.009	-8.175	35.339	1.00	44.47	C
ATOM	1390	CD1	LEU	B	267	19.878	-7.387	34.701	1.00	44.11	C
ATOM	1391	CD2	LEU	B	267	21.814	-8.856	34.252	1.00	45.78	C
ATOM	1392	C	LEU	B	267	22.777	-6.131	38.181	1.00	45.22	C
ATOM	1393	O	LEU	B	267	23.178	-5.067	37.720	1.00	46.14	O
ATOM	1394	N	LEU	B	268	23.378	-6.745	39.185	1.00	45.53	N
ATOM	1395	CA	LEU	B	268	24.621	-6.240	39.750	1.00	45.70	C
ATOM	1396	CB	LEU	B	268	24.530	-6.157	41.286	1.00	45.58	C
ATOM	1397	CG	LEU	B	268	25.739	-5.590	42.041	1.00	44.10	C
ATOM	1398	CD1	LEU	B	268	26.059	-4.158	41.626	1.00	40.63	C
ATOM	1399	CD2	LEU	B	268	25.508	-5.668	43.537	1.00	42.83	C
ATOM	1400	C	LEU	B	268	25.773	-7.148	39.359	1.00	46.42	C
ATOM	1401	O	LEU	B	268	25.740	-8.350	39.647	1.00	46.41	O
ATOM	1402	N	TYR	B	269	26.776	-6.569	38.699	1.00	47.09	N
ATOM	1403	CA	TYR	B	269	28.036	-7.251	38.431	1.00	47.83	C
ATOM	1404	CB	TYR	B	269	28.579	-6.877	37.059	1.00	47.25	C

Figure 2 Table 2a - 22

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ATOM   1405  CG  TYR B 269      27.881  -7.588  35.936  1.00 46.82      C
ATOM   1406  CD1 TYR B 269      26.580  -7.247  35.575  1.00 45.76      C
ATOM   1407  CE1 TYR B 269      25.925  -7.911  34.552  1.00 46.44      C
ATOM   1408  CZ  TYR B 269      26.569  -8.930  33.860  1.00 46.38      C
ATOM   1409  OH  TYR B 269      25.914  -9.575  32.832  1.00 45.90      O
ATOM   1410  CE2 TYR B 269      27.873  -9.286  34.190  1.00 46.24      C
ATOM   1411  CD2 TYR B 269      28.522  -8.610  35.228  1.00 45.95      C
ATOM   1412  C   TYR B 269      28.998  -6.816  39.506  1.00 48.87      C
ATOM   1413  O   TYR B 269      29.250  -5.621  39.673  1.00 49.23      O
ATOM   1414  N   LYS B 270      29.528  -7.799  40.224  1.00 50.06      N
ATOM   1415  CA  LYS B 270      30.287  -7.583  41.448  1.00 51.57      C
ATOM   1416  CB  LYS B 270      29.339  -7.717  42.663  1.00 51.80      C
ATOM   1417  CG  LYS B 270      29.955  -7.389  44.027  1.00 53.21      C
ATOM   1418  CD  LYS B 270      29.041  -7.731  45.218  1.00 54.09      C
ATOM   1419  CE  LYS B 270      29.858  -7.679  46.532  1.00 55.85      C
ATOM   1420  NZ  LYS B 270      29.069  -7.584  47.814  1.00 56.40      N
ATOM   1421  C   LYS B 270      31.435  -8.615  41.531  1.00 52.21      C
ATOM   1422  O   LYS B 270      31.199  -9.827  41.408  1.00 52.35      O
ATOM   1423  N   PRO B 271      32.680  -8.146  41.742  1.00 52.80      N
ATOM   1424  CA  PRO B 271      33.792  -9.071  42.001  1.00 53.58      C
ATOM   1425  CB  PRO B 271      35.009  -8.144  42.129  1.00 53.33      C
ATOM   1426  CG  PRO B 271      34.591  -6.854  41.548  1.00 53.08      C
ATOM   1427  CD  PRO B 271      33.123  -6.742  41.763  1.00 53.00      C
ATOM   1428  C   PRO B 271      33.614  -9.839  43.315  1.00 54.19      C
ATOM   1429  O   PRO B 271      32.814  -9.444  44.165  1.00 54.25      O
ATOM   1430  N   ILE B 272      34.352 -10.933  43.462  1.00 55.26      N
ATOM   1431  CA  ILE B 272      34.442 -11.654  44.728  1.00 56.36      C
ATOM   1432  CB  ILE B 272      34.300 -13.183  44.531  1.00 56.64      C
ATOM   1433  CG1 ILE B 272      33.019 -13.502  43.742  1.00 57.46      C
ATOM   1434  CD1 ILE B 272      32.838 -14.994  43.436  1.00 58.65      C
ATOM   1435  CG2 ILE B 272      34.321 -13.916  45.882  1.00 56.30      C
ATOM   1436  C   ILE B 272      35.774 -11.334  45.406  1.00 56.49      C
ATOM   1437  O   ILE B 272      35.908 -11.469  46.631  1.00 57.06      O
ATOM   1438  N   SER C  23       4.102  33.258  28.172  1.00 72.16      N
ATOM   1439  CA  SER C  23       4.567  32.163  27.306  1.00 71.96      C
ATOM   1440  CB  SER C  23       3.762  32.133  25.999  1.00 72.01      C
ATOM   1441  OG  SER C  23       2.378  31.947  26.269  1.00 71.60      O
ATOM   1442  C   SER C  23       6.065  32.299  27.007  1.00 71.79      C
ATOM   1443  O   SER C  23       6.848  32.650  27.893  1.00 71.63      O
ATOM   1444  N   ASN C  24       6.465  31.993  25.773  1.00 71.65      N
ATOM   1445  CA  ASN C  24       6.671  30.610  25.343  1.00 71.33      C
ATOM   1446  CB  ASN C  24       7.918  30.027  26.015  1.00 71.42      C
ATOM   1447  CG  ASN C  24       9.080  29.874  25.055  1.00 71.64      C
ATOM   1448  OD1 ASN C  24       9.245  30.671  24.127  1.00 70.85      O
ATOM   1449  ND2 ASN C  24       9.894  28.845  25.271  1.00 71.99      N
ATOM   1450  C   ASN C  24       5.481  29.692  25.593  1.00 70.86      C
ATOM   1451  O   ASN C  24       4.784  29.822  26.601  1.00 71.00      O
ATOM   1452  N   SER C  25       5.262  28.754  24.674  1.00 70.01      N
ATOM   1453  CA  SER C  25       4.192  27.776  24.822  1.00 68.94      C
ATOM   1454  CB  SER C  25       2.873  28.468  25.182  1.00 69.18      C
ATOM   1455  OG  SER C  25       2.231  27.805  26.262  1.00 69.24      O
ATOM   1456  C   SER C  25       4.022  26.952  23.553  1.00 68.04      C
ATOM   1457  O   SER C  25       3.169  27.245  22.715  1.00 68.40      O
ATOM   1458  N   SER C  26       4.844  25.919  23.416  1.00 66.68      N
ATOM   1459  CA  SER C  26       4.492  24.777  22.589  1.00 65.45      C
ATOM   1460  CB  SER C  26       5.726  23.914  22.317  1.00 65.66      C
ATOM   1461  OG  SER C  26       6.667  24.605  21.519  1.00 66.26      O
ATOM   1462  C   SER C  26       3.420  23.940  23.273  1.00 64.30      C
ATOM   1463  O   SER C  26       3.396  23.826  24.499  1.00 64.04      O
ATOM   1464  N   VAL C  27       2.537  23.355  22.470  1.00 63.00      N
ATOM   1465  CA  VAL C  27       1.961  22.053  22.787  1.00 61.98      C
ATOM   1466  CB  VAL C  27       1.298  21.416  21.547  1.00 61.90      C
ATOM   1467  CG1 VAL C  27       0.288  20.357  21.964  1.00 62.47      C
ATOM   1468  CG2 VAL C  27       0.624  22.485  20.700  1.00 62.08      C
ATOM   1469  C   VAL C  27       3.027  21.104  23.343  1.00 61.20      C
ATOM   1470  O   VAL C  27       2.707  20.100  23.984  1.00 61.05      O
ATOM   1471  N   TYR C  28       4.293  21.434  23.097  1.00 59.91      N
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Figure 2 Table 2a - 23

ATOM	1472	CA	TYR	C	28	5.408	20.618	23.567	1.00	58.82	C
ATOM	1473	CB	TYR	C	28	6.582	20.700	22.588	1.00	58.46	C
ATOM	1474	CG	TYR	C	28	6.346	19.985	21.280	1.00	57.81	C
ATOM	1475	CD1	TYR	C	28	5.773	20.643	20.199	1.00	57.35	C
ATOM	1476	CE1	TYR	C	28	5.555	19.992	18.998	1.00	57.12	C
ATOM	1477	CZ	TYR	C	28	5.914	18.665	18.868	1.00	57.11	C
ATOM	1478	OH	TYR	C	28	5.702	18.012	17.674	1.00	57.54	O
ATOM	1479	CE2	TYR	C	28	6.486	17.990	19.925	1.00	56.54	C
ATOM	1480	CD2	TYR	C	28	6.700	18.651	21.122	1.00	56.99	C
ATOM	1481	C	TYR	C	28	5.862	21.045	24.961	1.00	58.25	C
ATOM	1482	O	TYR	C	28	5.987	20.217	25.865	1.00	57.89	O
ATOM	1483	N	THR	C	29	6.115	22.340	25.123	1.00	57.54	N
ATOM	1484	CA	THR	C	29	6.669	22.867	26.366	1.00	57.00	C
ATOM	1485	CB	THR	C	29	7.086	24.348	26.212	1.00	57.19	C
ATOM	1486	OG1	THR	C	29	8.516	24.443	26.196	1.00	57.42	O
ATOM	1487	CG2	THR	C	29	6.541	25.189	27.360	1.00	57.66	C
ATOM	1488	C	THR	C	29	5.678	22.722	27.517	1.00	56.15	C
ATOM	1489	O	THR	C	29	6.071	22.492	28.659	1.00	55.97	O
ATOM	1490	N	THR	C	30	4.392	22.849	27.203	1.00	55.34	N
ATOM	1491	CA	THR	C	30	3.331	22.636	28.183	1.00	54.35	C
ATOM	1492	CB	THR	C	30	2.003	23.241	27.692	1.00	54.19	C
ATOM	1493	OG1	THR	C	30	2.159	24.659	27.589	1.00	53.30	O
ATOM	1494	CG2	THR	C	30	0.860	22.932	28.656	1.00	53.55	C
ATOM	1495	C	THR	C	30	3.173	21.152	28.511	1.00	54.01	C
ATOM	1496	O	THR	C	30	3.078	20.775	29.682	1.00	53.86	O
ATOM	1497	N	PHE	C	31	3.155	20.321	27.471	1.00	53.58	N
ATOM	1498	CA	PHE	C	31	3.136	18.865	27.615	1.00	53.21	C
ATOM	1499	CB	PHE	C	31	3.222	18.217	26.238	1.00	52.87	C
ATOM	1500	CG	PHE	C	31	3.139	16.725	26.257	1.00	52.44	C
ATOM	1501	CD1	PHE	C	31	4.283	15.952	26.445	1.00	51.88	C
ATOM	1502	CE1	PHE	C	31	4.215	14.576	26.463	1.00	50.62	C
ATOM	1503	CZ	PHE	C	31	3.000	13.943	26.271	1.00	50.48	C
ATOM	1504	CE2	PHE	C	31	1.858	14.687	26.070	1.00	50.99	C
ATOM	1505	CD2	PHE	C	31	1.925	16.085	26.065	1.00	51.73	C
ATOM	1506	C	PHE	C	31	4.277	18.370	28.507	1.00	53.19	C
ATOM	1507	O	PHE	C	31	4.053	17.593	29.431	1.00	53.35	O
ATOM	1508	N	MET	C	32	5.490	18.837	28.223	1.00	53.31	N
ATOM	1509	CA	MET	C	32	6.688	18.464	28.965	1.00	53.86	C
ATOM	1510	CB	MET	C	32	7.938	19.021	28.283	1.00	53.93	C
ATOM	1511	CG	MET	C	32	8.417	18.170	27.118	1.00	55.29	C
ATOM	1512	SD	MET	C	32	9.940	18.787	26.371	1.00	57.98	S
ATOM	1513	CE	MET	C	32	9.398	20.248	25.495	1.00	57.46	C
ATOM	1514	C	MET	C	32	6.661	18.895	30.421	1.00	53.78	C
ATOM	1515	O	MET	C	32	7.160	18.187	31.290	1.00	53.71	O
ATOM	1516	N	LYS	C	33	6.088	20.066	30.681	1.00	54.05	N
ATOM	1517	CA	LYS	C	33	5.971	20.580	32.047	1.00	54.00	C
ATOM	1518	CB	LYS	C	33	5.756	22.101	32.040	1.00	53.69	C
ATOM	1519	CG	LYS	C	33	7.014	22.870	31.670	1.00	54.10	C
ATOM	1520	CD	LYS	C	33	6.905	24.361	31.919	1.00	53.79	C
ATOM	1521	CE	LYS	C	33	8.134	25.067	31.356	1.00	54.37	C
ATOM	1522	NZ	LYS	C	33	8.275	26.472	31.843	1.00	55.06	N
ATOM	1523	C	LYS	C	33	4.865	19.879	32.839	1.00	53.92	C
ATOM	1524	O	LYS	C	33	4.847	19.949	34.066	1.00	53.48	O
ATOM	1525	N	SER	C	34	3.962	19.200	32.130	1.00	53.95	N
ATOM	1526	CA	SER	C	34	2.786	18.599	32.743	1.00	54.20	C
ATOM	1527	CB	SER	C	34	1.520	19.080	32.039	1.00	54.17	C
ATOM	1528	OG	SER	C	34	1.360	18.407	30.808	1.00	54.75	O
ATOM	1529	C	SER	C	34	2.831	17.069	32.775	1.00	54.44	C
ATOM	1530	O	SER	C	34	1.861	16.420	33.173	1.00	54.70	O
ATOM	1531	N	HIS	C	35	3.951	16.490	32.361	1.00	54.44	N
ATOM	1532	CA	HIS	C	35	4.147	15.055	32.512	1.00	54.72	C
ATOM	1533	CB	HIS	C	35	4.239	14.352	31.153	1.00	54.85	C
ATOM	1534	CG	HIS	C	35	2.916	14.192	30.474	1.00	55.73	C
ATOM	1535	ND1	HIS	C	35	2.344	15.191	29.717	1.00	56.27	N
ATOM	1536	CE1	HIS	C	35	1.172	14.779	29.264	1.00	56.50	C
ATOM	1537	NE2	HIS	C	35	0.967	13.547	29.698	1.00	57.10	N
ATOM	1538	CD2	HIS	C	35	2.040	13.158	30.463	1.00	56.44	C

Figure 2 Table 2a - 24

ATOM	1539	C	HIS	C	35	5.360	14.747	33.370	1.00	54.52	C
ATOM	1540	O	HIS	C	35	6.370	15.460	33.325	1.00	54.39	O
ATOM	1541	N	ARG	C	36	5.229	13.687	34.163	1.00	54.31	N
ATOM	1542	CA	ARG	C	36	6.288	13.206	35.029	1.00	53.95	C
ATOM	1543	CB	ARG	C	36	5.685	12.434	36.196	1.00	54.21	C
ATOM	1544	CG	ARG	C	36	4.715	13.179	37.082	1.00	54.70	C
ATOM	1545	CD	ARG	C	36	4.690	12.484	38.429	1.00	56.60	C
ATOM	1546	NE	ARG	C	36	3.743	13.034	39.400	1.00	59.79	N
ATOM	1547	CZ	ARG	C	36	3.882	14.193	40.049	1.00	61.83	C
ATOM	1548	NH1	ARG	C	36	4.924	14.990	39.815	1.00	62.05	N
ATOM	1549	NH2	ARG	C	36	2.957	14.574	40.931	1.00	62.44	N
ATOM	1550	C	ARG	C	36	7.200	12.261	34.256	1.00	53.71	C
ATOM	1551	O	ARG	C	36	6.776	11.627	33.296	1.00	53.58	O
ATOM	1552	N	CYS	C	37	8.445	12.147	34.700	1.00	53.60	N
ATOM	1553	CA	CYS	C	37	9.398	11.182	34.154	1.00	53.49	C
ATOM	1554	CB	CYS	C	37	10.740	11.301	34.869	1.00	53.59	C
ATOM	1555	SG	CYS	C	37	11.684	12.715	34.293	1.00	56.85	S
ATOM	1556	C	CYS	C	37	8.889	9.753	34.255	1.00	52.65	C
ATOM	1557	O	CYS	C	37	9.160	8.937	33.390	1.00	52.77	O
ATOM	1558	N	TYR	C	38	8.130	9.477	35.306	1.00	51.85	N
ATOM	1559	CA	TYR	C	38	7.540	8.171	35.544	1.00	50.84	C
ATOM	1560	CB	TYR	C	38	6.628	8.260	36.777	1.00	51.03	C
ATOM	1561	CG	TYR	C	38	5.782	7.030	37.012	1.00	49.89	C
ATOM	1562	CD1	TYR	C	38	4.439	6.993	36.611	1.00	48.88	C
ATOM	1563	CE1	TYR	C	38	3.658	5.861	36.814	1.00	49.09	C
ATOM	1564	CZ	TYR	C	38	4.221	4.754	37.434	1.00	49.48	C
ATOM	1565	OH	TYR	C	38	3.476	3.634	37.647	1.00	50.09	O
ATOM	1566	CE2	TYR	C	38	5.546	4.766	37.839	1.00	50.31	C
ATOM	1567	CD2	TYR	C	38	6.323	5.906	37.624	1.00	49.65	C
ATOM	1568	C	TYR	C	38	6.733	7.668	34.355	1.00	50.42	C
ATOM	1569	O	TYR	C	38	6.739	6.473	34.038	1.00	50.41	O
ATOM	1570	N	ASP	C	39	6.036	8.599	33.713	1.00	49.79	N
ATOM	1571	CA	ASP	C	39	5.121	8.299	32.631	1.00	49.23	C
ATOM	1572	CB	ASP	C	39	4.331	9.560	32.258	1.00	49.37	C
ATOM	1573	CG	ASP	C	39	3.410	10.045	33.378	1.00	50.27	C
ATOM	1574	OD1	ASP	C	39	3.051	9.242	34.280	1.00	50.96	O
ATOM	1575	OD2	ASP	C	39	3.028	11.242	33.342	1.00	51.37	O
ATOM	1576	C	ASP	C	39	5.801	7.740	31.384	1.00	48.97	C
ATOM	1577	O	ASP	C	39	5.118	7.223	30.514	1.00	49.61	O
ATOM	1578	N	LEU	C	40	7.125	7.870	31.269	1.00	48.37	N
ATOM	1579	CA	LEU	C	40	7.829	7.376	30.081	1.00	47.78	C
ATOM	1580	CB	LEU	C	40	8.920	8.336	29.589	1.00	48.06	C
ATOM	1581	CG	LEU	C	40	8.832	9.861	29.495	1.00	48.94	C
ATOM	1582	CD1	LEU	C	40	9.318	10.361	28.133	1.00	46.95	C
ATOM	1583	CD2	LEU	C	40	7.456	10.420	29.802	1.00	51.04	C
ATOM	1584	C	LEU	C	40	8.481	6.031	30.300	1.00	47.06	C
ATOM	1585	O	LEU	C	40	8.892	5.383	29.338	1.00	47.26	O
ATOM	1586	N	ILE	C	41	8.615	5.635	31.559	1.00	46.16	N
ATOM	1587	CA	ILE	C	41	9.183	4.341	31.930	1.00	45.09	C
ATOM	1588	CB	ILE	C	41	9.312	4.243	33.486	1.00	45.18	C
ATOM	1589	CG1	ILE	C	41	10.115	5.450	34.019	1.00	45.45	C
ATOM	1590	CD1	ILE	C	41	10.281	5.480	35.522	1.00	45.55	C
ATOM	1591	CG2	ILE	C	41	9.898	2.909	33.925	1.00	42.70	C
ATOM	1592	C	ILE	C	41	8.317	3.202	31.383	1.00	44.66	C
ATOM	1593	O	ILE	C	41	7.105	3.218	31.554	1.00	45.07	O
ATOM	1594	N	PRO	C	42	8.926	2.202	30.730	1.00	44.30	N
ATOM	1595	CA	PRO	C	42	8.092	1.110	30.261	1.00	44.17	C
ATOM	1596	CB	PRO	C	42	9.029	0.324	29.332	1.00	44.17	C
ATOM	1597	CG	PRO	C	42	10.365	0.604	29.818	1.00	44.24	C
ATOM	1598	CD	PRO	C	42	10.344	1.988	30.403	1.00	44.44	C
ATOM	1599	C	PRO	C	42	7.648	0.246	31.432	1.00	44.16	C
ATOM	1600	O	PRO	C	42	8.242	0.327	32.510	1.00	44.02	O
ATOM	1601	N	THR	C	43	6.614	-0.562	31.222	1.00	44.30	N
ATOM	1602	CA	THR	C	43	6.027	-1.371	32.282	1.00	44.79	C
ATOM	1603	CB	THR	C	43	4.823	-2.184	31.764	1.00	44.80	C
ATOM	1604	OG1	THR	C	43	3.777	-1.279	31.383	1.00	44.89	O
ATOM	1605	CG2	THR	C	43	4.284	-3.154	32.831	1.00	43.39	C

Figure 2 Table 2a - 25

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ATOM   1606  C   THR C  43       7.075  -2.295  32.874  1.00 45.60      C
ATOM   1607  O   THR C  43       7.055  -2.588  34.059  1.00 46.38      O
ATOM   1608  N   SER C  44       8.019  -2.707  32.041  1.00 46.40      N
ATOM   1609  CA  SER C  44       9.048  -3.646  32.421  1.00 46.95      C
ATOM   1610  CB  SER C  44       8.577  -5.040  32.054  1.00 47.13      C
ATOM   1611  OG  SER C  44       9.654  -5.934  32.139  1.00 49.65      O
ATOM   1612  C   SER C  44      10.364  -3.326  31.707  1.00 47.02      C
ATOM   1613  O   SER C  44      10.391  -3.210  30.487  1.00 46.75      O
ATOM   1614  N   SER C  45      11.445  -3.171  32.467  1.00 47.47      N
ATOM   1615  CA  SER C  45      12.764  -2.910  31.898  1.00 48.27      C
ATOM   1616  CB  SER C  45      13.054  -1.409  31.835  1.00 48.31      C
ATOM   1617  OG  SER C  45      13.138  -0.851  33.141  1.00 49.81      O
ATOM   1618  C   SER C  45      13.855  -3.596  32.697  1.00 48.54      C
ATOM   1619  O   SER C  45      13.634  -3.985  33.830  1.00 48.93      O
ATOM   1620  N   LYS C  46      15.030  -3.756  32.085  1.00 49.03      N
ATOM   1621  CA  LYS C  46      16.206  -4.263  32.781  1.00 48.82      C
ATOM   1622  CB  LYS C  46      16.799  -5.490  32.082  1.00 49.27      C
ATOM   1623  CG  LYS C  46      17.173  -5.312  30.623  1.00 51.14      C
ATOM   1624  CD  LYS C  46      17.843  -6.591  30.089  1.00 53.48      C
ATOM   1625  CE  LYS C  46      18.005  -6.545  28.557  1.00 55.88      C
ATOM   1626  NZ  LYS C  46      18.551  -7.843  28.035  1.00 57.50      N
ATOM   1627  C   LYS C  46      17.255  -3.178  32.945  1.00 47.85      C
ATOM   1628  O   LYS C  46      17.326  -2.247  32.152  1.00 47.83      O
ATOM   1629  N   LEU C  47      18.059  -3.311  33.989  1.00 46.94      N
ATOM   1630  CA  LEU C  47      19.064  -2.328  34.329  1.00 45.93      C
ATOM   1631  CB  LEU C  47      18.534  -1.452  35.458  1.00 45.95      C
ATOM   1632  CG  LEU C  47      19.338  -0.254  35.934  1.00 45.78      C
ATOM   1633  CD1 LEU C  47      19.174   0.910  34.966  1.00 45.84      C
ATOM   1634  CD2 LEU C  47      18.858   0.139  37.307  1.00 45.88      C
ATOM   1635  C   LEU C  47      20.313  -3.051  34.771  1.00 45.57      C
ATOM   1636  O   LEU C  47      20.248  -3.977  35.585  1.00 45.98      O
ATOM   1637  N   VAL C  48      21.454  -2.647  34.232  1.00 45.13      N
ATOM   1638  CA  VAL C  48      22.730  -3.273  34.599  1.00 44.90      C
ATOM   1639  CB  VAL C  48      23.565  -3.674  33.346  1.00 44.86      C
ATOM   1640  CG1 VAL C  48      24.903  -4.291  33.747  1.00 44.83      C
ATOM   1641  CG2 VAL C  48      22.796  -4.637  32.482  1.00 44.74      C
ATOM   1642  C   VAL C  48      23.535  -2.318  35.472  1.00 44.79      C
ATOM   1643  O   VAL C  48      23.809  -1.192  35.069  1.00 44.60      O
ATOM   1644  N   VAL C  49      23.897  -2.765  36.670  1.00 44.65      N
ATOM   1645  CA  VAL C  49      24.683  -1.945  37.585  1.00 44.77      C
ATOM   1646  CB  VAL C  49      23.965  -1.709  38.965  1.00 44.71      C
ATOM   1647  CG1 VAL C  49      24.835  -0.877  39.910  1.00 43.72      C
ATOM   1648  CG2 VAL C  49      22.612  -1.036  38.785  1.00 43.98      C
ATOM   1649  C   VAL C  49      26.058  -2.579  37.803  1.00 45.02      C
ATOM   1650  O   VAL C  49      26.166  -3.776  38.025  1.00 44.95      O
ATOM   1651  N   PHE C  50      27.098  -1.757  37.737  1.00 45.52      N
ATOM   1652  CA  PHE C  50      28.448  -2.202  38.021  1.00 46.18      C
ATOM   1653  CB  PHE C  50      29.401  -1.751  36.917  1.00 45.85      C
ATOM   1654  CG  PHE C  50      29.091  -2.333  35.570  1.00 45.42      C
ATOM   1655  CD1 PHE C  50      29.181  -1.545  34.428  1.00 43.35      C
ATOM   1656  CE1 PHE C  50      28.893  -2.072  33.177  1.00 45.06      C
ATOM   1657  CZ  PHE C  50      28.509  -3.412  33.056  1.00 46.03      C
ATOM   1658  CE2 PHE C  50      28.430  -4.215  34.199  1.00 45.81      C
ATOM   1659  CD2 PHE C  50      28.716  -3.671  35.445  1.00 44.09      C
ATOM   1660  C   PHE C  50      28.963  -1.685  39.361  1.00 46.73      C
ATOM   1661  O   PHE C  50      28.893  -0.474  39.636  1.00 46.99      O
ATOM   1662  N   ASP C  51      29.489  -2.596  40.179  1.00 46.61      N
ATOM   1663  CA  ASP C  51      30.250  -2.194  41.347  1.00 47.02      C
ATOM   1664  CB  ASP C  51      30.526  -3.401  42.265  1.00 47.28      C
ATOM   1665  CG  ASP C  51      31.252  -3.016  43.552  1.00 46.83      C
ATOM   1666  OD1 ASP C  51      30.679  -3.201  44.653  1.00 45.98      O
ATOM   1667  OD2 ASP C  51      32.397  -2.524  43.458  1.00 46.82      O
ATOM   1668  C   ASP C  51      31.544  -1.587  40.808  1.00 47.51      C
ATOM   1669  O   ASP C  51      32.147  -2.147  39.874  1.00 47.50      O
ATOM   1670  N   THR C  52      31.958  -0.444  41.368  1.00 47.86      N
ATOM   1671  CA  THR C  52      33.146   0.275  40.858  1.00 48.18      C
ATOM   1672  CB  THR C  52      33.285   1.743  41.403  1.00 47.90      C
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Figure 2 Table 2a - 26

ATOM	1673	OG1	THR	C	52	33.367	1.764	42.832	1.00	48.14	O
ATOM	1674	CG2	THR	C	52	32.114	2.600	40.956	1.00	48.10	C
ATOM	1675	C	THR	C	52	34.472	-0.511	40.989	1.00	48.49	C
ATOM	1676	O	THR	C	52	35.463	-0.171	40.349	1.00	48.82	O
ATOM	1677	N	SER	C	53	34.479	-1.569	41.791	1.00	48.74	N
ATOM	1678	CA	SER	C	53	35.664	-2.412	41.919	1.00	49.17	C
ATOM	1679	CB	SER	C	53	35.650	-3.118	43.265	1.00	48.80	C
ATOM	1680	OG	SER	C	53	34.572	-4.032	43.300	1.00	48.24	O
ATOM	1681	C	SER	C	53	35.758	-3.456	40.799	1.00	49.73	C
ATOM	1682	O	SER	C	53	36.628	-4.328	40.833	1.00	49.92	O
ATOM	1683	N	LEU	C	54	34.861	-3.373	39.821	1.00	50.32	N
ATOM	1684	CA	LEU	C	54	34.817	-4.334	38.725	1.00	50.80	C
ATOM	1685	CB	LEU	C	54	33.449	-4.298	38.041	1.00	50.65	C
ATOM	1686	CG	LEU	C	54	32.776	-5.563	37.490	1.00	50.43	C
ATOM	1687	CD1	LEU	C	54	31.994	-5.205	36.225	1.00	47.97	C
ATOM	1688	CD2	LEU	C	54	33.726	-6.712	37.220	1.00	49.83	C
ATOM	1689	C	LEU	C	54	35.868	-3.977	37.690	1.00	51.31	C
ATOM	1690	O	LEU	C	54	36.068	-2.798	37.376	1.00	51.00	O
ATOM	1691	N	GLN	C	55	36.517	-5.008	37.149	1.00	51.93	N
ATOM	1692	CA	GLN	C	55	37.422	-4.840	36.015	1.00	52.57	C
ATOM	1693	CB	GLN	C	55	38.067	-6.172	35.618	1.00	52.49	C
ATOM	1694	CG	GLN	C	55	39.304	-6.510	36.428	1.00	53.77	C
ATOM	1695	CD	GLN	C	55	40.155	-7.596	35.789	1.00	55.89	C
ATOM	1696	OE1	GLN	C	55	40.410	-8.634	36.400	1.00	57.17	O
ATOM	1697	NE2	GLN	C	55	40.607	-7.361	34.556	1.00	56.94	N
ATOM	1698	C	GLN	C	55	36.701	-4.205	34.818	1.00	52.54	C
ATOM	1699	O	GLN	C	55	35.644	-4.662	34.398	1.00	52.46	O
ATOM	1700	N	VAL	C	56	37.292	-3.138	34.300	1.00	53.09	N
ATOM	1701	CA	VAL	C	56	36.799	-2.422	33.116	1.00	53.70	C
ATOM	1702	CB	VAL	C	56	37.842	-1.370	32.687	1.00	53.38	C
ATOM	1703	CG1	VAL	C	56	37.838	-1.154	31.195	1.00	54.04	C
ATOM	1704	CG2	VAL	C	56	37.615	-0.071	33.443	1.00	53.75	C
ATOM	1705	C	VAL	C	56	36.446	-3.370	31.957	1.00	54.00	C
ATOM	1706	O	VAL	C	56	35.409	-3.210	31.303	1.00	53.82	O
ATOM	1707	N	LYS	C	57	37.305	-4.370	31.755	1.00	54.36	N
ATOM	1708	CA	LYS	C	57	37.202	-5.329	30.666	1.00	54.78	C
ATOM	1709	CB	LYS	C	57	38.437	-6.233	30.685	1.00	55.20	C
ATOM	1710	CG	LYS	C	57	38.844	-6.801	29.328	1.00	57.30	C
ATOM	1711	CD	LYS	C	57	40.124	-7.649	29.452	1.00	59.09	C
ATOM	1712	CE	LYS	C	57	40.564	-8.241	28.105	1.00	59.83	C
ATOM	1713	NZ	LYS	C	57	41.731	-9.163	28.265	1.00	59.65	N
ATOM	1714	C	LYS	C	57	35.946	-6.178	30.787	1.00	54.25	C
ATOM	1715	O	LYS	C	57	35.301	-6.499	29.792	1.00	54.15	O
ATOM	1716	N	LYS	C	58	35.615	-6.547	32.019	1.00	54.08	N
ATOM	1717	CA	LYS	C	58	34.450	-7.384	32.288	1.00	53.80	C
ATOM	1718	CB	LYS	C	58	34.563	-8.025	33.672	1.00	53.68	C
ATOM	1719	CG	LYS	C	58	35.782	-8.893	33.837	1.00	54.24	C
ATOM	1720	CD	LYS	C	58	36.093	-9.140	35.304	1.00	55.25	C
ATOM	1721	CE	LYS	C	58	37.188	-10.181	35.457	1.00	56.27	C
ATOM	1722	NZ	LYS	C	58	36.720	-11.538	35.024	1.00	57.57	N
ATOM	1723	C	LYS	C	58	33.172	-6.567	32.182	1.00	53.35	C
ATOM	1724	O	LYS	C	58	32.135	-7.075	31.758	1.00	53.38	O
ATOM	1725	N	ALA	C	59	33.274	-5.301	32.576	1.00	53.06	N
ATOM	1726	CA	ALA	C	59	32.170	-4.350	32.535	1.00	53.14	C
ATOM	1727	CB	ALA	C	59	32.569	-3.046	33.227	1.00	52.81	C
ATOM	1728	C	ALA	C	59	31.681	-4.082	31.112	1.00	53.33	C
ATOM	1729	O	ALA	C	59	30.480	-4.094	30.857	1.00	53.41	O
ATOM	1730	N	PHE	C	60	32.606	-3.859	30.185	1.00	53.60	N
ATOM	1731	CA	PHE	C	60	32.217	-3.607	28.801	1.00	54.08	C
ATOM	1732	CB	PHE	C	60	33.331	-2.901	28.025	1.00	54.48	C
ATOM	1733	CG	PHE	C	60	33.602	-1.514	28.531	1.00	55.49	C
ATOM	1734	CD1	PHE	C	60	34.826	-1.198	29.125	1.00	55.81	C
ATOM	1735	CE1	PHE	C	60	35.071	0.086	29.613	1.00	55.10	C
ATOM	1736	CZ	PHE	C	60	34.083	1.052	29.523	1.00	55.75	C
ATOM	1737	CE2	PHE	C	60	32.850	0.743	28.942	1.00	56.27	C
ATOM	1738	CD2	PHE	C	60	32.615	-0.532	28.453	1.00	55.49	C
ATOM	1739	C	PHE	C	60	31.700	-4.843	28.078	1.00	53.80	C

Figure 2 Table 2a - 27

ATOM	1740	O	PHE	C	60	30.847	-4.738	27.191	1.00	53.89	O
ATOM	1741	N	PHE	C	61	32.190	-6.009	28.478	1.00	53.17	N
ATOM	1742	CA	PHE	C	61	31.657	-7.249	27.955	1.00	52.99	C
ATOM	1743	CB	PHE	C	61	32.547	-8.431	28.348	1.00	53.31	C
ATOM	1744	CG	PHE	C	61	32.145	-9.743	27.707	1.00	54.73	C
ATOM	1745	CD1	PHE	C	61	32.331	-9.955	26.338	1.00	55.88	C
ATOM	1746	CE1	PHE	C	61	31.969	-11.168	25.741	1.00	55.96	C
ATOM	1747	CZ	PHE	C	61	31.424	-12.185	26.519	1.00	55.71	C
ATOM	1748	CE2	PHE	C	61	31.238	-11.988	27.890	1.00	56.24	C
ATOM	1749	CD2	PHE	C	61	31.600	-10.771	28.475	1.00	55.62	C
ATOM	1750	C	PHE	C	61	30.208	-7.459	28.415	1.00	52.27	C
ATOM	1751	O	PHE	C	61	29.407	-8.058	27.692	1.00	52.07	O
ATOM	1752	N	ALA	C	62	29.872	-6.948	29.600	1.00	51.58	N
ATOM	1753	CA	ALA	C	62	28.518	-7.094	30.153	1.00	50.96	C
ATOM	1754	CB	ALA	C	62	28.507	-6.820	31.638	1.00	50.58	C
ATOM	1755	C	ALA	C	62	27.492	-6.215	29.424	1.00	50.65	C
ATOM	1756	O	ALA	C	62	26.344	-6.623	29.228	1.00	50.56	O
ATOM	1757	N	LEU	C	63	27.907	-5.021	29.011	1.00	50.21	N
ATOM	1758	CA	LEU	C	63	27.058	-4.175	28.173	1.00	49.88	C
ATOM	1759	CB	LEU	C	63	27.770	-2.867	27.798	1.00	49.50	C
ATOM	1760	CG	LEU	C	63	28.162	-1.864	28.888	1.00	48.62	C
ATOM	1761	CD1	LEU	C	63	28.466	-0.526	28.271	1.00	48.17	C
ATOM	1762	CD2	LEU	C	63	27.073	-1.710	29.939	1.00	49.75	C
ATOM	1763	C	LEU	C	63	26.612	-4.940	26.921	1.00	50.11	C
ATOM	1764	O	LEU	C	63	25.412	-5.050	26.644	1.00	50.29	O
ATOM	1765	N	VAL	C	64	27.582	-5.492	26.189	1.00	50.11	N
ATOM	1766	CA	VAL	C	64	27.315	-6.300	24.990	1.00	49.97	C
ATOM	1767	CB	VAL	C	64	28.618	-6.849	24.364	1.00	49.85	C
ATOM	1768	CG1	VAL	C	64	28.306	-7.654	23.111	1.00	50.37	C
ATOM	1769	CG2	VAL	C	64	29.572	-5.726	24.041	1.00	49.71	C
ATOM	1770	C	VAL	C	64	26.388	-7.472	25.290	1.00	49.95	C
ATOM	1771	O	VAL	C	64	25.378	-7.654	24.613	1.00	50.09	O
ATOM	1772	N	THR	C	65	26.743	-8.258	26.305	1.00	50.08	N
ATOM	1773	CA	THR	C	65	25.986	-9.453	26.694	1.00	50.40	C
ATOM	1774	CB	THR	C	65	26.580	-10.098	27.971	1.00	50.59	C
ATOM	1775	OG1	THR	C	65	27.995	-9.901	27.995	1.00	51.27	O
ATOM	1776	CG2	THR	C	65	26.267	-11.594	28.029	1.00	50.75	C
ATOM	1777	C	THR	C	65	24.512	-9.140	26.961	1.00	50.17	C
ATOM	1778	O	THR	C	65	23.620	-9.908	26.592	1.00	50.09	O
ATOM	1779	N	ASN	C	66	24.281	-8.003	27.608	1.00	50.10	N
ATOM	1780	CA	ASN	C	66	22.952	-7.607	28.056	1.00	50.01	C
ATOM	1781	CB	ASN	C	66	23.060	-6.882	29.396	1.00	49.60	C
ATOM	1782	CG	ASN	C	66	23.448	-7.813	30.524	1.00	48.78	C
ATOM	1783	OD1	ASN	C	66	22.714	-8.748	30.839	1.00	47.50	O
ATOM	1784	ND2	ASN	C	66	24.601	-7.563	31.141	1.00	47.38	N
ATOM	1785	C	ASN	C	66	22.184	-6.764	27.047	1.00	50.30	C
ATOM	1786	O	ASN	C	66	20.987	-6.533	27.221	1.00	50.37	O
ATOM	1787	N	GLY	C	67	22.872	-6.317	26.000	1.00	50.71	N
ATOM	1788	CA	GLY	C	67	22.243	-5.552	24.929	1.00	51.16	C
ATOM	1789	C	GLY	C	67	21.861	-4.163	25.397	1.00	51.32	C
ATOM	1790	O	GLY	C	67	20.702	-3.759	25.311	1.00	51.48	O
ATOM	1791	N	VAL	C	68	22.818	-3.482	25.995	1.00	51.49	N
ATOM	1792	CA	VAL	C	68	22.547	-2.337	26.828	1.00	51.58	C
ATOM	1793	CB	VAL	C	68	22.436	-2.726	28.320	1.00	51.56	C
ATOM	1794	CG1	VAL	C	68	23.316	-1.896	29.180	1.00	50.51	C
ATOM	1795	CG2	VAL	C	68	21.044	-2.606	28.771	1.00	51.34	C
ATOM	1796	C	VAL	C	68	23.681	-1.381	26.606	1.00	52.08	C
ATOM	1797	O	VAL	C	68	24.697	-1.748	26.081	1.00	52.21	O
ATOM	1798	N	ARG	C	69	23.572	-0.383	27.465	1.00	52.75	N
ATOM	1799	CA	ARG	C	69	24.338	0.679	26.905	1.00	53.09	C
ATOM	1800	CB	ARG	C	69	23.389	1.694	26.328	1.00	53.82	C
ATOM	1801	CG	ARG	C	69	23.723	2.140	24.955	1.00	56.59	C
ATOM	1802	CD	ARG	C	69	23.235	1.098	24.016	1.00	61.97	C
ATOM	1803	NE	ARG	C	69	22.916	1.664	22.734	1.00	66.47	N
ATOM	1804	CZ	ARG	C	69	23.047	1.039	21.584	1.00	68.85	C
ATOM	1805	NH1	ARG	C	69	21.972	0.936	20.789	1.00	69.33	N
ATOM	1806	NH2	ARG	C	69	24.239	0.582	21.203	1.00	69.68	N

Figure 2 Table 2a - 28

ATOM	1807	C	ARG	C	69	25.068	1.356	27.993	1.00	52.74	C
ATOM	1808	O	ARG	C	69	26.153	1.839	27.828	1.00	53.98	O
ATOM	1809	N	ALA	C	70	24.279	1.837	28.638	1.00	51.61	N
ATOM	1810	CA	ALA	C	70	24.859	2.536	29.727	1.00	50.52	C
ATOM	1811	CB	ALA	C	70	24.246	3.895	29.846	1.00	50.29	C
ATOM	1812	C	ALA	C	70	24.579	1.700	30.945	1.00	49.80	C
ATOM	1813	O	ALA	C	70	23.587	1.017	31.020	1.00	49.34	O
ATOM	1814	N	ALA	C	71	25.479	1.736	31.897	1.00	49.21	N
ATOM	1815	CA	ALA	C	71	25.180	1.081	33.161	1.00	48.63	C
ATOM	1816	CB	ALA	C	71	25.866	-0.262	33.228	1.00	48.32	C
ATOM	1817	C	ALA	C	71	25.612	1.966	34.324	1.00	48.71	C
ATOM	1818	O	ALA	C	71	26.682	2.569	34.284	1.00	49.21	O
ATOM	1819	N	PRO	C	72	24.766	2.062	35.352	1.00	48.27	N
ATOM	1820	CA	PRO	C	72	25.086	2.871	36.529	1.00	47.72	C
ATOM	1821	CB	PRO	C	72	23.782	2.845	37.335	1.00	47.79	C
ATOM	1822	CG	PRO	C	72	22.720	2.632	36.318	1.00	48.25	C
ATOM	1823	CD	PRO	C	72	23.334	1.722	35.286	1.00	48.34	C
ATOM	1824	C	PRO	C	72	26.223	2.270	37.353	1.00	47.34	C
ATOM	1825	O	PRO	C	72	26.464	1.061	37.297	1.00	46.68	O
ATOM	1826	N	LEU	C	73	26.906	3.123	38.111	1.00	46.58	N
ATOM	1827	CA	LEU	C	73	28.064	2.708	38.880	1.00	45.36	C
ATOM	1828	CB	LEU	C	73	29.309	3.500	38.461	1.00	44.98	C
ATOM	1829	CG	LEU	C	73	29.761	3.375	37.004	1.00	44.07	C
ATOM	1830	CD1	LEU	C	73	30.952	4.282	36.715	1.00	43.53	C
ATOM	1831	CD2	LEU	C	73	30.079	1.946	36.617	1.00	42.04	C
ATOM	1832	C	LEU	C	73	27.793	2.878	40.364	1.00	45.03	C
ATOM	1833	O	LEU	C	73	27.391	3.944	40.822	1.00	44.63	O
ATOM	1834	N	TRP	C	74	28.029	1.803	41.104	1.00	44.79	N
ATOM	1835	CA	TRP	C	74	27.767	1.759	42.525	1.00	44.65	C
ATOM	1836	CB	TRP	C	74	26.889	0.548	42.832	1.00	44.06	C
ATOM	1837	CG	TRP	C	74	26.727	0.220	44.275	1.00	42.35	C
ATOM	1838	CD1	TRP	C	74	27.419	-0.723	44.985	1.00	41.43	C
ATOM	1839	NE1	TRP	C	74	26.986	-0.755	46.289	1.00	40.11	N
ATOM	1840	CE2	TRP	C	74	25.994	0.178	46.444	1.00	41.53	C
ATOM	1841	CD2	TRP	C	74	25.804	0.808	45.190	1.00	41.38	C
ATOM	1842	CE3	TRP	C	74	24.836	1.813	45.080	1.00	40.99	C
ATOM	1843	CZ3	TRP	C	74	24.088	2.146	46.215	1.00	40.94	C
ATOM	1844	CH2	TRP	C	74	24.294	1.504	47.436	1.00	39.88	C
ATOM	1845	CZ2	TRP	C	74	25.243	0.519	47.577	1.00	41.40	C
ATOM	1846	C	TRP	C	74	29.094	1.681	43.258	1.00	45.26	C
ATOM	1847	O	TRP	C	74	29.905	0.779	43.006	1.00	45.58	O
ATOM	1848	N	ASP	C	75	29.327	2.653	44.138	1.00	45.83	N
ATOM	1849	CA	ASP	C	75	30.500	2.644	45.007	1.00	46.28	C
ATOM	1850	CB	ASP	C	75	31.013	4.066	45.229	1.00	46.29	C
ATOM	1851	CG	ASP	C	75	32.353	4.107	45.948	1.00	47.46	C
ATOM	1852	OD1	ASP	C	75	33.170	4.987	45.597	1.00	47.93	O
ATOM	1853	OD2	ASP	C	75	32.597	3.280	46.865	1.00	49.88	O
ATOM	1854	C	ASP	C	75	30.123	1.985	46.331	1.00	46.38	C
ATOM	1855	O	ASP	C	75	29.394	2.554	47.148	1.00	46.48	O
ATOM	1856	N	SER	C	76	30.634	0.782	46.536	1.00	46.75	N
ATOM	1857	CA	SER	C	76	30.299	-0.006	47.720	1.00	47.18	C
ATOM	1858	CB	SER	C	76	30.832	-1.414	47.559	1.00	46.82	C
ATOM	1859	OG	SER	C	76	30.106	-2.267	48.398	1.00	48.55	O
ATOM	1860	C	SER	C	76	30.775	0.589	49.051	1.00	47.55	C
ATOM	1861	O	SER	C	76	30.084	0.479	50.072	1.00	47.47	O
ATOM	1862	N	LYS	C	77	31.957	1.211	49.040	1.00	48.07	N
ATOM	1863	CA	LYS	C	77	32.478	1.911	50.215	1.00	48.29	C
ATOM	1864	CB	LYS	C	77	33.914	2.377	49.971	1.00	48.68	C
ATOM	1865	CG	LYS	C	77	34.989	1.544	50.646	1.00	50.03	C
ATOM	1866	CD	LYS	C	77	36.376	2.060	50.280	1.00	52.20	C
ATOM	1867	CE	LYS	C	77	37.362	1.960	51.456	1.00	54.79	C
ATOM	1868	NZ	LYS	C	77	37.868	0.572	51.740	1.00	56.57	N
ATOM	1869	C	LYS	C	77	31.604	3.107	50.590	1.00	48.09	C
ATOM	1870	O	LYS	C	77	31.335	3.340	51.757	1.00	47.93	O
ATOM	1871	N	LYS	C	78	31.153	3.854	49.588	1.00	48.18	N
ATOM	1872	CA	LYS	C	78	30.376	5.068	49.825	1.00	48.14	C
ATOM	1873	CB	LYS	C	78	30.630	6.090	48.714	1.00	48.23	C

Figure 2 Table 2a - 29

ATOM	1874	CG	LYS	C	78	32.018	6.691	48.763	1.00	48.77	C
ATOM	1875	CD	LYS	C	78	32.258	7.627	47.604	1.00	51.10	C
ATOM	1876	CE	LYS	C	78	33.559	8.395	47.790	1.00	51.98	C
ATOM	1877	NZ	LYS	C	78	33.939	9.108	46.542	1.00	52.29	N
ATOM	1878	C	LYS	C	78	28.890	4.785	49.960	1.00	48.08	C
ATOM	1879	O	LYS	C	78	28.149	5.612	50.499	1.00	48.18	O
ATOM	1880	N	GLN	C	79	28.477	3.609	49.474	1.00	47.96	N
ATOM	1881	CA	GLN	C	79	27.072	3.151	49.458	1.00	47.68	C
ATOM	1882	CB	GLN	C	79	26.528	2.885	50.875	1.00	47.80	C
ATOM	1883	CG	GLN	C	79	27.195	1.721	51.637	1.00	47.42	C
ATOM	1884	CD	GLN	C	79	26.671	0.354	51.217	1.00	47.00	C
ATOM	1885	OE1	GLN	C	79	25.544	-0.026	51.552	1.00	45.75	O
ATOM	1886	NE2	GLN	C	79	27.493	-0.394	50.482	1.00	46.58	N
ATOM	1887	C	GLN	C	79	26.144	4.087	48.665	1.00	47.81	C
ATOM	1888	O	GLN	C	79	25.083	4.492	49.148	1.00	47.71	O
ATOM	1889	N	SER	C	80	26.552	4.414	47.437	1.00	47.62	N
ATOM	1890	CA	SER	C	80	25.767	5.272	46.562	1.00	47.54	C
ATOM	1891	CB	SER	C	80	25.838	6.736	47.018	1.00	47.89	C
ATOM	1892	OG	SER	C	80	26.976	7.395	46.503	1.00	48.47	O
ATOM	1893	C	SER	C	80	26.214	5.162	45.111	1.00	47.24	C
ATOM	1894	O	SER	C	80	27.317	4.692	44.806	1.00	47.26	O
ATOM	1895	N	PHE	C	81	25.344	5.595	44.213	1.00	46.77	N
ATOM	1896	CA	PHE	C	81	25.721	5.692	42.823	1.00	46.55	C
ATOM	1897	CB	PHE	C	81	24.493	5.854	41.935	1.00	46.34	C
ATOM	1898	CG	PHE	C	81	23.563	4.682	41.959	1.00	45.75	C
ATOM	1899	CD1	PHE	C	81	22.340	4.763	42.627	1.00	46.06	C
ATOM	1900	CE1	PHE	C	81	21.458	3.673	42.643	1.00	46.20	C
ATOM	1901	CZ	PHE	C	81	21.803	2.490	41.974	1.00	46.23	C
ATOM	1902	CE2	PHE	C	81	23.025	2.404	41.305	1.00	45.52	C
ATOM	1903	CD2	PHE	C	81	23.894	3.499	41.299	1.00	45.75	C
ATOM	1904	C	PHE	C	81	26.644	6.893	42.688	1.00	46.36	C
ATOM	1905	O	PHE	C	81	26.439	7.909	43.353	1.00	46.69	O
ATOM	1906	N	VAL	C	82	27.663	6.763	41.848	1.00	46.01	N
ATOM	1907	CA	VAL	C	82	28.661	7.823	41.683	1.00	45.84	C
ATOM	1908	CB	VAL	C	82	30.063	7.390	42.202	1.00	45.50	C
ATOM	1909	CG1	VAL	C	82	30.077	7.333	43.720	1.00	45.07	C
ATOM	1910	CG2	VAL	C	82	30.497	6.061	41.585	1.00	44.70	C
ATOM	1911	C	VAL	C	82	28.782	8.335	40.238	1.00	46.22	C
ATOM	1912	O	VAL	C	82	29.333	9.411	40.005	1.00	45.78	O
ATOM	1913	N	GLY	C	83	28.273	7.548	39.285	1.00	46.60	N
ATOM	1914	CA	GLY	C	83	28.336	7.878	37.871	1.00	46.81	C
ATOM	1915	C	GLY	C	83	27.792	6.807	36.947	1.00	47.34	C
ATOM	1916	O	GLY	C	83	27.100	5.871	37.377	1.00	47.51	O
ATOM	1917	N	MET	C	84	28.141	6.942	35.672	1.00	47.70	N
ATOM	1918	CA	MET	C	84	27.640	6.094	34.598	1.00	48.16	C
ATOM	1919	CB	MET	C	84	26.835	6.948	33.608	1.00	48.64	C
ATOM	1920	CG	MET	C	84	25.514	7.462	34.138	1.00	49.86	C
ATOM	1921	SD	MET	C	84	24.245	6.178	34.098	1.00	53.45	S
ATOM	1922	CE	MET	C	84	23.718	6.257	35.798	1.00	51.60	C
ATOM	1923	C	MET	C	84	28.811	5.487	33.853	1.00	48.20	C
ATOM	1924	O	MET	C	84	29.882	6.085	33.800	1.00	48.78	O
ATOM	1925	N	LEU	C	85	28.614	4.307	33.268	1.00	47.95	N
ATOM	1926	CA	LEU	C	85	29.579	3.768	32.318	1.00	47.94	C
ATOM	1927	CB	LEU	C	85	30.162	2.433	32.778	1.00	48.30	C
ATOM	1928	CG	LEU	C	85	31.417	1.969	32.017	1.00	49.08	C
ATOM	1929	CD1	LEU	C	85	32.646	2.773	32.448	1.00	49.85	C
ATOM	1930	CD2	LEU	C	85	31.670	0.485	32.203	1.00	48.61	C
ATOM	1931	C	LEU	C	85	28.905	3.609	30.972	1.00	47.83	C
ATOM	1932	O	LEU	C	85	27.960	2.829	30.837	1.00	47.73	O
ATOM	1933	N	THR	C	86	29.391	4.360	29.986	1.00	47.36	N
ATOM	1934	CA	THR	C	86	28.794	4.394	28.652	1.00	47.10	C
ATOM	1935	CB	THR	C	86	28.286	5.805	28.317	1.00	47.15	C
ATOM	1936	OG1	THR	C	86	29.398	6.701	28.168	1.00	48.13	O
ATOM	1937	CG2	THR	C	86	27.361	6.323	29.409	1.00	47.15	C
ATOM	1938	C	THR	C	86	29.782	3.922	27.572	1.00	46.77	C
ATOM	1939	O	THR	C	86	30.933	3.598	27.881	1.00	46.68	O
ATOM	1940	N	ILE	C	87	29.324	3.866	26.320	1.00	46.06	N

Figure 2 Table 2a - 30

ATOM	1941	CA	ILE	C	87	30.181	3.514	25.190	1.00	45.83	C
ATOM	1942	CB	ILE	C	87	29.395	3.418	23.851	1.00	46.12	C
ATOM	1943	CG1	ILE	C	87	28.104	2.612	24.017	1.00	46.21	C
ATOM	1944	CD1	ILE	C	87	28.318	1.188	24.404	1.00	47.71	C
ATOM	1945	CG2	ILE	C	87	30.286	2.875	22.718	1.00	45.31	C
ATOM	1946	C	ILE	C	87	31.305	4.537	25.013	1.00	45.60	C
ATOM	1947	O	ILE	C	87	32.403	4.186	24.581	1.00	45.24	O
ATOM	1948	N	THR	C	88	31.018	5.795	25.337	1.00	45.54	N
ATOM	1949	CA	THR	C	88	32.015	6.876	25.255	1.00	45.91	C
ATOM	1950	CB	THR	C	88	31.400	8.260	25.584	1.00	45.79	C
ATOM	1951	OG1	THR	C	88	30.198	8.420	24.834	1.00	46.98	O
ATOM	1952	CG2	THR	C	88	32.340	9.386	25.206	1.00	45.92	C
ATOM	1953	C	THR	C	88	33.216	6.583	26.159	1.00	45.62	C
ATOM	1954	O	THR	C	88	34.359	6.786	25.759	1.00	45.68	O
ATOM	1955	N	ASP	C	89	32.949	6.079	27.358	1.00	45.44	N
ATOM	1956	CA	ASP	C	89	34.008	5.667	28.264	1.00	45.63	C
ATOM	1957	CB	ASP	C	89	33.422	5.268	29.618	1.00	45.62	C
ATOM	1958	CG	ASP	C	89	32.548	6.360	30.213	1.00	45.98	C
ATOM	1959	OD1	ASP	C	89	31.350	6.110	30.455	1.00	46.24	O
ATOM	1960	OD2	ASP	C	89	33.050	7.484	30.413	1.00	46.87	O
ATOM	1961	C	ASP	C	89	34.799	4.523	27.648	1.00	45.60	C
ATOM	1962	O	ASP	C	89	36.026	4.502	27.696	1.00	45.76	O
ATOM	1963	N	PHE	C	90	34.080	3.583	27.050	1.00	45.82	N
ATOM	1964	CA	PHE	C	90	34.688	2.482	26.329	1.00	45.70	C
ATOM	1965	CB	PHE	C	90	33.603	1.580	25.761	1.00	46.26	C
ATOM	1966	CG	PHE	C	90	34.134	0.395	25.018	1.00	49.19	C
ATOM	1967	CD1	PHE	C	90	34.988	-0.519	25.651	1.00	50.54	C
ATOM	1968	CE1	PHE	C	90	35.476	-1.636	24.965	1.00	51.71	C
ATOM	1969	CZ	PHE	C	90	35.110	-1.848	23.632	1.00	51.63	C
ATOM	1970	CE2	PHE	C	90	34.260	-0.940	22.990	1.00	51.20	C
ATOM	1971	CD2	PHE	C	90	33.772	0.171	23.686	1.00	50.26	C
ATOM	1972	C	PHE	C	90	35.583	2.989	25.208	1.00	44.98	C
ATOM	1973	O	PHE	C	90	36.695	2.498	25.042	1.00	45.05	O
ATOM	1974	N	ILE	C	91	35.103	3.979	24.454	1.00	44.01	N
ATOM	1975	CA	ILE	C	91	35.890	4.557	23.376	1.00	43.30	C
ATOM	1976	CB	ILE	C	91	35.050	5.487	22.493	1.00	43.56	C
ATOM	1977	CG1	ILE	C	91	34.200	4.632	21.559	1.00	43.15	C
ATOM	1978	CD1	ILE	C	91	32.939	5.262	21.165	1.00	43.41	C
ATOM	1979	CG2	ILE	C	91	35.936	6.431	21.669	1.00	42.63	C
ATOM	1980	C	ILE	C	91	37.131	5.248	23.911	1.00	43.21	C
ATOM	1981	O	ILE	C	91	38.230	5.004	23.425	1.00	43.20	O
ATOM	1982	N	ASN	C	92	36.953	6.093	24.922	1.00	43.15	N
ATOM	1983	CA	ASN	C	92	38.066	6.739	25.608	1.00	43.06	C
ATOM	1984	CB	ASN	C	92	37.552	7.554	26.800	1.00	43.10	C
ATOM	1985	CG	ASN	C	92	36.860	8.841	26.375	1.00	44.36	C
ATOM	1986	OD1	ASN	C	92	36.733	9.129	25.192	1.00	45.77	O
ATOM	1987	ND2	ASN	C	92	36.415	9.622	27.344	1.00	46.35	N
ATOM	1988	C	ASN	C	92	39.131	5.746	26.064	1.00	43.14	C
ATOM	1989	O	ASN	C	92	40.324	5.995	25.902	1.00	43.02	O
ATOM	1990	N	ILE	C	93	38.684	4.616	26.610	1.00	43.30	N
ATOM	1991	CA	ILE	C	93	39.560	3.580	27.143	1.00	43.61	C
ATOM	1992	CB	ILE	C	93	38.760	2.593	28.086	1.00	43.87	C
ATOM	1993	CG1	ILE	C	93	38.608	3.209	29.478	1.00	44.18	C
ATOM	1994	CD1	ILE	C	93	37.353	2.828	30.228	1.00	45.21	C
ATOM	1995	CG2	ILE	C	93	39.438	1.230	28.210	1.00	42.72	C
ATOM	1996	C	ILE	C	93	40.309	2.837	26.031	1.00	43.81	C
ATOM	1997	O	ILE	C	93	41.500	2.534	26.179	1.00	43.90	O
ATOM	1998	N	LEU	C	94	39.613	2.534	24.935	1.00	43.78	N
ATOM	1999	CA	LEU	C	94	40.237	1.856	23.796	1.00	44.29	C
ATOM	2000	CB	LEU	C	94	39.200	1.465	22.759	1.00	44.39	C
ATOM	2001	CG	LEU	C	94	38.392	0.196	22.944	1.00	46.25	C
ATOM	2002	CD1	LEU	C	94	37.604	-0.021	21.663	1.00	48.01	C
ATOM	2003	CD2	LEU	C	94	39.278	-1.010	23.256	1.00	46.56	C
ATOM	2004	C	LEU	C	94	41.289	2.718	23.111	1.00	44.18	C
ATOM	2005	O	LEU	C	94	42.308	2.215	22.639	1.00	44.04	O
ATOM	2006	N	HIS	C	95	41.010	4.015	23.036	1.00	44.23	N
ATOM	2007	CA	HIS	C	95	41.954	4.974	22.496	1.00	44.46	C

Figure 2 Table 2a - 31

ATOM	2008	CB	HIS	C	95	41.318	6.352	22.419	1.00	43.76	C
ATOM	2009	CG	HIS	C	95	42.113	7.325	21.617	1.00	43.43	C
ATOM	2010	ND1	HIS	C	95	42.711	8.435	22.173	1.00	42.05	N
ATOM	2011	CE1	HIS	C	95	43.348	9.103	21.230	1.00	42.71	C
ATOM	2012	NE2	HIS	C	95	43.190	8.463	20.084	1.00	43.00	N
ATOM	2013	CD2	HIS	C	95	42.424	7.347	20.298	1.00	42.21	C
ATOM	2014	C	HIS	C	95	43.241	5.015	23.331	1.00	45.05	C
ATOM	2015	O	HIS	C	95	44.331	4.942	22.776	1.00	45.27	O
ATOM	2016	N	ARG	C	96	43.103	5.113	24.654	1.00	45.62	N
ATOM	2017	CA	ARG	C	96	44.251	5.103	25.562	1.00	46.70	C
ATOM	2018	CB	ARG	C	96	43.816	5.413	26.998	1.00	47.18	C
ATOM	2019	CG	ARG	C	96	44.058	6.847	27.431	1.00	49.64	C
ATOM	2020	CD	ARG	C	96	45.450	7.033	28.011	1.00	52.17	C
ATOM	2021	NE	ARG	C	96	45.454	8.129	28.972	1.00	55.63	N
ATOM	2022	CZ	ARG	C	96	45.726	8.002	30.273	1.00	58.76	C
ATOM	2023	NH1	ARG	C	96	46.050	6.817	30.800	1.00	59.95	N
ATOM	2024	NH2	ARG	C	96	45.697	9.073	31.055	1.00	60.09	N
ATOM	2025	C	ARG	C	96	45.021	3.788	25.550	1.00	46.43	C
ATOM	2026	O	ARG	C	96	46.236	3.786	25.668	1.00	46.37	O
ATOM	2027	N	TYR	C	97	44.303	2.674	25.438	1.00	46.58	N
ATOM	2028	CA	TYR	C	97	44.929	1.364	25.370	1.00	46.65	C
ATOM	2029	CB	TYR	C	97	43.876	0.248	25.413	1.00	47.64	C
ATOM	2030	CG	TYR	C	97	44.455	-1.117	25.096	1.00	49.80	C
ATOM	2031	CD1	TYR	C	97	45.057	-1.893	26.097	1.00	51.67	C
ATOM	2032	CE1	TYR	C	97	45.607	-3.138	25.806	1.00	52.85	C
ATOM	2033	CZ	TYR	C	97	45.564	-3.611	24.493	1.00	53.61	C
ATOM	2034	OH	TYR	C	97	46.102	-4.844	24.191	1.00	55.34	O
ATOM	2035	CE2	TYR	C	97	44.980	-2.858	23.482	1.00	52.18	C
ATOM	2036	CD2	TYR	C	97	44.430	-1.621	23.788	1.00	51.49	C
ATOM	2037	C	TYR	C	97	45.748	1.245	24.102	1.00	45.85	C
ATOM	2038	O	TYR	C	97	46.881	0.786	24.127	1.00	45.70	O
ATOM	2039	N	TYR	C	98	45.163	1.667	22.989	1.00	45.37	N
ATOM	2040	CA	TYR	C	98	45.825	1.578	21.705	1.00	44.50	C
ATOM	2041	CB	TYR	C	98	44.896	2.035	20.575	1.00	45.12	C
ATOM	2042	CG	TYR	C	98	45.580	2.046	19.228	1.00	46.42	C
ATOM	2043	CD1	TYR	C	98	45.753	0.859	18.511	1.00	48.04	C
ATOM	2044	CE1	TYR	C	98	46.395	0.845	17.273	1.00	49.06	C
ATOM	2045	CZ	TYR	C	98	46.887	2.030	16.746	1.00	49.30	C
ATOM	2046	OH	TYR	C	98	47.523	1.998	15.517	1.00	50.58	O
ATOM	2047	CE2	TYR	C	98	46.738	3.233	17.450	1.00	48.36	C
ATOM	2048	CD2	TYR	C	98	46.084	3.233	18.683	1.00	46.48	C
ATOM	2049	C	TYR	C	98	47.139	2.360	21.697	1.00	43.46	C
ATOM	2050	O	TYR	C	98	48.165	1.856	21.237	1.00	43.22	O
ATOM	2051	N	LYS	C	99	47.096	3.590	22.208	1.00	42.25	N
ATOM	2052	CA	LYS	C	99	48.267	4.471	22.195	1.00	41.19	C
ATOM	2053	CB	LYS	C	99	47.878	5.940	22.446	1.00	41.13	C
ATOM	2054	CG	LYS	C	99	47.054	6.595	21.328	1.00	41.78	C
ATOM	2055	CD	LYS	C	99	47.899	6.914	20.100	1.00	43.52	C
ATOM	2056	CE	LYS	C	99	47.061	7.520	18.985	1.00	44.34	C
ATOM	2057	NZ	LYS	C	99	47.882	7.850	17.785	1.00	45.69	N
ATOM	2058	C	LYS	C	99	49.290	4.004	23.217	1.00	39.94	C
ATOM	2059	O	LYS	C	99	50.479	4.069	22.973	1.00	40.16	O
ATOM	2060	N	SER	C	100	48.815	3.523	24.356	1.00	38.78	N
ATOM	2061	CA	SER	C	100	49.691	3.036	25.415	1.00	37.73	C
ATOM	2062	CB	SER	C	100	48.908	2.787	26.695	1.00	37.34	C
ATOM	2063	OG	SER	C	100	48.446	4.008	27.240	1.00	36.42	O
ATOM	2064	C	SER	C	100	50.446	1.786	25.007	1.00	37.18	C
ATOM	2065	O	SER	C	100	51.614	1.640	25.353	1.00	37.47	O
ATOM	2066	N	ALA	C	101	49.786	0.908	24.256	1.00	36.44	N
ATOM	2067	CA	ALA	C	101	50.394	-0.330	23.778	1.00	35.54	C
ATOM	2068	CB	ALA	C	101	49.374	-1.160	23.041	1.00	35.53	C
ATOM	2069	C	ALA	C	101	51.603	-0.054	22.892	1.00	35.13	C
ATOM	2070	O	ALA	C	101	52.611	-0.764	22.949	1.00	35.22	O
ATOM	2071	N	LEU	C	102	51.513	0.997	22.091	1.00	34.56	N
ATOM	2072	CA	LEU	C	102	52.592	1.358	21.176	1.00	34.28	C
ATOM	2073	CB	LEU	C	102	52.125	2.415	20.169	1.00	34.01	C
ATOM	2074	CG	LEU	C	102	51.170	1.950	19.064	1.00	33.61	C

Figure 2 Table 2a - 32

ATOM	2075	CD1	LEU	C	102	50.648	3.139	18.271	1.00	32.97	C
ATOM	2076	CD2	LEU	C	102	51.852	0.946	18.132	1.00	33.40	C
ATOM	2077	C	LEU	C	102	53.806	1.848	21.944	1.00	34.22	C
ATOM	2078	O	LEU	C	102	54.920	1.894	21.416	1.00	34.51	O
ATOM	2079	N	VAL	C	103	53.583	2.198	23.202	1.00	33.85	N
ATOM	2080	CA	VAL	C	103	54.639	2.712	24.041	1.00	33.88	C
ATOM	2081	CB	VAL	C	103	54.350	4.216	24.382	1.00	34.00	C
ATOM	2082	CG1	VAL	C	103	53.542	4.402	25.665	1.00	33.53	C
ATOM	2083	CG2	VAL	C	103	55.632	5.043	24.357	1.00	34.38	C
ATOM	2084	C	VAL	C	103	54.919	1.728	25.209	1.00	34.01	C
ATOM	2085	O	VAL	C	103	55.602	2.046	26.185	1.00	33.74	O
ATOM	2086	N	GLN	C	104	54.427	0.500	25.025	1.00	34.27	N
ATOM	2087	CA	GLN	C	104	54.632	-0.656	25.921	1.00	35.11	C
ATOM	2088	CB	GLN	C	104	56.094	-1.134	25.970	1.00	34.60	C
ATOM	2089	CG	GLN	C	104	56.681	-1.560	24.637	1.00	33.71	C
ATOM	2090	CD	GLN	C	104	57.054	-0.368	23.766	1.00	34.24	C
ATOM	2091	OE1	GLN	C	104	57.795	0.521	24.193	1.00	34.11	O
ATOM	2092	NE2	GLN	C	104	56.523	-0.330	22.549	1.00	34.89	N
ATOM	2093	C	GLN	C	104	54.062	-0.482	27.327	1.00	35.97	C
ATOM	2094	O	GLN	C	104	54.611	-0.991	28.290	1.00	35.42	O
ATOM	2095	N	ILE	C	105	52.951	0.242	27.415	1.00	37.79	N
ATOM	2096	CA	ILE	C	105	52.225	0.432	28.662	1.00	39.95	C
ATOM	2097	CB	ILE	C	105	52.017	1.948	29.005	1.00	39.82	C
ATOM	2098	CG1	ILE	C	105	53.377	2.613	29.289	1.00	39.69	C
ATOM	2099	CD1	ILE	C	105	53.376	4.122	29.317	1.00	37.75	C
ATOM	2100	CG2	ILE	C	105	51.062	2.116	30.200	1.00	39.01	C
ATOM	2101	C	ILE	C	105	50.907	-0.337	28.557	1.00	41.77	C
ATOM	2102	O	ILE	C	105	50.091	-0.063	27.686	1.00	42.04	O
ATOM	2103	N	TYR	C	106	50.714	-1.302	29.450	1.00	44.18	N
ATOM	2104	CA	TYR	C	106	49.606	-2.241	29.329	1.00	46.74	C
ATOM	2105	CB	TYR	C	106	50.127	-3.648	29.035	1.00	45.92	C
ATOM	2106	CG	TYR	C	106	51.010	-3.732	27.810	1.00	44.47	C
ATOM	2107	CD1	TYR	C	106	52.368	-4.004	27.927	1.00	42.54	C
ATOM	2108	CE1	TYR	C	106	53.179	-4.084	26.809	1.00	41.99	C
ATOM	2109	CZ	TYR	C	106	52.633	-3.890	25.557	1.00	41.58	C
ATOM	2110	OH	TYR	C	106	53.432	-3.968	24.442	1.00	41.04	O
ATOM	2111	CE2	TYR	C	106	51.289	-3.620	25.416	1.00	41.91	C
ATOM	2112	CD2	TYR	C	106	50.486	-3.542	26.537	1.00	41.93	C
ATOM	2113	C	TYR	C	106	48.748	-2.253	30.588	1.00	49.31	C
ATOM	2114	O	TYR	C	106	48.200	-3.288	30.965	1.00	50.21	O
ATOM	2115	N	GLU	C	107	48.637	-1.098	31.235	1.00	52.49	N
ATOM	2116	CA	GLU	C	107	47.782	-0.952	32.407	1.00	55.59	C
ATOM	2117	CB	GLU	C	107	47.897	0.459	32.986	1.00	55.65	C
ATOM	2118	CG	GLU	C	107	49.304	0.865	33.391	1.00	56.68	C
ATOM	2119	CD	GLU	C	107	49.404	2.340	33.732	1.00	57.15	C
ATOM	2120	OE1	GLU	C	107	48.973	3.173	32.905	1.00	57.39	O
ATOM	2121	OE2	GLU	C	107	49.915	2.666	34.825	1.00	57.19	O
ATOM	2122	C	GLU	C	107	46.329	-1.245	32.061	1.00	57.62	C
ATOM	2123	O	GLU	C	107	45.692	-2.104	32.673	1.00	57.66	O
ATOM	2124	N	LEU	C	108	45.816	-0.526	31.068	1.00	60.21	N
ATOM	2125	CA	LEU	C	108	44.409	-0.145	31.042	1.00	62.58	C
ATOM	2126	CB	LEU	C	108	44.033	0.436	29.675	1.00	62.54	C
ATOM	2127	CG	LEU	C	108	44.624	1.804	29.318	1.00	63.13	C
ATOM	2128	CD1	LEU	C	108	44.106	2.875	30.272	1.00	63.69	C
ATOM	2129	CD2	LEU	C	108	46.152	1.765	29.316	1.00	62.19	C
ATOM	2130	C	LEU	C	108	43.505	-1.323	31.383	1.00	64.13	C
ATOM	2131	O	LEU	C	108	42.535	-1.176	32.128	1.00	64.65	O
ATOM	2132	N	GLU	C	109	43.832	-2.491	30.840	1.00	65.79	N
ATOM	2133	CA	GLU	C	109	42.858	-3.567	30.712	1.00	67.44	C
ATOM	2134	CB	GLU	C	109	43.241	-4.500	29.562	1.00	67.64	C
ATOM	2135	CG	GLU	C	109	42.170	-4.626	28.485	1.00	69.17	C
ATOM	2136	CD	GLU	C	109	41.588	-3.283	28.066	1.00	70.53	C
ATOM	2137	OE1	GLU	C	109	40.968	-3.215	26.983	1.00	71.37	O
ATOM	2138	OE2	GLU	C	109	41.748	-2.296	28.816	1.00	70.70	O
ATOM	2139	C	GLU	C	109	42.695	-4.347	32.014	1.00	68.14	C
ATOM	2140	O	GLU	C	109	41.770	-5.149	32.155	1.00	68.70	O
ATOM	2141	N	GLU	C	110	43.593	-4.098	32.964	1.00	68.96	N

Figure 2 Table 2a - 33

ATOM	2142	CA	GLU	C	110	43.449	-4.621	34.323	1.00	69.34	C
ATOM	2143	CB	GLU	C	110	44.774	-5.205	34.820	1.00	69.62	C
ATOM	2144	CG	GLU	C	110	45.308	-6.350	33.971	1.00	71.44	C
ATOM	2145	CD	GLU	C	110	44.203	-7.144	33.296	1.00	74.11	C
ATOM	2146	OE1	GLU	C	110	43.339	-7.694	34.011	1.00	74.97	O
ATOM	2147	OE2	GLU	C	110	44.199	-7.215	32.049	1.00	74.75	O
ATOM	2148	C	GLU	C	110	42.951	-3.546	35.285	1.00	69.22	C
ATOM	2149	O	GLU	C	110	42.861	-3.774	36.492	1.00	69.03	O
ATOM	2150	N	HIS	C	111	42.632	-2.375	34.743	1.00	69.31	N
ATOM	2151	CA	HIS	C	111	41.978	-1.329	35.507	1.00	69.37	C
ATOM	2152	CB	HIS	C	111	41.709	-0.128	34.609	1.00	69.74	C
ATOM	2153	CG	HIS	C	111	42.854	0.830	34.500	1.00	71.66	C
ATOM	2154	ND1	HIS	C	111	44.166	0.421	34.389	1.00	73.39	N
ATOM	2155	CE1	HIS	C	111	44.946	1.482	34.300	1.00	74.28	C
ATOM	2156	NE2	HIS	C	111	44.186	2.564	34.332	1.00	73.91	N
ATOM	2157	CD2	HIS	C	111	42.875	2.183	34.453	1.00	73.11	C
ATOM	2158	C	HIS	C	111	40.655	-1.822	36.047	1.00	68.70	C
ATOM	2159	O	HIS	C	111	39.902	-2.483	35.360	1.00	68.55	O
ATOM	2160	N	LYS	C	112	40.361	-1.495	37.282	1.00	68.01	N
ATOM	2161	CA	LYS	C	112	38.983	-1.562	37.723	1.00	67.69	C
ATOM	2162	CB	LYS	C	112	38.856	-2.045	39.176	1.00	67.51	C
ATOM	2163	CG	LYS	C	112	39.633	-1.250	40.209	1.00	67.47	C
ATOM	2164	CD	LYS	C	112	40.499	-2.168	41.084	1.00	67.08	C
ATOM	2165	CE	LYS	C	112	39.681	-3.217	41.817	1.00	67.33	C
ATOM	2166	NZ	LYS	C	112	40.539	-4.188	42.547	1.00	67.56	N
ATOM	2167	C	LYS	C	112	38.347	-0.196	37.475	1.00	67.36	C
ATOM	2168	O	LYS	C	112	39.037	0.825	37.498	1.00	67.56	O
ATOM	2169	N	ILE	C	113	37.041	-0.185	37.229	1.00	66.71	N
ATOM	2170	CA	ILE	C	113	36.305	1.059	37.032	1.00	66.07	C
ATOM	2171	CB	ILE	C	113	34.787	0.846	37.193	1.00	65.81	C
ATOM	2172	CG1	ILE	C	113	34.257	-0.063	36.081	1.00	64.45	C
ATOM	2173	CD1	ILE	C	113	32.987	-0.798	36.437	1.00	61.31	C
ATOM	2174	CG2	ILE	C	113	34.057	2.181	37.195	1.00	65.61	C
ATOM	2175	C	ILE	C	113	36.776	2.136	38.006	1.00	66.24	C
ATOM	2176	O	ILE	C	113	37.103	3.252	37.600	1.00	66.05	O
ATOM	2177	N	GLU	C	114	36.810	1.791	39.290	1.00	66.22	N
ATOM	2178	CA	GLU	C	114	37.418	2.639	40.311	1.00	66.49	C
ATOM	2179	CB	GLU	C	114	37.866	1.789	41.505	1.00	66.44	C
ATOM	2180	CG	GLU	C	114	37.686	2.457	42.858	1.00	67.39	C
ATOM	2181	CD	GLU	C	114	37.724	1.465	44.010	1.00	69.58	C
ATOM	2182	OE1	GLU	C	114	38.154	0.312	43.793	1.00	71.05	O
ATOM	2183	OE2	GLU	C	114	37.325	1.838	45.135	1.00	70.52	O
ATOM	2184	C	GLU	C	114	38.604	3.422	39.753	1.00	66.43	C
ATOM	2185	O	GLU	C	114	38.615	4.654	39.776	1.00	66.16	O
ATOM	2186	N	THR	C	115	39.596	2.698	39.247	1.00	66.66	N
ATOM	2187	CA	THR	C	115	40.938	3.243	39.080	1.00	67.02	C
ATOM	2188	CB	THR	C	115	41.998	2.124	39.001	1.00	67.03	C
ATOM	2189	OG1	THR	C	115	41.497	1.041	38.209	1.00	67.68	O
ATOM	2190	CG2	THR	C	115	42.333	1.608	40.393	1.00	67.20	C
ATOM	2191	C	THR	C	115	41.033	4.121	37.838	1.00	67.11	C
ATOM	2192	O	THR	C	115	41.807	5.077	37.802	1.00	66.91	O
ATOM	2193	N	TRP	C	116	40.240	3.794	36.823	1.00	67.60	N
ATOM	2194	CA	TRP	C	116	40.190	4.594	35.604	1.00	68.14	C
ATOM	2195	CB	TRP	C	116	39.542	3.811	34.461	1.00	68.23	C
ATOM	2196	CG	TRP	C	116	39.534	4.566	33.162	1.00	70.14	C
ATOM	2197	CD1	TRP	C	116	40.581	4.727	32.298	1.00	70.62	C
ATOM	2198	NE1	TRP	C	116	40.192	5.486	31.220	1.00	71.27	N
ATOM	2199	CE2	TRP	C	116	38.874	5.831	31.371	1.00	71.23	C
ATOM	2200	CD2	TRP	C	116	38.426	5.270	32.585	1.00	70.55	C
ATOM	2201	CE3	TRP	C	116	37.098	5.478	32.974	1.00	70.62	C
ATOM	2202	CZ3	TRP	C	116	36.274	6.229	32.153	1.00	71.69	C
ATOM	2203	CH2	TRP	C	116	36.748	6.772	30.950	1.00	71.64	C
ATOM	2204	CZ2	TRP	C	116	38.042	6.585	30.543	1.00	72.00	C
ATOM	2205	C	TRP	C	116	39.448	5.906	35.832	1.00	68.15	C
ATOM	2206	O	TRP	C	116	39.871	6.958	35.354	1.00	68.10	O
ATOM	2207	N	ARG	C	117	38.341	5.838	36.564	1.00	68.46	N
ATOM	2208	CA	ARG	C	117	37.618	7.037	36.974	1.00	68.99	C

Figure 2 Table 2a - 34

ATOM	2209	CB	ARG	C	117	36.438	6.669	37.873	1.00	68.80	C
ATOM	2210	CG	ARG	C	117	35.144	6.414	37.117	1.00	67.96	C
ATOM	2211	CD	ARG	C	117	34.003	6.082	38.065	1.00	67.05	C
ATOM	2212	NE	ARG	C	117	33.616	7.224	38.889	1.00	65.39	N
ATOM	2213	CZ	ARG	C	117	32.837	8.219	38.473	1.00	64.68	C
ATOM	2214	NH1	ARG	C	117	32.358	8.223	37.237	1.00	64.00	N
ATOM	2215	NH2	ARG	C	117	32.538	9.214	39.297	1.00	64.56	N
ATOM	2216	C	ARG	C	117	38.534	8.023	37.691	1.00	69.73	C
ATOM	2217	O	ARG	C	117	38.299	9.231	37.670	1.00	69.77	O
ATOM	2218	N	GLU	C	118	39.576	7.499	38.326	1.00	64.36	N
ATOM	2219	CA	GLU	C	118	40.575	8.336	38.980	1.00	66.29	C
ATOM	2220	CB	GLU	C	118	41.271	7.557	40.099	1.00	66.41	C
ATOM	2221	CG	GLU	C	118	42.161	8.410	40.993	1.00	68.63	C
ATOM	2222	CD	GLU	C	118	41.403	9.028	42.154	1.00	71.51	C
ATOM	2223	OE1	GLU	C	118	40.551	8.332	42.750	1.00	72.43	O
ATOM	2224	OE2	GLU	C	118	41.661	10.210	42.473	1.00	72.10	O
ATOM	2225	C	GLU	C	118	41.602	8.855	37.977	1.00	67.09	C
ATOM	2226	O	GLU	C	118	42.118	9.963	38.122	1.00	67.06	O
ATOM	2227	N	VAL	C	119	41.893	8.047	36.961	1.00	68.46	N
ATOM	2228	CA	VAL	C	119	42.926	8.378	35.984	1.00	69.71	C
ATOM	2229	CB	VAL	C	119	43.313	7.152	35.130	1.00	69.62	C
ATOM	2230	CG1	VAL	C	119	43.667	7.572	33.709	1.00	69.57	C
ATOM	2231	CG2	VAL	C	119	44.469	6.398	35.774	1.00	69.40	C
ATOM	2232	C	VAL	C	119	42.487	9.522	35.074	1.00	70.81	C
ATOM	2233	O	VAL	C	119	43.318	10.272	34.564	1.00	71.00	O
ATOM	2234	N	TYR	C	120	41.179	9.654	34.878	1.00	72.27	N
ATOM	2235	CA	TYR	C	120	40.627	10.831	34.218	1.00	73.74	C
ATOM	2236	CB	TYR	C	120	39.532	10.438	33.226	1.00	74.22	C
ATOM	2237	CG	TYR	C	120	39.134	11.562	32.295	1.00	75.80	C
ATOM	2238	CD1	TYR	C	120	40.091	12.236	31.542	1.00	77.00	C
ATOM	2239	CE1	TYR	C	120	39.735	13.269	30.688	1.00	77.39	C
ATOM	2240	CZ	TYR	C	120	38.408	13.639	30.580	1.00	77.50	C
ATOM	2241	OH	TYR	C	120	38.052	14.664	29.731	1.00	77.49	O
ATOM	2242	CE2	TYR	C	120	37.438	12.984	31.317	1.00	77.34	C
ATOM	2243	CD2	TYR	C	120	37.806	11.951	32.170	1.00	77.16	C
ATOM	2244	C	TYR	C	120	40.089	11.841	35.226	1.00	74.37	C
ATOM	2245	O	TYR	C	120	40.706	12.880	35.464	1.00	74.63	O
ATOM	2246	N	LEU	C	121	38.937	11.535	35.812	1.00	75.06	N
ATOM	2247	CA	LEU	C	121	38.206	12.504	36.625	1.00	75.73	C
ATOM	2248	CB	LEU	C	121	36.860	11.924	37.070	1.00	75.71	C
ATOM	2249	CG	LEU	C	121	35.939	11.378	35.977	1.00	75.82	C
ATOM	2250	CD1	LEU	C	121	34.767	10.636	36.594	1.00	76.03	C
ATOM	2251	CD2	LEU	C	121	35.455	12.494	35.064	1.00	75.73	C
ATOM	2252	C	LEU	C	121	39.022	12.921	37.846	1.00	76.20	C
ATOM	2253	O	LEU	C	121	38.671	12.591	38.982	1.00	76.54	O
ATOM	2254	N	GLN	C	122	40.108	13.647	37.606	1.00	76.50	N
ATOM	2255	CA	GLN	C	122	41.091	13.925	38.649	1.00	76.71	C
ATOM	2256	CB	GLN	C	122	42.395	14.441	38.035	1.00	76.86	C
ATOM	2257	CG	GLN	C	122	42.769	13.784	36.716	1.00	77.70	C
ATOM	2258	CD	GLN	C	122	43.071	14.796	35.626	1.00	78.90	C
ATOM	2259	OE1	GLN	C	122	43.430	14.431	34.506	1.00	79.38	O
ATOM	2260	NE2	GLN	C	122	42.924	16.077	35.950	1.00	79.21	N
ATOM	2261	C	GLN	C	122	40.547	14.940	39.650	1.00	76.57	C
ATOM	2262	O	GLN	C	122	39.880	14.576	40.620	1.00	76.65	O
ATOM	2263	N	ASP	C	123	40.842	16.213	39.409	1.00	76.31	N
ATOM	2264	CA	ASP	C	123	40.126	17.306	40.056	1.00	76.03	C
ATOM	2265	CB	ASP	C	123	41.056	18.501	40.278	1.00	76.17	C
ATOM	2266	CG	ASP	C	123	42.487	18.085	40.559	1.00	76.70	C
ATOM	2267	OD1	ASP	C	123	43.142	17.544	39.643	1.00	77.22	O
ATOM	2268	OD2	ASP	C	123	42.958	18.300	41.696	1.00	77.26	O
ATOM	2269	C	ASP	C	123	38.920	17.725	39.220	1.00	75.60	C
ATOM	2270	O	ASP	C	123	37.998	18.369	39.726	1.00	75.74	O
ATOM	2271	N	SER	C	124	38.937	17.357	37.941	1.00	74.89	N
ATOM	2272	CA	SER	C	124	37.817	17.623	37.042	1.00	73.99	C
ATOM	2273	CB	SER	C	124	38.177	17.240	35.603	1.00	74.16	C
ATOM	2274	OG	SER	C	124	38.440	15.849	35.491	1.00	74.55	O
ATOM	2275	C	SER	C	124	36.566	16.874	37.494	1.00	73.05	C

Figure 2 Table 2a - 35

ATOM	2276	O	SER	C	124	36.186	15.861	36.903	1.00	73.10	O
ATOM	2277	N	PHE	C	125	35.931	17.381	38.546	1.00	75.61	N
ATOM	2278	CA	PHE	C	125	34.819	16.685	39.178	1.00	74.77	C
ATOM	2279	CB	PHE	C	125	34.549	17.257	40.572	1.00	75.05	C
ATOM	2280	CG	PHE	C	125	34.535	16.221	41.660	1.00	75.89	C
ATOM	2281	CD1	PHE	C	125	35.490	16.240	42.666	1.00	76.81	C
ATOM	2282	CE1	PHE	C	125	35.482	15.286	43.670	1.00	77.30	C
ATOM	2283	CZ	PHE	C	125	34.512	14.296	43.676	1.00	77.25	C
ATOM	2284	CE2	PHE	C	125	33.554	14.265	42.676	1.00	77.17	C
ATOM	2285	CD2	PHE	C	125	33.569	15.224	41.675	1.00	76.65	C
ATOM	2286	C	PHE	C	125	33.560	16.765	38.319	1.00	73.72	C
ATOM	2287	O	PHE	C	125	33.092	17.857	37.987	1.00	73.72	O
ATOM	2288	N	LYS	C	126	33.026	15.602	37.957	1.00	72.05	N
ATOM	2289	CA	LYS	C	126	31.692	15.517	37.371	1.00	70.28	C
ATOM	2290	CB	LYS	C	126	31.775	15.165	35.883	1.00	70.45	C
ATOM	2291	CG	LYS	C	126	32.758	16.018	35.097	1.00	70.17	C
ATOM	2292	CD	LYS	C	126	32.330	16.157	33.643	1.00	70.24	C
ATOM	2293	CE	LYS	C	126	32.938	17.398	33.006	1.00	69.51	C
ATOM	2294	NZ	LYS	C	126	32.371	18.649	33.581	1.00	69.02	N
ATOM	2295	C	LYS	C	126	30.843	14.488	38.109	1.00	68.89	C
ATOM	2296	O	LYS	C	126	30.909	13.293	37.815	1.00	69.05	O
ATOM	2297	N	PRO	C	127	30.049	14.956	39.071	1.00	67.31	N
ATOM	2298	CA	PRO	C	127	29.172	14.076	39.849	1.00	65.82	C
ATOM	2299	CB	PRO	C	127	28.564	15.022	40.887	1.00	65.87	C
ATOM	2300	CG	PRO	C	127	28.586	16.357	40.230	1.00	66.54	C
ATOM	2301	CD	PRO	C	127	29.835	16.379	39.396	1.00	67.23	C
ATOM	2302	C	PRO	C	127	28.071	13.465	38.986	1.00	64.23	C
ATOM	2303	O	PRO	C	127	27.826	13.936	37.875	1.00	64.24	O
ATOM	2304	N	LEU	C	128	27.419	12.426	39.497	1.00	62.28	N
ATOM	2305	CA	LEU	C	128	26.300	11.806	38.794	1.00	60.31	C
ATOM	2306	CB	LEU	C	128	25.874	10.493	39.461	1.00	60.00	C
ATOM	2307	CG	LEU	C	128	24.650	9.806	38.849	1.00	59.31	C
ATOM	2308	CD1	LEU	C	128	24.942	9.307	37.452	1.00	59.25	C
ATOM	2309	CD2	LEU	C	128	24.208	8.658	39.699	1.00	58.72	C
ATOM	2310	C	LEU	C	128	25.115	12.758	38.717	1.00	59.10	C
ATOM	2311	O	LEU	C	128	24.670	13.292	39.732	1.00	59.22	O
ATOM	2312	N	VAL	C	129	24.619	12.981	37.506	1.00	57.28	N
ATOM	2313	CA	VAL	C	129	23.371	13.706	37.332	1.00	55.39	C
ATOM	2314	CB	VAL	C	129	23.475	14.856	36.248	1.00	55.61	C
ATOM	2315	CG1	VAL	C	129	24.821	14.836	35.535	1.00	55.28	C
ATOM	2316	CG2	VAL	C	129	22.308	14.854	35.260	1.00	54.38	C
ATOM	2317	C	VAL	C	129	22.218	12.715	37.131	1.00	54.46	C
ATOM	2318	O	VAL	C	129	22.324	11.741	36.369	1.00	54.22	O
ATOM	2319	N	CYS	C	130	21.136	12.945	37.863	1.00	53.11	N
ATOM	2320	CA	CYS	C	130	19.973	12.067	37.811	1.00	52.02	C
ATOM	2321	CB	CYS	C	130	20.058	10.973	38.874	1.00	51.88	C
ATOM	2322	SG	CYS	C	130	20.058	11.613	40.557	1.00	49.74	S
ATOM	2323	C	CYS	C	130	18.713	12.865	38.028	1.00	51.56	C
ATOM	2324	O	CYS	C	130	18.764	14.048	38.334	1.00	51.07	O
ATOM	2325	N	ILE	C	131	17.578	12.191	37.907	1.00	51.29	N
ATOM	2326	CA	ILE	C	131	16.292	12.857	37.997	1.00	50.89	C
ATOM	2327	CB	ILE	C	131	15.779	13.294	36.589	1.00	50.45	C
ATOM	2328	CG1	ILE	C	131	14.746	14.403	36.705	1.00	51.37	C
ATOM	2329	CD1	ILE	C	131	14.911	15.494	35.654	1.00	50.63	C
ATOM	2330	CG2	ILE	C	131	15.227	12.137	35.808	1.00	50.70	C
ATOM	2331	C	ILE	C	131	15.302	11.979	38.760	1.00	50.38	C
ATOM	2332	O	ILE	C	131	15.348	10.766	38.674	1.00	50.14	O
ATOM	2333	N	SER	C	132	14.441	12.622	39.538	1.00	50.31	N
ATOM	2334	CA	SER	C	132	13.363	11.962	40.258	1.00	50.15	C
ATOM	2335	CB	SER	C	132	12.757	12.954	41.248	1.00	50.01	C
ATOM	2336	OG	SER	C	132	11.637	12.401	41.912	1.00	51.75	O
ATOM	2337	C	SER	C	132	12.287	11.481	39.278	1.00	49.75	C
ATOM	2338	O	SER	C	132	12.075	12.113	38.243	1.00	49.98	O
ATOM	2339	N	PRO	C	133	11.612	10.358	39.587	1.00	49.52	N
ATOM	2340	CA	PRO	C	133	10.445	9.939	38.785	1.00	49.49	C
ATOM	2341	CB	PRO	C	133	10.004	8.629	39.441	1.00	49.53	C
ATOM	2342	CG	PRO	C	133	10.632	8.621	40.779	1.00	49.00	C

Figure 2 Table 2a - 36

ATOM	2343	CD	PRO	C	133	11.904	9.406	40.669	1.00	49.20	C
ATOM	2344	C	PRO	C	133	9.287	10.936	38.811	1.00	49.90	C
ATOM	2345	O	PRO	C	133	8.447	10.901	37.905	1.00	50.35	O
ATOM	2346	N	ASN	C	134	9.253	11.812	39.825	1.00	49.86	N
ATOM	2347	CA	ASN	C	134	8.200	12.817	39.980	1.00	49.99	C
ATOM	2348	CB	ASN	C	134	7.868	13.011	41.456	1.00	49.88	C
ATOM	2349	CG	ASN	C	134	7.209	11.786	42.073	1.00	51.32	C
ATOM	2350	OD1	ASN	C	134	6.267	11.218	41.515	1.00	52.63	O
ATOM	2351	ND2	ASN	C	134	7.699	11.379	43.236	1.00	51.51	N
ATOM	2352	C	ASN	C	134	8.515	14.170	39.320	1.00	50.23	C
ATOM	2353	O	ASN	C	134	7.676	15.070	39.301	1.00	50.00	O
ATOM	2354	N	ALA	C	135	9.721	14.300	38.775	1.00	50.33	N
ATOM	2355	CA	ALA	C	135	10.145	15.521	38.109	1.00	50.28	C
ATOM	2356	CB	ALA	C	135	11.664	15.590	38.040	1.00	50.00	C
ATOM	2357	C	ALA	C	135	9.542	15.608	36.713	1.00	50.64	C
ATOM	2358	O	ALA	C	135	9.286	14.586	36.062	1.00	50.70	O
ATOM	2359	N	SER	C	136	9.321	16.839	36.259	1.00	50.62	N
ATOM	2360	CA	SER	C	136	8.770	17.081	34.937	1.00	50.84	C
ATOM	2361	CB	SER	C	136	8.482	18.568	34.736	1.00	50.73	C
ATOM	2362	OG	SER	C	136	9.674	19.285	34.473	1.00	50.29	O
ATOM	2363	C	SER	C	136	9.712	16.576	33.849	1.00	51.23	C
ATOM	2364	O	SER	C	136	10.936	16.509	34.031	1.00	51.41	O
ATOM	2365	N	LEU	C	137	9.123	16.215	32.717	1.00	51.42	N
ATOM	2366	CA	LEU	C	137	9.864	15.767	31.550	1.00	51.61	C
ATOM	2367	CB	LEU	C	137	8.879	15.219	30.526	1.00	51.34	C
ATOM	2368	CG	LEU	C	137	9.375	14.820	29.149	1.00	51.90	C
ATOM	2369	CD1	LEU	C	137	10.468	13.763	29.296	1.00	54.77	C
ATOM	2370	CD2	LEU	C	137	8.218	14.301	28.329	1.00	51.10	C
ATOM	2371	C	LEU	C	137	10.677	16.933	30.967	1.00	51.99	C
ATOM	2372	O	LEU	C	137	11.690	16.726	30.286	1.00	52.34	O
ATOM	2373	N	PHE	C	138	10.220	18.152	31.247	1.00	51.81	N
ATOM	2374	CA	PHE	C	138	10.945	19.366	30.898	1.00	52.05	C
ATOM	2375	CB	PHE	C	138	10.088	20.594	31.217	1.00	51.96	C
ATOM	2376	CG	PHE	C	138	10.739	21.899	30.872	1.00	52.08	C
ATOM	2377	CD1	PHE	C	138	10.441	22.539	29.679	1.00	51.86	C
ATOM	2378	CE1	PHE	C	138	11.043	23.750	29.355	1.00	51.55	C
ATOM	2379	CZ	PHE	C	138	11.947	24.326	30.232	1.00	51.61	C
ATOM	2380	CE2	PHE	C	138	12.248	23.698	31.435	1.00	51.31	C
ATOM	2381	CD2	PHE	C	138	11.644	22.496	31.749	1.00	52.22	C
ATOM	2382	C	PHE	C	138	12.265	19.418	31.670	1.00	52.02	C
ATOM	2383	O	PHE	C	138	13.330	19.665	31.095	1.00	52.17	O
ATOM	2384	N	ASP	C	139	12.185	19.187	32.974	1.00	51.81	N
ATOM	2385	CA	ASP	C	139	13.375	19.108	33.802	1.00	51.77	C
ATOM	2386	CB	ASP	C	139	13.014	18.807	35.260	1.00	51.98	C
ATOM	2387	CG	ASP	C	139	12.447	20.024	35.991	1.00	53.05	C
ATOM	2388	OD1	ASP	C	139	12.722	21.168	35.564	1.00	54.11	O
ATOM	2389	OD2	ASP	C	139	11.724	19.839	36.998	1.00	53.92	O
ATOM	2390	C	ASP	C	139	14.346	18.067	33.268	1.00	51.25	C
ATOM	2391	O	ASP	C	139	15.557	18.297	33.285	1.00	51.25	O
ATOM	2392	N	ALA	C	140	13.816	16.942	32.781	1.00	50.69	N
ATOM	2393	CA	ALA	C	140	14.642	15.874	32.200	1.00	50.06	C
ATOM	2394	CB	ALA	C	140	13.814	14.639	31.906	1.00	50.24	C
ATOM	2395	C	ALA	C	140	15.360	16.341	30.946	1.00	49.95	C
ATOM	2396	O	ALA	C	140	16.585	16.197	30.843	1.00	50.03	O
ATOM	2397	N	VAL	C	141	14.601	16.917	30.009	1.00	49.36	N
ATOM	2398	CA	VAL	C	141	15.169	17.475	28.779	1.00	48.63	C
ATOM	2399	CB	VAL	C	141	14.093	17.994	27.797	1.00	48.45	C
ATOM	2400	CG1	VAL	C	141	14.734	18.476	26.508	1.00	47.74	C
ATOM	2401	CG2	VAL	C	141	13.100	16.899	27.466	1.00	48.74	C
ATOM	2402	C	VAL	C	141	16.199	18.558	29.075	1.00	48.56	C
ATOM	2403	O	VAL	C	141	17.254	18.593	28.441	1.00	48.70	O
ATOM	2404	N	SER	C	142	15.914	19.422	30.049	1.00	48.37	N
ATOM	2405	CA	SER	C	142	16.848	20.489	30.409	1.00	48.47	C
ATOM	2406	CB	SER	C	142	16.199	21.485	31.364	1.00	48.49	C
ATOM	2407	OG	SER	C	142	14.861	21.716	30.976	1.00	50.02	O
ATOM	2408	C	SER	C	142	18.139	19.949	31.016	1.00	48.35	C
ATOM	2409	O	SER	C	142	19.212	20.487	30.766	1.00	48.66	O

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ATOM	2410	N	SER	C	143	18.034	18.885	31.809	1.00	48.21	N
ATOM	2411	CA	SER	C	143	19.192	18.267	32.433	1.00	48.19	C
ATOM	2412	CB	SER	C	143	18.733	17.283	33.523	1.00	48.48	C
ATOM	2413	OG	SER	C	143	19.784	16.443	33.973	1.00	48.48	O
ATOM	2414	C	SER	C	143	20.110	17.590	31.399	1.00	48.19	C
ATOM	2415	O	SER	C	143	21.334	17.688	31.492	1.00	47.77	O
ATOM	2416	N	LEU	C	144	19.512	16.919	30.414	1.00	48.39	N
ATOM	2417	CA	LEU	C	144	20.276	16.261	29.351	1.00	48.93	C
ATOM	2418	CB	LEU	C	144	19.371	15.393	28.469	1.00	48.63	C
ATOM	2419	CG	LEU	C	144	18.800	14.112	29.097	1.00	48.29	C
ATOM	2420	CD1	LEU	C	144	17.486	13.760	28.450	1.00	47.82	C
ATOM	2421	CD2	LEU	C	144	19.761	12.939	28.998	1.00	47.98	C
ATOM	2422	C	LEU	C	144	21.037	17.267	28.495	1.00	49.77	C
ATOM	2423	O	LEU	C	144	22.198	17.033	28.141	1.00	50.22	O
ATOM	2424	N	ILE	C	145	20.392	18.391	28.175	1.00	50.21	N
ATOM	2425	CA	ILE	C	145	21.011	19.395	27.321	1.00	50.82	C
ATOM	2426	CB	ILE	C	145	19.985	20.419	26.774	1.00	50.96	C
ATOM	2427	CG1	ILE	C	145	18.944	19.712	25.907	1.00	51.25	C
ATOM	2428	CD1	ILE	C	145	17.636	20.452	25.854	1.00	52.83	C
ATOM	2429	CG2	ILE	C	145	20.681	21.542	25.993	1.00	50.27	C
ATOM	2430	C	ILE	C	145	22.089	20.122	28.079	1.00	51.22	C
ATOM	2431	O	ILE	C	145	23.196	20.290	27.570	1.00	51.75	O
ATOM	2432	N	ARG	C	146	21.753	20.551	29.292	1.00	51.47	N
ATOM	2433	CA	ARG	C	146	22.615	21.412	30.092	1.00	51.82	C
ATOM	2434	CB	ARG	C	146	21.822	21.946	31.290	1.00	51.95	C
ATOM	2435	CG	ARG	C	146	22.575	22.832	32.251	1.00	52.02	C
ATOM	2436	CD	ARG	C	146	21.677	23.331	33.384	1.00	52.77	C
ATOM	2437	NE	ARG	C	146	21.222	22.260	34.266	1.00	53.76	N
ATOM	2438	CZ	ARG	C	146	19.964	21.831	34.340	1.00	54.18	C
ATOM	2439	NH1	ARG	C	146	19.022	22.388	33.592	1.00	55.26	N
ATOM	2440	NH2	ARG	C	146	19.646	20.847	35.165	1.00	54.73	N
ATOM	2441	C	ARG	C	146	23.891	20.678	30.521	1.00	51.91	C
ATOM	2442	O	ARG	C	146	24.971	21.266	30.564	1.00	52.11	O
ATOM	2443	N	ASN	C	147	23.770	19.388	30.806	1.00	52.14	N
ATOM	2444	CA	ASN	C	147	24.915	18.582	31.220	1.00	52.42	C
ATOM	2445	CB	ASN	C	147	24.505	17.589	32.303	1.00	52.01	C
ATOM	2446	CG	ASN	C	147	24.014	18.279	33.550	1.00	51.87	C
ATOM	2447	OD1	ASN	C	147	24.753	19.045	34.179	1.00	52.25	O
ATOM	2448	ND2	ASN	C	147	22.760	18.029	33.913	1.00	50.84	N
ATOM	2449	C	ASN	C	147	25.597	17.868	30.066	1.00	52.83	C
ATOM	2450	O	ASN	C	147	26.542	17.114	30.275	1.00	53.16	O
ATOM	2451	N	LYS	C	148	25.112	18.131	28.852	1.00	53.38	N
ATOM	2452	CA	LYS	C	148	25.674	17.597	27.600	1.00	53.64	C
ATOM	2453	CB	LYS	C	148	27.023	18.260	27.252	1.00	53.44	C
ATOM	2454	CG	LYS	C	148	26.966	19.788	27.253	1.00	53.41	C
ATOM	2455	CD	LYS	C	148	27.942	20.435	26.264	1.00	53.77	C
ATOM	2456	CE	LYS	C	148	27.726	21.955	26.223	1.00	54.45	C
ATOM	2457	NZ	LYS	C	148	28.259	22.632	24.998	1.00	55.13	N
ATOM	2458	C	LYS	C	148	25.744	16.073	27.669	1.00	53.69	C
ATOM	2459	O	LYS	C	148	26.782	15.448	27.462	1.00	53.77	O
ATOM	2460	N	ILE	C	149	24.591	15.493	27.951	1.00	54.18	N
ATOM	2461	CA	ILE	C	149	24.509	14.104	28.345	1.00	54.41	C
ATOM	2462	CB	ILE	C	149	24.391	14.039	29.900	1.00	54.47	C
ATOM	2463	CG1	ILE	C	149	25.232	12.910	30.471	1.00	55.56	C
ATOM	2464	CD1	ILE	C	149	26.709	13.330	30.614	1.00	55.99	C
ATOM	2465	CG2	ILE	C	149	22.954	14.220	30.427	1.00	54.27	C
ATOM	2466	C	ILE	C	149	23.415	13.337	27.584	1.00	54.58	C
ATOM	2467	O	ILE	C	149	22.402	13.916	27.177	1.00	54.30	O
ATOM	2468	N	HIS	C	150	23.649	12.041	27.367	1.00	55.18	N
ATOM	2469	CA	HIS	C	150	22.689	11.168	26.659	1.00	55.60	C
ATOM	2470	CB	HIS	C	150	23.373	10.467	25.481	1.00	55.61	C
ATOM	2471	CG	HIS	C	150	23.890	11.402	24.437	1.00	57.18	C
ATOM	2472	ND1	HIS	C	150	25.178	11.894	24.455	1.00	58.71	N
ATOM	2473	CE1	HIS	C	150	25.359	12.686	23.413	1.00	59.57	C
ATOM	2474	NE2	HIS	C	150	24.235	12.724	22.718	1.00	59.81	N
ATOM	2475	CD2	HIS	C	150	23.299	11.930	23.338	1.00	58.43	C
ATOM	2476	C	HIS	C	150	21.972	10.107	27.520	1.00	55.29	C

Figure 2 Table 2a - 38

ATOM	2477	O	HIS	C	150	21.150	9.356	27.011	1.00	56.05	O
ATOM	2478	N	ARG	C	151	22.288	10.019	28.805	1.00	54.69	N
ATOM	2479	CA	ARG	C	151	21.651	9.007	29.669	1.00	54.16	C
ATOM	2480	CB	ARG	C	151	22.580	7.809	29.921	1.00	54.13	C
ATOM	2481	CG	ARG	C	151	23.442	7.381	28.731	1.00	55.74	C
ATOM	2482	CD	ARG	C	151	22.698	6.444	27.802	1.00	57.36	C
ATOM	2483	NE	ARG	C	151	22.992	6.734	26.401	1.00	59.17	N
ATOM	2484	CZ	ARG	C	151	22.695	5.925	25.384	1.00	60.20	C
ATOM	2485	NH1	ARG	C	151	22.109	4.749	25.614	1.00	61.20	N
ATOM	2486	NH2	ARG	C	151	22.984	6.293	24.136	1.00	58.67	N
ATOM	2487	C	ARG	C	151	21.314	9.664	30.995	1.00	53.36	C
ATOM	2488	O	ARG	C	151	22.200	10.147	31.700	1.00	53.77	O
ATOM	2489	N	LEU	C	152	20.037	9.703	31.334	1.00	52.00	N
ATOM	2490	CA	LEU	C	152	19.631	10.292	32.589	1.00	50.61	C
ATOM	2491	CB	LEU	C	152	18.685	11.458	32.309	1.00	50.39	C
ATOM	2492	CG	LEU	C	152	18.207	12.378	33.435	1.00	49.44	C
ATOM	2493	CD1	LEU	C	152	19.359	12.962	34.240	1.00	46.41	C
ATOM	2494	CD2	LEU	C	152	17.359	13.467	32.825	1.00	47.45	C
ATOM	2495	C	LEU	C	152	18.960	9.218	33.436	1.00	49.92	C
ATOM	2496	O	LEU	C	152	17.835	8.836	33.142	1.00	50.35	O
ATOM	2497	N	PRO	C	153	19.658	8.694	34.464	1.00	49.29	N
ATOM	2498	CA	PRO	C	153	19.034	7.736	35.382	1.00	48.46	C
ATOM	2499	CB	PRO	C	153	20.172	7.352	36.322	1.00	47.93	C
ATOM	2500	CG	PRO	C	153	21.115	8.462	36.253	1.00	48.87	C
ATOM	2501	CD	PRO	C	153	21.060	8.952	34.832	1.00	49.24	C
ATOM	2502	C	PRO	C	153	17.896	8.355	36.180	1.00	48.28	C
ATOM	2503	O	PRO	C	153	18.032	9.450	36.757	1.00	48.29	O
ATOM	2504	N	VAL	C	154	16.793	7.644	36.212	1.00	48.12	N
ATOM	2505	CA	VAL	C	154	15.651	8.011	36.994	1.00	48.15	C
ATOM	2506	CB	VAL	C	154	14.375	7.609	36.289	1.00	48.38	C
ATOM	2507	CG1	VAL	C	154	13.197	7.943	37.127	1.00	47.61	C
ATOM	2508	CG2	VAL	C	154	14.289	8.274	34.951	1.00	46.54	C
ATOM	2509	C	VAL	C	154	15.724	7.271	38.290	1.00	48.69	C
ATOM	2510	O	VAL	C	154	15.761	6.070	38.306	1.00	48.69	O
ATOM	2511	N	ILE	C	155	15.748	8.017	39.380	1.00	49.09	N
ATOM	2512	CA	ILE	C	155	16.113	7.502	40.667	1.00	49.50	C
ATOM	2513	CB	ILE	C	155	17.460	8.019	41.110	1.00	49.66	C
ATOM	2514	CG1	ILE	C	155	18.539	7.560	40.160	1.00	49.75	C
ATOM	2515	CD1	ILE	C	155	19.887	7.722	40.706	1.00	48.54	C
ATOM	2516	CG2	ILE	C	155	17.800	7.482	42.441	1.00	48.77	C
ATOM	2517	C	ILE	C	155	15.088	7.908	41.684	1.00	49.94	C
ATOM	2518	O	ILE	C	155	14.864	9.075	41.899	1.00	49.77	O
ATOM	2519	N	ASP	C	156	14.479	6.916	42.312	1.00	50.42	N
ATOM	2520	CA	ASP	C	156	13.514	7.124	43.368	1.00	51.01	C
ATOM	2521	CB	ASP	C	156	12.773	5.837	43.654	1.00	51.22	C
ATOM	2522	CG	ASP	C	156	11.800	5.974	44.771	1.00	51.51	C
ATOM	2523	OD1	ASP	C	156	11.387	7.092	45.046	1.00	53.78	O
ATOM	2524	OD2	ASP	C	156	11.442	4.972	45.383	1.00	50.80	O
ATOM	2525	C	ASP	C	156	14.150	7.611	44.650	1.00	51.32	C
ATOM	2526	O	ASP	C	156	15.039	6.988	45.182	1.00	50.93	O
ATOM	2527	N	PRO	C	157	13.688	8.741	45.153	1.00	51.77	N
ATOM	2528	CA	PRO	C	157	14.347	9.336	46.295	1.00	51.81	C
ATOM	2529	CB	PRO	C	157	13.939	10.805	46.213	1.00	51.64	C
ATOM	2530	CG	PRO	C	157	12.827	10.858	45.347	1.00	51.70	C
ATOM	2531	CD	PRO	C	157	12.911	9.735	44.409	1.00	51.90	C
ATOM	2532	C	PRO	C	157	13.916	8.696	47.592	1.00	51.98	C
ATOM	2533	O	PRO	C	157	14.630	8.807	48.562	1.00	51.92	O
ATOM	2534	N	GLU	C	158	12.798	7.992	47.601	1.00	52.17	N
ATOM	2535	CA	GLU	C	158	12.479	7.149	48.743	1.00	52.44	C
ATOM	2536	CB	GLU	C	158	11.024	6.723	48.737	1.00	53.06	C
ATOM	2537	CG	GLU	C	158	10.059	7.871	48.630	1.00	56.43	C
ATOM	2538	CD	GLU	C	158	8.835	7.707	49.513	1.00	61.20	C
ATOM	2539	OE1	GLU	C	158	8.887	6.893	50.462	1.00	62.37	O
ATOM	2540	OE2	GLU	C	158	7.817	8.394	49.262	1.00	62.01	O
ATOM	2541	C	GLU	C	158	13.394	5.944	48.931	1.00	51.81	C
ATOM	2542	O	GLU	C	158	13.923	5.754	50.011	1.00	51.78	O
ATOM	2543	N	SER	C	159	13.576	5.142	47.880	1.00	51.10	N

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ATOM	2544	CA	SER	C	159	14.342	3.898	47.945	1.00 50.22	C
ATOM	2545	CB	SER	C	159	13.759	2.829	47.045	1.00 50.28	C
ATOM	2546	OG	SER	C	159	13.050	3.379	45.969	1.00 52.14	O
ATOM	2547	C	SER	C	159	15.786	4.058	47.591	1.00 49.26	C
ATOM	2548	O	SER	C	159	16.605	3.296	48.041	1.00 49.23	O
ATOM	2549	N	GLY	C	160	16.088	5.047	46.768	1.00 48.08	N
ATOM	2550	CA	GLY	C	160	17.425	5.225	46.225	1.00 46.90	C
ATOM	2551	C	GLY	C	160	17.641	4.409	44.958	1.00 46.23	C
ATOM	2552	O	GLY	C	160	18.713	4.476	44.355	1.00 46.13	O
ATOM	2553	N	ASN	C	161	16.625	3.634	44.569	1.00 45.55	N
ATOM	2554	CA	ASN	C	161	16.690	2.760	43.406	1.00 44.58	C
ATOM	2555	CB	ASN	C	161	15.546	1.742	43.417	1.00 44.13	C
ATOM	2556	CG	ASN	C	161	15.628	0.759	44.590	1.00 44.57	C
ATOM	2557	OD1	ASN	C	161	14.626	0.159	44.980	1.00 44.60	O
ATOM	2558	ND2	ASN	C	161	16.818	0.583	45.141	1.00 43.59	N
ATOM	2559	C	ASN	C	161	16.665	3.541	42.100	1.00 44.78	C
ATOM	2560	O	ASN	C	161	15.871	4.481	41.922	1.00 44.71	O
ATOM	2561	N	THR	C	162	17.563	3.157	41.197	1.00 44.31	N
ATOM	2562	CA	THR	C	162	17.471	3.560	39.823	1.00 44.29	C
ATOM	2563	CB	THR	C	162	18.766	3.285	39.071	1.00 44.03	C
ATOM	2564	OG1	THR	C	162	19.842	3.970	39.724	1.00 44.13	O
ATOM	2565	CG2	THR	C	162	18.663	3.782	37.622	1.00 44.09	C
ATOM	2566	C	THR	C	162	16.379	2.717	39.217	1.00 44.76	C
ATOM	2567	O	THR	C	162	16.389	1.480	39.340	1.00 45.13	O
ATOM	2568	N	LEU	C	163	15.434	3.391	38.569	1.00 45.07	N
ATOM	2569	CA	LEU	C	163	14.257	2.749	37.982	1.00 45.04	C
ATOM	2570	CB	LEU	C	163	13.026	3.644	38.193	1.00 44.75	C
ATOM	2571	CG	LEU	C	163	12.758	4.133	39.624	1.00 44.44	C
ATOM	2572	CD1	LEU	C	163	11.559	5.062	39.661	1.00 42.12	C
ATOM	2573	CD2	LEU	C	163	12.592	2.967	40.618	1.00 42.20	C
ATOM	2574	C	LEU	C	163	14.451	2.499	36.495	1.00 45.01	C
ATOM	2575	O	LEU	C	163	13.918	1.546	35.940	1.00 44.76	O
ATOM	2576	N	TYR	C	164	15.233	3.365	35.862	1.00 45.54	N
ATOM	2577	CA	TYR	C	164	15.252	3.460	34.416	1.00 45.94	C
ATOM	2578	CB	TYR	C	164	13.859	3.868	33.936	1.00 45.54	C
ATOM	2579	CG	TYR	C	164	13.671	3.841	32.449	1.00 45.20	C
ATOM	2580	CD1	TYR	C	164	13.763	2.634	31.719	1.00 45.17	C
ATOM	2581	CE1	TYR	C	164	13.595	2.626	30.339	1.00 43.27	C
ATOM	2582	CZ	TYR	C	164	13.304	3.831	29.701	1.00 44.34	C
ATOM	2583	OH	TYR	C	164	13.116	3.877	28.346	1.00 47.84	O
ATOM	2584	CE2	TYR	C	164	13.199	5.010	30.401	1.00 42.27	C
ATOM	2585	CD2	TYR	C	164	13.382	5.015	31.759	1.00 42.53	C
ATOM	2586	C	TYR	C	164	16.285	4.489	33.976	1.00 46.45	C
ATOM	2587	O	TYR	C	164	16.563	5.438	34.717	1.00 46.58	O
ATOM	2588	N	LEU	C	165	16.874	4.282	32.797	1.00 46.92	N
ATOM	2589	CA	LEU	C	165	17.735	5.303	32.172	1.00 47.42	C
ATOM	2590	CB	LEU	C	165	19.072	4.717	31.694	1.00 47.50	C
ATOM	2591	CG	LEU	C	165	19.701	3.710	32.678	1.00 48.01	C
ATOM	2592	CD1	LEU	C	165	20.952	3.065	32.117	1.00 47.85	C
ATOM	2593	CD2	LEU	C	165	20.034	4.369	34.011	1.00 49.50	C
ATOM	2594	C	LEU	C	165	16.991	5.943	31.021	1.00 47.28	C
ATOM	2595	O	LEU	C	165	16.630	5.278	30.049	1.00 47.09	O
ATOM	2596	N	LEU	C	166	16.765	7.242	31.145	1.00 47.74	N
ATOM	2597	CA	LEU	C	166	16.017	8.007	30.156	1.00 48.15	C
ATOM	2598	CB	LEU	C	166	15.308	9.149	30.852	1.00 48.12	C
ATOM	2599	CG	LEU	C	166	14.089	9.801	30.223	1.00 49.89	C
ATOM	2600	CD1	LEU	C	166	13.018	8.781	29.780	1.00 51.95	C
ATOM	2601	CD2	LEU	C	166	13.530	10.761	31.255	1.00 50.89	C
ATOM	2602	C	LEU	C	166	16.948	8.548	29.093	1.00 48.21	C
ATOM	2603	O	LEU	C	166	18.046	9.008	29.406	1.00 48.37	O
ATOM	2604	N	THR	C	167	16.505	8.469	27.839	1.00 48.47	N
ATOM	2605	CA	THR	C	167	17.279	8.911	26.681	1.00 48.44	C
ATOM	2606	CB	THR	C	167	17.748	7.705	25.805	1.00 49.00	C
ATOM	2607	OG1	THR	C	167	16.624	7.115	25.132	1.00 49.94	O
ATOM	2608	CG2	THR	C	167	18.460	6.630	26.651	1.00 47.96	C
ATOM	2609	C	THR	C	167	16.459	9.857	25.814	1.00 48.57	C
ATOM	2610	O	THR	C	167	15.238	9.897	25.918	1.00 48.54	O

Figure 2 Table 2a - 40

ATOM	2611	N	HIS	C	168	17.142	10.626	24.965	1.00	49.08	N
ATOM	2612	CA	HIS	C	168	16.515	11.465	23.948	1.00	48.80	C
ATOM	2613	CB	HIS	C	168	17.575	12.052	23.032	1.00	49.53	C
ATOM	2614	CG	HIS	C	168	18.439	13.088	23.671	1.00	52.03	C
ATOM	2615	ND1	HIS	C	168	19.718	12.820	24.104	1.00	54.54	N
ATOM	2616	CE1	HIS	C	168	20.248	13.923	24.604	1.00	54.04	C
ATOM	2617	NE2	HIS	C	168	19.363	14.898	24.498	1.00	53.15	N
ATOM	2618	CD2	HIS	C	168	18.226	14.405	23.912	1.00	53.20	C
ATOM	2619	C	HIS	C	168	15.565	10.677	23.062	1.00	48.30	C
ATOM	2620	O	HIS	C	168	14.464	11.142	22.781	1.00	48.51	O
ATOM	2621	N	LYS	C	169	16.005	9.510	22.583	1.00	47.68	N
ATOM	2622	CA	LYS	C	169	15.184	8.690	21.684	1.00	47.13	C
ATOM	2623	CB	LYS	C	169	15.899	7.385	21.314	1.00	47.19	C
ATOM	2624	CG	LYS	C	169	15.222	6.563	20.198	1.00	47.16	C
ATOM	2625	CD	LYS	C	169	15.950	5.268	19.886	1.00	46.87	C
ATOM	2626	CE	LYS	C	169	17.279	5.512	19.224	1.00	49.16	C
ATOM	2627	NZ	LYS	C	169	18.164	4.298	19.110	1.00	51.17	N
ATOM	2628	C	LYS	C	169	13.828	8.404	22.332	1.00	47.18	C
ATOM	2629	O	LYS	C	169	12.784	8.629	21.723	1.00	47.49	O
ATOM	2630	N	ARG	C	170	13.849	7.916	23.571	1.00	46.80	N
ATOM	2631	CA	ARG	C	170	12.626	7.658	24.313	1.00	46.37	C
ATOM	2632	CB	ARG	C	170	12.951	7.157	25.724	1.00	46.44	C
ATOM	2633	CG	ARG	C	170	11.752	6.724	26.543	1.00	46.02	C
ATOM	2634	CD	ARG	C	170	11.183	5.427	26.023	1.00	46.89	C
ATOM	2635	NE	ARG	C	170	10.139	4.913	26.910	1.00	49.35	N
ATOM	2636	CZ	ARG	C	170	9.402	3.819	26.685	1.00	47.05	C
ATOM	2637	NH1	ARG	C	170	9.567	3.094	25.579	1.00	45.44	N
ATOM	2638	NH2	ARG	C	170	8.484	3.464	27.571	1.00	44.31	N
ATOM	2639	C	ARG	C	170	11.765	8.900	24.413	1.00	46.04	C
ATOM	2640	O	ARG	C	170	10.580	8.845	24.147	1.00	46.74	O
ATOM	2641	N	ILE	C	171	12.357	10.011	24.826	1.00	45.60	N
ATOM	2642	CA	ILE	C	171	11.595	11.211	25.065	1.00	45.73	C
ATOM	2643	CB	ILE	C	171	12.482	12.328	25.631	1.00	45.70	C
ATOM	2644	CG1	ILE	C	171	12.981	11.946	27.023	1.00	43.49	C
ATOM	2645	CD1	ILE	C	171	14.122	12.797	27.547	1.00	39.35	C
ATOM	2646	CG2	ILE	C	171	11.732	13.686	25.607	1.00	45.39	C
ATOM	2647	C	ILE	C	171	10.896	11.687	23.773	1.00	46.59	C
ATOM	2648	O	ILE	C	171	9.712	12.034	23.805	1.00	47.11	O
ATOM	2649	N	LEU	C	172	11.616	11.688	22.649	1.00	46.58	N
ATOM	2650	CA	LEU	C	172	11.034	12.145	21.401	1.00	47.18	C
ATOM	2651	CB	LEU	C	172	12.072	12.310	20.287	1.00	46.93	C
ATOM	2652	CG	LEU	C	172	11.519	12.994	19.013	1.00	47.23	C
ATOM	2653	CD1	LEU	C	172	11.149	14.443	19.222	1.00	46.43	C
ATOM	2654	CD2	LEU	C	172	12.492	12.869	17.843	1.00	47.87	C
ATOM	2655	C	LEU	C	172	9.906	11.238	20.954	1.00	47.67	C
ATOM	2656	O	LEU	C	172	8.883	11.727	20.449	1.00	47.90	O
ATOM	2657	N	LYS	C	173	10.085	9.930	21.142	1.00	48.03	N
ATOM	2658	CA	LYS	C	173	9.058	8.968	20.754	1.00	48.50	C
ATOM	2659	CB	LYS	C	173	9.492	7.520	21.001	1.00	48.70	C
ATOM	2660	CG	LYS	C	173	8.614	6.541	20.255	1.00	49.29	C
ATOM	2661	CD	LYS	C	173	8.992	5.124	20.517	1.00	51.38	C
ATOM	2662	CE	LYS	C	173	8.183	4.205	19.623	1.00	52.15	C
ATOM	2663	NZ	LYS	C	173	8.543	2.793	19.884	1.00	53.10	N
ATOM	2664	C	LYS	C	173	7.784	9.237	21.524	1.00	48.48	C
ATOM	2665	O	LYS	C	173	6.686	9.182	20.968	1.00	48.40	O
ATOM	2666	N	PHE	C	174	7.948	9.516	22.814	1.00	48.70	N
ATOM	2667	CA	PHE	C	174	6.828	9.745	23.712	1.00	48.52	C
ATOM	2668	CB	PHE	C	174	7.337	9.925	25.131	1.00	48.34	C
ATOM	2669	CG	PHE	C	174	6.261	9.858	26.177	1.00	47.90	C
ATOM	2670	CD1	PHE	C	174	5.788	11.022	26.783	1.00	47.22	C
ATOM	2671	CE1	PHE	C	174	4.792	10.970	27.763	1.00	46.57	C
ATOM	2672	CZ	PHE	C	174	4.276	9.744	28.141	1.00	46.88	C
ATOM	2673	CE2	PHE	C	174	4.747	8.570	27.535	1.00	47.28	C
ATOM	2674	CD2	PHE	C	174	5.728	8.635	26.564	1.00	46.72	C
ATOM	2675	C	PHE	C	174	6.082	10.977	23.261	1.00	48.72	C
ATOM	2676	O	PHE	C	174	4.850	10.987	23.236	1.00	48.67	O
ATOM	2677	N	LEU	C	175	6.852	11.996	22.878	1.00	49.15	N

Figure 2 Table 2a - 41

ATOM	2678	CA	LEU	C	175	6.324	13.266	22.389	1.00	49.51	C
ATOM	2679	CB	LEU	C	175	7.452	14.275	22.187	1.00	49.52	C
ATOM	2680	CG	LEU	C	175	8.129	14.847	23.430	1.00	49.80	C
ATOM	2681	CD1	LEU	C	175	9.202	15.826	23.008	1.00	49.71	C
ATOM	2682	CD2	LEU	C	175	7.124	15.518	24.360	1.00	49.61	C
ATOM	2683	C	LEU	C	175	5.545	13.104	21.094	1.00	49.80	C
ATOM	2684	O	LEU	C	175	4.402	13.540	21.012	1.00	50.00	O
ATOM	2685	N	LYS	C	176	6.165	12.479	20.091	1.00	49.96	N
ATOM	2686	CA	LYS	C	176	5.491	12.164	18.836	1.00	50.31	C
ATOM	2687	CB	LYS	C	176	6.431	11.387	17.905	1.00	50.10	C
ATOM	2688	CG	LYS	C	176	5.773	10.592	16.780	1.00	49.39	C
ATOM	2689	CD	LYS	C	176	5.332	11.472	15.655	1.00	48.83	C
ATOM	2690	CE	LYS	C	176	4.206	10.833	14.850	1.00	48.45	C
ATOM	2691	NZ	LYS	C	176	3.627	11.805	13.862	1.00	46.40	N
ATOM	2692	C	LYS	C	176	4.159	11.439	19.060	1.00	51.17	C
ATOM	2693	O	LYS	C	176	3.166	11.755	18.418	1.00	51.29	O
ATOM	2694	N	LEU	C	177	4.131	10.504	20.001	1.00	52.41	N
ATOM	2695	CA	LEU	C	177	2.946	9.679	20.233	1.00	53.77	C
ATOM	2696	CB	LEU	C	177	3.315	8.389	20.974	1.00	53.90	C
ATOM	2697	CG	LEU	C	177	4.062	7.318	20.185	1.00	54.86	C
ATOM	2698	CD1	LEU	C	177	4.242	6.052	21.037	1.00	55.59	C
ATOM	2699	CD2	LEU	C	177	3.328	7.010	18.869	1.00	55.09	C
ATOM	2700	C	LEU	C	177	1.823	10.373	20.980	1.00	54.53	C
ATOM	2701	O	LEU	C	177	0.682	10.354	20.534	1.00	54.96	O
ATOM	2702	N	PHE	C	178	2.135	10.964	22.127	1.00	55.46	N
ATOM	2703	CA	PHE	C	178	1.085	11.446	23.018	1.00	56.18	C
ATOM	2704	CB	PHE	C	178	1.449	11.189	24.474	1.00	55.95	C
ATOM	2705	CG	PHE	C	178	1.344	9.757	24.863	1.00	55.57	C
ATOM	2706	CD1	PHE	C	178	2.455	8.926	24.799	1.00	55.49	C
ATOM	2707	CE1	PHE	C	178	2.362	7.583	25.158	1.00	55.45	C
ATOM	2708	CZ	PHE	C	178	1.147	7.063	25.588	1.00	55.35	C
ATOM	2709	CE2	PHE	C	178	0.024	7.888	25.650	1.00	55.73	C
ATOM	2710	CD2	PHE	C	178	0.129	9.228	25.288	1.00	55.60	C
ATOM	2711	C	PHE	C	178	0.703	12.894	22.789	1.00	57.08	C
ATOM	2712	O	PHE	C	178	-0.146	13.444	23.492	1.00	57.22	O
ATOM	2713	N	ILE	C	179	1.333	13.511	21.802	1.00	58.33	N
ATOM	2714	CA	ILE	C	179	0.845	14.777	21.294	1.00	59.60	C
ATOM	2715	CB	ILE	C	179	1.924	15.867	21.256	1.00	59.46	C
ATOM	2716	CG1	ILE	C	179	2.742	15.847	22.550	1.00	59.66	C
ATOM	2717	CD1	ILE	C	179	3.942	16.777	22.551	1.00	60.23	C
ATOM	2718	CG2	ILE	C	179	1.273	17.226	21.098	1.00	59.13	C
ATOM	2719	C	ILE	C	179	0.226	14.561	19.919	1.00	60.62	C
ATOM	2720	O	ILE	C	179	-0.375	15.479	19.386	1.00	60.79	O
ATOM	2721	N	THR	C	180	0.357	13.345	19.366	1.00	62.19	N
ATOM	2722	CA	THR	C	180	-0.308	12.962	18.100	1.00	63.13	C
ATOM	2723	CB	THR	C	180	-0.250	11.425	17.752	1.00	63.44	C
ATOM	2724	OG1	THR	C	180	1.108	10.990	17.567	1.00	63.69	O
ATOM	2725	CG2	THR	C	180	-1.040	11.130	16.456	1.00	63.42	C
ATOM	2726	C	THR	C	180	-1.751	13.414	18.184	1.00	63.69	C
ATOM	2727	O	THR	C	180	-2.639	12.704	18.685	1.00	64.13	O
ATOM	2728	N	GLU	C	181	-1.929	14.640	17.705	1.00	64.03	N
ATOM	2729	CA	GLU	C	181	-3.160	15.393	17.653	1.00	63.87	C
ATOM	2730	CB	GLU	C	181	-3.753	15.600	19.058	1.00	63.92	C
ATOM	2731	CG	GLU	C	181	-3.272	16.852	19.789	1.00	64.29	C
ATOM	2732	CD	GLU	C	181	-3.281	16.716	21.296	1.00	65.91	C
ATOM	2733	OE1	GLU	C	181	-4.065	17.449	21.935	1.00	66.42	O
ATOM	2734	OE2	GLU	C	181	-2.508	15.894	21.847	1.00	65.35	O
ATOM	2735	C	GLU	C	181	-2.535	16.672	17.133	1.00	63.96	C
ATOM	2736	O	GLU	C	181	-1.401	17.009	17.527	1.00	63.60	O
ATOM	2737	N	PHE	C	182	-3.204	17.368	16.214	1.00	63.84	N
ATOM	2738	CA	PHE	C	182	-2.621	18.623	15.774	1.00	63.61	C
ATOM	2739	CB	PHE	C	182	-1.698	18.530	14.515	1.00	63.97	C
ATOM	2740	CG	PHE	C	182	-1.647	17.169	13.816	1.00	65.01	C
ATOM	2741	CD1	PHE	C	182	-2.080	17.048	12.489	1.00	66.19	C
ATOM	2742	CE1	PHE	C	182	-2.010	15.825	11.808	1.00	66.09	C
ATOM	2743	CZ	PHE	C	182	-1.484	14.711	12.448	1.00	66.10	C
ATOM	2744	CE2	PHE	C	182	-1.023	14.819	13.766	1.00	66.54	C

Figure 2 Table 2a - 42

ATOM	2745	CD2	PHE	C	182	-1.088	16.049	14.435	1.00	65.81	C
ATOM	2746	C	PHE	C	182	-3.459	19.916	15.815	1.00	63.29	C
ATOM	2747	O	PHE	C	182	-4.017	20.353	14.787	1.00	63.17	O
ATOM	2748	N	PRO	C	183	-3.567	20.507	17.028	1.00	62.68	N
ATOM	2749	CA	PRO	C	183	-3.344	21.949	17.087	1.00	62.00	C
ATOM	2750	CB	PRO	C	183	-3.783	22.337	18.511	1.00	62.10	C
ATOM	2751	CG	PRO	C	183	-4.503	21.135	19.059	1.00	62.28	C
ATOM	2752	CD	PRO	C	183	-3.923	19.951	18.344	1.00	62.55	C
ATOM	2753	C	PRO	C	183	-1.821	22.071	16.894	1.00	61.25	C
ATOM	2754	O	PRO	C	183	-1.028	21.818	17.818	1.00	60.71	O
ATOM	2755	N	LYS	C	184	-1.435	22.385	15.659	1.00	60.19	N
ATOM	2756	CA	LYS	C	184	-0.049	22.280	15.222	1.00	59.17	C
ATOM	2757	CB	LYS	C	184	-0.001	21.663	13.819	1.00	59.21	C
ATOM	2758	CG	LYS	C	184	1.342	21.084	13.417	1.00	59.15	C
ATOM	2759	CD	LYS	C	184	1.313	20.597	11.970	1.00	60.27	C
ATOM	2760	CE	LYS	C	184	0.729	19.186	11.856	1.00	60.66	C
ATOM	2761	NZ	LYS	C	184	0.677	18.683	10.454	1.00	59.93	N
ATOM	2762	C	LYS	C	184	0.619	23.650	15.218	1.00	58.16	C
ATOM	2763	O	LYS	C	184	0.097	24.587	14.608	1.00	58.00	O
ATOM	2764	N	PRO	C	185	1.778	23.769	15.889	1.00	57.18	N
ATOM	2765	CA	PRO	C	185	2.519	25.026	15.864	1.00	56.66	C
ATOM	2766	CB	PRO	C	185	3.698	24.770	16.810	1.00	56.55	C
ATOM	2767	CG	PRO	C	185	3.368	23.526	17.558	1.00	56.72	C
ATOM	2768	CD	PRO	C	185	2.461	22.734	16.682	1.00	57.08	C
ATOM	2769	C	PRO	C	185	3.026	25.307	14.445	1.00	56.24	C
ATOM	2770	O	PRO	C	185	3.427	24.373	13.743	1.00	56.26	O
ATOM	2771	N	GLU	C	186	2.997	26.575	14.025	1.00	55.76	N
ATOM	2772	CA	GLU	C	186	3.464	26.950	12.684	1.00	55.16	C
ATOM	2773	CB	GLU	C	186	3.458	28.471	12.470	1.00	55.30	C
ATOM	2774	CG	GLU	C	186	2.076	29.109	12.409	1.00	56.89	C
ATOM	2775	CD	GLU	C	186	1.716	29.863	13.690	1.00	59.54	C
ATOM	2776	OE1	GLU	C	186	2.090	29.391	14.795	1.00	60.51	O
ATOM	2777	OE2	GLU	C	186	1.060	30.934	13.592	1.00	59.84	O
ATOM	2778	C	GLU	C	186	4.850	26.381	12.359	1.00	54.31	C
ATOM	2779	O	GLU	C	186	5.123	26.032	11.205	1.00	54.33	O
ATOM	2780	N	PHE	C	187	5.703	26.273	13.378	1.00	53.12	N
ATOM	2781	CA	PHE	C	187	7.097	25.888	13.176	1.00	52.43	C
ATOM	2782	CB	PHE	C	187	7.973	26.269	14.383	1.00	51.86	C
ATOM	2783	CG	PHE	C	187	7.685	25.488	15.638	1.00	51.86	C
ATOM	2784	CD1	PHE	C	187	7.990	24.124	15.727	1.00	52.23	C
ATOM	2785	CE1	PHE	C	187	7.730	23.405	16.885	1.00	51.03	C
ATOM	2786	CZ	PHE	C	187	7.182	24.048	17.979	1.00	51.02	C
ATOM	2787	CE2	PHE	C	187	6.884	25.406	17.908	1.00	50.89	C
ATOM	2788	CD2	PHE	C	187	7.139	26.115	16.746	1.00	50.87	C
ATOM	2789	C	PHE	C	187	7.297	24.423	12.741	1.00	52.17	C
ATOM	2790	O	PHE	C	187	8.333	24.077	12.172	1.00	52.44	O
ATOM	2791	N	MET	C	188	6.302	23.582	12.995	1.00	51.46	N
ATOM	2792	CA	MET	C	188	6.325	22.198	12.544	1.00	51.21	C
ATOM	2793	CB	MET	C	188	5.130	21.437	13.113	1.00	51.48	C
ATOM	2794	CG	MET	C	188	5.189	21.251	14.612	1.00	52.56	C
ATOM	2795	SD	MET	C	188	6.667	20.351	15.102	1.00	55.09	S
ATOM	2796	CE	MET	C	188	6.322	18.719	14.461	1.00	54.40	C
ATOM	2797	C	MET	C	188	6.319	22.082	11.025	1.00	50.56	C
ATOM	2798	O	MET	C	188	6.833	21.110	10.477	1.00	50.48	O
ATOM	2799	N	SER	C	189	5.734	23.081	10.366	1.00	49.62	N
ATOM	2800	CA	SER	C	189	5.656	23.145	8.914	1.00	49.07	C
ATOM	2801	CB	SER	C	189	4.294	23.694	8.486	1.00	49.22	C
ATOM	2802	OG	SER	C	189	3.246	23.000	9.144	1.00	49.55	O
ATOM	2803	C	SER	C	189	6.783	23.986	8.301	1.00	48.70	C
ATOM	2804	O	SER	C	189	6.776	24.265	7.102	1.00	48.78	O
ATOM	2805	N	LYS	C	190	7.736	24.390	9.131	1.00	48.34	N
ATOM	2806	CA	LYS	C	190	8.941	25.079	8.688	1.00	48.14	C
ATOM	2807	CB	LYS	C	190	9.304	26.154	9.698	1.00	48.13	C
ATOM	2808	CG	LYS	C	190	8.285	27.273	9.753	1.00	49.34	C
ATOM	2809	CD	LYS	C	190	8.731	28.373	10.705	1.00	52.11	C
ATOM	2810	CE	LYS	C	190	7.972	29.658	10.435	1.00	54.27	C
ATOM	2811	NZ	LYS	C	190	8.739	30.833	10.928	1.00	56.35	N

Figure 2 Table 2a - 43

ATOM	2812	C	LYS	C	190	10.102	24.097	8.507	1.00	48.00	C
ATOM	2813	O	LYS	C	190	10.094	23.010	9.089	1.00	47.42	O
ATOM	2814	N	SER	C	191	11.103	24.470	7.712	1.00	48.06	N
ATOM	2815	CA	SER	C	191	12.188	23.533	7.405	1.00	48.63	C
ATOM	2816	CB	SER	C	191	12.611	23.646	5.940	1.00	48.60	C
ATOM	2817	OG	SER	C	191	12.962	24.968	5.591	1.00	48.88	O
ATOM	2818	C	SER	C	191	13.391	23.665	8.329	1.00	48.89	C
ATOM	2819	O	SER	C	191	13.499	24.632	9.075	1.00	48.90	O
ATOM	2820	N	LEU	C	192	14.285	22.679	8.287	1.00	49.61	N
ATOM	2821	CA	LEU	C	192	15.524	22.722	9.076	1.00	50.46	C
ATOM	2822	CB	LEU	C	192	16.383	21.480	8.840	1.00	50.26	C
ATOM	2823	CG	LEU	C	192	15.827	20.095	9.169	1.00	49.98	C
ATOM	2824	CD1	LEU	C	192	16.777	19.045	8.617	1.00	49.95	C
ATOM	2825	CD2	LEU	C	192	15.622	19.891	10.670	1.00	49.32	C
ATOM	2826	C	LEU	C	192	16.336	23.962	8.730	1.00	51.03	C
ATOM	2827	O	LEU	C	192	16.912	24.614	9.615	1.00	51.19	O
ATOM	2828	N	GLU	C	193	16.371	24.267	7.434	1.00	51.79	N
ATOM	2829	CA	GLU	C	193	17.017	25.448	6.891	1.00	52.07	C
ATOM	2830	CB	GLU	C	193	16.623	25.590	5.428	1.00	52.47	C
ATOM	2831	CG	GLU	C	193	17.090	26.871	4.735	1.00	54.39	C
ATOM	2832	CD	GLU	C	193	18.379	26.662	3.981	1.00	57.29	C
ATOM	2833	OE1	GLU	C	193	19.335	26.127	4.591	1.00	59.78	O
ATOM	2834	OE2	GLU	C	193	18.431	27.014	2.778	1.00	58.27	O
ATOM	2835	C	GLU	C	193	16.589	26.682	7.667	1.00	52.11	C
ATOM	2836	O	GLU	C	193	17.421	27.358	8.262	1.00	52.59	O
ATOM	2837	N	GLU	C	194	15.289	26.961	7.674	1.00	51.97	N
ATOM	2838	CA	GLU	C	194	14.780	28.179	8.294	1.00	52.24	C
ATOM	2839	CB	GLU	C	194	13.458	28.610	7.666	1.00	52.47	C
ATOM	2840	CG	GLU	C	194	12.476	27.493	7.428	1.00	54.69	C
ATOM	2841	CD	GLU	C	194	11.187	27.978	6.765	1.00	56.69	C
ATOM	2842	OE1	GLU	C	194	10.764	29.135	7.049	1.00	57.76	O
ATOM	2843	OE2	GLU	C	194	10.602	27.196	5.970	1.00	57.09	O
ATOM	2844	C	GLU	C	194	14.665	28.144	9.819	1.00	51.62	C
ATOM	2845	O	GLU	C	194	14.645	29.179	10.460	1.00	51.79	O
ATOM	2846	N	LEU	C	195	14.589	26.957	10.402	1.00	51.46	N
ATOM	2847	CA	LEU	C	195	14.617	26.848	11.846	1.00	50.81	C
ATOM	2848	CB	LEU	C	195	13.800	25.653	12.316	1.00	50.09	C
ATOM	2849	CG	LEU	C	195	12.295	25.749	12.074	1.00	49.32	C
ATOM	2850	CD1	LEU	C	195	11.618	24.458	12.534	1.00	49.72	C
ATOM	2851	CD2	LEU	C	195	11.672	26.974	12.754	1.00	48.28	C
ATOM	2852	C	LEU	C	195	16.045	26.796	12.379	1.00	50.98	C
ATOM	2853	O	LEU	C	195	16.271	27.053	13.551	1.00	50.87	O
ATOM	2854	N	GLN	C	196	17.001	26.505	11.499	1.00	51.35	N
ATOM	2855	CA	GLN	C	196	18.414	26.308	11.873	1.00	51.67	C
ATOM	2856	CB	GLN	C	196	19.118	27.629	12.133	1.00	51.52	C
ATOM	2857	CG	GLN	C	196	19.611	28.223	10.853	1.00	52.65	C
ATOM	2858	CD	GLN	C	196	19.929	29.680	10.969	1.00	53.49	C
ATOM	2859	OE1	GLN	C	196	20.612	30.109	11.902	1.00	54.71	O
ATOM	2860	NE2	GLN	C	196	19.453	30.463	10.003	1.00	54.20	N
ATOM	2861	C	GLN	C	196	18.624	25.290	12.988	1.00	51.70	C
ATOM	2862	O	GLN	C	196	19.209	25.569	14.029	1.00	51.28	O
ATOM	2863	N	ILE	C	197	18.110	24.094	12.719	1.00	52.17	N
ATOM	2864	CA	ILE	C	197	18.280	22.935	13.558	1.00	52.17	C
ATOM	2865	CB	ILE	C	197	16.941	22.187	13.748	1.00	52.45	C
ATOM	2866	CG1	ILE	C	197	15.941	23.079	14.500	1.00	53.02	C
ATOM	2867	CD1	ILE	C	197	14.495	22.624	14.368	1.00	53.63	C
ATOM	2868	CG2	ILE	C	197	17.160	20.855	14.474	1.00	51.39	C
ATOM	2869	C	ILE	C	197	19.281	22.018	12.871	1.00	52.17	C
ATOM	2870	O	ILE	C	197	19.140	21.696	11.687	1.00	51.86	O
ATOM	2871	N	GLY	C	198	20.293	21.602	13.627	1.00	51.90	N
ATOM	2872	CA	GLY	C	198	21.311	20.716	13.111	1.00	51.14	C
ATOM	2873	C	GLY	C	198	22.633	21.434	13.028	1.00	50.85	C
ATOM	2874	O	GLY	C	198	22.731	22.630	13.301	1.00	50.67	O
ATOM	2875	N	THR	C	199	23.662	20.691	12.661	1.00	50.47	N
ATOM	2876	CA	THR	C	199	24.979	21.260	12.521	1.00	50.46	C
ATOM	2877	CB	THR	C	199	25.977	20.641	13.531	1.00	50.25	C
ATOM	2878	OG1	THR	C	199	25.509	20.866	14.867	1.00	51.93	O

Figure 2 Table 2a - 44

ATOM	2879	CG2	THR	C	199	27.288	21.282	13.402	1.00	50.73	C
ATOM	2880	C	THR	C	199	25.407	21.088	11.072	1.00	50.02	C
ATOM	2881	O	THR	C	199	25.273	19.983	10.510	1.00	49.98	O
ATOM	2882	N	TYR	C	200	25.898	22.190	10.489	1.00	49.06	N
ATOM	2883	CA	TYR	C	200	26.186	22.287	9.062	1.00	48.62	C
ATOM	2884	CB	TYR	C	200	25.177	23.219	8.372	1.00	48.11	C
ATOM	2885	CG	TYR	C	200	23.802	22.677	8.575	1.00	48.25	C
ATOM	2886	CD1	TYR	C	200	22.952	23.216	9.550	1.00	46.91	C
ATOM	2887	CE1	TYR	C	200	21.687	22.666	9.773	1.00	48.76	C
ATOM	2888	CZ	TYR	C	200	21.287	21.541	9.031	1.00	49.61	C
ATOM	2889	OH	TYR	C	200	20.044	20.967	9.233	1.00	50.44	O
ATOM	2890	CE2	TYR	C	200	22.132	20.984	8.069	1.00	48.21	C
ATOM	2891	CD2	TYR	C	200	23.374	21.541	7.856	1.00	47.98	C
ATOM	2892	C	TYR	C	200	27.618	22.673	8.757	1.00	48.85	C
ATOM	2893	O	TYR	C	200	27.943	22.979	7.622	1.00	49.24	O
ATOM	2894	N	ALA	C	201	28.473	22.648	9.772	1.00	49.12	N
ATOM	2895	CA	ALA	C	201	29.890	22.937	9.595	1.00	49.24	C
ATOM	2896	CB	ALA	C	201	30.183	24.405	9.923	1.00	49.39	C
ATOM	2897	C	ALA	C	201	30.767	22.006	10.434	1.00	49.36	C
ATOM	2898	O	ALA	C	201	30.302	21.424	11.425	1.00	49.26	O
ATOM	2899	N	ASN	C	202	32.024	21.860	10.013	1.00	49.50	N
ATOM	2900	CA	ASN	C	202	33.017	21.037	10.703	1.00	49.92	C
ATOM	2901	CB	ASN	C	202	33.483	21.716	12.000	1.00	50.37	C
ATOM	2902	CG	ASN	C	202	33.968	23.142	11.779	1.00	52.30	C
ATOM	2903	OD1	ASN	C	202	33.666	24.042	12.573	1.00	53.71	O
ATOM	2904	ND2	ASN	C	202	34.731	23.355	10.703	1.00	53.57	N
ATOM	2905	C	ASN	C	202	32.507	19.626	10.997	1.00	49.54	C
ATOM	2906	O	ASN	C	202	32.675	19.119	12.107	1.00	49.18	O
ATOM	2907	N	ILE	C	203	31.887	19.009	9.989	1.00	49.32	N
ATOM	2908	CA	ILE	C	203	31.268	17.695	10.125	1.00	48.82	C
ATOM	2909	CB	ILE	C	203	30.217	17.459	9.007	1.00	48.84	C
ATOM	2910	CG1	ILE	C	203	29.149	18.560	9.026	1.00	48.31	C
ATOM	2911	CD1	ILE	C	203	28.370	18.691	10.308	1.00	47.21	C
ATOM	2912	CG2	ILE	C	203	29.562	16.064	9.096	1.00	48.58	C
ATOM	2913	C	ILE	C	203	32.347	16.629	10.120	1.00	48.84	C
ATOM	2914	O	ILE	C	203	33.098	16.513	9.162	1.00	48.80	O
ATOM	2915	N	ALA	C	204	32.441	15.873	11.212	1.00	48.99	N
ATOM	2916	CA	ALA	C	204	33.429	14.803	11.314	1.00	49.38	C
ATOM	2917	CB	ALA	C	204	33.711	14.458	12.768	1.00	49.46	C
ATOM	2918	C	ALA	C	204	32.956	13.577	10.543	1.00	49.84	C
ATOM	2919	O	ALA	C	204	31.848	13.088	10.749	1.00	49.91	O
ATOM	2920	N	MET	C	205	33.817	13.099	9.645	1.00	50.44	N
ATOM	2921	CA	MET	C	205	33.478	12.082	8.645	1.00	50.49	C
ATOM	2922	CB	MET	C	205	33.114	12.741	7.315	1.00	50.31	C
ATOM	2923	CG	MET	C	205	31.977	13.704	7.372	1.00	50.74	C
ATOM	2924	SD	MET	C	205	31.667	14.349	5.736	1.00	53.02	S
ATOM	2925	CE	MET	C	205	32.774	15.769	5.686	1.00	51.94	C
ATOM	2926	C	MET	C	205	34.700	11.249	8.388	1.00	50.32	C
ATOM	2927	O	MET	C	205	35.815	11.696	8.626	1.00	50.67	O
ATOM	2928	N	VAL	C	206	34.494	10.046	7.869	1.00	50.40	N
ATOM	2929	CA	VAL	C	206	35.602	9.161	7.527	1.00	49.99	C
ATOM	2930	CB	VAL	C	206	35.702	7.983	8.512	1.00	50.10	C
ATOM	2931	CG1	VAL	C	206	36.015	8.482	9.926	1.00	49.64	C
ATOM	2932	CG2	VAL	C	206	34.430	7.122	8.483	1.00	49.44	C
ATOM	2933	C	VAL	C	206	35.447	8.668	6.090	1.00	50.05	C
ATOM	2934	O	VAL	C	206	34.443	8.945	5.443	1.00	49.88	O
ATOM	2935	N	ARG	C	207	36.449	7.957	5.585	1.00	50.30	N
ATOM	2936	CA	ARG	C	207	36.380	7.400	4.235	1.00	50.64	C
ATOM	2937	CB	ARG	C	207	37.569	7.867	3.389	1.00	50.77	C
ATOM	2938	CG	ARG	C	207	37.711	9.391	3.365	1.00	52.55	C
ATOM	2939	CD	ARG	C	207	38.193	9.951	2.031	1.00	55.10	C
ATOM	2940	NE	ARG	C	207	37.616	9.270	0.873	1.00	57.06	N
ATOM	2941	CZ	ARG	C	207	38.336	8.756	-0.126	1.00	58.86	C
ATOM	2942	NH1	ARG	C	207	39.664	8.856	-0.123	1.00	58.84	N
ATOM	2943	NH2	ARG	C	207	37.732	8.148	-1.143	1.00	59.54	N
ATOM	2944	C	ARG	C	207	36.301	5.888	4.275	1.00	50.53	C
ATOM	2945	O	ARG	C	207	36.739	5.263	5.242	1.00	50.64	O

Figure 2 Table 2a - 45

ATOM	2946	N	THR	C	208	35.718	5.309	3.232	1.00	50.61	N
ATOM	2947	CA	THR	C	208	35.697	3.853	3.020	1.00	50.93	C
ATOM	2948	CB	THR	C	208	35.713	3.543	1.514	1.00	50.75	C
ATOM	2949	OG1	THR	C	208	34.575	4.153	0.902	1.00	51.66	O
ATOM	2950	CG2	THR	C	208	35.672	2.050	1.251	1.00	51.91	C
ATOM	2951	C	THR	C	208	36.861	3.110	3.689	1.00	50.89	C
ATOM	2952	O	THR	C	208	36.652	2.078	4.336	1.00	51.12	O
ATOM	2953	N	THR	C	209	38.071	3.656	3.544	1.00	50.67	N
ATOM	2954	CA	THR	C	209	39.311	2.984	3.943	1.00	50.64	C
ATOM	2955	CB	THR	C	209	40.439	3.264	2.924	1.00	50.71	C
ATOM	2956	OG1	THR	C	209	40.927	4.600	3.102	1.00	50.92	O
ATOM	2957	CG2	THR	C	209	39.933	3.100	1.492	1.00	51.02	C
ATOM	2958	C	THR	C	209	39.841	3.338	5.343	1.00	50.43	C
ATOM	2959	O	THR	C	209	40.727	2.652	5.857	1.00	50.29	O
ATOM	2960	N	THR	C	210	39.315	4.409	5.940	1.00	50.15	N
ATOM	2961	CA	THR	C	210	39.790	4.913	7.235	1.00	49.84	C
ATOM	2962	CB	THR	C	210	38.893	6.078	7.741	1.00	49.65	C
ATOM	2963	OG1	THR	C	210	38.885	7.134	6.778	1.00	48.89	O
ATOM	2964	CG2	THR	C	210	39.391	6.632	9.051	1.00	49.37	C
ATOM	2965	C	THR	C	210	39.887	3.798	8.299	1.00	50.01	C
ATOM	2966	O	THR	C	210	38.901	3.125	8.580	1.00	50.44	O
ATOM	2967	N	PRO	C	211	41.081	3.586	8.878	1.00	49.75	N
ATOM	2968	CA	PRO	C	211	41.209	2.593	9.940	1.00	49.58	C
ATOM	2969	CB	PRO	C	211	42.691	2.669	10.311	1.00	49.79	C
ATOM	2970	CG	PRO	C	211	43.363	3.263	9.123	1.00	49.85	C
ATOM	2971	CD	PRO	C	211	42.369	4.233	8.575	1.00	49.80	C
ATOM	2972	C	PRO	C	211	40.354	2.925	11.162	1.00	49.40	C
ATOM	2973	O	PRO	C	211	40.077	4.097	11.424	1.00	49.88	O
ATOM	2974	N	VAL	C	212	39.950	1.896	11.901	1.00	48.92	N
ATOM	2975	CA	VAL	C	212	39.090	2.057	13.075	1.00	48.48	C
ATOM	2976	CB	VAL	C	212	38.692	0.677	13.664	1.00	48.49	C
ATOM	2977	CG1	VAL	C	212	38.027	0.808	15.035	1.00	48.20	C
ATOM	2978	CG2	VAL	C	212	37.776	-0.040	12.711	1.00	48.16	C
ATOM	2979	C	VAL	C	212	39.707	2.968	14.151	1.00	48.42	C
ATOM	2980	O	VAL	C	212	39.011	3.820	14.728	1.00	48.36	O
ATOM	2981	N	TYR	C	213	41.005	2.807	14.409	1.00	48.08	N
ATOM	2982	CA	TYR	C	213	41.682	3.643	15.407	1.00	47.91	C
ATOM	2983	CB	TYR	C	213	43.109	3.157	15.701	1.00	48.02	C
ATOM	2984	CG	TYR	C	213	44.085	3.278	14.552	1.00	48.56	C
ATOM	2985	CD1	TYR	C	213	44.220	2.252	13.619	1.00	49.54	C
ATOM	2986	CE1	TYR	C	213	45.127	2.348	12.568	1.00	49.71	C
ATOM	2987	CZ	TYR	C	213	45.906	3.482	12.440	1.00	49.80	C
ATOM	2988	OH	TYR	C	213	46.797	3.577	11.397	1.00	49.95	O
ATOM	2989	CE2	TYR	C	213	45.797	4.515	13.360	1.00	49.66	C
ATOM	2990	CD2	TYR	C	213	44.893	4.404	14.414	1.00	49.11	C
ATOM	2991	C	TYR	C	213	41.666	5.124	15.027	1.00	47.53	C
ATOM	2992	O	TYR	C	213	41.579	5.989	15.899	1.00	47.74	O
ATOM	2993	N	VAL	C	214	41.738	5.410	13.732	1.00	46.78	N
ATOM	2994	CA	VAL	C	214	41.654	6.779	13.260	1.00	46.07	C
ATOM	2995	CB	VAL	C	214	41.982	6.884	11.750	1.00	46.24	C
ATOM	2996	CG1	VAL	C	214	41.735	8.300	11.233	1.00	46.11	C
ATOM	2997	CG2	VAL	C	214	43.435	6.482	11.497	1.00	45.55	C
ATOM	2998	C	VAL	C	214	40.268	7.329	13.612	1.00	45.81	C
ATOM	2999	O	VAL	C	214	40.154	8.431	14.164	1.00	45.77	O
ATOM	3000	N	ALA	C	215	39.230	6.537	13.335	1.00	45.16	N
ATOM	3001	CA	ALA	C	215	37.851	6.869	13.730	1.00	44.63	C
ATOM	3002	CB	ALA	C	215	36.880	5.817	13.213	1.00	44.42	C
ATOM	3003	C	ALA	C	215	37.684	7.057	15.249	1.00	44.36	C
ATOM	3004	O	ALA	C	215	36.915	7.921	15.682	1.00	43.74	O
ATOM	3005	N	LEU	C	216	38.406	6.248	16.037	1.00	44.03	N
ATOM	3006	CA	LEU	C	216	38.437	6.390	17.494	1.00	43.78	C
ATOM	3007	CB	LEU	C	216	39.350	5.354	18.143	1.00	43.69	C
ATOM	3008	CG	LEU	C	216	38.867	3.926	18.329	1.00	43.54	C
ATOM	3009	CD1	LEU	C	216	39.849	3.200	19.222	1.00	41.92	C
ATOM	3010	CD2	LEU	C	216	37.474	3.908	18.920	1.00	43.81	C
ATOM	3011	C	LEU	C	216	38.932	7.754	17.904	1.00	43.90	C
ATOM	3012	O	LEU	C	216	38.270	8.456	18.672	1.00	44.10	O

Figure 2 Table 2a - 46

ATOM	3013	N	GLY	C	217	40.109	8.119	17.400	1.00	43.68	N
ATOM	3014	CA	GLY	C	217	40.691	9.424	17.665	1.00	43.83	C
ATOM	3015	C	GLY	C	217	39.729	10.555	17.348	1.00	43.93	C
ATOM	3016	O	GLY	C	217	39.662	11.537	18.083	1.00	43.83	O
ATOM	3017	N	ILE	C	218	38.978	10.404	16.261	1.00	43.93	N
ATOM	3018	CA	ILE	C	218	38.000	11.404	15.863	1.00	44.51	C
ATOM	3019	CB	ILE	C	218	37.519	11.154	14.408	1.00	44.69	C
ATOM	3020	CG1	ILE	C	218	38.649	11.476	13.424	1.00	44.14	C
ATOM	3021	CD1	ILE	C	218	38.613	10.626	12.159	1.00	44.45	C
ATOM	3022	CG2	ILE	C	218	36.270	11.964	14.076	1.00	44.19	C
ATOM	3023	C	ILE	C	218	36.847	11.477	16.881	1.00	44.92	C
ATOM	3024	O	ILE	C	218	36.408	12.581	17.257	1.00	45.02	O
ATOM	3025	N	PHE	C	219	36.390	10.309	17.339	1.00	45.01	N
ATOM	3026	CA	PHE	C	219	35.339	10.221	18.354	1.00	45.21	C
ATOM	3027	CB	PHE	C	219	34.999	8.764	18.697	1.00	44.90	C
ATOM	3028	CG	PHE	C	219	34.095	8.078	17.697	1.00	44.03	C
ATOM	3029	CD1	PHE	C	219	34.447	6.836	17.167	1.00	41.95	C
ATOM	3030	CE1	PHE	C	219	33.633	6.188	16.255	1.00	41.43	C
ATOM	3031	CZ	PHE	C	219	32.439	6.776	15.858	1.00	42.70	C
ATOM	3032	CE2	PHE	C	219	32.060	8.021	16.388	1.00	42.99	C
ATOM	3033	CD2	PHE	C	219	32.890	8.663	17.296	1.00	42.99	C
ATOM	3034	C	PHE	C	219	35.761	10.949	19.620	1.00	45.98	C
ATOM	3035	O	PHE	C	219	35.001	11.747	20.163	1.00	45.85	O
ATOM	3036	N	VAL	C	220	36.982	10.674	20.073	1.00	47.05	N
ATOM	3037	CA	VAL	C	220	37.521	11.270	21.296	1.00	48.01	C
ATOM	3038	CB	VAL	C	220	38.866	10.612	21.707	1.00	48.00	C
ATOM	3039	CG1	VAL	C	220	39.412	11.254	22.974	1.00	47.89	C
ATOM	3040	CG2	VAL	C	220	38.696	9.112	21.907	1.00	47.21	C
ATOM	3041	C	VAL	C	220	37.677	12.795	21.190	1.00	48.88	C
ATOM	3042	O	VAL	C	220	37.327	13.531	22.115	1.00	49.15	O
ATOM	3043	N	GLN	C	221	38.175	13.268	20.055	1.00	49.93	N
ATOM	3044	CA	GLN	C	221	38.459	14.680	19.896	1.00	50.95	C
ATOM	3045	CB	GLN	C	221	39.480	14.897	18.784	1.00	51.13	C
ATOM	3046	CG	GLN	C	221	40.201	16.232	18.892	1.00	52.92	C
ATOM	3047	CD	GLN	C	221	41.185	16.462	17.772	1.00	54.70	C
ATOM	3048	OE1	GLN	C	221	40.940	16.099	16.621	1.00	56.18	O
ATOM	3049	NE2	GLN	C	221	42.306	17.087	18.099	1.00	55.40	N
ATOM	3050	C	GLN	C	221	37.213	15.531	19.641	1.00	51.52	C
ATOM	3051	O	GLN	C	221	37.096	16.640	20.175	1.00	51.79	O
ATOM	3052	N	HIS	C	222	36.287	15.032	18.829	1.00	51.95	N
ATOM	3053	CA	HIS	C	222	35.122	15.840	18.461	1.00	52.60	C
ATOM	3054	CB	HIS	C	222	34.801	15.685	16.978	1.00	53.09	C
ATOM	3055	CG	HIS	C	222	35.922	16.094	16.079	1.00	54.98	C
ATOM	3056	ND1	HIS	C	222	35.927	17.287	15.391	1.00	58.06	N
ATOM	3057	CE1	HIS	C	222	37.041	17.384	14.685	1.00	58.68	C
ATOM	3058	NE2	HIS	C	222	37.762	16.298	14.896	1.00	58.68	N
ATOM	3059	CD2	HIS	C	222	37.084	15.473	15.765	1.00	57.11	C
ATOM	3060	C	HIS	C	222	33.891	15.578	19.333	1.00	52.46	C
ATOM	3061	O	HIS	C	222	32.949	16.378	19.336	1.00	52.11	O
ATOM	3062	N	ARG	C	223	33.922	14.473	20.083	1.00	52.49	N
ATOM	3063	CA	ARG	C	223	32.844	14.095	21.010	1.00	52.70	C
ATOM	3064	CB	ARG	C	223	32.792	15.004	22.244	1.00	52.86	C
ATOM	3065	CG	ARG	C	223	34.068	15.054	23.045	1.00	53.46	C
ATOM	3066	CD	ARG	C	223	33.897	15.997	24.200	1.00	55.60	C
ATOM	3067	NE	ARG	C	223	35.106	16.083	25.013	1.00	57.90	N
ATOM	3068	CZ	ARG	C	223	35.301	16.993	25.962	1.00	59.08	C
ATOM	3069	NH1	ARG	C	223	34.370	17.908	26.223	1.00	59.73	N
ATOM	3070	NH2	ARG	C	223	36.435	16.997	26.649	1.00	59.80	N
ATOM	3071	C	ARG	C	223	31.531	14.124	20.257	1.00	52.56	C
ATOM	3072	O	ARG	C	223	30.704	15.034	20.407	1.00	52.83	O
ATOM	3073	N	VAL	C	224	31.376	13.114	19.419	1.00	52.14	N
ATOM	3074	CA	VAL	C	224	30.319	13.054	18.439	1.00	51.81	C
ATOM	3075	CB	VAL	C	224	30.840	13.665	17.110	1.00	51.68	C
ATOM	3076	CG1	VAL	C	224	30.430	12.857	15.919	1.00	52.09	C
ATOM	3077	CG2	VAL	C	224	30.408	15.124	16.985	1.00	51.01	C
ATOM	3078	C	VAL	C	224	29.945	11.577	18.354	1.00	51.73	C
ATOM	3079	O	VAL	C	224	30.822	10.712	18.430	1.00	51.92	O

Figure 2 Table 2a - 47

ATOM	3080	N	SER	C	225	28.655	11.274	18.248	1.00	51.60	N
ATOM	3081	CA	SER	C	225	28.220	9.876	18.397	1.00	51.48	C
ATOM	3082	CB	SER	C	225	26.830	9.769	19.048	1.00	51.66	C
ATOM	3083	OG	SER	C	225	25.878	10.596	18.403	1.00	53.09	O
ATOM	3084	C	SER	C	225	28.319	9.018	17.135	1.00	50.86	C
ATOM	3085	O	SER	C	225	28.359	7.795	17.241	1.00	51.42	O
ATOM	3086	N	ALA	C	226	28.369	9.640	15.956	1.00	49.92	N
ATOM	3087	CA	ALA	C	226	28.508	8.882	14.702	1.00	49.16	C
ATOM	3088	CB	ALA	C	226	27.150	8.461	14.160	1.00	48.87	C
ATOM	3089	C	ALA	C	226	29.298	9.632	13.636	1.00	48.67	C
ATOM	3090	O	ALA	C	226	29.430	10.849	13.700	1.00	48.65	O
ATOM	3091	N	LEU	C	227	29.832	8.892	12.668	1.00	47.88	N
ATOM	3092	CA	LEU	C	227	30.616	9.470	11.592	1.00	47.57	C
ATOM	3093	CB	LEU	C	227	32.098	9.122	11.743	1.00	47.17	C
ATOM	3094	CG	LEU	C	227	32.752	9.460	13.080	1.00	46.73	C
ATOM	3095	CD1	LEU	C	227	34.144	8.859	13.160	1.00	45.33	C
ATOM	3096	CD2	LEU	C	227	32.776	10.977	13.319	1.00	47.10	C
ATOM	3097	C	LEU	C	227	30.097	8.998	10.240	1.00	47.54	C
ATOM	3098	O	LEU	C	227	30.015	7.800	9.999	1.00	47.90	O
ATOM	3099	N	PRO	C	228	29.695	9.941	9.374	1.00	47.49	N
ATOM	3100	CA	PRO	C	228	29.322	9.537	8.033	1.00	47.60	C
ATOM	3101	CB	PRO	C	228	28.880	10.855	7.389	1.00	47.33	C
ATOM	3102	CG	PRO	C	228	28.508	11.731	8.536	1.00	46.84	C
ATOM	3103	CD	PRO	C	228	29.510	11.387	9.580	1.00	47.02	C
ATOM	3104	C	PRO	C	228	30.527	8.952	7.306	1.00	48.12	C
ATOM	3105	O	PRO	C	228	31.641	9.483	7.414	1.00	48.47	O
ATOM	3106	N	VAL	C	229	30.308	7.848	6.602	1.00	48.39	N
ATOM	3107	CA	VAL	C	229	31.346	7.239	5.780	1.00	49.04	C
ATOM	3108	CB	VAL	C	229	31.308	5.695	5.874	1.00	49.10	C
ATOM	3109	CG1	VAL	C	229	32.425	5.070	5.067	1.00	48.98	C
ATOM	3110	CG2	VAL	C	229	31.367	5.239	7.331	1.00	48.97	C
ATOM	3111	C	VAL	C	229	31.110	7.702	4.343	1.00	49.63	C
ATOM	3112	O	VAL	C	229	30.041	7.465	3.771	1.00	49.97	O
ATOM	3113	N	VAL	C	230	32.098	8.380	3.772	1.00	50.14	N
ATOM	3114	CA	VAL	C	230	31.940	9.002	2.455	1.00	50.79	C
ATOM	3115	CB	VAL	C	230	32.121	10.541	2.518	1.00	50.80	C
ATOM	3116	CG1	VAL	C	230	31.105	11.183	3.474	1.00	50.34	C
ATOM	3117	CG2	VAL	C	230	33.555	10.903	2.912	1.00	50.53	C
ATOM	3118	C	VAL	C	230	32.904	8.432	1.412	1.00	51.34	C
ATOM	3119	O	VAL	C	230	33.923	7.831	1.756	1.00	51.45	O
ATOM	3120	N	ASP	C	231	32.566	8.624	0.139	1.00	51.96	N
ATOM	3121	CA	ASP	C	231	33.454	8.279	-0.965	1.00	52.56	C
ATOM	3122	CB	ASP	C	231	32.667	7.720	-2.166	1.00	52.45	C
ATOM	3123	CG	ASP	C	231	31.715	8.746	-2.795	1.00	52.60	C
ATOM	3124	OD1	ASP	C	231	30.682	8.308	-3.347	1.00	53.13	O
ATOM	3125	OD2	ASP	C	231	31.986	9.971	-2.760	1.00	51.76	O
ATOM	3126	C	ASP	C	231	34.306	9.484	-1.366	1.00	53.13	C
ATOM	3127	O	ASP	C	231	34.375	10.480	-0.639	1.00	53.13	O
ATOM	3128	N	GLU	C	232	34.931	9.389	-2.537	1.00	54.00	N
ATOM	3129	CA	GLU	C	232	35.873	10.408	-3.019	1.00	54.69	C
ATOM	3130	CB	GLU	C	232	36.741	9.865	-4.170	1.00	54.83	C
ATOM	3131	CG	GLU	C	232	35.987	9.047	-5.224	1.00	56.25	C
ATOM	3132	CD	GLU	C	232	36.914	8.175	-6.067	1.00	57.94	C
ATOM	3133	OE1	GLU	C	232	37.845	7.565	-5.485	1.00	59.07	O
ATOM	3134	OE2	GLU	C	232	36.706	8.091	-7.306	1.00	58.55	O
ATOM	3135	C	GLU	C	232	35.213	11.738	-3.395	1.00	54.39	C
ATOM	3136	O	GLU	C	232	35.854	12.791	-3.329	1.00	54.43	O
ATOM	3137	N	LYS	C	233	33.942	11.692	-3.780	1.00	54.11	N
ATOM	3138	CA	LYS	C	233	33.210	12.923	-4.062	1.00	53.79	C
ATOM	3139	CB	LYS	C	233	32.370	12.785	-5.336	1.00	53.96	C
ATOM	3140	CG	LYS	C	233	33.225	12.874	-6.597	1.00	54.34	C
ATOM	3141	CD	LYS	C	233	32.426	12.664	-7.867	1.00	55.52	C
ATOM	3142	CE	LYS	C	233	33.362	12.447	-9.053	1.00	55.89	C
ATOM	3143	NZ	LYS	C	233	32.621	12.189	-10.326	1.00	56.05	N
ATOM	3144	C	LYS	C	233	32.395	13.401	-2.855	1.00	53.28	C
ATOM	3145	O	LYS	C	233	31.579	14.308	-2.967	1.00	53.18	O
ATOM	3146	N	GLY	C	234	32.649	12.786	-1.701	1.00	52.89	N

Figure 2 Table 2a - 48

ATOM	3147	CA	GLY	C	234	32.025	13.181	-0.440	1.00	52.14	C
ATOM	3148	C	GLY	C	234	30.565	12.809	-0.322	1.00	51.66	C
ATOM	3149	O	GLY	C	234	29.832	13.414	0.460	1.00	51.32	O
ATOM	3150	N	ARG	C	235	30.152	11.821	-1.115	1.00	51.41	N
ATOM	3151	CA	ARG	C	235	28.815	11.246	-1.035	1.00	51.38	C
ATOM	3152	CB	ARG	C	235	28.419	10.593	-2.353	1.00	51.51	C
ATOM	3153	CG	ARG	C	235	28.044	11.542	-3.458	1.00	52.45	C
ATOM	3154	CD	ARG	C	235	27.823	10.770	-4.750	1.00	53.80	C
ATOM	3155	NE	ARG	C	235	29.086	10.501	-5.435	1.00	55.22	N
ATOM	3156	CZ	ARG	C	235	29.250	9.602	-6.401	1.00	55.80	C
ATOM	3157	NH1	ARG	C	235	28.233	8.851	-6.803	1.00	56.26	N
ATOM	3158	NH2	ARG	C	235	30.442	9.444	-6.959	1.00	55.97	N
ATOM	3159	C	ARG	C	235	28.799	10.183	0.050	1.00	51.17	C
ATOM	3160	O	ARG	C	235	29.684	9.322	0.094	1.00	51.13	O
ATOM	3161	N	VAL	C	236	27.787	10.237	0.917	1.00	50.78	N
ATOM	3162	CA	VAL	C	236	27.671	9.291	2.030	1.00	50.30	C
ATOM	3163	CB	VAL	C	236	26.714	9.824	3.150	1.00	49.96	C
ATOM	3164	CG1	VAL	C	236	25.285	9.900	2.668	1.00	49.39	C
ATOM	3165	CG2	VAL	C	236	26.806	8.970	4.387	1.00	49.73	C
ATOM	3166	C	VAL	C	236	27.276	7.895	1.521	1.00	49.96	C
ATOM	3167	O	VAL	C	236	26.347	7.757	0.726	1.00	49.65	O
ATOM	3168	N	VAL	C	237	28.012	6.880	1.964	1.00	49.91	N
ATOM	3169	CA	VAL	C	237	27.722	5.484	1.604	1.00	50.23	C
ATOM	3170	CB	VAL	C	237	28.838	4.843	0.722	1.00	49.90	C
ATOM	3171	CG1	VAL	C	237	28.889	5.502	-0.635	1.00	49.76	C
ATOM	3172	CG2	VAL	C	237	30.204	4.902	1.410	1.00	49.63	C
ATOM	3173	C	VAL	C	237	27.473	4.610	2.839	1.00	50.61	C
ATOM	3174	O	VAL	C	237	26.926	3.508	2.736	1.00	50.77	O
ATOM	3175	N	ASP	C	238	27.895	5.098	4.001	1.00	50.81	N
ATOM	3176	CA	ASP	C	238	27.659	4.389	5.246	1.00	51.27	C
ATOM	3177	CB	ASP	C	238	28.657	3.234	5.412	1.00	51.37	C
ATOM	3178	CG	ASP	C	238	28.045	2.012	6.094	1.00	51.65	C
ATOM	3179	OD1	ASP	C	238	27.185	2.167	6.988	1.00	52.47	O
ATOM	3180	OD2	ASP	C	238	28.431	0.887	5.734	1.00	50.89	O
ATOM	3181	C	ASP	C	238	27.760	5.342	6.420	1.00	51.62	C
ATOM	3182	O	ASP	C	238	27.930	6.556	6.250	1.00	51.49	O
ATOM	3183	N	ILE	C	239	27.648	4.776	7.614	1.00	52.10	N
ATOM	3184	CA	ILE	C	239	27.711	5.535	8.854	1.00	52.70	C
ATOM	3185	CB	ILE	C	239	26.272	6.006	9.296	1.00	52.48	C
ATOM	3186	CG1	ILE	C	239	26.303	6.801	10.595	1.00	52.45	C
ATOM	3187	CD1	ILE	C	239	26.164	8.255	10.399	1.00	51.47	C
ATOM	3188	CG2	ILE	C	239	25.305	4.845	9.423	1.00	52.63	C
ATOM	3189	C	ILE	C	239	28.441	4.684	9.907	1.00	53.16	C
ATOM	3190	O	ILE	C	239	28.196	3.480	10.020	1.00	53.05	O
ATOM	3191	N	TYR	C	240	29.342	5.312	10.659	1.00	53.86	N
ATOM	3192	CA	TYR	C	240	30.060	4.627	11.729	1.00	54.37	C
ATOM	3193	CB	TYR	C	240	31.573	4.688	11.494	1.00	54.52	C
ATOM	3194	CG	TYR	C	240	32.369	3.723	12.347	1.00	54.60	C
ATOM	3195	CD1	TYR	C	240	33.199	4.183	13.363	1.00	54.04	C
ATOM	3196	CE1	TYR	C	240	33.928	3.303	14.147	1.00	54.86	C
ATOM	3197	CZ	TYR	C	240	33.828	1.940	13.920	1.00	54.99	C
ATOM	3198	OH	TYR	C	240	34.548	1.058	14.699	1.00	53.47	O
ATOM	3199	CE2	TYR	C	240	33.009	1.459	12.918	1.00	54.78	C
ATOM	3200	CD2	TYR	C	240	32.287	2.348	12.138	1.00	54.84	C
ATOM	3201	C	TYR	C	240	29.708	5.219	13.089	1.00	54.87	C
ATOM	3202	O	TYR	C	240	30.047	6.366	13.383	1.00	54.74	O
ATOM	3203	N	SER	C	241	29.025	4.429	13.912	1.00	55.64	N
ATOM	3204	CA	SER	C	241	28.568	4.882	15.226	1.00	56.45	C
ATOM	3205	CB	SER	C	241	27.104	4.487	15.448	1.00	56.47	C
ATOM	3206	OG	SER	C	241	26.546	5.160	16.568	1.00	56.47	O
ATOM	3207	C	SER	C	241	29.435	4.322	16.353	1.00	57.05	C
ATOM	3208	O	SER	C	241	30.177	3.356	16.163	1.00	57.09	O
ATOM	3209	N	LYS	C	242	29.337	4.946	17.524	1.00	57.52	N
ATOM	3210	CA	LYS	C	242	29.957	4.419	18.737	1.00	58.08	C
ATOM	3211	CB	LYS	C	242	29.704	5.360	19.919	1.00	57.91	C
ATOM	3212	CG	LYS	C	242	30.191	6.778	19.690	1.00	57.22	C
ATOM	3213	CD	LYS	C	242	30.117	7.601	20.960	1.00	56.57	C

Figure 2

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ATOM	3214	CE	LYS	C	242	31.399	8.390	21.164	1.00	57.02	C
ATOM	3215	NZ	LYS	C	242	31.154	9.709	21.814	1.00	57.73	N
ATOM	3216	C	LYS	C	242	29.434	3.015	19.052	1.00	58.51	C
ATOM	3217	O	LYS	C	242	30.212	2.079	19.223	1.00	58.41	O
ATOM	3218	N	PHE	C	243	28.112	2.883	19.126	1.00	59.24	N
ATOM	3219	CA	PHE	C	243	27.451	1.586	19.007	1.00	60.12	C
ATOM	3220	CB	PHE	C	243	26.118	1.748	18.269	1.00	60.08	C
ATOM	3221	CG	PHE	C	243	25.221	0.542	18.357	1.00	60.31	C
ATOM	3222	CD1	PHE	C	243	24.073	0.577	19.130	1.00	60.79	C
ATOM	3223	CE1	PHE	C	243	23.234	-0.537	19.214	1.00	60.72	C
ATOM	3224	CZ	PHE	C	243	23.543	-1.694	18.518	1.00	60.17	C
ATOM	3225	CE2	PHE	C	243	24.687	-1.739	17.737	1.00	60.18	C
ATOM	3226	CD2	PHE	C	243	25.517	-0.624	17.655	1.00	60.18	C
ATOM	3227	C	PHE	C	243	28.337	0.571	18.281	1.00	60.77	C
ATOM	3228	O	PHE	C	243	28.705	-0.456	18.845	1.00	60.69	O
ATOM	3229	N	ASP	C	244	28.678	0.868	17.029	1.00	61.83	N
ATOM	3230	CA	ASP	C	244	29.426	-0.066	16.190	1.00	62.60	C
ATOM	3231	CB	ASP	C	244	29.610	0.503	14.779	1.00	62.68	C
ATOM	3232	CG	ASP	C	244	28.317	1.040	14.191	1.00	63.08	C
ATOM	3233	OD1	ASP	C	244	27.255	0.415	14.405	1.00	63.00	O
ATOM	3234	OD2	ASP	C	244	28.365	2.084	13.507	1.00	62.88	O
ATOM	3235	C	ASP	C	244	30.784	-0.381	16.802	1.00	63.12	C
ATOM	3236	O	ASP	C	244	31.647	-0.966	16.146	1.00	63.21	O
ATOM	3237	N	VAL	C	245	30.963	0.005	18.062	1.00	64.02	N
ATOM	3238	CA	VAL	C	245	32.285	0.017	18.684	1.00	64.95	C
ATOM	3239	CB	VAL	C	245	32.661	1.425	19.190	1.00	64.86	C
ATOM	3240	CG1	VAL	C	245	33.971	1.381	19.966	1.00	64.84	C
ATOM	3241	CG2	VAL	C	245	32.757	2.397	18.026	1.00	64.56	C
ATOM	3242	C	VAL	C	245	32.391	-0.989	19.828	1.00	65.43	C
ATOM	3243	O	VAL	C	245	33.447	-1.580	20.037	1.00	65.43	O
ATOM	3244	N	ILE	C	246	31.296	-1.181	20.562	1.00	66.42	N
ATOM	3245	CA	ILE	C	246	31.223	-2.250	21.562	1.00	67.64	C
ATOM	3246	CB	ILE	C	246	29.996	-2.110	22.497	1.00	67.66	C
ATOM	3247	CG1	ILE	C	246	28.872	-1.319	21.818	1.00	67.70	C
ATOM	3248	CD1	ILE	C	246	27.743	-2.191	21.286	1.00	67.40	C
ATOM	3249	CG2	ILE	C	246	30.405	-1.496	23.829	1.00	67.68	C
ATOM	3250	C	ILE	C	246	31.193	-3.630	20.916	1.00	68.28	C
ATOM	3251	O	ILE	C	246	31.315	-4.648	21.599	1.00	68.52	O
ATOM	3252	N	ASN	C	247	31.025	-3.657	19.599	1.00	69.16	N
ATOM	3253	CA	ASN	C	247	31.231	-4.873	18.827	1.00	70.09	C
ATOM	3254	CB	ASN	C	247	30.956	-4.612	17.346	1.00	70.32	C
ATOM	3255	CG	ASN	C	247	31.656	-5.606	16.446	1.00	71.23	C
ATOM	3256	OD1	ASN	C	247	32.716	-5.311	15.882	1.00	72.27	O
ATOM	3257	ND2	ASN	C	247	31.075	-6.801	16.319	1.00	71.62	N
ATOM	3258	C	ASN	C	247	32.641	-5.430	19.007	1.00	70.41	C
ATOM	3259	O	ASN	C	247	32.850	-6.641	18.951	1.00	70.34	O
ATOM	3260	N	LEU	C	248	33.602	-4.536	19.225	1.00	70.94	N
ATOM	3261	CA	LEU	C	248	34.988	-4.927	19.466	1.00	71.52	C
ATOM	3262	CB	LEU	C	248	35.904	-3.702	19.402	1.00	71.39	C
ATOM	3263	CG	LEU	C	248	36.130	-3.056	18.028	1.00	71.45	C
ATOM	3264	CD1	LEU	C	248	35.067	-3.471	17.016	1.00	71.08	C
ATOM	3265	CD2	LEU	C	248	36.191	-1.542	18.149	1.00	70.61	C
ATOM	3266	C	LEU	C	248	35.144	-5.638	20.810	1.00	72.04	C
ATOM	3267	O	LEU	C	248	36.128	-6.342	21.042	1.00	72.00	O
ATOM	3268	N	ALA	C	249	34.165	-5.449	21.690	1.00	72.67	N
ATOM	3269	CA	ALA	C	249	34.156	-6.108	22.993	1.00	73.24	C
ATOM	3270	CB	ALA	C	249	33.444	-5.244	24.038	1.00	73.12	C
ATOM	3271	C	ALA	C	249	33.531	-7.505	22.916	1.00	73.75	C
ATOM	3272	O	ALA	C	249	33.383	-8.183	23.940	1.00	73.92	O
ATOM	3273	N	ALA	C	250	33.168	-7.930	21.704	1.00	74.28	N
ATOM	3274	CA	ALA	C	250	32.695	-9.298	21.476	1.00	74.81	C
ATOM	3275	CB	ALA	C	250	31.705	-9.343	20.309	1.00	74.72	C
ATOM	3276	C	ALA	C	250	33.865	-10.263	21.242	1.00	75.14	C
ATOM	3277	O	ALA	C	250	33.848	-11.397	21.727	1.00	75.10	O
ATOM	3278	N	GLU	C	251	34.874	-9.792	20.506	1.00	75.61	N
ATOM	3279	CA	GLU	C	251	36.063	-10.580	20.143	1.00	75.98	C
ATOM	3280	CB	GLU	C	251	36.783	-9.937	18.949	1.00	75.98	C

Figure 2 Table 2a - 50

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ATOM   3281  CG  GLU C 251      36.822  -8.406  18.998  1.00 76.28      C
ATOM   3282  CD  GLU C 251      37.946  -7.787  18.175  1.00 76.96      C
ATOM   3283  OE1 GLU C 251      38.911  -8.505  17.829  1.00 76.92      O
ATOM   3284  OE2 GLU C 251      37.866  -6.568  17.885  1.00 76.98      O
ATOM   3285  C   GLU C 251      37.044 -10.755  21.308  1.00 76.18      C
ATOM   3286  O   GLU C 251      37.272  -9.824  22.085  1.00 76.16      O
ATOM   3287  N   LYS C 252      37.630 -11.949  21.412  1.00 76.45      N
ATOM   3288  CA  LYS C 252      38.601 -12.264  22.469  1.00 76.68      C
ATOM   3289  CB  LYS C 252      38.537 -13.754  22.823  1.00 76.69      C
ATOM   3290  CG  LYS C 252      37.394 -14.135  23.745  1.00 76.81      C
ATOM   3291  CD  LYS C 252      37.299 -15.644  23.893  1.00 76.72      C
ATOM   3292  CE  LYS C 252      36.395 -16.032  25.050  1.00 77.07      C
ATOM   3293  NZ  LYS C 252      37.035 -15.779  26.375  1.00 77.30      N
ATOM   3294  C   LYS C 252      40.042 -11.869  22.109  1.00 76.86      C
ATOM   3295  O   LYS C 252      40.991 -12.591  22.433  1.00 76.69      O
ATOM   3296  N   THR C 253      40.197 -10.717  21.449  1.00 77.16      N
ATOM   3297  CA  THR C 253      41.518 -10.218  21.033  1.00 77.35      C
ATOM   3298  CB  THR C 253      41.824 -10.513  19.530  1.00 77.38      C
ATOM   3299  OG1 THR C 253      40.702 -10.146  18.715  1.00 77.29      O
ATOM   3300  CG2 THR C 253      42.160 -11.994  19.313  1.00 77.34      C
ATOM   3301  C   THR C 253      41.736  -8.726  21.325  1.00 77.42      C
ATOM   3302  O   THR C 253      42.682  -8.371  22.036  1.00 77.40      O
ATOM   3303  N   TYR C 254      40.860  -7.875  20.777  1.00 77.59      N
ATOM   3304  CA  TYR C 254      40.961  -6.396  20.844  1.00 77.65      C
ATOM   3305  CB  TYR C 254      41.388  -5.902  22.239  1.00 77.81      C
ATOM   3306  CG  TYR C 254      40.257  -5.714  23.226  1.00 78.09      C
ATOM   3307  CD1 TYR C 254      40.090  -6.586  24.308  1.00 78.56      C
ATOM   3308  CE1 TYR C 254      39.046  -6.406  25.223  1.00 78.80      C
ATOM   3309  CZ  TYR C 254      38.166  -5.338  25.052  1.00 78.44      C
ATOM   3310  OH  TYR C 254      37.128  -5.131  25.934  1.00 78.28      O
ATOM   3311  CE2 TYR C 254      38.323  -4.467  23.989  1.00 78.32      C
ATOM   3312  CD2 TYR C 254      39.362  -4.656  23.088  1.00 78.16      C
ATOM   3313  C   TYR C 254      41.878  -5.782  19.777  1.00 77.52      C
ATOM   3314  O   TYR C 254      41.729  -4.605  19.427  1.00 77.52      O
ATOM   3315  N   ASN C 255      42.805  -6.594  19.267  1.00 77.32      N
ATOM   3316  CA  ASN C 255      43.880  -6.154  18.367  1.00 77.10      C
ATOM   3317  CB  ASN C 255      44.936  -7.265  18.227  1.00 77.11      C
ATOM   3318  CG  ASN C 255      45.584  -7.640  19.559  1.00 77.46      C
ATOM   3319  OD1 ASN C 255      45.975  -8.794  19.774  1.00 77.37      O
ATOM   3320  ND2 ASN C 255      45.706  -6.665  20.458  1.00 77.85      N
ATOM   3321  C   ASN C 255      43.441  -5.672  16.977  1.00 76.84      C
ATOM   3322  O   ASN C 255      44.170  -4.930  16.315  1.00 76.82      O
ATOM   3323  N   ASN C 256      42.255  -6.093  16.544  1.00 76.49      N
ATOM   3324  CA  ASN C 256      41.762  -5.781  15.204  1.00 76.23      C
ATOM   3325  CB  ASN C 256      40.670  -6.779  14.793  1.00 76.24      C
ATOM   3326  CG  ASN C 256      41.229  -8.130  14.393  1.00 76.25      C
ATOM   3327  OD1 ASN C 256      41.303  -8.457  13.207  1.00 76.11      O
ATOM   3328  ND2 ASN C 256      41.628  -8.925  15.383  1.00 76.65      N
ATOM   3329  C   ASN C 256      41.259  -4.340  15.030  1.00 76.00      C
ATOM   3330  O   ASN C 256      40.134  -4.125  14.575  1.00 76.01      O
ATOM   3331  N   LEU C 257      42.091  -3.361  15.385  1.00 75.69      N
ATOM   3332  CA  LEU C 257      41.713  -1.947  15.265  1.00 75.29      C
ATOM   3333  CB  LEU C 257      42.062  -1.162  16.539  1.00 75.36      C
ATOM   3334  CG  LEU C 257      41.427  -1.524  17.892  1.00 75.41      C
ATOM   3335  CD1 LEU C 257      41.986  -0.623  18.985  1.00 75.51      C
ATOM   3336  CD2 LEU C 257      39.906  -1.430  17.866  1.00 74.91      C
ATOM   3337  C   LEU C 257      42.355  -1.280  14.051  1.00 75.00      C
ATOM   3338  O   LEU C 257      41.967  -0.173  13.669  1.00 74.97      O
ATOM   3339  N   ASP C 258      43.332  -1.959  13.454  1.00 74.69      N
ATOM   3340  CA  ASP C 258      44.048  -1.433  12.290  1.00 74.45      C
ATOM   3341  CB  ASP C 258      45.430  -2.083  12.157  1.00 74.49      C
ATOM   3342  CG  ASP C 258      46.199  -2.102  13.468  1.00 74.68      C
ATOM   3343  OD1 ASP C 258      46.204  -1.075  14.183  1.00 74.63      O
ATOM   3344  OD2 ASP C 258      46.805  -3.151  13.779  1.00 74.88      O
ATOM   3345  C   ASP C 258      43.257  -1.614  10.997  1.00 74.16      C
ATOM   3346  O   ASP C 258      43.613  -1.042   9.961  1.00 74.22      O
ATOM   3347  N   VAL C 259      42.187  -2.409  11.068  1.00 73.71      N
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Figure 2 Table 2a - 51

ATOM	3348	CA	VAL	C	259	41.311	-2.679	9.921	1.00	73.27	C
ATOM	3349	CB	VAL	C	259	40.315	-3.843	10.207	1.00	73.32	C
ATOM	3350	CG1	VAL	C	259	41.060	-5.140	10.547	1.00	73.28	C
ATOM	3351	CG2	VAL	C	259	39.330	-3.472	11.317	1.00	73.30	C
ATOM	3352	C	VAL	C	259	40.534	-1.430	9.484	1.00	72.97	C
ATOM	3353	O	VAL	C	259	40.304	-0.522	10.290	1.00	72.79	O
ATOM	3354	N	SER	C	260	40.131	-1.397	8.212	1.00	72.59	N
ATOM	3355	CA	SER	C	260	39.367	-0.271	7.669	1.00	72.20	C
ATOM	3356	CB	SER	C	260	39.265	-0.351	6.137	1.00	72.22	C
ATOM	3357	OG	SER	C	260	38.037	-0.929	5.711	1.00	72.06	O
ATOM	3358	C	SER	C	260	37.975	-0.167	8.297	1.00	71.99	C
ATOM	3359	O	SER	C	260	37.503	-1.087	8.971	1.00	71.99	O
ATOM	3360	N	VAL	C	261	37.324	0.964	8.068	1.00	71.69	N
ATOM	3361	CA	VAL	C	261	36.009	1.221	8.628	1.00	71.44	C
ATOM	3362	CB	VAL	C	261	35.663	2.740	8.573	1.00	71.19	C
ATOM	3363	CG1	VAL	C	261	34.890	3.101	7.309	1.00	70.81	C
ATOM	3364	CG2	VAL	C	261	34.906	3.151	9.811	1.00	71.21	C
ATOM	3365	C	VAL	C	261	34.948	0.346	7.941	1.00	71.47	C
ATOM	3366	O	VAL	C	261	34.012	-0.129	8.592	1.00	71.52	O
ATOM	3367	N	THR	C	262	35.114	0.131	6.635	1.00	71.42	N
ATOM	3368	CA	THR	C	262	34.231	-0.741	5.868	1.00	71.41	C
ATOM	3369	CB	THR	C	262	34.667	-0.840	4.387	1.00	71.49	C
ATOM	3370	OG1	THR	C	262	34.429	0.414	3.738	1.00	71.15	O
ATOM	3371	CG2	THR	C	262	33.891	-1.935	3.657	1.00	71.33	C
ATOM	3372	C	THR	C	262	34.186	-2.126	6.499	1.00	71.43	C
ATOM	3373	O	THR	C	262	33.109	-2.628	6.822	1.00	71.45	O
ATOM	3374	N	LYS	C	263	35.355	-2.734	6.677	1.00	71.45	N
ATOM	3375	CA	LYS	C	263	35.441	-4.094	7.200	1.00	71.59	C
ATOM	3376	CB	LYS	C	263	36.886	-4.597	7.154	1.00	71.48	C
ATOM	3377	CG	LYS	C	263	37.014	-6.110	7.238	1.00	72.03	C
ATOM	3378	CD	LYS	C	263	38.430	-6.571	6.929	1.00	72.34	C
ATOM	3379	CE	LYS	C	263	38.502	-8.087	6.826	1.00	72.44	C
ATOM	3380	NZ	LYS	C	263	39.895	-8.569	6.610	1.00	72.36	N
ATOM	3381	C	LYS	C	263	34.895	-4.176	8.624	1.00	71.60	C
ATOM	3382	O	LYS	C	263	34.320	-5.191	9.018	1.00	71.55	O
ATOM	3383	N	ALA	C	264	35.087	-3.107	9.376	1.00	71.85	N
ATOM	3384	CA	ALA	C	264	34.585	-3.022	10.737	1.00	72.04	C
ATOM	3385	CB	ALA	C	264	35.022	-1.760	11.358	1.00	71.96	C
ATOM	3386	C	ALA	C	264	33.084	-3.118	10.802	1.00	72.22	C
ATOM	3387	O	ALA	C	264	32.527	-3.529	11.808	1.00	72.12	O
ATOM	3388	N	LEU	C	265	32.424	-2.732	9.712	1.00	72.45	N
ATOM	3389	CA	LEU	C	265	30.971	-2.608	9.697	1.00	72.61	C
ATOM	3390	CB	LEU	C	265	30.546	-1.362	8.915	1.00	72.27	C
ATOM	3391	CG	LEU	C	265	30.778	-0.018	9.610	1.00	71.81	C
ATOM	3392	CD1	LEU	C	265	30.735	1.118	8.604	1.00	71.03	C
ATOM	3393	CD2	LEU	C	265	29.762	0.207	10.722	1.00	70.94	C
ATOM	3394	C	LEU	C	265	30.306	-3.852	9.114	1.00	73.01	C
ATOM	3395	O	LEU	C	265	29.145	-4.138	9.408	1.00	73.00	O
ATOM	3396	N	GLN	C	266	31.048	-4.586	8.288	1.00	73.55	N
ATOM	3397	CA	GLN	C	266	30.593	-5.883	7.791	1.00	74.20	C
ATOM	3398	CB	GLN	C	266	31.693	-6.567	6.978	1.00	74.24	C
ATOM	3399	CG	GLN	C	266	31.860	-6.010	5.572	1.00	74.61	C
ATOM	3400	CD	GLN	C	266	33.243	-6.275	4.998	1.00	75.05	C
ATOM	3401	OE1	GLN	C	266	33.527	-5.919	3.854	1.00	75.04	O
ATOM	3402	NE2	GLN	C	266	34.110	-6.902	5.793	1.00	74.98	N
ATOM	3403	C	GLN	C	266	30.163	-6.776	8.948	1.00	74.44	C
ATOM	3404	O	GLN	C	266	29.127	-7.439	8.881	1.00	74.33	O
ATOM	3405	N	HIS	C	267	30.974	-6.792	10.001	1.00	74.98	N
ATOM	3406	CA	HIS	C	267	30.517	-6.378	11.318	1.00	75.59	C
ATOM	3407	CB	HIS	C	267	31.605	-6.516	12.367	1.00	75.64	C
ATOM	3408	CG	HIS	C	267	31.698	-7.887	12.960	1.00	76.09	C
ATOM	3409	ND1	HIS	C	267	31.741	-8.109	14.320	1.00	76.21	N
ATOM	3410	CE1	HIS	C	267	31.816	-9.408	14.551	1.00	76.27	C
ATOM	3411	NE2	HIS	C	267	31.821	-10.038	13.389	1.00	76.33	N
ATOM	3412	CD2	HIS	C	267	31.746	-9.110	12.379	1.00	76.19	C
ATOM	3413	C	HIS	C	267	29.199	-6.973	11.782	1.00	75.89	C
ATOM	3414	O	HIS	C	267	29.159	-7.816	12.680	1.00	75.94	O

Figure 2

Table 2a - 52

ATOM	3415	N	ARG	C	268	28.116	-6.521	11.151	1.00	76.27	N
ATOM	3416	CA	ARG	C	268	27.170	-5.625	11.813	1.00	76.64	C
ATOM	3417	CB	ARG	C	268	26.562	-4.657	10.794	1.00	76.53	C
ATOM	3418	CG	ARG	C	268	26.550	-3.206	11.246	1.00	76.74	C
ATOM	3419	CD	ARG	C	268	25.442	-2.424	10.554	1.00	76.85	C
ATOM	3420	NE	ARG	C	268	25.938	-1.650	9.419	1.00	76.47	N
ATOM	3421	CZ	ARG	C	268	26.118	-0.332	9.431	1.00	75.94	C
ATOM	3422	NH1	ARG	C	268	25.840	0.371	10.522	1.00	75.63	N
ATOM	3423	NH2	ARG	C	268	26.574	0.284	8.351	1.00	75.94	N
ATOM	3424	C	ARG	C	268	26.059	-6.382	12.533	1.00	76.96	C
ATOM	3425	O	ARG	C	268	25.420	-5.845	13.441	1.00	76.94	O
ATOM	3426	N	SER	C	269	25.837	-7.628	12.125	1.00	77.31	N
ATOM	3427	CA	SER	C	269	24.546	-8.282	12.320	1.00	77.58	C
ATOM	3428	CB	SER	C	269	24.442	-8.885	13.728	1.00	77.61	C
ATOM	3429	OG	SER	C	269	23.494	-8.186	14.523	1.00	77.49	O
ATOM	3430	C	SER	C	269	23.391	-7.315	12.063	1.00	77.78	C
ATOM	3431	O	SER	C	269	23.171	-6.370	12.824	1.00	77.77	O
ATOM	3432	N	HIS	C	270	22.667	-7.557	10.975	1.00	78.03	N
ATOM	3433	CA	HIS	C	270	21.252	-7.210	10.885	1.00	78.27	C
ATOM	3434	CB	HIS	C	270	20.894	-6.118	11.898	1.00	78.42	C
ATOM	3435	CG	HIS	C	270	19.770	-6.490	12.814	1.00	78.87	C
ATOM	3436	ND1	HIS	C	270	18.506	-6.798	12.356	1.00	79.40	N
ATOM	3437	CE1	HIS	C	270	17.726	-7.088	13.382	1.00	79.32	C
ATOM	3438	NE2	HIS	C	270	18.438	-6.978	14.490	1.00	79.42	N
ATOM	3439	CD2	HIS	C	270	19.719	-6.605	14.163	1.00	79.20	C
ATOM	3440	C	HIS	C	270	20.902	-6.753	9.471	1.00	78.26	C
ATOM	3441	O	HIS	C	270	21.236	-7.419	8.489	1.00	78.26	O
ATOM	3442	N	TYR	C	271	20.218	-5.619	9.383	1.00	78.15	N
ATOM	3443	CA	TYR	C	271	20.419	-4.676	8.291	1.00	77.86	C
ATOM	3444	CB	TYR	C	271	19.572	-5.061	7.076	1.00	78.10	C
ATOM	3445	CG	TYR	C	271	20.382	-5.556	5.897	1.00	78.63	C
ATOM	3446	CD1	TYR	C	271	21.761	-5.724	5.996	1.00	79.08	C
ATOM	3447	CE1	TYR	C	271	22.506	-6.176	4.921	1.00	79.15	C
ATOM	3448	CZ	TYR	C	271	21.874	-6.469	3.729	1.00	79.17	C
ATOM	3449	OH	TYR	C	271	22.611	-6.920	2.659	1.00	79.02	O
ATOM	3450	CE2	TYR	C	271	20.506	-6.312	3.605	1.00	78.98	C
ATOM	3451	CD2	TYR	C	271	19.769	-5.858	4.686	1.00	78.70	C
ATOM	3452	C	TYR	C	271	20.088	-3.262	8.758	1.00	77.46	C
ATOM	3453	O	TYR	C	271	19.496	-3.078	9.823	1.00	77.49	O
ATOM	3454	N	PHE	C	272	20.471	-2.263	7.968	1.00	76.83	N
ATOM	3455	CA	PHE	C	272	20.667	-2.420	6.544	1.00	76.00	C
ATOM	3456	CB	PHE	C	272	22.139	-2.350	6.174	1.00	76.13	C
ATOM	3457	CG	PHE	C	272	22.768	-1.017	6.469	1.00	76.48	C
ATOM	3458	CD1	PHE	C	272	22.699	-0.470	7.743	1.00	76.82	C
ATOM	3459	CE1	PHE	C	272	23.270	0.761	8.019	1.00	76.43	C
ATOM	3460	CZ	PHE	C	272	23.919	1.459	7.018	1.00	76.31	C
ATOM	3461	CE2	PHE	C	272	23.993	0.928	5.744	1.00	76.52	C
ATOM	3462	CD2	PHE	C	272	23.417	-0.304	5.474	1.00	76.86	C
ATOM	3463	C	PHE	C	272	19.836	-1.451	5.717	1.00	75.13	C
ATOM	3464	O	PHE	C	272	18.760	-1.023	6.142	1.00	75.12	O
ATOM	3465	N	GLU	C	273	20.336	-1.116	4.529	1.00	73.87	N
ATOM	3466	CA	GLU	C	273	19.502	-0.654	3.442	1.00	72.58	C
ATOM	3467	CB	GLU	C	273	18.203	-0.049	3.952	1.00	72.87	C
ATOM	3468	CG	GLU	C	273	17.698	1.098	3.075	1.00	73.65	C
ATOM	3469	CD	GLU	C	273	17.515	0.698	1.607	1.00	74.76	C
ATOM	3470	OE1	GLU	C	273	18.294	-0.128	1.089	1.00	75.06	O
ATOM	3471	OE2	GLU	C	273	16.586	1.217	0.962	1.00	74.85	O
ATOM	3472	C	GLU	C	273	20.275	0.433	2.786	1.00	71.19	C
ATOM	3473	O	GLU	C	273	20.729	0.296	1.653	1.00	71.37	O
ATOM	3474	N	GLY	C	274	20.388	1.527	3.528	1.00	69.26	N
ATOM	3475	CA	GLY	C	274	21.591	2.332	3.546	1.00	66.86	C
ATOM	3476	C	GLY	C	274	21.532	3.239	4.739	1.00	65.22	C
ATOM	3477	O	GLY	C	274	20.901	2.902	5.716	1.00	65.05	O
ATOM	3478	N	VAL	C	275	22.186	4.388	4.661	1.00	63.60	N
ATOM	3479	CA	VAL	C	275	22.127	5.355	5.738	1.00	62.00	C
ATOM	3480	CB	VAL	C	275	23.392	6.224	5.864	1.00	61.79	C
ATOM	3481	CG1	VAL	C	275	24.196	6.193	4.621	1.00	62.09	C

Figure 2 Table 2a - 53

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ATOM   3482  CG2 VAL C 275      23.048   7.605   6.220  1.00 60.82      C
ATOM   3483  C   VAL C 275      20.889   6.195   5.641  1.00 61.07      C
ATOM   3484  O   VAL C 275      20.392   6.462   4.568  1.00 61.42      O
ATOM   3485  N   LEU C 276      20.371   6.590   6.782  1.00 59.62      N
ATOM   3486  CA  LEU C 276      19.123   7.288   6.820  1.00 58.49      C
ATOM   3487  CB  LEU C 276      18.364   6.915   8.073  1.00 58.33      C
ATOM   3488  CG  LEU C 276      17.649   5.586   7.970  1.00 59.65      C
ATOM   3489  CD1 LEU C 276      17.774   4.834   9.264  1.00 60.41      C
ATOM   3490  CD2 LEU C 276      16.207   5.810   7.623  1.00 60.23      C
ATOM   3491  C   LEU C 276      19.363   8.781   6.745  1.00 57.58      C
ATOM   3492  O   LEU C 276      20.117   9.332   7.527  1.00 56.93      O
ATOM   3493  N   LYS C 277      18.712   9.415   5.778  1.00 56.69      N
ATOM   3494  CA  LYS C 277      19.145  10.696   5.267  1.00 55.88      C
ATOM   3495  CB  LYS C 277      19.606  10.558   3.824  1.00 56.04      C
ATOM   3496  CG  LYS C 277      20.983  10.002   3.690  1.00 56.89      C
ATOM   3497  CD  LYS C 277      21.309   9.708   2.270  1.00 58.61      C
ATOM   3498  CE  LYS C 277      20.363   8.703   1.686  1.00 58.92      C
ATOM   3499  NZ  LYS C 277      21.110   7.710   0.910  1.00 60.12      N
ATOM   3500  C   LYS C 277      18.028  11.688   5.326  1.00 55.03      C
ATOM   3501  O   LYS C 277      16.905  11.337   5.562  1.00 55.07      O
ATOM   3502  N   CYS C 278      18.344  12.939   5.082  1.00 53.81      N
ATOM   3503  CA  CYS C 278      17.313  13.943   4.909  1.00 52.84      C
ATOM   3504  CB  CYS C 278      16.765  14.391   6.264  1.00 52.59      C
ATOM   3505  SG  CYS C 278      17.975  15.227   7.304  1.00 53.39      S
ATOM   3506  C   CYS C 278      17.853  15.140   4.126  1.00 52.04      C
ATOM   3507  O   CYS C 278      19.037  15.195   3.789  1.00 51.77      O
ATOM   3508  N   TYR C 279      16.978  16.099   3.848  1.00 51.15      N
ATOM   3509  CA  TYR C 279      17.381  17.323   3.171  1.00 50.31      C
ATOM   3510  CB  TYR C 279      16.694  17.446   1.822  1.00 49.25      C
ATOM   3511  CG  TYR C 279      16.764  16.187   1.014  1.00 48.87      C
ATOM   3512  CD1 TYR C 279      15.712  15.274   1.023  1.00 49.26      C
ATOM   3513  CE1 TYR C 279      15.776  14.104   0.282  1.00 49.31      C
ATOM   3514  CZ  TYR C 279      16.909  13.843  -0.472  1.00 49.29      C
ATOM   3515  OH  TYR C 279      16.977  12.693  -1.215  1.00 50.98      O
ATOM   3516  CE2 TYR C 279      17.967  14.729  -0.492  1.00 47.51      C
ATOM   3517  CD2 TYR C 279      17.890  15.892   0.249  1.00 47.89      C
ATOM   3518  C   TYR C 279      17.066  18.528   4.037  1.00 50.12      C
ATOM   3519  O   TYR C 279      16.186  18.472   4.895  1.00 49.88      O
ATOM   3520  N   LEU C 280      17.808  19.605   3.790  1.00 50.14      N
ATOM   3521  CA  LEU C 280      17.717  20.862   4.526  1.00 49.91      C
ATOM   3522  CB  LEU C 280      18.681  21.871   3.905  1.00 50.82      C
ATOM   3523  CG  LEU C 280      20.077  22.130   4.450  1.00 52.29      C
ATOM   3524  CD1 LEU C 280      20.803  22.930   3.389  1.00 56.09      C
ATOM   3525  CD2 LEU C 280      19.987  22.939   5.728  1.00 54.97      C
ATOM   3526  C   LEU C 280      16.346  21.500   4.470  1.00 49.22      C
ATOM   3527  O   LEU C 280      16.019  22.324   5.318  1.00 49.39      O
ATOM   3528  N   HIS C 281      15.568  21.156   3.450  1.00 48.20      N
ATOM   3529  CA  HIS C 281      14.322  21.860   3.151  1.00 47.38      C
ATOM   3530  CB  HIS C 281      14.263  22.223   1.669  1.00 46.74      C
ATOM   3531  CG  HIS C 281      15.342  23.165   1.253  1.00 46.21      C
ATOM   3532  ND1 HIS C 281      15.227  24.533   1.385  1.00 46.78      N
ATOM   3533  CE1 HIS C 281      16.334  25.109   0.950  1.00 46.27      C
ATOM   3534  NE2 HIS C 281      17.163  24.163   0.546  1.00 46.31      N
ATOM   3535  CD2 HIS C 281      16.569  22.938   0.732  1.00 46.12      C
ATOM   3536  C   HIS C 281      13.091  21.070   3.566  1.00 47.21      C
ATOM   3537  O   HIS C 281      11.968  21.519   3.364  1.00 47.57      O
ATOM   3538  N   GLU C 282      13.315  19.896   4.139  1.00 46.99      N
ATOM   3539  CA  GLU C 282      12.261  19.127   4.810  1.00 47.12      C
ATOM   3540  CB  GLU C 282      12.752  17.705   5.148  1.00 46.82      C
ATOM   3541  CG  GLU C 282      13.304  16.945   3.946  1.00 47.39      C
ATOM   3542  CD  GLU C 282      13.145  15.448   4.066  1.00 48.38      C
ATOM   3543  OE1 GLU C 282      12.004  14.962   3.940  1.00 47.59      O
ATOM   3544  OE2 GLU C 282      14.169  14.757   4.268  1.00 48.20      O
ATOM   3545  C   GLU C 282      11.763  19.831   6.077  1.00 46.93      C
ATOM   3546  O   GLU C 282      12.552  20.449   6.811  1.00 47.15      O
ATOM   3547  N   THR C 283      10.455  19.741   6.320  1.00 46.26      N
ATOM   3548  CA  THR C 283       9.847  20.336   7.501  1.00 45.64      C
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Figure 2 Table 2a - 54

ATOM	3549	CB	THR	C	283	8.301	20.305	7.447	1.00	45.82	C
ATOM	3550	OG1	THR	C	283	7.850	18.944	7.542	1.00	45.39	O
ATOM	3551	CG2	THR	C	283	7.748	20.976	6.179	1.00	43.21	C
ATOM	3552	C	THR	C	283	10.282	19.563	8.749	1.00	45.86	C
ATOM	3553	O	THR	C	283	10.563	18.358	8.667	1.00	45.64	O
ATOM	3554	N	LEU	C	284	10.312	20.262	9.888	1.00	45.43	N
ATOM	3555	CA	LEU	C	284	10.590	19.675	11.185	1.00	45.66	C
ATOM	3556	CB	LEU	C	284	10.317	20.669	12.311	1.00	45.93	C
ATOM	3557	CG	LEU	C	284	11.266	20.789	13.512	1.00	45.92	C
ATOM	3558	CD1	LEU	C	284	10.499	21.155	14.774	1.00	45.36	C
ATOM	3559	CD2	LEU	C	284	12.126	19.572	13.737	1.00	45.30	C
ATOM	3560	C	LEU	C	284	9.706	18.468	11.424	1.00	46.19	C
ATOM	3561	O	LEU	C	284	10.184	17.431	11.906	1.00	46.31	O
ATOM	3562	N	GLU	C	285	8.419	18.612	11.109	1.00	46.14	N
ATOM	3563	CA	GLU	C	285	7.480	17.504	11.259	1.00	46.71	C
ATOM	3564	CB	GLU	C	285	6.075	17.904	10.809	1.00	46.92	C
ATOM	3565	CG	GLU	C	285	5.102	16.743	10.776	1.00	48.42	C
ATOM	3566	CD	GLU	C	285	3.661	17.185	10.827	1.00	50.70	C
ATOM	3567	OE1	GLU	C	285	3.245	17.981	9.966	1.00	51.42	O
ATOM	3568	OE2	GLU	C	285	2.936	16.724	11.730	1.00	53.20	O
ATOM	3569	C	GLU	C	285	7.940	16.250	10.514	1.00	46.55	C
ATOM	3570	O	GLU	C	285	7.969	15.155	11.104	1.00	46.51	O
ATOM	3571	N	ALA	C	286	8.295	16.413	9.233	1.00	45.99	N
ATOM	3572	CA	ALA	C	286	8.772	15.288	8.419	1.00	45.89	C
ATOM	3573	CB	ALA	C	286	9.099	15.726	6.996	1.00	45.26	C
ATOM	3574	C	ALA	C	286	9.975	14.587	9.054	1.00	45.82	C
ATOM	3575	O	ALA	C	286	10.051	13.363	9.046	1.00	46.09	O
ATOM	3576	N	ILE	C	287	10.899	15.374	9.596	1.00	45.90	N
ATOM	3577	CA	ILE	C	287	12.133	14.851	10.170	1.00	45.96	C
ATOM	3578	CB	ILE	C	287	13.217	15.964	10.320	1.00	46.52	C
ATOM	3579	CG1	ILE	C	287	13.912	16.218	8.988	1.00	46.73	C
ATOM	3580	CD1	ILE	C	287	13.386	17.363	8.285	1.00	50.52	C
ATOM	3581	CG2	ILE	C	287	14.304	15.554	11.320	1.00	46.85	C
ATOM	3582	C	ILE	C	287	11.887	14.127	11.497	1.00	45.49	C
ATOM	3583	O	ILE	C	287	12.448	13.063	11.730	1.00	45.41	O
ATOM	3584	N	ILE	C	288	11.037	14.690	12.349	1.00	45.17	N
ATOM	3585	CA	ILE	C	288	10.722	14.057	13.615	1.00	45.53	C
ATOM	3586	CB	ILE	C	288	9.783	14.924	14.495	1.00	45.54	C
ATOM	3587	CG1	ILE	C	288	10.534	16.118	15.069	1.00	45.60	C
ATOM	3588	CD1	ILE	C	288	9.647	17.118	15.817	1.00	45.60	C
ATOM	3589	CG2	ILE	C	288	9.185	14.091	15.650	1.00	46.64	C
ATOM	3590	C	ILE	C	288	10.121	12.679	13.337	1.00	45.58	C
ATOM	3591	O	ILE	C	288	10.555	11.680	13.924	1.00	45.77	O
ATOM	3592	N	ASN	C	289	9.153	12.624	12.418	1.00	45.31	N
ATOM	3593	CA	ASN	C	289	8.494	11.369	12.062	1.00	44.87	C
ATOM	3594	CB	ASN	C	289	7.395	11.581	11.021	1.00	44.75	C
ATOM	3595	CG	ASN	C	289	6.230	12.400	11.540	1.00	45.00	C
ATOM	3596	OD1	ASN	C	289	6.192	12.810	12.705	1.00	46.89	O
ATOM	3597	ND2	ASN	C	289	5.268	12.644	10.671	1.00	44.47	N
ATOM	3598	C	ASN	C	289	9.474	10.334	11.547	1.00	44.84	C
ATOM	3599	O	ASN	C	289	9.395	9.155	11.930	1.00	45.60	O
ATOM	3600	N	ARG	C	290	10.394	10.753	10.688	1.00	44.29	N
ATOM	3601	CA	ARG	C	290	11.372	9.812	10.134	1.00	44.69	C
ATOM	3602	CB	ARG	C	290	12.192	10.467	9.020	1.00	44.10	C
ATOM	3603	CG	ARG	C	290	13.122	9.515	8.328	1.00	44.03	C
ATOM	3604	CD	ARG	C	290	13.705	10.086	7.062	1.00	45.23	C
ATOM	3605	NE	ARG	C	290	12.684	10.789	6.288	1.00	46.74	N
ATOM	3606	CZ	ARG	C	290	12.900	11.927	5.642	1.00	45.85	C
ATOM	3607	NH1	ARG	C	290	14.106	12.478	5.664	1.00	45.78	N
ATOM	3608	NH2	ARG	C	290	11.913	12.513	4.980	1.00	46.28	N
ATOM	3609	C	ARG	C	290	12.291	9.232	11.219	1.00	44.85	C
ATOM	3610	O	ARG	C	290	12.525	8.015	11.275	1.00	44.90	O
ATOM	3611	N	LEU	C	291	12.785	10.121	12.076	1.00	45.28	N
ATOM	3612	CA	LEU	C	291	13.646	9.783	13.198	1.00	46.10	C
ATOM	3613	CB	LEU	C	291	14.038	11.072	13.862	1.00	46.55	C
ATOM	3614	CG	LEU	C	291	15.497	11.379	14.168	1.00	47.79	C
ATOM	3615	CD1	LEU	C	291	16.465	10.410	13.523	1.00	46.60	C

Figure 2 Table 2a - 55

ATOM	3616	CD2	LEU	C	291	15.735	12.816	13.738	1.00	46.77	C
ATOM	3617	C	LEU	C	291	12.966	8.863	14.220	1.00	46.65	C
ATOM	3618	O	LEU	C	291	13.498	7.798	14.567	1.00	46.54	O
ATOM	3619	N	VAL	C	292	11.782	9.266	14.686	1.00	47.07	N
ATOM	3620	CA	VAL	C	292	10.989	8.441	15.592	1.00	47.13	C
ATOM	3621	CB	VAL	C	292	9.647	9.115	15.979	1.00	47.10	C
ATOM	3622	CG1	VAL	C	292	8.715	8.119	16.685	1.00	46.90	C
ATOM	3623	CG2	VAL	C	292	9.886	10.326	16.862	1.00	45.85	C
ATOM	3624	C	VAL	C	292	10.736	7.044	15.016	1.00	48.14	C
ATOM	3625	O	VAL	C	292	10.985	6.031	15.704	1.00	48.56	O
ATOM	3626	N	GLU	C	293	10.248	6.952	13.780	1.00	48.69	N
ATOM	3627	CA	GLU	C	293	9.946	5.599	13.264	1.00	49.76	C
ATOM	3628	CB	GLU	C	293	8.803	5.571	12.226	1.00	49.72	C
ATOM	3629	CG	GLU	C	293	9.118	6.072	10.836	1.00	51.44	C
ATOM	3630	CD	GLU	C	293	7.878	6.653	10.140	1.00	53.94	C
ATOM	3631	OE1	GLU	C	293	6.856	5.932	10.054	1.00	54.97	O
ATOM	3632	OE2	GLU	C	293	7.925	7.829	9.675	1.00	56.96	O
ATOM	3633	C	GLU	C	293	11.172	4.779	12.835	1.00	49.45	C
ATOM	3634	O	GLU	C	293	11.080	3.569	12.728	1.00	49.65	O
ATOM	3635	N	ALA	C	294	12.311	5.443	12.635	1.00	49.63	N
ATOM	3636	CA	ALA	C	294	13.564	4.768	12.292	1.00	49.47	C
ATOM	3637	CB	ALA	C	294	14.442	5.662	11.439	1.00	49.46	C
ATOM	3638	C	ALA	C	294	14.322	4.330	13.532	1.00	49.52	C
ATOM	3639	O	ALA	C	294	15.182	3.453	13.452	1.00	49.61	O
ATOM	3640	N	GLU	C	295	14.013	4.952	14.667	1.00	49.66	N
ATOM	3641	CA	GLU	C	295	14.567	4.542	15.978	1.00	50.18	C
ATOM	3642	CB	GLU	C	295	14.106	3.124	16.383	1.00	49.94	C
ATOM	3643	CG	GLU	C	295	12.612	2.992	16.624	1.00	51.66	C
ATOM	3644	CD	GLU	C	295	12.158	1.548	16.733	1.00	55.37	C
ATOM	3645	OE1	GLU	C	295	11.418	1.106	15.825	1.00	58.91	O
ATOM	3646	OE2	GLU	C	295	12.536	0.840	17.708	1.00	56.03	O
ATOM	3647	C	GLU	C	295	16.091	4.659	16.000	1.00	49.62	C
ATOM	3648	O	GLU	C	295	16.798	3.791	16.522	1.00	49.33	O
ATOM	3649	N	VAL	C	296	16.570	5.770	15.446	1.00	49.42	N
ATOM	3650	CA	VAL	C	296	17.983	6.025	15.274	1.00	49.36	C
ATOM	3651	CB	VAL	C	296	18.345	5.834	13.771	1.00	49.70	C
ATOM	3652	CG1	VAL	C	296	18.536	7.160	13.029	1.00	49.13	C
ATOM	3653	CG2	VAL	C	296	19.528	4.896	13.621	1.00	50.16	C
ATOM	3654	C	VAL	C	296	18.328	7.417	15.841	1.00	49.58	C
ATOM	3655	O	VAL	C	296	17.450	8.284	15.952	1.00	49.30	O
ATOM	3656	N	HIS	C	297	19.590	7.631	16.207	1.00	49.64	N
ATOM	3657	CA	HIS	C	297	19.966	8.849	16.937	1.00	49.88	C
ATOM	3658	CB	HIS	C	297	21.218	8.627	17.806	1.00	50.66	C
ATOM	3659	CG	HIS	C	297	21.425	9.679	18.857	1.00	54.27	C
ATOM	3660	ND1	HIS	C	297	21.049	9.507	20.175	1.00	56.97	N
ATOM	3661	CE1	HIS	C	297	21.353	10.593	20.869	1.00	58.34	C
ATOM	3662	NE2	HIS	C	297	21.904	11.472	20.045	1.00	59.66	N
ATOM	3663	CD2	HIS	C	297	21.970	10.921	18.785	1.00	57.84	C
ATOM	3664	C	HIS	C	297	20.099	10.100	16.059	1.00	49.05	C
ATOM	3665	O	HIS	C	297	19.922	11.222	16.544	1.00	49.15	O
ATOM	3666	N	ARG	C	298	20.386	9.924	14.768	1.00	48.27	N
ATOM	3667	CA	ARG	C	298	20.495	11.068	13.858	1.00	47.25	C
ATOM	3668	CB	ARG	C	298	21.872	11.749	13.971	1.00	47.28	C
ATOM	3669	CG	ARG	C	298	22.970	11.235	13.008	1.00	47.59	C
ATOM	3670	CD	ARG	C	298	23.469	9.855	13.394	1.00	47.54	C
ATOM	3671	NE	ARG	C	298	24.013	9.825	14.749	1.00	46.11	N
ATOM	3672	CZ	ARG	C	298	23.986	8.760	15.541	1.00	45.36	C
ATOM	3673	NH1	ARG	C	298	23.428	7.631	15.124	1.00	46.59	N
ATOM	3674	NH2	ARG	C	298	24.505	8.830	16.756	1.00	44.70	N
ATOM	3675	C	ARG	C	298	20.242	10.730	12.404	1.00	46.83	C
ATOM	3676	O	ARG	C	298	20.360	9.574	11.991	1.00	45.95	O
ATOM	3677	N	LEU	C	299	19.925	11.777	11.640	1.00	46.51	N
ATOM	3678	CA	LEU	C	299	19.879	11.718	10.195	1.00	46.42	C
ATOM	3679	CB	LEU	C	299	18.607	12.382	9.680	1.00	46.27	C
ATOM	3680	CG	LEU	C	299	17.258	11.846	10.187	1.00	47.04	C
ATOM	3681	CD1	LEU	C	299	16.088	12.677	9.600	1.00	47.74	C
ATOM	3682	CD2	LEU	C	299	17.074	10.341	9.888	1.00	45.38	C

Figure 2 Table 2a - 56

ATOM	3683	C	LEU	C	299	21.101	12.412	9.608	1.00	46.60	C
ATOM	3684	O	LEU	C	299	21.551	13.449	10.120	1.00	46.92	O
ATOM	3685	N	VAL	C	300	21.636	11.856	8.527	1.00	46.52	N
ATOM	3686	CA	VAL	C	300	22.662	12.563	7.777	1.00	46.64	C
ATOM	3687	CB	VAL	C	300	23.617	11.611	7.029	1.00	46.76	C
ATOM	3688	CG1	VAL	C	300	24.732	12.417	6.354	1.00	45.50	C
ATOM	3689	CG2	VAL	C	300	24.203	10.540	7.980	1.00	46.42	C
ATOM	3690	C	VAL	C	300	21.994	13.497	6.769	1.00	47.14	C
ATOM	3691	O	VAL	C	300	21.250	13.037	5.891	1.00	47.45	O
ATOM	3692	N	VAL	C	301	22.265	14.796	6.896	1.00	47.08	N
ATOM	3693	CA	VAL	C	301	21.713	15.808	5.992	1.00	47.23	C
ATOM	3694	CB	VAL	C	301	21.682	17.231	6.634	1.00	47.16	C
ATOM	3695	CG1	VAL	C	301	20.993	18.216	5.712	1.00	45.24	C
ATOM	3696	CG2	VAL	C	301	20.982	17.187	7.986	1.00	45.91	C
ATOM	3697	C	VAL	C	301	22.497	15.843	4.683	1.00	47.84	C
ATOM	3698	O	VAL	C	301	23.728	15.913	4.669	1.00	47.72	O
ATOM	3699	N	VAL	C	302	21.772	15.830	3.576	1.00	48.61	N
ATOM	3700	CA	VAL	C	302	22.379	15.541	2.291	1.00	49.34	C
ATOM	3701	CB	VAL	C	302	22.145	14.014	1.986	1.00	49.40	C
ATOM	3702	CG1	VAL	C	302	21.487	13.753	0.659	1.00	48.56	C
ATOM	3703	CG2	VAL	C	302	23.436	13.200	2.210	1.00	48.49	C
ATOM	3704	C	VAL	C	302	21.881	16.530	1.223	1.00	50.21	C
ATOM	3705	O	VAL	C	302	20.859	17.180	1.419	1.00	50.54	O
ATOM	3706	N	ASP	C	303	22.611	16.688	0.120	1.00	51.06	N
ATOM	3707	CA	ASP	C	303	22.112	17.520	-0.982	1.00	51.91	C
ATOM	3708	CB	ASP	C	303	23.208	18.443	-1.525	1.00	51.69	C
ATOM	3709	CG	ASP	C	303	24.220	17.715	-2.405	1.00	52.62	C
ATOM	3710	OD1	ASP	C	303	24.240	16.460	-2.442	1.00	52.84	O
ATOM	3711	OD2	ASP	C	303	25.001	18.413	-3.082	1.00	54.46	O
ATOM	3712	C	ASP	C	303	21.527	16.642	-2.099	1.00	52.62	C
ATOM	3713	O	ASP	C	303	21.420	15.424	-1.929	1.00	52.46	O
ATOM	3714	N	GLU	C	304	21.165	17.269	-3.227	1.00	53.07	N
ATOM	3715	CA	GLU	C	304	20.609	16.584	-4.403	1.00	54.03	C
ATOM	3716	CB	GLU	C	304	20.606	17.532	-5.618	1.00	54.33	C
ATOM	3717	CG	GLU	C	304	19.658	18.724	-5.545	1.00	56.80	C
ATOM	3718	CD	GLU	C	304	20.103	19.816	-4.564	1.00	61.10	C
ATOM	3719	OE1	GLU	C	304	21.228	19.740	-4.012	1.00	61.84	O
ATOM	3720	OE2	GLU	C	304	19.311	20.765	-4.345	1.00	62.76	O
ATOM	3721	C	GLU	C	304	21.383	15.318	-4.795	1.00	54.03	C
ATOM	3722	O	GLU	C	304	20.827	14.395	-5.405	1.00	53.97	O
ATOM	3723	N	HIS	C	305	22.667	15.291	-4.453	1.00	54.09	N
ATOM	3724	CA	HIS	C	305	23.582	14.306	-5.008	1.00	54.10	C
ATOM	3725	CB	HIS	C	305	24.690	15.017	-5.796	1.00	54.06	C
ATOM	3726	CG	HIS	C	305	24.183	15.947	-6.858	1.00	54.38	C
ATOM	3727	ND1	HIS	C	305	23.662	15.503	-8.055	1.00	54.44	N
ATOM	3728	CE1	HIS	C	305	23.311	16.542	-8.794	1.00	54.06	C
ATOM	3729	NE2	HIS	C	305	23.595	17.645	-8.124	1.00	53.62	N
ATOM	3730	CD2	HIS	C	305	24.142	17.301	-6.911	1.00	54.86	C
ATOM	3731	C	HIS	C	305	24.191	13.374	-3.954	1.00	54.15	C
ATOM	3732	O	HIS	C	305	25.132	12.636	-4.256	1.00	54.39	O
ATOM	3733	N	ASP	C	306	23.640	13.397	-2.737	1.00	53.81	N
ATOM	3734	CA	ASP	C	306	24.114	12.576	-1.603	1.00	53.86	C
ATOM	3735	CB	ASP	C	306	24.208	11.088	-1.968	1.00	54.50	C
ATOM	3736	CG	ASP	C	306	22.871	10.367	-1.846	1.00	56.87	C
ATOM	3737	OD1	ASP	C	306	21.894	10.950	-1.303	1.00	58.78	O
ATOM	3738	OD2	ASP	C	306	22.806	9.202	-2.299	1.00	58.80	O
ATOM	3739	C	ASP	C	306	25.416	13.038	-0.943	1.00	53.05	C
ATOM	3740	O	ASP	C	306	25.980	12.338	-0.103	1.00	52.79	O
ATOM	3741	N	VAL	C	307	25.881	14.214	-1.333	1.00	52.24	N
ATOM	3742	CA	VAL	C	307	27.014	14.846	-0.687	1.00	51.83	C
ATOM	3743	CB	VAL	C	307	27.552	16.029	-1.560	1.00	51.76	C
ATOM	3744	CG1	VAL	C	307	28.721	16.742	-0.883	1.00	51.28	C
ATOM	3745	CG2	VAL	C	307	27.975	15.520	-2.923	1.00	50.72	C
ATOM	3746	C	VAL	C	307	26.536	15.319	0.691	1.00	51.61	C
ATOM	3747	O	VAL	C	307	25.468	15.935	0.794	1.00	51.51	O
ATOM	3748	N	VAL	C	308	27.296	15.012	1.745	1.00	51.43	N
ATOM	3749	CA	VAL	C	308	26.845	15.398	3.087	1.00	51.67	C

Figure 2 Table 2a - 57

ATOM	3750	CB	VAL	C	308	27.427	14.545	4.291	1.00	51.49	C
ATOM	3751	CG1	VAL	C	308	27.962	13.193	3.845	1.00	50.91	C
ATOM	3752	CG2	VAL	C	308	28.474	15.300	5.046	1.00	51.79	C
ATOM	3753	C	VAL	C	308	27.008	16.900	3.317	1.00	51.80	C
ATOM	3754	O	VAL	C	308	28.043	17.495	3.011	1.00	51.87	O
ATOM	3755	N	LYS	C	309	25.951	17.494	3.849	1.00	51.90	N
ATOM	3756	CA	LYS	C	309	25.894	18.909	4.108	1.00	52.20	C
ATOM	3757	CB	LYS	C	309	24.698	19.501	3.377	1.00	52.57	C
ATOM	3758	CG	LYS	C	309	25.028	19.975	1.955	1.00	56.36	C
ATOM	3759	CD	LYS	C	309	23.764	20.557	1.318	1.00	62.40	C
ATOM	3760	CE	LYS	C	309	23.998	21.894	0.615	1.00	65.34	C
ATOM	3761	NZ	LYS	C	309	22.675	22.568	0.393	1.00	67.95	N
ATOM	3762	C	LYS	C	309	25.812	19.176	5.605	1.00	51.75	C
ATOM	3763	O	LYS	C	309	26.093	20.276	6.062	1.00	51.96	O
ATOM	3764	N	GLY	C	310	25.435	18.161	6.373	1.00	51.07	N
ATOM	3765	CA	GLY	C	310	25.351	18.307	7.818	1.00	50.23	C
ATOM	3766	C	GLY	C	310	24.720	17.128	8.532	1.00	49.73	C
ATOM	3767	O	GLY	C	310	24.605	16.020	7.990	1.00	48.74	O
ATOM	3768	N	ILE	C	311	24.295	17.387	9.761	1.00	49.47	N
ATOM	3769	CA	ILE	C	311	23.724	16.355	10.605	1.00	49.33	C
ATOM	3770	CB	ILE	C	311	24.838	15.618	11.429	1.00	49.71	C
ATOM	3771	CG1	ILE	C	311	25.353	14.438	10.586	1.00	50.25	C
ATOM	3772	CD1	ILE	C	311	26.744	14.027	10.855	1.00	52.66	C
ATOM	3773	CG2	ILE	C	311	24.300	15.075	12.758	1.00	49.42	C
ATOM	3774	C	ILE	C	311	22.593	16.897	11.461	1.00	49.11	C
ATOM	3775	O	ILE	C	311	22.664	18.023	11.967	1.00	48.54	O
ATOM	3776	N	VAL	C	312	21.529	16.108	11.575	1.00	49.32	N
ATOM	3777	CA	VAL	C	312	20.449	16.437	12.486	1.00	49.93	C
ATOM	3778	CB	VAL	C	312	19.142	16.886	11.770	1.00	49.70	C
ATOM	3779	CG1	VAL	C	312	18.644	15.837	10.806	1.00	50.81	C
ATOM	3780	CG2	VAL	C	312	18.069	17.221	12.797	1.00	50.36	C
ATOM	3781	C	VAL	C	312	20.222	15.318	13.489	1.00	50.01	C
ATOM	3782	O	VAL	C	312	19.817	14.215	13.145	1.00	49.96	O
ATOM	3783	N	SER	C	313	20.487	15.644	14.738	1.00	50.32	N
ATOM	3784	CA	SER	C	313	20.499	14.688	15.825	1.00	51.00	C
ATOM	3785	CB	SER	C	313	21.793	14.882	16.606	1.00	50.99	C
ATOM	3786	OG	SER	C	313	21.767	14.197	17.839	1.00	55.48	O
ATOM	3787	C	SER	C	313	19.291	14.889	16.736	1.00	50.77	C
ATOM	3788	O	SER	C	313	18.676	15.960	16.723	1.00	50.95	O
ATOM	3789	N	LEU	C	314	18.958	13.860	17.524	1.00	50.53	N
ATOM	3790	CA	LEU	C	314	17.921	13.968	18.559	1.00	50.38	C
ATOM	3791	CB	LEU	C	314	17.816	12.669	19.365	1.00	50.37	C
ATOM	3792	CG	LEU	C	314	17.393	11.417	18.603	1.00	49.89	C
ATOM	3793	CD1	LEU	C	314	17.665	10.161	19.428	1.00	48.43	C
ATOM	3794	CD2	LEU	C	314	15.935	11.514	18.190	1.00	49.14	C
ATOM	3795	C	LEU	C	314	18.151	15.154	19.518	1.00	50.44	C
ATOM	3796	O	LEU	C	314	17.205	15.862	19.874	1.00	49.85	O
ATOM	3797	N	SER	C	315	19.407	15.353	19.926	1.00	50.56	N
ATOM	3798	CA	SER	C	315	19.791	16.487	20.756	1.00	51.19	C
ATOM	3799	CB	SER	C	315	21.304	16.504	21.007	1.00	51.01	C
ATOM	3800	OG	SER	C	315	21.830	15.202	21.210	1.00	52.24	O
ATOM	3801	C	SER	C	315	19.372	17.805	20.087	1.00	51.74	C
ATOM	3802	O	SER	C	315	18.830	18.696	20.759	1.00	52.13	O
ATOM	3803	N	ASP	C	316	19.617	17.925	18.776	1.00	51.28	N
ATOM	3804	CA	ASP	C	316	19.235	19.121	18.041	1.00	51.05	C
ATOM	3805	CB	ASP	C	316	19.641	19.015	16.569	1.00	51.03	C
ATOM	3806	CG	ASP	C	316	21.145	19.020	16.360	1.00	50.94	C
ATOM	3807	OD1	ASP	C	316	21.839	19.832	17.018	1.00	50.71	O
ATOM	3808	OD2	ASP	C	316	21.627	18.229	15.504	1.00	48.49	O
ATOM	3809	C	ASP	C	316	17.727	19.366	18.143	1.00	50.99	C
ATOM	3810	O	ASP	C	316	17.291	20.471	18.458	1.00	51.52	O
ATOM	3811	N	ILE	C	317	16.941	18.330	17.877	1.00	50.65	N
ATOM	3812	CA	ILE	C	317	15.489	18.450	17.884	1.00	50.67	C
ATOM	3813	CB	ILE	C	317	14.824	17.164	17.371	1.00	50.29	C
ATOM	3814	CG1	ILE	C	317	15.054	17.019	15.867	1.00	51.16	C
ATOM	3815	CD1	ILE	C	317	14.465	15.758	15.292	1.00	53.11	C
ATOM	3816	CG2	ILE	C	317	13.338	17.174	17.674	1.00	49.83	C

Figure 2 Table 2a - 58

ATOM	3817	C	ILE	C	317	14.944	18.784	19.271	1.00	51.03	C
ATOM	3818	O	ILE	C	317	14.072	19.642	19.412	1.00	51.19	O
ATOM	3819	N	LEU	C	318	15.458	18.104	20.291	1.00	51.35	N
ATOM	3820	CA	LEU	C	318	14.956	18.272	21.646	1.00	51.78	C
ATOM	3821	CB	LEU	C	318	15.412	17.113	22.538	1.00	52.21	C
ATOM	3822	CG	LEU	C	318	14.337	16.117	22.985	1.00	51.52	C
ATOM	3823	CD1	LEU	C	318	13.484	15.656	21.816	1.00	52.41	C
ATOM	3824	CD2	LEU	C	318	14.976	14.933	23.669	1.00	52.42	C
ATOM	3825	C	LEU	C	318	15.388	19.610	22.239	1.00	52.24	C
ATOM	3826	O	LEU	C	318	14.689	20.186	23.072	1.00	51.97	O
ATOM	3827	N	GLN	C	319	16.542	20.102	21.801	1.00	53.09	N
ATOM	3828	CA	GLN	C	319	16.973	21.451	22.142	1.00	53.98	C
ATOM	3829	CB	GLN	C	319	18.439	21.666	21.765	1.00	54.16	C
ATOM	3830	CG	GLN	C	319	18.879	23.120	21.833	1.00	56.65	C
ATOM	3831	CD	GLN	C	319	20.328	23.276	22.236	1.00	59.70	C
ATOM	3832	OE1	GLN	C	319	21.222	22.699	21.616	1.00	61.83	O
ATOM	3833	NE2	GLN	C	319	20.570	24.062	23.281	1.00	60.03	N
ATOM	3834	C	GLN	C	319	16.099	22.494	21.455	1.00	53.86	C
ATOM	3835	O	GLN	C	319	15.819	23.551	22.020	1.00	53.62	O
ATOM	3836	N	ALA	C	320	15.672	22.191	20.235	1.00	54.42	N
ATOM	3837	CA	ALA	C	320	14.761	23.071	19.510	1.00	55.27	C
ATOM	3838	CB	ALA	C	320	14.624	22.622	18.072	1.00	55.34	C
ATOM	3839	C	ALA	C	320	13.395	23.120	20.186	1.00	55.92	C
ATOM	3840	O	ALA	C	320	12.818	24.196	20.360	1.00	55.82	O
ATOM	3841	N	LEU	C	321	12.894	21.951	20.577	1.00	56.44	N
ATOM	3842	CA	LEU	C	321	11.542	21.830	21.113	1.00	57.15	C
ATOM	3843	CB	LEU	C	321	11.106	20.362	21.138	1.00	56.82	C
ATOM	3844	CG	LEU	C	321	10.868	19.701	19.778	1.00	55.57	C
ATOM	3845	CD1	LEU	C	321	10.491	18.246	19.963	1.00	54.99	C
ATOM	3846	CD2	LEU	C	321	9.793	20.447	18.998	1.00	54.41	C
ATOM	3847	C	LEU	C	321	11.422	22.433	22.506	1.00	57.98	C
ATOM	3848	O	LEU	C	321	10.333	22.815	22.931	1.00	57.74	O
ATOM	3849	N	VAL	C	322	12.546	22.518	23.209	1.00	59.66	N
ATOM	3850	CA	VAL	C	322	12.554	22.979	24.601	1.00	61.40	C
ATOM	3851	CB	VAL	C	322	13.510	22.122	25.486	1.00	61.05	C
ATOM	3852	CG1	VAL	C	322	14.881	22.776	25.639	1.00	61.00	C
ATOM	3853	CG2	VAL	C	322	12.891	21.869	26.837	1.00	60.76	C
ATOM	3854	C	VAL	C	322	12.844	24.478	24.747	1.00	62.94	C
ATOM	3855	O	VAL	C	322	12.349	25.122	25.667	1.00	63.01	O
ATOM	3856	N	LEU	C	323	13.647	25.030	23.844	1.00	65.07	N
ATOM	3857	CA	LEU	C	323	13.815	26.477	23.778	1.00	67.52	C
ATOM	3858	CB	LEU	C	323	15.186	26.853	23.199	1.00	67.53	C
ATOM	3859	CG	LEU	C	323	16.438	26.438	23.987	1.00	67.96	C
ATOM	3860	CD1	LEU	C	323	17.678	26.704	23.150	1.00	68.51	C
ATOM	3861	CD2	LEU	C	323	16.541	27.131	25.354	1.00	68.06	C
ATOM	3862	C	LEU	C	323	12.693	27.032	22.913	1.00	69.00	C
ATOM	3863	O	LEU	C	323	12.714	28.200	22.521	1.00	69.35	O
ATOM	3864	N	THR	C	324	11.715	26.167	22.640	1.00	70.86	N
ATOM	3865	CA	THR	C	324	10.590	26.418	21.729	1.00	72.42	C
ATOM	3866	CB	THR	C	324	9.790	27.690	22.090	1.00	72.46	C
ATOM	3867	OG1	THR	C	324	9.532	27.710	23.506	1.00	72.41	O
ATOM	3868	CG2	THR	C	324	8.468	27.726	21.313	1.00	72.59	C
ATOM	3869	C	THR	C	324	11.032	26.408	20.258	1.00	73.55	C
ATOM	3870	O	THR	C	324	11.941	27.155	19.868	1.00	74.09	O
ATOM	3871	N	GLY	C	325	10.392	25.543	19.466	1.00	74.47	N
ATOM	3872	CA	GLY	C	325	10.721	25.315	18.047	1.00	75.45	C
ATOM	3873	C	GLY	C	325	11.596	26.348	17.343	1.00	76.09	C
ATOM	3874	O	GLY	C	325	11.162	27.485	17.089	1.00	76.11	O
ATOM	3875	N	GLY	C	326	12.834	25.937	17.047	1.00	76.57	N
ATOM	3876	CA	GLY	C	326	13.802	26.725	16.263	1.00	76.82	C
ATOM	3877	C	GLY	C	326	14.055	28.142	16.751	1.00	76.97	C
ATOM	3878	O	GLY	C	326	14.246	29.053	15.942	1.00	77.00	O
ATOM	3879	O2A	ATP	E	1	23.451	5.448	17.772	1.00	47.20	O
ATOM	3880	PA	ATP	E	1	22.290	4.556	17.404	1.00	45.56	P
ATOM	3881	O1A	ATP	E	1	20.995	5.150	16.928	1.00	47.36	O
ATOM	3882	O3A	ATP	E	1	21.927	3.477	18.540	1.00	49.08	O
ATOM	3883	PB	ATP	E	1	21.736	3.882	20.079	1.00	49.02	P

Figure 2 Table 2a - 59

ATOM	3884	O1B	ATP	E	1	20.781	2.937	20.774	1.00	47.36	O
ATOM	3885	O2B	ATP	E	1	23.124	4.091	20.657	1.00	50.69	O
ATOM	3886	O3B	ATP	E	1	21.041	5.322	19.796	1.00	51.70	O
ATOM	3887	PG	ATP	E	1	20.703	6.389	20.961	1.00	52.64	P
ATOM	3888	O3G	ATP	E	1	19.863	5.606	21.961	1.00	51.28	O
ATOM	3889	O2G	ATP	E	1	22.087	6.834	21.401	1.00	52.41	O
ATOM	3890	O1G	ATP	E	1	19.932	7.469	20.232	1.00	53.65	O
ATOM	3891	O5*	ATP	E	1	22.827	3.517	16.309	1.00	46.73	O
ATOM	3892	C5*	ATP	E	1	22.355	2.166	16.300	1.00	44.80	C
ATOM	3893	C4*	ATP	E	1	22.779	1.546	14.984	1.00	44.78	C
ATOM	3894	C3*	ATP	E	1	24.277	1.726	14.756	1.00	45.46	C
ATOM	3895	O3*	ATP	E	1	24.895	0.453	14.481	1.00	46.89	O
ATOM	3896	C2*	ATP	E	1	24.401	2.677	13.581	1.00	44.21	C
ATOM	3897	O2*	ATP	E	1	25.338	2.234	12.594	1.00	44.82	O
ATOM	3898	C1*	ATP	E	1	23.011	2.752	12.977	1.00	43.51	C
ATOM	3899	O4*	ATP	E	1	22.093	2.247	13.946	1.00	44.44	O
ATOM	3900	N9	ATP	E	1	22.712	4.162	12.605	1.00	43.67	N
ATOM	3901	C4	ATP	E	1	22.299	4.537	11.391	1.00	42.78	C
ATOM	3902	C5	ATP	E	1	22.149	6.002	11.455	1.00	41.93	C
ATOM	3903	N7	ATP	E	1	22.498	6.395	12.699	1.00	41.84	N
ATOM	3904	C8	ATP	E	1	22.840	5.270	13.377	1.00	43.01	C
ATOM	3905	N3	ATP	E	1	22.011	3.865	10.236	1.00	42.22	N
ATOM	3906	C2	ATP	E	1	21.592	4.504	9.140	1.00	40.80	C
ATOM	3907	N1	ATP	E	1	21.438	5.844	9.135	1.00	42.78	N
ATOM	3908	C6	ATP	E	1	21.685	6.647	10.208	1.00	41.25	C
ATOM	3909	N6	ATP	E	1	21.508	7.983	10.136	1.00	40.46	N
ATOM	3910	O2A	ATP	E	2	26.293	9.465	28.074	1.00	38.81	O
ATOM	3911	PA	ATP	E	2	27.293	9.779	26.996	1.00	35.62	P
ATOM	3912	O1A	ATP	E	2	26.913	10.752	25.937	1.00	37.53	O
ATOM	3913	O3A	ATP	E	2	27.793	8.341	26.430	1.00	42.51	O
ATOM	3914	PB	ATP	E	2	26.987	7.680	25.206	1.00	46.30	P
ATOM	3915	O1B	ATP	E	2	27.132	6.177	24.980	1.00	47.74	O
ATOM	3916	O2B	ATP	E	2	25.599	8.193	25.517	1.00	50.44	O
ATOM	3917	O3B	ATP	E	2	27.708	8.537	24.050	1.00	51.03	O
ATOM	3918	PG	ATP	E	2	27.146	8.730	22.558	1.00	55.95	P
ATOM	3919	O3G	ATP	E	2	26.920	7.311	22.036	1.00	55.86	O
ATOM	3920	O2G	ATP	E	2	25.892	9.563	22.763	1.00	56.10	O
ATOM	3921	O1G	ATP	E	2	28.295	9.445	21.862	1.00	57.47	O
ATOM	3922	O5*	ATP	E	2	28.732	10.247	27.519	1.00	35.82	O
ATOM	3923	C5*	ATP	E	2	28.946	11.407	28.296	1.00	33.17	C
ATOM	3924	C4*	ATP	E	2	30.061	11.136	29.305	1.00	30.68	C
ATOM	3925	C3*	ATP	E	2	30.463	9.677	29.481	1.00	30.94	C
ATOM	3926	O3*	ATP	E	2	31.862	9.622	29.777	1.00	33.47	O
ATOM	3927	C2*	ATP	E	2	29.769	9.191	30.728	1.00	28.62	C
ATOM	3928	O2*	ATP	E	2	30.652	8.427	31.558	1.00	27.90	O
ATOM	3929	C1*	ATP	E	2	29.374	10.447	31.468	1.00	25.65	C
ATOM	3930	O4*	ATP	E	2	29.575	11.545	30.574	1.00	29.39	O
ATOM	3931	N9	ATP	E	2	27.934	10.363	31.784	1.00	22.79	N
ATOM	3932	C4	ATP	E	2	27.377	10.848	32.886	1.00	20.73	C
ATOM	3933	C5	ATP	E	2	25.944	10.558	32.774	1.00	20.69	C
ATOM	3934	N7	ATP	E	2	25.768	9.921	31.596	1.00	20.94	N
ATOM	3935	C8	ATP	E	2	26.977	9.819	31.001	1.00	21.20	C
ATOM	3936	N3	ATP	E	2	27.835	11.499	33.977	1.00	20.15	N
ATOM	3937	C2	ATP	E	2	27.003	11.872	34.968	1.00	20.41	C
ATOM	3938	N1	ATP	E	2	25.677	11.641	34.945	1.00	21.03	N
ATOM	3939	C6	ATP	E	2	25.089	11.010	33.897	1.00	21.10	C
ATOM	3940	N6	ATP	E	2	23.759	10.782	33.895	1.00	21.55	N
ATOM	3941	O3P	AMP	F	1	23.825	13.664	20.038	1.00	43.46	O
ATOM	3942	P	AMP	F	1	24.957	13.611	19.016	1.00	45.70	P
ATOM	3943	O1P	AMP	F	1	24.630	12.781	17.801	1.00	44.41	O
ATOM	3944	O2P	AMP	F	1	26.364	13.337	19.480	1.00	45.11	O
ATOM	3945	O5*	AMP	F	1	25.094	15.135	18.527	1.00	43.67	O
ATOM	3946	C5*	AMP	F	1	25.759	16.148	19.295	1.00	41.64	C
ATOM	3947	C4*	AMP	F	1	25.823	17.468	18.507	1.00	39.61	C
ATOM	3948	C3*	AMP	F	1	24.557	17.736	17.720	1.00	38.10	C
ATOM	3949	O3*	AMP	F	1	24.378	19.145	17.652	1.00	36.42	O
ATOM	3950	C2*	AMP	F	1	24.833	17.168	16.339	1.00	37.63	C

Figure 2 Table 2a - 60

ATOM	3951	O2*	AMP	F	1	24.130	17.881	15.307	1.00	37.33	O
ATOM	3952	C1*	AMP	F	1	26.341	17.297	16.207	1.00	36.76	C
ATOM	3953	O4*	AMP	F	1	26.866	17.410	17.524	1.00	39.11	O
ATOM	3954	N9	AMP	F	1	26.953	16.157	15.476	1.00	36.51	N
ATOM	3955	C4	AMP	F	1	27.986	16.288	14.641	1.00	36.45	C
ATOM	3956	C5	AMP	F	1	28.280	14.943	14.117	1.00	36.10	C
ATOM	3957	N7	AMP	F	1	27.392	14.106	14.684	1.00	34.69	N
ATOM	3958	C8	AMP	F	1	26.601	14.855	15.495	1.00	35.96	C
ATOM	3959	N3	AMP	F	1	28.751	17.338	14.246	1.00	36.89	N
ATOM	3960	C2	AMP	F	1	29.757	17.165	13.380	1.00	36.88	C
ATOM	3961	N1	AMP	F	1	30.078	15.968	12.855	1.00	36.99	N
ATOM	3962	C6	AMP	F	1	29.410	14.839	13.166	1.00	36.17	C
ATOM	3963	N6	AMP	F	1	29.774	13.659	12.611	1.00	36.65	N
ATOM	3964	MG	MG	G	1	26.238	5.466	22.898	1.00	60.66	MG
ATOM	3965	MG	MG	G	2	19.394	3.519	22.429	1.00	52.69	MG
ATOM	3966	O	HOH	W	1	18.365	7.233	49.589	1.00	28.13	O
ATOM	3967	O	HOH	W	2	18.597	-23.574	40.765	1.00	31.51	O
ATOM	3968	O	HOH	W	3	21.124	5.661	64.000	1.00	34.38	O
ATOM	3969	O	HOH	W	4	11.500	3.725	23.300	1.00	29.36	O
ATOM	3970	O	HOH	W	5	26.946	-15.014	39.994	1.00	27.28	O
ATOM	3971	O	HOH	W	6	-5.416	12.058	18.236	1.00	30.67	O
ATOM	3972	O	HOH	W	7	15.708	-8.796	25.642	1.00	38.52	O
ATOM	3973	O	HOH	W	8	7.357	-3.037	28.982	1.00	30.44	O
ATOM	3974	O	HOH	W	9	11.875	5.980	18.355	1.00	28.24	O
ATOM	3975	O	HOH	W	10	16.167	-12.527	36.431	1.00	28.03	O
ATOM	3976	O	HOH	W	11	10.525	-24.153	38.673	1.00	27.72	O
ATOM	3977	O	HOH	W	12	8.947	-4.831	44.348	1.00	26.17	O
ATOM	3978	O	HOH	W	13	13.180	-11.302	41.503	1.00	20.34	O
ATOM	3979	O	HOH	W	14	9.757	15.920	3.126	1.00	11.50	O
ATOM	3980	O	HOH	W	15	16.935	4.399	23.677	1.00	35.50	O
ATOM	3981	O	HOH	W	16	24.375	-4.416	61.189	1.00	23.42	O
ATOM	3982	O	HOH	W	17	8.854	18.207	4.521	1.00	23.47	O
ATOM	3983	O	HOH	W	18	10.313	-0.644	34.033	1.00	21.80	O
ATOM	3984	O	HOH	W	19	33.489	-1.381	15.111	1.00	34.84	O
ATOM	3985	O	HOH	W	20	20.585	2.187	-0.807	1.00	34.59	O
ATOM	3986	O	HOH	W	21	1.353	13.445	34.721	1.00	33.49	O
ATOM	3987	O	HOH	W	22	21.322	19.423	36.496	1.00	28.27	O
ATOM	3988	O	HOH	W	23	21.650	-0.367	32.410	1.00	26.84	O
ATOM	3989	O	HOH	W	24	2.997	14.460	17.482	1.00	28.85	O
ATOM	3990	O	HOH	W	25	25.201	-2.873	24.147	1.00	31.78	O
ATOM	3991	O	HOH	W	26	-2.523	11.266	20.638	1.00	32.39	O
ATOM	3992	O	HOH	W	27	33.679	-18.268	51.119	1.00	29.69	O
ATOM	3993	O	HOH	W	28	16.953	7.964	3.575	1.00	42.44	O
ATOM	3994	O	HOH	W	29	23.483	6.612	0.664	1.00	31.50	O
ATOM	3995	O	HOH	W	30	10.576	13.787	44.066	1.00	27.38	O
ATOM	3996	O	HOH	W	31	21.142	11.157	49.333	1.00	35.50	O
ATOM	3997	O	HOH	W	32	44.575	-4.872	13.362	1.00	35.74	O
ATOM	3998	O	HOH	W	33	32.508	22.889	6.976	1.00	20.66	O
ATOM	3999	O	HOH	W	34	32.846	0.046	45.174	1.00	23.53	O
ATOM	4000	O	HOH	W	35	13.153	25.994	3.108	1.00	18.21	O
ATOM	4001	O	HOH	W	36	12.076	32.803	27.670	1.00	36.94	O
ATOM	4002	O	HOH	W	37	7.528	-6.948	50.770	1.00	23.91	O
ATOM	4003	O	HOH	W	38	15.030	15.328	40.438	1.00	30.99	O
ATOM	4004	O	HOH	W	39	23.496	-29.067	62.499	1.00	23.52	O
ATOM	4005	O	HOH	W	40	9.214	11.828	5.570	1.00	28.24	O
ATOM	4006	O	HOH	W	41	22.740	19.870	21.010	1.00	30.47	O
ATOM	4007	O	HOH	W	42	32.891	6.861	34.906	1.00	27.00	O
ATOM	4008	O	HOH	W	43	23.541	-9.961	66.116	1.00	32.55	O
ATOM	4009	O	HOH	W	44	29.729	-5.330	50.062	1.00	44.15	O
ATOM	4010	O	HOH	W	45	12.718	-16.098	51.097	1.00	24.41	O
ATOM	4011	O	HOH	W	46	16.900	1.727	31.317	1.00	25.57	O
ATOM	4012	O	HOH	W	47	16.945	-0.899	40.690	1.00	21.76	O
ATOM	4013	O	HOH	W	48	16.447	-16.487	45.955	1.00	23.77	O
ATOM	4014	O	HOH	W	49	20.267	22.675	16.504	1.00	29.79	O
ATOM	4015	O	HOH	W	50	40.739	13.589	15.197	1.00	26.92	O
ATOM	4016	O	HOH	W	51	20.688	3.213	27.842	1.00	36.44	O
ATOM	4017	O	HOH	W	52	21.484	-0.989	11.839	1.00	53.09	O

Figure 2

Table 2a - 61

ATOM	4018	O	HOH W	53	54.811	-1.899	21.012	1.00	29.19	O
ATOM	4019	O	HOH W	54	27.511	-11.744	31.524	1.00	33.12	O
ATOM	4020	O	HOH W	55	40.871	-13.836	40.773	1.00	28.61	O
ATOM	4021	O	HOH W	56	14.971	-4.049	40.688	1.00	18.21	O
ATOM	4022	O	HOH W	57	10.535	-0.144	38.953	1.00	24.27	O
ATOM	4023	O	HOH W	58	28.445	11.683	21.829	1.00	35.41	O
ATOM	4024	O	HOH W	59	17.425	3.033	28.668	1.00	31.74	O
ATOM	4025	O	HOH W	60	8.323	-28.381	55.815	1.00	24.02	O
ATOM	4026	O	HOH W	61	9.711	19.041	38.121	1.00	27.30	O
ATOM	4027	O	HOH W	62	14.891	8.168	17.257	1.00	21.35	O
ATOM	4028	O	HOH W	63	46.575	-10.617	21.946	1.00	38.56	O
ATOM	4029	O	HOH W	64	13.807	-2.784	46.892	1.00	40.44	O
ATOM	4030	O	HOH W	65	30.981	10.593	46.295	1.00	35.22	O
ATOM	4031	O	HOH W	66	6.722	-29.417	54.137	1.00	33.62	O
ATOM	4032	O	HOH W	67	26.914	13.754	21.635	1.00	24.71	O
ATOM	4033	O	HOH W	68	16.920	5.589	2.360	1.00	37.87	O
ATOM	4034	O	HOH W	69	15.442	6.988	0.244	1.00	43.75	O
ATOM	4035	O	HOH W	70	12.633	-7.449	31.376	1.00	34.44	O
ATOM	4036	O	HOH W	71	12.524	-6.229	29.203	1.00	36.89	O
ATOM	4037	O	HOH W	72	24.070	7.854	20.110	1.00	20.69	O
ATOM	4038	O	HOH W	73	30.401	20.740	6.493	1.00	33.71	O
ATOM	4039	O	HOH W	74	30.643	18.776	5.006	1.00	24.92	O
ATOM	4040	O	HOH W	75	5.780	1.574	44.698	1.00	25.59	O
ATOM	4041	O	HOH W	76	6.060	3.931	45.838	1.00	34.69	O
ATOM	4042	O	HOH W	77	7.359	6.188	46.809	1.00	29.58	O
ATOM	4043	O	HOH W	78	1.906	-26.243	54.544	1.00	38.92	O
ATOM	4044	O	HOH W	79	4.135	-26.077	53.540	1.00	32.05	O
ATOM	4045	O	HOH W	80	14.983	-2.831	29.065	1.00	34.83	O
ATOM	4046	O	HOH W	81	38.017	-2.242	46.028	1.00	30.56	O
ATOM	4047	O	HOH W	82	1.955	29.043	29.008	1.00	42.28	O
ATOM	4048	O	HOH W	83	55.394	1.015	18.272	1.00	18.21	O
ATOM	4049	O	HOH W	84	36.989	-7.754	38.685	1.00	20.23	O
ATOM	4050	O	HOH W	85	32.820	-7.168	45.406	1.00	28.63	O
ATOM	4051	O	HOH W	86	21.773	6.449	-3.742	1.00	29.92	O
ATOM	4052	O	HOH W	87	12.503	8.528	18.894	1.00	20.66	O
ATOM	4053	O	HOH W	88	2.732	-24.050	36.691	1.00	40.86	O
ATOM	4054	O	HOH W	89	14.476	-1.673	41.810	1.00	23.71	O
ATOM	4055	O	HOH W	90	10.326	-17.821	49.529	1.00	25.15	O
ATOM	4056	O	HOH W	91	15.076	5.894	27.482	1.00	22.23	O
ATOM	4057	O	HOH W	92	42.653	10.095	14.682	1.00	21.56	O
ATOM	4058	O	HOH W	93	19.056	0.637	42.087	1.00	22.21	O
ATOM	4059	O	HOH W	94	16.362	-14.085	67.349	1.00	23.87	O
ATOM	4060	O	HOH W	95	16.775	6.650	-1.773	1.00	39.95	O
ATOM	4061	O	HOH W	96	34.926	-21.568	52.375	1.00	27.45	O
ATOM	4062	O	HOH W	97	8.596	24.632	21.357	1.00	29.51	O
ATOM	4063	O	HOH W	98	17.623	-32.090	58.938	1.00	36.98	O
ATOM	4064	O	HOH W	99	-3.218	23.600	13.574	1.00	27.32	O
ATOM	4065	O	HOH W	100	22.570	-4.293	62.585	1.00	30.20	O
ATOM	4066	O	HOH W	101	24.648	-21.768	64.224	1.00	20.89	O
ATOM	4067	O	HOH W	102	16.036	-0.879	65.466	1.00	30.14	O
ATOM	4068	O	HOH W	103	-1.786	-30.031	56.378	1.00	31.93	O
ATOM	4069	O	HOH W	104	16.136	-10.983	27.764	1.00	39.86	O
ATOM	4070	O	HOH W	105	32.824	19.327	7.046	1.00	25.91	O
ATOM	4071	O	HOH W	106	44.318	8.293	16.717	1.00	40.37	O
ATOM	4072	O	HOH W	107	27.410	-23.208	64.554	1.00	31.14	O
ATOM	4073	O	HOH W	108	36.784	16.537	31.336	1.00	30.98	O
ATOM	4074	O	HOH W	109	16.848	-2.239	8.623	1.00	29.74	O
ATOM	4075	O	HOH W	110	25.446	0.821	3.807	1.00	30.35	O
ATOM	4076	O	HOH W	111	26.076	7.553	-2.415	1.00	32.21	O
ATOM	4077	O	HOH W	112	37.824	13.772	39.203	1.00	38.15	O
ATOM	4078	O	HOH W	113	14.258	-17.900	24.309	1.00	36.91	O
ATOM	4079	O	HOH W	114	24.018	-36.577	59.278	1.00	24.93	O
ATOM	4080	O	HOH W	115	13.686	30.014	24.832	1.00	31.61	O
ATOM	4081	O	HOH W	116	9.376	3.895	46.916	1.00	25.43	O
ATOM	4082	O	HOH W	117	25.743	-31.448	55.510	1.00	20.43	O
ATOM	4083	O	HOH W	118	27.026	-34.130	55.449	1.00	23.50	O
ATOM	4084	O	HOH W	119	1.883	-0.799	54.442	1.00	34.52	O

Figure 2 Table 2a - 62

ATOM	4085	O	HOH W 120	31.546	-27.603	46.849	1.00	32.94	O
ATOM	4086	O	HOH W 121	17.008	-8.294	67.722	1.00	31.49	O
ATOM	4087	O	HOH W 122	18.793	-10.886	66.952	1.00	29.76	O
ATOM	4088	O	HOH W 123	7.660	-32.747	55.305	1.00	33.70	O
ATOM	4089	O	HOH W 124	25.331	6.260	19.040	1.00	31.36	O
ATOM	4090	O	HOH W 125	-1.076	15.609	32.285	1.00	32.90	O
ATOM	4091	O	HOH W 126	3.093	-29.472	63.852	1.00	33.29	O
ATOM	4092	O	HOH W 127	7.970	-20.982	55.029	1.00	27.96	O
ATOM	4093	O	HOH W 128	11.134	30.964	8.937	1.00	31.14	O
ATOM	4094	O	HOH W 129	19.671	1.784	23.901	1.00	33.24	O
ATOM	4095	O	HOH W 130	8.439	-25.348	37.436	1.00	34.04	O
ATOM	4096	O	HOH W 131	5.233	-2.667	50.933	1.00	33.33	O
ATOM	4097	O	HOH W 132	48.985	-7.276	26.393	1.00	34.18	O
ATOM	4098	O	HOH W 133	22.013	25.231	24.753	1.00	30.90	O
ATOM	4099	O	HOH W 134	42.583	-13.626	24.937	1.00	31.78	O
ATOM	4100	O	HOH W 135	10.611	32.640	22.726	1.00	33.61	O
ATOM	4101	O	HOH W 136	19.033	4.959	1.612	1.00	35.47	O

Table 2b

ATOM	1	N	SER	A	393	23.326	-12.767	29.053	1.00 63.54	N
ATOM	2	CA	SER	A	393	22.920	-13.398	30.343	1.00 63.51	C
ATOM	3	C	SER	A	393	21.800	-14.436	30.148	1.00 63.36	C
ATOM	4	O	SER	A	393	20.606	-14.108	30.233	1.00 63.45	O
ATOM	5	CB	SER	A	393	22.493	-12.321	31.342	1.00 63.59	C
ATOM	6	OG	SER	A	393	21.334	-11.641	30.887	1.00 63.95	O
ATOM	7	N	MET	A	394	22.197	-15.687	29.901	1.00 62.92	N
ATOM	8	CA	MET	A	394	21.255	-16.757	29.547	1.00 62.09	C
ATOM	9	C	MET	A	394	20.512	-17.392	30.728	1.00 60.77	C
ATOM	10	O	MET	A	394	19.325	-17.138	30.928	1.00 60.47	O
ATOM	11	CB	MET	A	394	21.947	-17.841	28.714	1.00 62.31	C
ATOM	12	CG	MET	A	394	21.657	-17.794	27.218	1.00 62.86	C
ATOM	13	SD	MET	A	394	21.459	-19.481	26.549	1.00 64.15	S
ATOM	14	CE	MET	A	394	22.254	-19.341	24.934	1.00 62.97	C
ATOM	15	N	ALA	A	395	21.203	-18.225	31.502	1.00 59.70	N
ATOM	16	CA	ALA	A	395	20.532	-19.068	32.497	1.00 58.21	C
ATOM	17	C	ALA	A	395	20.505	-18.463	33.895	1.00 57.27	C
ATOM	18	O	ALA	A	395	21.557	-18.277	34.498	1.00 57.39	O
ATOM	19	CB	ALA	A	395	21.165	-20.440	32.527	1.00 58.11	C
ATOM	20	N	TRP	A	396	19.301	-18.177	34.404	1.00 56.01	N
ATOM	21	CA	TRP	A	396	19.113	-17.653	35.771	1.00 55.01	C
ATOM	22	C	TRP	A	396	18.661	-18.710	36.780	1.00 54.93	C
ATOM	23	O	TRP	A	396	17.716	-19.456	36.538	1.00 54.84	O
ATOM	24	CB	TRP	A	396	18.106	-16.509	35.779	1.00 54.19	C
ATOM	25	CG	TRP	A	396	18.554	-15.354	34.990	1.00 53.69	C
ATOM	26	CD1	TRP	A	396	18.188	-15.044	33.709	1.00 51.97	C
ATOM	27	CD2	TRP	A	396	19.494	-14.353	35.397	1.00 53.00	C
ATOM	28	NE1	TRP	A	396	18.834	-13.911	33.301	1.00 51.59	N
ATOM	29	CE2	TRP	A	396	19.639	-13.458	34.315	1.00 52.42	C
ATOM	30	CE3	TRP	A	396	20.222	-14.119	36.572	1.00 52.43	C
ATOM	31	CZ2	TRP	A	396	20.486	-12.338	34.372	1.00 52.60	C
ATOM	32	CZ3	TRP	A	396	21.069	-13.014	36.627	1.00 52.17	C
ATOM	33	CH2	TRP	A	396	21.194	-12.137	35.536	1.00 52.42	C
ATOM	34	N	HIS	A	397	19.316	-18.755	37.929	1.00 54.80	N
ATOM	35	CA	HIS	A	397	18.922	-19.709	38.962	1.00 54.92	C
ATOM	36	C	HIS	A	397	18.345	-18.984	40.164	1.00 54.59	C
ATOM	37	O	HIS	A	397	18.906	-17.991	40.613	1.00 54.68	O
ATOM	38	CB	HIS	A	397	20.103	-20.605	39.347	1.00 54.88	C
ATOM	39	CG	HIS	A	397	20.766	-21.236	38.168	1.00 55.83	C
ATOM	40	ND1	HIS	A	397	21.715	-20.581	37.411	1.00 57.09	N
ATOM	41	CD2	HIS	A	397	20.573	-22.437	37.573	1.00 56.98	C
ATOM	42	CE1	HIS	A	397	22.096	-21.359	36.414	1.00 56.73	C
ATOM	43	NE2	HIS	A	397	21.421	-22.492	36.491	1.00 57.34	N
ATOM	44	N	LEU	A	398	17.202	-19.460	40.650	1.00 54.47	N
ATOM	45	CA	LEU	A	398	16.614	-18.922	41.868	1.00 54.67	C
ATOM	46	C	LEU	A	398	17.513	-19.297	43.037	1.00 54.82	C
ATOM	47	O	LEU	A	398	17.861	-20.454	43.186	1.00 55.03	O
ATOM	48	CB	LEU	A	398	15.200	-19.463	42.089	1.00 54.22	C
ATOM	49	CG	LEU	A	398	14.510	-18.925	43.350	1.00 54.55	C
ATOM	50	CD1	LEU	A	398	14.116	-17.453	43.175	1.00 52.18	C
ATOM	51	CD2	LEU	A	398	13.303	-19.775	43.707	1.00 53.13	C
ATOM	52	N	GLY	A	399	17.916	-18.304	43.828	1.00 55.20	N
ATOM	53	CA	GLY	A	399	18.776	-18.511	44.987	1.00 55.71	C
ATOM	54	C	GLY	A	399	20.050	-19.278	44.682	1.00 56.73	C
ATOM	55	O	GLY	A	399	20.627	-19.134	43.607	1.00 57.40	O
ATOM	56	N	ILE	A	400	20.484	-20.096	45.639	1.00 57.19	N
ATOM	57	CA	ILE	A	400	21.628	-20.985	45.475	1.00 57.31	C
ATOM	58	C	ILE	A	400	21.190	-22.355	45.961	1.00 57.57	C
ATOM	59	O	ILE	A	400	20.234	-22.468	46.734	1.00 58.46	O
ATOM	60	CB	ILE	A	400	22.881	-20.517	46.278	1.00 57.41	C
ATOM	61	CG1	ILE	A	400	22.626	-20.585	47.785	1.00 57.13	C
ATOM	62	CG2	ILE	A	400	23.305	-19.087	45.867	1.00 57.65	C
ATOM	63	CD1	ILE	A	400	23.754	-20.023	48.637	1.00 57.97	C
ATOM	64	N	ARG	A	401	21.890	-23.385	45.504	1.00 57.13	N

Figure 2 Table 2b - 2

ATOM	65	CA	ARG	A	401	21.558	-24.746	45.808	1.00	57.08	C
ATOM	66	C	ARG	A	401	22.712	-25.397	46.560	1.00	56.67	C
ATOM	67	O	ARG	A	401	23.875	-24.977	46.431	1.00	56.59	O
ATOM	68	CB	ARG	A	401	21.278	-25.525	44.517	1.00	57.52	C
ATOM	69	CG	ARG	A	401	19.979	-25.133	43.830	1.00	59.03	C
ATOM	70	CD	ARG	A	401	19.709	-25.934	42.573	1.00	58.31	C
ATOM	71	NE	ARG	A	401	20.937	-26.290	41.874	1.00	62.27	N
ATOM	72	CZ	ARG	A	401	21.476	-25.610	40.863	1.00	64.49	C
ATOM	73	NH1	ARG	A	401	20.910	-24.494	40.393	1.00	66.21	N
ATOM	74	NH2	ARG	A	401	22.600	-26.054	40.316	1.00	64.37	N
ATOM	75	N	SER	A	402	22.378	-26.428	47.333	1.00	55.51	N
ATOM	76	CA	SER	A	402	23.349	-27.145	48.131	1.00	54.93	C
ATOM	77	C	SER	A	402	22.876	-28.574	48.431	1.00	54.53	C
ATOM	78	O	SER	A	402	21.678	-28.834	48.576	1.00	54.22	O
ATOM	79	CB	SER	A	402	23.615	-26.391	49.433	1.00	54.83	C
ATOM	80	OG	SER	A	402	24.590	-27.058	50.217	1.00	55.13	O
ATOM	81	N	GLN	A	403	23.828	-29.496	48.505	1.00	53.94	N
ATOM	82	CA	GLN	A	403	23.531	-30.851	48.935	1.00	53.83	C
ATOM	83	C	GLN	A	403	24.028	-31.114	50.357	1.00	53.61	C
ATOM	84	O	GLN	A	403	24.164	-32.263	50.775	1.00	53.34	O
ATOM	85	CB	GLN	A	403	24.097	-31.868	47.946	1.00	53.94	C
ATOM	86	CG	GLN	A	403	23.315	-31.909	46.649	1.00	54.36	C
ATOM	87	CD	GLN	A	403	24.099	-32.493	45.506	1.00	54.75	C
ATOM	88	OE1	GLN	A	403	25.007	-33.299	45.700	1.00	55.70	O
ATOM	89	NE2	GLN	A	403	23.746	-32.093	44.295	1.00	56.46	N
ATOM	90	N	SER	A	404	24.279	-30.040	51.103	1.00	53.47	N
ATOM	91	CA	SER	A	404	24.599	-30.158	52.522	1.00	53.34	C
ATOM	92	C	SER	A	404	23.325	-30.476	53.291	1.00	53.10	C
ATOM	93	O	SER	A	404	22.220	-30.270	52.798	1.00	52.51	O
ATOM	94	CB	SER	A	404	25.249	-28.873	53.038	1.00	53.55	C
ATOM	95	OG	SER	A	404	26.334	-28.488	52.210	1.00	53.57	O
ATOM	96	N	ARG	A	405	23.476	-31.010	54.489	1.00	53.71	N
ATOM	97	CA	ARG	A	405	22.316	-31.316	55.321	1.00	54.66	C
ATOM	98	C	ARG	A	405	21.520	-30.048	55.639	1.00	54.52	C
ATOM	99	O	ARG	A	405	22.110	-29.027	55.992	1.00	54.63	O
ATOM	100	CB	ARG	A	405	22.761	-31.978	56.620	1.00	54.83	C
ATOM	101	CG	ARG	A	405	22.673	-33.468	56.635	1.00	56.45	C
ATOM	102	CD	ARG	A	405	23.274	-33.950	57.921	1.00	60.99	C
ATOM	103	NE	ARG	A	405	24.709	-34.225	57.791	1.00	64.51	N
ATOM	104	CZ	ARG	A	405	25.642	-33.863	58.673	1.00	65.51	C
ATOM	105	NH1	ARG	A	405	25.321	-33.166	59.760	1.00	65.80	N
ATOM	106	NH2	ARG	A	405	26.911	-34.182	58.454	1.00	65.59	N
ATOM	107	N	PRO	A	406	20.181	-30.109	55.513	1.00	54.59	N
ATOM	108	CA	PRO	A	406	19.319	-28.968	55.832	1.00	54.89	C
ATOM	109	C	PRO	A	406	19.667	-28.300	57.168	1.00	55.24	C
ATOM	110	O	PRO	A	406	19.821	-27.076	57.233	1.00	54.76	O
ATOM	111	CB	PRO	A	406	17.924	-29.590	55.894	1.00	54.53	C
ATOM	112	CG	PRO	A	406	17.996	-30.733	54.975	1.00	54.65	C
ATOM	113	CD	PRO	A	406	19.399	-31.269	55.049	1.00	54.68	C
ATOM	114	N	ASN	A	407	19.804	-29.112	58.211	1.00	55.78	N
ATOM	115	CA	ASN	A	407	20.110	-28.611	59.542	1.00	56.55	C
ATOM	116	C	ASN	A	407	21.472	-27.914	59.560	1.00	56.69	C
ATOM	117	O	ASN	A	407	21.639	-26.890	60.230	1.00	56.89	O
ATOM	118	CB	ASN	A	407	20.018	-29.724	60.588	1.00	56.70	C
ATOM	119	CG	ASN	A	407	20.469	-31.102	60.046	1.00	58.60	C
ATOM	120	OD1	ASN	A	407	20.168	-31.472	58.900	1.00	59.53	O
ATOM	121	ND2	ASN	A	407	21.171	-31.871	60.887	1.00	59.06	N
ATOM	122	N	ASP	A	408	22.430	-28.450	58.803	1.00	56.43	N
ATOM	123	CA	ASP	A	408	23.720	-27.780	58.640	1.00	56.46	C
ATOM	124	C	ASP	A	408	23.545	-26.412	57.952	1.00	56.15	C
ATOM	125	O	ASP	A	408	24.100	-25.407	58.403	1.00	56.00	O
ATOM	126	CB	ASP	A	408	24.697	-28.647	57.837	1.00	56.36	C
ATOM	127	CG	ASP	A	408	25.094	-29.929	58.556	1.00	57.52	C
ATOM	128	OD1	ASP	A	408	24.774	-30.099	59.758	1.00	59.15	O
ATOM	129	OD2	ASP	A	408	25.743	-30.781	57.906	1.00	58.18	O
ATOM	130	N	ILE	A	409	22.766	-26.378	56.873	1.00	55.81	N
ATOM	131	CA	ILE	A	409	22.606	-25.153	56.086	1.00	55.54	C

Figure 2 Table 2b - 3

ATOM	132	C	ILE	A	409	22.065	-24.036	56.964	1.00	55.84	C
ATOM	133	O	ILE	A	409	22.683	-22.973	57.073	1.00	55.70	O
ATOM	134	CB	ILE	A	409	21.675	-25.369	54.880	1.00	55.59	C
ATOM	135	CG1	ILE	A	409	22.258	-26.424	53.927	1.00	54.51	C
ATOM	136	CG2	ILE	A	409	21.443	-24.076	54.155	1.00	54.58	C
ATOM	137	CD1	ILE	A	409	21.263	-26.951	52.905	1.00	52.58	C
ATOM	138	N	MET	A	410	20.932	-24.307	57.613	1.00	56.01	N
ATOM	139	CA	MET	A	410	20.275	-23.356	58.488	1.00	56.41	C
ATOM	140	C	MET	A	410	21.156	-22.923	59.654	1.00	56.65	C
ATOM	141	O	MET	A	410	21.149	-21.759	60.042	1.00	56.76	O
ATOM	142	CB	MET	A	410	18.970	-23.929	59.022	1.00	56.54	C
ATOM	143	CG	MET	A	410	17.950	-24.245	57.972	1.00	57.47	C
ATOM	144	SD	MET	A	410	17.346	-22.818	57.060	1.00	59.58	S
ATOM	145	CE	MET	A	410	18.525	-22.668	55.747	1.00	61.64	C
ATOM	146	N	ALA	A	411	21.911	-23.858	60.213	1.00	56.74	N
ATOM	147	CA	ALA	A	411	22.801	-23.523	61.314	1.00	56.92	C
ATOM	148	C	ALA	A	411	23.899	-22.600	60.801	1.00	57.06	C
ATOM	149	O	ALA	A	411	24.218	-21.603	61.439	1.00	57.47	O
ATOM	150	CB	ALA	A	411	23.383	-24.778	61.967	1.00	56.30	C
ATOM	151	N	GLU	A	412	24.453	-22.908	59.634	1.00	57.13	N
ATOM	152	CA	GLU	A	412	25.520	-22.078	59.096	1.00	57.61	C
ATOM	153	C	GLU	A	412	25.068	-20.678	58.640	1.00	57.87	C
ATOM	154	O	GLU	A	412	25.838	-19.721	58.744	1.00	57.74	O
ATOM	155	CB	GLU	A	412	26.294	-22.806	57.997	1.00	57.61	C
ATOM	156	CG	GLU	A	412	27.323	-23.785	58.521	1.00	57.78	C
ATOM	157	CD	GLU	A	412	28.504	-23.123	59.232	1.00	59.28	C
ATOM	158	OE1	GLU	A	412	29.208	-22.304	58.603	1.00	59.49	O
ATOM	159	OE2	GLU	A	412	28.748	-23.451	60.418	1.00	60.17	O
ATOM	160	N	VAL	A	413	23.835	-20.536	58.161	1.00	58.34	N
ATOM	161	CA	VAL	A	413	23.373	-19.185	57.807	1.00	59.26	C
ATOM	162	C	VAL	A	413	23.214	-18.335	59.066	1.00	59.43	C
ATOM	163	O	VAL	A	413	23.515	-17.131	59.049	1.00	59.60	O
ATOM	164	CB	VAL	A	413	22.093	-19.133	56.898	1.00	59.37	C
ATOM	165	CG1	VAL	A	413	22.208	-20.116	55.718	1.00	59.29	C
ATOM	166	CG2	VAL	A	413	20.824	-19.392	57.695	1.00	60.59	C
ATOM	167	N	CYS	A	414	22.769	-18.986	60.143	1.00	59.34	N
ATOM	168	CA	CYS	A	414	22.567	-18.362	61.452	1.00	59.85	C
ATOM	169	C	CYS	A	414	23.864	-17.875	62.073	1.00	60.05	C
ATOM	170	O	CYS	A	414	23.914	-16.774	62.612	1.00	59.87	O
ATOM	171	CB	CYS	A	414	21.892	-19.340	62.415	1.00	59.73	C
ATOM	172	SG	CYS	A	414	20.120	-19.398	62.197	1.00	60.20	S
ATOM	173	N	ARG	A	415	24.904	-18.703	62.008	1.00	60.36	N
ATOM	174	CA	ARG	A	415	26.224	-18.273	62.440	1.00	60.87	C
ATOM	175	C	ARG	A	415	26.710	-17.129	61.552	1.00	60.75	C
ATOM	176	O	ARG	A	415	27.272	-16.165	62.057	1.00	61.00	O
ATOM	177	CB	ARG	A	415	27.224	-19.434	62.451	1.00	60.99	C
ATOM	178	CG	ARG	A	415	28.562	-19.108	63.140	1.00	61.42	C
ATOM	179	CD	ARG	A	415	29.684	-20.070	62.727	1.00	61.61	C
ATOM	180	NE	ARG	A	415	29.751	-20.229	61.274	1.00	63.56	N
ATOM	181	CZ	ARG	A	415	30.148	-19.281	60.426	1.00	65.07	C
ATOM	182	NH1	ARG	A	415	30.524	-18.088	60.879	1.00	65.94	N
ATOM	183	NH2	ARG	A	415	30.152	-19.516	59.118	1.00	65.13	N
ATOM	184	N	ALA	A	416	26.471	-17.218	60.245	1.00	60.84	N
ATOM	185	CA	ALA	A	416	26.826	-16.110	59.329	1.00	60.90	C
ATOM	186	C	ALA	A	416	26.125	-14.802	59.687	1.00	60.83	C
ATOM	187	O	ALA	A	416	26.769	-13.755	59.751	1.00	61.05	O
ATOM	188	CB	ALA	A	416	26.563	-16.476	57.885	1.00	60.38	C
ATOM	189	N	ILE	A	417	24.817	-14.868	59.933	1.00	60.83	N
ATOM	190	CA	ILE	A	417	24.052	-13.692	60.374	1.00	61.14	C
ATOM	191	C	ILE	A	417	24.678	-13.033	61.616	1.00	61.44	C
ATOM	192	O	ILE	A	417	24.943	-11.830	61.614	1.00	61.42	O
ATOM	193	CB	ILE	A	417	22.557	-14.039	60.636	1.00	61.07	C
ATOM	194	CG1	ILE	A	417	21.834	-14.378	59.326	1.00	60.43	C
ATOM	195	CG2	ILE	A	417	21.832	-12.875	61.304	1.00	61.39	C
ATOM	196	CD1	ILE	A	417	20.620	-15.308	59.512	1.00	59.29	C
ATOM	197	N	LYS	A	418	24.937	-13.832	62.651	1.00	61.87	N
ATOM	198	CA	LYS	A	418	25.476	-13.335	63.915	1.00	62.42	C

Figure 2 Table 2b - 4

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ATOM    199  C   LYS A 418      26.871 -12.739  63.751  1.00 62.88           C
ATOM    200  O   LYS A 418      27.172 -11.676  64.300  1.00 62.90           O
ATOM    201  CB  LYS A 418      25.483 -14.441  64.977  1.00 62.47           C
ATOM    202  CG  LYS A 418      25.542 -13.911  66.401  1.00 62.56           C
ATOM    203  CD  LYS A 418      25.669 -15.019  67.427  1.00 63.37           C
ATOM    204  CE  LYS A 418      25.881 -14.430  68.819  1.00 64.02           C
ATOM    205  NZ  LYS A 418      26.149 -15.470  69.853  1.00 64.61           N
ATOM    206  N   GLN A 419      27.716 -13.423  62.987  1.00 63.52           N
ATOM    207  CA  GLN A 419      29.051 -12.931  62.680  1.00 64.26           C
ATOM    208  C   GLN A 419      28.974 -11.543  62.030  1.00 64.48           C
ATOM    209  O   GLN A 419      29.764 -10.659  62.351  1.00 64.83           O
ATOM    210  CB  GLN A 419      29.769 -13.912  61.748  1.00 64.50           C
ATOM    211  CG  GLN A 419      31.286 -13.955  61.905  1.00 65.80           C
ATOM    212  CD  GLN A 419      31.735 -14.767  63.112  1.00 67.83           C
ATOM    213  OE1 GLN A 419      30.972 -15.572  63.663  1.00 69.27           O
ATOM    214  NE2 GLN A 419      32.984 -14.568  63.523  1.00 68.49           N
ATOM    215  N   LEU A 420      28.004 -11.356  61.135  1.00 64.43           N
ATOM    216  CA  LEU A 420      27.854 -10.109  60.391  1.00 64.23           C
ATOM    217  C   LEU A 420      27.189  -8.981  61.170  1.00 64.21           C
ATOM    218  O   LEU A 420      27.116  -7.850  60.672  1.00 64.40           O
ATOM    219  CB  LEU A 420      27.060 -10.367  59.106  1.00 64.39           C
ATOM    220  CG  LEU A 420      27.760 -10.530  57.749  1.00 64.56           C
ATOM    221  CD1 LEU A 420      29.196 -11.058  57.839  1.00 64.49           C
ATOM    222  CD2 LEU A 420      26.913 -11.410  56.841  1.00 64.31           C
ATOM    223  N   ASP A 421      26.699  -9.270  62.376  1.00 64.10           N
ATOM    224  CA  ASP A 421      25.966  -8.271  63.175  1.00 63.95           C
ATOM    225  C   ASP A 421      24.616  -7.897  62.568  1.00 63.50           C
ATOM    226  O   ASP A 421      24.136  -6.767  62.745  1.00 63.25           O
ATOM    227  CB  ASP A 421      26.792  -6.994  63.356  1.00 64.13           C
ATOM    228  CG  ASP A 421      27.560  -6.982  64.642  1.00 65.71           C
ATOM    229  OD1 ASP A 421      27.026  -7.492  65.660  1.00 67.23           O
ATOM    230  OD2 ASP A 421      28.696  -6.454  64.640  1.00 67.29           O
ATOM    231  N   TYR A 422      24.031  -8.830  61.820  1.00 62.78           N
ATOM    232  CA  TYR A 422      22.661  -8.677  61.343  1.00 62.01           C
ATOM    233  C   TYR A 422      21.771  -9.161  62.477  1.00 61.09           C
ATOM    234  O   TYR A 422      22.247  -9.837  63.386  1.00 61.14           O
ATOM    235  CB  TYR A 422      22.418  -9.509  60.083  1.00 62.42           C
ATOM    236  CG  TYR A 422      23.188  -9.081  58.853  1.00 62.70           C
ATOM    237  CD1 TYR A 422      22.904  -9.642  57.617  1.00 63.66           C
ATOM    238  CD2 TYR A 422      24.186  -8.105  58.918  1.00 63.96           C
ATOM    239  CE1 TYR A 422      23.608  -9.254  56.470  1.00 64.05           C
ATOM    240  CE2 TYR A 422      24.889  -7.707  57.778  1.00 63.37           C
ATOM    241  CZ  TYR A 422      24.592  -8.291  56.564  1.00 63.31           C
ATOM    242  OH  TYR A 422      25.284  -7.926  55.440  1.00 64.05           O
ATOM    243  N   GLU A 423      20.498  -8.792  62.459  1.00 59.93           N
ATOM    244  CA  GLU A 423      19.589  -9.315  63.464  1.00 59.05           C
ATOM    245  C   GLU A 423      18.536 -10.194  62.812  1.00 58.28           C
ATOM    246  O   GLU A 423      18.169  -9.989  61.652  1.00 57.89           O
ATOM    247  CB  GLU A 423      18.994  -8.209  64.339  1.00 59.12           C
ATOM    248  CG  GLU A 423      18.021  -7.269  63.671  1.00 58.98           C
ATOM    249  CD  GLU A 423      17.850  -5.965  64.469  1.00 60.02           C
ATOM    250  OE1 GLU A 423      17.882  -6.019  65.716  1.00 57.44           O
ATOM    251  OE2 GLU A 423      17.696  -4.883  63.841  1.00 61.85           O
ATOM    252  N   TRP A 424      18.086 -11.205  63.542  1.00 57.17           N
ATOM    253  CA  TRP A 424      17.205 -12.188  62.935  1.00 56.25           C
ATOM    254  C   TRP A 424      16.108 -12.715  63.843  1.00 55.07           C
ATOM    255  O   TRP A 424      16.153 -12.577  65.059  1.00 54.55           O
ATOM    256  CB  TRP A 424      18.014 -13.338  62.293  1.00 56.68           C
ATOM    257  CG  TRP A 424      18.608 -14.336  63.259  1.00 57.10           C
ATOM    258  CD1 TRP A 424      18.256 -15.650  63.391  1.00 57.19           C
ATOM    259  CD2 TRP A 424      19.656 -14.103  64.216  1.00 57.16           C
ATOM    260  NE1 TRP A 424      19.023 -16.255  64.367  1.00 57.33           N
ATOM    261  CE2 TRP A 424      19.888 -15.327  64.887  1.00 58.41           C
ATOM    262  CE3 TRP A 424      20.426 -12.986  64.563  1.00 56.98           C
ATOM    263  CZ2 TRP A 424      20.856 -15.459  65.892  1.00 58.80           C
ATOM    264  CZ3 TRP A 424      21.383 -13.117  65.562  1.00 57.32           C
ATOM    265  CH2 TRP A 424      21.589 -14.342  66.215  1.00 58.13           C
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Figure 2 Table 2b - 5

ATOM	266	N	LYS	A	425	15.117	-13.311	63.199	1.00 54.18	N
ATOM	267	CA	LYS	A	425	14.044	-14.014	63.850	1.00 53.53	C
ATOM	268	C	LYS	A	425	13.815	-15.317	63.123	1.00 53.02	C
ATOM	269	O	LYS	A	425	13.806	-15.364	61.892	1.00 53.44	O
ATOM	270	CB	LYS	A	425	12.781	-13.173	63.829	1.00 53.48	C
ATOM	271	CG	LYS	A	425	12.753	-12.174	64.943	1.00 54.15	C
ATOM	272	CD	LYS	A	425	11.569	-11.267	64.857	1.00 56.16	C
ATOM	273	CE	LYS	A	425	11.786	-10.069	65.773	1.00 57.17	C
ATOM	274	NZ	LYS	A	425	11.285	-8.847	65.119	1.00 59.88	N
ATOM	275	N	VAL	A	426	13.641	-16.379	63.895	1.00 52.58	N
ATOM	276	CA	VAL	A	426	13.328	-17.693	63.362	1.00 51.37	C
ATOM	277	C	VAL	A	426	11.814	-17.807	63.330	1.00 51.50	C
ATOM	278	O	VAL	A	426	11.166	-17.954	64.365	1.00 51.60	O
ATOM	279	CB	VAL	A	426	13.951	-18.800	64.249	1.00 51.48	C
ATOM	280	CG1	VAL	A	426	13.577	-20.209	63.748	1.00 49.36	C
ATOM	281	CG2	VAL	A	426	15.475	-18.609	64.347	1.00 49.89	C
ATOM	282	N	VAL	A	427	11.248	-17.680	62.140	1.00 51.66	N
ATOM	283	CA	VAL	A	427	9.816	-17.930	61.943	1.00 51.44	C
ATOM	284	C	VAL	A	427	9.562	-19.447	62.003	1.00 51.20	C
ATOM	285	O	VAL	A	427	8.786	-19.895	62.835	1.00 50.89	O
ATOM	286	CB	VAL	A	427	9.300	-17.316	60.598	1.00 51.56	C
ATOM	287	CG1	VAL	A	427	7.776	-17.327	60.523	1.00 50.79	C
ATOM	288	CG2	VAL	A	427	9.819	-15.896	60.416	1.00 50.57	C
ATOM	289	N	ASN	A	428	10.245	-20.195	61.123	1.00 51.10	N
ATOM	290	CA	ASN	A	428	10.232	-21.671	61.009	1.00 51.63	C
ATOM	291	C	ASN	A	428	11.639	-22.180	61.124	1.00 51.29	C
ATOM	292	O	ASN	A	428	12.573	-21.414	60.889	1.00 51.32	O
ATOM	293	CB	ASN	A	428	9.850	-22.102	59.580	1.00 52.38	C
ATOM	294	CG	ASN	A	428	8.415	-21.896	59.290	1.00 54.27	C
ATOM	295	OD1	ASN	A	428	7.560	-22.068	60.178	1.00 57.29	O
ATOM	296	ND2	ASN	A	428	8.113	-21.519	58.055	1.00 52.89	N
ATOM	297	N	PRO	A	429	11.810	-23.494	61.373	1.00 50.65	N
ATOM	298	CA	PRO	A	429	13.138	-24.060	61.140	1.00 50.51	C
ATOM	299	C	PRO	A	429	13.717	-23.780	59.744	1.00 50.68	C
ATOM	300	O	PRO	A	429	14.937	-23.867	59.575	1.00 51.21	O
ATOM	301	CB	PRO	A	429	12.916	-25.565	61.345	1.00 50.15	C
ATOM	302	CG	PRO	A	429	11.787	-25.641	62.285	1.00 49.04	C
ATOM	303	CD	PRO	A	429	10.872	-24.513	61.884	1.00 50.43	C
ATOM	304	N	TYR	A	430	12.886	-23.435	58.756	1.00 50.54	N
ATOM	305	CA	TYR	A	430	13.426	-23.141	57.408	1.00 50.46	C
ATOM	306	C	TYR	A	430	13.131	-21.745	56.891	1.00 51.25	C
ATOM	307	O	TYR	A	430	13.244	-21.486	55.693	1.00 51.27	O
ATOM	308	CB	TYR	A	430	12.956	-24.175	56.383	1.00 49.88	C
ATOM	309	CG	TYR	A	430	13.266	-25.567	56.827	1.00 48.97	C
ATOM	310	CD1	TYR	A	430	12.243	-26.436	57.164	1.00 48.39	C
ATOM	311	CD2	TYR	A	430	14.586	-25.988	56.987	1.00 46.40	C
ATOM	312	CE1	TYR	A	430	12.518	-27.704	57.609	1.00 49.78	C
ATOM	313	CE2	TYR	A	430	14.869	-27.247	57.432	1.00 48.60	C
ATOM	314	CZ	TYR	A	430	13.827	-28.103	57.740	1.00 48.92	C
ATOM	315	OH	TYR	A	430	14.072	-29.356	58.195	1.00 49.30	O
ATOM	316	N	TYR	A	431	12.768	-20.847	57.797	1.00 51.77	N
ATOM	317	CA	TYR	A	431	12.330	-19.537	57.398	1.00 52.63	C
ATOM	318	C	TYR	A	431	12.826	-18.483	58.394	1.00 53.16	C
ATOM	319	O	TYR	A	431	12.534	-18.527	59.606	1.00 52.93	O
ATOM	320	CB	TYR	A	431	10.807	-19.538	57.212	1.00 52.95	C
ATOM	321	CG	TYR	A	431	10.199	-18.220	56.816	1.00 54.30	C
ATOM	322	CD1	TYR	A	431	10.934	-17.262	56.107	1.00 55.21	C
ATOM	323	CD2	TYR	A	431	8.869	-17.941	57.111	1.00 54.81	C
ATOM	324	CE1	TYR	A	431	10.366	-16.063	55.733	1.00 54.94	C
ATOM	325	CE2	TYR	A	431	8.295	-16.733	56.750	1.00 55.45	C
ATOM	326	CZ	TYR	A	431	9.051	-15.801	56.065	1.00 55.84	C
ATOM	327	OH	TYR	A	431	8.484	-14.597	55.712	1.00 56.86	O
ATOM	328	N	LEU	A	432	13.611	-17.553	57.860	1.00 53.36	N
ATOM	329	CA	LEU	A	432	14.227	-16.521	58.652	1.00 53.75	C
ATOM	330	C	LEU	A	432	13.921	-15.159	58.091	1.00 54.64	C
ATOM	331	O	LEU	A	432	14.044	-14.915	56.882	1.00 54.22	O
ATOM	332	CB	LEU	A	432	15.734	-16.702	58.666	1.00 53.45	C

Figure 2 Table 2b - 6

ATOM	333	CG	LEU	A	432	16.356	-18.042	59.039	1.00	52.41	C
ATOM	334	CD1	LEU	A	432	17.842	-17.891	58.880	1.00	50.92	C
ATOM	335	CD2	LEU	A	432	16.003	-18.505	60.456	1.00	50.16	C
ATOM	336	N	ARG	A	433	13.510	-14.275	58.990	1.00	55.94	N
ATOM	337	CA	ARG	A	433	13.450	-12.845	58.732	1.00	56.68	C
ATOM	338	C	ARG	A	433	14.747	-12.239	59.264	1.00	56.40	C
ATOM	339	O	ARG	A	433	15.139	-12.540	60.385	1.00	56.18	O
ATOM	340	CB	ARG	A	433	12.247	-12.248	59.460	1.00	57.44	C
ATOM	341	CG	ARG	A	433	11.183	-11.668	58.535	1.00	60.62	C
ATOM	342	CD	ARG	A	433	10.037	-12.624	58.257	1.00	63.10	C
ATOM	343	NE	ARG	A	433	8.838	-12.262	59.021	1.00	65.18	N
ATOM	344	CZ	ARG	A	433	7.614	-12.742	58.776	1.00	66.38	C
ATOM	345	NH1	ARG	A	433	7.415	-13.605	57.775	1.00	66.20	N
ATOM	346	NH2	ARG	A	433	6.584	-12.370	59.535	1.00	64.53	N
ATOM	347	N	VAL	A	434	15.435	-11.429	58.458	1.00	56.55	N
ATOM	348	CA	VAL	A	434	16.663	-10.750	58.910	1.00	56.70	C
ATOM	349	C	VAL	A	434	16.635	-9.246	58.630	1.00	57.25	C
ATOM	350	O	VAL	A	434	15.985	-8.801	57.687	1.00	57.17	O
ATOM	351	CB	VAL	A	434	17.992	-11.399	58.384	1.00	56.64	C
ATOM	352	CG1	VAL	A	434	17.758	-12.803	57.842	1.00	56.87	C
ATOM	353	CG2	VAL	A	434	18.658	-10.554	57.355	1.00	56.60	C
ATOM	354	N	ARG	A	435	17.342	-8.486	59.475	1.00	57.62	N
ATOM	355	CA	ARG	A	435	17.368	-7.036	59.447	1.00	57.93	C
ATOM	356	C	ARG	A	435	18.792	-6.519	59.674	1.00	58.30	C
ATOM	357	O	ARG	A	435	19.555	-7.085	60.454	1.00	58.62	O
ATOM	358	CB	ARG	A	435	16.421	-6.505	60.512	1.00	58.24	C
ATOM	359	CG	ARG	A	435	16.202	-5.010	60.517	1.00	58.72	C
ATOM	360	CD	ARG	A	435	15.134	-4.663	61.530	1.00	60.66	C
ATOM	361	NE	ARG	A	435	15.041	-3.220	61.764	1.00	63.12	N
ATOM	362	CZ	ARG	A	435	15.390	-2.631	62.903	1.00	63.85	C
ATOM	363	NH1	ARG	A	435	15.849	-3.344	63.921	1.00	64.76	N
ATOM	364	NH2	ARG	A	435	15.271	-1.325	63.032	1.00	64.78	N
ATOM	365	N	ARG	A	436	19.149	-5.438	58.993	1.00	58.45	N
ATOM	366	CA	ARG	A	436	20.526	-4.993	58.950	1.00	58.70	C
ATOM	367	C	ARG	A	436	20.538	-3.492	59.114	1.00	59.03	C
ATOM	368	O	ARG	A	436	19.758	-2.811	58.454	1.00	59.60	O
ATOM	369	CB	ARG	A	436	21.108	-5.368	57.585	1.00	58.69	C
ATOM	370	CG	ARG	A	436	22.607	-5.234	57.447	1.00	59.50	C
ATOM	371	CD	ARG	A	436	23.037	-3.826	57.052	1.00	60.06	C
ATOM	372	NE	ARG	A	436	23.213	-3.649	55.612	1.00	61.24	N
ATOM	373	CZ	ARG	A	436	22.402	-2.945	54.818	1.00	60.60	C
ATOM	374	NH1	ARG	A	436	21.310	-2.355	55.306	1.00	59.33	N
ATOM	375	NH2	ARG	A	436	22.683	-2.843	53.525	1.00	59.12	N
ATOM	376	N	LYS	A	437	21.407	-2.964	59.976	1.00	59.16	N
ATOM	377	CA	LYS	A	437	21.613	-1.514	60.019	1.00	59.40	C
ATOM	378	C	LYS	A	437	22.794	-1.169	59.138	1.00	59.67	C
ATOM	379	O	LYS	A	437	23.863	-1.764	59.289	1.00	59.86	O
ATOM	380	CB	LYS	A	437	21.851	-0.993	61.434	1.00	59.29	C
ATOM	381	CG	LYS	A	437	21.951	0.526	61.507	1.00	59.74	C
ATOM	382	CD	LYS	A	437	22.299	1.009	62.903	1.00	59.73	C
ATOM	383	CE	LYS	A	437	22.255	2.518	62.980	1.00	60.02	C
ATOM	384	NZ	LYS	A	437	22.701	3.015	64.310	1.00	60.02	N
ATOM	385	N	ASN	A	438	22.590	-0.216	58.224	1.00	59.70	N
ATOM	386	CA	ASN	A	438	23.598	0.167	57.242	1.00	59.74	C
ATOM	387	C	ASN	A	438	24.718	1.037	57.835	1.00	60.06	C
ATOM	388	O	ASN	A	438	24.510	2.226	58.122	1.00	59.90	O
ATOM	389	CB	ASN	A	438	22.932	0.862	56.051	1.00	59.86	C
ATOM	390	CG	ASN	A	438	23.903	1.146	54.921	1.00	59.83	C
ATOM	391	OD1	ASN	A	438	24.655	2.118	54.959	1.00	58.91	O
ATOM	392	ND2	ASN	A	438	23.885	0.290	53.902	1.00	60.42	N
ATOM	393	N	PRO	A	439	25.926	0.454	57.980	1.00	60.29	N
ATOM	394	CA	PRO	A	439	27.022	1.099	58.713	1.00	60.36	C
ATOM	395	C	PRO	A	439	27.451	2.447	58.137	1.00	60.47	C
ATOM	396	O	PRO	A	439	28.202	3.178	58.789	1.00	60.71	O
ATOM	397	CB	PRO	A	439	28.168	0.075	58.630	1.00	60.30	C
ATOM	398	CG	PRO	A	439	27.823	-0.821	57.496	1.00	60.36	C
ATOM	399	CD	PRO	A	439	26.326	-0.857	57.429	1.00	60.26	C

Figure 2 Table 2b - 7

ATOM	400	N	VAL A 440	26.975	2.781	56.940	1.00	60.51	N
ATOM	401	CA	VAL A 440	27.276	4.086	56.335	1.00	60.37	C
ATOM	402	C	VAL A 440	26.078	5.041	56.406	1.00	60.30	C
ATOM	403	O	VAL A 440	26.202	6.160	56.895	1.00	60.48	O
ATOM	404	CB	VAL A 440	27.805	3.952	54.870	1.00	60.30	C
ATOM	405	CG1	VAL A 440	27.939	5.311	54.208	1.00	60.09	C
ATOM	406	CG2	VAL A 440	29.151	3.233	54.846	1.00	60.16	C
ATOM	407	N	THR A 441	24.923	4.584	55.940	1.00	60.42	N
ATOM	408	CA	THR A 441	23.744	5.437	55.799	1.00	60.72	C
ATOM	409	C	THR A 441	22.890	5.500	57.056	1.00	60.66	C
ATOM	410	O	THR A 441	22.122	6.452	57.232	1.00	60.44	O
ATOM	411	CB	THR A 441	22.842	4.949	54.648	1.00	60.83	C
ATOM	412	OG1	THR A 441	23.658	4.452	53.583	1.00	61.54	O
ATOM	413	CG2	THR A 441	21.981	6.090	54.119	1.00	61.12	C
ATOM	414	N	SER A 442	23.007	4.477	57.908	1.00	60.41	N
ATOM	415	CA	SER A 442	22.184	4.354	59.109	1.00	60.41	C
ATOM	416	C	SER A 442	20.743	3.974	58.770	1.00	60.36	C
ATOM	417	O	SER A 442	19.842	4.170	59.587	1.00	60.81	O
ATOM	418	CB	SER A 442	22.195	5.648	59.948	1.00	60.50	C
ATOM	419	OG	SER A 442	23.506	6.049	60.307	1.00	60.50	O
ATOM	420	N	THR A 443	20.518	3.451	57.568	1.00	59.98	N
ATOM	421	CA	THR A 443	19.200	2.934	57.205	1.00	59.66	C
ATOM	422	C	THR A 443	19.112	1.440	57.489	1.00	59.45	C
ATOM	423	O	THR A 443	20.132	0.762	57.670	1.00	59.20	O
ATOM	424	CB	THR A 443	18.859	3.180	55.731	1.00	59.81	C
ATOM	425	OG1	THR A 443	19.889	2.625	54.902	1.00	60.50	O
ATOM	426	CG2	THR A 443	18.714	4.676	55.448	1.00	59.57	C
ATOM	427	N	PHE A 444	17.888	0.931	57.530	1.00	59.12	N
ATOM	428	CA	PHE A 444	17.660	-0.469	57.843	1.00	58.66	C
ATOM	429	C	PHE A 444	17.107	-1.218	56.659	1.00	58.78	C
ATOM	430	O	PHE A 444	16.228	-0.714	55.962	1.00	58.45	O
ATOM	431	CB	PHE A 444	16.705	-0.609	59.022	1.00	58.46	C
ATOM	432	CG	PHE A 444	17.337	-0.302	60.336	1.00	58.79	C
ATOM	433	CD1	PHE A 444	17.242	0.980	60.887	1.00	58.61	C
ATOM	434	CD2	PHE A 444	18.048	-1.288	61.025	1.00	58.67	C
ATOM	435	CE1	PHE A 444	17.844	1.281	62.116	1.00	58.34	C
ATOM	436	CE2	PHE A 444	18.646	-1.005	62.251	1.00	58.53	C
ATOM	437	CZ	PHE A 444	18.545	0.288	62.800	1.00	58.63	C
ATOM	438	N	SER A 445	17.630	-2.425	56.445	1.00	58.86	N
ATOM	439	CA	SER A 445	17.133	-3.320	55.409	1.00	59.39	C
ATOM	440	C	SER A 445	16.718	-4.700	55.937	1.00	59.74	C
ATOM	441	O	SER A 445	17.398	-5.303	56.788	1.00	59.62	O
ATOM	442	CB	SER A 445	18.158	-3.469	54.297	1.00	59.29	C
ATOM	443	OG	SER A 445	17.871	-2.574	53.247	1.00	60.85	O
ATOM	444	N	LYS A 446	15.597	-5.183	55.411	1.00	59.78	N
ATOM	445	CA	LYS A 446	15.019	-6.452	55.812	1.00	59.90	C
ATOM	446	C	LYS A 446	14.914	-7.402	54.615	1.00	59.83	C
ATOM	447	O	LYS A 446	14.607	-6.973	53.489	1.00	59.20	O
ATOM	448	CB	LYS A 446	13.634	-6.235	56.419	1.00	59.97	C
ATOM	449	CG	LYS A 446	13.639	-5.570	57.777	1.00	62.19	C
ATOM	450	CD	LYS A 446	12.305	-5.734	58.515	1.00	65.03	C
ATOM	451	CE	LYS A 446	11.284	-4.705	58.046	1.00	68.01	C
ATOM	452	NZ	LYS A 446	10.309	-4.325	59.121	1.00	69.89	N
ATOM	453	N	MET A 447	15.176	-8.688	54.870	1.00	59.63	N
ATOM	454	CA	MET A 447	14.978	-9.746	53.874	1.00	60.06	C
ATOM	455	C	MET A 447	14.625	-11.085	54.523	1.00	59.30	C
ATOM	456	O	MET A 447	14.779	-11.258	55.718	1.00	58.82	O
ATOM	457	CB	MET A 447	16.197	-9.895	52.955	1.00	59.61	C
ATOM	458	CG	MET A 447	17.473	-10.335	53.645	1.00	60.63	C
ATOM	459	SD	MET A 447	18.635	-11.039	52.461	1.00	63.68	S
ATOM	460	CE	MET A 447	20.129	-11.134	53.421	1.00	62.42	C
ATOM	461	N	SER A 448	14.171	-12.021	53.697	1.00	58.90	N
ATOM	462	CA	SER A 448	13.708	-13.316	54.116	1.00	58.10	C
ATOM	463	C	SER A 448	14.602	-14.420	53.565	1.00	58.37	C
ATOM	464	O	SER A 448	14.992	-14.382	52.405	1.00	58.21	O
ATOM	465	CB	SER A 448	12.311	-13.525	53.568	1.00	57.91	C
ATOM	466	OG	SER A 448	11.340	-13.287	54.561	1.00	58.51	O

Figure 2 Table 2b - 8

ATOM	467	N	LEU	A	449	14.912	-15.411	54.394	1.00 58.26	N
ATOM	468	CA	LEU	A	449	15.531	-16.627	53.904	1.00 58.12	C
ATOM	469	C	LEU	A	449	14.585	-17.802	54.050	1.00 57.61	C
ATOM	470	O	LEU	A	449	13.995	-18.001	55.117	1.00 58.05	O
ATOM	471	CB	LEU	A	449	16.830	-16.906	54.634	1.00 58.68	C
ATOM	472	CG	LEU	A	449	18.021	-16.109	54.117	1.00 60.71	C
ATOM	473	CD1	LEU	A	449	18.182	-14.874	54.953	1.00 61.96	C
ATOM	474	CD2	LEU	A	449	19.264	-16.959	54.225	1.00 62.18	C
ATOM	475	N	GLN	A	450	14.434	-18.566	52.969	1.00 56.69	N
ATOM	476	CA	GLN	A	450	13.592	-19.756	52.943	1.00 55.84	C
ATOM	477	C	GLN	A	450	14.347	-20.887	52.255	1.00 55.67	C
ATOM	478	O	GLN	A	450	14.869	-20.711	51.139	1.00 54.99	O
ATOM	479	CB	GLN	A	450	12.275	-19.497	52.211	1.00 55.83	C
ATOM	480	CG	GLN	A	450	11.408	-20.746	52.005	1.00 56.43	C
ATOM	481	CD	GLN	A	450	10.755	-21.241	53.297	1.00 57.59	C
ATOM	482	OE1	GLN	A	450	9.787	-20.650	53.788	1.00 57.15	O
ATOM	483	NE2	GLN	A	450	11.295	-22.318	53.859	1.00 57.23	N
ATOM	484	N	LEU	A	451	14.405	-22.040	52.933	1.00 54.94	N
ATOM	485	CA	LEU	A	451	15.027	-23.220	52.369	1.00 54.06	C
ATOM	486	C	LEU	A	451	13.963	-24.146	51.816	1.00 54.34	C
ATOM	487	O	LEU	A	451	12.931	-24.378	52.451	1.00 54.18	O
ATOM	488	CB	LEU	A	451	15.912	-23.932	53.384	1.00 54.01	C
ATOM	489	CG	LEU	A	451	16.830	-25.054	52.864	1.00 52.34	C
ATOM	490	CD1	LEU	A	451	17.987	-24.508	52.036	1.00 51.00	C
ATOM	491	CD2	LEU	A	451	17.365	-25.865	54.012	1.00 50.22	C
ATOM	492	N	TYR	A	452	14.226	-24.652	50.616	1.00 54.47	N
ATOM	493	CA	TYR	A	452	13.305	-25.521	49.913	1.00 54.87	C
ATOM	494	C	TYR	A	452	14.008	-26.815	49.566	1.00 55.24	C
ATOM	495	O	TYR	A	452	15.232	-26.839	49.406	1.00 55.45	O
ATOM	496	CB	TYR	A	452	12.867	-24.873	48.604	1.00 55.18	C
ATOM	497	CG	TYR	A	452	11.890	-23.735	48.736	1.00 54.95	C
ATOM	498	CD1	TYR	A	452	12.277	-22.427	48.463	1.00 52.92	C
ATOM	499	CD2	TYR	A	452	10.562	-23.975	49.113	1.00 54.68	C
ATOM	500	CE1	TYR	A	452	11.370	-21.386	48.556	1.00 53.71	C
ATOM	501	CE2	TYR	A	452	9.655	-22.944	49.229	1.00 54.05	C
ATOM	502	CZ	TYR	A	452	10.060	-21.651	48.955	1.00 54.89	C
ATOM	503	OH	TYR	A	452	9.139	-20.632	49.073	1.00 56.04	O
ATOM	504	N	GLN	A	453	13.235	-27.889	49.443	1.00 55.50	N
ATOM	505	CA	GLN	A	453	13.746	-29.138	48.873	1.00 55.64	C
ATOM	506	C	GLN	A	453	13.463	-29.138	47.381	1.00 55.56	C
ATOM	507	O	GLN	A	453	12.344	-28.845	46.959	1.00 55.84	O
ATOM	508	CB	GLN	A	453	13.106	-30.351	49.546	1.00 55.46	C
ATOM	509	CG	GLN	A	453	13.588	-31.661	48.983	1.00 56.25	C
ATOM	510	CD	GLN	A	453	13.553	-32.830	49.953	1.00 56.68	C
ATOM	511	OE1	GLN	A	453	13.421	-32.672	51.171	1.00 58.44	O
ATOM	512	NE2	GLN	A	453	13.688	-34.022	49.406	1.00 57.73	N
ATOM	513	N	VAL	A	454	14.482	-29.424	46.578	1.00 55.56	N
ATOM	514	CA	VAL	A	454	14.296	-29.510	45.125	1.00 55.44	C
ATOM	515	C	VAL	A	454	14.619	-30.901	44.595	1.00 55.59	C
ATOM	516	O	VAL	A	454	14.179	-31.251	43.510	1.00 55.35	O
ATOM	517	CB	VAL	A	454	15.004	-28.358	44.307	1.00 55.38	C
ATOM	518	CG1	VAL	A	454	14.324	-27.034	44.564	1.00 55.42	C
ATOM	519	CG2	VAL	A	454	16.490	-28.246	44.621	1.00 55.17	C
ATOM	520	N	ASP	A	455	15.367	-31.680	45.381	1.00 56.03	N
ATOM	521	CA	ASP	A	455	15.594	-33.118	45.144	1.00 56.38	C
ATOM	522	C	ASP	A	455	15.575	-33.843	46.456	1.00 56.00	C
ATOM	523	O	ASP	A	455	15.595	-33.211	47.506	1.00 56.00	O
ATOM	524	CB	ASP	A	455	16.981	-33.370	44.585	1.00 56.64	C
ATOM	525	CG	ASP	A	455	17.039	-33.234	43.119	1.00 59.15	C
ATOM	526	OD1	ASP	A	455	15.965	-33.225	42.482	1.00 62.26	O
ATOM	527	OD2	ASP	A	455	18.167	-33.145	42.592	1.00 63.23	O
ATOM	528	N	SER	A	456	15.603	-35.172	46.397	1.00 55.36	N
ATOM	529	CA	SER	A	456	15.862	-35.974	47.593	1.00 55.14	C
ATOM	530	C	SER	A	456	17.229	-35.611	48.197	1.00 55.31	C
ATOM	531	O	SER	A	456	17.428	-35.704	49.408	1.00 54.86	O
ATOM	532	CB	SER	A	456	15.765	-37.482	47.289	1.00 54.88	C
ATOM	533	OG	SER	A	456	16.482	-37.846	46.116	1.00 52.83	O

Figure 2 Table 2b - 9

ATOM	534	N	ARG A 457	18.152	-35.164	47.346	1.00	55.69		N
ATOM	535	CA	ARG A 457	19.529	-34.892	47.760	1.00	56.38		C
ATOM	536	C	ARG A 457	19.828	-33.395	47.827	1.00	56.35		C
ATOM	537	O	ARG A 457	20.787	-32.986	48.481	1.00	56.45		O
ATOM	538	CB	ARG A 457	20.519	-35.579	46.807	1.00	56.08		C
ATOM	539	CG	ARG A 457	20.207	-37.058	46.536	1.00	57.55		C
ATOM	540	CD	ARG A 457	21.060	-37.647	45.406	1.00	58.65		C
ATOM	541	NE	ARG A 457	22.254	-38.345	45.897	1.00	60.72		N
ATOM	542	CZ	ARG A 457	23.431	-37.766	46.134	1.00	61.91		C
ATOM	543	NH1	ARG A 457	23.603	-36.459	45.944	1.00	63.24		N
ATOM	544	NH2	ARG A 457	24.447	-38.495	46.569	1.00	62.55		N
ATOM	545	N	THR A 458	18.997	-32.588	47.170	1.00	56.39		N
ATOM	546	CA	THR A 458	19.335	-31.186	46.894	1.00	56.90		C
ATOM	547	C	THR A 458	18.356	-30.179	47.497	1.00	56.95		C
ATOM	548	O	THR A 458	17.137	-30.372	47.446	1.00	56.93		O
ATOM	549	CB	THR A 458	19.435	-30.931	45.373	1.00	56.66		C
ATOM	550	OG1	THR A 458	19.904	-32.118	44.725	1.00	58.21		O
ATOM	551	CG2	THR A 458	20.387	-29.802	45.075	1.00	56.57		C
ATOM	552	N	TYR A 459	18.907	-29.099	48.051	1.00	57.16		N
ATOM	553	CA	TYR A 459	18.108	-28.001	48.621	1.00	57.42		C
ATOM	554	C	TYR A 459	18.455	-26.676	47.972	1.00	57.26		C
ATOM	555	O	TYR A 459	19.463	-26.569	47.269	1.00	57.17		O
ATOM	556	CB	TYR A 459	18.259	-27.933	50.144	1.00	57.32		C
ATOM	557	CG	TYR A 459	18.142	-29.310	50.765	1.00	58.15		C
ATOM	558	CD1	TYR A 459	19.281	-30.045	51.092	1.00	57.94		C
ATOM	559	CD2	TYR A 459	16.897	-29.899	50.966	1.00	57.79		C
ATOM	560	CE1	TYR A 459	19.185	-31.305	51.631	1.00	59.04		C
ATOM	561	CE2	TYR A 459	16.792	-31.163	51.506	1.00	58.98		C
ATOM	562	CZ	TYR A 459	17.939	-31.861	51.837	1.00	58.79		C
ATOM	563	OH	TYR A 459	17.843	-33.115	52.375	1.00	58.03		O
ATOM	564	N	LEU A 460	17.598	-25.684	48.204	1.00	57.07		N
ATOM	565	CA	LEU A 460	17.689	-24.391	47.561	1.00	56.60		C
ATOM	566	C	LEU A 460	17.389	-23.284	48.576	1.00	57.14		C
ATOM	567	O	LEU A 460	16.282	-23.194	49.140	1.00	57.19		O
ATOM	568	CB	LEU A 460	16.740	-24.363	46.363	1.00	56.59		C
ATOM	569	CG	LEU A 460	16.293	-23.148	45.513	1.00	56.75		C
ATOM	570	CD1	LEU A 460	16.801	-21.780	45.949	1.00	55.52		C
ATOM	571	CD2	LEU A 460	16.609	-23.416	44.044	1.00	54.54		C
ATOM	572	N	LEU A 461	18.397	-22.460	48.835	1.00	56.82		N
ATOM	573	CA	LEU A 461	18.217	-21.344	49.731	1.00	56.66		C
ATOM	574	C	LEU A 461	17.750	-20.146	48.909	1.00	57.32		C
ATOM	575	O	LEU A 461	18.345	-19.809	47.893	1.00	57.45		O
ATOM	576	CB	LEU A 461	19.505	-21.040	50.500	1.00	56.35		C
ATOM	577	CG	LEU A 461	19.437	-19.853	51.467	1.00	55.41		C
ATOM	578	CD1	LEU A 461	18.274	-20.005	52.458	1.00	54.87		C
ATOM	579	CD2	LEU A 461	20.765	-19.677	52.197	1.00	55.22		C
ATOM	580	N	ASP A 462	16.685	-19.508	49.372	1.00	57.73		N
ATOM	581	CA	ASP A 462	15.982	-18.508	48.609	1.00	57.57		C
ATOM	582	C	ASP A 462	15.941	-17.221	49.417	1.00	57.86		C
ATOM	583	O	ASP A 462	15.672	-17.232	50.624	1.00	57.97		O
ATOM	584	CB	ASP A 462	14.578	-19.024	48.306	1.00	57.41		C
ATOM	585	CG	ASP A 462	13.701	-17.989	47.673	1.00	59.08		C
ATOM	586	OD1	ASP A 462	14.118	-17.334	46.695	1.00	61.38		O
ATOM	587	OD2	ASP A 462	12.571	-17.825	48.156	1.00	61.83		O
ATOM	588	N	PHE A 463	16.237	-16.106	48.748	1.00	57.92		N
ATOM	589	CA	PHE A 463	16.349	-14.812	49.403	1.00	56.71		C
ATOM	590	C	PHE A 463	15.279	-13.909	48.824	1.00	57.18		C
ATOM	591	O	PHE A 463	15.122	-13.839	47.611	1.00	56.72		O
ATOM	592	CB	PHE A 463	17.708	-14.179	49.128	1.00	56.48		C
ATOM	593	CG	PHE A 463	18.891	-15.042	49.474	1.00	54.72		C
ATOM	594	CD1	PHE A 463	19.154	-16.204	48.779	1.00	55.46		C
ATOM	595	CD2	PHE A 463	19.794	-14.631	50.431	1.00	54.21		C
ATOM	596	CE1	PHE A 463	20.258	-16.997	49.095	1.00	55.35		C
ATOM	597	CE2	PHE A 463	20.895	-15.398	50.742	1.00	56.13		C
ATOM	598	CZ	PHE A 463	21.125	-16.597	50.072	1.00	54.40		C
ATOM	599	N	ARG A 464	14.552	-13.205	49.687	1.00	57.63		N
ATOM	600	CA	ARG A 464	13.522	-12.307	49.236	1.00	58.47		C

Figure 2 Table 2b - 10

ATOM	601	C	ARG	A	464	13.654	-10.979	49.971	1.00	58.80	C
ATOM	602	O	ARG	A	464	13.743	-10.947	51.203	1.00	59.63	O
ATOM	603	CB	ARG	A	464	12.157	-12.917	49.493	1.00	58.73	C
ATOM	604	CG	ARG	A	464	11.040	-12.171	48.813	1.00	61.08	C
ATOM	605	CD	ARG	A	464	9.685	-12.429	49.443	1.00	65.84	C
ATOM	606	NE	ARG	A	464	8.656	-11.665	48.730	1.00	70.74	N
ATOM	607	CZ	ARG	A	464	7.773	-12.190	47.879	1.00	72.57	C
ATOM	608	NH1	ARG	A	464	7.754	-13.508	47.637	1.00	73.00	N
ATOM	609	NH2	ARG	A	464	6.899	-11.394	47.271	1.00	72.20	N
ATOM	610	N	SER	A	465	13.670	-9.879	49.232	1.00	58.36	N
ATOM	611	CA	SER	A	465	13.738	-8.581	49.873	1.00	58.30	C
ATOM	612	C	SER	A	465	12.366	-8.189	50.376	1.00	58.49	C
ATOM	613	O	SER	A	465	11.344	-8.575	49.804	1.00	57.48	O
ATOM	614	CB	SER	A	465	14.301	-7.512	48.919	1.00	58.25	C
ATOM	615	OG	SER	A	465	13.388	-7.205	47.883	1.00	58.58	O
ATOM	616	N	ILE	A	466	12.348	-7.410	51.449	1.00	59.61	N
ATOM	617	CA	ILE	A	466	11.102	-7.016	52.064	1.00	61.43	C
ATOM	618	C	ILE	A	466	10.959	-5.499	51.998	1.00	63.09	C
ATOM	619	O	ILE	A	466	11.814	-4.753	52.485	1.00	63.36	O
ATOM	620	CB	ILE	A	466	10.976	-7.577	53.516	1.00	61.33	C
ATOM	621	CG1	ILE	A	466	11.057	-9.116	53.502	1.00	61.31	C
ATOM	622	CG2	ILE	A	466	9.663	-7.122	54.163	1.00	60.81	C
ATOM	623	CD1	ILE	A	466	11.239	-9.787	54.883	1.00	61.48	C
ATOM	624	N	ASP	A	467	9.868	-5.053	51.382	1.00	65.47	N
ATOM	625	CA	ASP	A	467	9.618	-3.635	51.136	1.00	67.69	C
ATOM	626	C	ASP	A	467	9.309	-2.826	52.389	1.00	69.06	C
ATOM	627	O	ASP	A	467	8.888	-3.374	53.408	1.00	69.05	O
ATOM	628	CB	ASP	A	467	8.483	-3.479	50.125	1.00	68.02	C
ATOM	629	CG	ASP	A	467	8.905	-3.835	48.707	1.00	70.09	C
ATOM	630	OD1	ASP	A	467	10.126	-3.823	48.412	1.00	72.07	O
ATOM	631	OD2	ASP	A	467	8.010	-4.120	47.878	1.00	72.60	O
ATOM	632	N	ASP	A	468	9.516	-1.510	52.286	1.00	71.09	N
ATOM	633	CA	ASP	A	468	9.244	-0.556	53.369	1.00	72.74	C
ATOM	634	C	ASP	A	468	7.775	-0.165	53.451	1.00	73.54	C
ATOM	635	O	ASP	A	468	7.057	-0.200	52.440	1.00	73.91	O
ATOM	636	CB	ASP	A	468	10.059	0.727	53.172	1.00	72.91	C
ATOM	637	CG	ASP	A	468	11.547	0.521	53.378	1.00	73.76	C
ATOM	638	OD1	ASP	A	468	12.244	1.540	53.586	1.00	74.95	O
ATOM	639	OD2	ASP	A	468	12.019	-0.640	53.323	1.00	73.29	O
ATOM	640	N	GLU	A	469	7.363	0.247	54.656	1.00	74.22	N
ATOM	641	CA	GLU	A	469	6.001	0.721	54.961	1.00	74.52	C
ATOM	642	C	GLU	A	469	4.896	-0.209	54.446	1.00	74.82	C
ATOM	643	O	GLU	A	469	5.085	-1.435	54.361	1.00	75.08	O
ATOM	644	CB	GLU	A	469	5.790	2.168	54.491	1.00	74.51	C
ATOM	645	CG	GLU	A	469	5.462	2.344	53.012	1.00	75.00	C
ATOM	646	CD	GLU	A	469	4.468	3.475	52.763	1.00	75.76	C
ATOM	647	OE1	GLU	A	469	3.344	3.179	52.301	1.00	75.59	O
ATOM	648	OE2	GLU	A	469	4.797	4.654	53.041	1.00	76.40	O
ATOM	649	N	VAL	A	524	21.380	17.944	40.562	1.00	65.02	N
ATOM	650	CA	VAL	A	524	20.688	16.872	41.274	1.00	64.98	C
ATOM	651	C	VAL	A	524	21.574	15.621	41.393	1.00	64.92	C
ATOM	652	O	VAL	A	524	21.720	14.850	40.431	1.00	64.83	O
ATOM	653	CB	VAL	A	524	19.313	16.540	40.619	1.00	64.96	C
ATOM	654	CG1	VAL	A	524	18.539	15.517	41.456	1.00	64.83	C
ATOM	655	CG2	VAL	A	524	18.486	17.812	40.427	1.00	64.65	C
ATOM	656	N	ALA	A	525	22.164	15.446	42.579	1.00	64.83	N
ATOM	657	CA	ALA	A	525	23.045	14.310	42.896	1.00	64.93	C
ATOM	658	C	ALA	A	525	22.348	13.271	43.793	1.00	64.73	C
ATOM	659	O	ALA	A	525	21.578	13.635	44.681	1.00	64.90	O
ATOM	660	CB	ALA	A	525	24.339	14.804	43.551	1.00	64.92	C
ATOM	661	N	PRO	A	526	22.614	11.972	43.569	1.00	64.55	N
ATOM	662	CA	PRO	A	526	21.873	10.935	44.322	1.00	64.38	C
ATOM	663	C	PRO	A	526	22.283	10.805	45.791	1.00	63.99	C
ATOM	664	O	PRO	A	526	21.425	10.884	46.680	1.00	64.03	O
ATOM	665	CB	PRO	A	526	22.200	9.643	43.566	1.00	64.13	C
ATOM	666	CG	PRO	A	526	23.547	9.897	42.978	1.00	64.95	C
ATOM	667	CD	PRO	A	526	23.587	11.383	42.628	1.00	64.58	C

Figure 2 Table 2b - 11

ATOM	668	N	ARG A 527	23.576	10.595	46.033	1.00	63.48	N
ATOM	669	CA	ARG A 527	24.110	10.398	47.387	1.00	63.01	C
ATOM	670	C	ARG A 527	23.397	9.196	48.103	1.00	61.78	C
ATOM	671	O	ARG A 527	22.486	8.599	47.526	1.00	61.40	O
ATOM	672	CB	ARG A 527	24.082	11.747	48.149	1.00	63.58	C
ATOM	673	CG	ARG A 527	25.431	12.200	48.774	1.00	65.04	C
ATOM	674	CD	ARG A 527	26.632	12.016	47.834	1.00	67.41	C
ATOM	675	NE	ARG A 527	27.694	11.224	48.470	1.00	68.85	N
ATOM	676	CZ	ARG A 527	28.879	11.696	48.862	1.00	69.11	C
ATOM	677	NH1	ARG A 527	29.193	12.978	48.684	1.00	68.95	N
ATOM	678	NH2	ARG A 527	29.759	10.875	49.430	1.00	68.94	N
ATOM	679	N	PRO A 528	23.802	8.847	49.348	1.00	60.85	N
ATOM	680	CA	PRO A 528	23.678	7.471	49.892	1.00	59.73	C
ATOM	681	C	PRO A 528	22.352	6.684	49.763	1.00	58.58	C
ATOM	682	O	PRO A 528	21.261	7.224	49.961	1.00	58.74	O
ATOM	683	CB	PRO A 528	24.034	7.654	51.371	1.00	59.69	C
ATOM	684	CG	PRO A 528	24.943	8.810	51.387	1.00	60.51	C
ATOM	685	CD	PRO A 528	24.374	9.755	50.365	1.00	60.85	C
ATOM	686	N	GLY A 529	22.475	5.400	49.451	1.00	56.99	N
ATOM	687	CA	GLY A 529	21.344	4.488	49.510	1.00	55.52	C
ATOM	688	C	GLY A 529	20.794	3.943	48.202	1.00	54.40	C
ATOM	689	O	GLY A 529	20.623	4.669	47.228	1.00	54.24	O
ATOM	690	N	SER A 530	20.516	2.646	48.193	1.00	53.56	N
ATOM	691	CA	SER A 530	19.652	2.022	47.191	1.00	52.53	C
ATOM	692	C	SER A 530	19.245	0.710	47.775	1.00	52.05	C
ATOM	693	O	SER A 530	20.080	-0.170	47.991	1.00	51.52	O
ATOM	694	CB	SER A 530	20.341	1.798	45.838	1.00	52.62	C
ATOM	695	OG	SER A 530	19.650	0.815	45.068	1.00	51.04	O
ATOM	696	N	HIS A 531	17.950	0.596	48.032	1.00	51.83	N
ATOM	697	CA	HIS A 531	17.375	-0.567	48.676	1.00	51.89	C
ATOM	698	C	HIS A 531	17.669	-1.835	47.880	1.00	51.49	C
ATOM	699	O	HIS A 531	18.123	-2.826	48.447	1.00	52.48	O
ATOM	700	CB	HIS A 531	15.881	-0.337	48.861	1.00	52.46	C
ATOM	701	CG	HIS A 531	15.202	-1.373	49.696	1.00	55.17	C
ATOM	702	ND1	HIS A 531	14.665	-2.523	49.158	1.00	56.76	N
ATOM	703	CD2	HIS A 531	14.959	-1.429	51.029	1.00	57.15	C
ATOM	704	CE1	HIS A 531	14.124	-3.246	50.123	1.00	58.00	C
ATOM	705	NE2	HIS A 531	14.292	-2.607	51.269	1.00	58.72	N
ATOM	706	N	THR A 532	17.452	-1.800	46.566	1.00	50.78	N
ATOM	707	CA	THR A 532	17.720	-2.951	45.701	1.00	49.74	C
ATOM	708	C	THR A 532	19.186	-3.377	45.708	1.00	50.04	C
ATOM	709	O	THR A 532	19.489	-4.565	45.822	1.00	50.33	O
ATOM	710	CB	THR A 532	17.275	-2.679	44.272	1.00	49.55	C
ATOM	711	OG1	THR A 532	15.856	-2.537	44.247	1.00	48.90	O
ATOM	712	CG2	THR A 532	17.660	-3.807	43.359	1.00	48.85	C
ATOM	713	N	ILE A 533	20.101	-2.421	45.577	1.00	49.98	N
ATOM	714	CA	ILE A 533	21.523	-2.750	45.620	1.00	49.67	C
ATOM	715	C	ILE A 533	21.968	-3.238	47.010	1.00	49.91	C
ATOM	716	O	ILE A 533	22.786	-4.162	47.133	1.00	50.48	O
ATOM	717	CB	ILE A 533	22.391	-1.591	45.120	1.00	49.42	C
ATOM	718	CG1	ILE A 533	21.893	-1.092	43.751	1.00	49.29	C
ATOM	719	CG2	ILE A 533	23.856	-2.012	45.056	1.00	49.18	C
ATOM	720	CD1	ILE A 533	21.900	-2.124	42.609	1.00	46.74	C
ATOM	721	N	GLU A 534	21.398	-2.662	48.059	1.00	49.79	N
ATOM	722	CA	GLU A 534	21.759	-3.088	49.410	1.00	49.87	C
ATOM	723	C	GLU A 534	21.295	-4.509	49.708	1.00	49.77	C
ATOM	724	O	GLU A 534	21.955	-5.244	50.441	1.00	50.12	O
ATOM	725	CB	GLU A 534	21.244	-2.093	50.451	1.00	49.61	C
ATOM	726	CG	GLU A 534	22.029	-0.776	50.458	1.00	49.88	C
ATOM	727	CD	GLU A 534	21.381	0.269	51.337	1.00	50.90	C
ATOM	728	OE1	GLU A 534	21.192	-0.015	52.553	1.00	54.22	O
ATOM	729	OE2	GLU A 534	21.049	1.356	50.821	1.00	46.91	O
ATOM	730	N	PHE A 535	20.157	-4.881	49.133	1.00	49.95	N
ATOM	731	CA	PHE A 535	19.647	-6.237	49.208	1.00	50.09	C
ATOM	732	C	PHE A 535	20.650	-7.211	48.586	1.00	50.53	C
ATOM	733	O	PHE A 535	20.970	-8.248	49.201	1.00	50.02	O
ATOM	734	CB	PHE A 535	18.281	-6.328	48.513	1.00	49.92	C

Figure 2 Table 2b - 12

ATOM	735	CG	PHE	A	535	17.786	-7.738	48.299	1.00	51.25	C
ATOM	736	CD1	PHE	A	535	17.555	-8.600	49.386	1.00	51.59	C
ATOM	737	CD2	PHE	A	535	17.554	-8.221	47.005	1.00	51.98	C
ATOM	738	CE1	PHE	A	535	17.087	-9.895	49.189	1.00	50.39	C
ATOM	739	CE2	PHE	A	535	17.091	-9.545	46.797	1.00	50.13	C
ATOM	740	CZ	PHE	A	535	16.846	-10.368	47.889	1.00	50.49	C
ATOM	741	N	PHE	A	536	21.149	-6.885	47.385	1.00	50.47	N
ATOM	742	CA	PHE	A	536	22.137	-7.764	46.734	1.00	50.75	C
ATOM	743	C	PHE	A	536	23.370	-7.946	47.613	1.00	51.66	C
ATOM	744	O	PHE	A	536	23.923	-9.040	47.672	1.00	51.48	O
ATOM	745	CB	PHE	A	536	22.572	-7.274	45.331	1.00	49.46	C
ATOM	746	CG	PHE	A	536	21.466	-7.262	44.308	1.00	47.95	C
ATOM	747	CD1	PHE	A	536	21.426	-6.276	43.324	1.00	45.81	C
ATOM	748	CD2	PHE	A	536	20.453	-8.209	44.337	1.00	45.06	C
ATOM	749	CE1	PHE	A	536	20.401	-6.249	42.386	1.00	45.50	C
ATOM	750	CE2	PHE	A	536	19.419	-8.174	43.410	1.00	44.96	C
ATOM	751	CZ	PHE	A	536	19.396	-7.195	42.431	1.00	45.74	C
ATOM	752	N	GLU	A	537	23.804	-6.873	48.279	1.00	52.89	N
ATOM	753	CA	GLU	A	537	25.011	-6.929	49.107	1.00	54.07	C
ATOM	754	C	GLU	A	537	24.812	-7.754	50.376	1.00	54.96	C
ATOM	755	O	GLU	A	537	25.699	-8.516	50.769	1.00	54.91	O
ATOM	756	CB	GLU	A	537	25.545	-5.528	49.418	1.00	53.94	C
ATOM	757	CG	GLU	A	537	26.034	-4.823	48.164	1.00	54.78	C
ATOM	758	CD	GLU	A	537	26.716	-3.500	48.427	1.00	55.08	C
ATOM	759	OE1	GLU	A	537	26.366	-2.834	49.419	1.00	55.33	O
ATOM	760	OE2	GLU	A	537	27.597	-3.122	47.625	1.00	55.25	O
ATOM	761	N	MET	A	538	23.645	-7.622	50.995	1.00	55.82	N
ATOM	762	CA	MET	A	538	23.298	-8.476	52.115	1.00	57.97	C
ATOM	763	C	MET	A	538	23.384	-9.943	51.718	1.00	57.37	C
ATOM	764	O	MET	A	538	24.036	-10.751	52.409	1.00	57.58	O
ATOM	765	CB	MET	A	538	21.901	-8.167	52.632	1.00	57.80	C
ATOM	766	CG	MET	A	538	21.821	-6.956	53.516	1.00	60.54	C
ATOM	767	SD	MET	A	538	20.263	-6.976	54.415	1.00	64.80	S
ATOM	768	CE	MET	A	538	19.137	-6.506	53.096	1.00	64.84	C
ATOM	769	N	CYS	A	539	22.729	-10.277	50.608	1.00	56.61	N
ATOM	770	CA	CYS	A	539	22.784	-11.623	50.069	1.00	56.27	C
ATOM	771	C	CYS	A	539	24.212	-12.062	49.847	1.00	55.98	C
ATOM	772	O	CYS	A	539	24.627	-13.102	50.339	1.00	56.01	O
ATOM	773	CB	CYS	A	539	22.023	-11.702	48.759	1.00	55.65	C
ATOM	774	SG	CYS	A	539	20.288	-11.562	48.998	1.00	57.11	S
ATOM	775	N	ALA	A	540	24.959	-11.252	49.110	1.00	55.82	N
ATOM	776	CA	ALA	A	540	26.329	-11.573	48.790	1.00	56.08	C
ATOM	777	C	ALA	A	540	27.100	-11.844	50.068	1.00	56.23	C
ATOM	778	O	ALA	A	540	27.855	-12.809	50.135	1.00	56.16	O
ATOM	779	CB	ALA	A	540	26.980	-10.454	48.000	1.00	55.21	C
ATOM	780	N	ASN	A	541	26.902	-10.990	51.073	1.00	56.64	N
ATOM	781	CA	ASN	A	541	27.598	-11.133	52.349	1.00	57.22	C
ATOM	782	C	ASN	A	541	27.221	-12.420	53.064	1.00	56.90	C
ATOM	783	O	ASN	A	541	28.088	-13.201	53.430	1.00	56.43	O
ATOM	784	CB	ASN	A	541	27.346	-9.930	53.248	1.00	57.53	C
ATOM	785	CG	ASN	A	541	28.028	-8.682	52.741	1.00	58.26	C
ATOM	786	OD1	ASN	A	541	29.167	-8.731	52.271	1.00	59.03	O
ATOM	787	ND2	ASN	A	541	27.335	-7.552	52.831	1.00	58.21	N
ATOM	788	N	LEU	A	542	25.921	-12.628	53.231	1.00	56.95	N
ATOM	789	CA	LEU	A	542	25.393	-13.861	53.776	1.00	57.01	C
ATOM	790	C	LEU	A	542	25.962	-15.104	53.110	1.00	57.17	C
ATOM	791	O	LEU	A	542	26.394	-16.016	53.808	1.00	57.52	O
ATOM	792	CB	LEU	A	542	23.882	-13.873	53.692	1.00	56.93	C
ATOM	793	CG	LEU	A	542	23.247	-13.549	55.033	1.00	58.43	C
ATOM	794	CD1	LEU	A	542	21.786	-13.274	54.848	1.00	59.08	C
ATOM	795	CD2	LEU	A	542	23.440	-14.737	56.000	1.00	60.56	C
ATOM	796	N	ILE	A	543	25.986	-15.134	51.779	1.00	56.65	N
ATOM	797	CA	ILE	A	543	26.496	-16.294	51.050	1.00	56.25	C
ATOM	798	C	ILE	A	543	27.996	-16.513	51.283	1.00	56.81	C
ATOM	799	O	ILE	A	543	28.425	-17.628	51.614	1.00	57.14	O
ATOM	800	CB	ILE	A	543	26.188	-16.204	49.551	1.00	55.93	C
ATOM	801	CG1	ILE	A	543	24.676	-16.270	49.327	1.00	55.62	C

Figure 2 Table 2b - 13

ATOM	802	CG2	ILE	A	543	26.895	-17.311	48.776	1.00 55.43	C
ATOM	803	CD1	ILE	A	543	24.224	-15.671	48.004	1.00 54.49	C
ATOM	804	N	LYS	A	544	28.789	-15.459	51.122	1.00 57.10	N
ATOM	805	CA	LYS	A	544	30.237	-15.555	51.270	1.00 57.58	C
ATOM	806	C	LYS	A	544	30.636	-16.062	52.659	1.00 58.00	C
ATOM	807	O	LYS	A	544	31.591	-16.842	52.812	1.00 57.93	O
ATOM	808	CB	LYS	A	544	30.880	-14.195	51.013	1.00 57.43	C
ATOM	809	CG	LYS	A	544	32.375	-14.176	51.261	1.00 58.54	C
ATOM	810	CD	LYS	A	544	32.967	-12.801	51.048	1.00 59.79	C
ATOM	811	CE	LYS	A	544	34.384	-12.755	51.590	1.00 60.50	C
ATOM	812	NZ	LYS	A	544	35.205	-11.788	50.822	1.00 61.72	N
ATOM	813	N	ASN	A	545	29.834	-15.684	53.743	1.00 56.42	N
ATOM	814	CA	ASN	A	545	30.173	-15.967	55.143	1.00 57.01	C
ATOM	815	CB	ASN	A	545	29.828	-14.756	56.015	1.00 56.91	C
ATOM	816	CG	ASN	A	545	30.903	-13.691	55.962	1.00 56.71	C
ATOM	817	OD1	ASN	A	545	31.897	-13.765	56.684	1.00 56.97	O
ATOM	818	ND2	ASN	A	545	30.721	-12.707	55.096	1.00 54.86	N
ATOM	819	C	ASN	A	545	29.594	-17.236	55.759	1.00 57.41	C
ATOM	820	O	ASN	A	545	29.972	-17.605	56.866	1.00 57.60	O
ATOM	821	N	SER	A	546	28.695	-17.911	55.051	1.00 58.32	N
ATOM	822	CA	SER	A	546	28.052	-19.105	55.589	1.00 59.65	C
ATOM	823	CB	SER	A	546	26.542	-18.912	55.601	1.00 59.05	C
ATOM	824	OG	SER	A	546	26.073	-18.761	54.281	1.00 59.12	O
ATOM	825	C	SER	A	546	28.360	-20.367	54.791	1.00 60.79	C
ATOM	826	O	SER	A	546	27.821	-21.437	55.076	1.00 61.57	O
ATOM	827	N	CYS	A	547	29.251	-20.261	53.822	1.00 61.96	N
ATOM	828	CA	CYS	A	547	29.030	-21.002	52.618	1.00 62.98	C
ATOM	829	CB	CYS	A	547	27.912	-20.235	51.930	1.00 63.42	C
ATOM	830	SG	CYS	A	547	27.225	-20.882	50.483	1.00 64.33	S
ATOM	831	C	CYS	A	547	30.281	-21.031	51.747	1.00 63.55	C
ATOM	832	O	CYS	A	547	31.017	-20.050	51.673	1.00 63.74	O
ATOM	833	N	THR	A	548	30.526	-22.161	51.095	1.00 64.15	N
ATOM	834	CA	THR	A	548	31.703	-22.310	50.240	1.00 64.87	C
ATOM	835	CB	THR	A	548	32.842	-23.044	50.993	1.00 64.82	C
ATOM	836	OG1	THR	A	548	33.615	-22.075	51.707	1.00 65.00	O
ATOM	837	CG2	THR	A	548	33.772	-23.810	50.055	1.00 64.82	C
ATOM	838	C	THR	A	548	31.338	-22.998	48.930	1.00 65.36	C
ATOM	839	O	THR	A	548	30.548	-23.937	48.935	1.00 65.59	O
ATOM	840	N	VAL	A	549	31.898	-22.518	47.818	1.00 65.88	N
ATOM	841	CA	VAL	A	549	31.641	-23.113	46.497	1.00 66.60	C
ATOM	842	CB	VAL	A	549	32.242	-22.258	45.332	1.00 66.53	C
ATOM	843	CG1	VAL	A	549	31.778	-22.779	43.973	1.00 66.09	C
ATOM	844	CG2	VAL	A	549	31.874	-20.786	45.483	1.00 66.50	C
ATOM	845	C	VAL	A	549	32.206	-24.539	46.430	1.00 67.19	C
ATOM	846	O	VAL	A	549	33.298	-24.802	46.949	1.00 67.24	O
ATOM	847	N	ASN	A	550	31.452	-25.449	45.809	1.00 68.05	N
ATOM	848	CA	ASN	A	550	31.944	-26.798	45.484	1.00 68.82	C
ATOM	849	CB	ASN	A	550	30.821	-27.836	45.585	1.00 68.93	C
ATOM	850	CG	ASN	A	550	30.496	-28.201	47.014	1.00 69.05	C
ATOM	851	OD1	ASN	A	550	31.399	-28.410	47.832	1.00 69.17	O
ATOM	852	ND2	ASN	A	550	29.200	-28.279	47.328	1.00 68.93	N
ATOM	853	C	ASN	A	550	32.531	-26.842	44.082	1.00 69.11	C
ATOM	854	O	ASN	A	550	31.787	-26.722	43.098	1.00 69.74	O
TER	855		ASN	A	550					
ATOM	856	N	GLY	B	190	-0.839	-36.149	92.802	1.00 61.08	N
ATOM	857	CA	GLY	B	190	-0.848	-35.248	91.606	1.00 61.12	C
ATOM	858	C	GLY	B	190	0.088	-35.709	90.500	1.00 61.17	C
ATOM	859	O	GLY	B	190	1.297	-35.476	90.566	1.00 61.32	O
ATOM	860	N	GLN	B	191	-0.483	-36.337	89.469	1.00 61.01	N
ATOM	861	CA	GLN	B	191	0.277	-37.030	88.412	1.00 60.82	C
ATOM	862	C	GLN	B	191	1.310	-36.164	87.683	1.00 60.48	C
ATOM	863	O	GLN	B	191	1.248	-34.934	87.724	1.00 60.74	O
ATOM	864	CB	GLN	B	191	-0.680	-37.690	87.396	1.00 60.78	C
ATOM	865	CG	GLN	B	191	0.012	-38.611	86.374	1.00 61.15	C
ATOM	866	CD	GLN	B	191	-0.878	-39.721	85.839	1.00 62.07	C
ATOM	867	OE1	GLN	B	191	-2.031	-39.494	85.472	1.00 62.92	O
ATOM	868	NE2	GLN	B	191	-0.333	-40.935	85.779	1.00 62.56	N

Figure 2 Table 2b - 14

ATOM	869	N	GLU	B	192	2.266	-36.827	87.033	1.00	59.93	N
ATOM	870	CA	GLU	B	192	3.168	-36.168	86.106	1.00	59.50	C
ATOM	871	C	GLU	B	192	2.399	-35.818	84.828	1.00	59.16	C
ATOM	872	O	GLU	B	192	1.288	-36.309	84.604	1.00	59.03	O
ATOM	873	CB	GLU	B	192	4.397	-37.043	85.803	1.00	59.53	C
ATOM	874	CG	GLU	B	192	4.150	-38.258	84.895	1.00	60.21	C
ATOM	875	CD	GLU	B	192	3.766	-39.522	85.659	1.00	62.00	C
ATOM	876	OE1	GLU	B	192	4.296	-39.753	86.773	1.00	62.42	O
ATOM	877	OE2	GLU	B	192	2.940	-40.305	85.137	1.00	63.00	O
ATOM	878	N	MET	B	193	2.982	-34.961	83.999	1.00	58.65	N
ATOM	879	CA	MET	B	193	2.344	-34.605	82.745	1.00	58.35	C
ATOM	880	C	MET	B	193	3.195	-35.008	81.553	1.00	58.34	C
ATOM	881	O	MET	B	193	4.419	-35.123	81.656	1.00	58.01	O
ATOM	882	CB	MET	B	193	1.950	-33.130	82.719	1.00	58.26	C
ATOM	883	CG	MET	B	193	0.856	-32.823	83.710	1.00	57.97	C
ATOM	884	SD	MET	B	193	-0.188	-31.456	83.234	1.00	58.11	S
ATOM	885	CE	MET	B	193	-1.360	-31.494	84.591	1.00	57.74	C
ATOM	886	N	TYR	B	194	2.527	-35.234	80.428	1.00	58.58	N
ATOM	887	CA	TYR	B	194	3.184	-35.758	79.238	1.00	59.04	C
ATOM	888	C	TYR	B	194	3.210	-34.760	78.069	1.00	59.60	C
ATOM	889	O	TYR	B	194	2.308	-33.942	77.904	1.00	59.30	O
ATOM	890	CB	TYR	B	194	2.550	-37.094	78.844	1.00	58.68	C
ATOM	891	CG	TYR	B	194	2.773	-38.193	79.870	1.00	58.31	C
ATOM	892	CD1	TYR	B	194	2.000	-38.267	81.028	1.00	58.10	C
ATOM	893	CD2	TYR	B	194	3.767	-39.155	79.683	1.00	58.14	C
ATOM	894	CE1	TYR	B	194	2.210	-39.270	81.970	1.00	58.06	C
ATOM	895	CE2	TYR	B	194	3.986	-40.160	80.612	1.00	57.69	C
ATOM	896	CZ	TYR	B	194	3.205	-40.214	81.754	1.00	57.68	C
ATOM	897	OH	TYR	B	194	3.419	-41.210	82.672	1.00	56.21	O
ATOM	898	N	ALA	B	195	4.275	-34.827	77.280	1.00	60.47	N
ATOM	899	CA	ALA	B	195	4.431	-33.957	76.136	1.00	61.76	C
ATOM	900	C	ALA	B	195	4.346	-34.737	74.830	1.00	62.69	C
ATOM	901	O	ALA	B	195	5.206	-35.565	74.515	1.00	62.73	O
ATOM	902	CB	ALA	B	195	5.744	-33.178	76.224	1.00	61.51	C
ATOM	903	N	PHE	B	196	3.287	-34.467	74.081	1.00	64.12	N
ATOM	904	CA	PHE	B	196	3.141	-34.987	72.741	1.00	65.53	C
ATOM	905	C	PHE	B	196	3.657	-33.909	71.812	1.00	67.46	C
ATOM	906	O	PHE	B	196	3.039	-32.852	71.651	1.00	67.66	O
ATOM	907	CB	PHE	B	196	1.680	-35.309	72.452	1.00	65.08	C
ATOM	908	CG	PHE	B	196	1.091	-36.316	73.385	1.00	63.71	C
ATOM	909	CD1	PHE	B	196	0.470	-35.914	74.554	1.00	62.22	C
ATOM	910	CD2	PHE	B	196	1.167	-37.665	73.100	1.00	62.91	C
ATOM	911	CE1	PHE	B	196	-0.065	-36.830	75.413	1.00	62.52	C
ATOM	912	CE2	PHE	B	196	0.623	-38.590	73.958	1.00	62.81	C
ATOM	913	CZ	PHE	B	196	0.011	-38.176	75.119	1.00	63.22	C
ATOM	914	N	ARG	B	197	4.815	-34.175	71.218	1.00	69.81	N
ATOM	915	CA	ARG	B	197	5.526	-33.162	70.461	1.00	72.01	C
ATOM	916	C	ARG	B	197	5.341	-33.337	68.964	1.00	73.57	C
ATOM	917	O	ARG	B	197	5.522	-34.438	68.425	1.00	73.50	O
ATOM	918	CB	ARG	B	197	7.004	-33.100	70.864	1.00	71.94	C
ATOM	919	CG	ARG	B	197	7.286	-31.995	71.887	1.00	72.30	C
ATOM	920	CD	ARG	B	197	8.748	-31.913	72.282	1.00	72.30	C
ATOM	921	NE	ARG	B	197	9.090	-32.854	73.348	1.00	73.34	N
ATOM	922	CZ	ARG	B	197	9.154	-32.550	74.648	1.00	73.99	C
ATOM	923	NH1	ARG	B	197	8.888	-31.322	75.077	1.00	73.46	N
ATOM	924	NH2	ARG	B	197	9.481	-33.488	75.531	1.00	74.28	N
ATOM	925	N	SER	B	198	4.990	-32.216	68.322	1.00	75.59	N
ATOM	926	CA	SER	B	198	4.488	-32.160	66.942	1.00	77.47	C
ATOM	927	C	SER	B	198	5.389	-32.903	65.964	1.00	78.79	C
ATOM	928	O	SER	B	198	5.006	-33.945	65.431	1.00	79.00	O
ATOM	929	CB	SER	B	198	4.298	-30.693	66.504	1.00	77.49	C
ATOM	930	OG	SER	B	198	3.819	-30.601	65.172	1.00	76.95	O
ATOM	931	N	GLU	B	199	6.590	-32.361	65.755	1.00	80.59	N
ATOM	932	CA	GLU	B	199	7.622	-32.969	64.906	1.00	82.07	C
ATOM	933	C	GLU	B	199	7.168	-33.158	63.464	1.00	82.73	C
ATOM	934	O	GLU	B	199	5.982	-33.009	63.137	1.00	82.83	O
ATOM	935	CB	GLU	B	199	8.122	-34.288	65.497	1.00	82.36	C

Figure 2 Table 2b - 15

ATOM	936	CG	GLU	B	199	9.582	-34.571	65.216	1.00	83.37	C
ATOM	937	CD	GLU	B	199	10.290	-35.101	66.439	1.00	84.88	C
ATOM	938	OE1	GLU	B	199	10.791	-34.261	67.223	1.00	84.79	O
ATOM	939	OE2	GLU	B	199	10.335	-36.347	66.618	1.00	85.12	O
ATOM	940	N	GLU	B	200	8.124	-33.488	62.603	1.00	83.60	N
ATOM	941	CA	GLU	B	200	7.910	-33.376	61.169	1.00	84.53	C
ATOM	942	C	GLU	B	200	7.204	-32.053	60.846	1.00	84.53	C
ATOM	943	O	GLU	B	200	7.380	-31.060	61.576	1.00	84.40	O
ATOM	944	CB	GLU	B	200	7.166	-34.599	60.609	1.00	84.78	C
ATOM	945	CG	GLU	B	200	7.990	-35.890	60.673	1.00	86.57	C
ATOM	946	CD	GLU	B	200	7.655	-36.891	59.562	1.00	88.60	C
ATOM	947	OE1	GLU	B	200	7.052	-36.496	58.520	1.00	89.99	O
ATOM	948	OE2	GLU	B	200	8.010	-38.085	59.733	1.00	89.94	O
ATOM	949	N	ARG	B	201	6.402	-32.046	59.778	1.00	84.50	N
ATOM	950	CA	ARG	B	201	5.990	-30.803	59.104	1.00	84.33	C
ATOM	951	C	ARG	B	201	7.217	-29.946	58.786	1.00	83.54	C
ATOM	952	O	ARG	B	201	7.338	-29.401	57.692	1.00	83.79	O
ATOM	953	CB	ARG	B	201	4.954	-30.008	59.919	1.00	84.75	C
ATOM	954	CG	ARG	B	201	4.416	-28.774	59.183	1.00	86.05	C
ATOM	955	CD	ARG	B	201	2.932	-28.553	59.457	1.00	88.24	C
ATOM	956	NE	ARG	B	201	2.182	-28.387	58.210	1.00	88.97	N
ATOM	957	CZ	ARG	B	201	1.442	-29.339	57.638	1.00	89.45	C
ATOM	958	NH1	ARG	B	201	1.328	-30.540	58.201	1.00	89.48	N
ATOM	959	NH2	ARG	B	201	0.807	-29.086	56.500	1.00	89.19	N
ATOM	960	N	PHE	B	202	8.082	-29.793	59.745	1.00	81.94	N
ATOM	961	CA	PHE	B	202	9.389	-29.189	59.530	1.00	80.74	C
ATOM	962	C	PHE	B	202	10.465	-30.273	59.630	1.00	79.96	C
ATOM	963	O	PHE	B	202	11.578	-30.035	60.109	1.00	80.07	O
ATOM	964	CB	PHE	B	202	9.586	-28.007	60.491	1.00	80.48	C
ATOM	965	CG	PHE	B	202	8.436	-27.035	60.461	1.00	79.82	C
ATOM	966	CD1	PHE	B	202	7.500	-27.009	61.493	1.00	79.03	C
ATOM	967	CD2	PHE	B	202	8.247	-26.196	59.354	1.00	79.16	C
ATOM	968	CE1	PHE	B	202	6.412	-26.133	61.446	1.00	79.60	C
ATOM	969	CE2	PHE	B	202	7.165	-25.317	59.294	1.00	78.88	C
ATOM	970	CZ	PHE	B	202	6.245	-25.283	60.343	1.00	79.57	C
ATOM	971	N	LYS	B	203	10.075	-31.463	59.140	1.00	77.26	N
ATOM	972	CA	LYS	B	203	10.971	-32.607	58.946	1.00	76.19	C
ATOM	973	C	LYS	B	203	11.934	-32.348	57.793	1.00	75.42	C
ATOM	974	O	LYS	B	203	13.138	-32.161	57.992	1.00	77.06	O
ATOM	975	CB	LYS	B	203	10.185	-33.910	58.670	1.00	76.32	C
ATOM	976	CG	LYS	B	203	8.858	-33.818	57.825	1.00	76.29	C
ATOM	977	CD	LYS	B	203	8.771	-32.660	56.794	1.00	74.29	C
ATOM	978	CE	LYS	B	203	7.601	-32.864	55.811	1.00	73.84	C
ATOM	979	NZ	LYS	B	203	7.361	-34.321	55.510	1.00	71.15	N
ATOM	980	N	SER	B	204	11.411	-32.389	56.599	1.00	75.47	N
ATOM	981	CA	SER	B	204	12.138	-31.937	55.443	1.00	74.23	C
ATOM	982	C	SER	B	204	11.656	-30.514	55.157	1.00	73.28	C
ATOM	983	O	SER	B	204	10.519	-30.173	55.496	1.00	73.27	O
ATOM	984	CB	SER	B	204	11.892	-32.884	54.256	1.00	74.29	C
ATOM	985	OG	SER	B	204	10.508	-33.116	54.044	1.00	74.07	O
ATOM	986	N	PRO	B	205	12.531	-29.662	54.579	1.00	72.25	N
ATOM	987	CA	PRO	B	205	12.113	-28.350	54.100	1.00	71.44	C
ATOM	988	C	PRO	B	205	11.014	-28.442	53.047	1.00	70.85	C
ATOM	989	O	PRO	B	205	10.935	-29.438	52.341	1.00	70.70	O
ATOM	990	CB	PRO	B	205	13.395	-27.795	53.477	1.00	71.53	C
ATOM	991	CG	PRO	B	205	14.493	-28.502	54.192	1.00	71.56	C
ATOM	992	CD	PRO	B	205	13.977	-29.874	54.387	1.00	71.99	C
ATOM	993	N	PRO	B	206	10.153	-27.420	52.932	1.00	70.95	N
ATOM	994	CA	PRO	B	206	9.091	-27.438	51.917	1.00	70.99	C
ATOM	995	C	PRO	B	206	9.621	-27.666	50.502	1.00	71.22	C
ATOM	996	O	PRO	B	206	10.705	-27.198	50.164	1.00	71.03	O
ATOM	997	CB	PRO	B	206	8.476	-26.034	52.024	1.00	70.87	C
ATOM	998	CG	PRO	B	206	9.506	-25.208	52.736	1.00	70.49	C
ATOM	999	CD	PRO	B	206	10.171	-26.150	53.680	1.00	70.72	C
ATOM	1000	N	ILE	B	207	8.866	-28.393	49.687	1.00	71.89	N
ATOM	1001	CA	ILE	B	207	9.207	-28.534	48.277	1.00	72.66	C
ATOM	1002	C	ILE	B	207	8.966	-27.203	47.590	1.00	73.19	C

Figure 2 Table 2b - 16

ATOM	1003	O	ILE	B	207	8.157	-26.400	48.055	1.00	73.24	O
ATOM	1004	CB	ILE	B	207	8.398	-29.648	47.569	1.00	72.66	C
ATOM	1005	CG1	ILE	B	207	6.896	-29.490	47.848	1.00	73.03	C
ATOM	1006	CG2	ILE	B	207	8.930	-31.025	47.969	1.00	72.38	C
ATOM	1007	CD1	ILE	B	207	5.990	-30.260	46.891	1.00	73.23	C
ATOM	1008	N	LEU	B	208	9.672	-26.966	46.491	1.00	74.03	N
ATOM	1009	CA	LEU	B	208	9.579	-25.684	45.806	1.00	74.87	C
ATOM	1010	C	LEU	B	208	8.186	-25.410	45.199	1.00	75.86	C
ATOM	1011	O	LEU	B	208	7.324	-24.906	45.912	1.00	75.82	O
ATOM	1012	CB	LEU	B	208.	10.732	-25.479	44.800	1.00	74.66	C
ATOM	1013	CG	LEU	B	208	10.869	-24.139	44.065	1.00	74.06	C
ATOM	1014	CD1	LEU	B	208	11.271	-23.020	44.998	1.00	72.97	C
ATOM	1015	CD2	LEU	B	208	11.879	-24.268	42.942	1.00	74.26	C
ATOM	1016	N	PRO	B	209	7.933	-25.822	43.932	1.00	77.06	N
ATOM	1017	CA	PRO	B	209	6.991	-25.074	43.074	1.00	77.87	C
ATOM	1018	C	PRO	B	209	5.618	-24.680	43.660	1.00	78.58	C
ATOM	1019	O	PRO	B	209	4.660	-25.458	43.538	1.00	78.75	O
ATOM	1020	CB	PRO	B	209	6.819	-25.995	41.852	1.00	77.62	C
ATOM	1021	CG	PRO	B	209	8.093	-26.744	41.784	1.00	77.36	C
ATOM	1022	CD	PRO	B	209	8.436	-27.023	43.233	1.00	77.08	C
ATOM	1023	N	PRO	B	210	5.522	-23.480	44.293	1.00	78.97	N
ATOM	1024	CA	PRO	B	210	4.188	-22.891	44.338	1.00	79.20	C
ATOM	1025	C	PRO	B	210	3.828	-22.466	42.903	1.00	79.25	C
ATOM	1026	O	PRO	B	210	2.928	-23.053	42.297	1.00	79.23	O
ATOM	1027	CB	PRO	B	210	4.359	-21.682	45.290	1.00	79.28	C
ATOM	1028	CG	PRO	B	210	5.668	-21.922	46.022	1.00	78.67	C
ATOM	1029	CD	PRO	B	210	6.507	-22.629	44.997	1.00	79.09	C
ATOM	1030	N	HIS	B	211	4.563	-21.486	42.372	1.00	79.38	N
ATOM	1031	CA	HIS	B	211	4.500	-21.065	40.964	1.00	79.44	C
ATOM	1032	C	HIS	B	211	5.814	-20.332	40.626	1.00	79.52	C
ATOM	1033	O	HIS	B	211	5.920	-19.620	39.615	1.00	79.68	O
ATOM	1034	CB	HIS	B	211	3.289	-20.153	40.724	1.00	79.46	C
ATOM	1035	CG	HIS	B	211	2.660	-20.321	39.372	1.00	79.73	C
ATOM	1036	ND1	HIS	B	211	1.464	-20.982	39.184	1.00	79.81	N
ATOM	1037	CD2	HIS	B	211	3.060	-19.915	38.143	1.00	79.83	C
ATOM	1038	CE1	HIS	B	211	1.154	-20.977	37.900	1.00	79.75	C
ATOM	1039	NE2	HIS	B	211	2.106	-20.336	37.246	1.00	79.95	N
ATOM	1040	N	LEU	B	212	6.811	-20.558	41.484	1.00	79.54	N
ATOM	1041	CA	LEU	B	212	8.085	-19.835	41.515	1.00	79.34	C
ATOM	1042	C	LEU	B	212	9.144	-20.622	40.757	1.00	78.98	C
ATOM	1043	O	LEU	B	212	9.481	-21.751	41.139	1.00	78.77	O
ATOM	1044	CB	LEU	B	212	8.535	-19.681	42.975	1.00	79.56	C
ATOM	1045	CG	LEU	B	212	8.875	-18.321	43.596	1.00	80.14	C
ATOM	1046	CD1	LEU	B	212	9.164	-18.533	45.080	1.00	80.64	C
ATOM	1047	CD2	LEU	B	212	10.034	-17.595	42.911	1.00	79.86	C
ATOM	1048	N	LEU	B	213	9.680	-20.025	39.695	1.00	78.56	N
ATOM	1049	CA	LEU	B	213	10.574	-20.761	38.792	1.00	78.12	C
ATOM	1050	C	LEU	B	213	12.004	-20.895	39.334	1.00	77.61	C
ATOM	1051	O	LEU	B	213	12.609	-19.914	39.775	1.00	77.79	O
ATOM	1052	CB	LEU	B	213	10.565	-20.160	37.376	1.00	78.06	C
ATOM	1053	CG	LEU	B	213	9.218	-20.029	36.659	1.00	77.73	C
ATOM	1054	CD1	LEU	B	213	9.308	-19.016	35.523	1.00	77.59	C
ATOM	1055	CD2	LEU	B	213	8.730	-21.369	36.150	1.00	78.03	C
ATOM	1056	N	GLN	B	214	12.505	-22.128	39.300	1.00	76.70	N
ATOM	1057	CA	GLN	B	214	13.855	-22.495	39.716	1.00	75.91	C
ATOM	1058	C	GLN	B	214	14.903	-21.950	38.755	1.00	75.61	C
ATOM	1059	O	GLN	B	214	15.968	-21.494	39.171	1.00	75.11	O
ATOM	1060	CB	GLN	B	214	13.937	-24.018	39.747	1.00	75.83	C
ATOM	1061	CG	GLN	B	214	15.252	-24.618	40.199	1.00	75.64	C
ATOM	1062	CD	GLN	B	214	15.107	-26.089	40.528	1.00	75.46	C
ATOM	1063	OE1	GLN	B	214	16.004	-26.888	40.266	1.00	76.59	O
ATOM	1064	NE2	GLN	B	214	13.962	-26.460	41.088	1.00	74.93	N
ATOM	1065	N	VAL	B	215	14.594	-22.037	37.465	1.00	75.61	N
ATOM	1066	CA	VAL	B	215	15.473	-21.571	36.403	1.00	75.68	C
ATOM	1067	C	VAL	B	215	14.733	-20.646	35.439	1.00	75.82	C
ATOM	1068	O	VAL	B	215	13.554	-20.843	35.152	1.00	75.56	O
ATOM	1069	CB	VAL	B	215	16.125	-22.743	35.613	1.00	75.67	C

Figure 2 Table 2b - 17

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ATOM   1070  CG1 VAL B 215      17.219 -23.404  36.436  1.00 75.05           C
ATOM   1071  CG2 VAL B 215      15.076 -23.760  35.155  1.00 75.75           C
ATOM   1072  N   ILE B 216      15.436 -19.627  34.960  1.00 76.39           N
ATOM   1073  CA  ILE B 216      14.904 -18.716  33.955  1.00 76.93           C
ATOM   1074  C   ILE B 216      15.882 -18.683  32.792  1.00 77.71           C
ATOM   1075  O   ILE B 216      17.001 -18.189  32.937  1.00 77.58           O
ATOM   1076  CB  ILE B 216      14.698 -17.270  34.512  1.00 76.78           C
ATOM   1077  CG1 ILE B 216      13.998 -17.282  35.879  1.00 75.99           C
ATOM   1078  CG2 ILE B 216      13.958 -16.391  33.501  1.00 76.36           C
ATOM   1079  CD1 ILE B 216      12.529 -17.634  35.855  1.00 74.74           C
ATOM   1080  N   LEU B 217      15.467 -19.247  31.658  1.00 78.94           N
ATOM   1081  CA  LEU B 217      16.245 -19.188  30.418  1.00 80.18           C
ATOM   1082  C   LEU B 217      15.933 -17.881  29.709  1.00 80.91           C
ATOM   1083  O   LEU B 217      14.793 -17.651  29.304  1.00 80.87           O
ATOM   1084  CB  LEU B 217      15.897 -20.363  29.486  1.00 80.27           C
ATOM   1085  CG  LEU B 217      16.635 -21.716  29.409  1.00 80.75           C
ATOM   1086  CD1 LEU B 217      17.849 -21.664  28.479  1.00 80.34           C
ATOM   1087  CD2 LEU B 217      17.012 -22.281  30.786  1.00 81.64           C
ATOM   1088  N   ASN B 218      16.935 -17.017  29.584  1.00 82.10           N
ATOM   1089  CA  ASN B 218      16.816 -15.804  28.766  1.00 83.24           C
ATOM   1090  C   ASN B 218      17.823 -15.793  27.611  1.00 84.22           C
ATOM   1091  O   ASN B 218      18.646 -14.879  27.485  1.00 84.49           O
ATOM   1092  CB  ASN B 218      16.892 -14.531  29.625  1.00 82.95           C
ATOM   1093  CG  ASN B 218      15.621 -14.299  30.448  1.00 82.88           C
ATOM   1094  OD1 ASN B 218      14.586 -14.925  30.211  1.00 82.66           O
ATOM   1095  ND2 ASN B 218      15.700 -13.390  31.415  1.00 82.15           N
ATOM   1096  N   LYS B 219      17.746 -16.840  26.787  1.00 85.39           N
ATOM   1097  CA  LYS B 219      18.503 -16.946  25.539  1.00 86.71           C
ATOM   1098  C   LYS B 219      18.075 -15.829  24.583  1.00 87.62           C
ATOM   1099  O   LYS B 219      18.793 -14.837  24.440  1.00 87.66           O
ATOM   1100  CB  LYS B 219      18.342 -18.363  24.933  1.00 86.68           C
ATOM   1101  CG  LYS B 219      18.286 -18.488  23.398  1.00 86.72           C
ATOM   1102  CD  LYS B 219      19.647 -18.604  22.727  1.00 86.30           C
ATOM   1103  CE  LYS B 219      19.478 -18.858  21.237  1.00 85.74           C
ATOM   1104  NZ  LYS B 219      20.769 -18.816  20.514  1.00 85.66           N
ATOM   1105  N   ASP B 220      16.902 -15.992  23.959  1.00 88.79           N
ATOM   1106  CA  ASP B 220      16.272 -14.983  23.082  1.00 89.90           C
ATOM   1107  C   ASP B 220      17.058 -14.596  21.811  1.00 90.52           C
ATOM   1108  O   ASP B 220      16.473 -14.032  20.878  1.00 90.68           O
ATOM   1109  CB  ASP B 220      15.895 -13.719  23.885  1.00 89.93           C
ATOM   1110  CG  ASP B 220      14.961 -14.017  25.055  1.00 90.52           C
ATOM   1111  OD1 ASP B 220      13.824 -14.482  24.812  1.00 91.11           O
ATOM   1112  OD2 ASP B 220      15.360 -13.777  26.219  1.00 90.97           O
ATOM   1113  N   THR B 221      18.350 -14.942  21.767  1.00 91.27           N
ATOM   1114  CA  THR B 221      19.364 -14.312  20.887  1.00 91.82           C
ATOM   1115  C   THR B 221      19.772 -12.955  21.515  1.00 92.22           C
ATOM   1116  O   THR B 221      19.903 -11.934  20.822  1.00 92.30           O
ATOM   1117  CB  THR B 221      18.909 -14.193  19.380  1.00 91.85           C
ATOM   1118  OG1 THR B 221      18.359 -15.442  18.942  1.00 91.90           O
ATOM   1119  CG2 THR B 221      20.077 -13.809  18.456  1.00 91.57           C
ATOM   1120  N   ASN B 222      19.979 -12.982  22.837  1.00 92.60           N
ATOM   1121  CA  ASN B 222      20.199 -11.787  23.671  1.00 92.98           C
ATOM   1122  C   ASN B 222      21.513 -11.059  23.374  1.00 92.98           C
ATOM   1123  O   ASN B 222      21.595  -9.831  23.480  1.00 92.94           O
ATOM   1124  CB  ASN B 222      20.128 -12.160  25.162  1.00 93.04           C
ATOM   1125  CG  ASN B 222      19.771 -10.977  26.057  1.00 93.76           C
ATOM   1126  OD1 ASN B 222      19.014 -10.082  25.666  1.00 94.55           O
ATOM   1127  ND2 ASN B 222      20.305 -10.981  27.276  1.00 94.07           N
ATOM   1128  N   PRO B 233       5.634 -10.510  33.123  1.00 81.85           N
ATOM   1129  CA  PRO B 233       4.342 -11.192  33.128  1.00 81.75           C
ATOM   1130  C   PRO B 233       4.202 -12.275  34.207  1.00 81.64           C
ATOM   1131  O   PRO B 233       3.169 -12.951  34.257  1.00 81.80           O
ATOM   1132  CB  PRO B 233       4.283 -11.816  31.729  1.00 81.83           C
ATOM   1133  CG  PRO B 233       5.120 -10.875  30.853  1.00 81.85           C
ATOM   1134  CD  PRO B 233       5.983 -10.021  31.775  1.00 81.95           C
ATOM   1135  N   ASN B 234       5.214 -12.417  35.069  1.00 81.35           N
ATOM   1136  CA  ASN B 234       5.220 -13.457  36.117  1.00 80.90           C
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Figure 2 Table 2b - 18

ATOM	1137	C	ASN	B	234	5.035	-12.958	37.564	1.00	80.38	C
ATOM	1138	O	ASN	B	234	5.482	-11.866	37.931	1.00	80.47	O
ATOM	1139	CB	ASN	B	234	6.467	-14.346	36.000	1.00	81.08	C
ATOM	1140	CG	ASN	B	234	6.244	-15.569	35.104	1.00	81.72	C
ATOM	1141	OD1	ASN	B	234	5.717	-15.469	33.987	1.00	81.47	O
ATOM	1142	ND2	ASN	B	234	6.665	-16.733	35.594	1.00	82.23	N
ATOM	1143	N	HIS	B	235	4.406	-13.792	38.385	1.00	79.38	N
ATOM	1144	CA	HIS	B	235	3.738	-13.327	39.604	1.00	78.26	C
ATOM	1145	C	HIS	B	235	4.641	-13.094	40.832	1.00	76.85	C
ATOM	1146	O	HIS	B	235	5.155	-11.988	41.038	1.00	76.89	O
ATOM	1147	CB	HIS	B	235	2.552	-14.262	39.961	1.00	78.92	C
ATOM	1148	CG	HIS	B	235	1.752	-14.728	38.776	1.00	80.11	C
ATOM	1149	ND1	HIS	B	235	1.400	-16.050	38.590	1.00	81.29	N
ATOM	1150	CD2	HIS	B	235	1.241	-14.052	37.717	1.00	80.96	C
ATOM	1151	CE1	HIS	B	235	0.706	-16.168	37.472	1.00	81.56	C
ATOM	1152	NE2	HIS	B	235	0.596	-14.969	36.922	1.00	81.61	N
ATOM	1153	N	VAL	B	236	4.808	-14.138	41.644	1.00	74.58	N
ATOM	1154	CA	VAL	B	236	5.433	-14.020	42.958	1.00	72.19	C
ATOM	1155	C	VAL	B	236	6.959	-14.231	42.925	1.00	70.17	C
ATOM	1156	O	VAL	B	236	7.570	-14.544	43.959	1.00	70.22	O
ATOM	1157	CB	VAL	B	236	4.723	-14.966	44.003	1.00	72.54	C
ATOM	1158	CG1	VAL	B	236	4.980	-16.448	43.687	1.00	72.72	C
ATOM	1159	CG2	VAL	B	236	5.111	-14.620	45.460	1.00	72.60	C
ATOM	1160	N	MET	B	237	7.580	-14.060	41.754	1.00	67.05	N
ATOM	1161	CA	MET	B	237	9.042	-14.088	41.696	1.00	64.03	C
ATOM	1162	C	MET	B	237	9.615	-12.700	41.944	1.00	61.36	C
ATOM	1163	O	MET	B	237	10.835	-12.518	41.974	1.00	60.68	O
ATOM	1164	CB	MET	B	237	9.607	-14.772	40.438	1.00	63.84	C
ATOM	1165	CG	MET	B	237	9.056	-14.362	39.091	1.00	64.44	C
ATOM	1166	SD	MET	B	237	9.321	-15.711	37.858	1.00	66.51	S
ATOM	1167	CE	MET	B	237	8.251	-16.976	38.556	1.00	66.62	C
ATOM	1168	N	LEU	B	238	8.717	-11.735	42.151	1.00	58.44	N
ATOM	1169	CA	LEU	B	238	9.098	-10.387	42.546	1.00	56.09	C
ATOM	1170	C	LEU	B	238	9.870	-10.435	43.850	1.00	54.30	C
ATOM	1171	O	LEU	B	238	9.525	-11.197	44.754	1.00	53.79	O
ATOM	1172	CB	LEU	B	238	7.872	-9.492	42.730	1.00	55.92	C
ATOM	1173	CG	LEU	B	238	7.142	-8.895	41.527	1.00	57.70	C
ATOM	1174	CD1	LEU	B	238	5.863	-8.216	42.011	1.00	58.59	C
ATOM	1175	CD2	LEU	B	238	8.003	-7.918	40.676	1.00	57.15	C
ATOM	1176	N	ASN	B	239	10.916	-9.622	43.921	1.00	52.35	N
ATOM	1177	CA	ASN	B	239	11.754	-9.478	45.112	1.00	51.54	C
ATOM	1178	C	ASN	B	239	12.715	-10.639	45.396	1.00	50.62	C
ATOM	1179	O	ASN	B	239	13.498	-10.571	46.332	1.00	50.55	O
ATOM	1180	CB	ASN	B	239	10.917	-9.125	46.372	1.00	51.49	C
ATOM	1181	CG	ASN	B	239	10.297	-7.726	46.310	1.00	51.39	C
ATOM	1182	OD1	ASN	B	239	10.046	-7.186	45.242	1.00	53.57	O
ATOM	1183	ND2	ASN	B	239	10.050	-7.143	47.465	1.00	53.46	N
ATOM	1184	N	HIS	B	240	12.658	-11.691	44.588	1.00	49.86	N
ATOM	1185	CA	HIS	B	240	13.496	-12.869	44.791	1.00	49.17	C
ATOM	1186	C	HIS	B	240	14.842	-12.749	44.122	1.00	49.23	C
ATOM	1187	O	HIS	B	240	14.951	-12.196	43.027	1.00	49.79	O
ATOM	1188	CB	HIS	B	240	12.787	-14.133	44.304	1.00	48.77	C
ATOM	1189	CG	HIS	B	240	11.722	-14.597	45.231	1.00	47.13	C
ATOM	1190	ND1	HIS	B	240	11.975	-15.458	46.277	1.00	46.68	N
ATOM	1191	CD2	HIS	B	240	10.410	-14.281	45.312	1.00	47.15	C
ATOM	1192	CE1	HIS	B	240	10.860	-15.659	46.958	1.00	46.36	C
ATOM	1193	NE2	HIS	B	240	9.892	-14.967	46.387	1.00	46.35	N
ATOM	1194	N	LEU	B	241	15.863	-13.288	44.776	1.00	48.90	N
ATOM	1195	CA	LEU	B	241	17.219	-13.251	44.240	1.00	48.80	C
ATOM	1196	C	LEU	B	241	17.441	-14.323	43.156	1.00	49.02	C
ATOM	1197	O	LEU	B	241	17.053	-15.500	43.309	1.00	48.91	O
ATOM	1198	CB	LEU	B	241	18.261	-13.372	45.374	1.00	48.68	C
ATOM	1199	CG	LEU	B	241	19.748	-13.209	45.036	1.00	48.46	C
ATOM	1200	CD1	LEU	B	241	20.072	-11.760	44.612	1.00	46.76	C
ATOM	1201	CD2	LEU	B	241	20.638	-13.669	46.177	1.00	47.35	C
ATOM	1202	N	TYR	B	242	18.038	-13.886	42.049	1.00	48.72	N
ATOM	1203	CA	TYR	B	242	18.491	-14.789	40.995	1.00	48.48	C

Figure 2 Table 2b - 19

ATOM	1204	C	TYR	B	242	19.954	-14.512	40.750	1.00	48.55	C
ATOM	1205	O	TYR	B	242	20.434	-13.394	40.994	1.00	48.90	O
ATOM	1206	CB	TYR	B	242	17.696	-14.576	39.708	1.00	48.42	C
ATOM	1207	CG	TYR	B	242	16.275	-15.072	39.811	1.00	48.57	C
ATOM	1208	CD1	TYR	B	242	15.295	-14.305	40.452	1.00	47.57	C
ATOM	1209	CD2	TYR	B	242	15.914	-16.321	39.301	1.00	46.90	C
ATOM	1210	CE1	TYR	B	242	13.999	-14.758	40.562	1.00	47.12	C
ATOM	1211	CE2	TYR	B	242	14.617	-16.784	39.406	1.00	46.41	C
ATOM	1212	CZ	TYR	B	242	13.665	-15.990	40.027	1.00	48.02	C
ATOM	1213	OH	TYR	B	242	12.374	-16.438	40.154	1.00	49.87	O
ATOM	1214	N	ALA	B	243	20.664	-15.535	40.290	1.00	48.20	N
ATOM	1215	CA	ALA	B	243	22.066	-15.400	39.951	1.00	48.04	C
ATOM	1216	C	ALA	B	243	22.438	-16.213	38.704	1.00	48.27	C
ATOM	1217	O	ALA	B	243	21.779	-17.204	38.362	1.00	47.73	O
ATOM	1218	CB	ALA	B	243	22.935	-15.785	41.138	1.00	47.40	C
ATOM	1219	N	LEU	B	244	23.473	-15.747	38.009	1.00	48.84	N
ATOM	1220	CA	LEU	B	244	24.162	-16.547	37.012	1.00	49.59	C
ATOM	1221	C	LEU	B	244	25.279	-17.271	37.729	1.00	50.33	C
ATOM	1222	O	LEU	B	244	25.749	-16.816	38.775	1.00	50.24	O
ATOM	1223	CB	LEU	B	244	24.785	-15.674	35.917	1.00	49.45	C
ATOM	1224	CG	LEU	B	244	23.947	-14.700	35.094	1.00	49.38	C
ATOM	1225	CD1	LEU	B	244	24.828	-13.990	34.050	1.00	48.50	C
ATOM	1226	CD2	LEU	B	244	22.781	-15.414	34.437	1.00	48.35	C
ATOM	1227	N	SER	B	245	25.704	-18.395	37.161	1.00	51.42	N
ATOM	1228	CA	SER	B	245	26.881	-19.113	37.633	1.00	52.60	C
ATOM	1229	C	SER	B	245	28.057	-18.148	37.727	1.00	52.95	C
ATOM	1230	O	SER	B	245	28.245	-17.304	36.839	1.00	53.33	O
ATOM	1231	CB	SER	B	245	27.237	-20.233	36.651	1.00	52.84	C
ATOM	1232	OG	SER	B	245	26.069	-20.882	36.172	1.00	54.44	O
ATOM	1233	N	ILE	B	246	28.833	-18.259	38.802	1.00	53.30	N
ATOM	1234	CA	ILE	B	246	30.070	-17.506	38.923	1.00	53.70	C
ATOM	1235	C	ILE	B	246	31.014	-17.924	37.795	1.00	54.55	C
ATOM	1236	O	ILE	B	246	31.296	-19.109	37.607	1.00	54.83	O
ATOM	1237	CB	ILE	B	246	30.716	-17.683	40.310	1.00	53.41	C
ATOM	1238	CG1	ILE	B	246	29.822	-17.049	41.385	1.00	53.82	C
ATOM	1239	CG2	ILE	B	246	32.107	-17.065	40.345	1.00	52.93	C
ATOM	1240	CD1	ILE	B	246	30.109	-17.515	42.803	1.00	53.32	C
ATOM	1241	N	LYS	B	247	31.459	-16.942	37.023	1.00	55.37	N
ATOM	1242	CA	LYS	B	247	32.380	-17.179	35.932	1.00	56.34	C
ATOM	1243	C	LYS	B	247	33.503	-16.158	35.982	1.00	56.81	C
ATOM	1244	O	LYS	B	247	33.248	-14.953	35.958	1.00	56.75	O
ATOM	1245	CB	LYS	B	247	31.651	-17.094	34.587	1.00	56.56	C
ATOM	1246	CG	LYS	B	247	31.286	-18.442	33.965	1.00	57.14	C
ATOM	1247	CD	LYS	B	247	31.010	-18.274	32.471	1.00	57.73	C
ATOM	1248	CE	LYS	B	247	31.066	-19.600	31.723	1.00	58.05	C
ATOM	1249	NZ	LYS	B	247	31.015	-19.394	30.246	1.00	57.15	N
ATOM	1250	N	ASP	B	248	34.740	-16.651	36.057	1.00	57.36	N
ATOM	1251	CA	ASP	B	248	35.946	-15.805	36.052	1.00	57.82	C
ATOM	1252	C	ASP	B	248	35.899	-14.727	37.147	1.00	57.93	C
ATOM	1253	O	ASP	B	248	36.138	-13.530	36.893	1.00	58.00	O
ATOM	1254	CB	ASP	B	248	36.196	-15.197	34.659	1.00	57.86	C
ATOM	1255	CG	ASP	B	248	37.654	-14.822	34.431	1.00	58.44	C
ATOM	1256	OD1	ASP	B	248	38.552	-15.629	34.766	1.00	59.44	O
ATOM	1257	OD2	ASP	B	248	37.904	-13.722	33.900	1.00	58.54	O
ATOM	1258	N	SER	B	249	35.558	-15.182	38.353	1.00	57.89	N
ATOM	1259	CA	SER	B	249	35.600	-14.391	39.587	1.00	58.16	C
ATOM	1260	C	SER	B	249	34.565	-13.266	39.699	1.00	58.20	C
ATOM	1261	O	SER	B	249	34.737	-12.359	40.517	1.00	58.33	O
ATOM	1262	CB	SER	B	249	37.019	-13.858	39.853	1.00	58.24	C
ATOM	1263	OG	SER	B	249	37.926	-14.906	40.180	1.00	58.77	O
ATOM	1264	N	VAL	B	250	33.495	-13.332	38.902	1.00	58.20	N
ATOM	1265	CA	VAL	B	250	32.427	-12.318	38.945	1.00	57.79	C
ATOM	1266	C	VAL	B	250	31.049	-12.884	39.346	1.00	57.45	C
ATOM	1267	O	VAL	B	250	30.619	-13.937	38.850	1.00	56.93	O
ATOM	1268	CB	VAL	B	250	32.362	-11.462	37.630	1.00	58.16	C
ATOM	1269	CG1	VAL	B	250	32.070	-12.317	36.404	1.00	58.76	C
ATOM	1270	CG2	VAL	B	250	31.336	-10.310	37.740	1.00	58.14	C

Figure 2 Table 2b - 20

ATOM	1271	N	MET B 251	30.395	-12.170	40.271	1.00	57.06	N
ATOM	1272	CA	MET B 251	29.032	-12.444	40.730	1.00	57.16	C
ATOM	1273	C	MET B 251	28.017	-11.605	39.972	1.00	56.13	C
ATOM	1274	O	MET B 251	28.145	-10.372	39.892	1.00	56.69	O
ATOM	1275	CB	MET B 251	28.882	-12.089	42.209	1.00	57.18	C
ATOM	1276	CG	MET B 251	29.221	-13.180	43.194	1.00	58.95	C
ATOM	1277	SD	MET B 251	28.263	-12.941	44.706	1.00	61.86	S
ATOM	1278	CE	MET B 251	28.762	-14.364	45.689	1.00	59.76	C
ATOM	1279	N	VAL B 252	26.990	-12.257	39.435	1.00	54.75	N
ATOM	1280	CA	VAL B 252	25.881	-11.529	38.829	1.00	53.04	C
ATOM	1281	C	VAL B 252	24.573	-11.814	39.565	1.00	52.27	C
ATOM	1282	O	VAL B 252	23.978	-12.887	39.439	1.00	51.76	O
ATOM	1283	CB	VAL B 252	25.756	-11.785	37.309	1.00	53.20	C
ATOM	1284	CG1	VAL B 252	24.738	-10.815	36.698	1.00	52.73	C
ATOM	1285	CG2	VAL B 252	27.106	-11.629	36.627	1.00	51.95	C
ATOM	1286	N	LEU B 253	24.148	-10.829	40.344	1.00	51.65	N
ATOM	1287	CA	LEU B 253	22.941	-10.911	41.150	1.00	51.05	C
ATOM	1288	C	LEU B 253	21.831	-10.129	40.484	1.00	51.21	C
ATOM	1289	O	LEU B 253	22.090	-9.117	39.845	1.00	52.03	O
ATOM	1290	CB	LEU B 253	23.207	-10.355	42.549	1.00	50.67	C
ATOM	1291	CG	LEU B 253	24.326	-11.071	43.331	1.00	49.96	C
ATOM	1292	CD1	LEU B 253	24.458	-10.468	44.727	1.00	47.90	C
ATOM	1293	CD2	LEU B 253	24.126	-12.611	43.387	1.00	45.82	C
ATOM	1294	N	SER B 254	20.597	-10.601	40.628	1.00	50.86	N
ATOM	1295	CA	SER B 254	19.461	-10.031	39.927	1.00	50.25	C
ATOM	1296	C	SER B 254	18.160	-10.279	40.669	1.00	49.43	C
ATOM	1297	O	SER B 254	18.030	-11.275	41.376	1.00	50.18	O
ATOM	1298	CB	SER B 254	19.387	-10.618	38.517	1.00	50.43	C
ATOM	1299	OG	SER B 254	18.070	-10.579	37.993	1.00	51.89	O
ATOM	1300	N	ALA B 255	17.206	-9.367	40.499	1.00	48.53	N
ATOM	1301	CA	ALA B 255	15.867	-9.463	41.088	1.00	47.72	C
ATOM	1302	C	ALA B 255	14.960	-8.453	40.396	1.00	47.42	C
ATOM	1303	O	ALA B 255	15.438	-7.456	39.863	1.00	46.87	O
ATOM	1304	CB	ALA B 255	15.918	-9.175	42.574	1.00	47.18	C
ATOM	1305	N	THR B 256	13.656	-8.698	40.407	1.00	47.28	N
ATOM	1306	CA	THR B 256	12.725	-7.733	39.851	1.00	47.33	C
ATOM	1307	C	THR B 256	11.947	-7.061	40.980	1.00	47.99	C
ATOM	1308	O	THR B 256	11.430	-7.736	41.882	1.00	48.68	O
ATOM	1309	CB	THR B 256	11.780	-8.389	38.841	1.00	47.47	C
ATOM	1310	OG1	THR B 256	12.552	-9.023	37.812	1.00	46.60	O
ATOM	1311	CG2	THR B 256	10.871	-7.352	38.195	1.00	47.26	C
ATOM	1312	N	HIS B 257	11.903	-5.731	40.952	1.00	47.85	N
ATOM	1313	CA	HIS B 257	11.176	-4.959	41.950	1.00	47.81	C
ATOM	1314	C	HIS B 257	10.154	-4.085	41.279	1.00	47.26	C
ATOM	1315	O	HIS B 257	10.203	-3.875	40.073	1.00	47.40	O
ATOM	1316	CB	HIS B 257	12.119	-4.095	42.785	1.00	47.98	C
ATOM	1317	CG	HIS B 257	12.926	-4.883	43.765	1.00	50.55	C
ATOM	1318	ND1	HIS B 257	14.096	-5.532	43.417	1.00	52.04	N
ATOM	1319	CD2	HIS B 257	12.714	-5.158	45.075	1.00	50.56	C
ATOM	1320	CE1	HIS B 257	14.578	-6.154	44.479	1.00	52.45	C
ATOM	1321	NE2	HIS B 257	13.759	-5.943	45.496	1.00	51.51	N
ATOM	1322	N	ARG B 258	9.248	-3.553	42.085	1.00	46.60	N
ATOM	1323	CA	ARG B 258	8.115	-2.812	41.597	1.00	45.92	C
ATOM	1324	C	ARG B 258	8.121	-1.421	42.209	1.00	45.30	C
ATOM	1325	O	ARG B 258	8.293	-1.264	43.419	1.00	44.62	O
ATOM	1326	CB	ARG B 258	6.854	-3.562	41.995	1.00	46.46	C
ATOM	1327	CG	ARG B 258	5.546	-2.967	41.554	1.00	46.91	C
ATOM	1328	CD	ARG B 258	4.431	-3.697	42.303	1.00	49.48	C
ATOM	1329	NE	ARG B 258	3.356	-2.792	42.697	1.00	51.16	N
ATOM	1330	CZ	ARG B 258	3.227	-2.241	43.899	1.00	51.64	C
ATOM	1331	NH1	ARG B 258	4.097	-2.503	44.865	1.00	52.01	N
ATOM	1332	NH2	ARG B 258	2.210	-1.432	44.137	1.00	52.62	N
ATOM	1333	N	TYR B 259	7.980	-0.423	41.341	1.00	44.43	N
ATOM	1334	CA	TYR B 259	7.708	0.945	41.732	1.00	43.82	C
ATOM	1335	C	TYR B 259	6.372	1.284	41.091	1.00	44.04	C
ATOM	1336	O	TYR B 259	6.242	1.316	39.858	1.00	44.07	O
ATOM	1337	CB	TYR B 259	8.823	1.914	41.274	1.00	42.95	C

Figure 2 Table 2b - 21

ATOM	1338	CG	TYR	B	259	8.595	3.365	41.682	1.00	41.98	C
ATOM	1339	CD1	TYR	B	259	8.803	3.790	42.997	1.00	41.00	C
ATOM	1340	CD2	TYR	B	259	8.153	4.309	40.759	1.00	40.74	C
ATOM	1341	CE1	TYR	B	259	8.589	5.116	43.369	1.00	40.38	C
ATOM	1342	CE2	TYR	B	259	7.937	5.634	41.122	1.00	38.78	C
ATOM	1343	CZ	TYR	B	259	8.155	6.036	42.424	1.00	40.19	C
ATOM	1344	OH	TYR	B	259	7.925	7.356	42.799	1.00	39.70	O
ATOM	1345	N	LYS	B	260	5.380	1.519	41.938	1.00	44.16	N
ATOM	1346	CA	LYS	B	260	4.011	1.740	41.497	1.00	44.36	C
ATOM	1347	C	LYS	B	260	3.588	0.667	40.491	1.00	44.37	C
ATOM	1348	O	LYS	B	260	3.392	-0.479	40.881	1.00	44.26	O
ATOM	1349	CB	LYS	B	260	3.836	3.151	40.961	1.00	44.31	C
ATOM	1350	CG	LYS	B	260	3.960	4.198	42.038	1.00	44.84	C
ATOM	1351	CD	LYS	B	260	4.027	5.593	41.456	1.00	45.61	C
ATOM	1352	CE	LYS	B	260	4.286	6.599	42.555	1.00	46.10	C
ATOM	1353	NZ	LYS	B	260	4.174	7.973	42.015	1.00	47.97	N
ATOM	1354	N	LYS	B	261	3.482	1.025	39.212	1.00	44.43	N
ATOM	1355	CA	LYS	B	261	3.050	0.075	38.173	1.00	44.29	C
ATOM	1356	C	LYS	B	261	4.195	-0.393	37.273	1.00	43.95	C
ATOM	1357	O	LYS	B	261	3.962	-1.076	36.263	1.00	43.85	O
ATOM	1358	CB	LYS	B	261	1.946	0.684	37.302	1.00	44.19	C
ATOM	1359	CG	LYS	B	261	0.702	1.131	38.042	1.00	45.36	C
ATOM	1360	CD	LYS	B	261	-0.127	-0.049	38.530	1.00	48.15	C
ATOM	1361	CE	LYS	B	261	-1.449	0.423	39.130	1.00	49.68	C
ATOM	1362	NZ	LYS	B	261	-2.111	1.415	38.227	1.00	51.02	N
ATOM	1363	N	LYS	B	262	5.423	-0.024	37.625	1.00	43.21	N
ATOM	1364	CA	LYS	B	262	6.548	-0.305	36.754	1.00	43.09	C
ATOM	1365	C	LYS	B	262	7.435	-1.337	37.416	1.00	43.17	C
ATOM	1366	O	LYS	B	262	7.613	-1.308	38.626	1.00	43.33	O
ATOM	1367	CB	LYS	B	262	7.366	0.953	36.441	1.00	42.70	C
ATOM	1368	CG	LYS	B	262	6.562	2.189	36.028	1.00	42.20	C
ATOM	1369	CD	LYS	B	262	5.953	2.124	34.643	1.00	41.09	C
ATOM	1370	CE	LYS	B	262	5.346	3.475	34.285	1.00	39.85	C
ATOM	1371	NZ	LYS	B	262	4.536	3.432	33.061	1.00	38.66	N
ATOM	1372	N	TYR	B	263	8.004	-2.221	36.598	1.00	42.79	N
ATOM	1373	CA	TYR	B	263	8.868	-3.286	37.055	1.00	42.28	C
ATOM	1374	C	TYR	B	263	10.215	-3.161	36.401	1.00	41.72	C
ATOM	1375	O	TYR	B	263	10.327	-2.959	35.199	1.00	42.33	O
ATOM	1376	CB	TYR	B	263	8.250	-4.646	36.712	1.00	42.73	C
ATOM	1377	CG	TYR	B	263	6.853	-4.825	37.270	1.00	42.99	C
ATOM	1378	CD1	TYR	B	263	5.752	-4.255	36.626	1.00	41.94	C
ATOM	1379	CD2	TYR	B	263	6.632	-5.545	38.453	1.00	41.19	C
ATOM	1380	CE1	TYR	B	263	4.466	-4.399	37.136	1.00	42.14	C
ATOM	1381	CE2	TYR	B	263	5.341	-5.695	38.969	1.00	40.86	C
ATOM	1382	CZ	TYR	B	263	4.271	-5.119	38.298	1.00	42.91	C
ATOM	1383	OH	TYR	B	263	2.990	-5.234	38.774	1.00	45.03	O
ATOM	1384	N	VAL	B	264	11.250	-3.272	37.201	1.00	41.48	N
ATOM	1385	CA	VAL	B	264	12.603	-3.251	36.691	1.00	40.80	C
ATOM	1386	C	VAL	B	264	13.377	-4.441	37.268	1.00	41.10	C
ATOM	1387	O	VAL	B	264	13.306	-4.740	38.467	1.00	40.36	O
ATOM	1388	CB	VAL	B	264	13.312	-1.897	37.002	1.00	40.37	C
ATOM	1389	CG1	VAL	B	264	13.534	-1.705	38.482	1.00	38.44	C
ATOM	1390	CG2	VAL	B	264	14.624	-1.809	36.269	1.00	40.99	C
ATOM	1391	N	THR	B	265	14.093	-5.116	36.385	1.00	41.76	N
ATOM	1392	CA	THR	B	265	14.984	-6.196	36.745	1.00	42.84	C
ATOM	1393	C	THR	B	265	16.375	-5.603	36.832	1.00	43.21	C
ATOM	1394	O	THR	B	265	16.907	-5.099	35.835	1.00	43.92	O
ATOM	1395	CB	THR	B	265	14.952	-7.264	35.643	1.00	43.14	C
ATOM	1396	OG1	THR	B	265	13.636	-7.819	35.568	1.00	43.47	O
ATOM	1397	CG2	THR	B	265	15.955	-8.375	35.917	1.00	43.79	C
ATOM	1398	N	THR	B	266	16.966	-5.654	38.016	1.00	43.30	N
ATOM	1399	CA	THR	B	266	18.274	-5.051	38.247	1.00	43.39	C
ATOM	1400	C	THR	B	266	19.363	-6.112	38.283	1.00	43.55	C
ATOM	1401	O	THR	B	266	19.200	-7.140	38.952	1.00	43.96	O
ATOM	1402	CB	THR	B	266	18.281	-4.262	39.582	1.00	43.65	C
ATOM	1403	OG1	THR	B	266	17.181	-3.335	39.608	1.00	43.04	O
ATOM	1404	CG2	THR	B	266	19.596	-3.498	39.755	1.00	43.49	C

Figure 2 Table 2b - 22

ATOM	1405	N	LEU	B	267	20.469	-5.870	37.582	1.00	43.15	N
ATOM	1406	CA	LEU	B	267	21.599	-6.793	37.617	1.00	43.38	C
ATOM	1407	C	LEU	B	267	22.786	-6.123	38.252	1.00	43.86	C
ATOM	1408	O	LEU	B	267	23.143	-5.011	37.881	1.00	44.89	O
ATOM	1409	CB	LEU	B	267	22.001	-7.238	36.204	1.00	43.17	C
ATOM	1410	CG	LEU	B	267	21.073	-8.147	35.399	1.00	42.62	C
ATOM	1411	CD1	LEU	B	267	19.925	-7.374	34.801	1.00	41.71	C
ATOM	1412	CD2	LEU	B	267	21.864	-8.816	34.298	1.00	43.97	C
ATOM	1413	N	LEU	B	268	23.422	-6.799	39.191	1.00	44.41	N
ATOM	1414	CA	LEU	B	268	24.651	-6.286	39.773	1.00	44.54	C
ATOM	1415	C	LEU	B	268	25.814	-7.161	39.377	1.00	45.26	C
ATOM	1416	O	LEU	B	268	25.790	-8.376	39.609	1.00	45.79	O
ATOM	1417	CB	LEU	B	268	24.552	-6.211	41.305	1.00	44.36	C
ATOM	1418	CG	LEU	B	268	25.766	-5.601	42.021	1.00	43.41	C
ATOM	1419	CD1	LEU	B	268	26.007	-4.133	41.627	1.00	40.75	C
ATOM	1420	CD2	LEU	B	268	25.604	-5.725	43.519	1.00	43.20	C
ATOM	1421	N	TYR	B	269	26.822	-6.546	38.765	1.00	45.84	N
ATOM	1422	CA	TYR	B	269	28.077	-7.222	38.476	1.00	46.45	C
ATOM	1423	C	TYR	B	269	29.037	-6.803	39.557	1.00	47.48	C
ATOM	1424	O	TYR	B	269	29.297	-5.614	39.735	1.00	48.15	O
ATOM	1425	CB	TYR	B	269	28.609	-6.831	37.099	1.00	45.65	C
ATOM	1426	CG	TYR	B	269	27.907	-7.542	35.974	1.00	44.88	C
ATOM	1427	CD1	TYR	B	269	26.583	-7.233	35.648	1.00	43.48	C
ATOM	1428	CD2	TYR	B	269	28.563	-8.527	35.225	1.00	43.77	C
ATOM	1429	CE1	TYR	B	269	25.923	-7.894	34.625	1.00	43.91	C
ATOM	1430	CE2	TYR	B	269	27.910	-9.198	34.186	1.00	44.17	C
ATOM	1431	CZ	TYR	B	269	26.585	-8.873	33.893	1.00	44.36	C
ATOM	1432	OH	TYR	B	269	25.923	-9.515	32.872	1.00	43.91	O
ATOM	1433	N	LYS	B	270	29.564	-7.794	40.263	1.00	48.67	N
ATOM	1434	CA	LYS	B	270	30.294	-7.597	41.503	1.00	49.94	C
ATOM	1435	C	LYS	B	270	31.435	-8.632	41.569	1.00	50.43	C
ATOM	1436	O	LYS	B	270	31.183	-9.834	41.466	1.00	50.62	O
ATOM	1437	CB	LYS	B	270	29.319	-7.798	42.686	1.00	49.98	C
ATOM	1438	CG	LYS	B	270	29.760	-7.189	44.008	1.00	50.88	C
ATOM	1439	CD	LYS	B	270	29.029	-7.797	45.204	1.00	51.19	C
ATOM	1440	CE	LYS	B	270	29.896	-7.650	46.459	1.00	52.32	C
ATOM	1441	NZ	LYS	B	270	29.141	-7.718	47.749	1.00	53.11	N
ATOM	1442	N	PRO	B	271	32.692	-8.179	41.752	1.00	50.91	N
ATOM	1443	CA	PRO	B	271	33.797	-9.131	41.927	1.00	51.51	C
ATOM	1444	C	PRO	B	271	33.671	-9.896	43.246	1.00	52.02	C
ATOM	1445	O	PRO	B	271	32.942	-9.462	44.136	1.00	52.05	O
ATOM	1446	CB	PRO	B	271	35.043	-8.236	41.997	1.00	51.21	C
ATOM	1447	CG	PRO	B	271	34.612	-6.892	41.589	1.00	51.17	C
ATOM	1448	CD	PRO	B	271	33.152	-6.785	41.843	1.00	51.04	C
ATOM	1449	N	ILE	B	272	34.369	-11.023	43.355	1.00	52.88	N
ATOM	1450	CA	ILE	B	272	34.541	-11.706	44.639	1.00	53.98	C
ATOM	1451	C	ILE	B	272	35.870	-11.287	45.288	1.00	54.14	C
ATOM	1452	O	ILE	B	272	36.051	-11.411	46.510	1.00	54.62	O
ATOM	1453	CB	ILE	B	272	34.481	-13.255	44.498	1.00	54.17	C
ATOM	1454	CG1	ILE	B	272	33.162	-13.687	43.836	1.00	54.87	C
ATOM	1455	CG2	ILE	B	272	34.648	-13.924	45.860	1.00	53.58	C
ATOM	1456	CD1	ILE	B	272	33.045	-15.195	43.592	1.00	54.63	C
TER	1457		ILE	B	272						
ATOM	1458	N	SER	E	23	3.006	29.030	17.721	1.00	66.01	N
ATOM	1459	CA	SER	E	23	4.383	28.469	17.927	1.00	65.70	C
ATOM	1460	C	SER	E	23	4.909	28.687	19.369	1.00	65.58	C
ATOM	1461	O	SER	E	23	5.318	27.733	20.043	1.00	65.44	O
ATOM	1462	CB	SER	E	23	5.353	29.057	16.880	1.00	65.69	C
ATOM	1463	OG	SER	E	23	5.003	28.676	15.555	1.00	64.49	O
ATOM	1464	N	ASN	E	24	4.854	29.948	19.814	1.00	65.55	N
ATOM	1465	CA	ASN	E	24	5.410	30.446	21.092	1.00	65.24	C
ATOM	1466	C	ASN	E	24	4.734	29.924	22.366	1.00	64.94	C
ATOM	1467	O	ASN	E	24	3.526	30.122	22.568	1.00	65.01	O
ATOM	1468	CB	ASN	E	24	5.398	31.990	21.102	1.00	65.29	C
ATOM	1469	CG	ASN	E	24	6.372	32.594	20.102	1.00	65.06	C
ATOM	1470	OD1	ASN	E	24	5.990	32.967	18.991	1.00	64.20	O
ATOM	1471	ND2	ASN	E	24	7.643	32.675	20.489	1.00	65.22	N

Figure 2 Table 2b - 23

ATOM	1472	N	SER	E	25	5.547	29.297	23.225	1.00 64.41	N
ATOM	1473	CA	SER	E	25	5.125	28.597	24.451	1.00 63.42	C
ATOM	1474	C	SER	E	25	4.834	27.142	24.141	1.00 62.79	C
ATOM	1475	O	SER	E	25	5.207	26.259	24.914	1.00 63.05	O
ATOM	1476	CB	SER	E	25	3.939	29.269	25.148	1.00 63.61	C
ATOM	1477	OG	SER	E	25	3.840	28.834	26.489	1.00 63.51	O
ATOM	1478	N	SER	E	26	4.158	26.898	23.020	1.00 61.66	N
ATOM	1479	CA	SER	E	26	4.133	25.577	22.385	1.00 60.75	C
ATOM	1480	C	SER	E	26	3.413	24.458	23.136	1.00 59.96	C
ATOM	1481	O	SER	E	26	3.510	24.324	24.356	1.00 59.70	O
ATOM	1482	CB	SER	E	26	5.563	25.136	22.037	1.00 60.94	C
ATOM	1483	OG	SER	E	26	5.652	23.749	21.760	1.00 60.87	O
ATOM	1484	N	VAL	E	27	2.720	23.639	22.353	1.00 59.13	N
ATOM	1485	CA	VAL	E	27	2.073	22.422	22.809	1.00 58.48	C
ATOM	1486	C	VAL	E	27	3.118	21.453	23.416	1.00 58.18	C
ATOM	1487	O	VAL	E	27	2.802	20.647	24.307	1.00 58.13	O
ATOM	1488	CB	VAL	E	27	1.270	21.761	21.639	1.00 58.48	C
ATOM	1489	CG1	VAL	E	27	0.355	20.642	22.137	1.00 58.47	C
ATOM	1490	CG2	VAL	E	27	0.421	22.810	20.912	1.00 58.41	C
ATOM	1491	N	TYR	E	28	4.363	21.552	22.952	1.00 57.24	N
ATOM	1492	CA	TYR	E	28	5.435	20.707	23.460	1.00 56.46	C
ATOM	1493	C	TYR	E	28	5.905	21.125	24.855	1.00 56.20	C
ATOM	1494	O	TYR	E	28	6.073	20.280	25.744	1.00 55.99	O
ATOM	1495	CB	TYR	E	28	6.617	20.693	22.494	1.00 56.17	C
ATOM	1496	CG	TYR	E	28	6.343	19.985	21.194	1.00 55.94	C
ATOM	1497	CD1	TYR	E	28	5.806	20.669	20.095	1.00 56.01	C
ATOM	1498	CD2	TYR	E	28	6.640	18.635	21.049	1.00 55.51	C
ATOM	1499	CE1	TYR	E	28	5.560	20.012	18.892	1.00 56.23	C
ATOM	1500	CE2	TYR	E	28	6.399	17.967	19.857	1.00 54.98	C
ATOM	1501	CZ	TYR	E	28	5.865	18.651	18.785	1.00 56.05	C
ATOM	1502	OH	TYR	E	28	5.642	17.970	17.607	1.00 56.15	O
ATOM	1503	N	THR	E	29	6.130	22.423	25.038	1.00 55.75	N
ATOM	1504	CA	THR	E	29	6.637	22.947	26.309	1.00 55.45	C
ATOM	1505	C	THR	E	29	5.664	22.714	27.483	1.00 54.73	C
ATOM	1506	O	THR	E	29	6.079	22.279	28.556	1.00 54.33	O
ATOM	1507	CB	THR	E	29	7.137	24.426	26.149	1.00 55.66	C
ATOM	1508	OG1	THR	E	29	8.567	24.425	26.053	1.00 55.95	O
ATOM	1509	CG2	THR	E	29	6.714	25.345	27.310	1.00 56.39	C
ATOM	1510	N	THR	E	30	4.377	22.962	27.247	1.00 54.18	N
ATOM	1511	CA	THR	E	30	3.327	22.701	28.229	1.00 53.40	C
ATOM	1512	C	THR	E	30	3.187	21.206	28.507	1.00 53.15	C
ATOM	1513	O	THR	E	30	3.121	20.788	29.664	1.00 53.10	O
ATOM	1514	CB	THR	E	30	1.984	23.290	27.768	1.00 53.29	C
ATOM	1515	OG1	THR	E	30	2.123	24.708	27.640	1.00 52.44	O
ATOM	1516	CG2	THR	E	30	0.868	22.976	28.768	1.00 52.68	C
ATOM	1517	N	PHE	E	31	3.153	20.405	27.446	1.00 52.84	N
ATOM	1518	CA	PHE	E	31	3.134	18.944	27.581	1.00 52.59	C
ATOM	1519	C	PHE	E	31	4.255	18.420	28.483	1.00 52.49	C
ATOM	1520	O	PHE	E	31	4.001	17.626	29.385	1.00 52.72	O
ATOM	1521	CB	PHE	E	31	3.219	18.291	26.209	1.00 52.30	C
ATOM	1522	CG	PHE	E	31	3.103	16.803	26.236	1.00 51.92	C
ATOM	1523	CD1	PHE	E	31	4.222	16.009	26.469	1.00 51.13	C
ATOM	1524	CD2	PHE	E	31	1.882	16.189	26.014	1.00 51.55	C
ATOM	1525	CE1	PHE	E	31	4.127	14.641	26.497	1.00 50.27	C
ATOM	1526	CE2	PHE	E	31	1.786	14.795	26.030	1.00 51.20	C
ATOM	1527	CZ	PHE	E	31	2.906	14.032	26.272	1.00 50.43	C
ATOM	1528	N	MET	E	32	5.480	18.869	28.226	1.00 52.58	N
ATOM	1529	CA	MET	E	32	6.660	18.467	28.990	1.00 53.32	C
ATOM	1530	C	MET	E	32	6.629	18.906	30.443	1.00 53.36	C
ATOM	1531	O	MET	E	32	7.128	18.197	31.317	1.00 53.61	O
ATOM	1532	CB	MET	E	32	7.937	18.987	28.331	1.00 53.17	C
ATOM	1533	CG	MET	E	32	8.388	18.152	27.149	1.00 54.11	C
ATOM	1534	SD	MET	E	32	9.895	18.770	26.372	1.00 55.88	S
ATOM	1535	CE	MET	E	32	9.386	20.340	25.688	1.00 55.42	C
ATOM	1536	N	LYS	E	33	6.056	20.080	30.698	1.00 53.54	N
ATOM	1537	CA	LYS	E	33	5.938	20.599	32.063	1.00 53.37	C
ATOM	1538	C	LYS	E	33	4.842	19.887	32.860	1.00 53.15	C

Figure 2 Table 2b - 24

ATOM	1539	O	LYS	E	33	4.825	19.953	34.089	1.00	52.81	O
ATOM	1540	CB	LYS	E	33	5.702	22.116	32.050	1.00	53.03	C
ATOM	1541	CG	LYS	E	33	6.940	22.902	31.659	1.00	53.70	C
ATOM	1542	CD	LYS	E	33	6.808	24.394	31.907	1.00	53.28	C
ATOM	1543	CE	LYS	E	33	8.102	25.103	31.535	1.00	53.67	C
ATOM	1544	NZ	LYS	E	33	8.201	26.463	32.162	1.00	55.56	N
ATOM	1545	N	SER	E	34	3.940	19.210	32.150	1.00	52.97	N
ATOM	1546	CA	SER	E	34	2.769	18.604	32.760	1.00	53.14	C
ATOM	1547	C	SER	E	34	2.799	17.076	32.742	1.00	53.22	C
ATOM	1548	O	SER	E	34	1.802	16.433	33.059	1.00	53.43	O
ATOM	1549	CB	SER	E	34	1.504	19.117	32.085	1.00	53.11	C
ATOM	1550	OG	SER	E	34	1.408	18.587	30.782	1.00	53.94	O
ATOM	1551	N	HIS	E	35	3.936	16.499	32.372	1.00	53.24	N
ATOM	1552	CA	HIS	E	35	4.132	15.055	32.506	1.00	53.46	C
ATOM	1553	C	HIS	E	35	5.355	14.729	33.360	1.00	53.25	C
ATOM	1554	O	HIS	E	35	6.390	15.404	33.284	1.00	52.87	O
ATOM	1555	CB	HIS	E	35	4.220	14.359	31.137	1.00	53.57	C
ATOM	1556	CG	HIS	E	35	2.892	14.170	30.472	1.00	54.56	C
ATOM	1557	ND1	HIS	E	35	2.302	15.144	29.693	1.00	55.59	N
ATOM	1558	CD2	HIS	E	35	2.029	13.125	30.484	1.00	55.92	C
ATOM	1559	CE1	HIS	E	35	1.134	14.708	29.255	1.00	55.62	C
ATOM	1560	NE2	HIS	E	35	0.945	13.485	29.718	1.00	56.61	N
ATOM	1561	N	ARG	E	36	5.210	13.695	34.185	1.00	53.19	N
ATOM	1562	CA	ARG	E	36	6.289	13.199	35.017	1.00	52.82	C
ATOM	1563	C	ARG	E	36	7.195	12.265	34.218	1.00	52.67	C
ATOM	1564	O	ARG	E	36	6.748	11.636	33.272	1.00	52.49	O
ATOM	1565	CB	ARG	E	36	5.700	12.421	36.179	1.00	53.13	C
ATOM	1566	CG	ARG	E	36	4.767	13.184	37.074	1.00	53.61	C
ATOM	1567	CD	ARG	E	36	4.768	12.527	38.429	1.00	55.25	C
ATOM	1568	NE	ARG	E	36	3.778	13.073	39.354	1.00	58.84	N
ATOM	1569	CZ	ARG	E	36	3.882	14.242	39.991	1.00	61.33	C
ATOM	1570	NH1	ARG	E	36	4.928	15.044	39.789	1.00	61.96	N
ATOM	1571	NH2	ARG	E	36	2.923	14.627	40.828	1.00	62.46	N
ATOM	1572	N	CYS	E	37	8.461	12.174	34.607	1.00	52.79	N
ATOM	1573	CA	CYS	E	37	9.386	11.173	34.069	1.00	53.40	C
ATOM	1574	C	CYS	E	37	8.842	9.749	34.190	1.00	52.54	C
ATOM	1575	O	CYS	E	37	8.990	8.939	33.282	1.00	52.71	O
ATOM	1576	CB	CYS	E	37	10.736	11.251	34.773	1.00	53.63	C
ATOM	1577	SG	CYS	E	37	11.702	12.698	34.295	1.00	57.69	S
ATOM	1578	N	TYR	E	38	8.187	9.469	35.304	1.00	51.80	N
ATOM	1579	CA	TYR	E	38	7.568	8.181	35.546	1.00	51.05	C
ATOM	1580	C	TYR	E	38	6.745	7.698	34.362	1.00	50.68	C
ATOM	1581	O	TYR	E	38	6.756	6.513	34.028	1.00	50.86	O
ATOM	1582	CB	TYR	E	38	6.664	8.285	36.782	1.00	51.05	C
ATOM	1583	CG	TYR	E	38	5.800	7.070	37.010	1.00	50.28	C
ATOM	1584	CD1	TYR	E	38	4.464	7.047	36.588	1.00	49.87	C
ATOM	1585	CD2	TYR	E	38	6.317	5.941	37.640	1.00	49.80	C
ATOM	1586	CE1	TYR	E	38	3.669	5.926	36.785	1.00	50.02	C
ATOM	1587	CE2	TYR	E	38	5.525	4.815	37.845	1.00	50.58	C
ATOM	1588	CZ	TYR	E	38	4.210	4.816	37.417	1.00	50.06	C
ATOM	1589	OH	TYR	E	38	3.443	3.708	37.624	1.00	50.31	O
ATOM	1590	N	ASP	E	39	6.029	8.624	33.738	1.00	50.21	N
ATOM	1591	CA	ASP	E	39	5.110	8.298	32.660	1.00	49.85	C
ATOM	1592	C	ASP	E	39	5.793	7.732	31.419	1.00	49.58	C
ATOM	1593	O	ASP	E	39	5.126	7.156	30.574	1.00	50.18	O
ATOM	1594	CB	ASP	E	39	4.309	9.532	32.269	1.00	49.88	C
ATOM	1595	CG	ASP	E	39	3.382	10.012	33.367	1.00	51.03	C
ATOM	1596	OD1	ASP	E	39	3.069	9.219	34.295	1.00	51.53	O
ATOM	1597	OD2	ASP	E	39	2.948	11.191	33.282	1.00	52.10	O
ATOM	1598	N	LEU	E	40	7.105	7.916	31.293	1.00	48.99	N
ATOM	1599	CA	LEU	E	40	7.826	7.433	30.116	1.00	48.69	C
ATOM	1600	C	LEU	E	40	8.465	6.076	30.332	1.00	47.85	C
ATOM	1601	O	LEU	E	40	8.934	5.462	29.374	1.00	47.94	O
ATOM	1602	CB	LEU	E	40	8.944	8.391	29.680	1.00	48.64	C
ATOM	1603	CG	LEU	E	40	8.812	9.908	29.548	1.00	50.72	C
ATOM	1604	CD1	LEU	E	40	9.269	10.373	28.163	1.00	49.21	C
ATOM	1605	CD2	LEU	E	40	7.419	10.459	29.861	1.00	52.74	C

Figure 2 Table 2b - 25

ATOM	1606	N	ILE	E	41	8.537	5.646	31.587	1.00	46.85	N
ATOM	1607	CA	ILE	E	41	9.137	4.365	31.948	1.00	46.23	C
ATOM	1608	C	ILE	E	41	8.293	3.210	31.410	1.00	45.36	C
ATOM	1609	O	ILE	E	41	7.080	3.199	31.598	1.00	45.65	O
ATOM	1610	CB	ILE	E	41	9.262	4.255	33.503	1.00	46.83	C
ATOM	1611	CG1	ILE	E	41	10.054	5.463	34.053	1.00	47.21	C
ATOM	1612	CG2	ILE	E	41	9.840	2.906	33.934	1.00	43.84	C
ATOM	1613	CD1	ILE	E	41	10.310	5.391	35.557	1.00	47.20	C
ATOM	1614	N	PRO	E	42	8.916	2.227	30.748	1.00	44.69	N
ATOM	1615	CA	PRO	E	42	8.083	1.134	30.272	1.00	44.49	C
ATOM	1616	C	PRO	E	42	7.658	0.261	31.444	1.00	44.54	C
ATOM	1617	O	PRO	E	42	8.260	0.349	32.519	1.00	44.23	O
ATOM	1618	CB	PRO	E	42	9.013	0.365	29.335	1.00	44.46	C
ATOM	1619	CG	PRO	E	42	10.364	0.663	29.808	1.00	44.17	C
ATOM	1620	CD	PRO	E	42	10.335	2.022	30.422	1.00	44.77	C
ATOM	1621	N	THR	E	43	6.629	-0.557	31.236	1.00	44.83	N
ATOM	1622	CA	THR	E	43	6.046	-1.385	32.286	1.00	45.49	C
ATOM	1623	C	THR	E	43	7.095	-2.303	32.880	1.00	46.11	C
ATOM	1624	O	THR	E	43	7.082	-2.573	34.063	1.00	46.84	O
ATOM	1625	CB	THR	E	43	4.854	-2.198	31.767	1.00	45.48	C
ATOM	1626	OG1	THR	E	43	3.784	-1.301	31.461	1.00	46.11	O
ATOM	1627	CG2	THR	E	43	4.357	-3.203	32.816	1.00	44.76	C
ATOM	1628	N	SER	E	44	8.040	-2.720	32.054	1.00	46.73	N
ATOM	1629	CA	SER	E	44	9.070	-3.643	32.451	1.00	47.24	C
ATOM	1630	C	SER	E	44	10.374	-3.308	31.729	1.00	47.30	C
ATOM	1631	O	SER	E	44	10.379	-3.148	30.510	1.00	47.27	O
ATOM	1632	CB	SER	E	44	8.614	-5.046	32.087	1.00	47.42	C
ATOM	1633	OG	SER	E	44	9.741	-5.872	31.935	1.00	49.89	O
ATOM	1634	N	SER	E	45	11.469	-3.190	32.476	1.00	47.46	N
ATOM	1635	CA	SER	E	45	12.781	-2.912	31.885	1.00	48.22	C
ATOM	1636	C	SER	E	45	13.877	-3.612	32.662	1.00	48.27	C
ATOM	1637	O	SER	E	45	13.667	-3.979	33.798	1.00	48.72	O
ATOM	1638	CB	SER	E	45	13.069	-1.409	31.846	1.00	48.14	C
ATOM	1639	OG	SER	E	45	13.203	-0.865	33.164	1.00	49.95	O
ATOM	1640	N	LYS	E	46	15.038	-3.811	32.034	1.00	48.62	N
ATOM	1641	CA	LYS	E	46	16.233	-4.289	32.727	1.00	48.39	C
ATOM	1642	C	LYS	E	46	17.232	-3.164	32.921	1.00	47.63	C
ATOM	1643	O	LYS	E	46	17.261	-2.212	32.151	1.00	47.83	O
ATOM	1644	CB	LYS	E	46	16.895	-5.469	32.005	1.00	48.53	C
ATOM	1645	CG	LYS	E	46	17.174	-5.309	30.512	1.00	49.73	C
ATOM	1646	CD	LYS	E	46	17.917	-6.560	29.972	1.00	51.25	C
ATOM	1647	CE	LYS	E	46	17.956	-6.595	28.432	1.00	54.03	C
ATOM	1648	NZ	LYS	E	46	18.243	-7.980	27.892	1.00	54.96	N
ATOM	1649	N	LEU	E	47	18.048	-3.287	33.958	1.00	46.77	N
ATOM	1650	CA	LEU	E	47	19.040	-2.292	34.286	1.00	45.92	C
ATOM	1651	C	LEU	E	47	20.278	-3.009	34.747	1.00	45.39	C
ATOM	1652	O	LEU	E	47	20.189	-3.932	35.552	1.00	46.31	O
ATOM	1653	CB	LEU	E	47	18.502	-1.410	35.406	1.00	46.08	C
ATOM	1654	CG	LEU	E	47	19.358	-0.258	35.916	1.00	45.93	C
ATOM	1655	CD1	LEU	E	47	19.230	0.933	34.976	1.00	44.77	C
ATOM	1656	CD2	LEU	E	47	18.906	0.112	37.307	1.00	46.05	C
ATOM	1657	N	VAL	E	48	21.433	-2.605	34.243	1.00	44.74	N
ATOM	1658	CA	VAL	E	48	22.705	-3.230	34.638	1.00	44.28	C
ATOM	1659	C	VAL	E	48	23.491	-2.285	35.546	1.00	44.27	C
ATOM	1660	O	VAL	E	48	23.739	-1.128	35.184	1.00	43.86	O
ATOM	1661	CB	VAL	E	48	23.581	-3.601	33.403	1.00	44.17	C
ATOM	1662	CG1	VAL	E	48	24.949	-4.121	33.831	1.00	44.36	C
ATOM	1663	CG2	VAL	E	48	22.892	-4.627	32.546	1.00	43.94	C
ATOM	1664	N	VAL	E	49	23.879	-2.771	36.723	1.00	43.97	N
ATOM	1665	CA	VAL	E	49	24.664	-1.951	37.644	1.00	43.87	C
ATOM	1666	C	VAL	E	49	26.044	-2.558	37.860	1.00	44.28	C
ATOM	1667	O	VAL	E	49	26.173	-3.758	38.080	1.00	44.52	O
ATOM	1668	CB	VAL	E	49	23.956	-1.739	39.017	1.00	43.66	C
ATOM	1669	CG1	VAL	E	49	24.830	-0.916	39.968	1.00	42.76	C
ATOM	1670	CG2	VAL	E	49	22.610	-1.077	38.845	1.00	42.21	C
ATOM	1671	N	PHE	E	50	27.071	-1.720	37.797	1.00	44.82	N
ATOM	1672	CA	PHE	E	50	28.428	-2.154	38.068	1.00	45.75	C

Figure 2 Table 2b - 26

ATOM	1673	C	PHE	E	50	28.955	-1.637	39.401	1.00	46.65	C
ATOM	1674	O	PHE	E	50	28.904	-0.427	39.670	1.00	47.17	O
ATOM	1675	CB	PHE	E	50	29.370	-1.690	36.969	1.00	45.21	C
ATOM	1676	CG	PHE	E	50	29.087	-2.291	35.623	1.00	45.01	C
ATOM	1677	CD1	PHE	E	50	29.211	-1.515	34.472	1.00	42.85	C
ATOM	1678	CD2	PHE	E	50	28.730	-3.635	35.504	1.00	43.47	C
ATOM	1679	CE1	PHE	E	50	28.961	-2.054	33.222	1.00	44.66	C
ATOM	1680	CE2	PHE	E	50	28.482	-4.193	34.258	1.00	44.77	C
ATOM	1681	CZ	PHE	E	50	28.586	-3.398	33.108	1.00	46.03	C
ATOM	1682	N	ASP	E	51	29.475	-2.548	40.221	1.00	46.75	N
ATOM	1683	CA	ASP	E	51	30.234	-2.148	41.391	1.00	47.46	C
ATOM	1684	C	ASP	E	51	31.529	-1.531	40.860	1.00	48.00	C
ATOM	1685	O	ASP	E	51	32.123	-2.063	39.904	1.00	48.11	O
ATOM	1686	CB	ASP	E	51	30.503	-3.365	42.299	1.00	47.73	C
ATOM	1687	CG	ASP	E	51	31.268	-3.008	43.568	1.00	47.78	C
ATOM	1688	OD1	ASP	E	51	30.696	-3.159	44.673	1.00	47.41	O
ATOM	1689	OD2	ASP	E	51	32.441	-2.580	43.457	1.00	48.40	O
ATOM	1690	N	THR	E	52	31.966	-0.414	41.454	1.00	48.40	N
ATOM	1691	CA	THR	E	52	33.163	0.290	40.945	1.00	48.75	C
ATOM	1692	C	THR	E	52	34.479	-0.513	41.061	1.00	49.22	C
ATOM	1693	O	THR	E	52	35.469	-0.176	40.418	1.00	49.76	O
ATOM	1694	CB	THR	E	52	33.325	1.765	41.478	1.00	48.38	C
ATOM	1695	OG1	THR	E	52	33.510	1.796	42.896	1.00	48.35	O
ATOM	1696	CG2	THR	E	52	32.117	2.600	41.119	1.00	48.96	C
ATOM	1697	N	SER	E	53	34.483	-1.581	41.851	1.00	49.47	N
ATOM	1698	CA	SER	E	53	35.669	-2.428	41.951	1.00	49.94	C
ATOM	1699	C	SER	E	53	35.780	-3.427	40.791	1.00	50.46	C
ATOM	1700	O	SER	E	53	36.707	-4.234	40.758	1.00	50.60	O
ATOM	1701	CB	SER	E	53	35.656	-3.188	43.269	1.00	49.61	C
ATOM	1702	OG	SER	E	53	34.532	-4.044	43.300	1.00	49.11	O
ATOM	1703	N	LEU	E	54	34.839	-3.378	39.852	1.00	51.09	N
ATOM	1704	CA	LEU	E	54	34.797	-4.341	38.762	1.00	51.55	C
ATOM	1705	C	LEU	E	54	35.864	-4.005	37.738	1.00	52.19	C
ATOM	1706	O	LEU	E	54	36.111	-2.829	37.450	1.00	52.06	O
ATOM	1707	CB	LEU	E	54	33.435	-4.306	38.070	1.00	51.34	C
ATOM	1708	CG	LEU	E	54	32.780	-5.593	37.555	1.00	51.01	C
ATOM	1709	CD1	LEU	E	54	32.141	-5.331	36.199	1.00	48.48	C
ATOM	1710	CD2	LEU	E	54	33.730	-6.768	37.468	1.00	50.66	C
ATOM	1711	N	GLN	E	55	36.485	-5.045	37.182	1.00	52.87	N
ATOM	1712	CA	GLN	E	55	37.418	-4.874	36.069	1.00	53.70	C
ATOM	1713	C	GLN	E	55	36.749	-4.247	34.829	1.00	53.59	C
ATOM	1714	O	GLN	E	55	35.769	-4.765	34.302	1.00	53.43	O
ATOM	1715	CB	GLN	E	55	38.102	-6.198	35.708	1.00	53.58	C
ATOM	1716	CG	GLN	E	55	39.406	-6.439	36.442	1.00	54.97	C
ATOM	1717	CD	GLN	E	55	40.205	-7.589	35.851	1.00	57.01	C
ATOM	1718	OE1	GLN	E	55	40.331	-8.648	36.468	1.00	58.19	O
ATOM	1719	NE2	GLN	E	55	40.740	-7.392	34.643	1.00	58.00	N
ATOM	1720	N	VAL	E	56	37.301	-3.125	34.384	1.00	54.19	N
ATOM	1721	CA	VAL	E	56	36.846	-2.416	33.174	1.00	54.94	C
ATOM	1722	C	VAL	E	56	36.491	-3.357	32.005	1.00	55.24	C
ATOM	1723	O	VAL	E	56	35.461	-3.186	31.350	1.00	55.03	O
ATOM	1724	CB	VAL	E	56	37.905	-1.377	32.749	1.00	54.63	C
ATOM	1725	CG1	VAL	E	56	37.946	-1.197	31.246	1.00	55.02	C
ATOM	1726	CG2	VAL	E	56	37.660	-0.063	33.465	1.00	55.21	C
ATOM	1727	N	LYS	E	57	37.340	-4.364	31.794	1.00	55.60	N
ATOM	1728	CA	LYS	E	57	37.212	-5.311	30.702	1.00	56.11	C
ATOM	1729	C	LYS	E	57	35.930	-6.117	30.824	1.00	55.55	C
ATOM	1730	O	LYS	E	57	35.202	-6.299	29.854	1.00	55.52	O
ATOM	1731	CB	LYS	E	57	38.416	-6.252	30.725	1.00	56.47	C
ATOM	1732	CG	LYS	E	57	38.838	-6.792	29.365	1.00	58.39	C
ATOM	1733	CD	LYS	E	57	40.055	-7.723	29.508	1.00	58.96	C
ATOM	1734	CE	LYS	E	57	40.651	-8.112	28.147	1.00	60.75	C
ATOM	1735	NZ	LYS	E	57	41.676	-9.192	28.292	1.00	60.65	N
ATOM	1736	N	LYS	E	58	35.659	-6.601	32.031	1.00	55.37	N
ATOM	1737	CA	LYS	E	58	34.472	-7.410	32.284	1.00	55.07	C
ATOM	1738	C	LYS	E	58	33.221	-6.557	32.134	1.00	54.60	C
ATOM	1739	O	LYS	E	58	32.206	-7.014	31.615	1.00	54.61	O

Figure 2 Table 2b - 27

ATOM	1740	CB	LYS	E	58	34.535	-8.036	33.679	1.00	55.03	C
ATOM	1741	CG	LYS	E	58	35.803	-8.818	33.939	1.00	55.56	C
ATOM	1742	CD	LYS	E	58	36.040	-9.000	35.428	1.00	56.42	C
ATOM	1743	CE	LYS	E	58	37.271	-9.846	35.685	1.00	57.42	C
ATOM	1744	NZ	LYS	E	58	36.992	-11.288	35.419	1.00	59.34	N
ATOM	1745	N	ALA	E	59	33.325	-5.312	32.585	1.00	54.25	N
ATOM	1746	CA	ALA	E	59	32.234	-4.349	32.539	1.00	54.22	C
ATOM	1747	C	ALA	E	59	31.760	-4.049	31.113	1.00	54.29	C
ATOM	1748	O	ALA	E	59	30.560	-3.962	30.861	1.00	54.36	O
ATOM	1749	CB	ALA	E	59	32.641	-3.065	33.257	1.00	54.00	C
ATOM	1750	N	PHE	E	60	32.691	-3.904	30.179	1.00	54.36	N
ATOM	1751	CA	PHE	E	60	32.295	-3.641	28.799	1.00	54.65	C
ATOM	1752	C	PHE	E	60	31.783	-4.881	28.087	1.00	54.20	C
ATOM	1753	O	PHE	E	60	30.936	-4.792	27.195	1.00	54.35	O
ATOM	1754	CB	PHE	E	60	33.403	-2.931	28.022	1.00	55.03	C
ATOM	1755	CG	PHE	E	60	33.698	-1.555	28.550	1.00	56.00	C
ATOM	1756	CD1	PHE	E	60	34.926	-1.268	29.149	1.00	55.97	C
ATOM	1757	CD2	PHE	E	60	32.729	-0.552	28.481	1.00	55.84	C
ATOM	1758	CE1	PHE	E	60	35.190	0.006	29.654	1.00	55.26	C
ATOM	1759	CE2	PHE	E	60	32.987	0.711	28.987	1.00	56.21	C
ATOM	1760	CZ	PHE	E	60	34.221	0.990	29.573	1.00	55.44	C
ATOM	1761	N	PHE	E	61	32.266	-6.039	28.508	1.00	53.41	N
ATOM	1762	CA	PHE	E	61	31.723	-7.276	27.996	1.00	52.92	C
ATOM	1763	C	PHE	E	61	30.265	-7.474	28.460	1.00	51.96	C
ATOM	1764	O	PHE	E	61	29.456	-8.070	27.744	1.00	51.64	O
ATOM	1765	CB	PHE	E	61	32.617	-8.458	28.379	1.00	53.30	C
ATOM	1766	CG	PHE	E	61	32.345	-9.705	27.578	1.00	54.61	C
ATOM	1767	CD1	PHE	E	61	32.883	-9.858	26.297	1.00	55.79	C
ATOM	1768	CD2	PHE	E	61	31.550	-10.726	28.100	1.00	54.51	C
ATOM	1769	CE1	PHE	E	61	32.630	-11.013	25.547	1.00	55.84	C
ATOM	1770	CE2	PHE	E	61	31.296	-11.880	27.366	1.00	55.00	C
ATOM	1771	CZ	PHE	E	61	31.835	-12.026	26.089	1.00	55.15	C
ATOM	1772	N	ALA	E	62	29.930	-6.942	29.636	1.00	50.99	N
ATOM	1773	CA	ALA	E	62	28.573	-7.062	30.186	1.00	50.10	C
ATOM	1774	C	ALA	E	62	27.544	-6.194	29.452	1.00	49.74	C
ATOM	1775	O	ALA	E	62	26.386	-6.598	29.283	1.00	49.62	O
ATOM	1776	CB	ALA	E	62	28.569	-6.758	31.658	1.00	50.04	C
ATOM	1777	N	LEU	E	63	27.961	-5.010	29.010	1.00	49.07	N
ATOM	1778	CA	LEU	E	63	27.100	-4.177	28.173	1.00	48.40	C
ATOM	1779	C	LEU	E	63	26.664	-4.952	26.921	1.00	48.40	C
ATOM	1780	O	LEU	E	63	25.466	-5.081	26.653	1.00	48.60	O
ATOM	1781	CB	LEU	E	63	27.787	-2.857	27.794	1.00	48.09	C
ATOM	1782	CG	LEU	E	63	28.188	-1.839	28.864	1.00	46.72	C
ATOM	1783	CD1	LEU	E	63	28.596	-0.564	28.190	1.00	47.23	C
ATOM	1784	CD2	LEU	E	63	27.058	-1.564	29.852	1.00	47.23	C
ATOM	1785	N	VAL	E	64	27.631	-5.488	26.177	1.00	48.21	N
ATOM	1786	CA	VAL	E	64	27.339	-6.290	24.975	1.00	47.86	C
ATOM	1787	C	VAL	E	64	26.407	-7.457	25.291	1.00	47.64	C
ATOM	1788	O	VAL	E	64	25.366	-7.608	24.652	1.00	47.77	O
ATOM	1789	CB	VAL	E	64	28.621	-6.850	24.320	1.00	47.79	C
ATOM	1790	CG1	VAL	E	64	28.274	-7.673	23.085	1.00	48.49	C
ATOM	1791	CG2	VAL	E	64	29.574	-5.736	23.963	1.00	47.48	C
ATOM	1792	N	THR	E	65	26.786	-8.265	26.283	1.00	47.46	N
ATOM	1793	CA	THR	E	65	26.030	-9.461	26.673	1.00	47.49	C
ATOM	1794	C	THR	E	65	24.559	-9.158	26.938	1.00	47.14	C
ATOM	1795	O	THR	E	65	23.675	-9.921	26.543	1.00	46.94	O
ATOM	1796	CB	THR	E	65	26.616	-10.100	27.954	1.00	47.66	C
ATOM	1797	OG1	THR	E	65	28.037	-9.957	27.953	1.00	48.60	O
ATOM	1798	CG2	THR	E	65	26.250	-11.579	28.045	1.00	47.66	C
ATOM	1799	N	ASN	E	66	24.318	-8.043	27.623	1.00	47.01	N
ATOM	1800	CA	ASN	E	66	22.981	-7.652	28.053	1.00	46.75	C
ATOM	1801	C	ASN	E	66	22.212	-6.811	27.043	1.00	47.03	C
ATOM	1802	O	ASN	E	66	21.008	-6.601	27.216	1.00	47.15	O
ATOM	1803	CB	ASN	E	66	23.070	-6.913	29.386	1.00	46.46	C
ATOM	1804	CG	ASN	E	66	23.388	-7.840	30.541	1.00	45.43	C
ATOM	1805	OD1	ASN	E	66	22.576	-8.694	30.895	1.00	43.47	O
ATOM	1806	ND2	ASN	E	66	24.566	-7.665	31.146	1.00	43.73	N

Figure 2 Table 2b - 28

ATOM	1807	N	GLY	E	67	22.909	-6.336	26.003	1.00	47.42	N
ATOM	1808	CA	GLY	E	67	22.313	-5.499	24.940	1.00	47.74	C
ATOM	1809	C	GLY	E	67	21.834	-4.176	25.504	1.00	47.94	C
ATOM	1810	O	GLY	E	67	20.643	-3.857	25.466	1.00	47.92	O
ATOM	1811	N	VAL	E	68	22.788	-3.419	26.034	1.00	48.11	N
ATOM	1812	CA	VAL	E	68	22.525	-2.255	26.859	1.00	48.22	C
ATOM	1813	C	VAL	E	68	23.642	-1.259	26.602	1.00	48.72	C
ATOM	1814	O	VAL	E	68	24.770	-1.652	26.291	1.00	48.89	O
ATOM	1815	CB	VAL	E	68	22.424	-2.667	28.359	1.00	48.31	C
ATOM	1816	CG1	VAL	E	68	23.276	-1.798	29.271	1.00	47.62	C
ATOM	1817	CG2	VAL	E	68	20.970	-2.690	28.803	1.00	48.23	C
ATOM	1818	N	ARG	E	69	23.321	0.026	26.718	1.00	48.87	N
ATOM	1819	CA	ARG	E	69	24.224	1.081	26.314	1.00	49.04	C
ATOM	1820	C	ARG	E	69	24.937	1.734	27.469	1.00	48.60	C
ATOM	1821	O	ARG	E	69	26.005	2.298	27.295	1.00	49.19	O
ATOM	1822	CB	ARG	E	69	23.450	2.161	25.556	1.00	49.57	C
ATOM	1823	CG	ARG	E	69	23.622	2.137	24.062	1.00	51.59	C
ATOM	1824	CD	ARG	E	69	23.072	0.855	23.469	1.00	55.91	C
ATOM	1825	NE	ARG	E	69	22.962	0.956	22.019	1.00	57.90	N
ATOM	1826	CZ	ARG	E	69	21.956	0.445	21.318	1.00	59.95	C
ATOM	1827	NH1	ARG	E	69	20.964	-0.199	21.939	1.00	60.28	N
ATOM	1828	NH2	ARG	E	69	21.932	0.597	19.995	1.00	60.91	N
ATOM	1829	N	ALA	E	70	24.327	1.708	28.640	1.00	48.17	N
ATOM	1830	CA	ALA	E	70	24.868	2.426	29.781	1.00	47.64	C
ATOM	1831	C	ALA	E	70	24.527	1.684	31.059	1.00	47.10	C
ATOM	1832	O	ALA	E	70	23.497	1.031	31.134	1.00	46.93	O
ATOM	1833	CB	ALA	E	70	24.318	3.860	29.813	1.00	47.51	C
ATOM	1834	N	ALA	E	71	25.390	1.799	32.061	1.00	46.91	N
ATOM	1835	CA	ALA	E	71	25.210	1.096	33.320	1.00	46.76	C
ATOM	1836	C	ALA	E	71	25.588	1.993	34.498	1.00	47.10	C
ATOM	1837	O	ALA	E	71	26.707	2.497	34.550	1.00	47.57	O
ATOM	1838	CB	ALA	E	71	26.045	-0.139	33.325	1.00	46.51	C
ATOM	1839	N	PRO	E	72	24.649	2.225	35.436	1.00	46.93	N
ATOM	1840	CA	PRO	E	72	24.999	2.973	36.640	1.00	46.66	C
ATOM	1841	C	PRO	E	72	26.174	2.357	37.402	1.00	46.69	C
ATOM	1842	O	PRO	E	72	26.400	1.136	37.341	1.00	45.99	O
ATOM	1843	CB	PRO	E	72	23.723	2.902	37.493	1.00	46.65	C
ATOM	1844	CG	PRO	E	72	22.623	2.692	36.527	1.00	46.84	C
ATOM	1845	CD	PRO	E	72	23.221	1.855	35.414	1.00	47.17	C
ATOM	1846	N	LEU	E	73	26.913	3.219	38.102	1.00	46.24	N
ATOM	1847	CA	LEU	E	73	28.060	2.783	38.878	1.00	45.55	C
ATOM	1848	C	LEU	E	73	27.772	2.934	40.356	1.00	45.37	C
ATOM	1849	O	LEU	E	73	27.322	3.985	40.804	1.00	45.09	O
ATOM	1850	CB	LEU	E	73	29.318	3.556	38.479	1.00	45.10	C
ATOM	1851	CG	LEU	E	73	29.741	3.375	37.019	1.00	44.95	C
ATOM	1852	CD1	LEU	E	73	30.937	4.253	36.673	1.00	45.23	C
ATOM	1853	CD2	LEU	E	73	30.038	1.927	36.698	1.00	43.79	C
ATOM	1854	N	TRP	E	74	28.038	1.863	41.099	1.00	45.22	N
ATOM	1855	CA	TRP	E	74	27.768	1.805	42.526	1.00	45.14	C
ATOM	1856	C	TRP	E	74	29.088	1.708	43.269	1.00	45.84	C
ATOM	1857	O	TRP	E	74	29.869	0.777	43.039	1.00	46.35	O
ATOM	1858	CB	TRP	E	74	26.872	0.604	42.831	1.00	44.36	C
ATOM	1859	CG	TRP	E	74	26.746	0.249	44.276	1.00	43.12	C
ATOM	1860	CD1	TRP	E	74	27.489	-0.671	44.965	1.00	42.41	C
ATOM	1861	CD2	TRP	E	74	25.811	0.788	45.214	1.00	42.27	C
ATOM	1862	NE1	TRP	E	74	27.079	-0.731	46.278	1.00	41.01	N
ATOM	1863	CE2	TRP	E	74	26.051	0.156	46.458	1.00	41.77	C
ATOM	1864	CE3	TRP	E	74	24.797	1.750	45.132	1.00	42.22	C
ATOM	1865	CZ2	TRP	E	74	25.307	0.455	47.607	1.00	42.10	C
ATOM	1866	CZ3	TRP	E	74	24.051	2.039	46.290	1.00	42.00	C
ATOM	1867	CH2	TRP	E	74	24.312	1.397	47.496	1.00	41.06	C
ATOM	1868	N	ASP	E	75	29.347	2.686	44.138	1.00	46.46	N
ATOM	1869	CA	ASP	E	75	30.534	2.666	44.999	1.00	46.78	C
ATOM	1870	C	ASP	E	75	30.174	2.038	46.347	1.00	46.72	C
ATOM	1871	O	ASP	E	75	29.455	2.630	47.160	1.00	46.82	O
ATOM	1872	CB	ASP	E	75	31.099	4.079	45.176	1.00	46.82	C
ATOM	1873	CG	ASP	E	75	32.400	4.107	45.978	1.00	48.50	C

Figure 2 Table 2b - 29

ATOM	1874	OD1	ASP	E	75	33.303	4.888	45.597	1.00	49.18	O
ATOM	1875	OD2	ASP	E	75	32.526	3.367	46.990	1.00	50.79	O
ATOM	1876	N	SER	E	76	30.694	0.840	46.579	1.00	46.81	N
ATOM	1877	CA	SER	E	76	30.356	0.056	47.767	1.00	46.90	C
ATOM	1878	C	SER	E	76	30.829	0.650	49.106	1.00	47.24	C
ATOM	1879	O	SER	E	76	30.124	0.562	50.123	1.00	46.94	O
ATOM	1880	CB	SER	E	76	30.898	-1.351	47.610	1.00	46.55	C
ATOM	1881	OG	SER	E	76	30.041	-2.235	48.280	1.00	47.45	O
ATOM	1882	N	LYS	E	77	32.026	1.238	49.102	1.00	47.69	N
ATOM	1883	CA	LYS	E	77	32.550	1.959	50.264	1.00	47.83	C
ATOM	1884	C	LYS	E	77	31.622	3.104	50.666	1.00	47.69	C
ATOM	1885	O	LYS	E	77	31.332	3.283	51.838	1.00	47.68	O
ATOM	1886	CB	LYS	E	77	33.946	2.509	49.962	1.00	48.12	C
ATOM	1887	CG	LYS	E	77	35.080	1.836	50.715	1.00	48.94	C
ATOM	1888	CD	LYS	E	77	36.424	2.128	50.061	1.00	50.41	C
ATOM	1889	CE	LYS	E	77	37.555	2.306	51.081	1.00	51.41	C
ATOM	1890	NZ	LYS	E	77	37.794	1.126	51.979	1.00	53.34	N
ATOM	1891	N	LYS	E	78	31.144	3.854	49.676	1.00	47.67	N
ATOM	1892	CA	LYS	E	78	30.350	5.061	49.915	1.00	47.59	C
ATOM	1893	C	LYS	E	78	28.857	4.788	50.004	1.00	47.39	C
ATOM	1894	O	LYS	E	78	28.105	5.631	50.498	1.00	47.61	O
ATOM	1895	CB	LYS	E	78	30.633	6.110	48.829	1.00	47.64	C
ATOM	1896	CG	LYS	E	78	32.039	6.685	48.894	1.00	48.03	C
ATOM	1897	CD	LYS	E	78	32.299	7.710	47.806	1.00	48.82	C
ATOM	1898	CE	LYS	E	78	33.664	8.361	48.006	1.00	49.63	C
ATOM	1899	NZ	LYS	E	78	34.079	9.116	46.798	1.00	50.08	N
ATOM	1900	N	GLN	E	79	28.442	3.610	49.527	1.00	47.16	N
ATOM	1901	CA	GLN	E	79	27.034	3.184	49.474	1.00	46.76	C
ATOM	1902	C	GLN	E	79	26.136	4.124	48.645	1.00	46.85	C
ATOM	1903	O	GLN	E	79	25.052	4.523	49.086	1.00	46.58	O
ATOM	1904	CB	GLN	E	79	26.450	2.948	50.881	1.00	47.12	C
ATOM	1905	CG	GLN	E	79	27.110	1.820	51.703	1.00	47.14	C
ATOM	1906	CD	GLN	E	79	26.679	0.426	51.263	1.00	47.43	C
ATOM	1907	OE1	GLN	E	79	25.545	0.000	51.508	1.00	47.07	O
ATOM	1908	NE2	GLN	E	79	27.593	-0.296	50.611	1.00	46.98	N
ATOM	1909	N	SER	E	80	26.589	4.462	47.435	1.00	46.60	N
ATOM	1910	CA	SER	E	80	25.796	5.278	46.530	1.00	46.43	C
ATOM	1911	C	SER	E	80	26.248	5.163	45.083	1.00	46.28	C
ATOM	1912	O	SER	E	80	27.356	4.701	44.774	1.00	46.31	O
ATOM	1913	CB	SER	E	80	25.821	6.749	46.953	1.00	46.66	C
ATOM	1914	OG	SER	E	80	26.896	7.433	46.356	1.00	46.68	O
ATOM	1915	N	PHE	E	81	25.376	5.597	44.192	1.00	45.72	N
ATOM	1916	CA	PHE	E	81	25.750	5.693	42.808	1.00	45.38	C
ATOM	1917	C	PHE	E	81	26.671	6.889	42.687	1.00	45.30	C
ATOM	1918	O	PHE	E	81	26.455	7.899	43.353	1.00	45.71	O
ATOM	1919	CB	PHE	E	81	24.515	5.863	41.944	1.00	45.02	C
ATOM	1920	CG	PHE	E	81	23.590	4.685	41.966	1.00	44.35	C
ATOM	1921	CD1	PHE	E	81	22.360	4.762	42.621	1.00	44.06	C
ATOM	1922	CD2	PHE	E	81	23.941	3.493	41.323	1.00	44.09	C
ATOM	1923	CE1	PHE	E	81	21.480	3.664	42.632	1.00	44.05	C
ATOM	1924	CE2	PHE	E	81	23.073	2.394	41.321	1.00	43.74	C
ATOM	1925	CZ	PHE	E	81	21.840	2.476	41.977	1.00	44.04	C
ATOM	1926	N	VAL	E	82	27.709	6.763	41.868	1.00	45.02	N
ATOM	1927	CA	VAL	E	82	28.693	7.837	41.706	1.00	44.88	C
ATOM	1928	C	VAL	E	82	28.838	8.309	40.252	1.00	45.51	C
ATOM	1929	O	VAL	E	82	29.457	9.341	39.991	1.00	44.98	O
ATOM	1930	CB	VAL	E	82	30.083	7.433	42.250	1.00	44.49	C
ATOM	1931	CG1	VAL	E	82	30.074	7.396	43.770	1.00	43.82	C
ATOM	1932	CG2	VAL	E	82	30.531	6.106	41.654	1.00	43.63	C
ATOM	1933	N	GLY	E	83	28.281	7.532	39.318	1.00	46.04	N
ATOM	1934	CA	GLY	E	83	28.351	7.846	37.903	1.00	46.52	C
ATOM	1935	C	GLY	E	83	27.806	6.776	36.979	1.00	47.02	C
ATOM	1936	O	GLY	E	83	27.107	5.853	37.408	1.00	47.23	O
ATOM	1937	N	MET	E	84	28.152	6.909	35.704	1.00	47.42	N
ATOM	1938	CA	MET	E	84	27.652	6.066	34.628	1.00	47.98	C
ATOM	1939	C	MET	E	84	28.828	5.431	33.914	1.00	48.01	C
ATOM	1940	O	MET	E	84	29.935	5.959	33.961	1.00	48.54	O

Figure 2 Table 2b - 30

ATOM	1941	CB	MET	E	84	26.878	6.928	33.617	1.00	48.19	C
ATOM	1942	CG	MET	E	84	25.533	7.434	34.107	1.00	49.52	C
ATOM	1943	SD	MET	E	84	24.234	6.173	34.029	1.00	53.60	S
ATOM	1944	CE	MET	E	84	23.723	6.185	35.733	1.00	50.87	C
ATOM	1945	N	LEU	E	85	28.596	4.296	33.258	1.00	47.82	N
ATOM	1946	CA	LEU	E	85	29.561	3.769	32.303	1.00	47.59	C
ATOM	1947	C	LEU	E	85	28.864	3.653	30.973	1.00	47.42	C
ATOM	1948	O	LEU	E	85	27.883	2.905	30.850	1.00	47.66	O
ATOM	1949	CB	LEU	E	85	30.103	2.400	32.721	1.00	47.87	C
ATOM	1950	CG	LEU	E	85	31.417	1.983	32.035	1.00	48.26	C
ATOM	1951	CD1	LEU	E	85	32.593	2.824	32.537	1.00	48.40	C
ATOM	1952	CD2	LEU	E	85	31.717	0.509	32.226	1.00	47.56	C
ATOM	1953	N	THR	E	86	29.359	4.403	29.988	1.00	46.60	N
ATOM	1954	CA	THR	E	86	28.778	4.422	28.645	1.00	46.09	C
ATOM	1955	C	THR	E	86	29.794	3.975	27.591	1.00	45.89	C
ATOM	1956	O	THR	E	86	30.961	3.721	27.911	1.00	45.85	O
ATOM	1957	CB	THR	E	86	28.258	5.821	28.274	1.00	45.89	C
ATOM	1958	OG1	THR	E	86	29.362	6.727	28.120	1.00	46.67	O
ATOM	1959	CG2	THR	E	86	27.319	6.351	29.328	1.00	45.86	C
ATOM	1960	N	ILE	E	87	29.347	3.871	26.338	1.00	45.30	N
ATOM	1961	CA	ILE	E	87	30.232	3.523	25.239	1.00	45.05	C
ATOM	1962	C	ILE	E	87	31.331	4.575	25.076	1.00	45.04	C
ATOM	1963	O	ILE	E	87	32.446	4.242	24.670	1.00	44.80	O
ATOM	1964	CB	ILE	E	87	29.470	3.374	23.899	1.00	45.48	C
ATOM	1965	CG1	ILE	E	87	28.196	2.542	24.077	1.00	45.47	C
ATOM	1966	CG2	ILE	E	87	30.392	2.835	22.782	1.00	44.29	C
ATOM	1967	CD1	ILE	E	87	28.415	1.181	24.639	1.00	47.70	C
ATOM	1968	N	THR	E	88	31.019	5.832	25.389	1.00	45.06	N
ATOM	1969	CA	THR	E	88	32.017	6.917	25.312	1.00	45.52	C
ATOM	1970	C	THR	E	88	33.226	6.603	26.197	1.00	45.33	C
ATOM	1971	O	THR	E	88	34.368	6.773	25.782	1.00	45.65	O
ATOM	1972	CB	THR	E	88	31.423	8.319	25.656	1.00	45.47	C
ATOM	1973	OG1	THR	E	88	30.255	8.550	24.868	1.00	46.11	O
ATOM	1974	CG2	THR	E	88	32.412	9.423	25.347	1.00	45.44	C
ATOM	1975	N	ASP	E	89	32.972	6.114	27.399	1.00	45.21	N
ATOM	1976	CA	ASP	E	89	34.058	5.718	28.276	1.00	45.50	C
ATOM	1977	C	ASP	E	89	34.836	4.573	27.648	1.00	45.49	C
ATOM	1978	O	ASP	E	89	36.069	4.562	27.653	1.00	45.68	O
ATOM	1979	CB	ASP	E	89	33.511	5.356	29.653	1.00	45.45	C
ATOM	1980	CG	ASP	E	89	32.613	6.442	30.204	1.00	45.95	C
ATOM	1981	OD1	ASP	E	89	31.397	6.210	30.362	1.00	46.10	O
ATOM	1982	OD2	ASP	E	89	33.120	7.557	30.428	1.00	47.48	O
ATOM	1983	N	PHE	E	90	34.103	3.631	27.071	1.00	45.64	N
ATOM	1984	CA	PHE	E	90	34.700	2.523	26.349	1.00	45.40	C
ATOM	1985	C	PHE	E	90	35.583	3.006	25.213	1.00	44.49	C
ATOM	1986	O	PHE	E	90	36.697	2.505	25.051	1.00	44.29	O
ATOM	1987	CB	PHE	E	90	33.616	1.609	25.804	1.00	46.27	C
ATOM	1988	CG	PHE	E	90	34.151	0.415	25.077	1.00	49.10	C
ATOM	1989	CD1	PHE	E	90	34.903	-0.549	25.755	1.00	50.23	C
ATOM	1990	CD2	PHE	E	90	33.905	0.245	23.710	1.00	50.29	C
ATOM	1991	CE1	PHE	E	90	35.398	-1.671	25.090	1.00	51.75	C
ATOM	1992	CE2	PHE	E	90	34.398	-0.872	23.028	1.00	51.53	C
ATOM	1993	CZ	PHE	E	90	35.148	-1.837	23.723	1.00	51.44	C
ATOM	1994	N	ILE	E	91	35.092	3.979	24.437	1.00	43.33	N
ATOM	1995	CA	ILE	E	91	35.879	4.550	23.351	1.00	42.35	C
ATOM	1996	C	ILE	E	91	37.109	5.242	23.888	1.00	42.29	C
ATOM	1997	O	ILE	E	91	38.206	5.006	23.399	1.00	42.33	O
ATOM	1998	CB	ILE	E	91	35.057	5.490	22.460	1.00	42.74	C
ATOM	1999	CG1	ILE	E	91	34.154	4.656	21.564	1.00	41.95	C
ATOM	2000	CG2	ILE	E	91	35.968	6.354	21.575	1.00	41.74	C
ATOM	2001	CD1	ILE	E	91	32.895	5.312	21.231	1.00	41.60	C
ATOM	2002	N	ASN	E	92	36.934	6.073	24.908	1.00	42.35	N
ATOM	2003	CA	ASN	E	92	38.067	6.701	25.591	1.00	42.52	C
ATOM	2004	C	ASN	E	92	39.130	5.710	26.063	1.00	42.65	C
ATOM	2005	O	ASN	E	92	40.320	5.959	25.904	1.00	42.36	O
ATOM	2006	CB	ASN	E	92	37.580	7.573	26.757	1.00	42.67	C
ATOM	2007	CG	ASN	E	92	36.928	8.866	26.281	1.00	43.62	C

Figure 2 Table 2b - 31

ATOM	2008	OD1	ASN	E	92	36.880	9.137	25.091	1.00	44.24	O
ATOM	2009	ND2	ASN	E	92	36.429	9.665	27.209	1.00	45.27	N
ATOM	2010	N	ILE	E	93	38.693	4.583	26.621	1.00	43.24	N
ATOM	2011	CA	ILE	E	93	39.595	3.561	27.147	1.00	43.84	C
ATOM	2012	C	ILE	E	93	40.332	2.822	26.027	1.00	44.09	C
ATOM	2013	O	ILE	E	93	41.531	2.530	26.158	1.00	44.22	O
ATOM	2014	CB	ILE	E	93	38.835	2.554	28.091	1.00	44.22	C
ATOM	2015	CG1	ILE	E	93	38.688	3.152	29.485	1.00	44.88	C
ATOM	2016	CG2	ILE	E	93	39.563	1.230	28.210	1.00	43.12	C
ATOM	2017	CD1	ILE	E	93	37.379	2.852	30.156	1.00	46.70	C
ATOM	2018	N	LEU	E	94	39.621	2.506	24.942	1.00	44.06	N
ATOM	2019	CA	LEU	E	94	40.253	1.845	23.799	1.00	44.54	C
ATOM	2020	C	LEU	E	94	41.292	2.727	23.128	1.00	44.37	C
ATOM	2021	O	LEU	E	94	42.345	2.249	22.711	1.00	44.22	O
ATOM	2022	CB	LEU	E	94	39.229	1.430	22.759	1.00	44.68	C
ATOM	2023	CG	LEU	E	94	38.419	0.165	22.955	1.00	46.21	C
ATOM	2024	CD1	LEU	E	94	37.729	-0.121	21.632	1.00	47.78	C
ATOM	2025	CD2	LEU	E	94	39.280	-1.026	23.399	1.00	46.39	C
ATOM	2026	N	HIS	E	95	40.975	4.014	23.010	1.00	44.58	N
ATOM	2027	CA	HIS	E	95	41.915	4.997	22.475	1.00	44.83	C
ATOM	2028	C	HIS	E	95	43.195	5.071	23.324	1.00	45.34	C
ATOM	2029	O	HIS	E	95	44.293	5.084	22.784	1.00	45.35	O
ATOM	2030	CB	HIS	E	95	41.253	6.364	22.381	1.00	44.27	C
ATOM	2031	CG	HIS	E	95	42.097	7.386	21.694	1.00	44.69	C
ATOM	2032	ND1	HIS	E	95	42.693	8.430	22.366	1.00	44.14	N
ATOM	2033	CD2	HIS	E	95	42.462	7.513	20.396	1.00	43.29	C
ATOM	2034	CE1	HIS	E	95	43.382	9.161	21.511	1.00	44.28	C
ATOM	2035	NE2	HIS	E	95	43.259	8.626	20.309	1.00	44.40	N
ATOM	2036	N	ARG	E	96	43.044	5.096	24.648	1.00	45.89	N
ATOM	2037	CA	ARG	E	96	44.187	5.135	25.558	1.00	46.70	C
ATOM	2038	C	ARG	E	96	44.968	3.832	25.576	1.00	46.54	C
ATOM	2039	O	ARG	E	96	46.183	3.839	25.734	1.00	46.34	O
ATOM	2040	CB	ARG	E	96	43.737	5.470	26.980	1.00	47.21	C
ATOM	2041	CG	ARG	E	96	44.056	6.885	27.419	1.00	49.54	C
ATOM	2042	CD	ARG	E	96	45.481	6.995	27.924	1.00	52.08	C
ATOM	2043	NE	ARG	E	96	45.584	8.020	28.955	1.00	55.52	N
ATOM	2044	CZ	ARG	E	96	45.806	7.774	30.247	1.00	58.79	C
ATOM	2045	NH1	ARG	E	96	45.977	6.528	30.699	1.00	59.39	N
ATOM	2046	NH2	ARG	E	96	45.881	8.787	31.102	1.00	60.52	N
ATOM	2047	N	TYR	E	97	44.259	2.714	25.447	1.00	46.63	N
ATOM	2048	CA	TYR	E	97	44.900	1.413	25.385	1.00	46.57	C
ATOM	2049	C	TYR	E	97	45.718	1.298	24.113	1.00	45.67	C
ATOM	2050	O	TYR	E	97	46.860	0.857	24.137	1.00	45.36	O
ATOM	2051	CB	TYR	E	97	43.867	0.285	25.438	1.00	47.78	C
ATOM	2052	CG	TYR	E	97	44.481	-1.067	25.152	1.00	49.82	C
ATOM	2053	CD1	TYR	E	97	45.103	-1.800	26.169	1.00	51.42	C
ATOM	2054	CD2	TYR	E	97	44.480	-1.597	23.854	1.00	51.09	C
ATOM	2055	CE1	TYR	E	97	45.691	-3.033	25.907	1.00	52.31	C
ATOM	2056	CE2	TYR	E	97	45.070	-2.828	23.577	1.00	51.37	C
ATOM	2057	CZ	TYR	E	97	45.670	-3.538	24.607	1.00	52.23	C
ATOM	2058	OH	TYR	E	97	46.252	-4.761	24.346	1.00	53.23	O
ATOM	2059	N	TYR	E	98	45.121	1.706	22.997	1.00	45.13	N
ATOM	2060	CA	TYR	E	98	45.782	1.602	21.712	1.00	44.25	C
ATOM	2061	C	TYR	E	98	47.093	2.381	21.688	1.00	43.10	C
ATOM	2062	O	TYR	E	98	48.115	1.873	21.217	1.00	42.90	O
ATOM	2063	CB	TYR	E	98	44.859	2.026	20.568	1.00	44.93	C
ATOM	2064	CG	TYR	E	98	45.581	2.062	19.241	1.00	46.33	C
ATOM	2065	CD1	TYR	E	98	45.929	0.875	18.589	1.00	47.68	C
ATOM	2066	CD2	TYR	E	98	45.954	3.279	18.652	1.00	46.70	C
ATOM	2067	CE1	TYR	E	98	46.613	0.890	17.369	1.00	48.29	C
ATOM	2068	CE2	TYR	E	98	46.646	3.305	17.436	1.00	47.73	C
ATOM	2069	CZ	TYR	E	98	46.970	2.102	16.798	1.00	48.10	C
ATOM	2070	OH	TYR	E	98	47.645	2.102	15.588	1.00	48.95	O
ATOM	2071	N	LYS	E	99	47.060	3.607	22.204	1.00	41.76	N
ATOM	2072	CA	LYS	E	99	48.247	4.461	22.209	1.00	40.57	C
ATOM	2073	C	LYS	E	99	49.257	3.954	23.224	1.00	39.37	C
ATOM	2074	O	LYS	E	99	50.446	3.997	22.985	1.00	39.56	O

Figure 2 Table 2b - 32

ATOM	2075	CB	LYS	E	99	47.891	5.935	22.477	1.00	40.54	C
ATOM	2076	CG	LYS	E	99	47.044	6.612	21.386	1.00	40.54	C
ATOM	2077	CD	LYS	E	99	47.861	6.973	20.156	1.00	41.63	C
ATOM	2078	CE	LYS	E	99	47.022	7.757	19.152	1.00	42.35	C
ATOM	2079	NZ	LYS	E	99	47.761	8.062	17.897	1.00	42.69	N
ATOM	2080	N	SER	E	100	48.776	3.466	24.354	1.00	38.47	N
ATOM	2081	CA	SER	E	100	49.659	2.961	25.402	1.00	37.68	C
ATOM	2082	C	SER	E	100	50.421	1.721	24.962	1.00	37.05	C
ATOM	2083	O	SER	E	100	51.603	1.588	25.261	1.00	37.29	O
ATOM	2084	CB	SER	E	100	48.885	2.680	26.684	1.00	37.48	C
ATOM	2085	OG	SER	E	100	48.318	3.870	27.202	1.00	37.24	O
ATOM	2086	N	ALA	E	101	49.746	0.831	24.239	1.00	36.28	N
ATOM	2087	CA	ALA	E	101	50.368	-0.381	23.720	1.00	35.34	C
ATOM	2088	C	ALA	E	101	51.571	-0.066	22.835	1.00	34.90	C
ATOM	2089	O	ALA	E	101	52.594	-0.753	22.879	1.00	34.79	O
ATOM	2090	CB	ALA	E	101	49.355	-1.194	22.955	1.00	35.44	C
ATOM	2091	N	LEU	E	102	51.456	0.988	22.043	1.00	34.18	N
ATOM	2092	CA	LEU	E	102	52.528	1.350	21.126	1.00	33.90	C
ATOM	2093	C	LEU	E	102	53.743	1.837	21.887	1.00	33.80	C
ATOM	2094	O	LEU	E	102	54.855	1.891	21.347	1.00	33.78	O
ATOM	2095	CB	LEU	E	102	52.056	2.395	20.115	1.00	33.81	C
ATOM	2096	CG	LEU	E	102	51.149	1.869	18.997	1.00	33.18	C
ATOM	2097	CD1	LEU	E	102	50.589	3.036	18.200	1.00	32.18	C
ATOM	2098	CD2	LEU	E	102	51.913	0.896	18.082	1.00	32.51	C
ATOM	2099	N	VAL	E	103	53.525	2.165	23.153	1.00	33.50	N
ATOM	2100	CA	VAL	E	103	54.588	2.675	23.987	1.00	33.60	C
ATOM	2101	C	VAL	E	103	54.884	1.710	25.161	1.00	33.76	C
ATOM	2102	O	VAL	E	103	55.583	2.043	26.117	1.00	33.73	O
ATOM	2103	CB	VAL	E	103	54.326	4.192	24.323	1.00	33.62	C
ATOM	2104	CG1	VAL	E	103	53.553	4.406	25.624	1.00	32.88	C
ATOM	2105	CG2	VAL	E	103	55.621	4.987	24.272	1.00	33.91	C
ATOM	2106	N	GLN	E	104	54.397	0.477	25.004	1.00	34.15	N
ATOM	2107	CA	GLN	E	104	54.615	-0.661	25.928	1.00	34.97	C
ATOM	2108	C	GLN	E	104	54.051	-0.481	27.338	1.00	35.84	C
ATOM	2109	O	GLN	E	104	54.647	-0.920	28.292	1.00	35.43	O
ATOM	2110	CB	GLN	E	104	56.084	-1.115	25.987	1.00	34.47	C
ATOM	2111	CG	GLN	E	104	56.677	-1.570	24.669	1.00	33.65	C
ATOM	2112	CD	GLN	E	104	57.072	-0.393	23.770	1.00	34.07	C
ATOM	2113	OE1	GLN	E	104	57.837	0.485	24.176	1.00	32.91	O
ATOM	2114	NE2	GLN	E	104	56.532	-0.363	22.554	1.00	34.32	N
ATOM	2115	N	ILE	E	105	52.895	0.167	27.434	1.00	37.91	N
ATOM	2116	CA	ILE	E	105	52.184	0.385	28.692	1.00	40.21	C
ATOM	2117	C	ILE	E	105	50.853	-0.377	28.612	1.00	42.06	C
ATOM	2118	O	ILE	E	105	50.010	-0.070	27.779	1.00	42.31	O
ATOM	2119	CB	ILE	E	105	51.965	1.916	28.994	1.00	40.19	C
ATOM	2120	CG1	ILE	E	105	53.317	2.620	29.208	1.00	40.26	C
ATOM	2121	CG2	ILE	E	105	51.032	2.125	30.206	1.00	39.62	C
ATOM	2122	CD1	ILE	E	105	53.248	4.122	29.355	1.00	39.33	C
ATOM	2123	N	TYR	E	106	50.672	-1.375	29.470	1.00	44.54	N
ATOM	2124	CA	TYR	E	106	49.521	-2.272	29.341	1.00	47.16	C
ATOM	2125	C	TYR	E	106	48.595	-2.273	30.550	1.00	49.76	C
ATOM	2126	O	TYR	E	106	47.820	-3.213	30.738	1.00	50.67	O
ATOM	2127	CB	TYR	E	106	49.994	-3.694	29.030	1.00	46.23	C
ATOM	2128	CG	TYR	E	106	50.956	-3.781	27.863	1.00	45.20	C
ATOM	2129	CD1	TYR	E	106	52.306	-4.072	28.067	1.00	43.52	C
ATOM	2130	CD2	TYR	E	106	50.515	-3.567	26.556	1.00	42.88	C
ATOM	2131	CE1	TYR	E	106	53.189	-4.156	26.995	1.00	43.00	C
ATOM	2132	CE2	TYR	E	106	51.389	-3.650	25.488	1.00	42.90	C
ATOM	2133	CZ	TYR	E	106	52.719	-3.941	25.712	1.00	42.83	C
ATOM	2134	OH	TYR	E	106	53.573	-4.016	24.645	1.00	43.13	O
ATOM	2135	N	GLU	E	107	48.672	-1.216	31.358	1.00	52.99	N
ATOM	2136	CA	GLU	E	107	47.840	-1.058	32.555	1.00	56.06	C
ATOM	2137	C	GLU	E	107	46.372	-1.231	32.219	1.00	57.95	C
ATOM	2138	O	GLU	E	107	45.654	-2.022	32.833	1.00	58.01	O
ATOM	2139	CB	GLU	E	107	47.981	0.353	33.135	1.00	56.08	C
ATOM	2140	CG	GLU	E	107	49.362	0.790	33.604	1.00	56.90	C
ATOM	2141	CD	GLU	E	107	49.396	2.288	33.885	1.00	56.88	C

Figure 2 Table 2b - 33

ATOM	2142	OE1	GLU	E	107	48.923	3.062	33.018	1.00	57.50	O
ATOM	2143	OE2	GLU	E	107	49.886	2.689	34.969	1.00	56.75	O
ATOM	2144	N	LEU	E	108	45.950	-0.476	31.213	1.00	60.51	N
ATOM	2145	CA	LEU	E	108	44.546	-0.190	30.987	1.00	62.88	C
ATOM	2146	C	LEU	E	108	43.627	-1.374	31.253	1.00	64.38	C
ATOM	2147	O	LEU	E	108	42.668	-1.246	32.017	1.00	65.10	O
ATOM	2148	CB	LEU	E	108	44.321	0.413	29.589	1.00	62.86	C
ATOM	2149	CG	LEU	E	108	44.776	1.865	29.370	1.00	63.23	C
ATOM	2150	CD1	LEU	E	108	44.037	2.802	30.341	1.00	63.36	C
ATOM	2151	CD2	LEU	E	108	46.317	2.038	29.466	1.00	62.49	C
ATOM	2152	N	GLU	E	109	43.935	-2.530	30.669	1.00	65.96	N
ATOM	2153	CA	GLU	E	109	42.970	-3.634	30.686	1.00	67.42	C
ATOM	2154	C	GLU	E	109	42.683	-4.257	32.063	1.00	67.95	C
ATOM	2155	O	GLU	E	109	41.595	-4.807	32.284	1.00	68.39	O
ATOM	2156	CB	GLU	E	109	43.295	-4.662	29.595	1.00	67.72	C
ATOM	2157	CG	GLU	E	109	42.290	-4.693	28.401	1.00	68.92	C
ATOM	2158	CD	GLU	E	109	41.606	-3.349	28.044	1.00	70.09	C
ATOM	2159	OE1	GLU	E	109	41.003	-3.270	26.948	1.00	71.03	O
ATOM	2160	OE2	GLU	E	109	41.642	-2.379	28.837	1.00	70.18	O
ATOM	2161	N	GLU	E	110	43.633	-4.114	32.990	1.00	68.61	N
ATOM	2162	CA	GLU	E	110	43.483	-4.593	34.378	1.00	68.76	C
ATOM	2163	C	GLU	E	110	42.958	-3.525	35.351	1.00	68.57	C
ATOM	2164	O	GLU	E	110	42.821	-3.781	36.547	1.00	68.56	O
ATOM	2165	CB	GLU	E	110	44.802	-5.193	34.892	1.00	69.00	C
ATOM	2166	CG	GLU	E	110	45.339	-6.362	34.062	1.00	70.51	C
ATOM	2167	CD	GLU	E	110	44.231	-7.189	33.415	1.00	72.95	C
ATOM	2168	OE1	GLU	E	110	43.475	-7.874	34.143	1.00	74.12	O
ATOM	2169	OE2	GLU	E	110	44.112	-7.142	32.170	1.00	73.93	O
ATOM	2170	N	HIS	E	111	42.667	-2.334	34.831	1.00	68.46	N
ATOM	2171	CA	HIS	E	111	42.044	-1.265	35.609	1.00	68.39	C
ATOM	2172	C	HIS	E	111	40.687	-1.728	36.116	1.00	67.77	C
ATOM	2173	O	HIS	E	111	39.914	-2.342	35.377	1.00	67.53	O
ATOM	2174	CB	HIS	E	111	41.824	-0.015	34.737	1.00	68.73	C
ATOM	2175	CG	HIS	E	111	43.006	0.907	34.646	1.00	70.32	C
ATOM	2176	ND1	HIS	E	111	44.232	0.631	35.218	1.00	71.98	N
ATOM	2177	CD2	HIS	E	111	43.150	2.097	34.010	1.00	71.57	C
ATOM	2178	CE1	HIS	E	111	45.071	1.619	34.957	1.00	72.61	C
ATOM	2179	NE2	HIS	E	111	44.440	2.520	34.223	1.00	72.33	N
ATOM	2180	N	LYS	E	112	40.394	-1.438	37.375	1.00	67.18	N
ATOM	2181	CA	LYS	E	112	39.008	-1.481	37.800	1.00	66.94	C
ATOM	2182	C	LYS	E	112	38.355	-0.139	37.472	1.00	66.66	C
ATOM	2183	O	LYS	E	112	39.043	0.880	37.361	1.00	66.64	O
ATOM	2184	CB	LYS	E	112	38.850	-1.882	39.275	1.00	66.90	C
ATOM	2185	CG	LYS	E	112	39.805	-1.224	40.256	1.00	67.23	C
ATOM	2186	CD	LYS	E	112	40.712	-2.253	40.951	1.00	66.71	C
ATOM	2187	CE	LYS	E	112	39.924	-3.375	41.608	1.00	67.03	C
ATOM	2188	NZ	LYS	E	112	40.807	-4.360	42.301	1.00	67.45	N
ATOM	2189	N	ILE	E	113	37.041	-0.155	37.268	1.00	66.10	N
ATOM	2190	CA	ILE	E	113	36.275	1.066	37.028	1.00	65.54	C
ATOM	2191	C	ILE	E	113	36.766	2.203	37.936	1.00	65.69	C
ATOM	2192	O	ILE	E	113	37.064	3.300	37.454	1.00	65.56	O
ATOM	2193	CB	ILE	E	113	34.758	0.814	37.204	1.00	65.24	C
ATOM	2194	CG1	ILE	E	113	34.271	-0.185	36.145	1.00	64.14	C
ATOM	2195	CG2	ILE	E	113	33.981	2.124	37.120	1.00	65.22	C
ATOM	2196	CD1	ILE	E	113	32.923	-0.798	36.409	1.00	61.28	C
ATOM	2197	N	GLU	E	114	36.857	1.906	39.236	1.00	65.62	N
ATOM	2198	CA	GLU	E	114	37.443	2.768	40.270	1.00	65.89	C
ATOM	2199	C	GLU	E	114	38.702	3.498	39.779	1.00	65.74	C
ATOM	2200	O	GLU	E	114	38.784	4.730	39.804	1.00	65.49	O
ATOM	2201	CB	GLU	E	114	37.801	1.886	41.479	1.00	65.73	C
ATOM	2202	CG	GLU	E	114	37.590	2.483	42.865	1.00	66.49	C
ATOM	2203	CD	GLU	E	114	37.738	1.434	43.990	1.00	68.10	C
ATOM	2204	OE1	GLU	E	114	38.344	0.360	43.751	1.00	70.05	O
ATOM	2205	OE2	GLU	E	114	37.250	1.672	45.123	1.00	69.13	O
ATOM	2206	N	THR	E	115	39.671	2.711	39.318	1.00	65.94	N
ATOM	2207	CA	THR	E	115	41.007	3.199	39.009	1.00	66.16	C
ATOM	2208	C	THR	E	115	41.056	3.990	37.710	1.00	66.28	C

Figure 2 Table 2b - 34

ATOM	2209	O	THR	E	115	41.870	4.903	37.580	1.00 66.17	O
ATOM	2210	CB	THR	E	115	42.066	2.054	39.007	1.00 66.21	C
ATOM	2211	OG1	THR	E	115	41.577	0.932	38.263	1.00 66.61	O
ATOM	2212	CG2	THR	E	115	42.368	1.591	40.435	1.00 66.37	C
ATOM	2213	N	TRP	E	116	40.188	3.646	36.756	1.00 66.61	N
ATOM	2214	CA	TRP	E	116	40.090	4.426	35.525	1.00 66.85	C
ATOM	2215	C	TRP	E	116	39.410	5.760	35.775	1.00 66.79	C
ATOM	2216	O	TRP	E	116	39.845	6.784	35.254	1.00 66.77	O
ATOM	2217	CB	TRP	E	116	39.398	3.689	34.375	1.00 67.16	C
ATOM	2218	CG	TRP	E	116	39.355	4.587	33.135	1.00 68.69	C
ATOM	2219	CD1	TRP	E	116	40.407	4.896	32.303	1.00 69.12	C
ATOM	2220	CD2	TRP	E	116	38.227	5.332	32.639	1.00 68.72	C
ATOM	2221	NE1	TRP	E	116	39.995	5.767	31.321	1.00 69.48	N
ATOM	2222	CE2	TRP	E	116	38.666	6.051	31.502	1.00 69.26	C
ATOM	2223	CE3	TRP	E	116	36.890	5.456	33.042	1.00 68.94	C
ATOM	2224	CZ2	TRP	E	116	37.808	6.878	30.754	1.00 69.96	C
ATOM	2225	CZ3	TRP	E	116	36.037	6.287	32.303	1.00 69.81	C
ATOM	2226	CH2	TRP	E	116	36.501	6.982	31.167	1.00 69.56	C
ATOM	2227	N	ARG	E	117	38.346	5.748	36.568	1.00 66.93	N
ATOM	2228	CA	ARG	E	117	37.691	6.984	36.973	1.00 67.28	C
ATOM	2229	C	ARG	E	117	38.651	7.918	37.698	1.00 67.85	C
ATOM	2230	O	ARG	E	117	38.603	9.126	37.508	1.00 67.80	O
ATOM	2231	CB	ARG	E	117	36.474	6.696	37.843	1.00 67.07	C
ATOM	2232	CG	ARG	E	117	35.222	6.428	37.037	1.00 66.34	C
ATOM	2233	CD	ARG	E	117	34.036	6.057	37.914	1.00 65.23	C
ATOM	2234	NE	ARG	E	117	33.672	7.096	38.881	1.00 63.33	N
ATOM	2235	CZ	ARG	E	117	32.931	8.166	38.605	1.00 62.01	C
ATOM	2236	NH1	ARG	E	117	32.467	8.380	37.380	1.00 60.91	N
ATOM	2237	NH2	ARG	E	117	32.656	9.030	39.565	1.00 61.45	N
ATOM	2238	N	GLU	E	118	39.530	7.352	38.517	1.00 68.67	N
ATOM	2239	CA	GLU	E	118	40.536	8.145	39.214	1.00 69.69	C
ATOM	2240	C	GLU	E	118	41.589	8.690	38.237	1.00 70.05	C
ATOM	2241	O	GLU	E	118	42.146	9.769	38.450	1.00 70.01	O
ATOM	2242	CB	GLU	E	118	41.182	7.324	40.334	1.00 69.65	C
ATOM	2243	CG	GLU	E	118	41.897	8.157	41.396	1.00 70.27	C
ATOM	2244	CD	GLU	E	118	42.256	7.358	42.651	1.00 70.94	C
ATOM	2245	OE1	GLU	E	118	41.473	6.455	43.051	1.00 71.32	O
ATOM	2246	OE2	GLU	E	118	43.323	7.651	43.246	1.00 71.23	O
ATOM	2247	N	VAL	E	119	41.839	7.947	37.165	1.00 70.69	N
ATOM	2248	CA	VAL	E	119	42.752	8.387	36.109	1.00 71.28	C
ATOM	2249	C	VAL	E	119	42.190	9.569	35.298	1.00 72.04	C
ATOM	2250	O	VAL	E	119	42.941	10.466	34.933	1.00 72.18	O
ATOM	2251	CB	VAL	E	119	43.213	7.190	35.207	1.00 71.25	C
ATOM	2252	CG1	VAL	E	119	43.539	7.621	33.778	1.00 70.75	C
ATOM	2253	CG2	VAL	E	119	44.405	6.475	35.838	1.00 70.92	C
ATOM	2254	N	TYR	E	120	40.883	9.595	35.035	1.00 72.96	N
ATOM	2255	CA	TYR	E	120	40.335	10.681	34.224	1.00 73.85	C
ATOM	2256	C	TYR	E	120	39.490	11.756	34.917	1.00 74.15	C
ATOM	2257	O	TYR	E	120	39.629	12.941	34.611	1.00 74.14	O
ATOM	2258	CB	TYR	E	120	39.638	10.172	32.965	1.00 74.35	C
ATOM	2259	CG	TYR	E	120	39.608	11.262	31.926	1.00 75.59	C
ATOM	2260	CD1	TYR	E	120	40.789	11.662	31.276	1.00 76.73	C
ATOM	2261	CD2	TYR	E	120	38.424	11.940	31.630	1.00 76.81	C
ATOM	2262	CE1	TYR	E	120	40.786	12.689	30.329	1.00 77.22	C
ATOM	2263	CE2	TYR	E	120	38.406	12.977	30.683	1.00 77.25	C
ATOM	2264	CZ	TYR	E	120	39.591	13.342	30.038	1.00 77.11	C
ATOM	2265	OH	TYR	E	120	39.581	14.358	29.108	1.00 77.21	O
ATOM	2266	N	LEU	E	121	38.613	11.361	35.832	1.00 74.65	N
ATOM	2267	CA	LEU	E	121	37.853	12.339	36.625	1.00 75.19	C
ATOM	2268	C	LEU	E	121	38.776	13.077	37.603	1.00 75.45	C
ATOM	2269	O	LEU	E	121	38.346	13.466	38.691	1.00 75.52	O
ATOM	2270	CB	LEU	E	121	36.720	11.649	37.406	1.00 75.16	C
ATOM	2271	CG	LEU	E	121	35.338	11.335	36.810	1.00 75.58	C
ATOM	2272	CD1	LEU	E	121	34.553	12.605	36.534	1.00 75.63	C
ATOM	2273	CD2	LEU	E	121	35.401	10.445	35.556	1.00 76.09	C
ATOM	2274	N	GLN	E	122	40.029	13.280	37.186	1.00 75.65	N
ATOM	2275	CA	GLN	E	122	41.156	13.654	38.059	1.00 76.01	C

Figure 2 Table 2b - 35

ATOM	2276	C	GLN	E	122	40.822	14.564	39.244	1.00	76.13	C
ATOM	2277	O	GLN	E	122	40.160	14.153	40.204	1.00	76.13	O
ATOM	2278	CB	GLN	E	122	42.284	14.292	37.234	1.00	76.03	C
ATOM	2279	CG	GLN	E	122	42.814	13.437	36.101	1.00	76.60	C
ATOM	2280	CD	GLN	E	122	44.324	13.525	35.976	1.00	77.33	C
ATOM	2281	OE1	GLN	E	122	45.057	13.030	36.837	1.00	77.43	O
ATOM	2282	NE2	GLN	E	122	44.799	14.150	34.900	1.00	76.96	N
ATOM	2283	N	ASP	E	123	41.335	15.791	39.176	1.00	76.25	N
ATOM	2284	CA	ASP	E	123	40.986	16.853	40.111	1.00	76.22	C
ATOM	2285	C	ASP	E	123	39.586	17.380	39.777	1.00	76.06	C
ATOM	2286	O	ASP	E	123	38.751	17.569	40.671	1.00	76.14	O
ATOM	2287	CB	ASP	E	123	42.036	17.978	40.067	1.00	76.23	C
ATOM	2288	CG	ASP	E	123	42.616	18.202	38.663	1.00	76.64	C
ATOM	2289	OD1	ASP	E	123	41.856	18.156	37.669	1.00	76.98	O
ATOM	2290	OD2	ASP	E	123	43.841	18.431	38.555	1.00	76.95	O
ATOM	2291	N	SER	E	124	39.340	17.563	38.490	1.00	75.66	N
ATOM	2292	CA	SER	E	124	38.055	18.080	38.015	1.00	75.13	C
ATOM	2293	C	SER	E	124	36.948	17.088	38.325	1.00	74.52	C
ATOM	2294	O	SER	E	124	37.000	15.928	37.903	1.00	74.67	O
ATOM	2295	CB	SER	E	124	38.099	18.382	36.508	1.00	75.27	C
ATOM	2296	OG	SER	E	124	38.158	17.192	35.737	1.00	75.50	O
ATOM	2297	N	PHE	E	125	35.955	17.547	39.076	1.00	73.61	N
ATOM	2298	CA	PHE	E	125	34.884	16.669	39.507	1.00	72.77	C
ATOM	2299	C	PHE	E	125	33.662	16.790	38.596	1.00	71.85	C
ATOM	2300	O	PHE	E	125	33.274	17.902	38.198	1.00	71.81	O
ATOM	2301	CB	PHE	E	125	34.511	16.948	40.966	1.00	73.01	C
ATOM	2302	CG	PHE	E	125	34.311	15.704	41.789	1.00	73.69	C
ATOM	2303	CD1	PHE	E	125	35.123	15.452	42.897	1.00	74.44	C
ATOM	2304	CD2	PHE	E	125	33.319	14.775	41.455	1.00	74.08	C
ATOM	2305	CE1	PHE	E	125	34.945	14.297	43.671	1.00	74.66	C
ATOM	2306	CE2	PHE	E	125	33.134	13.617	42.216	1.00	74.36	C
ATOM	2307	CZ	PHE	E	125	33.949	13.376	43.329	1.00	74.50	C
ATOM	2308	N	LYS	E	126	33.089	15.632	38.251	1.00	70.24	N
ATOM	2309	CA	LYS	E	126	31.805	15.551	37.557	1.00	68.55	C
ATOM	2310	C	LYS	E	126	30.922	14.565	38.308	1.00	67.22	C
ATOM	2311	O	LYS	E	126	31.065	13.353	38.133	1.00	67.44	O
ATOM	2312	CB	LYS	E	126	31.967	15.105	36.095	1.00	68.74	C
ATOM	2313	CG	LYS	E	126	32.594	16.137	35.158	1.00	68.51	C
ATOM	2314	CD	LYS	E	126	32.381	15.742	33.696	1.00	68.41	C
ATOM	2315	CE	LYS	E	126	33.194	16.623	32.747	1.00	67.99	C
ATOM	2316	NZ	LYS	E	126	32.763	18.045	32.807	1.00	67.02	N
ATOM	2317	N	PRO	E	127	30.007	15.079	39.154	1.00	65.70	N
ATOM	2318	CA	PRO	E	127	29.115	14.211	39.925	1.00	64.18	C
ATOM	2319	C	PRO	E	127	28.077	13.534	39.026	1.00	62.64	C
ATOM	2320	O	PRO	E	127	27.893	13.943	37.877	1.00	62.63	O
ATOM	2321	CB	PRO	E	127	28.437	15.187	40.891	1.00	64.27	C
ATOM	2322	CG	PRO	E	127	28.451	16.495	40.178	1.00	64.90	C
ATOM	2323	CD	PRO	E	127	29.748	16.510	39.419	1.00	65.62	C
ATOM	2324	N	LEU	E	128	27.415	12.502	39.537	1.00	60.67	N
ATOM	2325	CA	LEU	E	128	26.343	11.862	38.788	1.00	58.82	C
ATOM	2326	C	LEU	E	128	25.141	12.794	38.703	1.00	57.66	C
ATOM	2327	O	LEU	E	128	24.679	13.306	39.720	1.00	57.72	O
ATOM	2328	CB	LEU	E	128	25.936	10.530	39.430	1.00	58.51	C
ATOM	2329	CG	LEU	E	128	24.669	9.871	38.879	1.00	57.89	C
ATOM	2330	CD1	LEU	E	128	24.896	9.300	37.491	1.00	57.64	C
ATOM	2331	CD2	LEU	E	128	24.212	8.783	39.800	1.00	57.18	C
ATOM	2332	N	VAL	E	129	24.650	13.032	37.492	1.00	55.96	N
ATOM	2333	CA	VAL	E	129	23.387	13.741	37.336	1.00	54.24	C
ATOM	2334	C	VAL	E	129	22.256	12.732	37.151	1.00	53.56	C
ATOM	2335	O	VAL	E	129	22.379	11.756	36.399	1.00	53.38	O
ATOM	2336	CB	VAL	E	129	23.435	14.865	36.231	1.00	54.45	C
ATOM	2337	CG1	VAL	E	129	24.747	14.848	35.453	1.00	54.22	C
ATOM	2338	CG2	VAL	E	129	22.217	14.834	35.303	1.00	52.89	C
ATOM	2339	N	CYS	E	130	21.168	12.952	37.878	1.00	52.26	N
ATOM	2340	CA	CYS	E	130	20.024	12.059	37.817	1.00	51.13	C
ATOM	2341	C	CYS	E	130	18.769	12.849	38.048	1.00	50.50	C
ATOM	2342	O	CYS	E	130	18.823	14.022	38.372	1.00	49.92	O

Figure 2 Table 2b - 36

ATOM	2343	CB	CYS	E	130	20.123	10.966	38.879	1.00	51.15	C
ATOM	2344	SG	CYS	E	130	19.994	11.596	40.556	1.00	49.90	S
ATOM	2345	N	ILE	E	131	17.631	12.181	37.923	1.00	50.09	N
ATOM	2346	CA	ILE	E	131	16.362	12.866	38.043	1.00	49.76	C
ATOM	2347	C	ILE	E	131	15.352	11.997	38.793	1.00	49.16	C
ATOM	2348	O	ILE	E	131	15.354	10.788	38.665	1.00	48.89	O
ATOM	2349	CB	ILE	E	131	15.855	13.367	36.649	1.00	49.42	C
ATOM	2350	CG1	ILE	E	131	14.895	14.537	36.809	1.00	50.01	C
ATOM	2351	CG2	ILE	E	131	15.220	12.266	35.848	1.00	49.42	C
ATOM	2352	CD1	ILE	E	131	15.025	15.588	35.699	1.00	49.95	C
ATOM	2353	N	SER	E	132	14.530	12.642	39.606	1.00	49.04	N
ATOM	2354	CA	SER	E	132	13.427	12.003	40.297	1.00	49.39	C
ATOM	2355	C	SER	E	132	12.348	11.545	39.309	1.00	48.94	C
ATOM	2356	O	SER	E	132	12.130	12.205	38.300	1.00	49.48	O
ATOM	2357	CB	SER	E	132	12.831	13.008	41.277	1.00	49.37	C
ATOM	2358	OG	SER	E	132	11.667	12.485	41.887	1.00	52.28	O
ATOM	2359	N	PRO	E	133	11.674	10.413	39.584	1.00	48.70	N
ATOM	2360	CA	PRO	E	133	10.499	9.999	38.792	1.00	48.53	C
ATOM	2361	C	PRO	E	133	9.330	10.980	38.834	1.00	48.92	C
ATOM	2362	O	PRO	E	133	8.462	10.922	37.954	1.00	49.15	O
ATOM	2363	CB	PRO	E	133	10.058	8.693	39.462	1.00	48.58	C
ATOM	2364	CG	PRO	E	133	10.686	8.702	40.798	1.00	48.11	C
ATOM	2365	CD	PRO	E	133	11.986	9.434	40.634	1.00	48.48	C
ATOM	2366	N	ASN	E	134	9.302	11.861	39.841	1.00	49.00	N
ATOM	2367	CA	ASN	E	134	8.231	12.848	39.985	1.00	49.17	C
ATOM	2368	C	ASN	E	134	8.531	14.209	39.323	1.00	49.43	C
ATOM	2369	O	ASN	E	134	7.689	15.107	39.315	1.00	49.11	O
ATOM	2370	CB	ASN	E	134	7.869	13.024	41.454	1.00	48.98	C
ATOM	2371	CG	ASN	E	134	7.182	11.793	42.042	1.00	50.57	C
ATOM	2372	OD1	ASN	E	134	6.241	11.243	41.458	1.00	51.40	O
ATOM	2373	ND2	ASN	E	134	7.641	11.368	43.216	1.00	50.21	N
ATOM	2374	N	ALA	E	135	9.725	14.344	38.758	1.00	49.54	N
ATOM	2375	CA	ALA	E	135	10.142	15.582	38.121	1.00	49.83	C
ATOM	2376	C	ALA	E	135	9.543	15.687	36.725	1.00	50.28	C
ATOM	2377	O	ALA	E	135	9.315	14.676	36.056	1.00	50.67	O
ATOM	2378	CB	ALA	E	135	11.667	15.657	38.055	1.00	49.46	C
ATOM	2379	N	SER	E	136	9.302	16.917	36.284	1.00	50.57	N
ATOM	2380	CA	SER	E	136	8.757	17.166	34.955	1.00	50.76	C
ATOM	2381	C	SER	E	136	9.676	16.613	33.868	1.00	51.08	C
ATOM	2382	O	SER	E	136	10.897	16.516	34.043	1.00	51.30	O
ATOM	2383	CB	SER	E	136	8.532	18.661	34.739	1.00	50.48	C
ATOM	2384	OG	SER	E	136	9.728	19.297	34.324	1.00	50.08	O
ATOM	2385	N	LEU	E	137	9.079	16.249	32.742	1.00	51.36	N
ATOM	2386	CA	LEU	E	137	9.833	15.784	31.586	1.00	51.53	C
ATOM	2387	C	LEU	E	137	10.658	16.941	31.007	1.00	51.99	C
ATOM	2388	O	LEU	E	137	11.711	16.729	30.381	1.00	52.14	O
ATOM	2389	CB	LEU	E	137	8.867	15.226	30.554	1.00	51.09	C
ATOM	2390	CG	LEU	E	137	9.453	14.789	29.227	1.00	51.97	C
ATOM	2391	CD1	LEU	E	137	10.504	13.698	29.477	1.00	54.09	C
ATOM	2392	CD2	LEU	E	137	8.335	14.300	28.330	1.00	50.75	C
ATOM	2393	N	PHE	E	138	10.165	18.162	31.228	1.00	51.91	N
ATOM	2394	CA	PHE	E	138	10.887	19.374	30.888	1.00	52.11	C
ATOM	2395	C	PHE	E	138	12.225	19.405	31.623	1.00	52.38	C
ATOM	2396	O	PHE	E	138	13.280	19.633	31.018	1.00	52.56	O
ATOM	2397	CB	PHE	E	138	10.052	20.605	31.264	1.00	52.24	C
ATOM	2398	CG	PHE	E	138	10.714	21.908	30.933	1.00	51.65	C
ATOM	2399	CD1	PHE	E	138	10.442	22.548	29.733	1.00	51.42	C
ATOM	2400	CD2	PHE	E	138	11.620	22.490	31.818	1.00	51.45	C
ATOM	2401	CE1	PHE	E	138	11.063	23.754	29.418	1.00	50.97	C
ATOM	2402	CE2	PHE	E	138	12.243	23.687	31.514	1.00	50.50	C
ATOM	2403	CZ	PHE	E	138	11.964	24.319	30.310	1.00	51.00	C
ATOM	2404	N	ASP	E	139	12.172	19.178	32.930	1.00	52.33	N
ATOM	2405	CA	ASP	E	139	13.375	19.124	33.741	1.00	52.41	C
ATOM	2406	C	ASP	E	139	14.348	18.065	33.246	1.00	52.07	C
ATOM	2407	O	ASP	E	139	15.559	18.275	33.299	1.00	52.07	O
ATOM	2408	CB	ASP	E	139	13.031	18.889	35.213	1.00	52.67	C
ATOM	2409	CG	ASP	E	139	12.402	20.113	35.871	1.00	53.55	C

Figure 2 Table 2b - 37

ATOM	2410	OD1	ASP	E	139	12.595	21.238	35.359	1.00	54.44	O
ATOM	2411	OD2	ASP	E	139	11.709	19.952	36.904	1.00	54.48	O
ATOM	2412	N	ALA	E	140	13.820	16.939	32.762	1.00	51.69	N
ATOM	2413	CA	ALA	E	140	14.661	15.869	32.214	1.00	51.14	C
ATOM	2414	C	ALA	E	140	15.355	16.309	30.933	1.00	51.18	C
ATOM	2415	O	ALA	E	140	16.582	16.168	30.807	1.00	51.34	O
ATOM	2416	CB	ALA	E	140	13.859	14.615	31.979	1.00	51.48	C
ATOM	2417	N	VAL	E	141	14.580	16.863	29.996	1.00	50.40	N
ATOM	2418	CA	VAL	E	141	15.155	17.446	28.784	1.00	49.69	C
ATOM	2419	C	VAL	E	141	16.182	18.542	29.093	1.00	49.62	C
ATOM	2420	O	VAL	E	141	17.247	18.581	28.471	1.00	49.68	O
ATOM	2421	CB	VAL	E	141	14.080	17.979	27.815	1.00	49.71	C
ATOM	2422	CG1	VAL	E	141	14.726	18.484	26.528	1.00	49.08	C
ATOM	2423	CG2	VAL	E	141	13.063	16.899	27.486	1.00	49.62	C
ATOM	2424	N	SER	E	142	15.887	19.419	30.053	1.00	49.33	N
ATOM	2425	CA	SER	E	142	16.823	20.502	30.393	1.00	49.25	C
ATOM	2426	C	SER	E	142	18.121	19.981	31.009	1.00	48.97	C
ATOM	2427	O	SER	E	142	19.183	20.551	30.777	1.00	49.55	O
ATOM	2428	CB	SER	E	142	16.184	21.522	31.329	1.00	49.20	C
ATOM	2429	OG	SER	E	142	14.829	21.713	30.990	1.00	50.75	O
ATOM	2430	N	SER	E	143	18.036	18.906	31.787	1.00	48.33	N
ATOM	2431	CA	SER	E	143	19.207	18.316	32.414	1.00	47.98	C
ATOM	2432	C	SER	E	143	20.119	17.628	31.385	1.00	47.67	C
ATOM	2433	O	SER	E	143	21.342	17.721	31.481	1.00	47.10	O
ATOM	2434	CB	SER	E	143	18.776	17.363	33.547	1.00	48.48	C
ATOM	2435	OG	SER	E	143	19.810	16.477	33.953	1.00	48.44	O
ATOM	2436	N	LEU	E	144	19.525	16.952	30.402	1.00	47.71	N
ATOM	2437	CA	LEU	E	144	20.298	16.320	29.323	1.00	48.00	C
ATOM	2438	C	LEU	E	144	21.038	17.344	28.460	1.00	48.83	C
ATOM	2439	O	LEU	E	144	22.218	17.151	28.126	1.00	49.05	O
ATOM	2440	CB	LEU	E	144	19.418	15.417	28.452	1.00	47.81	C
ATOM	2441	CG	LEU	E	144	18.835	14.153	29.107	1.00	47.16	C
ATOM	2442	CD1	LEU	E	144	17.511	13.791	28.481	1.00	46.38	C
ATOM	2443	CD2	LEU	E	144	19.786	12.972	29.033	1.00	46.43	C
ATOM	2444	N	ILE	E	145	20.365	18.446	28.116	1.00	49.26	N
ATOM	2445	CA	ILE	E	145	21.003	19.462	27.286	1.00	49.65	C
ATOM	2446	C	ILE	E	145	22.102	20.106	28.080	1.00	50.01	C
ATOM	2447	O	ILE	E	145	23.238	20.169	27.615	1.00	50.49	O
ATOM	2448	CB	ILE	E	145	20.032	20.561	26.808	1.00	49.76	C
ATOM	2449	CG1	ILE	E	145	18.850	19.959	26.057	1.00	49.83	C
ATOM	2450	CG2	ILE	E	145	20.758	21.601	25.940	1.00	49.71	C
ATOM	2451	CD1	ILE	E	145	17.616	20.817	26.170	1.00	50.75	C
ATOM	2452	N	ARG	E	146	21.758	20.572	29.281	1.00	50.34	N
ATOM	2453	CA	ARG	E	146	22.639	21.435	30.073	1.00	50.60	C
ATOM	2454	C	ARG	E	146	23.888	20.691	30.558	1.00	50.50	C
ATOM	2455	O	ARG	E	146	24.976	21.262	30.619	1.00	50.48	O
ATOM	2456	CB	ARG	E	146	21.856	22.095	31.227	1.00	50.59	C
ATOM	2457	CG	ARG	E	146	22.705	22.699	32.346	1.00	50.96	C
ATOM	2458	CD	ARG	E	146	21.867	23.292	33.489	1.00	51.29	C
ATOM	2459	NE	ARG	E	146	21.256	22.283	34.351	1.00	52.08	N
ATOM	2460	CZ	ARG	E	146	19.979	21.916	34.282	1.00	52.41	C
ATOM	2461	NH1	ARG	E	146	19.168	22.477	33.398	1.00	53.57	N
ATOM	2462	NH2	ARG	E	146	19.509	20.988	35.097	1.00	52.62	N
ATOM	2463	N	ASN	E	147	23.737	19.410	30.870	1.00	50.71	N
ATOM	2464	CA	ASN	E	147	24.877	18.604	31.306	1.00	50.90	C
ATOM	2465	C	ASN	E	147	25.607	17.940	30.159	1.00	51.27	C
ATOM	2466	O	ASN	E	147	26.644	17.319	30.362	1.00	51.57	O
ATOM	2467	CB	ASN	E	147	24.449	17.586	32.348	1.00	50.40	C
ATOM	2468	CG	ASN	E	147	23.941	18.245	33.594	1.00	50.22	C
ATOM	2469	OD1	ASN	E	147	24.654	19.031	34.225	1.00	50.83	O
ATOM	2470	ND2	ASN	E	147	22.699	17.953	33.955	1.00	49.58	N
ATOM	2471	N	LYS	E	148	25.056	18.105	28.956	1.00	51.82	N
ATOM	2472	CA	LYS	E	148	25.651	17.629	27.698	1.00	52.20	C
ATOM	2473	C	LYS	E	148	25.742	16.114	27.745	1.00	52.34	C
ATOM	2474	O	LYS	E	148	26.805	15.513	27.615	1.00	52.29	O
ATOM	2475	CB	LYS	E	148	26.995	18.320	27.396	1.00	51.90	C
ATOM	2476	CG	LYS	E	148	26.907	19.843	27.452	1.00	51.96	C

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ATOM	2477	CD	LYS	E	148	27.888	20.554	26.520	1.00	51.98	C
ATOM	2478	CE	LYS	E	148	27.780	22.064	26.729	1.00	52.40	C
ATOM	2479	NZ	LYS	E	148	28.023	22.854	25.494	1.00	52.80	N
ATOM	2480	N	ILE	E	149	24.578	15.511	27.928	1.00	53.05	N
ATOM	2481	CA	ILE	E	149	24.489	14.125	28.321	1.00	53.30	C
ATOM	2482	C	ILE	E	149	23.373	13.375	27.590	1.00	53.69	C
ATOM	2483	O	ILE	E	149	22.338	13.958	27.241	1.00	53.38	O
ATOM	2484	CB	ILE	E	149	24.397	14.045	29.874	1.00	53.35	C
ATOM	2485	CG1	ILE	E	149	25.208	12.877	30.408	1.00	54.25	C
ATOM	2486	CG2	ILE	E	149	22.970	14.217	30.421	1.00	53.05	C
ATOM	2487	CD1	ILE	E	149	26.709	13.196	30.412	1.00	54.63	C
ATOM	2488	N	HIS	E	150	23.607	12.084	27.337	1.00	54.42	N
ATOM	2489	CA	HIS	E	150	22.616	11.221	26.666	1.00	54.97	C
ATOM	2490	C	HIS	E	150	21.949	10.161	27.558	1.00	54.79	C
ATOM	2491	O	HIS	E	150	21.116	9.397	27.085	1.00	55.34	O
ATOM	2492	CB	HIS	E	150	23.244	10.519	25.459	1.00	54.92	C
ATOM	2493	CG	HIS	E	150	23.808	11.451	24.436	1.00	56.16	C
ATOM	2494	ND1	HIS	E	150	25.126	11.850	24.445	1.00	57.09	N
ATOM	2495	CD2	HIS	E	150	23.241	12.041	23.354	1.00	56.84	C
ATOM	2496	CE1	HIS	E	150	25.348	12.650	23.418	1.00	58.05	C
ATOM	2497	NE2	HIS	E	150	24.223	12.777	22.736	1.00	58.30	N
ATOM	2498	N	ARG	E	151	22.317	10.087	28.832	1.00	54.64	N
ATOM	2499	CA	ARG	E	151	21.731	9.072	29.729	1.00	54.37	C
ATOM	2500	C	ARG	E	151	21.361	9.734	31.044	1.00	53.85	C
ATOM	2501	O	ARG	E	151	22.227	10.234	31.757	1.00	54.44	O
ATOM	2502	CB	ARG	E	151	22.716	7.924	29.995	1.00	54.40	C
ATOM	2503	CG	ARG	E	151	23.510	7.451	28.772	1.00	55.77	C
ATOM	2504	CD	ARG	E	151	22.665	6.572	27.868	1.00	57.70	C
ATOM	2505	NE	ARG	E	151	23.004	6.768	26.465	1.00	59.35	N
ATOM	2506	CZ	ARG	E	151	22.768	5.886	25.496	1.00	60.76	C
ATOM	2507	NH1	ARG	E	151	22.201	4.715	25.779	1.00	61.67	N
ATOM	2508	NH2	ARG	E	151	23.104	6.173	24.239	1.00	60.36	N
ATOM	2509	N	LEU	E	152	20.080	9.755	31.365	1.00	52.81	N
ATOM	2510	CA	LEU	E	152	19.648	10.344	32.613	1.00	51.73	C
ATOM	2511	C	LEU	E	152	18.969	9.267	33.457	1.00	51.18	C
ATOM	2512	O	LEU	E	152	17.837	8.898	33.174	1.00	51.86	O
ATOM	2513	CB	LEU	E	152	18.705	11.508	32.307	1.00	51.74	C
ATOM	2514	CG	LEU	E	152	18.139	12.406	33.413	1.00	51.71	C
ATOM	2515	CD1	LEU	E	152	19.224	13.043	34.276	1.00	49.62	C
ATOM	2516	CD2	LEU	E	152	17.264	13.456	32.780	1.00	50.79	C
ATOM	2517	N	PRO	E	153	19.669	8.723	34.474	1.00	50.63	N
ATOM	2518	CA	PRO	E	153	19.037	7.733	35.363	1.00	49.51	C
ATOM	2519	C	PRO	E	153	17.921	8.344	36.190	1.00	49.13	C
ATOM	2520	O	PRO	E	153	18.100	9.404	36.801	1.00	49.08	O
ATOM	2521	CB	PRO	E	153	20.173	7.315	36.284	1.00	49.06	C
ATOM	2522	CG	PRO	E	153	21.114	8.450	36.264	1.00	50.15	C
ATOM	2523	CD	PRO	E	153	21.069	8.972	34.860	1.00	50.49	C
ATOM	2524	N	VAL	E	154	16.770	7.689	36.164	1.00	48.88	N
ATOM	2525	CA	VAL	E	154	15.621	8.053	36.972	1.00	48.57	C
ATOM	2526	C	VAL	E	154	15.751	7.322	38.290	1.00	49.54	C
ATOM	2527	O	VAL	E	154	15.714	6.088	38.328	1.00	49.96	O
ATOM	2528	CB	VAL	E	154	14.302	7.642	36.278	1.00	48.64	C
ATOM	2529	CG1	VAL	E	154	13.100	7.923	37.169	1.00	47.94	C
ATOM	2530	CG2	VAL	E	154	14.155	8.345	34.925	1.00	46.87	C
ATOM	2531	N	ILE	E	155	15.911	8.085	39.368	1.00	49.87	N
ATOM	2532	CA	ILE	E	155	16.182	7.534	40.684	1.00	49.89	C
ATOM	2533	C	ILE	E	155	15.124	7.968	41.685	1.00	50.58	C
ATOM	2534	O	ILE	E	155	14.910	9.170	41.891	1.00	50.45	O
ATOM	2535	CB	ILE	E	155	17.571	7.970	41.210	1.00	50.02	C
ATOM	2536	CG1	ILE	E	155	18.674	7.542	40.236	1.00	49.77	C
ATOM	2537	CG2	ILE	E	155	17.819	7.398	42.595	1.00	48.91	C
ATOM	2538	CD1	ILE	E	155	20.085	7.883	40.692	1.00	48.82	C
ATOM	2539	N	ASP	E	156	14.480	6.975	42.302	1.00	51.11	N
ATOM	2540	CA	ASP	E	156	13.495	7.182	43.364	1.00	51.77	C
ATOM	2541	C	ASP	E	156	14.127	7.705	44.666	1.00	51.93	C
ATOM	2542	O	ASP	E	156	14.921	7.013	45.306	1.00	51.42	O
ATOM	2543	CB	ASP	E	156	12.752	5.869	43.640	1.00	52.00	C

Figure 2 Table 2b - 39

ATOM	2544	CG	ASP	E	156	11.814	5.960	44.843	1.00 52.62	C
ATOM	2545	OD1	ASP	E	156	11.158	7.006	45.019	1.00 54.25	O
ATOM	2546	OD2	ASP	E	156	11.730	4.975	45.610	1.00 53.33	O
ATOM	2547	N	PRO	E	157	13.773	8.935	45.065	1.00 52.35	N
ATOM	2548	CA	PRO	E	157	14.382	9.478	46.279	1.00 52.31	C
ATOM	2549	C	PRO	E	157	13.967	8.776	47.573	1.00 52.25	C
ATOM	2550	O	PRO	E	157	14.670	8.903	48.577	1.00 52.17	O
ATOM	2551	CB	PRO	E	157	13.956	10.953	46.271	1.00 52.18	C
ATOM	2552	CG	PRO	E	157	12.761	11.015	45.421	1.00 52.25	C
ATOM	2553	CD	PRO	E	157	12.856	9.896	44.425	1.00 52.68	C
ATOM	2554	N	GLU	E	158	12.872	8.016	47.552	1.00 52.37	N
ATOM	2555	CA	GLU	E	158	12.462	7.261	48.751	1.00 52.41	C
ATOM	2556	C	GLU	E	158	13.319	6.019	48.991	1.00 51.59	C
ATOM	2557	O	GLU	E	158	13.773	5.782	50.112	1.00 51.68	O
ATOM	2558	CB	GLU	E	158	10.986	6.860	48.691	1.00 53.03	C
ATOM	2559	CG	GLU	E	158	10.010	8.031	48.616	1.00 56.48	C
ATOM	2560	CD	GLU	E	158	8.748	7.820	49.462	1.00 61.51	C
ATOM	2561	OE1	GLU	E	158	8.832	7.161	50.540	1.00 62.56	O
ATOM	2562	OE2	GLU	E	158	7.672	8.329	49.052	1.00 62.79	O
ATOM	2563	N	SER	E	159	13.529	5.227	47.937	1.00 50.87	N
ATOM	2564	CA	SER	E	159	14.224	3.928	48.041	1.00 49.78	C
ATOM	2565	C	SER	E	159	15.696	4.006	47.645	1.00 49.12	C
ATOM	2566	O	SER	E	159	16.507	3.194	48.097	1.00 49.15	O
ATOM	2567	CB	SER	E	159	13.528	2.881	47.177	1.00 49.70	C
ATOM	2568	OG	SER	E	159	13.706	3.171	45.802	1.00 49.16	O
ATOM	2569	N	GLY	E	160	16.030	4.985	46.806	1.00 48.25	N
ATOM	2570	CA	GLY	E	160	17.373	5.123	46.262	1.00 47.58	C
ATOM	2571	C	GLY	E	160	17.581	4.330	44.981	1.00 47.23	C
ATOM	2572	O	GLY	E	160	18.662	4.363	44.396	1.00 47.30	O
ATOM	2573	N	ASN	E	161	16.549	3.610	44.548	1.00 46.79	N
ATOM	2574	CA	ASN	E	161	16.649	2.762	43.377	1.00 46.27	C
ATOM	2575	C	ASN	E	161	16.656	3.549	42.064	1.00 46.78	C
ATOM	2576	O	ASN	E	161	15.886	4.505	41.865	1.00 46.55	O
ATOM	2577	CB	ASN	E	161	15.529	1.727	43.362	1.00 45.89	C
ATOM	2578	CG	ASN	E	161	15.576	0.773	44.569	1.00 45.71	C
ATOM	2579	OD1	ASN	E	161	14.548	0.241	44.976	1.00 44.67	O
ATOM	2580	ND2	ASN	E	161	16.761	0.553	45.127	1.00 43.51	N
ATOM	2581	N	THR	E	162	17.565	3.152	41.182	1.00 46.53	N
ATOM	2582	CA	THR	E	162	17.477	3.542	39.809	1.00 46.21	C
ATOM	2583	C	THR	E	162	16.372	2.706	39.214	1.00 46.75	C
ATOM	2584	O	THR	E	162	16.378	1.470	39.335	1.00 47.35	O
ATOM	2585	CB	THR	E	162	18.778	3.269	39.086	1.00 46.15	C
ATOM	2586	OG1	THR	E	162	19.814	4.043	39.706	1.00 45.69	O
ATOM	2587	CG2	THR	E	162	18.668	3.658	37.605	1.00 45.57	C
ATOM	2588	N	LEU	E	163	15.414	3.387	38.593	1.00 47.05	N
ATOM	2589	CA	LEU	E	163	14.227	2.755	38.008	1.00 46.96	C
ATOM	2590	C	LEU	E	163	14.414	2.459	36.522	1.00 47.02	C
ATOM	2591	O	LEU	E	163	13.805	1.550	35.970	1.00 46.69	O
ATOM	2592	CB	LEU	E	163	13.020	3.677	38.195	1.00 46.37	C
ATOM	2593	CG	LEU	E	163	12.729	4.168	39.621	1.00 46.82	C
ATOM	2594	CD1	LEU	E	163	11.510	5.081	39.646	1.00 45.31	C
ATOM	2595	CD2	LEU	E	163	12.569	3.019	40.634	1.00 44.79	C
ATOM	2596	N	TYR	E	164	15.275	3.239	35.885	1.00 47.53	N
ATOM	2597	CA	TYR	E	164	15.253	3.379	34.439	1.00 47.76	C
ATOM	2598	C	TYR	E	164	16.262	4.430	34.006	1.00 47.66	C
ATOM	2599	O	TYR	E	164	16.612	5.331	34.776	1.00 47.50	O
ATOM	2600	CB	TYR	E	164	13.852	3.788	33.972	1.00 47.48	C
ATOM	2601	CG	TYR	E	164	13.683	3.798	32.476	1.00 48.25	C
ATOM	2602	CD1	TYR	E	164	13.755	2.604	31.725	1.00 48.26	C
ATOM	2603	CD2	TYR	E	164	13.442	4.994	31.798	1.00 46.43	C
ATOM	2604	CE1	TYR	E	164	13.605	2.625	30.342	1.00 47.72	C
ATOM	2605	CE2	TYR	E	164	13.278	5.018	30.430	1.00 45.52	C
ATOM	2606	CZ	TYR	E	164	13.363	3.849	29.712	1.00 47.98	C
ATOM	2607	OH	TYR	E	164	13.200	3.912	28.351	1.00 50.48	O
ATOM	2608	N	ILE	E	165	16.743	4.283	32.778	1.00 47.60	N
ATOM	2609	CA	ILE	E	165	17.654	5.247	32.187	1.00 47.54	C
ATOM	2610	C	ILE	E	165	16.956	5.922	31.031	1.00 47.66	C

Figure 2 Table 2b - 40

ATOM	2611	O	ILE	E	165	16.563	5.271	30.065	1.00	47.62	O
ATOM	2612	CB	ILE	E	165	18.947	4.593	31.733	1.00	47.56	C
ATOM	2613	CG1	ILE	E	165	19.624	3.915	32.933	1.00	46.89	C
ATOM	2614	CG2	ILE	E	165	19.862	5.637	31.094	1.00	46.65	C
ATOM	2615	CD1	ILE	E	165	20.915	3.208	32.587	1.00	46.28	C
ATOM	2616	N	LEU	E	166	16.787	7.233	31.151	1.00	48.18	N
ATOM	2617	CA	LEU	E	166	16.029	8.004	30.184	1.00	48.73	C
ATOM	2618	C	LEU	E	166	16.964	8.526	29.119	1.00	48.88	C
ATOM	2619	O	LEU	E	166	18.089	8.930	29.429	1.00	49.16	O
ATOM	2620	CB	LEU	E	166	15.343	9.151	30.898	1.00	49.00	C
ATOM	2621	CG	LEU	E	166	14.147	9.837	30.259	1.00	50.84	C
ATOM	2622	CD1	LEU	E	166	13.038	8.833	29.876	1.00	53.27	C
ATOM	2623	CD2	LEU	E	166	13.636	10.858	31.253	1.00	51.57	C
ATOM	2624	N	THR	E	167	16.511	8.485	27.866	1.00	49.14	N
ATOM	2625	CA	THR	E	167	17.306	8.916	26.709	1.00	49.15	C
ATOM	2626	C	THR	E	167	16.502	9.840	25.812	1.00	49.30	C
ATOM	2627	O	THR	E	167	15.276	9.842	25.859	1.00	49.26	O
ATOM	2628	CB	THR	E	167	17.787	7.711	25.857	1.00	49.59	C
ATOM	2629	OG1	THR	E	167	16.676	7.137	25.144	1.00	50.73	O
ATOM	2630	CG2	THR	E	167	18.448	6.636	26.729	1.00	48.26	C
ATOM	2631	N	HIS	E	168	17.199	10.631	24.994	1.00	50.09	N
ATOM	2632	CA	HIS	E	168	16.580	11.485	23.978	1.00	49.74	C
ATOM	2633	C	HIS	E	168	15.601	10.719	23.108	1.00	49.27	C
ATOM	2634	O	HIS	E	168	14.503	11.210	22.836	1.00	49.46	O
ATOM	2635	CB	HIS	E	168	17.639	12.036	23.047	1.00	50.49	C
ATOM	2636	CG	HIS	E	168	18.542	13.042	23.672	1.00	52.80	C
ATOM	2637	ND1	HIS	E	168	19.758	12.702	24.221	1.00	55.77	N
ATOM	2638	CD2	HIS	E	168	18.428	14.386	23.803	1.00	53.57	C
ATOM	2639	CE1	HIS	E	168	20.346	13.794	24.679	1.00	55.45	C
ATOM	2640	NE2	HIS	E	168	19.560	14.828	24.436	1.00	53.16	N
ATOM	2641	N	LYS	E	169	16.013	9.538	22.637	1.00	48.54	N
ATOM	2642	CA	LYS	E	169	15.195	8.746	21.708	1.00	48.14	C
ATOM	2643	C	LYS	E	169	13.831	8.452	22.312	1.00	48.21	C
ATOM	2644	O	LYS	E	169	12.801	8.663	21.675	1.00	48.64	O
ATOM	2645	CB	LYS	E	169	15.898	7.442	21.326	1.00	48.01	C
ATOM	2646	CG	LYS	E	169	15.168	6.615	20.253	1.00	48.44	C
ATOM	2647	CD	LYS	E	169	15.876	5.306	19.931	1.00	48.10	C
ATOM	2648	CE	LYS	E	169	17.177	5.520	19.201	1.00	49.76	C
ATOM	2649	NZ	LYS	E	169	18.056	4.296	19.145	1.00	52.12	N
ATOM	2650	N	ARG	E	170	13.833	7.955	23.544	1.00	48.04	N
ATOM	2651	CA	ARG	E	170	12.609	7.678	24.267	1.00	47.36	C
ATOM	2652	C	ARG	E	170	11.786	8.942	24.395	1.00	46.87	C
ATOM	2653	O	ARG	E	170	10.607	8.949	24.078	1.00	47.58	O
ATOM	2654	CB	ARG	E	170	12.943	7.134	25.662	1.00	47.75	C
ATOM	2655	CG	ARG	E	170	11.753	6.736	26.491	1.00	47.17	C
ATOM	2656	CD	ARG	E	170	11.169	5.469	25.962	1.00	47.93	C
ATOM	2657	NE	ARG	E	170	10.176	4.925	26.879	1.00	50.08	N
ATOM	2658	CZ	ARG	E	170	9.454	3.825	26.659	1.00	47.50	C
ATOM	2659	NH1	ARG	E	170	9.602	3.128	25.537	1.00	46.11	N
ATOM	2660	NH2	ARG	E	170	8.579	3.434	27.569	1.00	44.54	N
ATOM	2661	N	ILE	E	171	12.398	10.014	24.872	1.00	46.28	N
ATOM	2662	CA	ILE	E	171	11.640	11.225	25.105	1.00	46.38	C
ATOM	2663	C	ILE	E	171	10.960	11.696	23.799	1.00	47.03	C
ATOM	2664	O	ILE	E	171	9.765	12.005	23.802	1.00	47.34	O
ATOM	2665	CB	ILE	E	171	12.525	12.338	25.672	1.00	46.51	C
ATOM	2666	CG1	ILE	E	171	13.019	11.958	27.066	1.00	44.04	C
ATOM	2667	CG2	ILE	E	171	11.778	13.686	25.654	1.00	46.10	C
ATOM	2668	CD1	ILE	E	171	14.131	12.844	27.602	1.00	40.58	C
ATOM	2669	N	LEU	E	172	11.702	11.724	22.690	1.00	46.74	N
ATOM	2670	CA	LEU	E	172	11.110	12.159	21.438	1.00	47.31	C
ATOM	2671	C	LEU	E	172	9.964	11.265	20.992	1.00	47.76	C
ATOM	2672	O	LEU	E	172	8.936	11.771	20.503	1.00	47.97	O
ATOM	2673	CB	LEU	E	172	12.143	12.321	20.322	1.00	47.09	C
ATOM	2674	CG	LEU	E	172	11.580	13.045	19.082	1.00	47.47	C
ATOM	2675	CD1	LEU	E	172	11.205	14.476	19.352	1.00	47.31	C
ATOM	2676	CD2	LEU	E	172	12.542	12.977	17.907	1.00	48.26	C
ATOM	2677	N	LYS	E	173	10.133	9.950	21.156	1.00	47.99	N

Figure 2 Table 2b - 41

ATOM	2678	CA	LYS	E	173	9.098	8.991	20.752	1.00	48.35	C
ATOM	2679	C	LYS	E	173	7.814	9.245	21.505	1.00	48.34	C
ATOM	2680	O	LYS	E	173	6.718	9.203	20.931	1.00	48.09	O
ATOM	2681	CB	LYS	E	173	9.521	7.546	21.016	1.00	48.68	C
ATOM	2682	CG	LYS	E	173	8.643	6.565	20.286	1.00	48.94	C
ATOM	2683	CD	LYS	E	173	9.071	5.160	20.529	1.00	51.04	C
ATOM	2684	CE	LYS	E	173	8.273	4.217	19.652	1.00	51.69	C
ATOM	2685	NZ	LYS	E	173	8.592	2.826	20.036	1.00	52.81	N
ATOM	2686	N	PHE	E	174	7.965	9.480	22.806	1.00	48.38	N
ATOM	2687	CA	PHE	E	174	6.837	9.719	23.691	1.00	48.05	C
ATOM	2688	C	PHE	E	174	6.106	10.964	23.239	1.00	47.94	C
ATOM	2689	O	PHE	E	174	4.875	10.973	23.184	1.00	47.75	O
ATOM	2690	CB	PHE	E	174	7.337	9.881	25.113	1.00	48.11	C
ATOM	2691	CG	PHE	E	174	6.258	9.847	26.146	1.00	48.32	C
ATOM	2692	CD1	PHE	E	174	5.822	11.020	26.747	1.00	48.70	C
ATOM	2693	CD2	PHE	E	174	5.689	8.640	26.537	1.00	48.50	C
ATOM	2694	CE1	PHE	E	174	4.822	10.998	27.724	1.00	48.87	C
ATOM	2695	CE2	PHE	E	174	4.703	8.604	27.507	1.00	49.02	C
ATOM	2696	CZ	PHE	E	174	4.268	9.791	28.108	1.00	48.73	C
ATOM	2697	N	LEU	E	175	6.879	11.995	22.889	1.00	48.19	N
ATOM	2698	CA	LEU	E	175	6.340	13.272	22.402	1.00	48.55	C
ATOM	2699	C	LEU	E	175	5.560	13.116	21.111	1.00	48.74	C
ATOM	2700	O	LEU	E	175	4.417	13.546	21.035	1.00	48.76	O
ATOM	2701	CB	LEU	E	175	7.449	14.301	22.205	1.00	48.53	C
ATOM	2702	CG	LEU	E	175	8.120	14.873	23.452	1.00	48.85	C
ATOM	2703	CD1	LEU	E	175	9.153	15.910	23.047	1.00	48.47	C
ATOM	2704	CD2	LEU	E	175	7.096	15.474	24.408	1.00	48.58	C
ATOM	2705	N	LYS	E	176	6.181	12.495	20.107	1.00	48.96	N
ATOM	2706	CA	LYS	E	176	5.510	12.181	18.854	1.00	49.32	C
ATOM	2707	C	LYS	E	176	4.186	11.439	19.056	1.00	50.19	C
ATOM	2708	O	LYS	E	176	3.212	11.728	18.380	1.00	50.40	O
ATOM	2709	CB	LYS	E	176	6.462	11.429	17.918	1.00	49.17	C
ATOM	2710	CG	LYS	E	176	5.820	10.622	16.797	1.00	48.74	C
ATOM	2711	CD	LYS	E	176	5.305	11.498	15.694	1.00	47.62	C
ATOM	2712	CE	LYS	E	176	4.269	10.778	14.839	1.00	47.17	C
ATOM	2713	NZ	LYS	E	176	3.676	11.714	13.811	1.00	46.11	N
ATOM	2714	N	LEU	E	177	4.138	10.522	20.015	1.00	51.54	N
ATOM	2715	CA	LEU	E	177	2.963	9.670	20.215	1.00	52.84	C
ATOM	2716	C	LEU	E	177	1.816	10.323	20.953	1.00	53.65	C
ATOM	2717	O	LEU	E	177	0.667	10.221	20.531	1.00	54.30	O
ATOM	2718	CB	LEU	E	177	3.341	8.384	20.951	1.00	52.99	C
ATOM	2719	CG	LEU	E	177	4.005	7.279	20.136	1.00	53.77	C
ATOM	2720	CD1	LEU	E	177	4.231	6.037	21.015	1.00	54.92	C
ATOM	2721	CD2	LEU	E	177	3.168	6.943	18.895	1.00	53.09	C
ATOM	2722	N	PHE	E	178	2.117	10.966	22.072	1.00	54.58	N
ATOM	2723	CA	PHE	E	178	1.062	11.451	22.952	1.00	55.16	C
ATOM	2724	C	PHE	E	178	0.661	12.886	22.701	1.00	55.81	C
ATOM	2725	O	PHE	E	178	-0.240	13.412	23.351	1.00	55.79	O
ATOM	2726	CB	PHE	E	178	1.434	11.221	24.407	1.00	55.02	C
ATOM	2727	CG	PHE	E	178	1.292	9.809	24.825	1.00	54.73	C
ATOM	2728	CD1	PHE	E	178	2.379	8.951	24.784	1.00	55.13	C
ATOM	2729	CD2	PHE	E	178	0.056	9.316	25.234	1.00	55.15	C
ATOM	2730	CE1	PHE	E	178	2.246	7.614	25.169	1.00	54.86	C
ATOM	2731	CE2	PHE	E	178	-0.088	7.984	25.617	1.00	55.10	C
ATOM	2732	CZ	PHE	E	178	1.014	7.134	25.586	1.00	54.73	C
ATOM	2733	N	ILE	E	179	1.328	13.522	21.753	1.00	56.95	N
ATOM	2734	CA	ILE	E	179	0.834	14.791	21.249	1.00	58.01	C
ATOM	2735	C	ILE	E	179	0.215	14.609	19.868	1.00	59.01	C
ATOM	2736	O	ILE	E	179	-0.467	15.505	19.399	1.00	59.37	O
ATOM	2737	CB	ILE	E	179	1.891	15.899	21.258	1.00	57.77	C
ATOM	2738	CG1	ILE	E	179	2.688	15.852	22.561	1.00	57.77	C
ATOM	2739	CG2	ILE	E	179	1.208	17.245	21.145	1.00	57.30	C
ATOM	2740	CD1	ILE	E	179	3.854	16.817	22.611	1.00	58.52	C
ATOM	2741	N	THR	E	180	0.436	13.444	19.239	1.00	60.56	N
ATOM	2742	CA	THR	E	180	-0.265	13.059	17.993	1.00	61.33	C
ATOM	2743	C	THR	E	180	-1.710	13.475	18.162	1.00	61.85	C
ATOM	2744	O	THR	E	180	-2.468	12.888	18.948	1.00	62.27	O

Figure 2 Table 2b - 42

ATOM	2745	CB	THR	E	180	-0.235	11.517	17.661	1.00	61.73	C
ATOM	2746	OG1	THR	E	180	1.114	11.025	17.573	1.00	61.77	O
ATOM	2747	CG2	THR	E	180	-0.967	11.232	16.330	1.00	61.26	C
ATOM	2748	N	GLU	E	181	-2.056	14.494	17.385	1.00	62.21	N
ATOM	2749	CA	GLU	E	181	-3.207	15.363	17.544	1.00	62.17	C
ATOM	2750	C	GLU	E	181	-2.521	16.633	17.077	1.00	62.25	C
ATOM	2751	O	GLU	E	181	-1.348	16.875	17.444	1.00	61.78	O
ATOM	2752	CB	GLU	E	181	-3.641	15.517	19.013	1.00	62.21	C
ATOM	2753	CG	GLU	E	181	-3.304	16.883	19.624	1.00	62.48	C
ATOM	2754	CD	GLU	E	181	-3.169	16.879	21.131	1.00	63.59	C
ATOM	2755	OE1	GLU	E	181	-3.717	17.819	21.739	1.00	64.34	O
ATOM	2756	OE2	GLU	E	181	-2.514	15.970	21.703	1.00	61.82	O
ATOM	2757	N	PHE	E	182	-3.191	17.427	16.240	1.00	62.02	N
ATOM	2758	CA	PHE	E	182	-2.575	18.688	15.873	1.00	61.87	C
ATOM	2759	C	PHE	E	182	-3.390	19.998	15.924	1.00	61.60	C
ATOM	2760	O	PHE	E	182	-3.926	20.467	14.898	1.00	61.52	O
ATOM	2761	CB	PHE	E	182	-1.609	18.617	14.653	1.00	62.27	C
ATOM	2762	CG	PHE	E	182	-1.706	17.359	13.794	1.00	63.46	C
ATOM	2763	CD1	PHE	E	182	-2.389	17.381	12.572	1.00	64.64	C
ATOM	2764	CD2	PHE	E	182	-1.029	16.187	14.153	1.00	64.21	C
ATOM	2765	CE1	PHE	E	182	-2.445	16.242	11.750	1.00	64.77	C
ATOM	2766	CE2	PHE	E	182	-1.086	15.043	13.340	1.00	64.44	C
ATOM	2767	CZ	PHE	E	182	-1.793	15.072	12.139	1.00	63.82	C
ATOM	2768	N	PRO	E	183	-3.492	20.576	17.143	1.00	60.96	N
ATOM	2769	CA	PRO	E	183	-3.244	22.012	17.195	1.00	60.22	C
ATOM	2770	C	PRO	E	183	-1.720	22.105	17.000	1.00	59.37	C
ATOM	2771	O	PRO	E	183	-0.930	21.865	17.930	1.00	58.80	O
ATOM	2772	CB	PRO	E	183	-3.682	22.413	18.614	1.00	60.40	C
ATOM	2773	CG	PRO	E	183	-4.426	21.219	19.166	1.00	60.59	C
ATOM	2774	CD	PRO	E	183	-3.848	20.029	18.463	1.00	60.88	C
ATOM	2775	N	LYS	E	184	-1.337	22.376	15.755	1.00	58.29	N
ATOM	2776	CA	LYS	E	184	0.043	22.281	15.299	1.00	57.35	C
ATOM	2777	C	LYS	E	184	0.677	23.664	15.293	1.00	56.37	C
ATOM	2778	O	LYS	E	184	0.119	24.587	14.701	1.00	56.20	O
ATOM	2779	CB	LYS	E	184	0.063	21.698	13.880	1.00	57.32	C
ATOM	2780	CG	LYS	E	184	1.390	21.107	13.443	1.00	57.27	C
ATOM	2781	CD	LYS	E	184	1.331	20.612	11.994	1.00	57.92	C
ATOM	2782	CE	LYS	E	184	0.674	19.236	11.891	1.00	58.76	C
ATOM	2783	NZ	LYS	E	184	0.735	18.643	10.532	1.00	58.33	N
ATOM	2784	N	PRO	E	185	1.842	23.811	15.945	1.00	55.51	N
ATOM	2785	CA	PRO	E	185	2.559	25.080	15.913	1.00	55.18	C
ATOM	2786	C	PRO	E	185	3.084	25.348	14.501	1.00	55.00	C
ATOM	2787	O	PRO	E	185	3.549	24.420	13.838	1.00	55.07	O
ATOM	2788	CB	PRO	E	185	3.732	24.853	16.874	1.00	55.00	C
ATOM	2789	CG	PRO	E	185	3.436	23.609	17.609	1.00	54.87	C
ATOM	2790	CD	PRO	E	185	2.560	22.794	16.727	1.00	55.53	C
ATOM	2791	N	GLU	E	186	3.010	26.600	14.039	1.00	54.86	N
ATOM	2792	CA	GLU	E	186	3.485	26.946	12.695	1.00	54.34	C
ATOM	2793	C	GLU	E	186	4.844	26.326	12.358	1.00	53.66	C
ATOM	2794	O	GLU	E	186	5.088	25.950	11.203	1.00	53.53	O
ATOM	2795	CB	GLU	E	186	3.541	28.459	12.479	1.00	54.52	C
ATOM	2796	CG	GLU	E	186	2.198	29.107	12.185	1.00	56.25	C
ATOM	2797	CD	GLU	E	186	1.648	29.866	13.384	1.00	58.92	C
ATOM	2798	OE1	GLU	E	186	1.985	29.484	14.534	1.00	60.28	O
ATOM	2799	OE2	GLU	E	186	0.891	30.850	13.176	1.00	58.84	O
ATOM	2800	N	PHE	E	187	5.711	26.212	13.365	1.00	52.74	N
ATOM	2801	CA	PHE	E	187	7.100	25.815	13.139	1.00	52.35	C
ATOM	2802	C	PHE	E	187	7.290	24.349	12.722	1.00	52.14	C
ATOM	2803	O	PHE	E	187	8.330	23.987	12.175	1.00	52.54	O
ATOM	2804	CB	PHE	E	187	8.009	26.206	14.317	1.00	51.83	C
ATOM	2805	CG	PHE	E	187	7.694	25.504	15.609	1.00	52.14	C
ATOM	2806	CD1	PHE	E	187	7.968	24.139	15.777	1.00	52.58	C
ATOM	2807	CD2	PHE	E	187	7.165	26.210	16.681	1.00	51.71	C
ATOM	2808	CE1	PHE	E	187	7.693	23.496	16.974	1.00	51.15	C
ATOM	2809	CE2	PHE	E	187	6.891	25.571	17.885	1.00	51.48	C
ATOM	2810	CZ	PHE	E	187	7.157	24.209	18.029	1.00	51.36	C
ATOM	2811	N	MET	E	188	6.280	23.523	12.963	1.00	51.41	N

Figure 2

Table 2b - 43

ATOM	2812	CA	MET	E	188	6.305	22.146	12.518	1.00	51.17	C
ATOM	2813	C	MET	E	188	6.332	22.059	10.999	1.00	50.61	C
ATOM	2814	O	MET	E	188	6.916	21.133	10.435	1.00	50.48	O
ATOM	2815	CB	MET	E	188	5.092	21.401	13.063	1.00	51.59	C
ATOM	2816	CG	MET	E	188	5.136	21.194	14.565	1.00	52.39	C
ATOM	2817	SD	MET	E	188	6.634	20.313	15.024	1.00	55.10	S
ATOM	2818	CE	MET	E	188	6.230	18.639	14.542	1.00	54.26	C
ATOM	2819	N	SER	E	189	5.708	23.043	10.356	1.00	49.55	N
ATOM	2820	CA	SER	E	189	5.641	23.129	8.911	1.00	48.90	C
ATOM	2821	C	SER	E	189	6.760	24.001	8.318	1.00	48.69	C
ATOM	2822	O	SER	E	189	6.703	24.392	7.152	1.00	48.68	O
ATOM	2823	CB	SER	E	189	4.265	23.648	8.486	1.00	49.03	C
ATOM	2824	OG	SER	E	189	3.238	22.940	9.161	1.00	48.99	O
ATOM	2825	N	LYS	E	190	7.773	24.297	9.124	1.00	48.45	N
ATOM	2826	CA	LYS	E	190	8.948	25.036	8.683	1.00	48.36	C
ATOM	2827	C	LYS	E	190	10.133	24.100	8.502	1.00	48.28	C
ATOM	2828	O	LYS	E	190	10.144	22.998	9.052	1.00	47.89	O
ATOM	2829	CB	LYS	E	190	9.278	26.117	9.698	1.00	48.45	C
ATOM	2830	CG	LYS	E	190	8.260	27.233	9.715	1.00	49.59	C
ATOM	2831	CD	LYS	E	190	8.736	28.371	10.601	1.00	52.34	C
ATOM	2832	CE	LYS	E	190	8.070	29.671	10.206	1.00	54.35	C
ATOM	2833	NZ	LYS	E	190	8.809	30.812	10.801	1.00	56.68	N
ATOM	2834	N	SER	E	191	11.137	24.518	7.738	1.00	48.29	N
ATOM	2835	CA	SER	E	191	12.194	23.574	7.380	1.00	49.02	C
ATOM	2836	C	SER	E	191	13.406	23.647	8.293	1.00	49.32	C
ATOM	2837	O	SER	E	191	13.547	24.596	9.059	1.00	49.19	O
ATOM	2838	CB	SER	E	191	12.588	23.723	5.907	1.00	49.07	C
ATOM	2839	OG	SER	E	191	13.206	24.962	5.639	1.00	49.04	O
ATOM	2840	N	LEU	E	192	14.266	22.631	8.228	1.00	50.11	N
ATOM	2841	CA	LEU	E	192	15.525	22.653	8.982	1.00	51.02	C
ATOM	2842	C	LEU	E	192	16.323	23.921	8.657	1.00	51.63	C
ATOM	2843	O	LEU	E	192	16.846	24.590	9.558	1.00	51.89	O
ATOM	2844	CB	LEU	E	192	16.379	21.408	8.718	1.00	50.73	C
ATOM	2845	CG	LEU	E	192	15.899	19.997	9.102	1.00	51.05	C
ATOM	2846	CD1	LEU	E	192	16.864	18.970	8.543	1.00	50.74	C
ATOM	2847	CD2	LEU	E	192	15.754	19.785	10.611	1.00	50.53	C
ATOM	2848	N	GLU	E	193	16.390	24.246	7.367	1.00	52.41	N
ATOM	2849	CA	GLU	E	193	17.040	25.447	6.863	1.00	52.85	C
ATOM	2850	C	GLU	E	193	16.628	26.689	7.658	1.00	53.01	C
ATOM	2851	O	GLU	E	193	17.474	27.361	8.248	1.00	53.30	O
ATOM	2852	CB	GLU	E	193	16.652	25.622	5.406	1.00	53.16	C
ATOM	2853	CG	GLU	E	193	17.080	26.929	4.756	1.00	55.11	C
ATOM	2854	CD	GLU	E	193	18.291	26.733	3.887	1.00	57.93	C
ATOM	2855	OE1	GLU	E	193	19.310	26.231	4.421	1.00	60.02	O
ATOM	2856	OE2	GLU	E	193	18.217	27.055	2.676	1.00	58.28	O
ATOM	2857	N	GLU	E	194	15.329	26.977	7.675	1.00	52.84	N
ATOM	2858	CA	GLU	E	194	14.818	28.199	8.286	1.00	53.41	C
ATOM	2859	C	GLU	E	194	14.692	28.173	9.813	1.00	52.70	C
ATOM	2860	O	GLU	E	194	14.649	29.213	10.450	1.00	52.59	O
ATOM	2861	CB	GLU	E	194	13.493	28.612	7.647	1.00	53.50	C
ATOM	2862	CG	GLU	E	194	12.501	27.494	7.468	1.00	55.33	C
ATOM	2863	CD	GLU	E	194	11.204	27.950	6.800	1.00	56.75	C
ATOM	2864	OE1	GLU	E	194	10.818	29.145	6.976	1.00	58.78	O
ATOM	2865	OE2	GLU	E	194	10.574	27.105	6.109	1.00	57.61	O
ATOM	2866	N	LEU	E	195	14.634	26.984	10.397	1.00	52.57	N
ATOM	2867	CA	LEU	E	195	14.653	26.866	11.838	1.00	51.86	C
ATOM	2868	C	LEU	E	195	16.085	26.784	12.348	1.00	52.02	C
ATOM	2869	O	LEU	E	195	16.333	27.011	13.519	1.00	52.17	O
ATOM	2870	CB	LEU	E	195	13.830	25.670	12.294	1.00	51.16	C
ATOM	2871	CG	LEU	E	195	12.325	25.742	12.055	1.00	50.21	C
ATOM	2872	CD1	LEU	E	195	11.670	24.467	12.562	1.00	50.47	C
ATOM	2873	CD2	LEU	E	195	11.711	26.953	12.726	1.00	49.24	C
ATOM	2874	N	GLN	E	196	17.023	26.493	11.453	1.00	52.24	N
ATOM	2875	CA	GLN	E	196	18.431	26.275	11.813	1.00	52.65	C
ATOM	2876	C	GLN	E	196	18.627	25.243	12.920	1.00	52.59	C
ATOM	2877	O	GLN	E	196	19.203	25.517	13.964	1.00	52.47	O
ATOM	2878	CB	GLN	E	196	19.146	27.589	12.093	1.00	52.77	C

Figure 2 Table 2b - 44

ATOM	2879	CG	GLN	E	196	19.613	28.231	10.807	1.00	54.60	C
ATOM	2880	CD	GLN	E	196	19.967	29.675	10.967	1.00	57.25	C
ATOM	2881	OE1	GLN	E	196	20.668	30.058	11.910	1.00	59.49	O
ATOM	2882	NE2	GLN	E	196	19.506	30.499	10.028	1.00	58.30	N
ATOM	2883	N	ILE	E	197	18.114	24.045	12.651	1.00	52.54	N
ATOM	2884	CA	ILE	E	197	18.296	22.894	13.502	1.00	52.01	C
ATOM	2885	C	ILE	E	197	19.314	21.971	12.844	1.00	51.65	C
ATOM	2886	O	ILE	E	197	19.168	21.575	11.684	1.00	51.38	O
ATOM	2887	CB	ILE	E	197	16.954	22.150	13.744	1.00	52.24	C
ATOM	2888	CG1	ILE	E	197	15.994	23.051	14.538	1.00	52.54	C
ATOM	2889	CG2	ILE	E	197	17.192	20.826	14.477	1.00	51.78	C
ATOM	2890	CD1	ILE	E	197	14.539	22.654	14.429	1.00	52.72	C
ATOM	2891	N	GLY	E	198	20.357	21.645	13.597	1.00	51.01	N
ATOM	2892	CA	GLY	E	198	21.350	20.711	13.129	1.00	49.96	C
ATOM	2893	C	GLY	E	198	22.681	21.393	12.998	1.00	49.44	C
ATOM	2894	O	GLY	E	198	22.813	22.578	13.273	1.00	49.45	O
ATOM	2895	N	THR	E	199	23.676	20.627	12.582	1.00	49.05	N
ATOM	2896	CA	THR	E	199	25.018	21.137	12.433	1.00	48.47	C
ATOM	2897	C	THR	E	199	25.394	21.024	10.963	1.00	48.58	C
ATOM	2898	O	THR	E	199	25.247	19.926	10.358	1.00	48.67	O
ATOM	2899	CB	THR	E	199	25.995	20.336	13.291	1.00	48.28	C
ATOM	2900	OG1	THR	E	199	25.468	20.242	14.618	1.00	48.15	O
ATOM	2901	CG2	THR	E	199	27.363	21.012	13.331	1.00	48.04	C
ATOM	2902	N	TYR	E	200	25.884	22.146	10.416	1.00	47.33	N
ATOM	2903	CA	TYR	E	200	26.171	22.290	8.993	1.00	47.11	C
ATOM	2904	C	TYR	E	200	27.609	22.671	8.678	1.00	47.33	C
ATOM	2905	O	TYR	E	200	27.937	22.944	7.534	1.00	47.50	O
ATOM	2906	CB	TYR	E	200	25.153	23.232	8.338	1.00	46.73	C
ATOM	2907	CG	TYR	E	200	23.779	22.685	8.570	1.00	47.03	C
ATOM	2908	CD1	TYR	E	200	22.943	23.224	9.557	1.00	45.43	C
ATOM	2909	CD2	TYR	E	200	23.341	21.548	7.859	1.00	47.11	C
ATOM	2910	CE1	TYR	E	200	21.680	22.672	9.802	1.00	47.64	C
ATOM	2911	CE2	TYR	E	200	22.094	20.986	8.098	1.00	47.70	C
ATOM	2912	CZ	TYR	E	200	21.269	21.540	9.074	1.00	48.43	C
ATOM	2913	OH	TYR	E	200	20.033	20.970	9.291	1.00	48.67	O
ATOM	2914	N	ALA	E	201	28.469	22.673	9.687	1.00	47.70	N
ATOM	2915	CA	ALA	E	201	29.887	22.933	9.470	1.00	48.09	C
ATOM	2916	C	ALA	E	201	30.767	22.031	10.345	1.00	48.40	C
ATOM	2917	O	ALA	E	201	30.290	21.475	11.341	1.00	48.23	O
ATOM	2918	CB	ALA	E	201	30.204	24.415	9.711	1.00	48.13	C
ATOM	2919	N	ASN	E	202	32.037	21.884	9.954	1.00	48.80	N
ATOM	2920	CA	ASN	E	202	33.023	21.093	10.694	1.00	49.37	C
ATOM	2921	C	ASN	E	202	32.542	19.673	10.969	1.00	49.11	C
ATOM	2922	O	ASN	E	202	32.704	19.162	12.075	1.00	48.69	O
ATOM	2923	CB	ASN	E	202	33.384	21.778	12.020	1.00	49.81	C
ATOM	2924	CG	ASN	E	202	34.027	23.134	11.828	1.00	51.72	C
ATOM	2925	OD1	ASN	E	202	33.861	24.037	12.659	1.00	53.29	O
ATOM	2926	ND2	ASN	E	202	34.780	23.287	10.737	1.00	52.99	N
ATOM	2927	N	ILE	E	203	31.944	19.053	9.952	1.00	49.20	N
ATOM	2928	CA	ILE	E	203	31.312	17.749	10.094	1.00	48.80	C
ATOM	2929	C	ILE	E	203	32.378	16.673	10.094	1.00	48.81	C
ATOM	2930	O	ILE	E	203	33.147	16.575	9.153	1.00	48.86	O
ATOM	2931	CB	ILE	E	203	30.277	17.525	8.983	1.00	48.67	C
ATOM	2932	CG1	ILE	E	203	29.215	18.623	9.021	1.00	48.36	C
ATOM	2933	CG2	ILE	E	203	29.614	16.140	9.080	1.00	49.49	C
ATOM	2934	CD1	ILE	E	203	28.402	18.698	10.287	1.00	47.20	C
ATOM	2935	N	ALA	E	204	32.439	15.893	11.171	1.00	48.92	N
ATOM	2936	CA	ALA	E	204	33.403	14.801	11.279	1.00	49.29	C
ATOM	2937	C	ALA	E	204	32.922	13.574	10.510	1.00	49.68	C
ATOM	2938	O	ALA	E	204	31.804	13.106	10.700	1.00	49.77	O
ATOM	2939	CB	ALA	E	204	33.674	14.461	12.728	1.00	49.20	C
ATOM	2940	N	MET	E	205	33.793	13.066	9.643	1.00	50.25	N
ATOM	2941	CA	MET	E	205	33.463	12.066	8.627	1.00	50.50	C
ATOM	2942	C	MET	E	205	34.700	11.254	8.376	1.00	50.02	C
ATOM	2943	O	MET	E	205	35.804	11.716	8.629	1.00	50.31	O
ATOM	2944	CB	MET	E	205	33.112	12.743	7.297	1.00	50.18	C
ATOM	2945	CG	MET	E	205	31.994	13.737	7.358	1.00	50.84	C

Figure 2

Table 2b - 45

ATOM	2946	SD	MET	E	205	31.671	14.433	5.738	1.00	53.20	S
ATOM	2947	CE	MET	E	205	32.965	15.680	5.599	1.00	51.29	C
ATOM	2948	N	VAL	E	206	34.523	10.053	7.842	1.00	49.88	N
ATOM	2949	CA	VAL	E	206	35.654	9.193	7.508	1.00	49.38	C
ATOM	2950	C	VAL	E	206	35.485	8.657	6.089	1.00	49.49	C
ATOM	2951	O	VAL	E	206	34.465	8.896	5.449	1.00	49.44	O
ATOM	2952	CB	VAL	E	206	35.786	8.038	8.506	1.00	49.42	C
ATOM	2953	CG1	VAL	E	206	36.163	8.561	9.893	1.00	48.90	C
ATOM	2954	CG2	VAL	E	206	34.499	7.198	8.544	1.00	48.31	C
ATOM	2955	N	ARG	E	207	36.479	7.937	5.590	1.00	49.71	N
ATOM	2956	CA	ARG	E	207	36.388	7.388	4.241	1.00	50.23	C
ATOM	2957	C	ARG	E	207	36.316	5.873	4.257	1.00	50.15	C
ATOM	2958	O	ARG	E	207	36.767	5.237	5.211	1.00	50.37	O
ATOM	2959	CB	ARG	E	207	37.554	7.888	3.383	1.00	50.46	C
ATOM	2960	CG	ARG	E	207	37.621	9.420	3.334	1.00	52.21	C
ATOM	2961	CD	ARG	E	207	38.336	9.970	2.114	1.00	55.25	C
ATOM	2962	NE	ARG	E	207	37.796	9.459	0.856	1.00	56.82	N
ATOM	2963	CZ	ARG	E	207	38.523	8.827	-0.066	1.00	58.50	C
ATOM	2964	NH1	ARG	E	207	39.826	8.631	0.123	1.00	58.99	N
ATOM	2965	NH2	ARG	E	207	37.951	8.394	-1.186	1.00	59.02	N
ATOM	2966	N	THR	E	208	35.721	5.304	3.214	1.00	50.16	N
ATOM	2967	CA	THR	E	208	35.741	3.853	2.969	1.00	50.52	C
ATOM	2968	C	THR	E	208	36.903	3.122	3.660	1.00	50.42	C
ATOM	2969	O	THR	E	208	36.685	2.114	4.341	1.00	50.63	O
ATOM	2970	CB	THR	E	208	35.830	3.568	1.464	1.00	50.38	C
ATOM	2971	OG1	THR	E	208	34.840	4.336	0.780	1.00	51.54	O
ATOM	2972	CG2	THR	E	208	35.609	2.102	1.170	1.00	51.66	C
ATOM	2973	N	THR	E	209	38.122	3.645	3.499	1.00	50.15	N
ATOM	2974	CA	THR	E	209	39.344	2.959	3.951	1.00	50.14	C
ATOM	2975	C	THR	E	209	39.894	3.355	5.329	1.00	49.90	C
ATOM	2976	O	THR	E	209	40.831	2.728	5.816	1.00	49.66	O
ATOM	2977	CB	THR	E	209	40.491	3.141	2.934	1.00	50.31	C
ATOM	2978	OG1	THR	E	209	40.672	4.539	2.672	1.00	50.16	O
ATOM	2979	CG2	THR	E	209	40.193	2.395	1.622	1.00	50.50	C
ATOM	2980	N	THR	E	210	39.325	4.389	5.945	1.00	49.74	N
ATOM	2981	CA	THR	E	210	39.834	4.922	7.215	1.00	49.55	C
ATOM	2982	C	THR	E	210	39.959	3.827	8.298	1.00	49.64	C
ATOM	2983	O	THR	E	210	38.974	3.183	8.652	1.00	49.98	O
ATOM	2984	CB	THR	E	210	38.953	6.104	7.714	1.00	49.39	C
ATOM	2985	OG1	THR	E	210	38.869	7.110	6.700	1.00	48.95	O
ATOM	2986	CG2	THR	E	210	39.526	6.730	8.959	1.00	49.46	C
ATOM	2987	N	PRO	E	211	41.177	3.599	8.817	1.00	49.44	N
ATOM	2988	CA	PRO	E	211	41.329	2.626	9.894	1.00	49.22	C
ATOM	2989	C	PRO	E	211	40.423	2.928	11.080	1.00	49.01	C
ATOM	2990	O	PRO	E	211	40.139	4.094	11.364	1.00	49.53	O
ATOM	2991	CB	PRO	E	211	42.790	2.795	10.306	1.00	49.36	C
ATOM	2992	CG	PRO	E	211	43.471	3.291	9.084	1.00	49.49	C
ATOM	2993	CD	PRO	E	211	42.467	4.204	8.438	1.00	49.55	C
ATOM	2994	N	VAL	E	212	39.974	1.879	11.760	1.00	48.56	N
ATOM	2995	CA	VAL	E	212	39.091	2.006	12.917	1.00	48.06	C
ATOM	2996	C	VAL	E	212	39.689	2.907	14.007	1.00	48.05	C
ATOM	2997	O	VAL	E	212	38.995	3.778	14.551	1.00	48.06	O
ATOM	2998	CB	VAL	E	212	38.724	0.610	13.486	1.00	48.02	C
ATOM	2999	CG1	VAL	E	212	38.071	0.707	14.865	1.00	47.46	C
ATOM	3000	CG2	VAL	E	212	37.814	-0.103	12.528	1.00	47.52	C
ATOM	3001	N	TYR	E	213	40.970	2.714	14.312	1.00	47.76	N
ATOM	3002	CA	TYR	E	213	41.623	3.537	15.328	1.00	47.65	C
ATOM	3003	C	TYR	E	213	41.606	5.023	14.970	1.00	47.23	C
ATOM	3004	O	TYR	E	213	41.493	5.869	15.856	1.00	47.56	O
ATOM	3005	CB	TYR	E	213	43.040	3.053	15.647	1.00	47.93	C
ATOM	3006	CG	TYR	E	213	44.042	3.174	14.524	1.00	48.69	C
ATOM	3007	CD1	TYR	E	213	44.250	2.121	13.635	1.00	49.92	C
ATOM	3008	CD2	TYR	E	213	44.808	4.326	14.369	1.00	49.65	C
ATOM	3009	CE1	TYR	E	213	45.183	2.216	12.607	1.00	49.85	C
ATOM	3010	CE2	TYR	E	213	45.738	4.437	13.341	1.00	50.03	C
ATOM	3011	CZ	TYR	E	213	45.918	3.378	12.464	1.00	49.88	C
ATOM	3012	OH	TYR	E	213	46.838	3.479	11.448	1.00	50.08	O

Figure 2

Table 2b - 46

ATOM	3013	N	VAL	E	214	41.703	5.337	13.679	1.00	46.19	N
ATOM	3014	CA	VAL	E	214	41.649	6.722	13.240	1.00	45.10	C
ATOM	3015	C	VAL	E	214	40.263	7.284	13.567	1.00	44.56	C
ATOM	3016	O	VAL	E	214	40.147	8.405	14.078	1.00	44.43	O
ATOM	3017	CB	VAL	E	214	42.041	6.883	11.741	1.00	45.29	C
ATOM	3018	CG1	VAL	E	214	41.829	8.313	11.271	1.00	45.20	C
ATOM	3019	CG2	VAL	E	214	43.501	6.504	11.529	1.00	44.68	C
ATOM	3020	N	ALA	E	215	39.225	6.488	13.321	1.00	43.57	N
ATOM	3021	CA	ALA	E	215	37.862	6.871	13.702	1.00	42.96	C
ATOM	3022	C	ALA	E	215	37.699	7.085	15.216	1.00	42.79	C
ATOM	3023	O	ALA	E	215	36.925	7.952	15.635	1.00	42.24	O
ATOM	3024	CB	ALA	E	215	36.856	5.860	13.195	1.00	42.58	C
ATOM	3025	N	LEU	E	216	38.432	6.296	16.017	1.00	42.44	N
ATOM	3026	CA	LEU	E	216	38.443	6.452	17.470	1.00	42.16	C
ATOM	3027	C	LEU	E	216	38.941	7.815	17.875	1.00	42.36	C
ATOM	3028	O	LEU	E	216	38.271	8.528	18.632	1.00	42.64	O
ATOM	3029	CB	LEU	E	216	39.328	5.409	18.151	1.00	42.11	C
ATOM	3030	CG	LEU	E	216	38.864	3.965	18.257	1.00	41.41	C
ATOM	3031	CD1	LEU	E	216	39.715	3.275	19.286	1.00	40.43	C
ATOM	3032	CD2	LEU	E	216	37.400	3.893	18.630	1.00	41.67	C
ATOM	3033	N	GLY	E	217	40.128	8.170	17.385	1.00	42.17	N
ATOM	3034	CA	GLY	E	217	40.697	9.489	17.636	1.00	42.43	C
ATOM	3035	C	GLY	E	217	39.720	10.613	17.314	1.00	42.49	C
ATOM	3036	O	GLY	E	217	39.652	11.608	18.036	1.00	42.49	O
ATOM	3037	N	ILE	E	218	38.953	10.442	16.245	1.00	42.22	N
ATOM	3038	CA	ILE	E	218	37.965	11.427	15.861	1.00	42.87	C
ATOM	3039	C	ILE	E	218	36.815	11.471	16.881	1.00	43.19	C
ATOM	3040	O	ILE	E	218	36.382	12.565	17.293	1.00	43.25	O
ATOM	3041	CB	ILE	E	218	37.484	11.178	14.414	1.00	42.98	C
ATOM	3042	CG1	ILE	E	218	38.629	11.470	13.441	1.00	42.92	C
ATOM	3043	CG2	ILE	E	218	36.267	12.017	14.074	1.00	42.50	C
ATOM	3044	CD1	ILE	E	218	38.630	10.558	12.220	1.00	44.21	C
ATOM	3045	N	PHE	E	219	36.352	10.292	17.303	1.00	43.20	N
ATOM	3046	CA	PHE	E	219	35.311	10.185	18.332	1.00	43.29	C
ATOM	3047	C	PHE	E	219	35.731	10.914	19.597	1.00	43.95	C
ATOM	3048	O	PHE	E	219	34.960	11.687	20.153	1.00	43.74	O
ATOM	3049	CB	PHE	E	219	34.989	8.721	18.670	1.00	43.07	C
ATOM	3050	CG	PHE	E	219	34.067	8.039	17.680	1.00	42.19	C
ATOM	3051	CD1	PHE	E	219	34.411	6.804	17.136	1.00	40.53	C
ATOM	3052	CD2	PHE	E	219	32.865	8.629	17.297	1.00	41.70	C
ATOM	3053	CE1	PHE	E	219	33.583	6.158	16.228	1.00	40.46	C
ATOM	3054	CE2	PHE	E	219	32.019	7.992	16.390	1.00	43.11	C
ATOM	3055	CZ	PHE	E	219	32.386	6.745	15.847	1.00	42.12	C
ATOM	3056	N	VAL	E	220	36.965	10.674	20.031	1.00	45.01	N
ATOM	3057	CA	VAL	E	220	37.507	11.286	21.246	1.00	46.00	C
ATOM	3058	C	VAL	E	220	37.672	12.810	21.128	1.00	46.85	C
ATOM	3059	O	VAL	E	220	37.287	13.561	22.030	1.00	47.27	O
ATOM	3060	CB	VAL	E	220	38.860	10.640	21.657	1.00	46.03	C
ATOM	3061	CG1	VAL	E	220	39.429	11.308	22.916	1.00	45.61	C
ATOM	3062	CG2	VAL	E	220	38.699	9.152	21.871	1.00	45.29	C
ATOM	3063	N	GLN	E	221	38.236	13.271	20.022	1.00	47.79	N
ATOM	3064	CA	GLN	E	221	38.518	14.686	19.880	1.00	48.57	C
ATOM	3065	C	GLN	E	221	37.270	15.524	19.617	1.00	49.02	C
ATOM	3066	O	GLN	E	221	37.182	16.661	20.086	1.00	49.35	O
ATOM	3067	CB	GLN	E	221	39.546	14.919	18.783	1.00	48.67	C
ATOM	3068	CG	GLN	E	221	40.411	16.132	19.040	1.00	50.28	C
ATOM	3069	CD	GLN	E	221	41.200	16.556	17.822	1.00	52.24	C
ATOM	3070	OE1	GLN	E	221	40.717	16.481	16.687	1.00	53.30	O
ATOM	3071	NE2	GLN	E	221	42.419	17.017	18.051	1.00	52.69	N
ATOM	3072	N	HIS	E	222	36.306	14.984	18.875	1.00	49.37	N
ATOM	3073	CA	HIS	E	222	35.135	15.785	18.494	1.00	49.95	C
ATOM	3074	C	HIS	E	222	33.892	15.530	19.356	1.00	49.84	C
ATOM	3075	O	HIS	E	222	32.970	16.355	19.376	1.00	49.43	O
ATOM	3076	CB	HIS	E	222	34.809	15.617	17.008	1.00	50.42	C
ATOM	3077	CG	HIS	E	222	35.883	16.110	16.092	1.00	51.79	C
ATOM	3078	ND1	HIS	E	222	35.697	17.173	15.233	1.00	54.79	N
ATOM	3079	CD2	HIS	E	222	37.152	15.681	15.890	1.00	53.37	C

Figure 2 Table 2b - 47

ATOM	3080	CE1	HIS	E	222	36.808	17.384	14.547	1.00	55.14	C
ATOM	3081	NE2	HIS	E	222	37.708	16.494	14.930	1.00	54.84	N
ATOM	3082	N	ARG	E	223	33.889	14.404	20.076	1.00	49.99	N
ATOM	3083	CA	ARG	E	223	32.784	14.017	20.977	1.00	50.33	C
ATOM	3084	C	ARG	E	223	31.496	14.109	20.199	1.00	50.34	C
ATOM	3085	O	ARG	E	223	30.729	15.076	20.301	1.00	50.73	O
ATOM	3086	CB	ARG	E	223	32.721	14.872	22.253	1.00	50.38	C
ATOM	3087	CG	ARG	E	223	34.048	15.028	22.944	1.00	51.06	C
ATOM	3088	CD	ARG	E	223	33.950	15.931	24.133	1.00	52.77	C
ATOM	3089	NE	ARG	E	223	35.251	16.037	24.783	1.00	55.48	N
ATOM	3090	CZ	ARG	E	223	35.523	16.847	25.802	1.00	57.08	C
ATOM	3091	NH1	ARG	E	223	34.581	17.637	26.308	1.00	57.77	N
ATOM	3092	NH2	ARG	E	223	36.746	16.870	26.313	1.00	57.77	N
ATOM	3093	N	VAL	E	224	31.295	13.087	19.388	1.00	50.19	N
ATOM	3094	CA	VAL	E	224	30.251	13.062	18.402	1.00	49.93	C
ATOM	3095	C	VAL	E	224	29.874	11.592	18.299	1.00	50.01	C
ATOM	3096	O	VAL	E	224	30.752	10.722	18.342	1.00	50.08	O
ATOM	3097	CB	VAL	E	224	30.801	13.654	17.085	1.00	49.85	C
ATOM	3098	CG1	VAL	E	224	30.398	12.829	15.898	1.00	50.38	C
ATOM	3099	CG2	VAL	E	224	30.389	15.116	16.946	1.00	48.72	C
ATOM	3100	N	SER	E	225	28.581	11.301	18.216	1.00	50.11	N
ATOM	3101	CA	SER	E	225	28.130	9.913	18.393	1.00	50.21	C
ATOM	3102	C	SER	E	225	28.302	9.022	17.166	1.00	49.67	C
ATOM	3103	O	SER	E	225	28.345	7.804	17.307	1.00	50.45	O
ATOM	3104	CB	SER	E	225	26.697	9.847	18.931	1.00	50.34	C
ATOM	3105	OG	SER	E	225	25.871	10.829	18.328	1.00	51.87	O
ATOM	3106	N	ALA	E	226	28.409	9.617	15.980	1.00	48.81	N
ATOM	3107	CA	ALA	E	226	28.548	8.849	14.733	1.00	48.15	C
ATOM	3108	C	ALA	E	226	29.338	9.603	13.664	1.00	47.74	C
ATOM	3109	O	ALA	E	226	29.488	10.821	13.740	1.00	47.70	O
ATOM	3110	CB	ALA	E	226	27.184	8.457	14.192	1.00	47.81	C
ATOM	3111	N	LEU	E	227	29.846	8.870	12.676	1.00	46.93	N
ATOM	3112	CA	LEU	E	227	30.596	9.463	11.586	1.00	46.68	C
ATOM	3113	C	LEU	E	227	30.060	8.980	10.240	1.00	46.94	C
ATOM	3114	O	LEU	E	227	29.954	7.777	10.015	1.00	47.41	O
ATOM	3115	CB	LEU	E	227	32.078	9.133	11.704	1.00	46.25	C
ATOM	3116	CG	LEU	E	227	32.746	9.423	13.041	1.00	45.79	C
ATOM	3117	CD1	LEU	E	227	34.119	8.783	13.080	1.00	44.43	C
ATOM	3118	CD2	LEU	E	227	32.815	10.934	13.298	1.00	45.77	C
ATOM	3119	N	PRO	E	228	29.678	9.916	9.359	1.00	46.87	N
ATOM	3120	CA	PRO	E	228	29.311	9.524	8.017	1.00	47.13	C
ATOM	3121	C	PRO	E	228	30.528	8.954	7.293	1.00	47.76	C
ATOM	3122	O	PRO	E	228	31.635	9.517	7.399	1.00	48.02	O
ATOM	3123	CB	PRO	E	228	28.878	10.846	7.378	1.00	46.98	C
ATOM	3124	CG	PRO	E	228	28.512	11.717	8.525	1.00	46.50	C
ATOM	3125	CD	PRO	E	228	29.517	11.364	9.565	1.00	46.51	C
ATOM	3126	N	VAL	E	229	30.329	7.834	6.598	1.00	47.82	N
ATOM	3127	CA	VAL	E	229	31.374	7.230	5.774	1.00	48.47	C
ATOM	3128	C	VAL	E	229	31.147	7.704	4.339	1.00	48.86	C
ATOM	3129	O	VAL	E	229	30.060	7.516	3.777	1.00	49.21	O
ATOM	3130	CB	VAL	E	229	31.332	5.678	5.853	1.00	48.66	C
ATOM	3131	CG1	VAL	E	229	32.467	5.056	5.071	1.00	48.50	C
ATOM	3132	CG2	VAL	E	229	31.362	5.201	7.308	1.00	48.58	C
ATOM	3133	N	VAL	E	230	32.156	8.343	3.758	1.00	49.08	N
ATOM	3134	CA	VAL	E	230	32.002	8.959	2.436	1.00	49.57	C
ATOM	3135	C	VAL	E	230	32.949	8.385	1.378	1.00	49.97	C
ATOM	3136	O	VAL	E	230	33.940	7.728	1.706	1.00	50.14	O
ATOM	3137	CB	VAL	E	230	32.171	10.507	2.488	1.00	49.61	C
ATOM	3138	CG1	VAL	E	230	31.155	11.146	3.450	1.00	48.88	C
ATOM	3139	CG2	VAL	E	230	33.601	10.888	2.856	1.00	49.00	C
ATOM	3140	N	ASP	E	231	32.625	8.641	0.111	1.00	50.47	N
ATOM	3141	CA	ASP	E	231	33.486	8.283	-1.018	1.00	50.91	C
ATOM	3142	C	ASP	E	231	34.347	9.477	-1.434	1.00	51.36	C
ATOM	3143	O	ASP	E	231	34.435	10.468	-0.706	1.00	51.41	O
ATOM	3144	CB	ASP	E	231	32.657	7.755	-2.205	1.00	50.83	C
ATOM	3145	CG	ASP	E	231	31.712	8.806	-2.797	1.00	50.97	C
ATOM	3146	OD1	ASP	E	231	30.673	8.401	-3.358	1.00	51.74	O

Figure 2

Table 2b - 48

ATOM	3147	OD2	ASP	E	231	31.996	10.024	-2.718	1.00	50.43	O
ATOM	3148	N	GLU	E	232	34.959	9.381	-2.614	1.00	51.97	N
ATOM	3149	CA	GLU	E	232	35.901	10.401	-3.105	1.00	52.50	C
ATOM	3150	C	GLU	E	232	35.245	11.733	-3.488	1.00	52.14	C
ATOM	3151	O	GLU	E	232	35.904	12.778	-3.468	1.00	52.31	O
ATOM	3152	CB	GLU	E	232	36.777	9.863	-4.252	1.00	52.48	C
ATOM	3153	CG	GLU	E	232	36.029	9.106	-5.351	1.00	53.42	C
ATOM	3154	CD	GLU	E	232	36.958	8.585	-6.443	1.00	54.41	C
ATOM	3155	OE1	GLU	E	232	38.132	8.275	-6.130	1.00	55.93	O
ATOM	3156	OE2	GLU	E	232	36.519	8.481	-7.616	1.00	55.49	O
ATOM	3157	N	LYS	E	233	33.963	11.700	-3.833	1.00	51.72	N
ATOM	3158	CA	LYS	E	233	33.228	12.941	-4.069	1.00	51.26	C
ATOM	3159	C	LYS	E	233	32.408	13.363	-2.846	1.00	50.72	C
ATOM	3160	O	LYS	E	233	31.572	14.261	-2.925	1.00	50.72	O
ATOM	3161	CB	LYS	E	233	32.399	12.860	-5.355	1.00	51.34	C
ATOM	3162	CG	LYS	E	233	33.277	12.973	-6.590	1.00	51.31	C
ATOM	3163	CD	LYS	E	233	32.502	12.918	-7.889	1.00	51.78	C
ATOM	3164	CE	LYS	E	233	33.465	12.839	-9.067	1.00	51.91	C
ATOM	3165	NZ	LYS	E	233	32.769	12.547	-10.356	1.00	52.35	N
ATOM	3166	N	GLY	E	234	32.673	12.708	-1.714	1.00	50.11	N
ATOM	3167	CA	GLY	E	234	32.064	13.058	-0.435	1.00	49.25	C
ATOM	3168	C	GLY	E	234	30.590	12.751	-0.330	1.00	48.69	C
ATOM	3169	O	GLY	E	234	29.882	13.361	0.470	1.00	48.25	O
ATOM	3170	N	ARG	E	235	30.128	11.819	-1.156	1.00	48.51	N
ATOM	3171	CA	ARG	E	235	28.777	11.299	-1.046	1.00	48.66	C
ATOM	3172	C	ARG	E	235	28.766	10.248	0.050	1.00	48.47	C
ATOM	3173	O	ARG	E	235	29.691	9.437	0.146	1.00	48.61	O
ATOM	3174	CB	ARG	E	235	28.335	10.651	-2.347	1.00	48.81	C
ATOM	3175	CG	ARG	E	235	28.028	11.609	-3.467	1.00	49.80	C
ATOM	3176	CD	ARG	E	235	27.778	10.841	-4.755	1.00	51.54	C
ATOM	3177	NE	ARG	E	235	29.032	10.446	-5.394	1.00	53.14	N
ATOM	3178	CZ	ARG	E	235	29.121	9.705	-6.493	1.00	53.79	C
ATOM	3179	NH1	ARG	E	235	28.026	9.252	-7.090	1.00	54.25	N
ATOM	3180	NH2	ARG	E	235	30.313	9.412	-6.995	1.00	54.12	N
ATOM	3181	N	VAL	E	236	27.724	10.263	0.877	1.00	48.09	N
ATOM	3182	CA	VAL	E	236	27.621	9.320	1.992	1.00	47.61	C
ATOM	3183	C	VAL	E	236	27.230	7.918	1.483	1.00	47.33	C
ATOM	3184	O	VAL	E	236	26.320	7.777	0.660	1.00	46.94	O
ATOM	3185	CB	VAL	E	236	26.663	9.856	3.106	1.00	47.21	C
ATOM	3186	CG1	VAL	E	236	25.236	9.946	2.605	1.00	46.78	C
ATOM	3187	CG2	VAL	E	236	26.730	8.986	4.334	1.00	46.98	C
ATOM	3188	N	VAL	E	237	27.949	6.899	1.950	1.00	47.33	N
ATOM	3189	CA	VAL	E	237	27.640	5.494	1.606	1.00	47.74	C
ATOM	3190	C	VAL	E	237	27.480	4.592	2.837	1.00	48.38	C
ATOM	3191	O	VAL	E	237	27.014	3.453	2.730	1.00	48.57	O
ATOM	3192	CB	VAL	E	237	28.687	4.855	0.646	1.00	47.28	C
ATOM	3193	CG1	VAL	E	237	28.628	5.501	-0.713	1.00	46.95	C
ATOM	3194	CG2	VAL	E	237	30.097	4.922	1.228	1.00	46.62	C
ATOM	3195	N	ASP	E	238	27.896	5.095	3.995	1.00	48.87	N
ATOM	3196	CA	ASP	E	238	27.690	4.394	5.248	1.00	49.67	C
ATOM	3197	C	ASP	E	238	27.831	5.349	6.416	1.00	50.27	C
ATOM	3198	O	ASP	E	238	28.069	6.556	6.242	1.00	50.22	O
ATOM	3199	CB	ASP	E	238	28.682	3.233	5.394	1.00	49.96	C
ATOM	3200	CG	ASP	E	238	28.074	2.008	6.084	1.00	50.28	C
ATOM	3201	OD1	ASP	E	238	27.312	2.153	7.065	1.00	51.04	O
ATOM	3202	OD2	ASP	E	238	28.373	0.889	5.645	1.00	49.94	O
ATOM	3203	N	ILE	E	239	27.684	4.794	7.611	1.00	50.87	N
ATOM	3204	CA	ILE	E	239	27.745	5.558	8.846	1.00	51.55	C
ATOM	3205	C	ILE	E	239	28.439	4.687	9.891	1.00	52.06	C
ATOM	3206	O	ILE	E	239	28.148	3.495	9.997	1.00	52.26	O
ATOM	3207	CB	ILE	E	239	26.310	6.019	9.281	1.00	51.46	C
ATOM	3208	CG1	ILE	E	239	26.341	6.800	10.586	1.00	51.43	C
ATOM	3209	CG2	ILE	E	239	25.344	4.848	9.404	1.00	51.45	C
ATOM	3210	CD1	ILE	E	239	26.104	8.236	10.413	1.00	50.66	C
ATOM	3211	N	TYR	E	240	29.382	5.265	10.633	1.00	52.78	N
ATOM	3212	CA	TYR	E	240	30.097	4.527	11.682	1.00	53.18	C
ATOM	3213	C	TYR	E	240	29.820	5.138	13.056	1.00	53.65	C

Figure 2

Table 2b - 49

ATOM	3214	O	TYR	E	240	30.287	6.240	13.359	1.00	53.45	O
ATOM	3215	CB	TYR	E	240	31.602	4.469	11.382	1.00	53.37	C
ATOM	3216	CG	TYR	E	240	32.394	3.568	12.308	1.00	53.67	C
ATOM	3217	CD1	TYR	E	240	33.223	4.104	13.293	1.00	53.56	C
ATOM	3218	CD2	TYR	E	240	32.312	2.174	12.199	1.00	54.22	C
ATOM	3219	CE1	TYR	E	240	33.954	3.275	14.146	1.00	54.31	C
ATOM	3220	CE2	TYR	E	240	33.027	1.336	13.051	1.00	54.27	C
ATOM	3221	CZ	TYR	E	240	33.852	1.886	14.022	1.00	54.35	C
ATOM	3222	OH	TYR	E	240	34.562	1.052	14.870	1.00	53.07	O
ATOM	3223	N	SER	E	241	29.054	4.412	13.875	1.00	54.32	N
ATOM	3224	CA	SER	E	241	28.598	4.899	15.190	1.00	55.13	C
ATOM	3225	C	SER	E	241	29.440	4.397	16.365	1.00	55.65	C
ATOM	3226	O	SER	E	241	30.189	3.417	16.241	1.00	55.54	O
ATOM	3227	CB	SER	E	241	27.132	4.512	15.428	1.00	55.23	C
ATOM	3228	OG	SER	E	241	26.591	5.142	16.587	1.00	54.97	O
ATOM	3229	N	LYS	E	242	29.303	5.086	17.502	1.00	56.10	N
ATOM	3230	CA	LYS	E	242	29.837	4.608	18.785	1.00	56.72	C
ATOM	3231	C	LYS	E	242	29.320	3.190	19.120	1.00	56.99	C
ATOM	3232	O	LYS	E	242	30.087	2.331	19.538	1.00	56.77	O
ATOM	3233	CB	LYS	E	242	29.525	5.605	19.918	1.00	56.59	C
ATOM	3234	CG	LYS	E	242	30.291	6.909	19.815	1.00	56.44	C
ATOM	3235	CD	LYS	E	242	30.260	7.734	21.089	1.00	56.49	C
ATOM	3236	CE	LYS	E	242	31.394	8.756	21.042	1.00	56.86	C
ATOM	3237	NZ	LYS	E	242	31.425	9.736	22.164	1.00	58.01	N
ATOM	3238	N	PHE	E	243	28.026	2.954	18.913	1.00	57.81	N
ATOM	3239	CA	PHE	E	243	27.445	1.618	19.036	1.00	58.75	C
ATOM	3240	C	PHE	E	243	28.232	0.573	18.231	1.00	59.22	C
ATOM	3241	O	PHE	E	243	28.434	-0.540	18.695	1.00	59.22	O
ATOM	3242	CB	PHE	E	243	25.965	1.626	18.621	1.00	58.81	C
ATOM	3243	CG	PHE	E	243	25.356	0.246	18.485	1.00	59.72	C
ATOM	3244	CD1	PHE	E	243	24.765	-0.382	19.579	1.00	60.44	C
ATOM	3245	CD2	PHE	E	243	25.381	-0.431	17.265	1.00	59.61	C
ATOM	3246	CE1	PHE	E	243	24.202	-1.658	19.455	1.00	60.57	C
ATOM	3247	CE2	PHE	E	243	24.824	-1.701	17.135	1.00	59.81	C
ATOM	3248	CZ	PHE	E	243	24.234	-2.315	18.230	1.00	60.09	C
ATOM	3249	N	ASP	E	244	28.685	0.940	17.033	1.00	60.12	N
ATOM	3250	CA	ASP	E	244	29.447	0.019	16.186	1.00	60.78	C
ATOM	3251	C	ASP	E	244	30.797	-0.275	16.809	1.00	61.28	C
ATOM	3252	O	ASP	E	244	31.575	-1.061	16.271	1.00	61.42	O
ATOM	3253	CB	ASP	E	244	29.644	0.590	14.773	1.00	60.77	C
ATOM	3254	CG	ASP	E	244	28.338	1.015	14.116	1.00	61.09	C
ATOM	3255	OD1	ASP	E	244	27.311	0.312	14.274	1.00	60.38	O
ATOM	3256	OD2	ASP	E	244	28.346	2.054	13.427	1.00	61.31	O
ATOM	3257	N	VAL	E	245	31.064	0.356	17.950	1.00	62.05	N
ATOM	3258	CA	VAL	E	245	32.364	0.238	18.615	1.00	62.94	C
ATOM	3259	C	VAL	E	245	32.415	-0.814	19.737	1.00	63.39	C
ATOM	3260	O	VAL	E	245	33.462	-1.416	19.943	1.00	63.27	O
ATOM	3261	CB	VAL	E	245	32.886	1.612	19.100	1.00	62.77	C
ATOM	3262	CG1	VAL	E	245	34.237	1.468	19.785	1.00	62.82	C
ATOM	3263	CG2	VAL	E	245	32.991	2.570	17.929	1.00	62.77	C
ATOM	3264	N	ILE	E	246	31.307	-1.041	20.447	1.00	64.31	N
ATOM	3265	CA	ILE	E	246	31.247	-2.159	21.419	1.00	65.47	C
ATOM	3266	C	ILE	E	246	31.186	-3.536	20.767	1.00	65.97	C
ATOM	3267	O	ILE	E	246	31.198	-4.557	21.458	1.00	66.14	O
ATOM	3268	CB	ILE	E	246	30.086	-2.063	22.467	1.00	65.60	C
ATOM	3269	CG1	ILE	E	246	28.822	-1.410	21.879	1.00	66.02	C
ATOM	3270	CG2	ILE	E	246	30.579	-1.438	23.778	1.00	65.66	C
ATOM	3271	CD1	ILE	E	246	27.800	-2.419	21.334	1.00	65.81	C
ATOM	3272	N	ASN	E	247	31.100	-3.560	19.442	1.00	66.68	N
ATOM	3273	CA	ASN	E	247	31.276	-4.789	18.688	1.00	67.38	C
ATOM	3274	C	ASN	E	247	32.692	-5.337	18.883	1.00	67.58	C
ATOM	3275	O	ASN	E	247	32.910	-6.544	18.805	1.00	67.46	O
ATOM	3276	CB	ASN	E	247	30.989	-4.539	17.207	1.00	67.64	C
ATOM	3277	CG	ASN	E	247	31.964	-5.260	16.291	1.00	68.36	C
ATOM	3278	OD1	ASN	E	247	32.800	-4.626	15.641	1.00	69.06	O
ATOM	3279	ND2	ASN	E	247	31.878	-6.592	16.253	1.00	67.70	N
ATOM	3280	N	LEU	E	248	33.641	-4.436	19.142	1.00	67.87	N

Figure 2

Table 2b - 50

ATOM	3281	CA	LEU	E	248	35.036	-4.801	19.404	1.00	68.38	C
ATOM	3282	C	LEU	E	248	35.195	-5.533	20.748	1.00	68.92	C
ATOM	3283	O	LEU	E	248	36.260	-6.079	21.058	1.00	68.92	O
ATOM	3284	CB	LEU	E	248	35.920	-3.553	19.350	1.00	68.22	C
ATOM	3285	CG	LEU	E	248	36.243	-2.874	17.999	1.00	68.18	C
ATOM	3286	CD1	LEU	E	248	35.476	-3.417	16.791	1.00	67.95	C
ATOM	3287	CD2	LEU	E	248	36.060	-1.377	18.097	1.00	67.28	C
ATOM	3288	N	ALA	E	249	34.121	-5.537	21.535	1.00	69.45	N
ATOM	3289	CA	ALA	E	249	34.062	-6.282	22.784	1.00	69.92	C
ATOM	3290	C	ALA	E	249	33.415	-7.662	22.576	1.00	70.38	C
ATOM	3291	O	ALA	E	249	33.182	-8.405	23.539	1.00	70.45	O
ATOM	3292	CB	ALA	E	249	33.327	-5.474	23.863	1.00	69.79	C
ATOM	3293	N	ALA	E	250	33.134	-8.002	21.316	1.00	70.85	N
ATOM	3294	CA	ALA	E	250	32.710	-9.359	20.953	1.00	71.26	C
ATOM	3295	C	ALA	E	250	33.923	-10.289	20.805	1.00	71.50	C
ATOM	3296	O	ALA	E	250	33.933	-11.399	21.344	1.00	71.44	O
ATOM	3297	CB	ALA	E	250	31.867	-9.348	19.667	1.00	71.12	C
ATOM	3298	N	GLU	E	251	34.936	-9.811	20.079	1.00	71.86	N
ATOM	3299	CA	GLU	E	251	36.168	-10.560	19.799	1.00	72.14	C
ATOM	3300	C	GLU	E	251	36.972	-10.887	21.064	1.00	72.31	C
ATOM	3301	O	GLU	E	251	36.973	-10.111	22.019	1.00	72.41	O
ATOM	3302	CB	GLU	E	251	37.042	-9.770	18.812	1.00	72.10	C
ATOM	3303	CG	GLU	E	251	37.274	-8.308	19.212	1.00	72.06	C
ATOM	3304	CD	GLU	E	251	38.113	-7.528	18.211	1.00	72.44	C
ATOM	3305	OE1	GLU	E	251	39.116	-8.081	17.710	1.00	72.38	O
ATOM	3306	OE2	GLU	E	251	37.774	-6.350	17.936	1.00	72.70	O
ATOM	3307	N	LYS	E	252	37.648	-12.036	21.061	1.00	72.51	N
ATOM	3308	CA	LYS	E	252	38.544	-12.427	22.160	1.00	72.63	C
ATOM	3309	C	LYS	E	252	39.990	-11.955	21.938	1.00	72.78	C
ATOM	3310	O	LYS	E	252	40.940	-12.610	22.382	1.00	72.53	O
ATOM	3311	CB	LYS	E	252	38.508	-13.943	22.366	1.00	72.59	C
ATOM	3312	CG	LYS	E	252	37.379	-14.426	23.254	1.00	72.65	C
ATOM	3313	CD	LYS	E	252	37.419	-15.936	23.405	1.00	72.64	C
ATOM	3314	CE	LYS	E	252	36.611	-16.396	24.604	1.00	72.95	C
ATOM	3315	NZ	LYS	E	252	37.264	-16.032	25.894	1.00	73.18	N
ATOM	3316	N	THR	E	253	40.143	-10.811	21.262	1.00	73.06	N
ATOM	3317	CA	THR	E	253	41.464	-10.273	20.892	1.00	73.21	C
ATOM	3318	C	THR	E	253	41.680	-8.798	21.269	1.00	73.26	C
ATOM	3319	O	THR	E	253	42.612	-8.486	22.017	1.00	73.16	O
ATOM	3320	CB	THR	E	253	41.784	-10.481	19.376	1.00	73.24	C
ATOM	3321	OG1	THR	E	253	40.697	-9.999	18.571	1.00	73.06	O
ATOM	3322	CG2	THR	E	253	42.047	-11.961	19.063	1.00	73.14	C
ATOM	3323	N	TYR	E	254	40.819	-7.914	20.748	1.00	73.50	N
ATOM	3324	CA	TYR	E	254	40.923	-6.439	20.895	1.00	73.58	C
ATOM	3325	C	TYR	E	254	41.840	-5.765	19.860	1.00	73.47	C
ATOM	3326	O	TYR	E	254	41.705	-4.563	19.593	1.00	73.52	O
ATOM	3327	CB	TYR	E	254	41.344	-6.017	22.319	1.00	73.78	C
ATOM	3328	CG	TYR	E	254	40.202	-5.756	23.282	1.00	74.02	C
ATOM	3329	CD1	TYR	E	254	40.040	-6.530	24.436	1.00	74.65	C
ATOM	3330	CD2	TYR	E	254	39.291	-4.729	23.047	1.00	74.05	C
ATOM	3331	CE1	TYR	E	254	38.987	-6.284	25.326	1.00	74.83	C
ATOM	3332	CE2	TYR	E	254	38.243	-4.477	23.924	1.00	74.22	C
ATOM	3333	CZ	TYR	E	254	38.093	-5.251	25.059	1.00	74.28	C
ATOM	3334	OH	TYR	E	254	37.046	-4.985	25.916	1.00	74.12	O
ATOM	3335	N	ASN	E	255	42.749	-6.549	19.279	1.00	73.25	N
ATOM	3336	CA	ASN	E	255	43.837	-6.041	18.431	1.00	73.01	C
ATOM	3337	C	ASN	E	255	43.451	-5.660	16.991	1.00	72.84	C
ATOM	3338	O	ASN	E	255	44.249	-5.049	16.274	1.00	72.83	O
ATOM	3339	CB	ASN	E	255	45.003	-7.044	18.415	1.00	72.98	C
ATOM	3340	CG	ASN	E	255	45.583	-7.308	19.806	1.00	73.14	C
ATOM	3341	OD1	ASN	E	255	46.204	-8.349	20.045	1.00	72.76	O
ATOM	3342	ND2	ASN	E	255	45.385	-6.365	20.727	1.00	73.23	N
ATOM	3343	N	ASN	E	256	42.237	-6.014	16.576	1.00	72.53	N
ATOM	3344	CA	ASN	E	256	41.790	-5.785	15.201	1.00	72.31	C
ATOM	3345	C	ASN	E	256	41.328	-4.352	14.907	1.00	72.10	C
ATOM	3346	O	ASN	E	256	40.327	-4.151	14.215	1.00	72.10	O
ATOM	3347	CB	ASN	E	256	40.684	-6.783	14.824	1.00	72.34	C

Figure 2 Table 2b - 51

ATOM	3348	CG	ASN	E	256	41.232	-8.113	14.347	1.00	72.48	C
ATOM	3349	OD1	ASN	E	256	41.281	-8.381	13.145	1.00	72.55	O
ATOM	3350	ND2	ASN	E	256	41.648	-8.957	15.289	1.00	72.81	N
ATOM	3351	N	LEU	E	257	42.059	-3.361	15.415	1.00	71.81	N
ATOM	3352	CA	LEU	E	257	41.656	-1.957	15.266	1.00	71.44	C
ATOM	3353	C	LEU	E	257	42.323	-1.278	14.072	1.00	71.23	C
ATOM	3354	O	LEU	E	257	41.950	-0.161	13.702	1.00	71.15	O
ATOM	3355	CB	LEU	E	257	41.920	-1.161	16.553	1.00	71.45	C
ATOM	3356	CG	LEU	E	257	41.266	-1.603	17.873	1.00	71.42	C
ATOM	3357	CD1	LEU	E	257	41.878	-0.865	19.053	1.00	71.56	C
ATOM	3358	CD2	LEU	E	257	39.756	-1.418	17.863	1.00	70.61	C
ATOM	3359	N	ASP	E	258	43.296	-1.960	13.470	1.00	70.97	N
ATOM	3360	CA	ASP	E	258	44.035	-1.412	12.331	1.00	70.80	C
ATOM	3361	C	ASP	E	258	43.294	-1.562	11.002	1.00	70.58	C
ATOM	3362	O	ASP	E	258	43.678	-0.944	10.004	1.00	70.71	O
ATOM	3363	CB	ASP	E	258	45.432	-2.031	12.234	1.00	70.78	C
ATOM	3364	CG	ASP	E	258	46.241	-1.844	13.504	1.00	70.93	C
ATOM	3365	OD1	ASP	E	258	46.360	-0.693	13.980	1.00	70.71	O
ATOM	3366	OD2	ASP	E	258	46.765	-2.853	14.024	1.00	71.07	O
ATOM	3367	N	VAL	E	259	42.237	-2.374	10.998	1.00	70.17	N
ATOM	3368	CA	VAL	E	259	41.426	-2.620	9.795	1.00	69.75	C
ATOM	3369	C	VAL	E	259	40.610	-1.387	9.386	1.00	69.39	C
ATOM	3370	O	VAL	E	259	40.338	-0.516	10.217	1.00	69.22	O
ATOM	3371	CB	VAL	E	259	40.472	-3.842	9.966	1.00	69.79	C
ATOM	3372	CG1	VAL	E	259	41.263	-5.126	10.249	1.00	69.94	C
ATOM	3373	CG2	VAL	E	259	39.430	-3.587	11.056	1.00	69.70	C
ATOM	3374	N	SER	E	260	40.223	-1.331	8.110	1.00	68.99	N
ATOM	3375	CA	SER	E	260	39.426	-0.219	7.582	1.00	68.50	C
ATOM	3376	C	SER	E	260	38.029	-0.179	8.203	1.00	68.28	C
ATOM	3377	O	SER	E	260	37.542	-1.175	8.745	1.00	68.39	O
ATOM	3378	CB	SER	E	260	39.334	-0.275	6.048	1.00	68.51	C
ATOM	3379	OG	SER	E	260	38.130	-0.885	5.606	1.00	68.30	O
ATOM	3380	N	VAL	E	261	37.395	0.984	8.115	1.00	67.86	N
ATOM	3381	CA	VAL	E	261	36.065	1.194	8.665	1.00	67.51	C
ATOM	3382	C	VAL	E	261	35.024	0.348	7.918	1.00	67.42	C
ATOM	3383	O	VAL	E	261	34.054	-0.122	8.519	1.00	67.43	O
ATOM	3384	CB	VAL	E	261	35.696	2.713	8.671	1.00	67.34	C
ATOM	3385	CG1	VAL	E	261	35.066	3.147	7.353	1.00	67.19	C
ATOM	3386	CG2	VAL	E	261	34.789	3.038	9.829	1.00	67.25	C
ATOM	3387	N	THR	E	262	35.247	0.150	6.616	1.00	67.31	N
ATOM	3388	CA	THR	E	262	34.382	-0.688	5.788	1.00	67.10	C
ATOM	3389	C	THR	E	262	34.373	-2.108	6.331	1.00	66.97	C
ATOM	3390	O	THR	E	262	33.304	-2.665	6.570	1.00	66.97	O
ATOM	3391	CB	THR	E	262	34.793	-0.653	4.291	1.00	67.19	C
ATOM	3392	OG1	THR	E	262	34.283	0.546	3.695	1.00	66.86	O
ATOM	3393	CG2	THR	E	262	34.240	-1.858	3.524	1.00	66.91	C
ATOM	3394	N	LYS	E	263	35.558	-2.669	6.560	1.00	66.83	N
ATOM	3395	CA	LYS	E	263	35.665	-4.024	7.098	1.00	66.83	C
ATOM	3396	C	LYS	E	263	35.017	-4.126	8.484	1.00	66.77	C
ATOM	3397	O	LYS	E	263	34.341	-5.109	8.784	1.00	66.69	O
ATOM	3398	CB	LYS	E	263	37.120	-4.509	7.113	1.00	66.74	C
ATOM	3399	CG	LYS	E	263	37.250	-6.021	7.264	1.00	67.21	C
ATOM	3400	CD	LYS	E	263	38.530	-6.576	6.648	1.00	67.68	C
ATOM	3401	CE	LYS	E	263	38.432	-8.096	6.490	1.00	68.01	C
ATOM	3402	NZ	LYS	E	263	39.646	-8.715	5.884	1.00	67.91	N
ATOM	3403	N	ALA	E	264	35.200	-3.092	9.302	1.00	66.88	N
ATOM	3404	CA	ALA	E	264	34.605	-3.029	10.644	1.00	67.03	C
ATOM	3405	C	ALA	E	264	33.078	-3.098	10.645	1.00	67.18	C
ATOM	3406	O	ALA	E	264	32.483	-3.744	11.511	1.00	67.12	O
ATOM	3407	CB	ALA	E	264	35.060	-1.781	11.366	1.00	66.94	C
ATOM	3408	N	LEU	E	265	32.451	-2.425	9.681	1.00	67.37	N
ATOM	3409	CA	LEU	E	265	30.992	-2.385	9.601	1.00	67.50	C
ATOM	3410	C	LEU	E	265	30.378	-3.669	9.038	1.00	67.84	C
ATOM	3411	O	LEU	E	265	29.219	-3.974	9.320	1.00	67.81	O
ATOM	3412	CB	LEU	E	265	30.515	-1.150	8.830	1.00	67.13	C
ATOM	3413	CG	LEU	E	265	30.621	0.162	9.610	1.00	66.86	C
ATOM	3414	CD1	LEU	E	265	30.490	1.350	8.676	1.00	66.46	C

Figure 2

Table 2b - 52

ATOM	3415	CD2	LEU	E	265	29.587	0.243	10.736	1.00	66.26	C
ATOM	3416	N	GLN	E	266	31.159	-4.425	8.266	1.00	68.31	N
ATOM	3417	CA	GLN	E	266	30.709	-5.709	7.711	1.00	68.86	C
ATOM	3418	C	GLN	E	266	30.198	-6.656	8.795	1.00	69.04	C
ATOM	3419	O	GLN	E	266	29.316	-7.476	8.547	1.00	68.95	O
ATOM	3420	CB	GLN	E	266	31.831	-6.381	6.915	1.00	68.88	C
ATOM	3421	CG	GLN	E	266	32.088	-5.749	5.545	1.00	69.02	C
ATOM	3422	CD	GLN	E	266	33.392	-6.210	4.886	1.00	69.33	C
ATOM	3423	OE1	GLN	E	266	33.867	-5.579	3.937	1.00	69.38	O
ATOM	3424	NE2	GLN	E	266	33.970	-7.308	5.382	1.00	69.00	N
ATOM	3425	N	HIS	E	267	30.744	-6.509	9.999	1.00	69.48	N
ATOM	3426	CA	HIS	E	267	30.423	-7.371	11.131	1.00	70.05	C
ATOM	3427	C	HIS	E	267	29.091	-7.022	11.825	1.00	70.24	C
ATOM	3428	O	HIS	E	267	28.715	-7.674	12.803	1.00	70.27	O
ATOM	3429	CB	HIS	E	267	31.589	-7.351	12.133	1.00	70.15	C
ATOM	3430	CG	HIS	E	267	31.834	-8.666	12.814	1.00	70.61	C
ATOM	3431	ND1	HIS	E	267	31.888	-8.796	14.186	1.00	70.88	N
ATOM	3432	CD2	HIS	E	267	32.043	-9.906	12.310	1.00	70.81	C
ATOM	3433	CE1	HIS	E	267	32.117	-10.060	14.499	1.00	71.00	C
ATOM	3434	NE2	HIS	E	267	32.214	-10.754	13.379	1.00	71.05	N
ATOM	3435	N	ARG	E	268	28.379	-6.014	11.314	1.00	70.49	N
ATOM	3436	CA	ARG	E	268	27.100	-5.565	11.897	1.00	70.72	C
ATOM	3437	C	ARG	E	268	26.074	-6.673	12.140	1.00	70.88	C
ATOM	3438	O	ARG	E	268	26.030	-7.676	11.424	1.00	70.76	O
ATOM	3439	CB	ARG	E	268	26.448	-4.467	11.042	1.00	70.66	C
ATOM	3440	CG	ARG	E	268	26.511	-3.066	11.652	1.00	70.96	C
ATOM	3441	CD	ARG	E	268	25.404	-2.147	11.105	1.00	71.42	C
ATOM	3442	NE	ARG	E	268	25.686	-1.667	9.750	1.00	71.51	N
ATOM	3443	CZ	ARG	E	268	25.999	-0.411	9.431	1.00	71.45	C
ATOM	3444	NH1	ARG	E	268	26.065	0.542	10.356	1.00	70.54	N
ATOM	3445	NH2	ARG	E	268	26.241	-0.106	8.165	1.00	71.65	N
ATOM	3446	N	SER	E	269	25.249	-6.458	13.155	1.00	71.07	N
ATOM	3447	CA	SER	E	269	24.106	-7.313	13.426	1.00	71.23	C
ATOM	3448	C	SER	E	269	22.907	-6.761	12.658	1.00	71.40	C
ATOM	3449	O	SER	E	269	22.647	-5.552	12.687	1.00	71.40	O
ATOM	3450	CB	SER	E	269	23.822	-7.349	14.928	1.00	71.24	C
ATOM	3451	OG	SER	E	269	22.832	-8.310	15.238	1.00	71.03	O
ATOM	3452	N	HIS	E	270	22.191	-7.656	11.975	1.00	71.65	N
ATOM	3453	CA	HIS	E	270	21.089	-7.314	11.050	1.00	71.89	C
ATOM	3454	C	HIS	E	270	21.617	-6.822	9.698	1.00	71.90	C
ATOM	3455	O	HIS	E	270	22.784	-6.423	9.581	1.00	72.00	O
ATOM	3456	CB	HIS	E	270	20.130	-6.261	11.639	1.00	72.02	C
ATOM	3457	CG	HIS	E	270	19.464	-6.679	12.914	1.00	72.45	C
ATOM	3458	ND1	HIS	E	270	18.390	-7.546	12.946	1.00	73.02	N
ATOM	3459	CD2	HIS	E	270	19.705	-6.332	14.201	1.00	72.80	C
ATOM	3460	CE1	HIS	E	270	18.007	-7.725	14.198	1.00	72.99	C
ATOM	3461	NE2	HIS	E	270	18.788	-6.999	14.980	1.00	73.16	N
ATOM	3462	N	TYR	E	271	20.755	-6.846	8.679	1.00	71.77	N
ATOM	3463	CA	TYR	E	271	21.080	-6.183	7.415	1.00	71.64	C
ATOM	3464	C	TYR	E	271	20.863	-4.659	7.508	1.00	71.17	C
ATOM	3465	O	TYR	E	271	20.491	-4.136	8.566	1.00	71.12	O
ATOM	3466	CB	TYR	E	271	20.347	-6.814	6.220	1.00	71.88	C
ATOM	3467	CG	TYR	E	271	21.291	-7.126	5.077	1.00	72.47	C
ATOM	3468	CD1	TYR	E	271	21.744	-8.429	4.862	1.00	72.96	C
ATOM	3469	CD2	TYR	E	271	21.762	-6.112	4.231	1.00	72.87	C
ATOM	3470	CE1	TYR	E	271	22.626	-8.721	3.824	1.00	73.37	C
ATOM	3471	CE2	TYR	E	271	22.646	-6.388	3.192	1.00	73.04	C
ATOM	3472	CZ	TYR	E	271	23.073	-7.696	2.994	1.00	73.35	C
ATOM	3473	OH	TYR	E	271	23.945	-7.984	1.968	1.00	73.36	O
ATOM	3474	N	PHE	E	272	21.096	-3.957	6.400	1.00	70.61	N
ATOM	3475	CA	PHE	E	272	21.291	-2.509	6.432	1.00	70.01	C
ATOM	3476	C	PHE	E	272	20.746	-1.839	5.162	1.00	69.29	C
ATOM	3477	O	PHE	E	272	21.358	-1.925	4.092	1.00	69.46	O
ATOM	3478	CB	PHE	E	272	22.791	-2.232	6.625	1.00	70.12	C
ATOM	3479	CG	PHE	E	272	23.138	-0.785	6.769	1.00	70.89	C
ATOM	3480	CD1	PHE	E	272	22.826	-0.090	7.937	1.00	71.29	C
ATOM	3481	CD2	PHE	E	272	23.805	-0.117	5.747	1.00	71.28	C

Figure 2

Table 2b - 53

ATOM	3482	CE1	PHE	E	272	23.151	1.250	8.072	1.00	71.04	C
ATOM	3483	CE2	PHE	E	272	24.140	1.224	5.875	1.00	70.87	C
ATOM	3484	CZ	PHE	E	272	23.813	1.909	7.036	1.00	71.17	C
ATOM	3485	N	GLU	E	273	19.593	-1.179	5.290	1.00	68.15	N
ATOM	3486	CA	GLU	E	273	18.896	-0.568	4.147	1.00	66.98	C
ATOM	3487	C	GLU	E	273	19.498	0.792	3.743	1.00	65.90	C
ATOM	3488	O	GLU	E	273	18.783	1.706	3.327	1.00	65.97	O
ATOM	3489	CB	GLU	E	273	17.382	-0.478	4.448	1.00	67.16	C
ATOM	3490	CG	GLU	E	273	16.509	0.303	3.437	1.00	67.70	C
ATOM	3491	CD	GLU	E	273	16.651	-0.177	1.991	1.00	68.18	C
ATOM	3492	OE1	GLU	E	273	16.253	-1.325	1.691	1.00	67.77	O
ATOM	3493	OE2	GLU	E	273	17.151	0.607	1.151	1.00	68.06	O
ATOM	3494	N	GLY	E	274	20.817	0.918	3.853	1.00	64.63	N
ATOM	3495	CA	GLY	E	274	21.509	2.175	3.571	1.00	63.02	C
ATOM	3496	C	GLY	E	274	21.434	3.122	4.753	1.00	61.96	C
ATOM	3497	O	GLY	E	274	20.688	2.877	5.702	1.00	61.69	O
ATOM	3498	N	VAL	E	275	22.215	4.200	4.707	1.00	61.02	N
ATOM	3499	CA	VAL	E	275	22.173	5.219	5.764	1.00	59.93	C
ATOM	3500	C	VAL	E	275	20.908	6.059	5.647	1.00	59.26	C
ATOM	3501	O	VAL	E	275	20.458	6.359	4.543	1.00	59.62	O
ATOM	3502	CB	VAL	E	275	23.478	6.088	5.849	1.00	59.68	C
ATOM	3503	CG1	VAL	E	275	24.235	6.089	4.543	1.00	60.18	C
ATOM	3504	CG2	VAL	E	275	23.184	7.493	6.297	1.00	59.12	C
ATOM	3505	N	LEU	E	276	20.320	6.401	6.788	1.00	58.25	N
ATOM	3506	CA	LEU	E	276	19.108	7.205	6.822	1.00	57.62	C
ATOM	3507	C	LEU	E	276	19.432	8.698	6.688	1.00	56.98	C
ATOM	3508	O	LEU	E	276	20.192	9.264	7.492	1.00	56.59	O
ATOM	3509	CB	LEU	E	276	18.298	6.887	8.081	1.00	57.45	C
ATOM	3510	CG	LEU	E	276	17.534	5.560	7.944	1.00	58.59	C
ATOM	3511	CD1	LEU	E	276	17.741	4.630	9.152	1.00	58.88	C
ATOM	3512	CD2	LEU	E	276	16.045	5.811	7.671	1.00	58.90	C
ATOM	3513	N	LYS	E	277	18.852	9.315	5.658	1.00	56.24	N
ATOM	3514	CA	LYS	E	277	19.208	10.678	5.234	1.00	55.57	C
ATOM	3515	C	LYS	E	277	18.037	11.636	5.280	1.00	54.90	C
ATOM	3516	O	LYS	E	277	16.890	11.223	5.471	1.00	54.99	O
ATOM	3517	CB	LYS	E	277	19.741	10.659	3.795	1.00	55.62	C
ATOM	3518	CG	LYS	E	277	21.063	9.930	3.636	1.00	56.21	C
ATOM	3519	CD	LYS	E	277	21.323	9.560	2.195	1.00	57.42	C
ATOM	3520	CE	LYS	E	277	20.347	8.500	1.713	1.00	57.25	C
ATOM	3521	NZ	LYS	E	277	21.062	7.518	0.884	1.00	57.73	N
ATOM	3522	N	CYS	E	278	18.335	12.916	5.077	1.00	53.86	N
ATOM	3523	CA	CYS	E	278	17.302	13.919	4.889	1.00	53.29	C
ATOM	3524	C	CYS	E	278	17.839	15.132	4.120	1.00	52.38	C
ATOM	3525	O	CYS	E	278	19.030	15.215	3.795	1.00	51.89	O
ATOM	3526	CB	CYS	E	278	16.724	14.348	6.236	1.00	53.29	C
ATOM	3527	SG	CYS	E	278	17.895	15.211	7.281	1.00	55.00	S
ATOM	3528	N	TYR	E	279	16.958	16.078	3.841	1.00	51.43	N
ATOM	3529	CA	TYR	E	279	17.377	17.297	3.166	1.00	50.67	C
ATOM	3530	C	TYR	E	279	17.088	18.516	4.016	1.00	50.48	C
ATOM	3531	O	TYR	E	279	16.200	18.497	4.873	1.00	50.39	O
ATOM	3532	CB	TYR	E	279	16.710	17.427	1.808	1.00	49.77	C
ATOM	3533	CG	TYR	E	279	16.767	16.166	0.992	1.00	49.15	C
ATOM	3534	CD1	TYR	E	279	15.677	15.297	0.949	1.00	49.68	C
ATOM	3535	CD2	TYR	E	279	17.908	15.833	0.263	1.00	47.43	C
ATOM	3536	CE1	TYR	E	279	15.720	14.133	0.199	1.00	49.48	C
ATOM	3537	CE2	TYR	E	279	17.963	14.679	-0.490	1.00	47.14	C
ATOM	3538	CZ	TYR	E	279	16.867	13.837	-0.514	1.00	49.36	C
ATOM	3539	OH	TYR	E	279	16.906	12.696	-1.262	1.00	51.09	O
ATOM	3540	N	LEU	E	280	17.862	19.570	3.759	1.00	50.11	N
ATOM	3541	CA	LEU	E	280	17.778	20.837	4.470	1.00	49.41	C
ATOM	3542	C	LEU	E	280	16.391	21.447	4.461	1.00	48.44	C
ATOM	3543	O	LEU	E	280	16.066	22.233	5.339	1.00	48.50	O
ATOM	3544	CB	LEU	E	280	18.714	21.844	3.808	1.00	50.25	C
ATOM	3545	CG	LEU	E	280	20.053	22.258	4.403	1.00	51.63	C
ATOM	3546	CD1	LEU	E	280	20.671	23.275	3.448	1.00	54.31	C
ATOM	3547	CD2	LEU	E	280	19.836	22.904	5.753	1.00	54.18	C
ATOM	3548	N	HIS	E	281	15.587	21.099	3.464	1.00	47.13	N

Figure 2

Table 2b - 54

ATOM	3549	CA	HIS	E	281	14.347	21.819	3.189	1.00	46.50	C
ATOM	3550	C	HIS	E	281	13.119	21.045	3.605	1.00	46.44	C
ATOM	3551	O	HIS	E	281	12.000	21.491	3.395	1.00	46.69	O
ATOM	3552	CB	HIS	E	281	14.261	22.191	1.710	1.00	45.78	C
ATOM	3553	CG	HIS	E	281	15.339	23.121	1.275	1.00	45.10	C
ATOM	3554	ND1	HIS	E	281	15.211	24.492	1.346	1.00	45.80	N
ATOM	3555	CD2	HIS	E	281	16.578	22.883	0.787	1.00	45.09	C
ATOM	3556	CE1	HIS	E	281	16.320	25.059	0.902	1.00	44.98	C
ATOM	3557	NE2	HIS	E	281	17.163	24.106	0.550	1.00	44.73	N
ATOM	3558	N	GLU	E	282	13.338	19.874	4.181	1.00	46.74	N
ATOM	3559	CA	GLU	E	282	12.271	19.109	4.835	1.00	47.05	C
ATOM	3560	C	GLU	E	282	11.728	19.833	6.077	1.00	46.92	C
ATOM	3561	O	GLU	E	282	12.497	20.463	6.823	1.00	47.15	O
ATOM	3562	CB	GLU	E	282	12.773	17.704	5.208	1.00	46.84	C
ATOM	3563	CG	GLU	E	282	13.419	16.953	4.046	1.00	47.40	C
ATOM	3564	CD	GLU	E	282	13.151	15.466	4.077	1.00	48.22	C
ATOM	3565	OE1	GLU	E	282	11.975	15.071	3.895	1.00	47.05	O
ATOM	3566	OE2	GLU	E	282	14.127	14.699	4.262	1.00	48.14	O
ATOM	3567	N	THR	E	283	10.410	19.755	6.285	1.00	46.22	N
ATOM	3568	CA	THR	E	283	9.797	20.325	7.478	1.00	45.47	C
ATOM	3569	C	THR	E	283	10.248	19.524	8.697	1.00	45.85	C
ATOM	3570	O	THR	E	283	10.517	18.321	8.590	1.00	45.63	O
ATOM	3571	CB	THR	E	283	8.253	20.266	7.463	1.00	45.70	C
ATOM	3572	OG1	THR	E	283	7.827	18.896	7.602	1.00	45.26	O
ATOM	3573	CG2	THR	E	283	7.637	20.943	6.213	1.00	42.82	C
ATOM	3574	N	LEU	E	284	10.300	20.208	9.843	1.00	45.49	N
ATOM	3575	CA	LEU	E	284	10.614	19.626	11.121	1.00	45.63	C
ATOM	3576	C	LEU	E	284	9.720	18.426	11.384	1.00	46.45	C
ATOM	3577	O	LEU	E	284	10.190	17.379	11.858	1.00	46.36	O
ATOM	3578	CB	LEU	E	284	10.365	20.638	12.227	1.00	45.76	C
ATOM	3579	CG	LEU	E	284	11.319	20.752	13.417	1.00	46.04	C
ATOM	3580	CD1	LEU	E	284	10.526	21.082	14.663	1.00	45.22	C
ATOM	3581	CD2	LEU	E	284	12.192	19.535	13.635	1.00	45.84	C
ATOM	3582	N	GLU	E	285	8.432	18.583	11.091	1.00	46.62	N
ATOM	3583	CA	GLU	E	285	7.487	17.498	11.281	1.00	47.45	C
ATOM	3584	C	GLU	E	285	7.921	16.235	10.518	1.00	47.71	C
ATOM	3585	O	GLU	E	285	7.885	15.125	11.078	1.00	48.05	O
ATOM	3586	CB	GLU	E	285	6.072	17.929	10.886	1.00	47.51	C
ATOM	3587	CG	GLU	E	285	5.109	16.779	10.696	1.00	48.86	C
ATOM	3588	CD	GLU	E	285	3.666	17.207	10.777	1.00	50.83	C
ATOM	3589	OE1	GLU	E	285	3.208	17.965	9.905	1.00	51.41	O
ATOM	3590	OE2	GLU	E	285	2.980	16.771	11.719	1.00	53.40	O
ATOM	3591	N	ALA	E	286	8.340	16.405	9.262	1.00	47.35	N
ATOM	3592	CA	ALA	E	286	8.777	15.267	8.453	1.00	47.33	C
ATOM	3593	C	ALA	E	286	10.007	14.589	9.062	1.00	47.22	C
ATOM	3594	O	ALA	E	286	10.112	13.367	9.057	1.00	47.54	O
ATOM	3595	CB	ALA	E	286	9.034	15.682	6.990	1.00	46.49	C
ATOM	3596	N	ILE	E	287	10.926	15.391	9.584	1.00	47.27	N
ATOM	3597	CA	ILE	E	287	12.151	14.876	10.177	1.00	47.30	C
ATOM	3598	C	ILE	E	287	11.876	14.155	11.498	1.00	47.01	C
ATOM	3599	O	ILE	E	287	12.473	13.119	11.756	1.00	47.36	O
ATOM	3600	CB	ILE	E	287	13.214	16.002	10.373	1.00	47.66	C
ATOM	3601	CG1	ILE	E	287	14.004	16.228	9.092	1.00	47.91	C
ATOM	3602	CG2	ILE	E	287	14.246	15.621	11.428	1.00	47.84	C
ATOM	3603	CD1	ILE	E	287	13.381	17.159	8.198	1.00	50.35	C
ATOM	3604	N	ILE	E	288	10.977	14.689	12.323	1.00	46.51	N
ATOM	3605	CA	ILE	E	288	10.692	14.067	13.599	1.00	46.68	C
ATOM	3606	C	ILE	E	288	10.124	12.675	13.331	1.00	46.80	C
ATOM	3607	O	ILE	E	288	10.584	11.686	13.915	1.00	46.74	O
ATOM	3608	CB	ILE	E	288	9.741	14.910	14.490	1.00	46.74	C
ATOM	3609	CG1	ILE	E	288	10.504	16.040	15.165	1.00	46.38	C
ATOM	3610	CG2	ILE	E	288	9.081	14.025	15.586	1.00	47.26	C
ATOM	3611	CD1	ILE	E	288	9.605	17.077	15.834	1.00	46.13	C
ATOM	3612	N	ASN	E	289	9.153	12.607	12.419	1.00	46.58	N
ATOM	3613	CA	ASN	E	289	8.528	11.345	12.037	1.00	46.10	C
ATOM	3614	C	ASN	E	289	9.527	10.341	11.496	1.00	46.18	C
ATOM	3615	O	ASN	E	289	9.457	9.152	11.834	1.00	47.03	O

Figure 2 Table 2b - 55

ATOM	3616	CB	ASN	E	289	7.409	11.563	11.018	1.00 45.83	C
ATOM	3617	CG	ASN	E	289	6.251	12.360	11.579	1.00 45.68	C
ATOM	3618	OD1	ASN	E	289	6.247	12.747	12.747	1.00 47.36	O
ATOM	3619	ND2	ASN	E	289	5.262	12.617	10.744	1.00 44.74	N
ATOM	3620	N	ARG	E	290	10.463	10.787	10.673	1.00 45.75	N
ATOM	3621	CA	ARG	E	290	11.428	9.834	10.125	1.00 46.23	C
ATOM	3622	C	ARG	E	290	12.309	9.247	11.235	1.00 46.21	C
ATOM	3623	O	ARG	E	290	12.488	8.028	11.326	1.00 46.13	O
ATOM	3624	CB	ARG	E	290	12.273	10.461	9.020	1.00 45.73	C
ATOM	3625	CG	ARG	E	290	13.087	9.450	8.255	1.00 46.13	C
ATOM	3626	CD	ARG	E	290	13.665	10.023	6.976	1.00 48.12	C
ATOM	3627	NE	ARG	E	290	12.669	10.827	6.267	1.00 49.09	N
ATOM	3628	CZ	ARG	E	290	12.944	11.961	5.637	1.00 47.59	C
ATOM	3629	NH1	ARG	E	290	14.190	12.411	5.603	1.00 47.17	N
ATOM	3630	NH2	ARG	E	290	11.974	12.634	5.035	1.00 47.48	N
ATOM	3631	N	LEU	E	291	12.827	10.139	12.072	1.00 46.50	N
ATOM	3632	CA	LEU	E	291	13.654	9.812	13.224	1.00 47.02	C
ATOM	3633	C	LEU	E	291	12.959	8.891	14.230	1.00 47.36	C
ATOM	3634	O	LEU	E	291	13.494	7.839	14.600	1.00 47.22	O
ATOM	3635	CB	LEU	E	291	13.987	11.108	13.910	1.00 47.39	C
ATOM	3636	CG	LEU	E	291	15.439	11.461	14.170	1.00 48.27	C
ATOM	3637	CD1	LEU	E	291	16.391	10.519	13.489	1.00 48.19	C
ATOM	3638	CD2	LEU	E	291	15.599	12.865	13.693	1.00 47.17	C
ATOM	3639	N	VAL	E	292	11.763	9.285	14.665	1.00 47.58	N
ATOM	3640	CA	VAL	E	292	10.968	8.456	15.558	1.00 47.75	C
ATOM	3641	C	VAL	E	292	10.738	7.054	14.983	1.00 48.82	C
ATOM	3642	O	VAL	E	292	11.035	6.053	15.658	1.00 49.58	O
ATOM	3643	CB	VAL	E	292	9.621	9.114	15.926	1.00 47.71	C
ATOM	3644	CG1	VAL	E	292	8.664	8.083	16.574	1.00 47.02	C
ATOM	3645	CG2	VAL	E	292	9.841	10.315	16.839	1.00 46.08	C
ATOM	3646	N	GLU	E	293	10.226	6.942	13.758	1.00 49.39	N
ATOM	3647	CA	GLU	E	293	9.945	5.579	13.260	1.00 50.34	C
ATOM	3648	C	GLU	E	293	11.167	4.759	12.830	1.00 50.02	C
ATOM	3649	O	GLU	E	293	11.086	3.545	12.785	1.00 50.30	O
ATOM	3650	CB	GLU	E	293	8.787	5.508	12.248	1.00 50.49	C
ATOM	3651	CG	GLU	E	293	9.073	5.985	10.853	1.00 52.18	C
ATOM	3652	CD	GLU	E	293	7.812	6.506	10.169	1.00 55.53	C
ATOM	3653	OE1	GLU	E	293	6.884	5.703	9.921	1.00 56.47	O
ATOM	3654	OE2	GLU	E	293	7.747	7.725	9.880	1.00 58.34	O
ATOM	3655	N	ALA	E	294	12.291	5.419	12.564	1.00 50.12	N
ATOM	3656	CA	ALA	E	294	13.541	4.728	12.247	1.00 50.04	C
ATOM	3657	C	ALA	E	294	14.304	4.325	13.499	1.00 50.19	C
ATOM	3658	O	ALA	E	294	15.220	3.504	13.430	1.00 50.23	O
ATOM	3659	CB	ALA	E	294	14.422	5.584	11.355	1.00 49.99	C
ATOM	3660	N	GLU	E	295	13.939	4.912	14.638	1.00 50.47	N
ATOM	3661	CA	GLU	E	295	14.509	4.524	15.943	1.00 51.14	C
ATOM	3662	C	GLU	E	295	16.035	4.670	15.979	1.00 50.80	C
ATOM	3663	O	GLU	E	295	16.747	3.800	16.508	1.00 50.31	O
ATOM	3664	CB	GLU	E	295	14.064	3.102	16.350	1.00 50.87	C
ATOM	3665	CG	GLU	E	295	12.636	3.045	16.854	1.00 52.32	C
ATOM	3666	CD	GLU	E	295	12.045	1.648	16.878	1.00 53.88	C
ATOM	3667	OE1	GLU	E	295	11.033	1.450	16.173	1.00 57.28	O
ATOM	3668	OE2	GLU	E	295	12.561	0.751	17.594	1.00 55.29	O
ATOM	3669	N	VAL	E	296	16.514	5.790	15.428	1.00 50.73	N
ATOM	3670	CA	VAL	E	296	17.942	6.060	15.300	1.00 50.80	C
ATOM	3671	C	VAL	E	296	18.309	7.451	15.861	1.00 51.09	C
ATOM	3672	O	VAL	E	296	17.440	8.324	15.994	1.00 50.79	O
ATOM	3673	CB	VAL	E	296	18.378	5.818	13.826	1.00 51.07	C
ATOM	3674	CG1	VAL	E	296	18.652	7.118	13.057	1.00 51.38	C
ATOM	3675	CG2	VAL	E	296	19.554	4.866	13.772	1.00 51.61	C
ATOM	3676	N	HIS	E	297	19.580	7.659	16.198	1.00 51.40	N
ATOM	3677	CA	HIS	E	297	19.981	8.864	16.936	1.00 51.96	C
ATOM	3678	C	HIS	E	297	20.108	10.118	16.065	1.00 51.51	C
ATOM	3679	O	HIS	E	297	19.934	11.240	16.562	1.00 51.60	O
ATOM	3680	CB	HIS	E	297	21.258	8.613	17.760	1.00 52.83	C
ATOM	3681	CG	HIS	E	297	21.549	9.669	18.790	1.00 56.27	C
ATOM	3682	ND1	HIS	E	297	21.204	9.536	20.118	1.00 59.52	N

Figure 2

Table 2b - 56

ATOM	3683	CD2	HIS	E	297	22.174	10.870	18.687	1.00	60.02	C
ATOM	3684	CE1	HIS	E	297	21.592	10.608	20.789	1.00	60.86	C
ATOM	3685	NE2	HIS	E	297	22.172	11.441	19.940	1.00	62.13	N
ATOM	3686	N	ARG	E	298	20.388	9.947	14.770	1.00	51.03	N
ATOM	3687	CA	ARG	E	298	20.523	11.093	13.861	1.00	49.96	C
ATOM	3688	C	ARG	E	298	20.276	10.749	12.401	1.00	49.63	C
ATOM	3689	O	ARG	E	298	20.413	9.592	11.998	1.00	49.05	O
ATOM	3690	CB	ARG	E	298	21.914	11.730	13.984	1.00	50.13	C
ATOM	3691	CG	ARG	E	298	22.999	11.176	13.025	1.00	50.42	C
ATOM	3692	CD	ARG	E	298	23.444	9.778	13.406	1.00	49.93	C
ATOM	3693	NE	ARG	E	298	24.034	9.727	14.740	1.00	48.60	N
ATOM	3694	CZ	ARG	E	298	23.982	8.667	15.538	1.00	48.39	C
ATOM	3695	NH1	ARG	E	298	23.352	7.566	15.149	1.00	48.66	N
ATOM	3696	NH2	ARG	E	298	24.551	8.710	16.734	1.00	48.38	N
ATOM	3697	N	LEU	E	299	19.932	11.779	11.624	1.00	48.86	N
ATOM	3698	CA	LEU	E	299	19.881	11.707	10.177	1.00	48.46	C
ATOM	3699	C	LEU	E	299	21.089	12.402	9.596	1.00	48.26	C
ATOM	3700	O	LEU	E	299	21.519	13.457	10.099	1.00	48.43	O
ATOM	3701	CB	LEU	E	299	18.623	12.386	9.653	1.00	48.36	C
ATOM	3702	CG	LEU	E	299	17.288	11.873	10.208	1.00	49.92	C
ATOM	3703	CD1	LEU	E	299	16.107	12.686	9.627	1.00	50.64	C
ATOM	3704	CD2	LEU	E	299	17.097	10.351	9.972	1.00	47.67	C
ATOM	3705	N	VAL	E	300	21.635	11.839	8.527	1.00	47.88	N
ATOM	3706	CA	VAL	E	300	22.658	12.557	7.778	1.00	47.99	C
ATOM	3707	C	VAL	E	300	22.004	13.504	6.771	1.00	48.44	C
ATOM	3708	O	VAL	E	300	21.251	13.052	5.898	1.00	48.92	O
ATOM	3709	CB	VAL	E	300	23.601	11.613	7.035	1.00	48.12	C
ATOM	3710	CG1	VAL	E	300	24.707	12.426	6.355	1.00	46.33	C
ATOM	3711	CG2	VAL	E	300	24.184	10.545	8.008	1.00	47.73	C
ATOM	3712	N	VAL	E	301	22.285	14.805	6.897	1.00	48.27	N
ATOM	3713	CA	VAL	E	301	21.740	15.809	5.973	1.00	48.25	C
ATOM	3714	C	VAL	E	301	22.506	15.814	4.653	1.00	48.67	C
ATOM	3715	O	VAL	E	301	23.737	15.890	4.617	1.00	48.63	O
ATOM	3716	CB	VAL	E	301	21.696	17.248	6.577	1.00	48.23	C
ATOM	3717	CG1	VAL	E	301	21.026	18.195	5.607	1.00	45.77	C
ATOM	3718	CG2	VAL	E	301	20.949	17.242	7.905	1.00	47.42	C
ATOM	3719	N	VAL	E	302	21.770	15.765	3.562	1.00	49.07	N
ATOM	3720	CA	VAL	E	302	22.385	15.469	2.288	1.00	50.09	C
ATOM	3721	C	VAL	E	302	21.908	16.453	1.208	1.00	51.03	C
ATOM	3722	O	VAL	E	302	20.906	17.145	1.401	1.00	51.28	O
ATOM	3723	CB	VAL	E	302	22.151	13.935	1.991	1.00	50.34	C
ATOM	3724	CG1	VAL	E	302	21.350	13.666	0.741	1.00	48.65	C
ATOM	3725	CG2	VAL	E	302	23.467	13.157	2.073	1.00	49.71	C
ATOM	3726	N	ASP	E	303	22.627	16.562	0.096	1.00	51.91	N
ATOM	3727	CA	ASP	E	303	22.140	17.420	-0.999	1.00	52.81	C
ATOM	3728	C	ASP	E	303	21.538	16.559	-2.114	1.00	53.43	C
ATOM	3729	O	ASP	E	303	21.411	15.342	-1.943	1.00	53.45	O
ATOM	3730	CB	ASP	E	303	23.235	18.358	-1.519	1.00	52.44	C
ATOM	3731	CG	ASP	E	303	24.237	17.657	-2.422	1.00	53.62	C
ATOM	3732	OD1	ASP	E	303	24.327	16.407	-2.407	1.00	54.96	O
ATOM	3733	OD2	ASP	E	303	24.938	18.367	-3.170	1.00	55.99	O
ATOM	3734	N	GLU	E	304	21.178	17.192	-3.238	1.00	53.82	N
ATOM	3735	CA	GLU	E	304	20.595	16.516	-4.407	1.00	54.69	C
ATOM	3736	C	GLU	E	304	21.377	15.274	-4.827	1.00	54.73	C
ATOM	3737	O	GLU	E	304	20.811	14.325	-5.374	1.00	54.60	O
ATOM	3738	CB	GLU	E	304	20.542	17.473	-5.612	1.00	54.94	C
ATOM	3739	CG	GLU	E	304	19.590	18.654	-5.476	1.00	57.00	C
ATOM	3740	CD	GLU	E	304	20.103	19.769	-4.560	1.00	60.59	C
ATOM	3741	OE1	GLU	E	304	21.189	19.623	-3.944	1.00	60.96	O
ATOM	3742	OE2	GLU	E	304	19.402	20.803	-4.452	1.00	62.16	O
ATOM	3743	N	HIS	E	305	22.681	15.297	-4.570	1.00	54.97	N
ATOM	3744	CA	HIS	E	305	23.590	14.294	-5.090	1.00	55.17	C
ATOM	3745	C	HIS	E	305	24.182	13.405	-3.994	1.00	55.27	C
ATOM	3746	O	HIS	E	305	25.147	12.685	-4.245	1.00	55.56	O
ATOM	3747	CB	HIS	E	305	24.713	14.970	-5.882	1.00	55.12	C
ATOM	3748	CG	HIS	E	305	24.229	15.928	-6.925	1.00	55.67	C
ATOM	3749	ND1	HIS	E	305	23.738	15.517	-8.145	1.00	55.98	N

Figure 2 Table 2b - 57

ATOM	3750	CD2	HIS	E	305	24.176	17.282	-6.936	1.00	56.40	C
ATOM	3751	CE1	HIS	E	305	23.396	16.576	-8.860	1.00	56.13	C
ATOM	3752	NE2	HIS	E	305	23.655	17.660	-8.150	1.00	55.33	N
ATOM	3753	N	ASP	E	306	23.601	13.451	-2.795	1.00	55.11	N
ATOM	3754	CA	ASP	E	306	24.036	12.616	-1.654	1.00	55.20	C
ATOM	3755	C	ASP	E	306	25.344	13.041	-0.980	1.00	54.31	C
ATOM	3756	O	ASP	E	306	25.879	12.317	-0.140	1.00	53.92	O
ATOM	3757	CB	ASP	E	306	24.118	11.132	-2.038	1.00	55.96	C
ATOM	3758	CG	ASP	E	306	22.804	10.399	-1.838	1.00	58.61	C
ATOM	3759	OD1	ASP	E	306	21.824	11.020	-1.344	1.00	60.37	O
ATOM	3760	OD2	ASP	E	306	22.759	9.190	-2.177	1.00	60.63	O
ATOM	3761	N	VAL	E	307	25.853	14.208	-1.362	1.00	53.28	N
ATOM	3762	CA	VAL	E	307	27.011	14.803	-0.707	1.00	52.47	C
ATOM	3763	C	VAL	E	307	26.553	15.298	0.671	1.00	52.00	C
ATOM	3764	O	VAL	E	307	25.455	15.857	0.796	1.00	51.71	O
ATOM	3765	CB	VAL	E	307	27.609	15.956	-1.581	1.00	52.35	C
ATOM	3766	CG1	VAL	E	307	28.858	16.557	-0.943	1.00	51.59	C
ATOM	3767	CG2	VAL	E	307	27.944	15.437	-2.963	1.00	51.61	C
ATOM	3768	N	VAL	E	308	27.362	15.077	1.707	1.00	51.50	N
ATOM	3769	CA	VAL	E	308	26.900	15.445	3.049	1.00	51.51	C
ATOM	3770	C	VAL	E	308	27.046	16.947	3.326	1.00	51.52	C
ATOM	3771	O	VAL	E	308	28.096	17.553	3.109	1.00	51.23	O
ATOM	3772	CB	VAL	E	308	27.444	14.533	4.234	1.00	51.25	C
ATOM	3773	CG1	VAL	E	308	27.992	13.209	3.738	1.00	50.90	C
ATOM	3774	CG2	VAL	E	308	28.470	15.240	5.062	1.00	51.22	C
ATOM	3775	N	LYS	E	309	25.955	17.527	3.801	1.00	51.58	N
ATOM	3776	CA	LYS	E	309	25.870	18.939	4.079	1.00	52.09	C
ATOM	3777	C	LYS	E	309	25.727	19.189	5.581	1.00	51.75	C
ATOM	3778	O	LYS	E	309	25.949	20.291	6.063	1.00	52.03	O
ATOM	3779	CB	LYS	E	309	24.708	19.540	3.292	1.00	52.34	C
ATOM	3780	CG	LYS	E	309	25.088	19.926	1.846	1.00	55.69	C
ATOM	3781	CD	LYS	E	309	24.001	20.821	1.239	1.00	60.80	C
ATOM	3782	CE	LYS	E	309	24.582	21.962	0.418	1.00	63.93	C
ATOM	3783	NZ	LYS	E	309	23.556	23.028	0.177	1.00	66.33	N
ATOM	3784	N	GLY	E	310	25.363	18.159	6.326	1.00	51.19	N
ATOM	3785	CA	GLY	E	310	25.322	18.266	7.777	1.00	50.64	C
ATOM	3786	C	GLY	E	310	24.718	17.073	8.503	1.00	50.03	C
ATOM	3787	O	GLY	E	310	24.603	15.974	7.954	1.00	49.11	O
ATOM	3788	N	ILE	E	311	24.310	17.327	9.740	1.00	49.83	N
ATOM	3789	CA	ILE	E	311	23.724	16.322	10.603	1.00	49.68	C
ATOM	3790	C	ILE	E	311	22.608	16.890	11.465	1.00	49.52	C
ATOM	3791	O	ILE	E	311	22.683	18.027	11.937	1.00	49.18	O
ATOM	3792	CB	ILE	E	311	24.819	15.610	11.447	1.00	49.80	C
ATOM	3793	CG1	ILE	E	311	25.287	14.368	10.671	1.00	50.44	C
ATOM	3794	CG2	ILE	E	311	24.271	15.146	12.792	1.00	49.61	C
ATOM	3795	CD1	ILE	E	311	26.755	14.138	10.680	1.00	51.29	C
ATOM	3796	N	VAL	E	312	21.557	16.096	11.637	1.00	49.81	N
ATOM	3797	CA	VAL	E	312	20.483	16.448	12.541	1.00	50.02	C
ATOM	3798	C	VAL	E	312	20.254	15.318	13.523	1.00	50.32	C
ATOM	3799	O	VAL	E	312	19.833	14.227	13.157	1.00	50.31	O
ATOM	3800	CB	VAL	E	312	19.191	16.872	11.803	1.00	49.73	C
ATOM	3801	CG1	VAL	E	312	18.697	15.778	10.889	1.00	49.87	C
ATOM	3802	CG2	VAL	E	312	18.119	17.267	12.805	1.00	49.34	C
ATOM	3803	N	SER	E	313	20.545	15.610	14.779	1.00	50.71	N
ATOM	3804	CA	SER	E	313	20.549	14.633	15.855	1.00	50.96	C
ATOM	3805	C	SER	E	313	19.328	14.836	16.738	1.00	50.69	C
ATOM	3806	O	SER	E	313	18.660	15.868	16.643	1.00	51.04	O
ATOM	3807	CB	SER	E	313	21.841	14.805	16.641	1.00	50.92	C
ATOM	3808	OG	SER	E	313	21.707	14.433	18.001	1.00	56.14	O
ATOM	3809	N	LEU	E	314	19.017	13.847	17.579	1.00	50.58	N
ATOM	3810	CA	LEU	E	314	17.951	13.985	18.573	1.00	50.35	C
ATOM	3811	C	LEU	E	314	18.184	15.171	19.529	1.00	50.50	C
ATOM	3812	O	LEU	E	314	17.242	15.890	19.862	1.00	50.22	O
ATOM	3813	CB	LEU	E	314	17.775	12.688	19.370	1.00	50.54	C
ATOM	3814	CG	LEU	E	314	17.397	11.451	18.554	1.00	50.17	C
ATOM	3815	CD1	LEU	E	314	17.566	10.184	19.387	1.00	48.90	C
ATOM	3816	CD2	LEU	E	314	15.987	11.569	17.982	1.00	48.35	C

Figure 2 Table 2b - 58

ATOM	3817	N	SER	E	315	19.430	15.374	19.958	1.00	50.44	N
ATOM	3818	CA	SER	E	315	19.777	16.527	20.784	1.00	50.95	C
ATOM	3819	C	SER	E	315	19.352	17.836	20.085	1.00	51.51	C
ATOM	3820	O	SER	E	315	18.763	18.725	20.726	1.00	51.90	O
ATOM	3821	CB	SER	E	315	21.278	16.571	21.082	1.00	50.75	C
ATOM	3822	OG	SER	E	315	21.849	15.280	21.171	1.00	51.46	O
ATOM	3823	N	ASP	E	316	19.641	17.954	18.783	1.00	50.93	N
ATOM	3824	CA	ASP	E	316	19.266	19.140	18.030	1.00	50.31	C
ATOM	3825	C	ASP	E	316	17.763	19.392	18.149	1.00	50.45	C
ATOM	3826	O	ASP	E	316	17.338	20.490	18.504	1.00	51.02	O
ATOM	3827	CB	ASP	E	316	19.658	18.993	16.564	1.00	50.05	C
ATOM	3828	CG	ASP	E	316	21.155	19.008	16.354	1.00	49.54	C
ATOM	3829	OD1	ASP	E	316	21.839	19.824	17.022	1.00	48.22	O
ATOM	3830	OD2	ASP	E	316	21.640	18.215	15.501	1.00	46.29	O
ATOM	3831	N	ILE	E	317	16.969	18.367	17.873	1.00	50.11	N
ATOM	3832	CA	ILE	E	317	15.516	18.461	17.954	1.00	49.97	C
ATOM	3833	C	ILE	E	317	14.979	18.776	19.359	1.00	50.22	C
ATOM	3834	O	ILE	E	317	14.139	19.666	19.521	1.00	50.16	O
ATOM	3835	CB	ILE	E	317	14.869	17.189	17.394	1.00	49.55	C
ATOM	3836	CG1	ILE	E	317	15.122	17.118	15.891	1.00	50.65	C
ATOM	3837	CG2	ILE	E	317	13.378	17.175	17.649	1.00	49.39	C
ATOM	3838	CD1	ILE	E	317	14.637	15.849	15.278	1.00	53.53	C
ATOM	3839	N	LEU	E	318	15.445	18.045	20.370	1.00	50.34	N
ATOM	3840	CA	LEU	E	318	14.978	18.258	21.726	1.00	50.53	C
ATOM	3841	C	LEU	E	318	15.407	19.624	22.251	1.00	50.98	C
ATOM	3842	O	LEU	E	318	14.666	20.278	22.988	1.00	50.55	O
ATOM	3843	CB	LEU	E	318	15.441	17.124	22.657	1.00	50.81	C
ATOM	3844	CG	LEU	E	318	14.420	16.042	23.035	1.00	49.65	C
ATOM	3845	CD1	LEU	E	318	13.861	15.329	21.834	1.00	49.65	C
ATOM	3846	CD2	LEU	E	318	15.067	15.048	23.948	1.00	51.07	C
ATOM	3847	N	GLN	E	319	16.597	20.058	21.854	1.00	51.88	N
ATOM	3848	CA	GLN	E	319	17.039	21.421	22.138	1.00	52.99	C
ATOM	3849	C	GLN	E	319	16.135	22.450	21.464	1.00	53.18	C
ATOM	3850	O	GLN	E	319	15.858	23.504	22.027	1.00	52.92	O
ATOM	3851	CB	GLN	E	319	18.485	21.644	21.712	1.00	52.98	C
ATOM	3852	CG	GLN	E	319	18.844	23.110	21.658	1.00	54.89	C
ATOM	3853	CD	GLN	E	319	20.210	23.395	22.196	1.00	57.49	C
ATOM	3854	OE1	GLN	E	319	21.216	23.092	21.554	1.00	59.49	O
ATOM	3855	NE2	GLN	E	319	20.262	23.989	23.386	1.00	57.51	N
ATOM	3856	N	ALA	E	320	15.679	22.139	20.260	1.00	54.15	N
ATOM	3857	CA	ALA	E	320	14.788	23.042	19.542	1.00	55.43	C
ATOM	3858	C	ALA	E	320	13.426	23.090	20.216	1.00	56.22	C
ATOM	3859	O	ALA	E	320	12.901	24.176	20.482	1.00	56.39	O
ATOM	3860	CB	ALA	E	320	14.649	22.627	18.091	1.00	55.26	C
ATOM	3861	N	LEU	E	321	12.883	21.911	20.517	1.00	56.95	N
ATOM	3862	CA	LEU	E	321	11.547	21.776	21.097	1.00	57.76	C
ATOM	3863	C	LEU	E	321	11.406	22.377	22.487	1.00	58.65	C
ATOM	3864	O	LEU	E	321	10.303	22.725	22.899	1.00	58.42	O
ATOM	3865	CB	LEU	E	321	11.129	20.300	21.128	1.00	57.56	C
ATOM	3866	CG	LEU	E	321	10.893	19.610	19.785	1.00	56.11	C
ATOM	3867	CD1	LEU	E	321	10.510	18.164	20.014	1.00	55.73	C
ATOM	3868	CD2	LEU	E	321	9.822	20.340	18.981	1.00	55.27	C
ATOM	3869	N	VAL	E	322	12.524	22.503	23.195	1.00	60.36	N
ATOM	3870	CA	VAL	E	322	12.515	22.961	24.584	1.00	62.18	C
ATOM	3871	C	VAL	E	322	12.807	24.453	24.729	1.00	63.77	C
ATOM	3872	O	VAL	E	322	12.295	25.105	25.638	1.00	63.77	O
ATOM	3873	CB	VAL	E	322	13.479	22.122	25.465	1.00	61.90	C
ATOM	3874	CG1	VAL	E	322	14.840	22.795	25.613	1.00	61.88	C
ATOM	3875	CG2	VAL	E	322	12.866	21.876	26.818	1.00	61.72	C
ATOM	3876	N	LEU	E	323	13.634	24.993	23.840	1.00	65.89	N
ATOM	3877	CA	LEU	E	323	13.869	26.429	23.815	1.00	68.26	C
ATOM	3878	C	LEU	E	323	12.810	27.067	22.924	1.00	69.62	C
ATOM	3879	O	LEU	E	323	12.973	28.192	22.444	1.00	69.98	O
ATOM	3880	CB	LEU	E	323	15.288	26.745	23.322	1.00	68.38	C
ATOM	3881	CG	LEU	E	323	16.452	26.321	24.232	1.00	69.05	C
ATOM	3882	CD1	LEU	E	323	17.773	26.482	23.496	1.00	69.78	C
ATOM	3883	CD2	LEU	E	323	16.475	27.092	25.565	1.00	69.54	C

Figure 2

Table 2b - 59

ATOM	3884	N	THR E 324	11.716	26.323	22.743	1.00	71.25	N
ATOM	3885	CA	THR E 324	10.607	26.636	21.832	1.00	72.64	C
ATOM	3886	C	THR E 324	11.034	26.611	20.354	1.00	73.70	C
ATOM	3887	O	THR E 324	11.801	27.471	19.902	1.00	74.15	O
ATOM	3888	CB	THR E 324	9.850	27.933	22.216	1.00	72.72	C
ATOM	3889	OG1	THR E 324	9.495	27.887	23.611	1.00	72.87	O
ATOM	3890	CG2	THR E 324	8.585	28.092	21.358	1.00	72.69	C
ATOM	3891	N	GLY E 325	10.533	25.607	19.628	1.00	74.51	N
ATOM	3892	CA	GLY E 325	10.859	25.345	18.211	1.00	75.48	C
ATOM	3893	C	GLY E 325	11.694	26.351	17.422	1.00	76.05	C
ATOM	3894	O	GLY E 325	11.273	27.500	17.213	1.00	76.15	O
ATOM	3895	N	GLY E 326	12.875	25.901	16.989	1.00	76.49	N
ATOM	3896	CA	GLY E 326	13.774	26.663	16.110	1.00	76.65	C
ATOM	3897	C	GLY E 326	14.191	28.027	16.628	1.00	76.89	C
ATOM	3898	O	GLY E 326	14.234	28.998	15.869	1.00	76.88	O
TER	3899		GLY E 326						
HETATM	3900	PG	ATP E1327	20.739	6.432	21.029	1.00	61.14	P
HETATM	3901	O1G	ATP E1327	19.739	5.671	22.054	1.00	59.79	O
HETATM	3902	O2G	ATP E1327	22.105	6.726	21.611	1.00	61.35	O
HETATM	3903	O3G	ATP E1327	19.919	7.578	20.497	1.00	62.12	O
HETATM	3904	PB	ATP E1327	21.675	4.014	19.943	1.00	58.29	P
HETATM	3905	O1B	ATP E1327	23.131	4.146	20.574	1.00	58.41	O
HETATM	3906	O2B	ATP E1327	20.757	3.008	20.794	1.00	58.14	O
HETATM	3907	O3B	ATP E1327	20.887	5.410	19.797	1.00	60.32	O
HETATM	3908	PA	ATP E1327	22.297	4.550	17.293	1.00	52.38	P
HETATM	3909	O1A	ATP E1327	23.430	5.430	17.756	1.00	52.86	O
HETATM	3910	O2A	ATP E1327	21.117	5.200	16.639	1.00	53.86	O
HETATM	3911	O3A	ATP E1327	21.729	3.555	18.418	1.00	55.80	O
HETATM	3912	O5'	ATP E1327	22.918	3.429	16.334	1.00	52.91	O
HETATM	3913	C5'	ATP E1327	22.368	2.110	16.281	1.00	51.23	C
HETATM	3914	C4'	ATP E1327	22.749	1.501	14.943	1.00	51.13	C
HETATM	3915	O4'	ATP E1327	22.093	2.259	13.923	1.00	51.11	O
HETATM	3916	C3'	ATP E1327	24.254	1.612	14.702	1.00	51.59	C
HETATM	3917	O3'	ATP E1327	24.819	0.339	14.333	1.00	51.81	O
HETATM	3918	C2'	ATP E1327	24.416	2.641	13.598	1.00	50.64	C
HETATM	3919	O2'	ATP E1327	25.397	2.257	12.631	1.00	51.06	O
HETATM	3920	C1'	ATP E1327	23.037	2.744	12.966	1.00	50.66	C
HETATM	3921	N9	ATP E1327	22.736	4.151	12.585	1.00	51.32	N
HETATM	3922	C8	ATP E1327	22.862	5.258	13.351	1.00	50.89	C
HETATM	3923	N7	ATP E1327	22.505	6.373	12.673	1.00	50.01	N
HETATM	3924	C5	ATP E1327	22.148	5.987	11.438	1.00	50.35	C
HETATM	3925	C6	ATP E1327	21.671	6.638	10.197	1.00	50.37	C
HETATM	3926	N6	ATP E1327	21.492	7.975	10.128	1.00	49.93	N
HETATM	3927	N1	ATP E1327	21.418	5.843	9.124	1.00	51.20	N
HETATM	3928	C2	ATP E1327	21.581	4.505	9.139	1.00	50.26	C
HETATM	3929	N3	ATP E1327	22.012	3.855	10.227	1.00	50.96	N
HETATM	3930	C4	ATP E1327	22.306	4.523	11.379	1.00	51.20	C
HETATM	3931	PG	ATP E1328	26.316	8.566	22.704	1.00	62.07	P
HETATM	3932	O1G	ATP E1328	26.290	7.039	22.169	1.00	61.46	O
HETATM	3933	O2G	ATP E1328	24.909	8.950	23.120	1.00	62.32	O
HETATM	3934	O3G	ATP E1328	27.043	9.374	21.653	1.00	63.76	O
HETATM	3935	PB	ATP E1328	26.894	7.836	25.399	1.00	53.88	P
HETATM	3936	O1B	ATP E1328	25.455	8.202	25.964	1.00	56.82	O
HETATM	3937	O2B	ATP E1328	26.965	6.242	25.185	1.00	57.08	O
HETATM	3938	O3B	ATP E1328	27.281	8.528	23.993	1.00	58.58	O
HETATM	3939	PA	ATP E1328	27.490	9.901	27.082	1.00	39.75	P
HETATM	3940	O1A	ATP E1328	26.483	9.609	28.146	1.00	42.39	O
HETATM	3941	O2A	ATP E1328	27.145	10.939	26.077	1.00	41.89	O
HETATM	3942	O3A	ATP E1328	27.928	8.485	26.425	1.00	47.83	O
HETATM	3943	O5'	ATP E1328	28.939	10.266	27.654	1.00	39.92	O
HETATM	3944	C5'	ATP E1328	29.257	11.485	28.305	1.00	36.14	C
HETATM	3945	C4'	ATP E1328	30.280	11.244	29.415	1.00	32.38	C
HETATM	3946	O4'	ATP E1328	29.680	11.629	30.645	1.00	31.07	O
HETATM	3947	C3'	ATP E1328	30.708	9.800	29.617	1.00	31.99	C
HETATM	3948	O3'	ATP E1328	32.076	9.780	30.042	1.00	33.91	O
HETATM	3949	C2'	ATP E1328	29.901	9.278	30.779	1.00	29.67	C
HETATM	3950	O2'	ATP E1328	30.693	8.453	31.641	1.00	29.29	O

Figure 2

Table 2b - 60

HETATM	3951	C1'	ATP	E1328	29.479	10.521	31.531	1.00 25.99 C
HETATM	3952	N9	ATP	E1328	28.038	10.433	31.843	1.00 23.39 N
HETATM	3953	C8	ATP	E1328	27.085	9.894	31.052	1.00 21.92 C
HETATM	3954	N7	ATP	E1328	25.871	9.995	31.641	1.00 21.67 N
HETATM	3955	C5	ATP	E1328	26.039	10.621	32.823	1.00 21.23 C
HETATM	3956	C6	ATP	E1328	25.176	11.064	33.941	1.00 21.80 C
HETATM	3957	N6	ATP	E1328	23.847	10.837	33.929	1.00 21.77 N
HETATM	3958	N1	ATP	E1328	25.755	11.686	34.996	1.00 22.26 N
HETATM	3959	C2	ATP	E1328	27.080	11.917	35.029	1.00 22.00 C
HETATM	3960	N3	ATP	E1328	27.921	11.555	34.042	1.00 21.28 N
HETATM	3961	C4	ATP	E1328	27.472	10.910	32.944	1.00 21.49 C
HETATM	3962	P	AMP	E1329	24.959	13.644	19.028	1.00 43.12 P
HETATM	3963	O1P	AMP	E1329	23.812	13.680	20.033	1.00 40.21 O
HETATM	3964	O2P	AMP	E1329	24.673	12.784	17.825	1.00 41.76 O
HETATM	3965	O3P	AMP	E1329	26.373	13.404	19.489	1.00 42.46 O
HETATM	3966	O5'	AMP	E1329	25.054	15.164	18.510	1.00 41.64 O
HETATM	3967	C5'	AMP	E1329	25.801	16.180	19.200	1.00 40.01 C
HETATM	3968	C4'	AMP	E1329	25.829	17.501	18.404	1.00 38.29 C
HETATM	3969	O4'	AMP	E1329	26.860	17.478	17.406	1.00 38.12 O
HETATM	3970	C3'	AMP	E1329	24.560	17.774	17.631	1.00 36.64 C
HETATM	3971	O3'	AMP	E1329	24.396	19.186	17.644	1.00 35.63 O
HETATM	3972	C2'	AMP	E1329	24.823	17.250	16.224	1.00 36.68 C
HETATM	3973	O2'	AMP	E1329	24.173	18.008	15.189	1.00 36.06 O
HETATM	3974	C1'	AMP	E1329	26.328	17.339	16.085	1.00 36.89 C
HETATM	3975	N9	AMP	E1329	26.942	16.166	15.400	1.00 36.84 N
HETATM	3976	C8	AMP	E1329	26.610	14.861	15.468	1.00 36.55 C
HETATM	3977	N7	AMP	E1329	27.420	14.091	14.691	1.00 35.44 N
HETATM	3978	C5	AMP	E1329	28.307	14.911	14.108	1.00 36.74 C
HETATM	3979	C6	AMP	E1329	29.450	14.795	13.168	1.00 36.94 C
HETATM	3980	N6	AMP	E1329	29.854	13.616	12.652	1.00 37.05 N
HETATM	3981	N1	AMP	E1329	30.101	15.926	12.822	1.00 38.01 N
HETATM	3982	C2	AMP	E1329	29.747	17.131	13.302	1.00 37.47 C
HETATM	3983	N3	AMP	E1329	28.728	17.314	14.148	1.00 36.79 N
HETATM	3984	C4	AMP	E1329	27.983	16.270	14.577	1.00 36.76 C
HETATM	3985	MG	MG	E1330	19.409	3.633	22.244	1.00 58.69 MG
HETATM	3986	MG	MG	E1331	26.614	5.347	23.333	1.00 60.65 MG
HETATM	3987	O	HOH	A2001	27.090	-22.781	64.105	1.00 34.08 O
HETATM	3988	O	HOH	A2002	7.532	-7.137	62.483	1.00 36.80 O
HETATM	3989	O	HOH	A2003	18.847	-22.478	63.361	1.00 39.07 O
HETATM	3990	O	HOH	A2004	18.503	-23.440	40.944	1.00 37.98 O
HETATM	3991	O	HOH	A2005	24.374	-36.590	59.330	1.00 26.71 O
HETATM	3992	O	HOH	A2006	27.166	-34.123	55.478	1.00 17.11 O
HETATM	3993	O	HOH	A2007	17.400	-31.983	59.134	1.00 52.09 O
HETATM	3994	O	HOH	A2008	23.400	-28.838	62.722	1.00 20.39 O
HETATM	3995	O	HOH	A2009	26.058	-31.370	55.433	1.00 21.50 O
HETATM	3996	O	HOH	A2010	24.532	-21.747	64.183	1.00 13.24 O
HETATM	3997	O	HOH	A2011	24.509	-4.399	61.134	1.00 20.22 O
HETATM	3998	O	HOH	A2012	22.991	-9.979	66.203	1.00 30.76 O
HETATM	3999	O	HOH	A2013	17.158	-8.555	67.535	1.00 31.24 O
HETATM	4000	O	HOH	A2014	16.336	-13.851	67.789	1.00 22.26 O
HETATM	4001	O	HOH	A2015	18.992	-10.854	66.684	1.00 18.02 O
HETATM	4002	O	HOH	A2016	9.809	-7.252	63.380	1.00 31.24 O
HETATM	4003	O	HOH	A2017	16.694	-23.047	62.210	1.00 40.33 O
HETATM	4004	O	HOH	A2018	15.584	-1.057	65.676	1.00 28.35 O
HETATM	4005	O	HOH	A2019	21.215	5.294	64.276	1.00 33.26 O
HETATM	4006	O	HOH	A2020	22.556	-3.943	62.456	1.00 24.02 O
HETATM	4007	O	HOH	A2021	12.729	-16.101	51.217	1.00 21.65 O
HETATM	4008	O	HOH	A2022	7.996	-20.883	55.217	1.00 7.81 O
HETATM	4009	O	HOH	A2023	16.517	-16.353	46.119	1.00 15.46 O
HETATM	4010	O	HOH	A2024	10.394	-17.864	49.448	1.00 26.01 O
HETATM	4011	O	HOH	A2025	7.567	-6.894	50.818	1.00 21.76 O
HETATM	4012	O	HOH	A2026	5.374	-2.774	50.752	1.00 42.53 O
HETATM	4013	O	HOH	A2027	2.027	-0.479	55.000	1.00 46.42 O
HETATM	4014	O	HOH	A2028	21.537	19.481	38.706	1.00 42.33 O
HETATM	4015	O	HOH	A2029	20.912	11.592	49.559	1.00 26.07 O
HETATM	4016	O	HOH	A2030	18.445	7.214	49.623	1.00 30.68 O
HETATM	4017	O	HOH	A2031	13.617	-2.866	46.979	1.00 46.91 O

Figure 2 Table 2b - 61

HETATM	4018	O	HOH A2032	14.762	-1.710	41.851	1.00 23.16	O
HETATM	4019	O	HOH A2033	33.931	-18.206	51.356	1.00 33.47	O
HETATM	4020	O	HOH B2001	3.240	-29.235	63.460	1.00 32.98	O
HETATM	4021	O	HOH B2002	8.437	-28.365	55.740	1.00 21.17	O
HETATM	4022	O	HOH B2003	6.780	-29.361	54.111	1.00 32.49	O
HETATM	4023	O	HOH B2004	1.796	-26.195	54.691	1.00 45.84	O
HETATM	4024	O	HOH B2005	-1.598	-30.301	55.944	1.00 38.03	O
HETATM	4025	O	HOH B2006	13.552	-29.361	62.165	1.00 34.93	O
HETATM	4026	O	HOH B2007	2.872	-23.533	36.593	1.00 60.08	O
HETATM	4027	O	HOH B2008	10.532	-24.076	38.707	1.00 28.81	O
HETATM	4028	O	HOH B2009	14.311	-18.097	24.320	1.00 63.32	O
HETATM	4029	O	HOH B2010	16.418	-11.265	27.557	1.00 53.65	O
HETATM	4030	O	HOH B2011	16.009	-8.949	25.729	1.00 40.65	O
HETATM	4031	O	HOH B2012	13.193	-11.372	41.603	1.00 14.43	O
HETATM	4032	O	HOH B2013	27.019	-14.939	39.961	1.00 25.35	O
HETATM	4033	O	HOH B2014	40.676	-14.034	40.715	1.00 26.46	O
HETATM	4034	O	HOH B2015	16.148	-12.557	36.308	1.00 29.23	O
HETATM	4035	O	HOH B2016	8.862	-4.834	44.335	1.00 19.80	O
HETATM	4036	O	HOH B2017	5.730	1.712	44.688	1.00 24.39	O
HETATM	4037	O	HOH B2018	10.481	-0.194	39.072	1.00 20.07	O
HETATM	4038	O	HOH B2019	10.414	-0.574	33.957	1.00 17.34	O
HETATM	4039	O	HOH B2020	14.938	-4.056	40.618	1.00 12.58	O
HETATM	4040	O	HOH B2021	16.998	-0.876	40.679	1.00 15.92	O
HETATM	4041	O	HOH B2022	27.364	-11.729	31.514	1.00 32.80	O
HETATM	4042	O	HOH B2023	29.619	-5.645	49.468	1.00 46.59	O
HETATM	4043	O	HOH B2024	32.854	-7.000	45.355	1.00 35.12	O
HETATM	4044	O	HOH B2025	3.943	-26.365	53.348	1.00 26.45	O
HETATM	4045	O	HOH B2026	9.031	-25.414	37.439	1.00 48.06	O
HETATM	4046	O	HOH B2027	6.047	3.908	45.981	1.00 36.67	O
HETATM	4047	O	HOH E2001	10.580	32.271	22.874	1.00 47.01	O
HETATM	4048	O	HOH E2002	6.231	31.699	25.296	1.00 30.87	O
HETATM	4049	O	HOH E2003	-1.011	15.712	32.107	1.00 42.68	O
HETATM	4050	O	HOH E2004	1.275	13.299	34.845	1.00 37.22	O
HETATM	4051	O	HOH E2005	12.591	-6.091	29.233	1.00 42.48	O
HETATM	4052	O	HOH E2006	12.995	-7.652	31.242	1.00 31.85	O
HETATM	4053	O	HOH E2007	15.094	-2.926	29.076	1.00 40.50	O
HETATM	4054	O	HOH E2008	36.999	-7.590	38.776	1.00 15.06	O
HETATM	4055	O	HOH E2009	25.234	-2.908	23.897	1.00 33.32	O
HETATM	4056	O	HOH E2010	21.623	-0.423	32.360	1.00 26.94	O
HETATM	4057	O	HOH E2011	32.869	-0.012	45.185	1.00 21.90	O
HETATM	4058	O	HOH E2012	31.055	10.645	46.161	1.00 37.75	O
HETATM	4059	O	HOH E2013	49.563	-7.249	25.986	1.00 49.04	O
HETATM	4060	O	HOH E2014	44.660	8.170	16.885	1.00 69.64	O
HETATM	4061	O	HOH E2015	56.191	-2.877	29.045	1.00 23.14	O
HETATM	4062	O	HOH E2016	54.576	-1.753	21.385	1.00 24.25	O
HETATM	4063	O	HOH E2017	38.110	-2.133	45.990	1.00 28.73	O
HETATM	4064	O	HOH E2018	32.879	6.903	34.847	1.00 39.71	O
HETATM	4065	O	HOH E2019	36.755	15.994	31.326	1.00 47.59	O
HETATM	4066	O	HOH E2020	36.698	14.033	40.390	1.00 68.08	O
HETATM	4067	O	HOH E2021	15.244	15.254	40.376	1.00 25.05	O
HETATM	4068	O	HOH E2022	10.500	13.606	43.984	1.00 23.03	O
HETATM	4069	O	HOH E2023	9.605	18.998	38.200	1.00 26.73	O
HETATM	4070	O	HOH E2024	21.183	19.416	36.232	1.00 26.97	O
HETATM	4071	O	HOH E2025	20.455	3.500	27.618	1.00 33.63	O
HETATM	4072	O	HOH E2026	9.250	4.047	46.811	1.00 23.42	O
HETATM	4073	O	HOH E2027	7.506	6.260	46.806	1.00 26.80	O
HETATM	4074	O	HOH E2028	19.060	0.762	42.076	1.00 21.68	O
HETATM	4075	O	HOH E2029	12.949	1.329	26.742	1.00 41.08	O
HETATM	4076	O	HOH E2030	16.855	2.003	31.137	1.00 26.93	O
HETATM	4077	O	HOH E2031	15.233	5.857	27.540	1.00 17.32	O
HETATM	4078	O	HOH E2032	17.293	3.096	28.618	1.00 28.45	O
HETATM	4079	O	HOH E2033	15.255	4.359	23.730	1.00 46.04	O
HETATM	4080	O	HOH E2034	12.677	8.496	18.760	1.00 17.72	O
HETATM	4081	O	HOH E2035	6.459	1.581	18.456	1.00 14.34	O
HETATM	4082	O	HOH E2036	2.988	14.200	17.282	1.00 31.42	O
HETATM	4083	O	HOH E2037	-5.464	12.195	18.318	1.00 31.94	O
HETATM	4084	O	HOH E2038	-2.441	10.858	20.383	1.00 46.05	O

Figure 2 Table 2b - 62

```
HETATM 4085  O   HOH E2039      -3.334  23.681  13.424  1.00 24.03           O
HETATM 4086  O   HOH E2040      13.181  25.734   3.023  1.00  5.87           O
HETATM 4087  O   HOH E2041      11.504  30.916   9.034  1.00 28.69           O
HETATM 4088  O   HOH E2042      20.155  22.573  16.588  1.00 22.98           O
HETATM 4089  O   HOH E2043      30.749  20.719   6.914  1.00 43.41           O
HETATM 4090  O   HOH E2044      32.660  22.849   7.037  1.00 14.66           O
HETATM 4091  O   HOH E2045      32.932  19.145   7.175  1.00 28.42           O
HETATM 4092  O   HOH E2046      42.599  10.262  14.968  1.00 19.67           O
HETATM 4093  O   HOH E2047      40.559  13.766  15.328  1.00 27.37           O
HETATM 4094  O   HOH E2048      25.741   7.740  -2.257  1.00 53.26           O
HETATM 4095  O   HOH E2049      25.816   0.867   3.695  1.00 47.44           O
HETATM 4096  O   HOH E2050      33.562  -1.404  15.092  1.00 35.65           O
HETATM 4097  O   HOH E2051      42.441 -13.555  24.944  1.00 29.27           O
HETATM 4098  O   HOH E2052      46.702 -10.712  21.932  1.00 32.59           O
HETATM 4099  O   HOH E2053      44.503  -4.625  13.650  1.00 48.17           O
HETATM 4100  O   HOH E2054      21.975  -0.918  11.326  1.00 47.98           O
HETATM 4101  O   HOH E2055      17.203  -2.186   8.238  1.00 40.36           O
HETATM 4102  O   HOH E2056      20.684   2.074  -0.551  1.00 42.93           O
HETATM 4103  O   HOH E2057      19.367   4.885   1.866  1.00 44.47           O
HETATM 4104  O   HOH E2058      23.625   6.650   0.673  1.00 30.43           O
HETATM 4105  O   HOH E2059      17.234   8.108   3.831  1.00 31.92           O
HETATM 4106  O   HOH E2060       9.656  15.921   3.103  1.00  5.43           O
HETATM 4107  O   HOH E2061       8.795  18.269   4.602  1.00 15.22           O
HETATM 4108  O   HOH E2062       9.274  11.674   5.450  1.00 25.76           O
HETATM 4109  O   HOH E2063      11.856   5.902  18.360  1.00 34.28           O
HETATM 4110  O   HOH E2064      14.947   8.184  17.230  1.00 17.44           O
HETATM 4111  O   HOH E2065      21.822   6.324  -3.889  1.00 33.94           O
HETATM 4112  O   HOH E2066      30.564  18.912   5.076  1.00 25.00           O
HETATM 4113  O   HOH E2067      21.541  25.182  24.850  1.00 18.98           O
HETATM 4114  O   HOH E2068      22.691  19.807  21.046  1.00 34.82           O
HETATM 4115  O   HOH E2069      13.610  29.706  24.815  1.00 40.85           O
HETATM 4116  O   HOH E2070       8.112  29.381  25.394  1.00 37.32           O
HETATM 4117  O   HOH E2071       8.501  24.651  21.412  1.00 30.51           O
HETATM 4118  O   HOH E2072      12.255   4.192  23.125  1.00 27.68           O
HETATM 4119  O   HOH E2073      16.426   6.181   1.859  1.00 44.73           O
HETATM 4120  O   HOH E2074      19.838   2.294  23.626  1.00 43.58           O
HETATM 4121  O   HOH E2075      25.412   6.223  18.948  1.00 25.37           O
HETATM 4122  O   HOH E2076      23.875   7.742  20.133  1.00 13.57           O
HETATM 4123  O   HOH E2077      17.652   4.323  23.235  1.00 37.42           O
HETATM 4124  O   HOH E2078      25.204   4.774  21.906  1.00 50.96           O
HETATM 4125  O   HOH E2079      28.130  11.737  21.410  1.00 35.00           O
HETATM 4126  O   HOH E2080      26.776  13.844  21.778  1.00 18.88           O
END
```

Figure 3

```
1     MEsVaa-eSa PApENEHSQE TPESNSSVYT tFMKSHRCYD LIPTSSKLVV FDTSLQVKKA
1     MEtVissdSs PAvENEHPQE TPESNNSVYT sFMKSHRCYD LIPTSSKLVV FDTSLQVKKA

60    FFALVTNGVR AAPLWDSKKQ SFVGMLTITD FINILHRYYK SALVQIYELE EHKIETWREV
61    FFALVTNGVR AAPLWDSKKQ SFVGMLTITD FINILHRYYK SALVQIYELE EHKIETWREV

120   YLQDSFKPLV CISPNASLFD AVSSLIRNKI HRLPVIDPES GNTLYILTHK RILKFLKLFI
121   YLQDSFKPLV CISPNASLFD AVSSLIRNKI HRLPVIDPES GNTLYILTHK RILKFLKLFI

180   TEFPKPEFMS KSLEELQIGT YANIAMVRTT TPVYVALGIF VQHRVSALPV VDEKGRVVDI
181   TEFPKPEFMS KSLEELQIGT YANIAMVRTT TPVYVALGIF VQHRVSALPV VDEKGRVVDI

240   YSKFDVINLA AEKTYNNLDV SVTKALQHRS HYFEGVLKCY LHETLEAIIN RLVEAEVHRL
241   YSKFDVINLA AEKTYNNLDV SVTKALQHRS HYFEGVLKCY LHETLETIIN RLVEAEVHRL

300   VVVDEHDVVK GIVSLSDILQ ALVLTGGEKK P    (SEQ ID NO:1)
301   VVVDENDVVK GIVSLSDILQ ALVLTGGEKK P    (SEQ ID NO:2)
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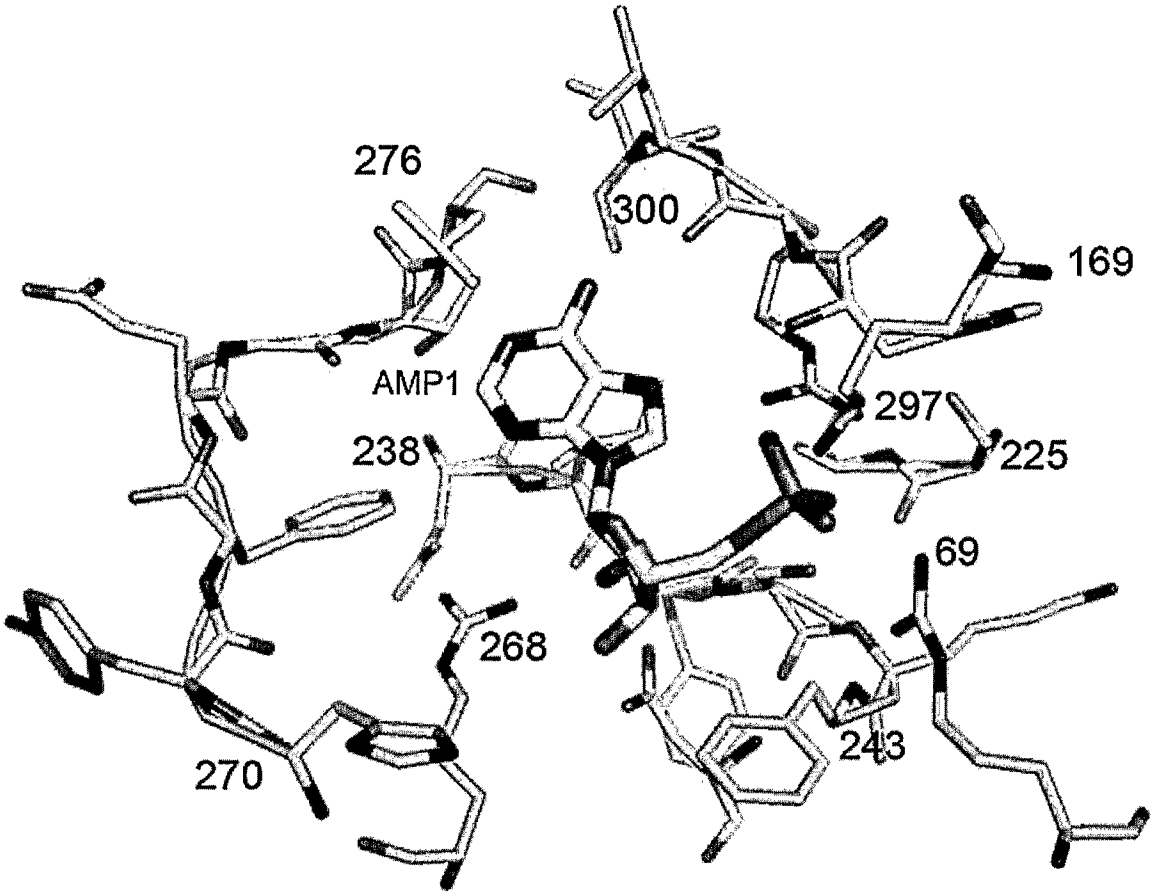


Figure 4

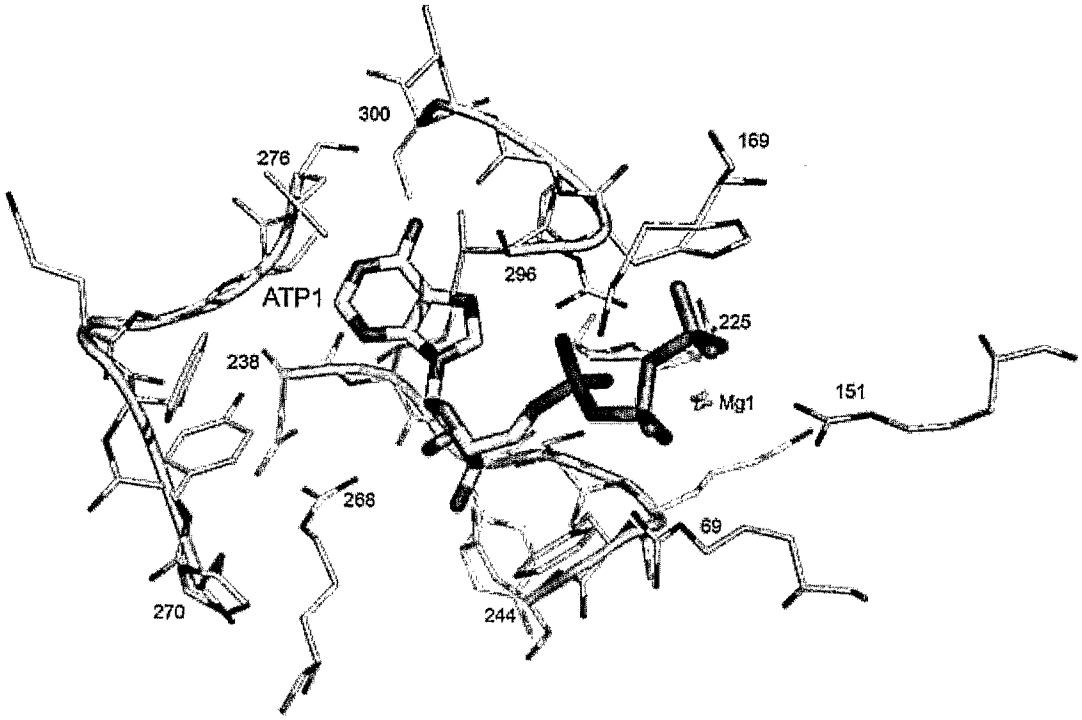


Figure 5

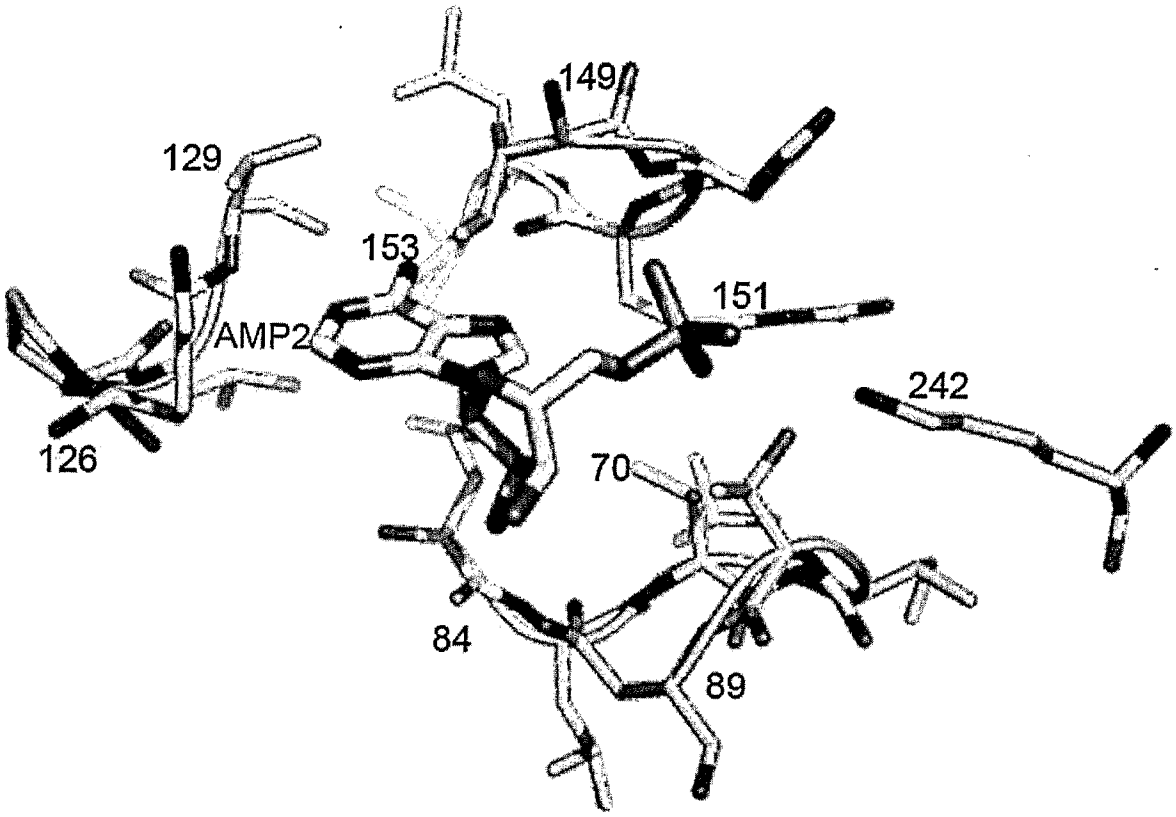


Figure 6

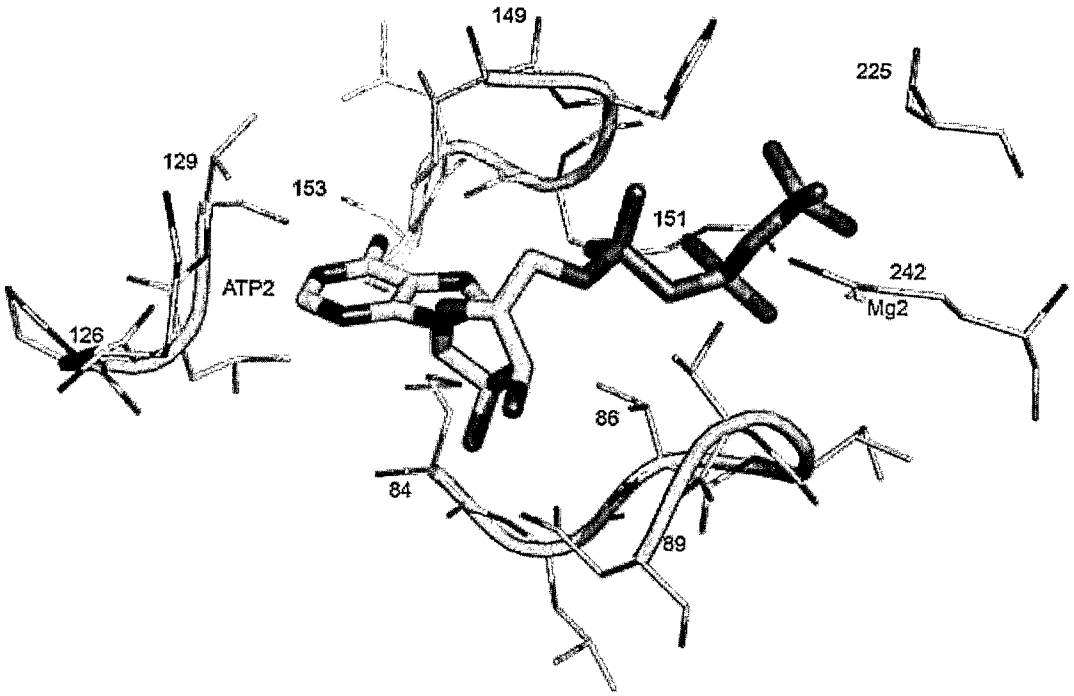


Figure 7

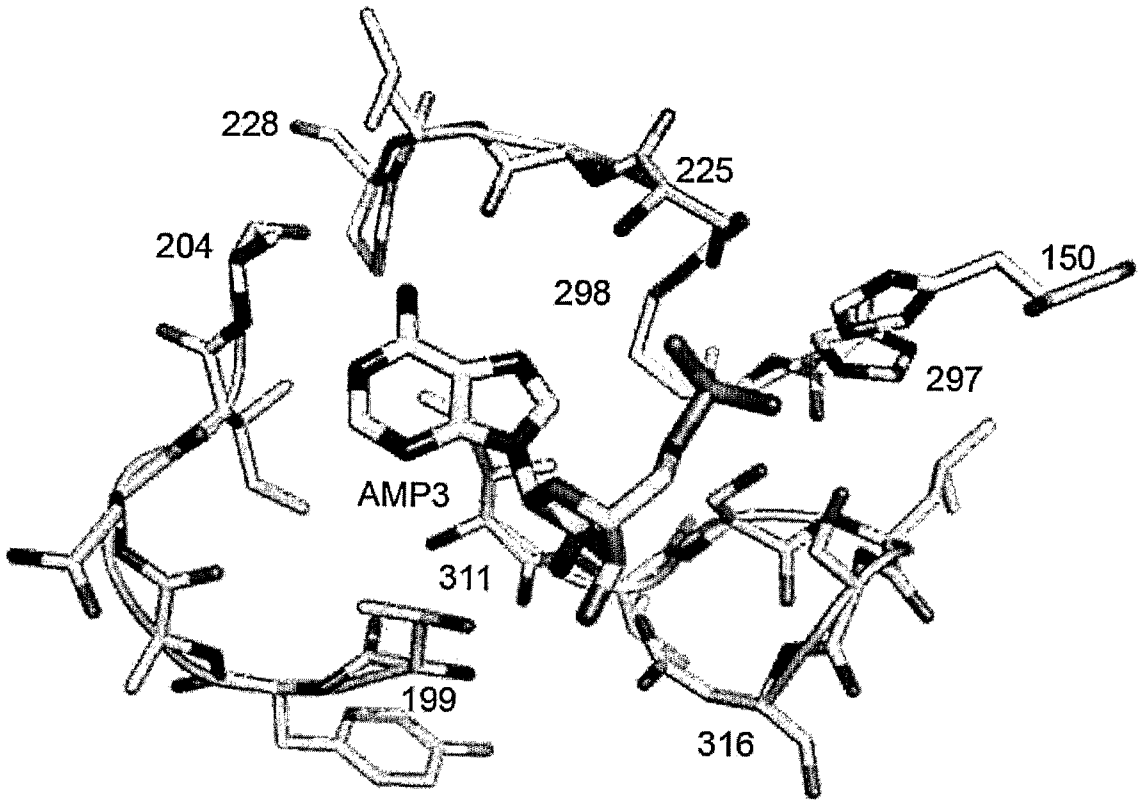


Figure 8

INTERNATIONAL SEARCH REPORT

International application No
PCT/GB2008/002688

A. CLASSIFICATION OF SUBJECT MATTER
INV. C12N9/12 C07K14/47 C12N15/09 C12N15/12 G06F19/00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
C12N C07K G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
EPO-Internal, Sequence Search, WPI Data, BIOSIS, EMBASE

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	TOWNLEY ROBERT ET AL: "Crystal structures of the adenylate sensor from fission yeast AMP-activated protein kinase." SCIENCE (NEW YORK, N.Y.) 23 MAR 2007, vol. 315, no. 5819, 23 March 2007 (2007-03-23), pages 1726-1729, XP002508091 ISSN: 1095-9203	1-17,22, 23,26-30
X	disclosure of an alpha-beta-gamma heterotrimer of fission yeast AMPK homolog the whole document	26
	----- -/--	

[X] Further documents are listed in the continuation of Box C. [X] See patent family annex.

* Special categories of cited documents :

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"E" earlier document but published on or after the international filing date
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"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
19 December 2008	13/01/2009

Name and mailing address of the ISA/	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Fax: (+31-70) 340-3016	Vix, Olivier

Form PCT/ISA/210 (second sheet) (April 2005)

INTERNATIONAL SEARCH REPORT

International application No
PCT/GB2008/002688

C(Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
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Y	WO 97/25341 A (ST VINCENTS INST MED RES [AU]; DARTMOUTH COLLEGE [US]; KEMP BRUCE E [A) 17 July 1997 (1997-07-17) see page 7-13, 18-19 and examples 1-3, claims 6, 14 and 20 the whole document	1-17,22, 23,26-30
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Y	BERI R K ET AL: "MOLECULAR CLONING, EXPRESSION AND CHROMOSOMAL LOCALISATION OF HUMAN AMP-ACTIVATED PROTEIN KINASE" FEBS LETTERS, ELSEVIER, AMSTERDAM, NL, vol. 356, 1 January 1994 (1994-01-01), pages 117-121, XP002907312 ISSN: 0014-5793 the whole document	1-17, 26-30
Y	WO 2004/024942 A (UNIV DUNDEE [GB]; HARDIE GRAHAME [GB]) 25 March 2004 (2004-03-25) in particular see claims 1-6 and pages 30-32 the whole document	28-30
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INTERNATIONAL SEARCH REPORT

International application No
PCT/GB2008/002688

C(Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	TOPALIS DIMITRI ET AL: "Nucleotide binding to human UMP-CMP kinase using fluorescent derivatives -- a screening based on affinity for the UMP-CMP binding site." THE FEBS JOURNAL JUL 2007, vol. 274, no. 14, July 2007 (2007-07), pages 3704-3714, XP002508263 ISSN: 1742-464X the whole document	28-30
Y	BLUNDELL T L ET AL: "HIGH-THROUGHPUT CRYSTALLOGRAPHY FOR LEAD DISCOVERY IN DRUG DESIGN" NATURE REVIEWS. DRUG DISCOVERY, NATURE PUBLISHING GROUP, BASINGSTOKE, GB, vol. 1, no. 1, 1 January 2002 (2002-01-01), pages 45-54, XP009023187 ISSN: 1474-1784 the whole document	1-17,26, 27
Y	WONG KELLY A ET AL: "A revised model for AMP-activated protein kinase structure: The alpha-subunit binds to both the beta- and gamma-subunits although there is no direct binding between the beta- and gamma-subunits." THE JOURNAL OF BIOLOGICAL CHEMISTRY 24 NOV 2006, vol. 281, no. 47, 24 November 2006 (2006-11-24), pages 36434-36442, XP002508092 ISSN: 0021-9258 the whole document	1-17,22, 23,26-30
P,X	XIAO BING ET AL: "Structural basis for AMP binding to mammalian AMP-activated protein kinase" NATURE (LONDON), vol. 449, no. 7161, September 2007 (2007-09), pages 496-501, XP002508093 ISSN: 0028-0836 the whole document	1-17,22, 23,26-30
P,X	JIN ET AL: "Structural Insight into AMPK Regulation: ADP Comes into Play" STRUCTURE, CURRENT BIOLOGY LTD., PHILADELPHIA, PA, US, vol. 15, no. 10, 16 October 2007 (2007-10-16), pages 1285-1295, XP022368318 ISSN: 0969-2126 the whole document	1-17,22, 23,26-30

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box II.1

Claims Nos.: 18-21,24-25

Rule 39.1(v) PCT - Presentation of information
Concerning claims 18-21 and 24-25 applicant's attention is drawn to Rule 39.1(v) PCT. The subject-matter of claims 18-21 and 24-25 refers to the presentation of structure data (3D atomic structure model of AMPK) and is not regarded as patentable invention within the meaning of Rule 67 (v) PCT since it relates to a presentation of information (protein model structure coordinates or computer generated model) as a coordinate listings (or structure factor data) on a storage medium, or information stored on a computer (e.g. data storage device storing data on a computer, computer system comprising this data) or computer readable media. Thus, the above mentioned claims will not be searched.

INTERNATIONAL SEARCH REPORT

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PCT/GB2008/002688

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. [X] Claims Nos.: 18-21, 24-25
because they relate to subject matter not required to be searched by this Authority, namely:

see FURTHER INFORMATION sheet PCT/ISA/210

2. [ ] Claims Nos.:
because they relate to parts of the International application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. [ ] Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. [ ] As all required additional search fees were timely paid by the applicant, this international search report covers allsearchable claims.

2. [ ] As all searchable claims could be searched without effort justifying an additional fees, this Authority did not invite payment of additional fees.

3. [ ] As only some of the required additional search fees were timely paid by the applicant, this international search reportcovers only those claims for which fees were paid, specifically claims Nos.:

4. [ ] No required additional search fees were timely paid by the applicant. Consequently, this International search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

[ ] The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.

[ ] The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.

[ ] No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No
PCT/GB2008/002688

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