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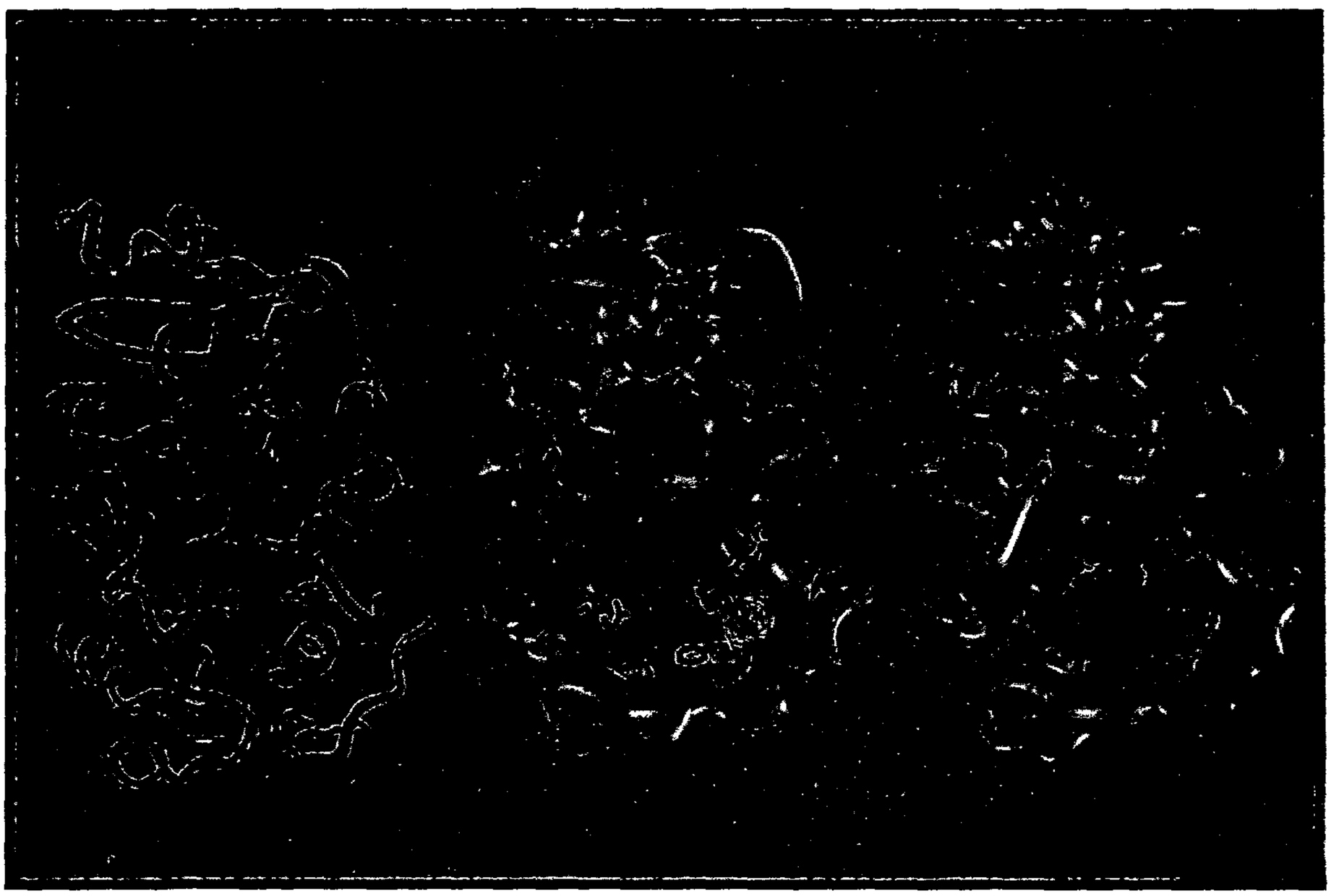
(54) Title: DESIGNING MODULATORS FOR GLYCOSYLTRANSFERASES



(57) Abrégé/Abstract:
The invention relates to structures and models of glycosyltransferases and ligand binding domains of glycosyltransferases, and complexes of the glycosyltransferases and ligand binding domains with ligands. The structural coordinates that define the structures and models enable the determination of homologues, the structures of polypeptides with unknown structure, and the identification of modulators of the glycosyltransferases. The invention also relates to structures and models of nucleotide-sugar donors and acceptors for the glycosyltransferases, and the design of modulators for the glycosyltransferases based on the properties of these structures and models.

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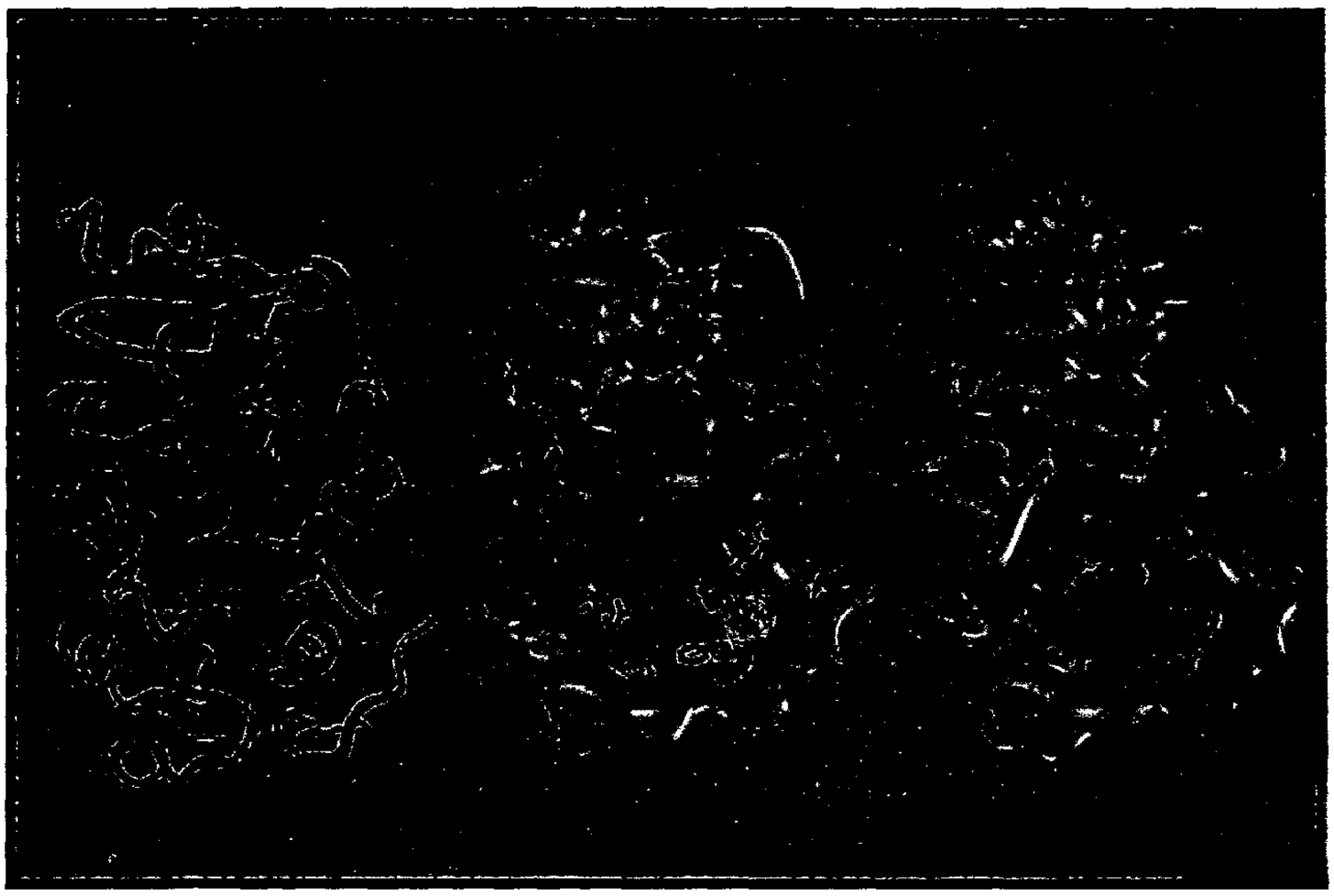

(57) Abstract: The invention relates to structures and models of glycosyltransferases and ligand binding domains of glycosyltransferases, and complexes of the glycosyltransferases and ligand binding domains with ligands. The structural coordinates that define the structures and models enable the determination of homologues, the structures of polypeptides with unknown structure, and the identification of modulators of the glycosyltransferases. The invention also relates to structures and models of nucleotide-sugar donors and acceptors for the glycosyltransferases, and the design of modulators for the glycosyltransferases based on the properties of these structures and models.

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TITLE: Designing Modulators for Glycosyltransferases

FIELD OF THE INVENTION

The invention relates to structures and models of glycosyltransferases and ligand binding domains of glycosyltransferases, and complexes of the glycosyltransferases and ligand binding domains with ligands. The structural coordinates that define the structures and models enable the determination of homologues, the structures of polypeptides with unknown structure, and the identification of modulators of the glycosyltransferases. The invention also relates to structures and models of nucleotide-sugar donors and acceptors for the glycosyltransferases, and the design of modulators for the glycosyltransferases based on the properties of these structures and models.

BACKGROUND OF THE INVENTION

Glycosyltransferases (GTs, a general nomenclature for glycosyltransferases is EC 2.4.x.y) comprise a group of enzymes that are involved in the biosynthesis of complex oligosaccharides (1-4). The result of the reaction catalyzed by these enzymes is the formation of a new glycosidic linkage and it appears that there is at least one distinct glycosyltransferase for every type of glycosidic linkage. Glycosylation proceeds in a stepwise manner and, therefore, the expression and specificity of the enzymes represent key regulatory factors in defining the repertoire of biosynthesized oligosaccharides. During oligosaccharide processing, oligosaccharides are converted into hybrid and complex oligosaccharides by addition of *N*-acetylglucosaminyl residues (GlcNAc, 2-acetamido-2-deoxy-α-D-glucopyranosyl). These modifications in the oligosaccharide chains of *N*- and *O*-linked glycoproteins accompany many physiological and pathological cell processes (5). The transfer of GlcNAc is catalyzed by *N*-acetylglucosaminyltransferases (GlcNAc-Ts or GnTs). In such a transfer, the donor of the GlcNAc residue is UDP-GlcNAc [uridine 5'-(2-acetamido-2-deoxy-α-D-glucopyranosyl pyrophosphate)] while the acceptor is one of the hydroxyl groups located at a particular position of a variety of oligosaccharides. *N*-acetylglucosaminyltransferases show a decisive specificity for the oligosaccharide-acceptor and they generally require the presence of a metal cofactor (6). There are at least eight different GlcNAc-Ts involved in the biosynthesis of complex and hybrid *N*-glycans (GlcNAc-T I – GlcNAc-T VIII), five in the biosynthesis of *O*-glycans (Core 2 – Core 4 GnTs, Core 1 and Core 2 elongation GnTs), and two in the biosynthesis of antigen determinants (blood group i and blood group I) (1, 2,4, 7). Though some of these GlcNAc-Ts have already been cloned, the origin of their specificity remains unknown due to the lack of experimental structures of GlcNAc-Ts or any other mammalian glycosyltransferase.

In spite of their large abundance in nature, crystal structures of glycosyltransferases are rare. Until recently, the only structure of glycosyltransferase available was that of a DNA-modifying β-glucosyltransferase from bacteriophage T4 and its complex with UDP-Glc (8). However, that enzyme is somewhat different from other glycosyltransferases since the acceptor involved in the reaction with this enzyme is not a carbohydrate. Indeed, this enzyme catalyses the transfer of a glucose moiety from UDP-glucose to hydroxymethylated cytosines of DNA. The DNA-modifying β-glucosyltransferase from bacteriophage T4 presents no sequence homology to any other glycosyltransferase (9) though the structure of this enzyme has been used as a template to predict the structure of other glycosyltransferases (10). Recently, a decisive breakthrough in this field has been achieved with the resolution of the X-ray structures of two bacterial glycosyltransferases in their native and nucleotide-complexed forms, the SpsA (11), for which the substrate specificity is undefined, and the β1,4-galactosyltransferase T1 (12).

The reaction catalyzed by GlcNAc-Ts can be regarded as a nucleophilic displacement of the UDP (uridine 5'-pyrophosphate) functional group at the anomeric carbon C1 of the GlcNAc (2-acetamido-2-deoxy-α-D-glucopyranose) residue of UDP-GlcNAc by a hydroxyl group of a specific oligosaccharide-acceptor (Figure 36). The

enzymatic reaction of all known GlcNAc-Ts, except the α-1,4-GlcNAc-T (13), leads to an inversion of the anomeric configuration. There is a clear resemblance between the enzymatic action of glycosyltransferases and the enzymatic action of glycoside hydrolases, mechanisms of which have largely been characterized in detail (14-21). Many aspects of the functions and catalytic mechanisms of *N*-acetylglucosaminyltransferases are, however, still unknown since only few mechanistic studies on *N*-acetylglucosaminyltransferases have been reported to date (6,22). In the absence of experimental data, high-level *ab initio* calculations can be used to gain some insight into many characteristics of the enzymatic reaction catalyzed by *N*-acetylglucosaminyltransferases. They can provide the description on an atomic level of the discrete intermediates and transition states found along the enzyme-catalyzed reaction pathway.

SUMMARY OF THE INVENTION

The applicants have produced high-level *ab initio* quantum chemical results on a model of the GlcNAc transfer reaction catalyzed by N-acetylglucosaminyltransferases and, based on the results additionally developed homology models for glycosyltransferases and ligand binding domains thereof, and complexes of the enzymes or ligand binding domains with ligands including sugar nucleotide donors and acceptors. In particular, applicants have produced models and structures for GnT1, GnTV, core 2L, core 2b/M, and core 3, ligand binding domains thereof, and complexes of the enzymes, for example with UDP, UDP-GlcNAc and acceptors. Models and structures have also been produced for transition states of GnT1 and core 2L.

Therefore, the invention provides a model or secondary, tertiary, and/or quanternary structure of a ligand binding domain of a glycosyltransferase. Binding domains are of significant utility in drug discovery. The association of natural ligands and substrates with the ligand binding domains of glycosyltransferases is the basis of biological mechanisms. The associations may occur with all or any parts of a ligand binding domain. An understanding of these associations is the basis for the design and optimization of drugs having more favorable associations with their target enzyme and thus provide improved biological effects. Therefore, information about the shape and structure of glycosyltransferases and their ligand-binding domains is invaluable in designing potential modulators of glycosyltransferases for use in treating diseases and conditions associated with or modulated by the glycosyltransferases.

Ligand binding domains include one or more of the binding domains for a disphosphate group or pyrophosphate of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a nitrogeneous heterocyclic base (preferably a pyrimidine base, more preferably uracil) of a sugar nucleotide donor, a sugar of the nucleotide of a sugar nucleotide donor, a selected sugar of a sugar nucleotide donor that is transferred to an acceptor, and/or an acceptor. The structure of a ligand binding domain may be defined by selected binding sites or atomic interactions in the domain.

In accordance with aspects of the invention, a ligand binding domain is defined by (a) one or more (preferably all) amino acid residues of a GnT1 shown in Table 10; (b) one or more (preferably all) amino acid residues of a GnTV shown in Table 11; (c) one or more (preferably all) amino acid residues of a core 2L/T1 shown in Table 12; and (d) one or more (preferably all) amino acid residues of a core 2b/2M/T2 shown in Table 13. The invention also relates to a model or secondary, tertiary, and/or quanternary structure of a ligand binding domain of a glycosyltransferase defined by the structural coordinates of one or more of the atomic contacts or atomic interactions as shown in Table 10, Table 11, Table 12, or Table 13. Each of the atomic interactions is defined in Table 10, 11,

12, or 13 by an atomic contact (more preferably a specific atom where indicated) on the sugar nucleotide donor or part thereof, and an atomic contact (more preferably a specific atom where indicated) on the glycosyltransferase.

The invention also provides a model of a ligand binding domain designed in accordance with a method of the invention.

The invention further provides a model or secondary, tertiary and/or quanternary structure of a glycosyltransferase or a transition state of a glycosyltransferase.

The invention contemplates a model or secondary, tertiary and/or quanternary structure of a glycosyltransferase or ligand binding domain in association with a ligand or substrate.

The structures and models of the invention provide information about the atomic contacts involved in the interaction between the enzyme and a known ligand which can be used to screen for unknown ligands. Therefore the present invention provides a method of screening for a ligand capable of binding a glycosyltransferase ligand binding domain, comprising the use of a secondary, tertiary or quanternary structure or a model of the invention. For example, the method may comprise the step of contacting a ligand binding domain with a test compound, and determining if the test compound binds to the ligand.

A structure or model of the invention may be used to design, evaluate, and identify ligands of glycosyltransferase other than ligands that associate with a glycosyltransferase. The ligands may be based on the shape and structure of a glycosyltransferase, or a ligand binding domain or atomic interactions, or atomic contacts thereof. Therefore, ligands, in particular modulators, may be derived from ligand binding domains or analogues or parts thereof.

The present invention also contemplates a ligand identified by a method of the invention. A ligand may be a competitive or non-competitive inhibitor of a glycosyltransferase. Preferably, the ligand is a modulator that is capable of modulating the activity of a glycosyltransferase enzyme. Thus, the methods of the invention permit the identification early in the drug development cycle of compounds that have advantageous properties.

In an embodiment, the present invention contemplates a method of identifying a modulator of a glycosyltransferase or a ligand binding domain or binding site thereof, comprising the step of using the structural coordinates of a glycosyltransferase or a ligand binding domain or binding site thereof, or a model of the invention to computationally evaluate a test compound for its ability to associate with the glycosyltransferase or ligand binding domain or binding site thereof. Use of the structural coordinates of a glycosyltransferase structure, ligand binding domain, or binding site thereof, of the invention to identify a ligand or modulator is also provided.

In another embodiment of the invention, a method is provided for identifying a potential modulator of a glycosyltransferase by determining binding interactions between a test compound and atomic contacts of a ligand binding domain of a glycosyltransferase defined in accordance with the invention comprising:

(a) generating the atomic contacts on a computer screen;

(b) generating test compounds with their spatial structure on the computer screen; and

(c) determining whether the compounds associate or interact with the atomic contacts defining the glycosyltransferase;

(d) identifying test compounds that are potential modulators by their ability to enter into a selected number of atomic contacts.

Another aspect of the invention provides methods for identifying a potential modulator of a glycosyltransferase function by docking a computer representation of a test compound with a computer

representation of a structure of a glycosyltransferase or a ligand binding domain thereof that is defined as described herein. In an embodiment the method comprises the following steps:

(a) docking a computer representation of a compound from a computer data base with a computer representation of atomic interactions or atomic contacts of a ligand binding domain of a glycosyltransferase to obtain a complex;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying test compounds that best fit the atomic interactions or contacts as potential modulators of the glycosyltransferase.

In another embodiment the method comprises the following steps:

(a) modifying a computer representation of a test compound complexed with a ligand binding domain of a glycosyltransferase by deleting or adding a chemical group or groups;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying a test compound that best fits the ligand binding domain as a potential modulator of a glycosyltransferase.

In still another embodiment the method comprises the following steps:

(a) selecting a computer representation of a test compound complexed with atomic contacts or atomic interactions of a binding domain of a glycosyltransferase; and

(b) searching for molecules in a data base that are similar to the test compound using a searching computer program, or replacing portions of the test compound with similar chemical structures from a data base using a compound building computer program.

The ligands or compounds identified according to the methods of the invention preferably have structures such that they are able to enter into an association with a ligand binding domain. Selected ligands or compounds may be characterized by their suitability for binding to particular ligand binding domains. A ligand binding domain or binding site may be regarded as a type of negative template with which the compounds correlate as positives in the manner described herein and thus the compounds are unambiguously defined. Therefore, it is possible to describe the structure of a compound suitable as a modulator of a glycosyltransferase by accurately defining the atomic interactions to which the compound binds to a ligand binding domain and deriving the structure of the compound from the spacial structure of the target.

The invention contemplates a method for the design of ligands, in particular modulators, for glycosyltransferase based on the secondary, tertiary or quanternary structure of a sugar nucleotide donor (or part thereof) defined in relation to its spatial association with the three dimensional structure of the glycosyltransferase or a ligand binding domain thereof. Generally, a method is provided for designing potential inhibitors of a glycosyltransferase comprising the step of using the structural coordinates of a sugar nucleotide donor or part thereof, defined in relation to its spatial association with the secondary, tertiary or quanternary tructure or model of a glycosyltransferase or a ligand binding domain thereof, to generate a compound for associating with the ligand binding domain of the glycosyltransferase. The following steps are employed in a particular method of the invention: (a) generating a computer representation of a sugar nucleotide donor, or part thereof, defined in relation to its spatial association with the three dimensional structure of a glycosyltransferase or a ligand binding domain thereof; (b)

searching for molecules in a data base that are similar to the defined sugar nucleotide donor, or part thereof, using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

Therefore, the invention further contemplates classes of ligands, in particular modulators, of a glycosyltransferase based on the secondary, tertiary or quanternary structure of a sugar nucleotide donor, or part thereof, defined in relation to the sugar nucleotide donor's spatial association with a three dimensional structure of a glycosyltransferase.

It will be appreciated that a ligand or modulator of a glycosyltransferase may be identified by generating an actual secondary or three-dimensional model of a ligand binding domain or binding site, synthesizing a compound, and examining the components to find whether the required interaction occurs.

Modulators which are capable of modulating the activity of glycosyltransferases have therapeutic and prophylactic potential. Therefore, the methods of the invention for identifying modulators may comprise one or more of the following additional steps:

(a) testing whether the ligand is a modulator of the activity of a glycosyltransferase, preferably testing the activity of the modulator in cellular assays and animal model assays;

(b) modifying the modulator;

(c) optionally rerunning steps (a) or (b); and

(d) preparing a pharmaceutical composition comprising the modulator.

Steps (a), (b) (c) and (d) may be carried out in any order, at different points in time, and they need not be sequential.

Still another aspect of the invention provides a method of conducting a drug discovery business comprising:

(a) providing one or more systems or methods for identifying modulators based on a model or structure of the present invention, preferably a method using a computer as described herein;

(b) conducting therapeutic profiling of modulators identified in step (a), or further analogs thereof, for efficacy and toxicity in animals; and

(c) formulating a pharmaceutical composition including one or more agents identified in step (b) as having an acceptable therapeutic profile.

In certain embodiments, the subject method may also include a step of establishing a distribution system for distributing the pharmaceutical composition for sale, and may optionally include establishing a sales group for marketing the pharmaceutical composition.

In yet another aspect of the invention, a method of conducting a target discovery business is provided comprising:

(a) providing one or more system or method for identifying modulators based on a model or structure of the present invention, preferably a method using a computer as described herein;

(b) optionally conducting therapeutic profiling of modulators identified in (a) for efficacy and toxicity in animals; and

(c) licensing to a third party the rights for further drug development and/or sales for agents identified in step (a), or analogs thereof.

There is also provided a pharmaceutical composition comprising a modulator, and a method of treating and/or preventing disease associated with a glycosyltransferase comprising the step of administering a modulator or pharmaceutical composition comprising a modulator to a patient.

In an aspect, the invention contemplates a method of treating a disease associated with a glycosyltransferase with inappropriate activity in a cellular organism, comprising:

(a) administering a modulator identified using the methods of the invention in an acceptable pharmaceutical preparation; and

(b) activating or inhibiting a glycosyltransferase to treat the disease.

The invention provides for the use of a modulator identified by the methods of the invention in the preparation of a medicament to treat a disease associated with a glycosyltransferase with inappropriate activity in a cellular organism. Use of the structural coordinates of a glycosyltransferase structure of the invention to manufacture a medicament is also provided.

Another aspect of the invention provides machine readable media encoded with data representing a model of the invention or the coordinates of a structure of a glycosyltransferase or ligand binding domain or binding site thereof as defined herein, or the three dimensional structure of a sugar nucleotide donor or part thereof defined in relation to its spatial association with a three dimensional structure of a glycosyltransferase as defined herein. The invention also provides computerized representations of a model of the invention or the secondary, tertiary or quanternary structures of the invention , including any electronic, magnetic, or electromagnetic storage forms of the data needed to define the structures such that the data will be computer readable for purposes of display and/or manipulation. The invention further provides a computer programmed with a homology model of a ligand binding domain of a glycosyltransferase. The invention still further contemplates the use of a homology model of the invention as input to a computer programmed for drug design and/or database searching and/or molecular graphic imaging in order to identify new ligands or modulators for glycosyltransferases.

These and other aspects of the present invention will become evident upon reference to the following detailed description and attached drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

The invention will now be described in relation to the drawings in which:

Figure 1. (a) Potential Energy Surface calculated at the HF/6-31G* level and corresponding to the mechanism involving only a catalytic base to assist the nucleophilic attack followed by the proton transfer to the base (3-A); (b) Geometrical representation of the different stationary points calculated at the DFT/B3LYP/6-31G* level. Numbers in italic represent relative energies (in kcal/mol) at DFT/B3LYP/6-31++G**//DFT/B3LYP/6-31G* level. R, TS, INT, and PC represent the reactants, transition states, intermediates, and products, respectively.

Figure 2. (a) Potential Energy Surface calculated at the HF/6-31G* level and corresponding to the mechanism involving a pair of catalytic amino acids to assist the proton transfer to O1 and the nucleophilic attack. In this mechanism, the proton Ha is located at the acceptor (Scheme 3-B). (b) Geometrical representation of the different stationary points calculated at the DFT/B3LYP/6-31G* level. Numbers in italic represent relative energies (in kcal/mol) at DFT/B3LYP/6-31++G**//DFT/B3LYP/6-31G* level. R, TS, INT, and PC represent the reactants, transition states, intermediates, and products, respectively.

Figure 3. (a) Potential Energy Surface calculated at the HF/6-31G* level and corresponding to the mechanism involving a pair of catalytic amino acids to assist the proton transfer to O1 and the nucleophilic attack. In this mechanism, the proton Ha is positioned at the base (Scheme 3-B). (b) Geometrical representation of the different stationary points calculated at the DFT/B3LYP/6-31G* level. Numbers in italic represent relative energies (in

kcal/mol) at DFT/B3LYP/6-31++G**//DFT/B3LYP/6-31G* level. R, TS, INT, and PC represent the reactants, transition states, intermediates, and products, respectively.

Figure 4. (a) Crystal structures of SpsA and GnT I. (b) Superimposition of SpsA and GnT I structures.

Figure 5. Sequence alignment of GnTI and Core 2L Gn T. Relevant amino acid residues of the GnT I binding site are highlighted.

Figure 6. Homology models of Core 2L (left), Core 2b/M GnT (middle), and GnTV (right) based on the structure of GnT I.

Figure 7. Representation of the electrostatic potential surface of GnT I and the favored binding modes of UDP docked within the enzyme.

Figure 8. Representation of UDP binding interactions in the experimental structures of GnTs.

Figure 9. Representation of the four top scoring UDP-Core2L GnT complexes. Amino acids interacting with the uridine part as described herein are shown in tube.

Figure 10. Representation of the predicted lowest energy docking mode of the acceptor heptasaccharide into GnT I-UDPGlcNAc complex model. (a) enlarged view of the GlcNAc binding site. (b) overall view of the Transition state-GnT I complex.

Figure 11. Predicted binding mode of the transition state in the Core2L GnT model.

Figure 12. Representation of the electrostatic potential surface of the Core2L GnT model and UDP in its prominent binding mode. GlcNAc acceptor (GalNAc-Gal) binding regions are outlined in green.

Figure 13. GnT V model complexed with the transition state of UDP-GlcNAc and the acceptor oligosaccharide.

Figure 14. Predicted binding mode of GD500 in the model of Core2L GnT.

Figure 15. Predicted binding modes for a fragment of GD0541 (in yellow) and an analogue where the GD0541 fragment is attached to Tacrine (in white).

Figure 16. (a) Structure of Tetrahydroaminoacaridine (Tacrine). (b) Structure of a potential GD0541 analogue having the so-called Tacrine molecule attached to a fragment of GD0541 through an etheric linkage.

Figure 17: A view showing a superimposition of GT's. The Figure shows the superimposition of the main chain atoms of GnT I (red), Core 2L GnT (green), SpsA (magenta), α-1,3-GalT (cyan) and GnT V (black).

Figure 18a-d: The UDP recognition domain of a) Core 2L GnT; b) GalT; c) SpsA (Davies and co-workers); and d) GnT I (Rini and co-workers).

Figure 18e: Overlay of the trace of the UDP recognition domain of GnT I and SpsA. The binding conformation of UDP is shown in tubes.

Figure 19A shows the formula of the heptasaccharide acceptor for GnTV, which provides the basis for a potential modulator based on the acceptor for GnT V. The reactive groups in the molecule can be substituted with the list of groups set out elsewhere in the application.

Figure 19B shows the formula of (1,6)-linked N-acetylglucosylamine linked to the heptasaccharide acceptor for GnT V. This is the product after the reaction with the enzyme.

Figure 20 represents the schematic view of the resulting homology model of GnT V (right). For comparison the scheme of the GnT I template (left) is also shown. The overall shape of the binding pocket of GnT V in the center of the enzyme resembles the binding pocket of GnT I and as a result the docking of UDPGlcNAc is assumed to be similar.

Figure 21 shows UDPGlcNAc in the active site of GnT V.

Figure 22 shows UDP in the active site of GnT V.

Figure 23 illustrates the orientation of the ligand in the binding pocket of GnT V complexed with UDPGlcNAc (top view). The uridine part of the molecule is stabilized (localized at the bottom part of the pocket) with hydrogen bonds and stacking interactions.

Figure 24 shows the amino acids involved in the interactions with the UDPGlcNAc ligand. There are two low energy conformations presented from the top-ranking clusters of UDPGlcNAc. The Figure also illustrates the flexibility around the diphosphate linkages.

Figure 25a shows the active site residues of the GnT I-UDP complex.

Figure 25b shows a superimposition of the Core 2L GnT model (green) and the GnT I structure (red). The active site residues of Core 2L GnT are shown in tubes. The core region contains many of the common alpha helix and beta strand elements, including the active site residues Asp99 (Core 2L)/Asp144(GnT I), His 131 (Core 2L)/His190 (GnT I), Ile133 (Core 2L)/Ile187(GnT I), Glu159 (Core 2L)/Asp213 (GnT I). It is clear that the active site architectures and the residues that constitute the active site of Core 2L GnT and GnT I are highly conserved.

Figure 26 shows the computed low energy docking modes of UDP to Core 2L GnT. The lowest energy-binding mode is shown as a thick tube. In all the top ranking binding modes of UDP shown in this Figure, the uridine group assumes a similar binding conformation.

Figure 27 shows the lowest energy-docking mode of UDP on the solvent-excluded surface of the Core 2L GnT. The potential residues that interact with the uridine ring are shown in blue colored surface. The ribose ring and pyrophosphate groups of UDP are covered by the loop structure of Core 2L GnT.

Figure 28 shows a view of the lowest energy-binding mode of UDP-GlcNAc to the Core 2L GnT. The Core 2L GnT is shown in a solvent excluded surface representation and the UDP-GlcNAc is shown in tubes.

Figure 29 shows a close-up view of the sugar binding pocket. The sugar group of the UDP-GlcNAc occupies a site that is close to the hydrophobic region.

Figure 30 shows an overall view of GlcNAc binding to the transition state of Core 2L GnT showing the hydrophobic pocket.

Figure 31 shows a view of GlcNAc binding to the transition state of Core 2L GnT showing the hydrophobic pocket.

Figure 32 shows the binding of the pyrophosphate of UDP-GlcNAc to the loop structure of Core 2L GnT.

Figure 33 shows a GnT I acceptor.

Figure 34 is a schematic energetic representation (in kcal/mol) of the possible reaction pathways observed in the different PESs for the transfer of GlcNAc catalyzed by inverting *N*-acetylglucosaminyltransferases. Relative energies are calculated at DFT/B3LYP/6-31++G**//DFT/B3LYP/6-31G* level.

Figure 35 is a geometrical representation of the transition states TS1-TS11 calculated at the DFT/B3LYP/6-31G* level. Transition states are clustered by similarities in their C1-Oa and C1-O1 bond lengths. Average C1-Oa and C1-O1 distances, calculated for each group, are noted on the figure. (A) TS2, TS5 and TS8 structures exhibit short C1-Oa (1.4-1.6 Å) and long C1-O1 bond lengths (2.8-3.2 Å). TS11 has been omitted from the structure superimposition for clarity purpose. (B) TS3, TS4 and TS9 structures display long C1-Oa (2.4-2.7 Å) and short C1-O1 (1.5-2.1 Å) bond lengths. TS10 has been omitted from the structure superimposition for clarity. (C) TS1, TS6 and TS7 structures exhibit elongated C1-Oa (2.1-2.4 Å) and C1-O1 (2.5-2.7 Å) bond lengths.

Figure 36 is a schematic representation of the *N*-acetylglucosaminyltransferases involved in the biosynthesis of *N*-glycans (GlcNAc-T I-VIII), *O*-glycans (Core 2-4 and Core 1-2 elongation GnTs) and antigen determinants (blood groups i and I).

Figure 37 is a schematic representation of the structural model used to describe the GlcNAc transfer by inverting *N*-acetylglucosaminyltransferases.

Figure 38 is a schematic representation of the two different types of mechanism investigated for the transfer of GlcNAc by inverting *N*-acetylglucosaminyltransferases. Mechanism A involves only a catalytic base while two catalytic amino acids are implicated in mechanism B.

DESCRIPTION OF THE TABLES

Table 1 – Structural coordinates for GnT1.

Table 2 – Structural coordinates for GnTV.

Table 3 – Structural coordinates for core 2L or T1 (human).

Table 4 – Structural coordinates for core 2L or T1(mouse)

Table 5 – Structural coordinates for core 2L (bovine)

Table 6 – Structural coordinates for core 2b/core M/core 2 T2.

Table 7 – Structural coordinates for core 2C (human)

Table 8 – Structural coordinates for core 3.

Table 9 – consensus polar and hydrophobic interactions in the UDP binding sites of GT-UDP complexes (the first columns are uracil atoms).

Table 10 - Atomic interactions between a GnT1 and a nucleotide sugar donor.

Table 11 – Atomic interactions between a GnTV and a nucleotide sugar donor.

Table 12 – Atomic interactions between a core 2L or T1 and a nucleotide sugar donor.

Table 13 – Atomic interactions between a core 2B and a nucleotide sugar donor.

Table 14 – Structural coordinates for conformations of UDP in association with a GNT1/ground state.

Table 15 – Structural coordinates for conformations of UDP in association with GnTV.

Table 16 – Structural coordinates for conformations of UDP in association with core 2L.

Table 17 – Structural coordinates for conformations of UDPGlcNAc in association with a GnT1 transition state.

Table 18 – Structural coordinates for conformations of UDPGlcNAc in association with GnTV.

Table 19 – Structural coordinates for conformations of UDPGlcNAc in association with a core 2L/transition state.

Table 20 – Structural coordinates for conformations of an oligosaccharide acceptor in association with a GnT1.

Table 21 – Structural coordinates for the loop structure for a GnT1.

Table 22 – Structural coordinates for the loop structure for a Core 2L.

Table 23 – Structural coordinates for the loop structure for a GnTV.

Table 24 is a list of N-acetylglucosylaminotransferases, and their sugar nucleotide donors and acceptors.

Table 25 – Ab initio calculated Geometrical Parameters of the points observed on PESs described in Figures 1-3 at the HFG/6-31G* and DFT/B3YLYP/6-31G* levels.

Table 26 – Comparison of the ab initio relative energies (kcal/mol) calculated by various methods for the points observed on PESs described on Figures 1-3.

In Tables 2 through 9 inclusive, from the left, the second column identifies the atom number; the third identifies the atom type; the fourth identifies the amino acid type; the fifth identifies the residue number; the sixth identifies the x coordinates; the seventh identifies the y coordinates; and the eighth identifies the z coordinates.

DETAILED DESCRIPTION OF PREFERRED EMBODIMENTS

Definitions:

Unless otherwise indicated, all terms used herein have the same meaning as they would to one skilled in the art of the present invention. Practitioners are particularly directed to Current Protocols in Molecular Biology (Ansubel) for definitions and terms of the art. Abbreviations for amino acid residues are the standard 3-letter and/or 1-letter codes used in the art to refer to one of the 20 common L-amino acids.

The term "associate", "association" or "associating" refers to a condition of proximity between a ligand, chemical entity, or compound, or portions or fragments thereof, and a glycosyltransferase, or portions or fragments thereof (e.g. ligand binding domain). The association may be non-covalent i.e. where the juxtaposition is energetically favored by for example, hydrogen-bonding, van der Waals, or electrostatic or hydrophobic interactions, or it may be covalent.

The term "glycosyltransferase" refers to an enzyme that catalyzes the transfer of a single monosaccharide unit from a donor to the hydroxyl group of an acceptor substrate. The acceptor can be either a free saccharide, glycoprotein, glycolipid, or polysaccharide. The donor can be a nucleotide–sugar, preferably UDP-GlcNAc. Glycosyltransferases show a precise specificity for both the sugar acceptor and donor and generally require the presence of a metal cofactor. Glycosyltransferases include but are not limited to eukaryotic glycosyltransferases involved in the biosynthesis of glycoproteins, glycolipids, glycosylphosphatidylinositols and other complex glycoconjugates, and prokaryotic glycosyltransferases involved in the synthesis of carbohydrate structures of bacteria and viruses, such as enzymes involved in LOS and lipopolysaccharide biosynthesis.

Glycosyltransferases are derivable from a variety of sources, including viruses, bacteria, fungi, plants, and animals. In a preferred embodiment the glycosyltransferases are derivable from an animal, preferably a mammal including but not limited to bovine, ovine, porcine, murine equine, most preferably a human. The enzyme may be from any source, whether natural, synthetic, semi-synthetic, or recombinant

Examples of glycosyltransferases are N-acetylglucosaminyltransferases, including N-acetylglucosaminyltransferases I through VIII ("GnT1" through "GnTVIII") involved in the biosynthesis of complex and hybrid N-glycans; UDP-N-acetylglucosamine: N-acetyl galactosamine β-1,6-N-acetylgucosaminyl transferases (core 2 GlcNAc transferases), Core 3 GlcNAc transferase, Core 4 GlcNAc transferase, and Core 1 and Core 2 elongation GnTs involved in the biosynthesis of *O*-glycans, and the GnTs involved in the biosynthesis of antigen determinants (blood group i and blood group I) (Schachter, H. *Curr. Opin. Struct. Biol.* 1991, *1*, 755-765; Montreuil, J.; Vliegenthart, J. F. G.; Schachter, H. *Glycoproteins*; Neuberger, A. and van Deenen, L. L. M., Ed.; Elsevier: Amsterdam, 1995; Vol. 29a; and Raju, T. S.; Stanley, P. *J. Biol. Chem.* 1998, *273*, 14090-14098). Table 24 provides examples of eukaryotic glycosyltransferases, and their sugar nucleotide donors, and acceptors.

A number of core 2 GlcNAc transferases have been identified and cloned: Core 2 GnT1 (Core 2 GnT, Core 2 GnT-L, Core 2L/T1); Core 2 GnT2 (Core 2/4 GnT, Core 2 GnT-M, Core 2b/T2/M); and Core 2 GnT3 (Core 2c/T3) (Bierhuizen, I. and Fukuda, M. 1999, Proc. Natl. Acad, Sci. U.S.A. 89, 9326-9330; Schwientek, T. et al,

1999, J. Biol. Chem. 274, 4504-4512; Yeh, J.C. et al, 1999, J. Biol. Chem. 274, 3215-3221; and Schwientek et al, 2000, J. Biol. Chem. 275, 11106-11113). Acceptors for Core 2 GnT-M include oligosaccharides, glycoproteins, O-linked core 1-glycopeptides, and glycosphingolipids comprising the sequences Galβ1-3GalNAc, or Glcβ1-3GalNAc. Acceptors for Core 2 GnT3 include oligosaccharides, glycoproteins, O-linked core 1 and core 3-glycopeptides, and glycosphingolipids comprising the sequences Galβ1-3GalNAc, GlcNAc 1-3GalNAc, or Glc 1-3GalNAc.

In preferred embodiments of the invention, the glycosyltransferases are GnT1, GnTV, Core 2L/T1, Core 2b/T2/M, Core 2c/T3, and Core 3; and the invention provides preferred models and structures for these enzymes and methods of using the models and structures.

A glycosyltransferase or part thereof in the present invention may be a wild type enzyme, or part thereof, or a mutant, variant or homologue of such an enzyme.

The term "wild type" refers to a polypeptide having a primary amino acid sequence which is identical with the native enzyme (for example, the mammalian enzyme).

The term "mutant" refers to a polypeptide having a primary amino acid sequence which differs from the wild type sequence by one or more amino acid additions, substitutions or deletions. Preferably, the mutant has at least 90% sequence identity with the wild type sequence. Preferably, the mutant has 20 mutations or less over the whole wild-type sequence. More preferably the mutant has 10 mutations or less, most preferably 5 mutations or less over the whole wild-type sequence. A mutant may or may not be functional.

The term "variant" refers to a naturally occurring polypeptide which differs from a wild-type sequence. A variant may be found within the same species (i.e. if there is more than one isoform of the enzyme) or may be found within a different species. Preferably the variant has at least 90% sequence identity with the wild type sequence. Preferably, the variant has 20 mutations or less over the whole wild-type sequence. More preferably, the variant has 10 mutations or less, most preferably 5 mutations or less over the whole wild-type sequence.

The term "part" indicates that the polypeptide comprises a fraction of the wild-type amino acid sequence. It may comprise one or more large contiguous sections of sequence or a plurality of small sections. The "part" may comprise a ligand binding domain as described herein. The polypeptide may also comprise other elements of sequence, for example, it may be a fusion protein with another protein. Preferably the polypeptide comprises at least 50%, more preferably at least 65%, most preferably at least 80% of the wild-type sequence.

The term "homologue" means a polypeptide having a degree of homology with the wild-type amino acid sequence. The term "homology" can be equated with "identity".

In the present context, a homologous sequence is taken to include an amino acid sequence which may be at least 75, 85 or 90% identical, preferably at least 95 or 98% identical to the wild-type sequence. Typically, the homologues will comprise the same sites (for example, ligand binding domains) as the subject amino acid sequence. Although homology can also be considered in terms of similarity (i.e. amino acid residues having similar chemical properties/functions), in the context of the present invention it is preferred to express homology in terms of sequence identity.

Homology comparisons can be conducted by eye, or more usually, with the aid of readily available sequence comparison programs. These commercially available computer programs can calculate % homology between two or more sequences (e.g. Wilbur, W.J. and Lipman, D. J. Proc. Natl. Acad. Sci. USA (1983), 80:726-730).

The term "function" refers to the ability of a modulator to enhance or inhibit the association between a glycosyltransferase and a ligand or substrate, or the activity of the glycosyltransferase.

"Ligand binding domain" refers to a region of a molecule or molecular complex that as a result of its shape, favourably associates with a ligand or a part thereof. For example, it may be a region of a glycosyltransferase that is responsible for binding a ligand, substrate, or known modulator. With reference to the models and structures of the invention, residues in a ligand binding domain may be defined by their spatial proximity to a ligand in the model or structure.

The term "ligand binding domain" includes homologues of a ligand binding domain or portions thereof. As used herein, the term "homologue" in reference to a ligand binding domain refers to a ligand binding domain or a portion thereof which may have deletions, insertions or substitutions of amino acid residues as long as the binding specificity of the molecule is retained. In this regard, deliberate amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues as long as the binding specificity of the ligand binding domain is retained.

As used herein, the term "portion thereof" means the structural coordinates corresponding to a sufficient number of amino acid residues of a glycosyltransferase ligand binding domain (or homologues thereof) that are capable of associating or interacting with a ligand, substrate, modulator, or test compound that binds to the ligand binding domain. This term includes glycosyltransferase ligand binding domain amino acid residues having amino acid residues from about 4Å to about 5Å of a bound compound or fragment thereof. Thus, for example, the structural coordinates provided in the structure may contain a subset of the amino acid residues in the ligand binding domain which may be useful in the modeling and design of compounds that bind to the ligand binding domain.

A ligand binding domain may be defined by its association with a ligand. With reference to the structures and models of the invention, residues in the ligand binding domain may be defined by their spatial proximity to a ligand. For example, such may be defined by their proximity to a substrate or modulator.

"Ligand" refers to a compound or entity that associates with a ligand binding domain, including substrates or analogues or parts thereof. A ligand may be designed rationally using a model according to the invention. A ligand may be a modulator.

"Modulator" refers to a molecule which changes or alters the biological activity of a glycosyltransferase. A modulator may increase or decrease glycosyltransferase activity, or change its characteristics, or functional or immunological properties. It may be an inhibitor that decreases the biological or immunological activity of the protein. A modulator may include but is not limited to peptides, members of random peptide libraries and combinatorial chemistry-derived molecular libraries, phosphopeptides (including members of random or partially degenerate, directed phosphopeptide libraries), antibodies, carbohydrates, monosaccharides, oligosaccharides, polysaccharides, glycolipids, heterocyclic compounds, nucleosides or nucleotides or parts thereof, and small organic or inorganic molecules. A modulator may be an endogenous physiological compound or it may be a natural or synthetic compound. The term "modulator" also includes a chemically modified ligand or compound, and includes isomers and racemic forms.

The term "structural coordinates" as used herein refers to a set of values that define the position of one or more amino acid residues or molecules with reference to a system of axes. A data set of structural coordinates defines the three dimensional structure of a molecule or molecules. Structural coordinates can be slightly modified and still render nearly identical three dimensional structures. A measure of a unique set of structural coordinates is

the root-mean-square deviation of the resulting structure. Structural coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 2 Å, preferably less than 0.5 Å, more preferably less than 0.3 Å, may be viewed by a person of ordinary skill in the art as identical.

Variations in structural coordinates may be generated because of mathematical manipulations of the structural coordinates of a glycosyltransferase described herein. For example, the structural coordinates of Tables 1-8 and 14-23 may be manipulated by crystallographic permutations of the structural coordinates, fractionalization of the structural coordinates, integer additions or substractions to sets of the structural coordinates, inversion of the structural coordinates or any combination of the above.

Variations in structure due to mutations, additions, substitutions, and/or deletions of the amino acids, or other changes in any of the components that make up a structure of the invention may also account for modifications in structural coordinates. If such modifications are within an acceptable standard error as compared to the original structural coordinates, the resulting structure may be the same. Therefore, a ligand that bound to a ligand binding domain of a glycosyltransferase would also be expected to bind to another ligand binding domain whose structural coordinates defined a shape that fell within the acceptable error. Such modified structures of a ligand binding domain are also within the scope of the invention.

Various computational analyses may be used to determine whether a ligand or a ligand binding domain thereof is sufficiently similar to all or parts of a ligand or ligand binding domain of the invention. Such analyses may be carried out using conventional software applications and methods as described herein.

The term "modeling" includes the quantitative and qualitative analysis of molecular structure and/or function based on atomic structural information and interaction models. The term includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry, and other structure-based constraint models. Preferably modeling is performed using a computer and may be optimized using known methods. This is called modeling optimization.

The term "substrate" refers to molecules that associate with a glycosyltransferase as it catalyzes the transfer of a selected sugar from a nucleotide sugar donor to an acceptor that leads to the formation of a new glycosidic linkage. A substrate includes the nucleotide sugar donor and acceptor and parts thereof.

A "sugar nucleotide donor" refers to a nucleotide coupled to a selected sugar that is transferred by a glycosyltransferase to an acceptor. The selected sugar may be a monosaccharide or disaccharide, preferably a monosaccharide. A suitable selected sugar includes GlcNAc. The GlcNAc may be modified for example, the hydroxyls may be blocked with acetonide, acylated, or alkylated or substituted with other groups such as halogen. The nucleotide is preferably UDP. The heterocyclic amine base in the nucleotide may be modified. For example, when the base is uridine it may be modified at the C-5 or C-6 position with groups including but not limited to alkyl, aryl, gallic acid, and with electron donating and electron withdrawing groups. The sugar in the nucleotide (e.g. ribose) may be modified at the 2' or 3' position with groups including but not limited to alkyl, aryl, gallic acid, and with electron donating and electron withdrawing groups.

An "acceptor" refers to the part of a carbohydrate structure (e.g. glycoprotein, glycolipid) where the selected sugar of a sugar nucleotide donor is transferred by the glycosyltransferase.

The term "alkyl", alone or in combination, refers to a branched or linear hydrocarbon radical, typically containing from 1 through 20 carbon atoms, preferably 1 through 10 carbon atoms, more preferably 1 to 6 carbon

atoms. Typical alkyl groups include but are not limited to methyl, ethyl, 1-propyl, 2-propyl, 1-butyl, 2-butyl, tert-butyl, pentyl, hexyl, heptyl, octyl, nonyl, decyl, and the like.

The term "alkenyl", alone or in combination, refers to an unsaturated branched or linear group typically having from 2 to 20 carbon atoms and at least one double bond. Examples of such groups include but are not limited to ethenyl, 1-propenyl, 2-propenyl, 1-butenyl, 1,3-butadienyl, 1-hexenyl, 2-hexenyl, 1-pentenyl, 2-pentenyl, and the like.

The term "alkynyl", alone or in combination, refers to an unsaturated branched or linear group having 2 to 20 carbon atoms and at least one triple bond. Examples of such groups include but are not limited to ethynyl, 1-propynyl, 2-propynyl, 1-butynyl, 2-butynyl, 1-pentynyl, and the like.

The term "cycloalkyl" refers to cyclic hydrocarbon groups and includes but is not limited to cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, cycloheptyl, and cyclooctyl.

The term "aryl", alone or in combination, refers to a monocyclic or polycyclic group, preferably a monocyclic or bicyclic group. An aryl group may optionally be substituted as described herein. Examples of aryl groups and substituted aryl groups are phenyl, benzyl, p-nitrobenzyl, p-methoxybenzyl, biphenyl, and naphthyl.

The term "alkoxy" alone or in combination, refers to an alkyl or cycloalkyl linked to the parent molecular moiety through an oxygen atom. The term "aryloxy" refers to an aryl linked to the parent molecular moiety through an oxygen atom. Examples of alkoxy groups are methoxy, ethoxy, propoxy, vinyloxy, allyloxy, butoxy, pentoxy, hexoxy, cyclopentoxy, and cyclohexoxy. Examples of aryloxy groups are phenyloxy, O-benzyl i.e. benzyloxy, O-p-nitrobenzyl and O-p-methyl-benzyl, 4-nitrophenyloxy, 4-chlorophenyloxy, and the like.

The term "halo" or "halogen", alone or in combination, means fluoro, chloro, bromo, or iodo.

The term "amino", alone or in combination, refers to a chemical functional group where a nitrogen atom (N) is bonded to three substituents being any combination of hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, or aryl with the general chemical formula $-NR_{14}R_{16}$ where R_{14} and R_{16} can be any combination of hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, or aryl. Optionally one substituent on the nitrogen atom can be a hydroxyl group (-OH) to give an amine known as a hydroxylamine. Examples of amino groups are amino ($-NH_2$), methylamine, ethylamine, dimethylamine, 2-propylamine, butylamine, isobutylamine, cyclopropylamine, benzylamine, allylamine, hydroxylamine, cyclohexylamino ($-NHCH(CH_2)_5$), piperidine ($-N(CH_2)_5$) and benzylamino ($-NHCH_2C_6H_5$).

The term "thioalkyl", alone or in combination, refers to a chemical functional group where a sulfur atom (S) is bonded to an alkyl. Examples of thioalkyl groups are thiomethyl, thioethyl, and thiopropyl.

The term "thioaryl", alone or in combination, refers to a chemical functional group where a sulfur atom (S) is bonded to an aryl group with the general chemical formula $-SR_{16}$ where R_{16} is an aryl group which may be substituted. Examples of thioaryl groups and substituted thioaryl groups are thiophenyl, para-chlorothiophenyl, thiobenzyl, 4-methoxy-thiophenyl, 4-nitro-thiophenyl, and para-nitrothiobenzyl.

Heterocyclic rings are molecular rings where one or more carbon atoms have been replaced by hetero atoms (atoms not being carbon) such as for example, oxygen (O), nitrogen (N) or sulfur (S), or combinations thereof. Examples of heterocyclic rings include ethylene oxide, tetrahydrofuran, thiophene, piperidine (piperidinyl group), pyridine (pyridinyl group), and caprolactam. A carbocyclic or heterocyclic group may be optionally substituted at carbon or nitrogen atoms with for example, alkyl, phenyl, benzyl or thienyl, or a carbon atom in the heterocyclic group together with an oxygen atom may form a carbonyl group, or a heterocyclic group may be fused with a phenyl group.

"Antibody" includes intact monoclonal or polyclonal molecules, and immunologically active fragments (e.g. a Fab or $(Fab)_2$ fragment), an antibody heavy chain, an antibody light chain, a genetically engineered single chain F_V molecule (Ladner et al, U.S. Pat. No. 4,946,778), a humanized antibody or a chimeric antibody, for example, an antibody which contains the binding specificity of a murine antibody, but in which the remaining portions are of human origin. Antibodies including monoclonal and polyclonal antibodies, fragments and chimeras, may be prepared using methods known to those skilled in the art. Antibodies that bind a peptide of the invention can be prepared using intact peptides or fragments containing an immunizing antigen of interest. The polypeptide or oligopeptide used to immunize an animal may be obtained from the translation of RNA or synthesized chemically and can be conjugated to a carrier protein, if desired. Suitable carriers that may be chemically coupled to peptides include bovine serum albumin and thyroglobulin, and keyhole limpet hemocyanin. The coupled peptide may then be used to immunize the animal (e.g., a mouse, a rat, or a rabbit).

By being "derived from" a ligand binding domain is meant any molecular entity which is identical or substantially equivalent to a native ligand binding domain of a molecule i.e. a loop structure of a glycosyltransferase. A peptide derived from a specific ligand binding domain may encompass the amino acid sequence of a naturally occurring ligand binding domain, any portion of that domain, or other molecular entity that functions to associate with an associated molecule. A peptide derived from such a ligand binding domain will interact directly or indirectly with an associated molecule in such a way as to mimic a native ligand binding domain. Such peptides may include competitive inhibitors, peptide mimetics, and the like.

"Peptide mimetics" are structures which serve as substitutes for peptides in interactions between molecules (See Morgan et al (1989), Ann. Reports Med. Chem. 24:243-252 for a review). Peptide mimetics include synthetic structures which may or may not contain amino acids and/or peptide bonds but retain the structural and functional features of a peptide, or agonist, or antagonist. Peptide mimetics also include peptoids, oligopeptoids (Simon et al (1972) Proc. Natl. Acad, Sci USA 89:9367); and peptide libraries containing peptides of a designed length representing all possible sequences of amino acids corresponding to a peptide, or agonist or antagonist of the invention.

Three Dimensional Structure of Glycosyltransferases and Binding Domains of Same

The present invention provides a glycosyltransferase secondary, tertiary and/or quanternary structure. The invention also provides a homology model that represents the secondary, tertiary, and/or quanternary structure of a glycosyltransferase. A model may, for example, be a structural model (or representation thereof), or a computer model. The model itself may be in two or three dimensions. It is possible for a computer model to be in three dimensions despite the constraints imposed by a conventional computer screen, if it is possible to scroll along at least a pair of axes, causing "rotation" of the image. A model or structure of a glycosyltransferase may be defined by the structural coordinates of each of Tables 1 through 8.

In accordance with an aspect of the invention a method is provided for designing a homology model of a ligand binding domain of a glycosytransferase wherein the homology model may be displayed as a three-dimensional image, the method comprising:

(i) providing an amino acid sequence and structural coordinates of a ligand binding domain structure of a glycosyltransferase, preferably a GnT1 glycosytransferase;

(ii) modifying said structure to take into account differences between the amino acid configuration of the ligand binding domains of the glycosyltransferase on the one hand and the glycosyltransferase on the other hand to generate a homology model, and

(iii) if required refining the homology model.

The method may further comprise comparing the homology model with the structures of other, similar, proteins.

Models or structures of preferred glycosyltransferases of the invention comprise the following atomic structural coordinates:

Table 1 – Structural coordinates for GnT1.

Table 2 – Structural coordinates for GnTV.

Table 3 – Structural coordinates for core 2L or T1 (human).

Table 4 – Structural coordinates for core 2L or T1(mouse)

Table 5 – Structural coordinates for core 2L (bovine)

Table 6 – Structural coordinates for core 2b/core M/core 2 T2.

Table 7 – Structural coordinates for core 2C (human)

Table 8 – Structural coordinates for core 3.

Computer representations of exemplary structures or models of the invention are illustrated in the Figures. For example, Figure 6 illustrates homology models for GnTV, Core 2L, and Core 2b/M; Figure 17 shows a superimposition of main chain atoms of various structures; Figure 20 shows a homology model of GnTV; and Figure 25b shows a Core 2L model.

The structural coordinates in a structure or model of the invention may comprise the amino acid residues of a glycosyltransferase ligand binding domain, or a portion or homolog thereof useful in the modeling and design of test compounds capable of binding to the glycosyltransferase. Therefore, the invention also relates to a secondary, tertiary, or quanternary structure or model of a ligand binding domain of a glycosyltransferase. Ligand binding domains include the ligand binding domains for a disphosphate group of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a nitrogeneous heterocyclic base (preferably a pyrimidine base, more preferably uracil) of a sugar nucleotide donor, and/or a sugar (e.g. GlcNAc) of a sugar nucleotide donor.

A structure of a ligand binding domain may be defined by selected atomic interactions or contacts in the ligand binding domain, as follows:

(a) one or more of atomic interactions or atomic contacts for GnT1 shown in Table 10;

(b) one or more of atomic interactions or atomic contacts for GnTV shown in Table 11;

(c) one or more of atomic interactions or atomic contacts for Core 2L/T1 shown in Table 12; or

(d) one or more of atomic interactions or atomic contacts for Core 2b/T shown in Table 13.

Computer representations of exemplary structures or models of ligand binding domains (and ligands) of the invention are illustrated in the Figures. For example, Figures 18, 22, 25a, 26, and 27 show models of a UDP ligand binding domain; Figures 21, 23, 24, 28 show models of a UDP-GlcNAc ligand binding domain; and Figure 29 shows a sugar ligand binding domain.

It is understood that a structure or model of the invention includes a structure where at least one amino acid residue is replaced with a different amino acid residue or by adding or deleting amino acid residues, and having substantially the same three dimensional structure as the glycosyltransferase as described herein, or the ligand

binding domains as described herein, i.e. having a set of atomic structural coordinates that have a root mean square deviation of less than or equal to about 2Å, preferably less than 0.5Å, most preferably less than 0.3Å, when superimposed with the atomic structure coordinates of a glycosyltransferase as described herein or a ligand binding domain as described herein when at least 50% to 100% of the atoms of the ligand binding domain or binding domains of components thereof as the case may be, are included in the superimposition.

The invention also features a secondary, tertiary, or quanternary structure or model of a glycosyltransferase in association with one or more molecules (e.g. substrates such as UDP-GlcNac, uridine-ribose, monophophate-Mn^{2+}, or diphosphate-Mn^{2+}). The association may be covalent or non-covalent. The molecule may be any organic molecule, and it may modulate the function of a glycosyltransferase by, for example, inhibiting or enhancing its function, or it may be an acceptor or donor for the glycosyltransferase. It is preferred that the geometry of the compound and the interactions formed between the compound and the glycosyltransferase provide high affinity binding between the two molecules.

The structure and model of a glycosyltransferase decribed herein has allowed the identification and characterization of ligand binding domains of UDP and UDP-GlcNAc. The UDP-GlcNAc binding domain has been subdivided into sub-sites (the uracil binding domain, ribose binding domain, pyrophosphate binding domain, GlcNAc binding domain) and characterized.

In an embodiment of the invention, a secondary, tertiary, and/or quanternary structure or model of a ligand binding domain of a glycosyltransferase that associates with a diphosphate of a sugar nucleotide donor is provided comprising (a) atomic interaction 7 listed in Table 10 (GnT1 Table); (b) at least two of atomic interactions 9, 10, 11, 12, and 13 listed in Table 12 (Core 2L Table); (c) at least two of atomic interactions 11, 12, 13, 14, or 15 listed in Table 13 (Core2b/M); or (d) atomic interaction 8 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the diphosphate of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase. Preferably, a ligand binding domain is defined by atomic interaction 7 listed in Table 10 (GnT1 Table); atomic interactions 9, 10, 11, 12, and 13 listed in Table 12 (Core 2L Table), atomic interactions 11, 12, 13, 14, and 15 listed in Table 13 (Core2b/M), or atomic interaction 8 listed in Table 11 (GNTV Table). Most preferably, a ligand binding domain is defined by the atoms of the amino acid residues of the atomic interactions having the structural coordinates for the atoms listed in Table 1 for GnT1, Table 3, 4, or 5 for Core 2L, Table 6 for Core 2b(M), and Table 2 for GnTV.

The three dimensional structure of a complex of a ligand binding domain of a glycosyltransferase in association with a disphosphate can also be defined as described above.

In an embodiment of the invention, a secondary, tertiary, and/or quanternary structure or model of a ligand binding domain of a glycosyltransferase that associates with a heterocyclic amine base (preferably uracil) of a sugar nucleotide donor is provided comprising at least two of the following atomic interactions (a) 1, 2, 3, and 4 listed in Table 10 (GnT1 Table); (b) 1, 2, 3, 4, and 5 listed in Table 12 (Core 2L Table); (c) 1, 2, 3, and 4 listed in Table 13 (Core2b/M); or (d) 1, 2, 3, and 4 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the heterocyclic amine base of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase. Preferably, a ligand binding domain is defined by atomic interactions 1, 2, 3, and 4 listed in Table 10 (GnT1 Table); atomic interactions 1, 2, 3, 4, and 5, listed in Table 12 (Core 2L Table), atomic interactions 1, 2, 3, and 4 listed in Table 13 (Core2b/M), or atomic interactions 1, 2, 3, and 4, listed in Table 11 (GNTV Table). Most preferably, a ligand

binding domain is defined by the atoms of the amino acid residues in the atomic interactions having the structural coordinates for the atoms listed in Table 1 for GnT1, Table 3, 4, or 5 for Core 2L, Table 6 for Core 2b(M), and Table 2 for GnTV. The three dimensional structure of a complex of a ligand binding domain of a glycosyltransferase in association with a heterocyclic amine base (preferably uracil) can also be defined as described above.

In an embodiment of the invention, a secondary, tertiary, and/or quanternary structure or model of a ligand binding domain of a glycosyltransferase that associates with the sugar (preferably ribose) of the nucleotide of a sugar nucleotide donor is provided comprising atomic interaction 5 or 6 listed in Table 10 (GnT1 Table); at least two of atomic interactions 6, 7, and 8 listed in Table 12 (Core 2L Table), or atomic interaction 5 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the sugar of the nucleotide of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase. Preferably, a ligand binding domain is defined by atomic interactions 5 and 6 listed in Table 10 (GnT1 Table); atomic interactions 6, 7, and 8 listed in Table 12 (Core 2L Table), or atomic interaction 5 listed in Table 11 (GNTV Table). Most preferably, a ligand binding domain is defined by the atoms of the amino acid residues in the atomic interactions having the structural coordinates for the atoms listed in Table 1 for GnT1, Table 3, 4, or 5 for Core 2L, Table 6 for Core 2b(M), and Table 2 for GnTV. The three dimensional structure of a complex of a ligand binding domain of a glycosyltransferase in association with a sugar (preferably ribose) can also be defined as described above.

In an embodiment of the invention, a secondary, tertiary, and/or quanternary structure or model of a ligand binding domain of a glycosyltransferase that associates with the sugar (GlcNAc) of a sugar nucleotide donor is provided comprising at least two of atomic interactions 8, 9, 10, 11, and 12 listed in Table 10 (GnT1 Table); at least two of atomic interactions 14, 15, 16, 17, and 18 listed in Table 12 (Core 2L Table), atomic interactions 16 or 17 listed in Table 13 (Core2b/M), or at least two of atomic interactions 9, 10, 11, 12, and 13 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the sugar of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase. Preferably, the ligand binding domain is defined by atomic interactions 8, 9, 10, 11 and 12 listed in Table 10 (GnT1 Table); atomic interactions 14, 15, 16, 17, and 18 listed in Table 12 (Core 2L Table); atomic interactions 16 and 17 listed in Table 13 (Core2b/M), or atomic interactions 9, 10, 11, 12, and 13 listed in Table 11 (GNTV Table). Most preferably, a ligand binding domain is defined by the atoms of the amino acid residues in the atomic interactions having the structural coordinates for the atoms listed in Table 1 for GnT1, Table 3, 4, or 5 for Core 2L, Table 6 for Core 2b(M), and Table 2 for GnTV. The three dimensional structure of a complex of a ligand binding domain of a glycosyltransferase in association with a sugar (GlcNAc) of a sugar nucleotide donor can also be defined as described above.

A secondary, tertiary, and/or quanternary structure or model of a ligand binding domain of a glycosyltransferase that binds UDP is provided characterized by (a) a hydrogen bond between an Asp side chain of the glycosyltransferase with position 3 of the uracil ring of UDP; (b) a stacking interaction between either a disulfide or an aromatic group (Phe or Tyr) of the glycosyltransferase and the uracil ring of the UDP; (c) a stacking interaction between either an Ile or a Thr of the glycosyltransferase and the ribose ring of the UDP; and (d) metal mediated charge interactions between a well-conserved Asp/Glu of the glycosyltransferase and a pyrophosphate oxygen of the UDP.

In an embodiment of the invention, a secondary, tertiary, and/or quanternary structure or model of a ligand binding domain of a glycosyltransferase that associates with a nucleotide (preferably UDP) of a sugar nucleotide donor is provided comprising at least two of (a) atomic interactions 1, 2, 3, 4, 5, 6, and 7 listed in Table 10 (GnT1 Table); (b) atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13 listed in Table 12 (Core 2L Table); (c) atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14 and 15 listed in Table 13 (Core2b/M); or (d) atomic interactions 1, 2, 3, 4, 5, 6, 7, and 8, listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the nucleotide of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase. Preferably, a ligand binding domain is defined by atomic interactions 1, 2, 3, 4, 5, 6, and 7 listed in Table 10 (GnT1 Table); atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13 listed in Table 12 (Core 2L Table); atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, and 15 listed in Table 13 (Core2b/M); or, atomic interactions 1, 2, 3, 4, 5, 6, 7, and 8 listed in Table 11 (GNTV Table). Most preferably, a ligand binding domain is defined by the atoms of the amino acid residues in the atomic interactions having the structural coordinates for the atoms listed in Table 1 for GnT1, Table 3, 4, or 5 for Core 2L, Table 6 for Core 2b(M), and Table 2 for GnTV. The three dimensional structure of a complex of the ligand binding domain of a glycosyltransferase in association with a nucleotide (e.g. UDP) of a sugar nucleotide donor can also be defined as described above.

In an embodiment of the invention, a secondary, tertiary, and/or quanternary structure or model of a ligand binding domain of a glycosyltransferase that associates with a sugar nucleotide donor (e.g. UDP-GlcNAc) is provided comprising at least two of (a) atomic interactions 1, 2,3, 4, 5, 6, 7, 8, 9, 10, 11, and 12 listed in Table 10 (GnT1 Table); (b) atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, and 18 listed in Table 12 (Core 2L Table); (c) atomic interactions 1, 2, 3, 4, 5, 6, 9, 10, 11, 12, 13, 14, 15, 16, and 17 listed in Table 13 (Core2b/M), or (d) atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase. Preferably, a ligand binding domain is defined by atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, and 12 listed in Table 10 (GnT1 Table); atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, and 18 listed in Table 12 (Core 2L Table); atomic interactions 1, 2, 3, 4, 5, 6, 9, 10, 11, 12, 13, 14, 15, 16, and 17 listed in Table 13 (Core2b/M); or atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13 listed in Table 11 (GNTV Table). Most preferably, a ligand binding domain is defined by the atoms of the amino acid residues in the atomic interactions having the structural coordinates for the atoms listed in Table 1 for GnT1, Table 3, 4, or 5 for Core 2L, Table 6 for Core 2b(M), and Table 2 for GnTV. The three dimensional structure of a complex of a ligand binding domain of a glycosyltransferase in association with a sugar nucleotide donor (e.g. UDP-GlcNAc) can also be defined as described above.

The three dimensional structure of glycostyltransferases are characterized by a "loop" structure. The loop folds on top of the pyrophosphate after the sugar nucleotide donor associates with the active site of the glycosyltransferase. The loop has a similar amino acid motif in glycosyltransferases but in Core 2 transferases the loop is hydrophilic and in GNT1 and GNTV the loop is hydrophobic. Molecules that associate with the loop are highly specific inhibitors of the enzymes. In an embodiment of the invention, a secondary, tertiary, or quanternary structure or model of a loop structure of a glycosyltransferase that binds a pyrophosphate of a sugar nucleotide donor

is provided comprising the structural coordinates for the loop structure of GnT1 listed in Table 21; Core 2L listed in Table 22; or GnTV listed in Table 23.

Figure 32 illustrates a model of the pyrophosphate of UDP-GlcNAc interacting with the loop structure of Core 2L.

Transition State Ligand Binding Domains

The invention also provides a secondary, tertiary, and/or quanternary structure or model of a ligand binding domain of a transition state of a reaction catalyzed by a glycosyltransferase. In particular, the invention provides a secondary, tertiary, and/or quanternary structure or model of a sugar transition state ligand binding domain, preferably a GlcNAc transition state ligand binding domain, of a glycosyltransferase comprising a hydrophobic pocket that is 1.9 to 3.5 Å, preferably 2.2 to 3.0Å, from the pyrophosphate binding cavity for the glycosyltransferase. The amino acid residues in the domain that associate with the C2 and C4 positions of the sugar preferably have the structural coordinates of Leu-331, and Leu 269 in Table 1 (GNT1 Table), or the structural coordinates of Leu –116 and Val-81 of Table 3, 4, or 5 (Core 2L coordinates).

The sugar transition ligand binding domain preferably comprises atomic interactions 14 to 18 in Table 12 (Core 2L Table) or atomic interactions 9 to 12 of Table 10 (GnT1 Table), or the particular structural coordinates for the atomic contacts of the atomic interactions as set out in Tables 1 (GnT1) or 3, 4, or 5 (Core 2L).

Figure 31 shows a model of the binding of GlcNAc to the transition state of Core 2L showing a hydrophobic ligand binding domain.

Identification of Homologues

The knowledge of the structures and models of the invention enables one skilled in the art to identify homologues of glycosyltransferases. This is achieved by searches of three-dimensional databases. Since structural folds are conserved to a greater extent than sequence, one may identify homologues with very little sequence identity or similarity. Programs that provide this type of database searching are known in the art and include Dal and the Fold recognition server located at UCLA (8). The structural coordinates of a protein structure are submitted and the program performs a multiple structural alignment with proteins in the protein data bank. Homologues identified in accordance with the present invention may be used in the methods of the invention described herein.

Computer Format of Structures/Models

Information derivable from the structures of the present invention (for example the structural coordinates) or a model of the present invention may be provided in a computer-readable format.

Therefore, the invention provides a computer readable medium or a machine readable storage medium which comprises the models of the invention or structural coordinates of a glycosyltransferase including all or any parts of the glycosyltransferase (e.g ligand binding domain), ligands including portions thereof, or substrates including portions thereof. Such storage medium or storage medium encoded with these data are capable of displaying on a computer screen or similar viewing device, a three-dimensional graphical representation of a molecule or molecular complex which comprises the enzyme or ligand binding domains or similarly shaped homologous enzymes or ligand binding domains. Thus, the invention also provides computerized representations of a model or structure of the invention, including any electronic, magnetic, or electromagnetic storage forms of the data needed to define the structures such that the data will be computer readable for purposes of display and/or manipulation.

In an aspect the invention provides a computer for producing a model or three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a glycosyltransferase or ligand binding domain thereof defined by structural coordinates of glycosyltransferase amino acids or a ligand binding domain thereof, or comprises structural coordinates of atoms of a ligand or substrate, or a three-dimensional representation of a homologue of said molecule or molecular complex, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates of glycosyltransferase amino acids according to any one of Tables 1-8 or a ligand binding domain thereof according to Table 21, 22, or 23, or a ligand according to any one of Tables 14-20;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

A homologue may comprise a glycosyltransferase or ligand binding domain thereof, or ligand or substrate that has a root mean square deviation from the backbone atoms of not more than 1.5 angstroms.

The invention also provides a computer for determining at least a portion of the structural coordinates corresponding to an X-ray diffraction pattern of a molecule or molecular complex wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates according to any one of Tables 1-8, and 14-23;

(b) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises an X-ray diffraction pattern of said molecule or molecular complex;

(c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);

(d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structural coordinates; and

(e) a display coupled to said central-processing unit for displaying said structural coordinates of said molecule or molecular complex.

The invention also contemplates a computer programmed with a homology model of a ligand binding domain according to the invention; a machine-readable data-storage medium on which has been stored in machine-readable form a homology model of a ligand binding domain of a glycosyltransferase; and the use of a homology model as input to a computer programmed for drug design and/or database searching and/or molecular graphic imaging in order to identify new ligands or modulators for glycosyltransferases.

Structural Determinations

The present invention also provides a method for determining the secondary and/or tertiary structures of a polypeptide by using a model according to the invention. The polypeptide may be any polypeptide for which the

secondary and or tertiary structure is uncharacterised or incompletely characterised. In a preferred embodiment the polypeptide shares (or is predicted to share) some structural or functional homology to a glycosyltransferase. For example, the polypeptide may show a degree of structural homology over some or all parts of the primary amino acid sequence. For example the polypeptide may have one or more domains which show homology with a glycosyltransferase domain.

The polypeptide may be a glycosyltransferase with a different specificity for a ligand or substrate. The polypeptide may be a glycosyltransferase which requires a different metal cofactor. Alternatively (or in addition) the polypeptide may be a glycosyltransferase from a different species.

The polypeptide may be a mutant of the wild-type glycosyltransferase. A mutant may arise naturally, or may be made artificially (for example using molecular biology techniques). The mutant may also not be "made" at all in the conventional sense, but merely tested theoretically using the model of the present invention. A mutant may or may not be functional.

Thus, using a model of the present invention, the effect of a particular mutation on the overall two and/or three dimensional structure of a glycosyltransferase and/or the interaction between the enzyme and a ligand or substrate can be investigated. Alternatively, the polypeptide may perform an analogous function or be suspected to show a similar catalytic mechanism to the glycosyltransferase enzyme. For example, the polypeptide may transfer a sugar residue from a sugar nucleotide donor.

The polypeptide may also be the same as a polypeptide described herein, but in association with a different ligand (for example, modulator or inhibitor) or cofactor. In this way it is possible to investigate the effect of altering a ligand or compound with which the polypeptide is associated on the structure of a ligand binding domain.

Secondary or tertiary structure may be determined by applying the structural coordinates of the model of the present invention to other data such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Homology modeling, molecular replacement, and nuclear magnetic resonance methods using these other data sets are described below.

Homology modeling (also known as comparative modeling or knowledge-based modeling) methods develop a three dimensional model from a polypeptide sequence based on the structures of known proteins (e.g. native or mutated glycosyltransferases). In the present invention the method utilizes a computer representation of the structure of a glycosyltransferase, or a binding domain or complex of same as described herein, a computer representation of the amino acid sequence of a polypeptide with an unknown structure (additional native or mutated glycosyltransferases), and standard computer representations of the structures of amino acids. The method in particular comprises the steps of; (a) identifying structurally conserved and variable regions in the known structure; (b) aligning the amino acid sequences of the known structure and unknown structure (c) generating coordinates of main chain atoms and side chain atoms in structurally conserved and variable regions of the unknown structure based on the coordinates of the known structure thereby obtaining a homology model; and (d) refining the homology model to obtain a three dimensional structure for the unknown structure. This method is well known to those skilled in the art (Greer, 1985, Science 228, 1055; Bundell et al 1988, Eur. J. Biochem. 172, 513; Knighton et al., 1992, Science 258:130-135, http://biochem.vt.edu/courses/modeling/ homology.htn). Computer programs that can be used in homology modeling are Quanta and the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc, or MODELLER (Rockefeller University, www.iucr.ac.uk/sinris-top/logical/prg-modeller.html).

In step (a) of the homology modeling method, a known glycosyltransferase structure is examined to identify the structurally conserved regions (SCRs) from which an average structure, or framework, can be constructed for these regions of the protein. Variable regions (VRs), in which known structures may differ in conformation, also must be identified. SCRs generally correspond to the elements of secondary structure, such as alpha-helices and beta-sheets, and to ligand- and substrate-binding sites (e.g. acceptor and donor binding sites). The VRs usually lie on the surface of the proteins and form the loops where the main chain turns.

Many methods are available for sequence alignment of known structures and unknown structures. Sequence alignments generally are based on the dynamic programming algorithm of Needleman and Wunsch [J. Mol. Biol. 48: 442-453, 1970]. Current methods include FASTA, Smith-Waterman, and BLASTP, with the BLASTP method differing from the other two in not allowing gaps. Scoring of alignments typically involves construction of a 20x20 matrix in which identical amino acids and those of similar character (i.e., conservative substitutions) may be scored higher than those of different character. Substitution schemes which may be used to score alignments include the scoring matrices PAM (Dayhoff et al., Meth. Enzymol. 91: 524-545, 1983), and BLOSUM (Henikoff and Henikoff, Proc. Nat. Acad. Sci. USA 89: 10915-`0919, 1992), and the matrices based on alignments derived from three-dimensional structures including that of Johnson and Overington (JO matrices) (J. Mol. Biol. 233: 716-738, 1993).

Alignment based solely on sequence may be used, though other structural features also may be taken into account. In Quanta, multiple sequence alignment algorithms are available that may be used when aligning a sequence of the unknown with the known structures. Four scoring systems (i.e. sequence homology, secondary structure homology, residue accessibility homology, CA-CA distance homology) are available, each of which may be evaluated during an alignment so that relative statistical weights may be assigned.

When generating coordinates for the unknown structure, main chain atoms and side chain atoms, both in SCRs and VRs need to be modeled. A variety of approaches may be used to assign coordinates to the unknown. In particular, the coordinates of the main chain atoms of SCRs will be transferred to the unknown structure. VRs correspond most often to the loops on the surface of the polypeptide and if a loop in the known structure is a good model for the unknown, then the main chain coordinates of the known structure may be copied. Side chain coordinates of SCRs and VRs are copied if the residue type in the unknown is identical to or very similar to that in the known structure. For other side chain coordinates, a side chain rotamer library may be used to define the side chain coordinates. When a good model for a loop cannot be found fragment databases may be searched for loops in other proteins that may provide a suitable model for the unknown. If desired, the loop may then be subjected to conformational searching to identify low energy conformers if desired.

Once a homology model has been generated it is analyzed to determine its correctness. A computer program available to assist in this analysis is the Protein Health module in Quanta which provides a variety of tests. Other programs that provide structure analysis along with output include PROCHECK and 3D-Profiler [Luthy R. et al, Nature 356: 83-85, 1992; and Bowie, J.U. et al, Science 253: 164-170, 1991]. Once any irregularities have been resolved, the entire structure may be further refined. Refinement may consist of energy minimization with restraints, especially for the SCRs. Restraints may be gradually removed for subsequent minimizations. Molecular dynamics may also be applied in conjunction with energy minimization.

The structural coordinates of a glycosyltransferase structure may be applied to nuclear magnetic resonance (NMR) data to determine the three dimensional structures of polypeptides in solution (e.g. additional native or mutated glycosyltransferases). (See for example, Wuthrich, 1986, John Wiley and Sons, New York: 176-199;

Pflugrath et al., 1986, J. Molecular Biology 189: 383-386; Kline et al., 1986 J. Molecular Biology 189:377-382). While the secondary structure of a polypeptide may often be determined by NMR data, the spatial connections between individual pieces of secondary structure are not as readily determined. The structural coordinates of a polypeptide can guide the NMR spectroscopist to an understanding of the spatical interactions between secondary structural elements in a polypeptide of related structure. Information on spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from two-dimensional NMR experiments. In addition, applying the structural coordinates after the determination of secondary structure by NMR techniques simplifies the assignment of NOE's relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure.

In an embodiment, the invention relates to a method of determining three dimensional structures of polypeptides with unknown structures, preferably a native or mutated glycosyltransferase, by applying the structural coordinates of a glycosyltransferase structure, or ligand binding domain or complex thereof described herein to nuclear magnetic resonance (NMR) data of the unknown structure. This method comprises the steps of: (a) determining the secondary structure of an unknown structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The term " through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence. The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

Screening Method

The present invention also provides a method of screening for a ligand that associates with a ligand binding domain and/or modulates the function of a glycosyltransferase, by using a structure or a model according to the present invention. The method may involve investigating whether a test compound is capable of associating with or binding a ligand binding domain.

In accordance with an aspect of the present invention, a method is provided for screening for a ligand capable of binding to a ligand binding domain, wherein said method comprises the use of a structure or model according to the invention.

In another aspect, the invention relates to a method of screening for a ligand capable of binding to a ligand binding domain, wherein the ligand binding domain is defined by the amino acid residue structural coordinates given herein, the method comprising contacting the ligand binding domain with a test compound and determining if said test compound binds to said ligand binding domain.

In one embodiment, the present invention provides a method of screening for a test compound capable of interacting with one or more key amino acid residue of the ligand binding domain of a glycosyltransferase.

Another aspect of the invention provides a process comprising the steps of:

(a) performing a method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a ligand binding domain; and

(c) preparing a quantity of said one or more ligands.

A further aspect of the invention provides a process comprising the steps of:

(a) performing the method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a ligand binding domain; and

(c) preparing a pharmaceutical composition comprising said one or more ligands.

Once a test compound capable of interacting with a key amino acid residue in a glycosyltransferase ligand binding domain has been identified, further steps may be carried out either to select and/or to modify compounds and/or to modify existing compounds, to modulate the interaction with key amino acid residues in the glycosyltransferase ligand binding domain.

Yet another aspect of the invention provides a process comprising the steps of:

(a) performing a method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a ligand binding domain;

(c) modifying said one or more ligands capable of binding to a ligand binding domain;

(d) performing said method of screening for a ligand as described above;

(e) optionally preparing a pharmaceutical composition comprising said one or more ligands.

As used herein, the term "test compound" means any compound which is potentially capable of associating with a ligand binding domain. If, after testing, it is determined that the test compound does bind to the ligand binding domain, it is known as a "ligand".

A "test compound" includes, but is not limited to, a compound which may be obtainable from or produced by any suitable source, whether natural or not. The test compound may be designed or obtained from a library of compounds which may comprise peptides, as well as other compounds, such as small organic molecules and particularly new lead compounds. By way of example, the test compound may be a natural substance, a biological macromolecule, or an extract made from biological materials such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic test compound, a semi-synthetic test compound, a carbohydrate, a monosaccharide, an oligosaccharide or polysaccharide, a glycolipid, a glycopeptide, a saponin, a heterocyclic compound, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised test compound, a peptide cleaved from a whole protein, or a peptide synthesised synthetically (such as, by way of example, either using a peptide synthesizer or by recombinant techniques or combinations thereof), a recombinant test compound, a natural or a non-natural test compound, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof.

The test compound may be screened as part of a library or a data base of molecules. Data bases which may be used include ACD (Molecular Designs Limited), NCI (National Cancer Institute), CCDC (Cambridge Crystallographic Data Center), CAST (Chemical Abstract Service), Derwent (Derwent Information Limited), Maybridge (Maybridge Chemical Company Ltd), Aldrich (Aldrich Chemical Company), DOCK (University of California in San Francisco), and the Directory of Natural Products (Chapman & Hall). Computer programs such as CONCORD (Tripos Associates) or DB-Converter (Molecular Simulations Limited) can be used to convert a data set represented in two dimensions to one represented in three dimensions.

Test compounds may be tested for their capacity to fit spatially into a glycosyltransferase ligand binding domain. As used herein, the term "fits spatially" means that the three-dimensional structure of the test compound is accommodated geometrically in a glycosyltransferase ligand binding domain. The test compound can then be considered to be a ligand.

A favourable geometric fit occurs when the surface area of the test compound is in close proximity with the surface area of the cavity or pocket without forming unfavorable interactions. A favourable complementary interaction occurs where the test compound interacts by hydrophobic, aromatic, ionic, dipolar, or hydrogen donating

and accepting forces. Unfavourable interactions may be steric hindrance between atoms in the test compound and atoms in the binding site.

In an embodiment of the invention, a method is provided for identifying potential modulators of a glycosyltransferase function. The method utilizes the structural coordinates or model of a glycosyltransferase three dimensional structure, or binding domain thereof. The method comprises the steps of (a) docking a computer representation of a test compound from a computer data base with a computer model of a ligand binding domain of a glycosyltransferase; (b) determining a conformation of a complex between the test compound and binding domain with a favourable geometric fit or favorable complementary interactions; and (c) identifying test compounds that best fit the glycosyltransferase ligand binding domain as potential modulators of glycosyltransferase function. The initial glycosyltransferase structure may or may not have substrates bound to it. A favourable complementary interaction occurs where a compound in a compound-glycosyltransferase complex interacts by hydrophobic, ionic, or hydrogen donating and accepting forces, with the active-site or binding domain of a glycosyltransferase without forming unfavorable interactions.

If a model of the present invention is a computer model, the test compounds may be positioned in a ligand binding domain through computational docking. If, on the other hand, the model of the present invention is a structural model, the test compounds may be positioned in the ligand binding domain by, for example, manual docking.

As used herein the term "docking" refers to a process of placing a compound in close proximity with a glycosyltransferase ligand binding domain, or a process of finding low energy conformations of a test compound/ glycosyltransferase complex.

A screening method of the present invention may comprise the following steps:

(i) generating a computer model of a glycosyltransferase or a ligand binding domain thereof according to the first aspect of the invention;

(ii) docking a computer representation of a test compound with the computer model;

(iii) analysing the fit of the compound in the glycosyltransferase or ligand binding domain thereof.

In an aspect of the invention a method is provided comprising the following steps:

(a) docking a computer representation of a structure of a test compound into a computer representation of a ligand binding domain of a glycosyltransferase defined in accordance with the invention using a computer program, or by interactively moving the representation of the test compound into the representation of the binding domain;

(b) characterizing the geometry and the complementary interactions formed between the atoms of the ligand binding domain and the compound; optionally

(c) searching libraries for molecular fragments which can fit into the empty space between the compound and ligand binding domain and can be linked to the compound; and

(d) linking the fragments found in (c) to the compound and evaluating the new modified compound.

In an embodiment of the invention a method is provided which comprises the following steps:

(a) docking a computer representation of a test compound from a computer data base with a computer representation of a selected site (e.g. an inhibitor binding domain) on a glycosyltransferase structure or model defined in accordance with the invention to obtain a complex;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying test compounds that best fit the selected site as potential modulators of the glycosyltransferase.

A method of the invention may be applied to a plurality of test compounds, to identify those that best fit the selected site.

The model used in the screening method may comprise a glycosyltransferase or ligand binding domain thereof either alone or in association with one or more ligands and/or cofactors. For example, the model may comprise a ligand binding domain in association with a ligand, substrate, or analogue thereof.

If the model comprises an unassociated ligand binding domain, then the selected site under investigation may be the ligand binding domain itself. The test compound may, for example, mimic a known substrate for the enzyme in order to interact with the ligand binding domain. The selected site may alternatively be another site on the enzyme.

If the model comprises an associated ligand binding domain, for example a ligand binding domain in association with a ligand, substrate molecule or analogue thereof, the selected site may be the ligand binding domain or a site made up of the ligand binding domain and the complexed ligand, or a site on the ligand itself. The test compound may be investigated for its capacity to modulate the interaction with the associated molecule.

A test compound (or plurality of test compounds) may be selected on the basis of its similarity to a known ligand for the glycosyltransferase. For example, the screening method may comprise the following steps:

(i) generating a computer model of a glycosyltransferase ligand binding domain in complex with a ligand;

(ii) searching for a test compound with a similar three dimensional structure and/or similar chemical groups; and

(iii) evaluating the fit of the test compound in the ligand binding domain.

Searching may be carried out using a database of computer representations of potential compounds, using methods known in the art.

The present invention also provides a method for designing ligands for a glycosyltransferase. It is well known in the art to use a screening method as described above to identify a test compound with promising fit, but then to use this test compound as a starting point to design a ligand with improved fit to the model. A known modulator can also be modified to enhance its fit with a model of the invention. Such techniques are known as "structure–based ligand design" (See Kuntz et al., 1994, Acc. Chem. Res. 27:117; Guida, 1994, Current Opinion in Struc. Biol. 4: 777; and Colman, 1994, Current Opinion in Struc. Biol. 4: 868, for reviews of structure-based drug design and identification;and Kuntz et al 1982, J. Mol. Biol. 162:269; Kuntz et al., 1994, Acc. Chem. Res. 27: 117; Meng et al., 1992, J. Compt. Chem. 13: 505; Bohm, 1994, J. Comp. Aided Molec. Design 8: 623 for methods of structure-based modulator design).

Examples of computer programs that may be used for structure-based ligand design are CAVEAT (Bartlett et al., 1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M. Ley, S.V.; Campbell, N.M. eds; Royal Society of Chemistry: Cambridge, pp 182-196); FLOG (Miller et al., 1994, J. Comp. Aided Molec. Design 8:153); PRO Modulator (Clark et al., 1995 J. Comp. Aided Molec. Design 9:13); MCSS (Miranker and

Karplus, 1991, Proteins: Structure, Function, and Genetics 8:195); and, GRID (Goodford, 1985, J. Med. Chem. 28:849).

The method may comprise the following steps:

(i) docking a model of a test compound with a model of a selected ligand binding domain;

(ii) identifying one or more groups on the test compound which may be modified to improve their fit in the selected ligand binding domain;

(iii) replacing one or more identified groups to produce a modified test compound model; and

(iv) docking the modified test compound model with the model of the selected ligand binding domain.

Evaluation of fit may comprise the following steps:

(a) mapping chemical features of a test compound such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites; and

(b) adding geometric constraints to selected mapped features.

The fit of the modified test compound may then be evaluated using the same criteria.

The chemical modification of a group may either enhance or reduce hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between the test compound and the key amino acid residue(s) of the selected site. Preferably the group modifications involve the addition, removal, or replacement of substituents onto the test compound such that the substituents are positioned to collide or to bind preferentially with one or more amino acid residues that correspond to the key amino acid residues of the selected site.

Identified groups in a test compound may be substituted with, for example, alkyl, alkoxy, hydroxyl, aryl, cycloalkyl, alkenyl, alkynyl, thiol, thioalkyl, thioaryl, amino, or halo groups. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided.

If a modified test compound model has an improved fit, then it may bind to the selected site and be considered to be a "ligand". Rational modification of groups may be made with the aid of libraries of molecular fragments which may be screened for their capacity to fit into the available space and to interact with the appropriate atoms. Databases of computer representations of libraries of chemical groups are available commercially, for this purpose.

A test compound may also be modified "*in situ*" (i.e. once docked into the potential binding domain), enabling immediate evaluation of the effect of replacing selected groups. The computer representation of the test compound may be modified by deleting a chemical group or groups, replacing chemical groups, or by adding a chemical group or groups. After each modification to a compound, the atoms of the modified compound and potential binding site can be shifted in conformation and the distance between the modulator and the active site atoms may be scored on the basis of geometric fit and favourable complementary interactions between the molecules. This technique is described in detail in Molecular Simulations User Manual, 1995 in LUDI.

Examples of ligand building and/or searching computer programs include programs in the Molecular Simulations Package (Catalyst), ISIS/HOST, ISIS/BASE, and ISIS/DRAW (Molecular Designs Limited), and UNITY (Tripos Associates).

The "starting point" for rational ligand design may be a known ligand for the enzyme. For example, in order to identify potential modulators of a glycosyltransferase, a logical approach would be to start with a known ligand (for example a substrate molecule or inhibitor) to produce a molecule which mimics the binding of the ligand. Such a molecule may, for example, act as a competitive inhibitor for the true ligand, or may bind so strongly that the interaction (and inhibition) is effectively irreversible. Such a method may comprise the following steps:

(i) generating a computer model of a glycosyltransferase ligand binding domain in complex with a ligand;

(ii) replacing one or more groups on the ligand computer model to produce a modified ligand; and

(iii) evaluating the fit of the modified ligand in the ligand binding domain.

The replacement groups could be selected and replaced using a compound construction program which replaces computer representations of chemical groups with groups from a computer database, where the representations of the compounds are defined by structural coordinates.

In an embodiment, a screening method is provided for identifying a ligand of a glycosyltransferase comprising the step of using the structural coordinates or model of a substrate molecule or component thereof, defined in relation to its spatial association with a glycosyltransferase structure or a ligand binding domain, to generate a compound that is capable of associating with the glycosyltransferase or ligand binding domain.

The screening methods of the present invention may be used to identify compounds or entities that associate with a molecule that associates with a glycosyltransferase enzyme (for example, a substrate molecule).

Compounds and entities (e.g. ligands) of a glycosyltransferase identified using the above-described methods may be prepared using methods described in standard reference sources utilized by those skilled in the art. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill.

Test compounds and ligands which are identified using a model of the present invention can be screened in assays such as those well known in the art. Screening can be, for example, *in vitro*, in cell culture, and/or *in vivo*. Biological screening assays preferably centre on activity-based response models, binding assays (which measure how well a compound binds), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity-high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity. The biological assay, may also be an assay for the ligand binding activity of a compound that selectively binds to the ligand binding domain compared to other enzymes.

The invention contemplates a method for the design of modulators for a glycosyltransferase based on a structure or model of a sugar nucleotide donor (or parts thereof) or an acceptor defined in related to its association with a ligand binding domain.

In accordance with particular aspects of the invention, a method is provided for designing potential inhibitors of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L GnT, comprising the step of using one or more (preferably all) of the structural coordinates of uracil, uridine, ribose, pyrophosphate, or UDP of Tables 14, 15 or 16, as follows:

Table 14 for GnT1 Ground State

Table 15 for GntV

Table 16 for core 2L

to generate a compound for associating with a ligand binding domain of a glycosyltransferase that associates with uracil, uridine, ribose, pyrophosphate, or UDP.

To generate a compound for associating with the active site of a glycosyltransferase, the following steps are employed in a particular method of the invention: (a) generating a computer representation of uracil, uridine, or UDP defined by structural coordinates of Tables 14, 15 or 16; (b) searching for molecules in a data base that are structurally or chemically similar to the defined uracil, uridine, or UDP using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound-building computer program.

In another embodiment of the invention, a method is provided for designing potential inhibitors of a glycosyltransferase preferably GnT I, GnT V,. and/or Core 2L GnT, said method comprising the step of using one or more (preferably all) of the structural coordinates of UDP-GlcNAc of Tables 17, 18, or 19 as follows:

Table 17 for GnT1 transition state

Table 18 for GnTV

Table 19 for core 2 L transition state

to generate a compound for associating with a ligand binding domain of a glycosyltransferase that associates with UDP-GlcNAc.

The following steps are employed in a particular method of the invention: (a) generating a computer representation of UDP-GlcNAc defined by one or more (preferably all) of the structural coordinates of Table 17, 18, or 19 appropriate for a specific glycosyltransferase; (b) searching for molecules in a data base that are structurally or chemically similar to the defined UDP-GlcNAc using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

In another embodiment of the invention, a method is provided for designing potential inhibitors of GnT I, said method comprising the step of using one or more (preferably all) of the structural coordinates of Table 20 for an oligosaccharide acceptor, to generate a compound for associating with a ligand binding domain of a glycosyltransferase that associates with the acceptor.

The following steps are employed in a particular method of the invention: (a) generating a computer representation of an oligosaccharide acceptor defined by the one or more (preferably all) of the structural coordinates of Table 20 appropriate for a specific glycosyltransferase; (b) searching for molecules in a data base that are structurally or chemically similar to the defined oligosaccharide acceptor using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

Potential modulators of glycosyltransferases identified using the above-described methods may be prepared using methods described in standard reference sources utilized by those skilled in the art. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill.

Ligands/Modulators

The present invention provides a ligand or compound or entity identified by a screening method of the present invention. A ligand or compound may have been designed rationally by using a model according to the present invention. A ligand or compound identified using the screening methods of the invention specifically associate with a target compound. In the present invention the target compound may be a glycosyltransferase or a

molecule that is capable of associating with a glycosyltransferase (for example a ligand or substrate molecule). In a preferred embodiment the ligand is capable of binding to the ligand binding domain of a glycosyltransferase.

A ligand or compound identified using a screening method of the invention may act as a "modulator", i.e. a compound which affects the activity of a glycosyltransferase. A modulator may reduce, enhance or alter the biological function of a glycosyltransferase. For example a modulator may modulate the capacity of the enzyme to transfer a sugar from a nucleotide sugar donor to a specific hydroxyl of various saccharide acceptors that leads to the formation of a new glycosidic linkage. An alteration in biological function may be characterised by a change in specificity. For example, a modulator may cause the enzyme to accept a different substrate molecule, to transfer a different sugar, or to work with a different metal cofactor. In order to exert its function, a modulator commonly binds to a ligand binding domain.

A modulator which is capable of reducing the biological function of the enzyme may also be known as an inhibitor. Preferably an inhibitor reduces or blocks the capacity of the enzyme to form new glycosidic linkages. The inhibitor may mimic the binding of a substrate molecule, for example, it may be a substrate analogue. A substrate analogue may be designed by considering the interactions between the substrate molecule and the enzyme (for example by using information derivable from a model of the invention) and specifically altering one or more groups.

In a highly preferred embodiment, a modulator acts as an inhibitor of a glycosyltransferase and is capable of inhibiting N- or O-glycan biosynthesis.

The present invention also provides a method for modulating the activity of a glycosyltransferase within a cell using a modulator according to the present invention. It would be possible to monitor the expression of N-glycans on the cell surface following such treatment by a number of methods known in the art (for example by detecting expression with an N-and O-glycan specific antibody).

In another preferred embodiment, the modulator modulates the catalytic mechanism of a glycosyltransferase.

A modulator may be an agonist, partial agonist, partial inverse agonist or antagonist of a glycosyltransferase.

The term "agonist" includes any ligand, which is capable of binding to a glycosyltransferse or ligand binding domain thereof, and which is capable of increasing a proportion of active enzyme, resulting in an increased biological response. The term includes partial agonists and inverse agonists.

The term "partial agonist" includes an agonist that is unable to evoke the maximal response of a biological system, even at a concentration sufficient to saturate a specific glycosyltransferase or ligand binding domain thereof.

The term "partial inverse agonist" includes an inverse agonist that evokes a submaximal response to a biological system, even at a concentration sufficient to saturate the specific receptors. At high concentrations, it will diminish the actions of a full inverse agonist.

The invention relates to a glycosyltransferase ligand binding domain antagonist, wherein said ligand binding domain is that defined by the amino acid structural coordinates described herein. For example the ligand may antagonise the inhibition of glycosyltransferase by an inhibitor.

The term "antagonist" includes any agent that reduces the action of another agent, such as an agonist. The antagonist may act at the same site as the agonist (competitive antagonism). The antagonistic action may result from a combination of the substance being antagonised (chemical antagonism) or the production of an opposite effect through a different molecule (functional antagonism or physiological antagonism) or as a consequence of

competition for the binding site of an intermediate that links the enzyme to the effect observed (indirect antagonism).

The term "competitive antagonism" refers to the competition between an agonist and an antagonist for a glycosyltransferase or ligand binding domain thereof that occurs when the binding of agonist and antagonist becomes mutually exclusive. This may be because the agonist and antagonist compete for the same binding site or combine with adjacent but overlapping sites. A third possibility is that different sites are involved but that they influence the glycosyltransferase or ligand binding domain in such a way that agonist and antagonist molecules cannot be bound at the same time. If the agonist and antagonist form only short lived combinations with a glycosyltransferase or ligand binding domain thereof so that equilibrium between agonist, antagonist and glycosyltransferase and ligand binding domain thereof is reached during the presence of the agonist, the antagonism will be surmountable over a wide range of concentrations. In contrast, some antagonists, when in close enough proximity to their binding site, may form a stable covalent bond with it and the antagonism becomes insurmountable when no spare ligand binding domain remains.

As mentioned above, an identified ligand or compound may act as a ligand model (for example, a template) for the development of other compounds. A modulator may be a mimetic of a ligand or ligand binding domain. A mimetic of a ligand may compete with a natural ligand for a glycosyltransferase or ligand binding domain thereof, and antagonize a physiological effect of the enzyme in an animal. A mimetic of a ligand may be an organically synthesized compound. A mimetic of a ligand binding domain, may be either a peptide or other biopharmaceutical (such as an organically synthesized compound) that specifically binds to a natural substrate molecule for a glycosyltransferase and antagonize a physiological effect of the enzyme in an animal.

Once a ligand has been optimally selected or designed, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to a glycosyltransferase ligand binding domain by the same computer methods described above.

Preferably, positions for substitution are selected based on the predicted binding orientation of a ligand to a glycosyltransferase ligand binding domain.

A technique suitable for preparing a modulator will depend on its chemical nature. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill. Peptides can be synthesized by solid phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with the instructions provided by the manufacturer. Once cleaved from the resin, the peptide may be purified by preparative high performance liquid chromatography (e.g., Creighton (1983) Proteins Structures and Molecular Principles, WH Freeman and Co, New York NY). The composition of the synthetic peptides may be confirmed by amino acid analysis or sequencing (e.g., the Edman degradation procedure; Creighton, *supra*).

If a modulator is a nucleotide, or a polypeptide expressable therefrom, it may be synthesized, in whole or in part, using chemical methods well known in the art (see Caruthers MH *et al* (1980) Nuc Acids Res Symp Ser 215-

23, Horn T *et al* (1980) Nuc Acids Res Symp Ser 225-232), or it may be prepared using recombinant techniques well known in the art.

Direct synthesis of a ligand or mimetics thereof can be performed using various solid-phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with the instructions provided by the manufacturer. Additionally, the amino acid sequences obtainable from the ligand, or any part thereof, may be altered during direct synthesis and/or combined using chemical methods with a sequence from other subunits, or any part thereof, to produce a variant ligand.

In an alternative embodiment of the invention, the coding sequence of a ligand or mimetics thereof may be synthesized, in whole or in part, using chemical methods well known in the art (see Caruthers MH *et al* (1980) Nuc Acids Res Symp Ser 215-23, Horn T *et al* (1980) Nuc Acids Res Symp Ser 225-232).

A wide variety of host cells can be employed for expression of the nucleotide sequences encoding a ligand of the present invention. These cells may be both prokaryotic and eukaryotic host cells. Suitable host cells include bacteria such as *E. coli*, yeast, filamentous fungi, insect cells, mammalian cells, typically immortalized, e.g., mouse, CHO, human and monkey cell lines and derivatives thereof. Preferred host cells are able to process the expression products to produce an appropriate mature polypeptide. Processing includes but is not limited to glycosylation, ubiquitination, disulfide bond formation and general post-translational modification.

In an embodiment of the present invention, the ligand may be a derivative of, or a chemically modified ligand. The term "derivative" or “derivatised” as used herein includes the chemical modification of a ligand.

A chemical modification of a ligand and/or a key amino acid residue of a ligand binding domain of the present invention may either enhance or reduce hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between the ligand and the key amino acid residue(s) of a glycosyltransferase ligand binding domain.

Preferably such modifications involve the addition of substituents onto a test compound such that the substituents are positioned to collide or to bind preferentially with one or more amino acid residues that correspond to the key amino acid residues of a glycosyltransferase ligand binding domain. Typical modifications may include, for example, the replacement of a hydrogen by a halo group, an alkyl group, an acyl group or an amino group.

The invention also relates to classes of modulators of a glycosyltransferase based on the structure and shape of a substrate, defined in relation to the substrate molecule’s spatial association with a glycosyltransferase structure of the invention or part thereof. Therefore, a modulator may comprise a substrate molecule having the shape or structure, preferably the structural coordinates, of a substrate molecule in an active site or ligand binding domain of a reaction catalyzed by a glycosyltransferase.

Modulators Based on the 3D Structure of a Nucleotide Sugar Donor

One class of modulators (i.e. inhibitors) of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L GnT, comprise the structure of uracil, uridine, ribose, pyrophosphate, or UDP with one or more (preferably all) of the structural coordinates of uracil, uridine, ribose, pyrophosphate, or UDP of Tables 14, 15 or 16 as follows:

Table 14 for Gnt1 Ground State

Table 15 for GnTV

Table 16 for core 2L

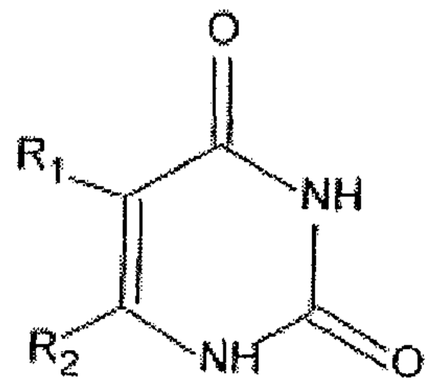
In an embodiment, the invention provides inhibitors of a glycosyltransferase, preferably GnT I, GnT V. and/or Core 2L GnT, comprising the structure of UDP-GlcNAc and having one or more (preferably all) of the structural coordinates of UDP-GlcNAc of Tables 17, 18, or 19 as follows:

Table 17 for GnT1 transition state

Table 18 for GnTV,

Table 19 for core 2L

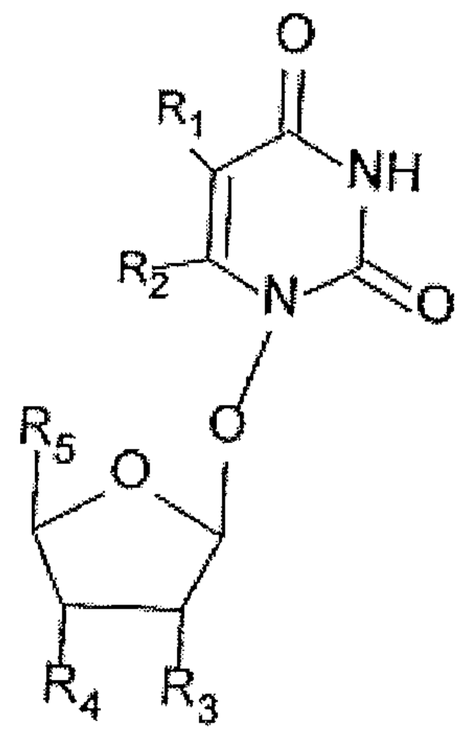
Another class of modulators defined by the invention are compounds of the Formula I having the structural coordinates of uracil of Table 14, 15 or 16, preferably the first conformation in each Table:



wherein R_1 and R_2 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, pyrophophate, gallic acid, phosphonates, thioamide, and $-OR_{10}$ where R_{10} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring;

and salts and optically active and racemic forms of a compound of the formula I.

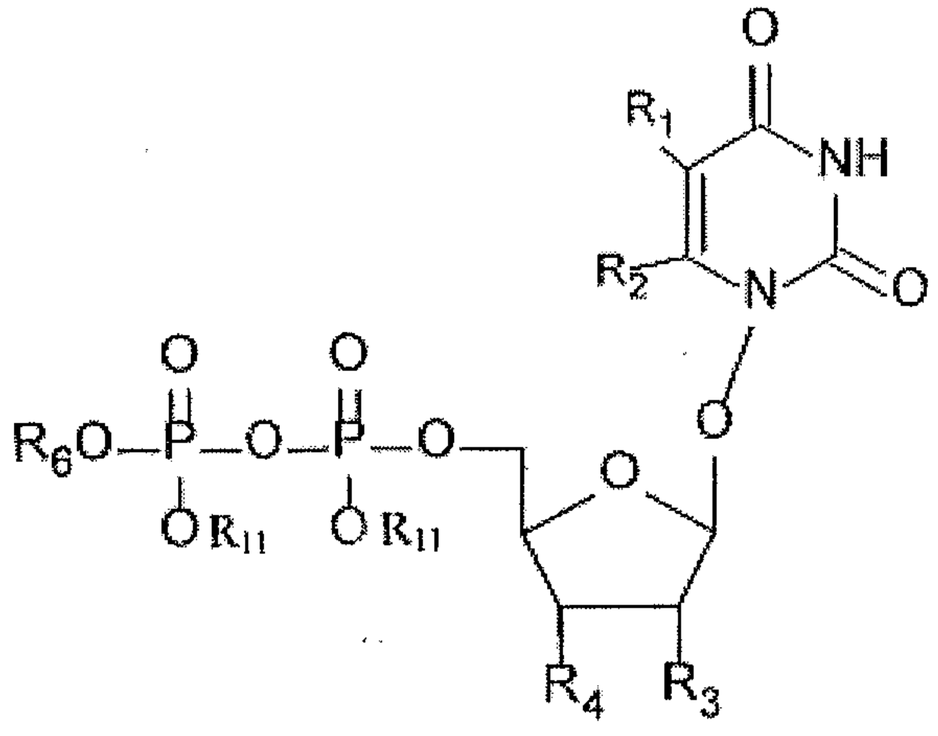
Yet another class of modulators defined by the invention are compounds of the formula II having the structural coordinates of uridine of Table 14, 15, or 16, preferably, the first conformation in each Table:



wherein R_1, R_2, R_3, R_4, and R_5 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, pyrophosphate, gallic acid, phosphonates, thioamide, and $-OR_{10}$ where R_{10} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring,

and salts and optically active and racemic forms of a compound of the formula II.

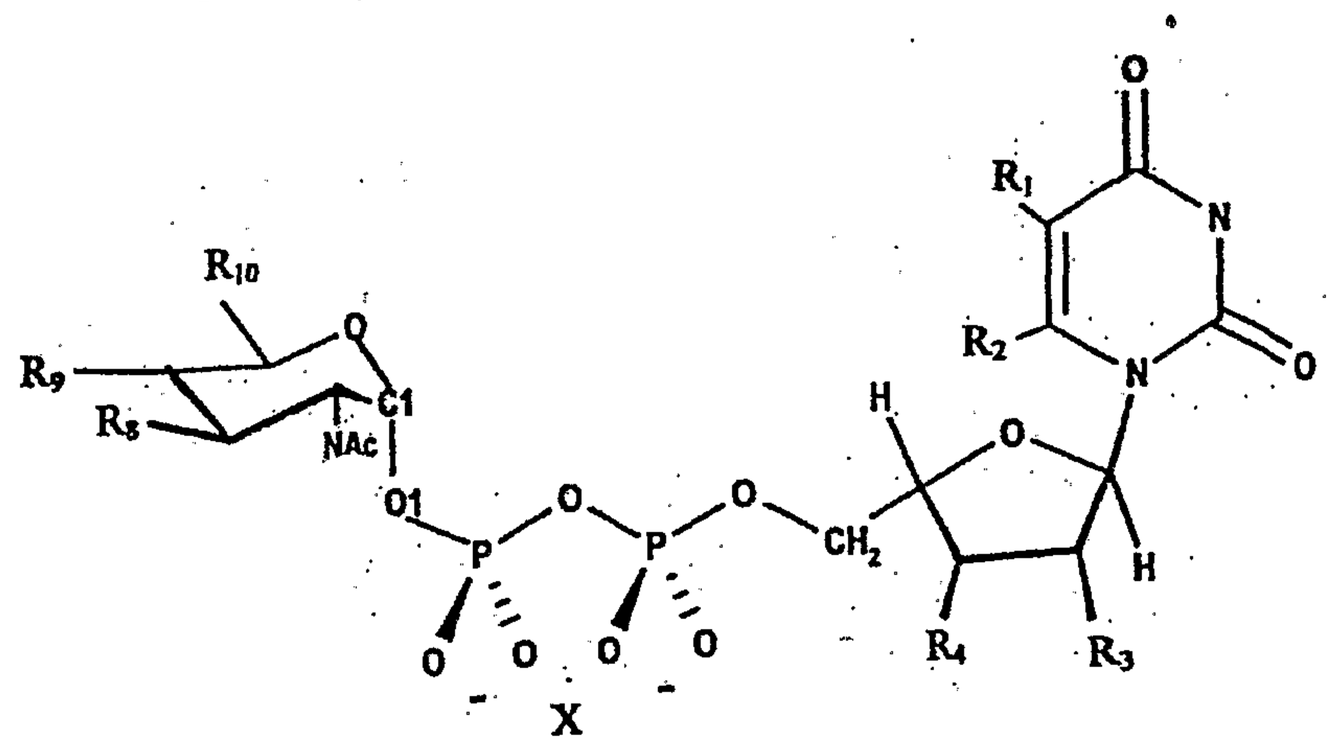
Yet another class of modulators identified by the invention are compounds of the formula III having the structural coordinates of UDP of Tables 14, 15, or 16, preferably the first conformation in each Table:



wherein R_1, R_2, R_3, R_4, R_5, and R_6 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, gallic acid, phosphonates, thioamide, and $-OR_{10}$ where R_{10} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring, R_6 may be a monosaccharide or disaccharide, preferably a monosaccharide, including GlcNAc, glucose, and mannose,

and salts and optically active and racemic forms of a compound of the formula III.

Yet another class of modulators are compounds of the formula IV having the structural coordinates of UDP-GlcNAc of Table 17, 18, or 19, preferably the first conformation in each Table:



wherein R_1, R_2, R_3, R_4, and R_5 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, gallic acid, phosphonates, thioamide, and $-OR_{10}$ where R_{10} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring,

and salts and optically active and racemic forms of a compound of the formula IV.

One or more of R_1, R_2, R_3, R_4, R_5, and/or R_6, alone or together, which contain available functional groups as described herein, may be substituted with for example one or more of the following: alkyl, alkoxy, hydroxyl, aryl, cycloalkyl, alkenyl, alkynyl, thiol, thioalkyl, thioaryl, amino, or halo. The term "one or more" used herein preferably refers to from 1 to 2 substituents.

Modulators (e.g. inhibitors) are also contemplated that have the structure of an acceptor of a glycosyltransferase, and are characterized by the structural coordinates of an acceptor for a glycosyltransferase of Table 20. The acceptor may have the structure as shown in Figure 19A or 33. Functional groups in the acceptor structure may be substituted with for example, alkyl, alkoxy, hydroxyl, aryl, cycloalkyl, alkenyl, alkynyl, thiol, thioalkyl, thioaryl, amino, or halo, or they may be modified using techniques known in the art.

Modulators Derived from the Transition State Sugar Binding Cavity

A class of modulators defined by the invention are compounds comprising the structural coordinates of GlcNAc in the transition state of a reaction catalyzed by a glycosyltransferase, preferably Core 2 GnT-L and GnT-I. The GlcNAc has a half chair or distorted chair conformation, a partial double bond between C1 and 05, and a hybridization Sp^2 at C1.

Yet another class of modulators defined by the invention are compounds comprising a pyrophosphate group directly or indirectly linked to GlcNAc having the structural coordinates of GlcNAc in the transition state of a reaction catalyzed by a glycosyltransferase, preferably Core 2 GnT-L and GnT-I. The GlcNAc component has a half chair or distorted chair conformation, a partial double bond between C1 and 05, and a hybridization Sp^2 at C1. The distance between the pyrophosphate group and the GlcNAc is about 1.9 to 3.5 Å, preferably 2.2 to 3.0Å.

The compounds may comprise analogues and derivatives of GlcNAc or the pyrophosphate group. For example, reactive groups of the GlcNAc or pyrophosphate group may be modified or they may be substituted with alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof (e.g. $-CH_2OH$), amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, gallic acid, phosphonates, thioamide, and $-OR_{12}$ where R_{12} is alkyl, cycloalkyl, alkenyl, alkynyl, or a heterocyclic ring. The GlcNAc and pyrophosphate may be linked via any molecules suitable for linking a sugar and phosphate group.

The present invention contemplates all optical isomers and racemic forms thereof of the compounds (modulators) of the invention described herein, and the formulas of the compounds shown herein are intended to encompass all possible optical isomers of the compounds so depicted.

The present invention also contemplates salts and esters of the compounds (modulators) of the invention described herein. In particular, the present invention includes pharmaceutically acceptable salts. By pharmaceutically acceptable salts is meant those salts which are suitable for use in contact with the tissues of humans and lower animals without undue toxicity, irritation, allergic response and the like, and are commensurate with a reasonable

benefit/risk ratio. Pharmaceutically acceptable salts are well known in the art and are described for example, in S. M. Berge, et al., J. Pharmaceutical Sciences, 1977, 66:1-19.

Peptide Modulators Derived from the Loop Structure of a Glycosyltransferase

The invention provides peptides that are derived from the loop structure of a glycosyltransferase. For example, peptides of the invention include the amino acids EER, HVNT, or VSHG that bind to a pyrophosphate group of a sugar nucleotide donor. Other proteins containing these binding domain sequences may be identified with a protein homology search, for example by searching available databases such as GenBank or SwissProt and various search algorithms and/or programs may be used including FASTA, BLAST (available as a part of the GCG sequence analysis package, University of Wisconsin, Madison, Wis.), or ENTREZ (National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, MD).

In accordance with an embodiment of the invention, specific peptides are contemplated that mediate the association of the loop structure of a Core 2 transferase and a pyrophosphate group of a sugar nucleotide donor for the Core 2 transferase. In particular, a peptide of the following formula is provided which interferes with the association of the loop structure of a Core 2 transferase and a pyrophosphate group of a sugar nucleotide donor for the Core 2 transferase:

$$X\text{-}X^1\text{-}X^2\text{-}X^3\text{-}X^4$$

wherein X represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids, X^1 and X^2 independently represent an amino acid with a charged polar group, preferably Glu, Asp, Asn, or Gln, X^3 represents a basic amino acid, preferably Arg, His, or Lys, and X^4 represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids. In specific embodiments, X^1 and X^2 are Glu, and X^3 is Arg.

In an embodiment of the present invention a peptide is provided where X represents X^5-SHK where X^5 represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids, or X^4 represents X^6-NRKRYE where X^6 represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids.

Preferred peptides of the invention include SHKEERNRKRYE, SHKDERNRKRYE, SHKEDRNRYE, SHKEENNRKRYE, SHKDDRNRKRYE, and SHKNERNRKRYE.

In accordance with another embodiment of the invention, specific peptides are contemplated that mediate the association of the loop structure of a GnT-I to V transferase and a pyrophosphate group of a sugar nucleotide donor for the transferase. In particular, a peptide of the following formula is provided which interferes with the association of the loop structure of a GnT-I to V transferase and a pyrophosphate group of a sugar nucleotide donor for the transferase:

$$X^7\text{-}X^8\text{-}X^9\text{-}X^{10}\text{-}X^{11}\text{-}X^{12}$$

wherein X^7 represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids, X^8 represents Val or His, X^9 represents Val or Ser, X^{10} represents Asn, or His, X^{11} represents Thr or Gly, and X^{12} represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids.

In an embodiment of the present invention a peptide is provided where X^7 represents X^{13}-FIGRP or X^{13}-GRKG where X^{13} represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids, or X^{12} represents X^{14}-DLN or X^{14}-QFF, where X^{14} represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids.

Preferred peptides of the invention include FIGRPHVNTDLN, and GRKGVSHGQFF.

All of the peptides of the invention, as well as molecules substantially homologous, complementary or otherwise functionally or structurally equivalent to these peptides may be used for purposes of the present invention. In addition to full-length peptides of the invention, truncations of the peptides are contemplated in the present invention. Truncated peptides may comprise peptides of about 7 to 10 amino acid residues

The truncated peptides may have an amino group (-NH2), a hydrophobic group (for example, carbobenzoxyl, dansyl, or T-butyloxycarbonyl), an acetyl group, a 9-fluorenylmethoxy-carbonyl (PMOC) group, or a macromolecule including but not limited to lipid-fatty acid conjugates, polyethylene glycol, or carbohydrates at the amino terminal end. The truncated peptides may have a carboxyl group, an amido group, a T-butyloxycarbonyl group, or a macromolecule including but not limited to lipid-fatty acid conjugates, polyethylene glycol, or carbohydrates at the carboxy terminal end.

The peptides of the invention may also include analogs of a peptide of the invention and/or truncations of a peptide, which may include, but are not limited to a peptide of the invention containing one or more amino acid insertions, additions, or deletions, or both. Analogs of a peptide of the invention exhibit the activity characteristic of a peptide e.g. interference with the interaction of a loop structure of a glycosyltransferase and a pyrophosphate of a sugar nucleotide donor, and may further possess additional advantageous features such as increased bioavailability, stability, or reduced host immune recognition. One or more amino acid insertions may be introduced into a peptide of the invention. Amino acid insertions may consist of a single amino acid residue or sequential amino acids.

One or more amino acids, preferably one to five amino acids, may be added to the right or left termini of a peptide of the invention. Deletions may consist of the removal of one or more amino acids, or discrete portions from the peptide sequence. The deleted amino acids may or may not be contiguous. The lower limit length of the resulting analog with a deletion mutation is about 7 amino acids.

It is anticipated that if amino acids are inserted or deleted in sequences outside an X^1-X^2-X^3 or X^8-X^9-X^{10}-X^{11} sequence that the resulting analog of the peptide will exhibit the activity of a peptide of the invention.

The invention also includes a peptide conjugated with a selected protein, or a selectable marker (see below) to produce fusion proteins.

The peptides of the invention may be prepared using recombinant DNA methods. Accordingly, nucleic acid molecules which encode a peptide of the invention may be incorporated in a known manner into an appropriate expression vector which ensures good expression of the peptide. Possible expression vectors include but are not limited to cosmids, plasmids, or modified viruses so long as the vector is compatible with the host cell used. The expression vectors contain a nucleic acid molecule encoding a peptide of the invention and the necessary regulatory sequences for the transcription and translation of the inserted protein-sequence. Suitable regulatory sequences may be obtained from a variety of sources, including bacterial, fungal, viral, mammalian, or insect genes. (For example, see the regulatory sequences described in Goeddel, Gene Expression Technology: Methods in Enzymology 185, Academic Press, San Diego, CA (1990). Selection of appropriate regulatory sequences is dependent on the host cell chosen, and may be readily accomplished by one of ordinary skill in the art. Other sequences, such as an origin of

replication, additional DNA restriction sites, enhancers, and sequences conferring inducibility of transcription may also be incorporated into the expression vector.

The recombinant expression vectors may also contain a selectable marker gene which facilitates the selection of transformed or transfected host cells. Suitable selectable marker genes are genes encoding proteins such as G418 and hygromycin which confer resistance to certain drugs, β-galactosidase, chloramphenicol acetyltransferase, firefly luciferase, or an immunoglobulin or portion thereof such as the Fc portion of an immunoglobulin preferably IgG. The selectable markers may be introduced on a separate vector from the nucleic acid of interest encoding a peptide of the invention.

The recombinant expression vectors may also contain genes that encode a fusion portion which provides increased expression of the recombinant peptide; increased solubility of the recombinant peptide; and/or aid in the purification of the recombinant peptide by acting as a ligand in affinity purification. For example, a proteolytic cleavage site may be inserted in the recombinant peptide to allow separation of the recombinant peptide from the fusion portion after purification of the fusion protein. Examples of fusion expression vectors include pGEX (Amrad Corp., Melbourne, Australia), pMAL (New England Biolabs, Beverly, MA) and pRIT5 (Pharmacia, Piscataway, NJ) which fuse glutathione S-transferase (GST), maltose E binding protein, or protein A, respectively, to the recombinant protein.

Recombinant expression vectors may be introduced into host cells to produce a transformant host cell. Transformant host cells include prokaryotic and eukaryotic cells which have been transformed or transfected with a recombinant expression vector of the invention. The terms "transformed with", "transfected with", "transformation" and "transfection" are intended to include the introduction of nucleic acid (e.g. a vector) into a cell by one of many techniques known in the art. For example, prokaryotic cells can be transformed with nucleic acid by electroporation or calcium-chloride mediated transformation. Nucleic acid can be introduced into mammalian cells using conventional techniques such as calcium phosphate or calcium chloride co-precipitation, DEAE-dextran-mediated transfection, lipofectin, electroporation or microinjection. Suitable methods for transforming and transfecting host cells may be found in Sambrook et al. (Molecular Cloning: A Laboratory Manual, 2nd Edition, Cold Spring Harbor Laboratory press (1989)), and other laboratory textbooks.

Suitable host cells include a wide variety of prokaryotic and eukaryotic host cells. For example, the peptides of the invention may be expressed in bacterial cells such as *E. coli*, insect cells (using baculovirus), yeast cells or mammalian cells. Other suitable host cells can be found in Goeddel, Gene Expression Technology: Methods in Enzymology 185, Academic Press, San Diego, CA (1991).

The peptides of the invention may be synthesized by chemical synthesis using solid phase peptide synthesis. These methods employ either solid or solution phase synthesis methods (see for example, J. M. Stewart, and J.D. Young, Solid Phase Peptide Synthesis, 2nd Ed., Pierce Chemical Co., Rockford III. (1984) and G. Barany and R.B. Merrifield, The Peptides: Analysis Synthesis, Biology editors E. Gross and J. Meienhofer Vol. 2 Academic Press, New York, 1980, pp. 3-254 for solid phase synthesis techniques; and M Bodansky, Principles fo Peptide Synthesis, Springer-Verlag, Berlin 1984, and E. Gross and J. Meienhofer, Eds., The Peptides: Analysis, Synthesis, Biologu, suprs, Vol 1, for classical solution synthesis).

N-terminal or C-terminal fusion proteins comprising a peptide of the invention conjugated with other molecules may be prepared by fusing, through recombinant techniques, the N-terminal or C-terminal of the peptide, and the sequence of a selected protein or selectable marker with a desired biological function. The resultant fusion

proteins contain the peptide fused to the selected protein or marker protein as described herein. Examples of proteins which may be used to prepare fusion proteins include immunoglobulins, glutathione-S-transferase (GST), hemagglutinin (HA), and truncated myc.

Cyclic derivatives of the peptides of the invention are also part of the present invention. Cyclization may allow the peptide to assume a more favorable conformation for association with a ligand binding domain. Cyclization may be achieved using techniques known in the art. For example, disulfide bonds may be formed between two appropriately spaced components having free sulfhydryl groups, or an amide bond may be formed between an amino group of one component and a carboxyl group of another component. Cyclization may also be achieved using an azobenzene-containing amino acid as described by Ulysse, L., et al., J. Am. Chem. Soc. 1995, 117, 8466-8467. The side chains of Tyr and Asn may be linked to form cyclic peptides. The components that form the bonds may be side chains of amino acids, non-amino acid components or a combination of the two. In aspects of the invention, cyclic peptides may have a beta-turn in the right position. Beta-turns may be introduced into the peptides of the invention by adding the amino acids Pro-Gly at the right position.

It may be desirable to produce a cyclic peptide that is more flexible than the cyclic peptides containing peptide bond linkages as described above. A more flexible peptide may be prepared by introducing cysteines at the right and left position of the peptide and forming a disulphide bridge between the two cysteines. The peptide is more flexible as a result of the length of the disulfide linkage and the smaller number of hydrogen bonds in the beta-sheet portion. The relative flexibility of a cyclic peptide can be determined by molecular dynamics simulations.

Peptide mimetics may be designed based on information obtained by systematic replacement of L-amino acids by D-amino acids, replacement of side chains with groups having different electronic properties, and by systematic replacement of peptide bonds with amide bond replacements. Local conformational constraints can also be introduced to determine conformational requirements for activity of a candidate peptide mimetic. The mimetics may include isosteric amide bonds, or D-amino acids to stabilize or promote reverse turn conformations and to help stabilize the molecule. Cyclic amino acid analogues may be used to constrain amino acid residues to particular conformational states. The mimetics can also include mimics of inhibitor peptide secondary structures. These structures can model the 3-dimensional orientation of amino acid residues into the known secondary conformations of proteins. Peptoids may also be used which are oligomers of N-substituted amino acids and can be used as motifs for the generation of chemically diverse libraries of novel molecules.

Combined with certain formulations, peptides can be effective intracellular agents. However, in order to increase the efficacy of peptides, a fusion peptide can be prepared comprising a second peptide which promotes "transcytosis", e.g. uptake of the peptide by epithelial cells. To illustrate, a peptide of the invention can be provided as part of a fusion polypeptide with all or a fragment of the N-terminal domain of the HIV protein Tat, e.g. residues 1-72 of Tat or a smaller fragment thereof which can promote transcytosis. In other embodiments, a peptide of the invention can be provided as a fusion polypeptide with all or a portion of an antennapedia protein. To further illustrate, a peptide of the invention can be provided as a chimeric peptide which includes a heterologous peptide sequence ("internalizing peptide") which drives the translocation of an extracellular form of a peptide sequence across a cell membrane in order to facilitate intracellular localization of the peptide.

The peptides may be developed using a biological expression system. The use of these systems allows the production of large libraries of random peptide sequences and the screening of these libraries for peptide sequences that bind to the loop structure. Libraries may be produced by cloning synthetic DNA that encodes random peptide

sequences into appropriate expression vectors. (see Christian et al 1992, J. Mol. Biol. 227:711; Devlin et al, 1990 Science 249:404; Cwirla et al 1990, Proc. Natl. Acad, Sci. USA, 87:6378). Libraries may also be constructed by concurrent synthesis of overlapping peptides (see U.S. Pat. No. 4,708,871).

Peptides of the invention may be used to identify lead compounds for drug development. The structure of the peptides described herein can be readily determined by a number of methods such as NMR and X-ray crystallography. A comparison of the structures of peptides similar in sequence, but differing in the biological activities they elicit in target molecules can provide information about the structure-activity relationship of the target. Information obtained from the examination of structure-activity relationships can be used to design either modified peptides, or other small molecules or lead compounds which can be tested for predicted properties as related to the target molecule (i.e. glycosyltranaferases or ligand binding domain thereof). The activity of the lead compounds can be evaluated using assays similar to those described herein.

Information about structure-activity relationships may also be obtained from co-crystallization studies. In these studies, a peptide with a desired activity is crystallized in association with a target molecule, and the X-ray structure of the complex is determined. The structure can then be compared to the structure of the target molecule in its native state, and information from such a comparison may be used to design compounds expected to possess desired activities.

The peptides of the invention may be used to prepare antibodies. Conventional methods can be used to prepare the antibodies.

The peptides and antibodies specific for the peptides of the invention may be labelled using conventional methods with various enzymes, fluorescent materials, luminescent materials and radioactive materials. Suitable enzymes, fluorescent materials, luminescent materials, and radioactive material are well known to the skilled artisan. Antibodies and labeled antibodies specific for the peptides of the invention may be used to screen for proteins containing loop structures or they may be used to modulate the activity of a glycosyltransferase.

Computer modelling techniques known in the art may also be used to observe the interaction of a peptide of the invention, and truncations and analogs thereof with a pyrophosphate of a sugar nucleotide donor (for example, Homology Insight II and Discovery available from BioSym/Molecular Simulations, San Diego, California, U.S.A.). If computer modelling indicates a strong interaction, the peptide can be synthesized and tested for its ability to interfere with the binding of the molecules of a complex discussed herein.

The present invention also contemplates salts and esters of the peptides of the invention. In particular, the present invention includes pharmaceutically acceptable salts. By pharmaceutically acceptable salts is meant those salts which are suitable for use in contact with the tissues of humans and lower animals without undue toxicity, irritation, allergic response and the like, and are commensurate with a reasonable benefit/risk ratio. Pharmaceutically acceptable salts are well known in the art and are described for example, in S. M. Berge, et al., J. Pharmaceutical Sciences, 1977, 66:1-19.

The peptides of the invention may be converted into pharmaceutical salts by reacting with inorganic acids such as hydrochloric acid, sulfuric acid, hydrobromic acid, phosphoric acid, etc., or organic acids such as formic acid, acetic acid, propionic acid, glycolic acid, lactic acid, pyruvic acid, oxalic acid, succinic acid, malic acid, tartaric acid, citric acid, benzoic acid, salicylic acid, benezenesulfonic acid, and toluenesulfonic acids.

Compositions and Methods of Treatment

A secondary, tertiary, or quanternary glycosyltransferase structure or models of the invention and the modulators identified using the methods of the invention may be used to modulate the biological activity of a glycosyltransferase in a cell, including modulating a pathway in a cell regulated by the glycosyltransferase or modulating a glycosyltransferase with inappropriate activity in a cellular organism.

The modulators can be administered for prophylactic and/or therapeutic treatments. In therapeutic applications, compositions are administered to a patient already suffering from a condition, in an amount sufficient to cure or at least alleviate the symptoms of the disease and its complications. In prophylactic applications, modulators are administered to a patient susceptible to or otherwise at risk of a particular condition.

Cellular assays, as well as animal model assays *in vivo*, may be used to test the activity of a potential modulator of a glycosyltransferase as well as diagnose a disease associated with inappropriate glycosyltransferase activity. *In vivo* assays are also useful for testing the bioactivity of a potential modulator designed by the methods of the invention.

The modulators (e.g. inhibitors) identified using the methods of the invention can be useful in the treatment and prophylaxis of tumor growth and metastasis of tumors. Anti-metastatic effects of inhibitors can be demonstrated using a lung colonization assay. For example, melanoma cells treated with an inhibitor may be injected into mice and the ability of the melanoma cells to colonize the lungs of the mice may be examined by counting tumor nodules on the lungs after death. Suppression of tumor growth in mice by the inhibitor administered orally or intravenously may be examined by measuring tumor volume.

An inhibitor identified using the invention can have particular application in the prevention of tumor recurrence after surgery i.e. as an adjuvant therapy.

An inhibitor can be especially useful in the treatment of various forms of neoplasia such as leukemias, lymphomas, melanomas, adenomas, sarcomas, and carcinomas of solid tissues in patients. In particular, inhibitors can be used for treating malignant melanoma, pancreatic cancer, cervico-uterine cancer, ovarian cancer, cancer of the kidney such as metastatic renal cell carcinoma, stomach, lung, rectum, breast, bowel, gastric, liver, thyroid, head and neck cancers such as unresectable head and neck cancers, lymphangitis carcinamatosis, cancers of the cervix, breast, salivary gland, leg, tongue, lip, bile duct, pelvis, mediastinum, urethra, bronchogenic, bladder, esophagus and colon, non-small cell lung cancer, and Kaposi's Sarcoma which is a form of cancer associated with HIV-infected patients with Acquired Immune Deficiency Syndrome (AIDS). The inhibitors may also be used for other anti-proliferative conditions such as bacterial and viral infections, in particular AIDS.

An inhibitor identified in accordance with the present invention can be used to treat immunocompromised subjects. For example, they can be used in a subject infected with HIV, or other viruses or infectious agents including bacteria, fungi, and parasites, in a subject undergoing bone marrow transplants, and in subjects with chemical or tumor-induced immune suppression.

Inhibitors may be used as hemorestorative agents and in particular to stimulate bone marrow cell proliferation, in particular following chemotherapy or radiotherapy. The myeloproliferative activity of an inhibitor of the invention may be determined by injecting the inhibitor into mice, sacrificing the mice, removing bone marrow cells and measuring the ability of the inhibitor to stimulate bone marrow proliferation by directly counting bone marrow cells and by measuring clonogenic progenitor cells in methylcellulose assays. The inhibitors can also be used as chemoprotectants and in particular to protect mucosal epithelium following chemotherapy.

An inhibitor identified in accordance with the invention also may be used as an antiviral agent in particular on membrane enveloped viruses such as retroviruses, influenza viruses, cytomegaloviruses and herpes viruses. A small molecule inhibitor can also be used to treat bacterial, fungal, and parasitic infections. For example, a small molecule inhibitor can be used to prevent or treat infections caused by the following: *Neisseria* species such as *Neisseria meningitidis*, and *N. gonorrheae*; *Chlamydia* species such as *Chlamydia pneumoniae, Chlamydia psittaci, Chlamydia trichomatis*; *Escherichia coli*, *Haemophilus* species such as *Haemophilus influenza*; *Yersinia enterocolitica*; *Salmonella* species such as *S.typhimurium*; *Shigella* species such as *Shigella flexneri*; *Streptococcus* species such as *S.agalactiae* and *S. pneumoniae*; *Bacilllus* species such as *Bacillus subtilis*; *Branhamella catarrhalis*; *Borrelia burgdorfer*; *Pseudomonas aeruginosa*; *Coxiella burnetti*; *Campylobacter* species such as *C.hyoilei*; *Helicobacter pylori*; and, *Klebsiella* species such as *Klebsiella pneumoniae.*

An inhibitor can also be used in the treatment of inflammatory diseases such as rheumatoid arthritis, asthma, inflammatory bowel disease, and atherosclerosis. In particular, an inhibitor of core 2Lmay be used in the treatment of inflammatory diseases.

An inhibitor can also be used to augment the anti-cancer effects of agents such as interleukin-2 and poly-IC, to augment natural killer and macrophage tumoricidal activity, induce cytokine synthesis and secretion, enhance expression of LAK and HLA class I specific antigens; activate protein kinase C, stimulate bone marrow cell proliferation including hematopoietic progenitor cell proliferation, and increase engraftment efficiency and colony-forming unit activity, to confer protection against chemotherapy and radiation therapy (e.g. chemoprotective and radioprotective agents), and to accelerate recovery of bone marrow cellularity particularly when used in combination with chemical agents commonly used in the treatment of human diseases including cancer and acquired immune deficiency syndrome (AIDS). For example, an inhibitor can be used as a chemoprotectant in combination with anti-cancer agents including doxorubicin, 5-fluorouracil, cyclophosphamide, and methotrexate, and in combination with isoniazid or NSAID.

The present invention thus provides a method for treating the above-mentioned conditions in a subject comprising administering to a subject an effective amount of a modulator identified using the methods of the invention. The invention also contemplates a method for stimulating or inhibiting tumor growth or metastasis in a subject comprising administering to a subject an effective amount of a modulator identified using the methods of the invention. The invention further contemplates the use of a modulator to treat the above-mentioned conditions in a subject.

The invention still further relates to a pharmaceutical composition which comprises a glycosyltransferase structure of the invention or a ligand binding domain thereof (e.g. a loop structure, a hydrophobic pocket), or a modulator identified using the methods of the invention in an amount effective to regulate one or more of the above-mentioned conditions (e.g. tumor growth or metastasis) and a pharmaceutically acceptable carrier, diluent or excipient. The invention contemplates the use of a modulator in the preparation of a pharmaceutical composition.

The compositions of the invention are administered to subjects in a biologically compatible form suitable for pharmaceutical administration *in vivo*. By "biologically compatible form suitable for administration *in vivo*" is meant a form of the protein to be administered in which any toxic effects are outweighed by the therapeutic effects of the protein. The terms “subject” or “individual” are intended to include mammals and includes humans, dogs, cats, mice, rats, and transgenic species thereof. Administration of a therapeutically active amount of the pharmaceutical compositions of the present invention is defined as an amount effective, at dosages and for periods of

time necessary to achieve the desired result. For example, a therapeutically active amount of a three dimensional glycosyltransferase structure of the invention or modulators of the invention may vary according to factors such as the condition, age, sex, and weight of the individual. Dosage regimes may be adjusted to provide the optimum therapeutic response. For example, several divided doses may be administered daily or the dose may be proportionally reduced as indicated by the exigencies of the therapeutic situation.

The active compound may be administered in a convenient manner such as by injection (subcutaneous, intravenous, etc.), oral administration, inhalation, transdermal application, or intracerebral administration.

A pharmaceutical composition of the invention can be administered to a subject in an appropriate carrier or diluent, co-administered with enzyme inhibitors or in an appropriate carrier such as microporous or solid beads or liposomes. The term "pharmaceutically acceptable carrier" as used herein is intended to include diluents such as saline and aqueous buffer solutions. Liposomes include water-in-oil-in-water emulsions as well as conventional liposomes (Strejan et al., (1984) J. Neuroimmunol 7:27). The active compound may also be administered parenterally or intraperitoneally. Dispersions can also be prepared in glycerol, liquid polyethylene glycols, and mixtures thereof and in oils. Under ordinary conditions of storage and use, these preparations may contain a preservative to prevent the growth of microorganisms. Depending on the route of administration, the active compound may be coated to protect the compound from the action of enzymes, acids, and other natural conditions which may inactivate the compound.

Therapeutic administration of polypeptides may also be accomplished using gene therapy. A nucleic acid including a promoter operatively linked to a heterologous polypeptide may be used to produce high-level expression of the polypeptide in cells transfected with the nucleic acid. DNA or isolated nucleic acids may be introduced into cells of a subject by conventional nucleic acid delivery systems. Suitable delivery systems include liposomes, naked DNA, and receptor-mediated delivery systems, and viral vectors such as retroviruses, herpes viruses, and adenoviruses.

The therapeutic efficacy and safety of a modulator or composition of the invention can be determined by standard pharmaceutical procedures in cell cultures or animal models. Therapeutic efficacy and toxicity may be determined by standard pharmaceutical procedures in cell cultures or with experimental animals, such as by calculating the ED_{50} (the dose therapeutically effective in 50% of the population) or LD_{50} (the dose lethal to 50% of the population) statistics. The therapeutic index is the dose ratio of therapeutic to toxic effects and it can be expressed as the ED_{50}/LD_{50} ratio. Pharmaceutical compositions which exhibit large therapeutic indices are preferred.

EXAMPLES

The following non-limiting examples illustrate the invention:

Example 1

Model and Computational Procedures

The structural model used in this investigation to analyze the GlcNAc transfer by an *N*-acetylglucosaminyltransferase enzymatic mechanism computationally consists of all the essential molecules or their fragments, assumed to be involved in the enzymatic mechanism (Figure 37). The reaction site model contains a complete sugar-donor molecule, UDP-GlcNAc, a hydroxyl group of the oligosaccharide-acceptor modeled by methanol, a divalent metal cofactor modeled by Mg^{2+}, as well as the essential parts of the catalytic acid (A) and catalytic base (B) represented by acetic acid and acetate molecules. Such a model of the active site allows all the required electronic rearrangements occurring during the enzymatic reaction such as the proton transfers between the

active site components and the substrates. This model consists of 86 atoms and has an overall charge of minus one. In the construction of this model, the relative position of the different participants was an important issue that could not be restricted by the usual means of crystallographic data since no structure of a N-acetylglucosaminyltransferase complexed with the entire UDP-GlcNAc substrate was available. As a consequence, the conformation of the UDP-GlcNAc used in the model is based on previous extensive calculations on sugar-phosphate and diphosphate models (23-25). The two catalytic amino acids present in the model were placed in an arrangement that emulates their orientation in the active site of inverting glycosyl hydrolases (16) where the two carboxylates are located 6.5 Å to 9.5 Å apart. In the model, the two amino acids are located about 5.0 Å away from the anomeric carbon C1. The methanol oxygen atom Oa, representing the reactive hydroxyl of the sugar-acceptor, was initially placed at 3.0 Å from the anomeric carbon C1 and at 3.0 Å from the oxygen OB of the amino acid noted B on Figure 37. Geometrical constraints applied to fix the relative position of the different components are another important element to consider in building a physically meaningful model. Because the whole structure of the enzyme is not used in the model, these constraints are essential to prevent movement of residues to unrealistic positions with respect to the substrates. The positions of the relevant oxygen atoms of both the catalytic base and catalytic acid have been restricted in the model.

In addition to the nucleophilic attack, the transfer of either one or two protons can be involved in the catalytic reaction of GlcNAc-Ts. Consequently, three distances were used as reaction coordinates in order to follow the mechanism (Figure 37): the distance r_{HA-O1} between the proton HA of the catalytic acid and the glycosidic oxygen O1; the distance r_{Ha-OB} between the proton Ha of the sugar-acceptor and the oxygen OB of the catalytic base; and the r_{C1-Oa} distance between the anomeric carbon C1 and the oxygen Oa of the acceptor hydroxyl group. These geometrical parameters reflect the proton transfer process from the catalytic acid to the sugar-donor, the proton transfer process from the sugar-acceptor to the catalytic base, and the nucleophilic attack of the sugar-acceptor on the anomeric C1-O1 linkage. The energy of the model calculated as a function of these three reaction-coordinates gives the Potential Energy Surface (PES). Each calculated point on the PES corresponds to the optimized structure and arrangement of the model for the given r_{HA-O1}, r_{Ha-OB}, and r_{C1-Oa} distances. These distances were varied by 0.2 Å increments within the 0.9 Å to 2.1 Å range for r_{Ha-OB}, 0.9 Å to 1.9 Å range for r_{HA-O1} and within the 3.0 Å to 1.3 Å range for r_{C1-Oa}. During the optimization, all geometrical parameters were optimized with exception of the location of two amino acids. As a result, each point on the PES represented by fixed values of the r_{HA-O1}, r_{Ha-OB}, and r_{C1-Oa} distances have all their geometrical variables adjusted to their most stable values. Since, the calculation of such maps requires an extremely large amount of CPU time, the calculation of the PESs was divided into two parts. The first PES corresponds to the energy calculated as a function of the r_{Ha-OB} and r_{C1-Oa} distances whereas for the second PES, the energy was computed as a function of the r_{HA-O1}, and r_{C1-Oa} distances. The location of the local minima and transition barriers on the PESs is only approximate and for that reason a further optimization of the stationary points with no constraints on the r_{Ha-O1}, r_{Ha-OB}, and r_{C1-Oa} distances is required. These stationary points represent structures of the intermediates and transition states found on the different PESs and along the different reaction pathways. However, in order to avoid any confusion, the same acronyms TSi, and INTi respectively are used herein for the barriers located on PESs and for the stationary points that follow.

The *ab initio* calculations were carried out with the Jaguar program (26). The optimization of the geometry was performed at the SCF level with the 6-31G* (834 basis functions) basis set. Full optimizations were accomplished using the gradient optimization routines of the program without any symmetry constraints. To better

characterize the individual reaction paths, the location and structure of the diverse transition states were calculated using three nearest points to the particular barrier on the PES using the QST-guided search of the Jaguar software (26). The geometry of all stationary points on PESs was then fully optimized using the 6-31G* basis set. The effects of electron correlation on the potential energy surface were estimated using the B3LYP density functional method (27). Ultimately, selected geometries were used to estimate the effect of the basis set by calculating their single point energy with the 6-31++G** basis set (1178 basic functions).

Results and Discussion

The only experimental data available to date on the mechanism of *N*-acetylglucosaminyltransferases are kinetic studies on GlcNAc-T I and GlcNAc-T II (6, 22). They indicate an ordered sequential mechanism and the prerequisite of a metal cofactor for the enzyme activity. A metal cofactor has been shown to be generally required by these *N*-acetylglucosaminyltransferases, presumably to increase the leaving ability of the pyrophosphate group. This metal ion binds to the enzyme prior to the donor nucleotide-sugar. Then, before any of the products leaves the enzyme, a sugar-acceptor has to be bound in order to proceed to the transfer of the sugar. For some galactosyltransferases (28), the metal cofactor was found to be released from the enzyme in the form of a complex with the nucleotide-diphosphate.

By analogy with the reaction mechanism of the inverting glycosyl hydrolases (18-20), one can assume two different types of mechanism for the inverting GlcNAc-Ts (Figure 38). In the first type (Scheme A), only a carboxylate acting as a general base catalyst is involved in the catalytic mechanism. Such a catalytic base assists the nucleophilic attack of the acceptor oxygen Oa on the anomeric carbon C1 of the donor to form a new glycosidic linkage C1-Oa. A pair of carboxylic acids is involved in the second type of catalytic mechanism (Figure 38, Scheme B). This mechanism consists of an electrophilic attack of a carboxylic acid on the target oxygen O1 of the donor that cleaves the bond, followed by the nucleophilic attack of the acceptor oxygen Oa on the anomeric carbon C1 of the donor. Here, one catalytic acid behaves as a general acid catalyst protonating the glycosidic oxygen atom O1 while the second carboxylate acts as a general base catalyst deprotonating the nucleophilic oxygen Oa of the acceptor. Both types of catalytic reaction described above may proceed via one or several transition states and, in terms of course of events, both mechanisms can proceed either in a concerted or stepwise manner. In the absence of experimental information on the reaction pathway, calculation of the potential energy surfaces (PESs) describing these mechanisms would provide valuable insight on the kinetic importance of a particular pathway and on the structure and energy of stationary points, intermediates and transition states observed on these PESs.

The HF/6-31G* calculated potential energy surfaces of the catalytic reactions are represented in the form of two-dimensional reaction-coordinate contour diagrams in Figures 1a –3a. The distances along the x-axis determine the formation and scission of a new glycosidic linkage C1-Oa, and corresponding to the nucleophilic attack of the acceptor Oa on anomeric C1, while the distances along the y-axis characterize the proton transfer processes. Different reaction pathways can generally be identified on these potential energy surfaces. The reaction pathways parallel to the vertical and horizontal axes describe particular steps in a stepwise mechanism while the reaction pathways following the diagonal across the PES represent a concerted mechanism. The profile of the PESs depends on the relative acidity of the different molecules involved. The calculated two-dimensional PESs only represent a section of the potential energy hypersurface (PEHS) describing the entire complex reaction. Nevertheless, several conclusions can be formulated from the calculated two-dimensional PESs displayed on Figures 1a – 3a and they will be discussed below. Optimized structures of the different stationary points found along the reaction pathways, and

determined at the DFT/B3LYP/6-31G* level, are given in Figures 1b-3b. Analysis of the stationary point structures along the reaction pathways calculated at DFT/B3LYP/6-31G* level revealed features qualitatively similar to those found on the PESs calculated at HF/6-31G* level. As previously observed (23-25), the inclusion of the electron correlation results in slightly different magnitudes of bond lengths and the increase of the basis set decreases the relative energy of minima. For that reason, the discussion will essentially be based on the structures calculated at DFT/B3LYP/6-31G* level and their energy estimated at DFT/B3LYP/6-31++G**//DFT/B3LYP/6-31G*. More detailed structural information on each stationary point is given for reference in Table 25 while their relative energy (ΔE) determined at various levels is listed in Table 26. Figure 34 shows a scheme of various possible reaction pathways observed for the transfer of GlcNAc catalyzed by *N*-acetylglucosaminyltransferases.

3.1 Potential energy surfaces

PES as a function of the $r_{Ha\text{-}OB}$ and $r_{C1\text{-}Oa}$ distances. – The first reaction mechanism studied (Figure 38, Scheme A) characterizes the nucleophilic attack of the methanol (sugar-acceptor) on the anomeric carbon C1 of UDP-GlcNAc (sugar-donor) either followed or preceded by the proton transfer from the methanol (acceptor) to the catalytic base (B). As mentioned earlier, only one carboxylate (catalytic base noted B on Figure 37, Scheme 2) is involved in this reaction mechanism but for the sake of energy comparison with other reaction pathways, the second catalytic acid (noted A on Figure 37, Scheme 2) was kept in the model in a constrained position. The PES corresponding to such reaction mechanism and calculated at HF/6-31G* level is given on Figure 1a. Distances plotted along both axes of the contour map describe horizontally the nucleophilic attack of the methanol oxygen Oa on the anomeric carbon C1 of GlcNAc and vertically the proton (Ha) transfer from the hydroxyl group of the methanol to the catalytic base (B). This PES shows two intermediates (INT1 and INT2) and four energy barriers (TS1 – TS4) located in valleys along the borders of the contour map. An energy maximum, with no saddle point, is observed in the central region of the map. Thus, a concerted mechanism appears to be impossible in this model and the reaction must proceed through a stepwise mechanism from the reactants (R) to the product complex (PC1) with the proton transfer and the nucleophilic attack as two distinct steps.

The stepwise mechanism observed on the contour map of Figure 1a, offers two distinct pathways leading to the same product complex (PC1) but differing in the sequence of the individual steps. In the first pathway (R → TS1 → INT1 → TS2 → PC1), the enzymatic reaction starts with the nucleophilic attack (along the horizontal axis) of the methanol oxygen Oa on the anomeric carbon C1 of UDP-GlcNAc, followed by the proton (Ha) transfer (along the vertical axis) from the methanol to the catalytic base (B). In the second pathway (R → TS3 → INT2 → TS4 → PC1), the order of the steps is reversed with the proton transfer occurring before the nucleophilic attack. Comparison of the energy barriers required to proceed along these two pathways (Figure 34) reveals that the process starting by the nucleophilic attack is less energy demanding. From Figure 1a and Table 26, both intermediates (INT1 and INT2) appear to have also higher relative energy compared to the reactants or the products. As a consequence, the transition states are located in asymmetric positions next to the intermediates.

The energy of the proton transfer from methanol to the catalytic base depends on the stage of the nucleophilic attack and reflects the different acidity of both participants. As the nucleophilic attack proceeds, acid strength of the attacking methanol changes from about 15 for methanol to an approximate value of –5 for the protonated glycosidic oxygen in INT1 (29). The changes in the calculated proton transfer energy are consistent with this variation of the pK_a. When the methanol is in the starting position ($r_{C1\text{-}Oa}$ = 2.8 Å), not attacking the anomeric carbon of UDP-GlcNAc, the proton transfer energy is 36.3 kcal/mol, which is in reasonable agreement with the

experimental estimate of ΔH = 44 kcal/mol for the $HCOO^- + C_2H_5OH \rightarrow HCOOH + C_2H_5O^-$ process in the gas phase (29). The proton transfer energy then gradually decreases as the methanol oxygen Oa attacks the anomeric carbon C1 to finally end up with an energy around –22.4 kcal/mol in the final stage of the nucleophilic attack ($r_{C1\text{-}Oa}$ = 1.5 Å). The examination of the PES indicates that along the different pathways, the points located at equal $r_{C1\text{-}Oa}$ = 2.0 Å but with distinct position of the proton Ha, $r_{Ha\text{-}OB}$ = 1.0 Å and 2.0 Å respectively, appear to have roughly the same energy. This suggests that at such an $r_{C1\text{-}Oa}$ distance, the acidity of the methanol and the catalytic base are very similar. The hydroxyl group of the methanol used in the model probably has higher acidity compared to the hydroxyl group that would be present in the real oligosaccharide substrate. It can, therefore, be expected that a weaker acid ROH of this type would increase the transition barrier and move TS1 and TS3 toward the products. Similarly, an increase of the strength of the catalytic base would move the TSs closer to INT2 or INT1.

Since the general reaction can be considered as a simple nucleophilic displacement at the anomeric carbon with inversion of configuration, the reaction path must involve the deprotonation of the acceptor oxygen and a change of the absolute configuration at the anomeric carbon. These changes are clearly seen in the structure of the discrete points along both reaction pathways (Figure 1b). The analysis of these geometrical changes revealed that while the proton transfer only marginally influences the structure of the reactants, the nucleophilic attack results in a significant alteration of the UDP-GlcNAc structure. Along the reaction path: R → TS1 (13.4 kcal/mol) → INT1 (7.6) → TS2 (14.7) → PC1 (-22.4), the C1-O1 bond length between the anomeric carbon C1 and the leaving group, UDP, gradually elongates from 1.519 Å to 3.260 Å as the distance between the anomeric carbon and the attacking oxygen $r_{C1\text{-}Oa}$ decreases. The transition state for the nucleophilic attack occurring as a first step in the reaction, TS1, undergoes significant geometrical changes compared to the starting structure, R. As the C1-Oa reaction coordinate gets close to 2.16 Å such as in TS1, the C1-O1 scissile bond increases drastically by 1 Å going from 1.519 Å to 2.535 Å and the C1-O5 bond shortens from 1.371 Å to 1.290 Å. In INT1, the C1-Oa and C1-O1 bonds have value of 1.532 Å and 2.829 Å, respectively. During the second step of the reaction, the proton Ha of TS2 is positioned closer to the oxygen Oa with $r_{Ha\text{-}Oa}$ = 1.361 Å. The C1-O1 distance slightly stretches to 3.014 Å whereas the C1-Oa bond shortens to 1.499 Å but in overall, only small changes were found between the relevant bonds of TS2 and INT1.

The geometry of the starting active site model (R) is characterized by the values of 1.519 Å and 1.371 Å for, respectively, the C1-O1 and C1-O5 bond lengths. The pyranoid ring of the GlcNAc is initially in the $^4C_1$ chair conformation characterized by the ring-puckering parameters ϕ=246.2, θ=14.1 and Q=0.54. Along the reaction coordinate, the conformation of the pyranoid ring continuously changes from the $^4C_1$ chair through the $^4H_3$ half-chair and the ^4E envelope conformations where the proton H1 is at a quasi-planar position and back to the $^4C_1$ chair conformation. During this process, the H1 atom moves from the equatorial position through the position in the plane defined by C2-C1-O5 atoms to the axial position. Interestingly, no boat conformations of the transferred sugar, as earlier described for β-1,4-xylanases (30) or suggested for chitinases (31), were found on the PES. These modifications in the six-membered ring conformation of GlcNAc are accompanied by changes in the orientation of the leaving and attacking groups with respect to the six-membered ring. As the ring shape shifts to the envelope conformation, the atoms attached to the anomeric carbon become coplanar with the sp^2 character at the reaction center, C1. The delocalization of the ring oxygen lone-pair electrons into the empty p orbital at the C1 atom stabilizes the oxocarbenium ion-like character of GlcNAc. The formation of such an oxocarbenium ion requires an alteration of the GlcNAc ring conformation, from chair to half-chair or envelope, to accommodate the partial double-bond character. A consequence of the charge delocalization is the shortening of the C1-O5 bond length from its

equilibrium value of 1.371 Å observed in R. This change is more pronounced in TS1 with $r_{C1\text{-}Oa}$ = 2.158 Å and where the C1-O5 bond length, $r_{C1\text{-}O5}$ = 1.290 Å, developed a partial double bond character. The orientation of both the leaving and the attacking groups, is also influenced by the tendency to optimize interactions between the C1 carbon p orbital and the lone pairs of the connecting oxygen atoms of these groups. The most efficient interactions clearly occur when these oxygen atoms are located in the direction of this p orbital oriented perpendicularly to the O5-C1-C2 plane. A stronger nucleophilic character of the methanolate should result in a larger stabilization of such oxocarbenium species. Indeed, it appears that in the case of methanol, the O1 and Oa atoms adopt a quasi-orthogonal orientation regarding the O5-C1-C2 plane with the O5-C1-O1/Oa bond angles close to 90° at $r_{C1\text{-}Oa}$ = 2.158 Å, whereas in the case of methanolate (the alternative pathway described on the map), this situation occurs earlier at larger C1-Oa distance ($r_{C1\text{-}Oa}$ = 2.426 Å).

For the alternative reaction pathway described on the map, R → TS3 (36.3) → INT2 (30.4) → TS4 (32.2)→ PC1 (-22.4), the conversion of the reactants into the intermediate INT2 during the proton transfer occurs through the transition state TS3 at $r_{Ha\text{-}Oa}$ = 1.638 Å. The geometry of GlcNAc does not exhibit any important change along this reaction step. The C1-O1 bond is a good illustration of this behavior since this bond remains almost unchanged with lengths of 1.519, 1.524 and 1.529 Å in respectively the R, TS3 and INT2 stationary points.

As in the first pathway, the main geometrical changes are connected with the nucleophilic attack occurring along the horizontal axis of the contour map. Several interesting differences between the TS1 and TS4 structures can be noticed. In TS4, the distance C1-Oa of 2.426 Å is longer compared to the 2.158 Å found for TS1. On the contrary, the length of the C1-O1 scissile bond is considerably shorter in TS4, 1.863 Å versus 2.535 Å in TS1. Using these distances as a criterion to describe the extent of the transfer reaction, one can assume TS4 is an earlier transition state because its geometry is closer to the reactants, in contrast to TS1 that might be characterized as a late transition state since the structure is nearer to that of the products. Both TS1 and TS4 structures have a significant sp^2 character at the C1 atom.

A comparison of the orientations of the *N*-acetyl group located at C2 shows that for all points on the PES, the acetamido group remains in the most stable conformation called *Z*-trans (32). This indicates that the *N*-acetyl group does not participate in the catalytic mechanism through the so-called substrate assisted catalysis by stabilizing the developing oxocarbenium character on C1 as proposed earlier for some retaining hydrolases (33). This is not surprising given the difference in stereochemical outcome. For some early points along the R → TS1 → INT1 → TS2 → PC1 reaction pathway, the N-acetyl group is brought closer to the leaving UDP group. However, the weak (N)-H…O1 hydrogen bond formed disappears as the C1-O1 distance increases.

PESs as a function of the $r_{HA\text{-}O1}$, and $r_{C1\text{-}Oa}$ distances. – The mechanism considered here describes the proton transfer from the catalytic acid (A) to the glycosidic oxygen O1 and the nucleophilic attack of the acceptor oxygen Oa on the anomeric carbon C1 (Figure 38, Scheme B). Results on the mechanism earlier described showed that the nucleophilic attack and the proton transfer from the acceptor to the catalytic base (B) proceed in distinct steps. The question then was whether or not this behavior also remained for pathways where the HA proton of a second catalytic acid (A) is attacking the glycosidic oxygen. Preliminary calculations of the PES as a function of the $r_{HA\text{-}O1}$ and $r_{C1\text{-}Oa}$ distances indicated a conservation of these features. However, the optimization led to structures with the Ha proton located either at the acceptor oxygen atom (Oa) or at the catalytic base oxygen (OB) depending on the starting position. For that reason, two different PESs were calculated in order to describe the present mechanism. In the first PES (Figure 2a), the Ha is initially located at the acceptor oxygen Oa while in the second PES (Figure 3a),

the proton Ha is positioned at the catalytic base oxygen OB. The analyses of the results support the previous findings and they reveal that on both potential energy surfaces, the Ha proton always remains in its same starting location. Some assumptions are implicitly included in these two models used to describe the reaction mechanisms. For the first PES (Ha located at the acceptor), the proton transfer from the acceptor to the catalytic base is the final step completing the reaction. However, in the second PES (Ha located at the catalytic base), the proton transfer from the acceptor to the base (B) precedes the nucleophilic attack and the proton transfer from catalytic acid (A) to the glycosidic oxygen O1.

Both PESs corresponding to the type of mechanism described on Scheme 3-B and calculated at the HF/6-31G* level, are given on Figures 2a and 3a. The distances $r_{C1\text{-}Oa}$ and $r_{Ha\text{-}O1}$ represented along both axes of the contour map characterize horizontally the nucleophilic attack of the methanol oxygen Oa on the anomeric carbon C1 of GlcNAc and vertically, the proton (HA) transfer from the catalytic acid (A) to the glycosidic oxygen O1. Though the proton transfer processes represented on the vertical axes of Figure 1 and Figures 2 - 3 refer to a transfer between different molecules, all maps exhibit similar features. They all indicate that a concerted mechanism is impossible in this model. As a consequence, the reaction must proceed by a stepwise mechanism through different reaction channels with the proton transfer and the nucleophilic attack occurring as two distinct steps. In all maps, the transition states are similarly located in asymmetric positions near the intermediates.

Two different pathways are observed on each of the PESs, namely INT2 → TS4 → PC1 → TS5 → PC2 and INT2 → TS6 → INT3 → TS7 → PC2 on Figure 2 and R → TS1 → INT1 → TS8 → INT5 and R → TS9 → INT4 → TS10 → INT5 on Figure 3. Three intermediates and four transition states are encountered in valleys along the borders of each contour map. It should be pointed out that some points of these PESs, corresponding to the nucleophilic attack with the HA proton located at the catalytic acid, coincide with points shown on Figure 1. This was possible because the second catalytic acid (A) was kept in the model in a constrained position though it is not involved in the mechanism illustrated on Figure 1. In this way, a consistent comparison between the energies required by the diverse reaction pathways was achieved.

The calculated PESs show that the HA proton must pass through a relatively large energetic barrier during its transfer from the catalytic acid (A) to the glycosidic oxygen O1. In general, this step is the most energy demanding among all the steps occurring along a particular reaction pathway. When this process is the starting step of a reaction mechanism, the energy barrier calculated at the 6-31G* level is particularly high. For example, in the pathway R → TS9 (26.2 kcal/mol) → INT4 (25.8) → TS10 (37.7)→ INT5 (17.3) (Figure 3a), the barrier for the proton transfer from the catalytic acid to the glycosidic oxygen (R → INT4) approaches 37.6 kcal/mol. A similar magnitude for the energy barrier between R→ INT2 (36.3 kcal/mol) was observed in the mechanism earlier described and corresponding to the Ha proton transfer (Figure 1). This suggests that in the present mechanism, the probability of protonation of the glycosidic oxygen might be too low to be kinetically productive. As on Figure 1, the more favorable pathways found on Figures 2 and 3 are those starting with the nucleophilic attack.

The difference between the nucleophilic character of methanol and methanolate oxygen atoms is clearly reflected in the location of the transition barriers on PESs given in Figures 2a and 3a. When the nucleophile is methanolate (Figure 2a), the reaction barriers for the nucleophilic attack are closer to the starting reactants (INT2), whereas, in the case of nucleophilic attack by methanol (Figure 3a), the TSs are closer to the products. Barriers for the proton (HA) transfer from the catalytic acid (A) to the glycosidic oxygen O1 are located asymmetrically on the bottom part of the maps, closer to the final intermediates, and are therefore exhibiting a character of late transition

states. The location of these energy barriers results from the fact that the glycosidic oxygen O1 in UDP-GlcNAc might have a p*K*a value (34) of approximately -10 and that the pyrophosphate group is a very strong acid. The activation energy of the reverse reaction in solution (the proton transfer from O1 to the catalytic acid) is an exothermic process assumed to be a diffused-controlled reaction with an activation barrier of about 5 kcal/mol (35), which is in reasonable agreement with the energy barriers of about 6 kcal/mol calculated on these maps, with however, an exception for the proton transfer between INT4→ TS9.

As expected, the analysis of the geometrical changes observed along the reaction pathways and shown on Figures 2b and 3b reveals that the nucleophilic attack alters the structure in a similar fashion to the mechanism described on Figure 1. However, the proton transfer from the catalytic acid to O1 is more significantly influencing the structure of UDP-GlcNAc than was in Figure 1, the proton transfer from the acceptor to the catalytic base. The modifications in the structure of UDP-GlcNAc caused by the proton transfer can be illustrated by the bond distance $r_{C1\text{-}O1}$ between the anomeric carbon C1 and the oxygen O1 that gradually elongates as the HA proton approaches the O1 atom. Such a process is observed on Figure 3a during the R → INT4 step, where the value of the C1-O1 bond length changes from the equilibrium position of 1.519 Å through 1.950 Å in TS9 to 3.733 Å in INT4. In the INT2 → INT3 step described in Figure 2a, the elongation of the glycosidic bond gets more pronounced with the C1-O1 distance increasing from 1.529 Å to 2.663 Å. The reverse trend is however observed for the C1-O5 bond that is shortening from 1.371 Å to 1.259 Å along R → INT4 and from 1.381 Å to 1.253 Å along INT2 → INT3. The changes in the bond lengths observed during this proton transfer process are accompanied by an alteration of the six-membered ring conformation. The conformation of the pyranoid ring continuously changes from the $^4C_1$ chair to the $^4H_3$ half-chair and back to the $^4C_1$ conformation. During this process, the H1 atom moves from the equatorial position through the position in the plane defined by C2-C1-O5 atoms to reach ultimately the axial position. These results show that the structure around the reaction center is very sensitive to the nucleophilic attack and the proton transfer to the glycosidic oxygen. Moreover, they suggest that geometric changes caused by these two processes are comparable, both leading to the cleavage of the C1-O1 bond and the alteration of the GlcNAc ring conformation leading to inversion of the anomeric configuration of the transferred sugar. The energetic requirements for the two processes are very different and they indicate that the nucleophilic attack is the less energy-demanding operation.

Using information coming from the three calculated PESs, various possible reaction pathways for the transfer of GlcNAc catalyzed by *N*-acetylglucosaminyltransferases could be established. They are schematized in Figure 34. Among them, four distinct stepwise reaction pathways exist to describe the transfer of GlcNAc using mechanisms involving jointly a catalytic acid and a catalytic base. Two pathways, R → TS3 (36.3) → INT2 (30.4) → TS4 (32.2)→ PC1 (-22.4) → TS5 (-0.2) → PC2 (-3) and R → TS3 (36.3) → INT2 (30.4) → TS6 (59.8)→ INT3 (54.4) → TS7 (54.7)→ PC2 (-3), start with the proton transfer from the acceptor to the catalytic base, R → TS3 → INT2, and as such, have their first step (noted in bold) identical to the mechanism previously discussed and involving only the catalytic base. In two other pathways, R → TS1 (13.4) → INT1 (7.6) → TS8 (26.4)→ INT5 (17.3) → TS11 (34.4)→ PC2 (-3) and R → TS9 (37.6) → INT4 (25.8) → TS10 (37.7)→ INT5 (17.3) → TS11 (34.4) → PC2 (-3), the final step of the reaction, INT5 → TS11 → PC2, is the proton transfer from the acceptor to the catalytic base. In the first of these two pathways, the proton transfer to O1 occurs as the second step after the nucleophilic attack and it proceeds from INT1 to the intermediate INT5 via TS8. Both TS8 and INT5 structures have the GlcNAc ring in a $^4H_3$ conformation and the C1-O5 bond length around 1.33 Å. The C1-O1 bond length differs though for these structures with 2.843 Å versus 3.467 Å for TS8 and INT5, respectively. In the second pathway, the

proton transfer happens as the first step, from R to INT4 via TS9, and it is energetically less favorable. In this case, the C1-O1 and C1-O5 bonds of TS9 are 1.950 Å and 1.286 Å, respectively. For all points on the PESs, the acetamido group remains in the most stable conformation called Z-trans (32).

Several changes described above resemble those assumed in reactions catalyzed by glycosyl hydrolases. The calculated potential energy surface for a general acid catalyzed reaction of lysozyme (35) has suggested for the transition state [RC1-O1(H+)-R], C1-O1 bond lengths in the range of 2.5 – 2.6 Å. It was assumed that the larger values calculated for the C1-O1 bond lengths of UDP-GlcNAc reflect the better leaving character of the UDP group compared to sugar aglycons. The comparison of the six-membered ring conformational rearrangements calculated in the present study with those observed in reactions catalyzed by glycosidases is of particular interest. Enforced by either the protonation of the glycosidic oxygen or the nucleophilic attack on the anomeric carbon, the changes observed in the GlcNAc ring conformation of UDP-GlcNAc resemble to some extent those calculated for 2-oxanol (36). This molecule was used as a hexopyranose model in the investigation of transition state structures during the glycoside hydrolysis mechanism. Some major features, however, distinguish glycosidases from glycosyltransferases. For example, it is clear from the analysis of all the points located on the PESs that the GlcNAc ring does not adopt any of the boat conformations sometimes described for glycosidase mechanism (30, 31). Most likely, the restraints associated with the nucleophilic attack of the acceptor and with the inversion of configuration at the C1 atom prevent any large ring conformational changes along the reaction pathways, which is in agreement with the assumption of the least motion effect (37). Complexes of glycosidases with a substrate or a product, in which a sugar ring is substantially deformed, have been experimentally observed (30, 31, 38). Ring distortion induced by these enzymes in ground states has been assumed to be crucial for their reaction mechanism. On the other side, circular dichroism studies in solution of *N*-acetylglucosaminyltransferase V and its complex with UDP-GlcNAc (39) suggested that the UDP part alone of UDP-GlcNAc is tightly bound to the enzyme while the GlcNAc residue is simply weakly interacting with the enzyme. These findings are supported by X-ray structural data available on complexes of glycosyltransferases with UDP-sugars (8, 11, 12) showing only the location of the UDP part in the binding pocket. The position of the transferred sugar moiety could never directly be determined from experiments, which suggests that in the ground state, the GlcNAc residue, initially observed in the $^4C_1$ conformation, is only loosely bound to the enzyme.

The inclusion of the electron correlation by means of the DFT/B3LYP method at the 6-31G* level usually reduces the relative energy of the stationary points determined on PESs compared to HF calculations (Table 26). The largest shifts are usually found for the structures along the proton transfer process, what indicates the importance of the use of electron correlation to describe systems with hydrogen bonds. The relative energy of the stationary points at the best theory DFT/B3LYP/6-31++G**//DFT/B3LYP/6-31G* is further decreased usually by about 3 kcal/mol and in few cases as much as 8 kcal/mol compared to DFT/B3LYP/6-31G*//DFT/B3LYP/6-31G*. The inclusion of electron correlation also affects the geometry of the molecules by increasing the bond lengths by approximately 0.3 Å (Table 5) as has earlier been observed for similar compounds (23-25).

Reaction pathways.

The calculated PESs show altogether the presence of five intermediates (INT1 – INT5) and 11 energy barriers indicating thus the existence of 11 transition states (TS1 – TS11). Considering the structures of the stationary points described on Figures 1b-3b and Table 25 as well as the relative energetic data listed in Table 26 and

schematically shown in Figure 34, a number of results on the mechanism of inverting *N*-acetylglucosaminyltransferases become immediately apparent:

A maximum of energy is observed in the central region of all the calculated PESs indicating that a concerted mechanism is impossible in this model of GlcNAc transfer reaction. Therefore, in order to move from reactants (R) to the product complex, the reaction has to proceed through a stepwise mechanism. To avoid confusion, it is emphasized that this concerns only the $r_{C1\text{-}Oa}$, $r_{Ha\text{-}OB}$, and $r_{HA\text{-}O1}$ reaction coordinates used to define the reaction mechanism. The C1-O1 bond has not been considered as a reaction coordinate since it is assumed here that changes in this bond length are a consequence of the nucleophilic attack or the proton transfer. The results clearly show that the C1-O1 distance varies in a continuous manner with the $r_{C1\text{-}Oa}$ and $r_{HA\text{-}O1}$ distances as a result of the nucleophilic attack at C1 or the proton transfer to O1. Whether the prolongation of the C1-O1 bond and the nucleophilic attack at C1 and proton transfer to O1 proceed in concerted manner remains to be explored.

There exist a number of transition states and intermediates connected by several pathways associated with proton transfer between the enzyme and the substrates and the nucleophilic attack of the acceptor. From the six possible pathways described here, only one [R → TS3 (36.3) → INT2 (30.4) → TS6 (59.8) → INT3 (54.4) → TS7 (54.7) → PC2 (-3)] appears very unlikely. In this pathway, the catalytic reaction begins with two consecutive energetically unfavorable proton transfers.

The overall activation energy of 38 kcal/mol calculated for the preferred pathway of the mechanism requiring the participation of a pair of carboxylic acids [R → TS9 (37.6) → INT4 (25.8) → TS10 (37.7) → INT5 (17.3) → TS11 (34.4) → PC2 (-3)] is relatively high. This mechanism involves the proton transfer from a catalytic acid to the glycosidic oxygen. However, the energy results shown on Figure 34, apparently suggest that for some enzymes, the involvement of this catalytic acid in the reaction mechanism might not be essential for the enzymatic catalysis. These conclusions are supported by experimental findings reported for the inverting mechanism of human fucosyltransferase V, where only one carboxylate residue functions as a general base catalyst. It has been shown (40, 41) that a single proton is "in flight" at the rate determining transition state. The secondary deuterium kinetic isotope effect for this reaction is consistent with a large degree of S_N1 character at the transition state and therefore a largely dissociative mechanism.

The GlcNAc transfer mechanism assuming the enrolment of only a catalytic base [R → TS1 (13.4) → INT1 (7.6) → TS2 (14.7) → PC1 (-22.4)] appears to be the less energy-demanding pathway represented on Figure 34. The overall activation energy calculated at the DFT/B3LYP/6-31++G** //DFT/B3LYP/6-31G* level is approximately 15 kcal/mol. The alternative pathway with the proton transfer to the catalytic base occurring as first step [R → TS3 (36.3) → INT4 (25.8) → TS4 (32.2) → PC1 (-22.4)] requires considerably higher overall activation energy (about 36 kcal/mol).

The comparison of the calculated reaction barriers with experimental data would be very instructive but, unfortunately, values of the rate constant k_{cat} determined for the various GTs are not available in the literature. Only k_{cat} values for blood group A and B glycosyltransferases(42) and for FucT V (40) have been reported. These k_{cat} values are in the range between 50 s^{-1} and 0.1 s^{-1}. Using the phenomenological definition associating k_{cat} with the activation free energy, $\Delta G^{act} = -RT\ln(hk_{cat}/k_BT)$, activation barriers between 15 kcal/mol and 19 kcal/mol have been determined. These estimates are in reasonable agreement with the overall activation energy of about 15 kcal/mol calculated for the GlcNAc transfer mechanism via the [R → TS1 (13.4) → INT1 (7.6) → TS2 (14.7) → PC1 (-22.4)] pathway. This further supports the assumption that inverting *N*-acetylglucosaminyltransferases would prefer a

general base catalyzed mechanism represented by such a pathway. However, without any additional experiment and because this agreement could be only fortuitous, it would be premature to completely exclude the possibility for the reaction to proceed via another pathway. Especially when similar activation barriers were calculated for several reaction pathways indicating that subtle changes in the microenvironment of the active site could change the overall reaction barrier of any of the pathways.

Transition state structures associated with the different reaction pathways exhibit significant variations in their C1-Oa and C1-O1 bond lengths (Table 25). Using these distances as criteria, the multiple transition states could be clustered into three groups presenting common structural features. The difference in C1-Oa and C1-O1 bonds of the TSs associated with different stages of the reaction and distinct pathways can be as large as 1.2 and 1.5 Å respectively. Superposition of the TSs belonging to each group is represented on Figure 35. The first group (Figure 35-A) is characterized by structures, such as TS2, TS5, TS8 and TS11, having short C1-Oa bonds within the range of 1.4-1.6 Å and long C1-O1 distances between 2.8 and 3.2 Å. The geometry of these stationary points is close to the structure of the final products, PC1 or PC2, where the C1-Oa bond created from the nucleophilic attack of the acceptor on C1 almost reached its final length of 1.42 Å and the UDP group is leaving the reaction site. These structures can therefore be described as "late transition states". The second group (Figure 35-B) is represented by structures, such as TS3, TS4, TS9 and TS10 with long C1-Oa bonds located within the range of 2.4-2.7 Å and short C1-O1 distances comprised between 1.5 and 2.1 Å. The geometries of these stationary points have not been yet altered by the reaction and thus, are very comparable to the initial reactants. These structures can be termed as "early transition states". The third group (Figure 35-C) corresponds to intermediate structures such as TS1, TS6 and TS7 where both C1-Oa and C1-O1 are elongated compared to their initial values but where the structures did not reach yet the final arrangement observed in the products, PC1 and PC2. Compared to the $^4C_1$ chair conformation in the reactants, the shape of the GlcNAc ring in most of the transition states changes to half-chair. These variations in C1-Oa and C1-O1 bond lengths and in the ring shape of the GlcNAc residue clearly demonstrate that the design of a transition state analog inhibitor is dependent on the actual mechanism of a particular enzyme.

Though the active site model consists of all the molecules that may directly be involved in the mechanism, it does only represent a model of the real active site and as such it has its internal limitations and several factors can influence the calculated relative energies. The actual arrangement of the relevant molecules as well as their conformation in the real active site might differ from the model considered but it can also vary from enzyme to enzyme. The real location of the catalytic acids in a particular enzyme may be different compared to the model. This may result, for example, in a smaller $r_{Oa\text{-}OB}$ distance between the catalytic base and the hydroxyl group of the oxygen of the acceptor. As a consequence, the reaction barrier for the proton transfer from the acceptor to the catalytic base might be lower.(43) Reaction barriers for proton transfer and nucleophilic attack processes may also be drastically influenced by the presence in the vicinity (up to 6Å) of the reaction center of ionized amino acid residues despite the fact that they might not participate in the reaction.(44) The influence of the catalytic metal on the conformation of the substrates is also a parameter to consider. An earlier study (25) showed that the relative stability of sugar-pyrophosphate conformations is sensitive to the occupancy of the metal coordination shell by interactions with surrounding elements present in the enzyme active site. This can be observed for instance, in the crystal structure of a nucleotide-complexed form of nucleotide-diphospho-sugar transferase SpsA, (11) where the coordination of the metal present in the active site, Mn^{2+}, involves a neighboring aspartate residue.

Albeit ΔG values would be more appropriate for description of reaction processes, the conclusions were based on the energy values. For such a complex system like the reaction model, the determination of the ΔG for each individual step of the catalytic reaction would require enormous computational resources. On the basis of previous model compounds (23-25) that suggested inclusion of the ZPE and thermodynamic contributions to the calculated energies would only barely decrease energy differences, these calculations were not done. Therefore, it might be presumed that the calculated ΔE values could slightly be overestimated compared to ΔG values.

On the catalytic reaction mechanism of inverting *N*-acetylglucosaminyltransferases.

On the basis of the available experimental data and these calculation results, a mechanism of inverting *N*-acetylglucosaminyltransferases is suggested.

Experimental studies have revealed a sequential mechanism for GnT I and GnT II (6, 22) where UDP-GlcNAc binds first either to an enzyme.Mn^{2+} complex or as a Mn^{2+}.UDP-GlcNAc complex followed by the binding of the acceptor substrate. Already observed in crystal (8) and in solution, (39) the binding of the sugar-donor appears to be associated with conformational changes of the enzyme upon binding of the sugar-acceptor. The binding of the nucleotide-sugar by the enzyme therefore triggers the conformational change that will bring to a proper distance the donor- and acceptor-binding sites in order to start the enzymatic reaction. Crystal structures of glycosyltransferases (8, 11, 12) and a solution study on GnT V (39) revealed however, that only the UDP part is observable in the nucleotide-sugar.enzyme complex. The sugar residue of the donor would then just be loosely bound in the ground state complex. Thus only the UDP-binding domain may be present or accessible in the sugar-donor.enzyme complex. This hypothesis can be supported by inhibition studies of GlcNAc-T II (6) indicating that neither GlcNAc nor GlcNAc-α-1-phosphate binds to the enzyme, whereas UDP-Glc, UDP-Gal, and UDP-GalNAc do bind into the enzyme though they are not substrates for GnT II. These results show how crucial is the UDP part for the binding of the donor into the enzyme, whereas it is mostly during the sugar transfer reaction that the enzyme recognizes the GlcNAc residue. UDP-GlcNAc being the GlcNAc-donor substrate of all GnTs, it is believed that the specificity of the enzyme must ensue from the structure of the transition state-binding domain that includes also specific information on the sugar-acceptor substrate.

In view of these different elements, one can therefore speculate that the sugar donor-binding site in *N*-acetylglucosaminyltransferases consists of two separate pockets: one pocket serving to accommodate the UDP part of the donor and a second for the binding of the sugar residue that will be transferred during the reaction. Only the UDP pocket would be occupied in the ground state. The sugar pocket of the donor-binding site would become accessible only after the reaction starts and the C1-O1 bond is elongated. Then only, in the transition state of the reaction, would the pocket be fully occupied. This pocket could more precisely be termed as the "sugar transition state pocket". The UDP and sugar pockets should be separated by a distance corresponding approximately to the C1-O1 bond length in the transition state, which can be as large as 3.2 Å based on the calculations.

The architecture of the uridine-binding site, commonly known as a nucleotide recognition domain (NRD)(45), has been well described for many nucleotide-binding enzymes. A network of interactions involving the uracil and ribose rings with some conserved amino acids characterizes this region.(8, 11, 12) Therefore, it can be envisaged that the topology of the UDP-binding site may be fairly comparable in all concerned glycosyltransferases. An important feature in the UDP pocket is the presence of a metal cofactor, usually Mn^{2+}, which is required by most of the UDP-dependent transferases for activity. The exceptions might appear to be β-1,6-GlcNAc-Ts, since their activity does not depend on the addition of a metal cofactor to the medium, however, it is assumed that these

enzymes already contain a tightly bound metal ion.(1-4) The divalent cation contributes to the binding of UDP-GlcNAc in the binding site through strong interactions with the pyrophosphate group of the nucleotide. The nature of these interactions presumably determines the conformation adopted by the pyrophosphate group during the reaction. Without a doubt, the metal also plays an important role in the stabilization of the leaving group, UDP, which sees its formal charge changing from 0 to -1 as the C1-O1 bond is cleaved. It has been shown that a particular aspartate from the D*X*D motif, contained in many glycosyltransferases and involved in the binding of the nucleotide-sugar, is crucial for binding the divalent ion associated with the nucleotide. (46) A complex of UDP.Mn^{2+} was found in the products of galactosyltransferase reactions (28), leading to the notion that this particular Asp residue may also play an important role in the removal of the UDP-metal complex from the reaction site.

During the nucleophilic attack of the acceptor on the anomeric carbon, calculation of reaction pathways clearly showed the elongation of the C1-O1 linkage accompanied by conformational rearrangement of the glucopyranose ring. As the catalytic reaction proceeds, modifications at the reaction center move the sugar residue closer to the sugar-binding pocket. Interactions between the sugar and the enzyme benefit from this movement. As reactants get closer to the transition state, interactions with the enzyme increase and become crucial for the stabilization of the TS during the rate-limiting step. Relevant structural features within the enzyme active site should reflect the specificity and the structure of the transition state for a particular enzyme. The specificity for a particular sugar residue that differentiates UDP-GlcNAc, UDP-Glc, UDP-GalNAc, and UDP-Gal is likely produced by a sensitive array of hydrogen bonds, hydrophobic, and electrostatic interactions. Though the structure of the "sugar transition state pocket" is not experimentally known, one can hypothesize that this pocket will likely accommodate specific interactions with the proton-rich part of the half-chair sugar ring. Some amino acid residues located in the neighborhood of the *N*-acetyl group at C2 could also be responsible for the specificity of the enzyme, distinguishing for example between UDP-GlcNAc and UDP-Glc substrates. In the case of A/B glycosyltransferases, (42) the difference for the donor specificity, UDP-Gal vs. UDP-GalNAc, has been shown to reside in the different nature of a single amino acid, e.g. methionine vs. leucine, interacting favorably with the *N*-acetyl group of the donor. In the same way, properly oriented amino acids should preferentially interact with the equatorially oriented hydroxyl group at the C4 atom of GlcNAc and not with the axially oriented OH4 of GalNAc.

Concerning the acceptor-binding site, it should reflect the differences appearing in the oligosaccharide-acceptor structures, specific for each *N*-acetylglucosaminyltransferase, and what contributes to the specificity of the enzyme. In the case of a general base mechanism, a catalytic base, presumably an aspartate or a glutamate residue, is likely to be positioned at a proper distance from the hydroxyl group of the oligosaccharide-acceptor where the sugar transfer will occur. Inhibition studies of GlcNAc-T V revealed (47) that the α-D-mannopyranosyl residue to which GlcNAc-T V transfers is not tightly bound to the enzyme prior to the transfer of GlcNAc from the donor. This flexibility may allow the α-D-mannopyranosyl residue to adopt the optimal position for the nucleophilic attack.

Conclusion

Despite their extreme importance, the mechanism of glycosyltransferases has not yet been resolved but the results of this investigation have enlarged the understanding of this process. The present work explores the potential energy surface for the transfer of GlcNAc catalyzed by inverting *N*-acetylglucosaminyltransferases using *ab initio* quantum chemical methods. The structural model of the reaction site used in this study consists of all essential molecules assumed to be involved in the mechanism. All stationary points, transition states, and intermediates revealed from the calculated PESs were characterized at HF/6-31G*, HF/31++G**//HF/6-31G*, DFT/B3LYP/6-

31G*, and DFT/B3LYP/6-31++G**// DFT/B3LYP/6-31G* levels. The multiple transition states along the different reaction pathways were grouped into three groups having common structural features relating them to different stages of the reaction. These geometrical differences clearly demonstrate that the design of a transition state analog inhibitor is dependent on the actual mechanism of a particular enzyme. Among the six different reaction pathways analyzed, a stepwise reaction pathway assuming the enrolment of only a catalytic base [R → TS1 (13.4) → INT1 (7.6) → TS2 (14.7) → PC1 (-22.4)] appeared to be the most probable reaction path, and is consistent with the existing experimental data. The mechanism described by such a pathway starts with the nucleophilic attack of the acceptor hydroxyl on the anomeric carbon C1 of the transferred GlcNAc, followed by proton transfer from the acceptor to the catalytic base.

The use of *ab initio* methods to study enzyme reactions presents a great challenge due to the high complexity and dimensionality of the potential energy surfaces describing this type of mechanism. Nevertheless, the recent progress in computational methods and technology makes possible to study more and more complex systems such as those presented in this work. The results obtained by these methods can supplement experimental data and provide unique information about reaction pathways and structure of the relevant stationary points observed along the reaction coordinate. Needless to say, such information is vital for the design of drugs inhibiting these enzymes.

Example 2

Structural Modeling of *N*-acetylglucosaminyltransferases

The structure of the enzyme is another relevant asset to design inhibitors in a rational way. In the absence of X-ray data, the modeling of the three-dimensional structure of some GnTs (Core2L and Core2b/M GnTs; GnT V; GnT Vb) provides an alternative to get insight on structural features of the active site. The modeling of these GnTs was carried out using computational procedures in the following systematic way:

(a) Search for homologous sequences in protein amino acid sequence databases and alignment of the amino acid sequences.

(b) Structural modeling of the protein using either the Threading or Homology approach.

(c) Refinement of the models using molecular mechanics.

(d) Docking of ligands into the active site of the enzyme.

(e) Analysis and description of the binding interactions for ligands.

(f) Search for ligand mimics in databases of protein-ligand complexes.

Information from the ab initio molecular orbital study described in Example 1 was also used in the modeling of the the glycosyltransferases.

Computational procedures. – Two different modeling procedures were used to generate models of GnTs. The first approach is so-called "protein threading". This method has been used to successfully predict protein structures prior to their experimental studies. The appraisal of such approach is periodically reviewed at the "meetings on the Critical Assessment of Techniques for Protein Structure Prediction (CASP)".(50) The threading approach is generally used when there is no structural or functional information on the sequence of interest. In this approach, a query amino acid sequence of a particular protein, in particular GnT, is mapped onto all the experimentally observed protein folds by using the publicly available Fold Recognition Server (51, 52). The fitness of such mapping is computationally based on a heuristic-scoring scheme that takes into account experimentally observed amino acid interactions. Based on their score, the best matching folds are selected, and the corresponding structural fragments are retrieved from the PDB database. (53) Subsequently, the protein sequence is mapped onto

the different fragmentary structures. Though the generation of protein models using such procedure contains large risks, site-directed mutagenesis experiments and exhaustive docking calculations can validate the reliability of a particular model. The threading modeling approach has been used in the early stage of the investigation for generating models of GnTs. However, since the X-ray coordinates of SpsA glycosyltransferase (11) and GnT I (49) structures were obtained another approach, called "homology modeling", has been used to predict the protein structures.

The homology procedure exploits the structural similarities between proteins by constructing a three-dimensional structure of a given sequence using as a template the structure of a similar and known protein. In this procedure, the amino acid sequence of the protein is matched onto the protein selected to be the template. The Needleman-Wunch alignment algorithm (54) was applied to align the two sequences of amino acids and the homology module from MSI (55) was used to construct the enzyme models. First, the SpsA glycosyltransferase structure (11) was utilized as a template model for generating the homology models of GnTs. Subsequently the crystal structure of GnT I (49) became available, and it was used in the computational studies. In the created models, the atomic charges were assigned using the cvff91 force field and the essential hydrogen atoms fixed.

Topology of known GnTs. – The X-ray structures of GnT I and SpsA are shown on Figure 4.a. The architecture of their binding sites appears somewhat similar. An exception is a loop consisting of amino acids 318-329 that is not clearly seen in the electron density map of GnT I (Figure 4.b). In the SpsA structure, a loop similar to the sequence 318-329 of GnT I is folded into the active site and interacts with the nucleotide. The nucleotide-binding domain of SpsA is very similar to others, such as in pyruvate kinase and in 5'-3' exonuclease domain of *Thermus aquaticus* DNA polymerase. The location of UDP was then determined using a docking procedure. Sequence alignments were performed for all GnT V, GnT Vb, Core2L and Core2b/M GnT enzymes. The best identity alignment, usually ~30%, was used for further studies. To illustrate such procedure, the sequence alignment of Core2L GnT with GnT I is displayed on Figure 5. On this Figure, the relevant amino acid residues of the GnT I binding site are highlighted.

Homology modeling of Core2L GnT, Core2b/M GnT and GnT V. – Figure 6 shows the comparison of the homology models obtained for GnT V, Core2L and Core2b/M GnTs using as a template the GnT I structure. On this Figure, few relevant amino acid residues constituting the nucleotide-binding site accommodating the UDP part of the sugar-donor are shown in the form of tubes. The architecture of the active site was found to be similar for all three enzymes. Of course, some differences in the amino acid residues that form the active sites exist and they are discussed below.

Modeling of *N*-acetylglucosaminyltransferase-Ligand Complexes

Insight on the crucial interactions between the enzyme and the natural substrates in the binding site is a prerequisite for understanding the catalytic mechanism of the enzyme and designing a specific inhibitor. To determine the interactions responsible for the binding of the ligands, the structure of GnT-ligand complexes was investigated using the docking approach.

Computational methods. – The protein-ligand docking calculations were performed using the AutoDock suite of programs (56). The position and orientation of the ligand into the protein was not constrained. All the freely rotatable bonds of the ligands were allowed to vary during the optimization runs of docking. About 100 docking runs were performed for every ligand. Each of these runs consists of about 1 million energy evaluations. Subsequently, the calculated complexes were clustered using a RMS tolerance of 2.5Å and the top ranked clusters analyzed.

4.a. Critical Binding Sites for the Natural Substrates

The docking of the natural substrates into the active site of GnTs has been performed in a systematic manner. After docking UDP into the enzyme active site, the prominent binding modes for the nucleotide were identified and the lowest energy binding mode was used. Subsequently, the GlcNAc residue and the oligosaccharide-acceptor were docked into the protein active site. Three of the sub sites constituting the enzyme active sites, the UDP sub site, the GlcNAc sub site and the acceptor sub site, are briefly described in the following.

UDP-binding site. – Docking calculations of the UDP molecule onto the surface of the GnT I structure were undertaken. Guided by the SpsA structure were undertaken, the metal cation had earlier been placed in the active site of GnT I. Several possible binding modes for UDP were predicted. Figure 7 shows the lowest energy binding modes of UDP within the electrostatic potential surface of GnT I. As it can be clearly seen from this Figure, UDP (shown in colored lines) binds into the well-formed electronegative groove where several interactions between the uridine and the side chains of GnT I stabilize the UDP location. A list of the predicted interactions is given in Table 10, 11, 12, and 13. This funnel shaped groove restricts the conformation of the uracil ring in a narrow pocket. While in most of the lowest energy binding modes calculated for UDP, the uracil group appears to prefer a similar and characteristic binding mode, at least three different conformations are observed for the pyrophosphate moiety. A comparison of the atomic details described therein on the GnT I-UDP complex with the model of the complex obtained by docking revealed that the predicted intermolecular interactions described in Table 10 are in agreement with the interactions experimentally observed. Similarly to the procedure above described for GnT I, the different homology models of GnTs were used to determine and characterize the binding site of the nucleotide sugar. A similar electronegative groove with the uracil part of UDP bound deeply into the pocket is commonly seen in the known X-ray structures of glycosyltransferases. Comparison of the observed and predicted interactions revealed that a characteristic pattern of interactions is conserved in all GnTs and suggests that this region is relevant for the recognition and binding of UDP-GlcNAc. This is illustrated on Figure 8 where the interactions between the enzyme and UDP are displayed.

Based on the docking results, the UDP-binding site in Core2L GnT can be described in detail. A representation of the four top scoring Core2L GnT complexes with UDP is shown on Figure 9. In the conformations displayed on this Figure, the uridine part of UDP favors a similar binding mode comparable to the one observed in GnT I, but the diphosphate moiety adopts two different conformations. In both of these phosphate conformations, the phosphoryl oxygens located the closest to the uridine are in the vicinity of a glutamate (Glu-159 in Core2L GnT) that is conserved in the pyrophosphate sub site through all the different GnTs investigated (Table 10, 11, 12, and 13) Residues Ile-57 and His-131 located in the surroundings of the ribose-binding pocket arrest the ribose in a definite location. These interactions, together with stacking interactions of the Cys59-Cys100 disulfide bond with the uracil, assist in restricting the uridine group in a favorable position to the protein. The conformational preferences observed for the pyrophosphate group indicate a possible flexibility of the pyrophosphate moiety. This flexibility may play an important role in the removal of the products from the active site.

Results from the docking of UDP into the homology model of GnT V gave a set of conformations that overlapped with the predicted UDP-Core2L GnT complex (Table 11, 12). However, the stacking interactions of the uracil group with the Cys59-Cys 100 disulfide bond were not observed in GnT I. This seems to be the most relevant difference between the UDP-binding sites of GnT V and Core2L GnT.

Transition state-binding site. – As an isolated molecule, GlcNAc appears to dock in many regions of the GnT I surface. The surface representation of GnT I is shown on Figure 10. In GnT I, the most significant binding site

of the GlcNAc molecule corresponds to a specific hydrophobic pocket. The predicted lowest energy docking modes calculated for the acceptor heptasaccharide into the enzyme are shown on Figure 10. The terminal mannose, to which the GlcNAc is transferred, is buried into the binding site, in the vicinity of the GlcNAc-binding site. Several docking modes for the acceptor are observed. The location of the amino acid Asp-291 in the vicinity of GlcNAc and the acceptor oligosaccharide suggests a possible function of catalytic base for this amino acid. Some of the low energy docking modes resemble the lowest energy complex displayed on Figure 10, however, different arrangements of the other sugar units are observed, that creates distinct local interactions.

As for GnT I, the GlcNAc molecule in the isolated form, appears to dock in many regions of the Core2L GnT surface. Figure 11 shows one of the predicted binding modes for the UDP-GlcNAc-Acceptor (GalNAc-Gal) complex. The most significant binding site of the GlcNAc molecule is a hydrophobic rich region located about 3 Å apart from UDP. The estimation of this distance is done using the (GlcNAc)C1…OP(UDP) distance. For Core2L GnT, the Glu-253 residue is assumed to play the role of the catalytic base in the reaction mechanism. On Figure 11 the protein surface is color coded by the chemical nature of the atom. It is clear from this Figure that the entire ligand molecules dock into the cavity formed at the Core2L GnT surface. It is also noteworthy that the arrangement of the reactants in this binding mode resembles the structure of the late transition state predicted by the *ab initio* calculations.

To summarize, the active site of the modeled Core2L GnT appears to have at least three prominent sub sites where the UDP, the GlcNAc and the oligosaccharide-acceptor can easily be accommodated. The GlcNAc and the oligosaccharide-acceptor regions are outlined in green on the electrostatic potential surface of the modeled Core2L GnT presented in Figure 12. In this Figure, the UDP is shown in its preferred binding mode. The sub site located on the top of the ribose ring is the hydrophobic region where the GlcNAc binds. The other sub site corresponds to the region where the disaccharide-acceptor (GalNac-Gal) binds.

The results revealed that the UDP-binding site of the modeled Core2b/M GnT has similar features to those earlier described for Core2L GnT. The similar architecture of the active site in all GnTs studied is documented in Tables 10, 11, 12, and 13, where some relevant amino acid residues forming three sub sites of the active site are listed together with the predicted catalytic base residue.

At the moment, results on the GnT V-transition state complexes are based on the model of GnT V issued from the SpsA structure. These results are given on Figure 13 and they resemble the results on other GnTs revealing three distinct sub sites in the enzyme active site.

4.b. Binding of Selected Compounds into the Active Site of *N*-acetylglucosaminyltransferases

As a first step in understanding the potency and specificity of the GD compounds, several compounds were docked into the Core2L GnT model. Preliminary results indicate that GD compounds with a UDP-like group prefer to dock into a well defined pocket through two strong hydrogen bonds with Asp-99 and His-131 and a strong stacking interaction with the hydrophobic amino acid residue, Ile-57, located at the bottom of the pocket. To illustrate the potential of the method used, the results obtained for GD0500, a fragment of GD0541 and a potential inhibitor are described.

Binding mode of GD0500. – GD0500 is an analogue of the uridine molecule bearing a small modification at the C5 position of the uracil ring. The docking of this simple molecule into the active site of Core2L GnT led to four prominent binding regions. A location of the top ranking binding mode resulting from the docking calculations corresponds to the earlier described UDP-binding pocket of Core2L GnT (Figure 14). This binding mode involves

all the interactions observed for the binding of the uridine part of UDP. However, the orientation of GD0500 in the binding site is slightly different than for UDP. The substituent at the C5 position of the uracil ring of GD0500 favors a hydrogen bond interaction with Tyr-97 from Core2L GnT. This interaction might be responsible for the small shift in the orientation of GD0500 compared to UDP. In addition, this hydrogen bond interaction may perhaps be the reason for the specific inhibition of Core2L GnT. In fact, preliminary results show that Tyr-97 is not present in the models of GnT I and GnT V. The absence of this interaction in the enzyme-GD0500 complexes may explain the different inhibitory results of this compound against the different enzymes.

Binding mode of a GD0541 fragment. – GD0541 was found to be a potent inhibitor of Core2L GnT. Docking of a fragment of this molecule in the Core2L GnT model revealed various possible binding modes in several regions of the protein surface (represented in yellow color on Figure 15). A detailed analysis of the docking calculations revealed the presence of a conformational cluster of the GD0541 fragment overlapped with the predicted binding region of UDP. In these computed GD0541 fragment-Core2L GnT complexes, the hydroxyl groups attached to the benzyl group of GD0541 fragment are situated in close distance to the metal ion. Independently, a structural database search revealed that similar hydroxyl groups attached to a benzyl ring generally favor interactions with a bound metal ion.

Binding mode of a potential GD0541 analogue. – Extensive database searches revealed that tetrahydroaminoacridine (Tacrine, Figure 16.a) and its structural analogues prefer to dock into hydrophobic rich region. Interestingly, Tacrine is a drug already used for the treatment of Alzheimer's disease as an inhibitor of acetylcholinesterase. A close resemblance was detected between the GlcNAc-binding site in Core2L GnT and the Tacrine-binding sites in various protein complexes. This suggests that Tacrine could presumably occupy the hydrophobic region of GlcNAc. As a result of these observations, a molecule was built on the assumption that a combination of the GD0541 structural features with the hydrophobic moiety contained in Tacrine might lead to a significant restriction of the binding modes observed for the GD0541 fragment. Computational modification of GD0541 resulted in a new potential molecule having the Tacrine molecule attached to the fragment of GD0541 through an etheric linkage (Figure 16.b). The docking results show that unlike the GD0541 fragment alone, this combination of fragments, displayed on Figure 15 in white color, favors indeed the docking in a single region of the Core2L GnT model. This region appears also to be the prominent site where UDP binds. In the top scoring complexes, the Tacrine fragment binds into the GlcNAc-binding site while the hydroxyls of the GD0541 fragment interact with Glu-159 and Asp-160 via a metal ion. This suggests that this type of molecule could be tested as a potential lead for developing new inhibitors of Core2L GnT.

Discussion and Conclusions

The present results shed some light on the mechanism of inverting *N*-acetylglucosaminyltransferases, the structure of the transition states, the structure and character of the catalytic site of GnTs, and the binding of natural substrates and inhibitors into the GnTs. As a result, the following conclusions can be drawn:

Among the six different reaction pathways analyzed, a stepwise reaction pathway assuming the enrolment of only a catalytic base appears to be the most probable reaction path that is consistent with the existing experimental data. A mechanism described by such pathway starts with the nucleophilic attack of the acceptor reactive hydroxyl on the anomeric carbon C1 of the transferred GlcNAc, followed by the proton transfer from the acceptor to the catalytic base. The structure of the rate determining transition state for this pathway corresponds to the "late transition state".

The multiple transition states found along the different reaction pathways were classified into three groups having common structural features relating them to different stages of the reaction. During the reaction, the structure of the donor, UDP-GlcNAc, undergoes significant structural changes. The geometry of the so-called "late transition states" is close to the final products, where the C1-Oa bond (1.5 Å) created during the reaction almost reached the length of the C-O glycosidic bond (1.42 Å). The UDP group that is leaving the reaction site is characterized by the C1-O1 distance ~3 Å. The structural characterization of the late transition state offers us an opportunity to create a pharmacophore and to design late transition state analogue inhibitors.

The binding interactions of the natural substrates (UDP-GlcNAc and acceptor-oligosaccharide) within the homology models of Core2L GnT, GnT V and GnT I were described. Based on the complex models, it is proposed that the binding sites of these enzymes possess at least three prominent binding sites. The models allowed the prediction of the position of an amino acid residue that functions as the catalytic base in the catalytic reaction mechanism. The characterization of the structure and interactions in each of the three binding sub sites can be used in a sub site-directed pharmacophore search.

In all the GnTs, the binding conformation of the uracil group in UDP is restricted because of the size of the funnel shaped groove and the nature of the amino acid residues forming the narrow groove. In all the predicted binding modes of UDP, the carbonyl oxygen atoms (O2, O4) and the amide hydrogen (N3H) of the uracil ring interact with the protein while the C5 position of the ring is exposed to the exterior.

The ribose ring prefers a very defined conformation in the active site of all GnTs. A hydrophobic residue at the bottom of the UDP-binding site pocket arrests the conformation of the ribose by favorable stacking interactions.

A "hydrophobic pocket" corresponding to the GlcNAc transition state-binding site has been identified. In all GnTs, the GlcNAc prefers to dock into this well-defined hydrophobic pocket, which is approximately 3 Å distant from the pyrophosphate-binding sub site.

Models of Core2L GnT complexed with some drug hits provide some structural explanation for their inhibitory activity.

Proposed catalytic mechanism of glycosyltransferases. – On the basis of the available experimental data, protein-ligand modeling, reaction pathways and transition state structure calculations, the mechanism of inverting *N*-acetylglucosaminyltransferases.

Experimental studies have revealed a sequential mechanism for GnT I and GnT II (6, 22) where UDP-GlcNAc binds first either to an enzyme.Mn^{2+} complex or as a Mn^{2+}.UDP-GlcNAc complex followed by the binding of the acceptor substrate. Already observed in crystal (8) and in solution, (39) the binding of the sugar-donor appears to be associated with conformational changes of the enzyme upon binding of the sugar-acceptor. The binding of the nucleotide-sugar by the enzyme therefore triggers the conformational change that will bring to a proper distance the donor- and the acceptor-binding sites in order to start the enzymatic reaction. Crystal structures of glycosyltransferases (8, 11, 12) and a solution study on GnT V (39) revealed however, that only the UDP part is observable in the nucleotide-sugar.enzyme complex. The sugar residue of the donor would then just be loosely bound in the ground state complex. Therefore only the UDP binding domain may be present or accessible in the sugar-donor.enzyme complex. This hypothesis can be supported by inhibition studies of GlcNAc-T II (6) indicating that neither GlcNAc nor GlcNAc-α-1-phosphate binds to the enzyme, whereas UDP-Glc, UDP-Gal, and UDP-GalNAc do bind into the enzyme though they are not substrates for GnT II. These results show how crucial is the UDP part for the binding of the donor into the enzyme, whereas it is mostly during the sugar transfer reaction that

the enzyme recognizes the GlcNAc residue. Since UDP-GlcNAc is the GlcNAc-donor substrate of all GnTs, the specificity of the enzyme must ensue from the structure of the transition state binding domain that includes also specific information on the sugar-acceptor substrate.

In view of these different elements and results of the molecular modeling, one can therefore consider that the sugar-donor binding site in *N*-acetylglucosaminyltransferases consists of two separate pockets. One pocket serving to accommodate the UDP part of the donor and a second for the binding of the sugar residue that will be transferred during the reaction. Only the UDP pocket would be occupied in the ground state. The sugar-binding pocket of the donor would only become accessible after the reaction starts and the C1-O1 bond is elongated. Only in the transition state of the reaction, would the pocket be fully occupied. This pocket could more precisely be termed as the "sugar transition state pocket". The GnT homology structures complexed with ligands show that the GlcNAc pocket is very hydrophobic and separated by about 3 Å from the UDP pocket. This separation corresponds approximately to the average C1-O1 bond length of 3.1 Å observed in the late transition states that was independently calculated using *ab initio* methods.

The architecture of the uridine-binding site, commonly known as a nucleotide recognition domain (NRD)(45), has been well described for many nucleotide-binding enzymes. A network of interactions involving the uracil and ribose rings with some conserved amino acids characterizes this region. (8, 11, 12). The docking calculations with different GnTs show similar nucleotide-binding interactions where the uracil and ribose moieties are tightly bound to the enzyme. Therefore, it can be envisaged that the topology of the UDP-binding site may be quite comparable in the concerned glycosyltransferases. An important feature in the UDP pocket is the presence of a metal cofactor, usually Mn^{2+}, which is required by most of the UDP-dependent transferases for activity. The exceptions might appear to be β-1,6-GlcNAc-Ts, since their activity does not depend on the addition of a metal cofactor to the medium, however, it is assumed that these enzymes already contain a tightly bound metal ion. (1-4). The divalent cation contributes to the binding of UDP-GlcNAc in the binding site through strong interactions with the pyrophosphate group of the nucleotide. The nature of these interactions presumably determines the conformation adopted by the pyrophosphate group during the reaction. Without a doubt, the metal also plays an important role in the stabilization of the leaving group, UDP, which sees its formal charge changing from 0 to -1 as the C1-O1 bond is cleaved. It has been shown that a particular aspartate from the D*X*D motif, contained in many glycosyltransferases and involved in the binding of the nucleotide-sugar, is crucial for binding the divalent ion associated with the nucleotide. (46) In agreement with these data, the GnT homology models (Tables 10 and 11) have usually a glutamate residue in the vicinity of the pyrophosphate-binding site. A complex of UDP.Mn^{2+} was found in the products of galactosyltransferase reactions, (28) which indicates that this particular aspartate residue may as well play an important role in the removal of the UDP-metal complex from the reaction site.

During the nucleophilic attack of the acceptor on the anomeric carbon, calculation of reaction pathways clearly showed the elongation of the C1-O1 linkage accompanied by conformational rearrangement of the glucopyranose ring. As the catalytic reaction proceeds, modifications at the reaction center move the sugar residue closer to the sugar-binding pocket. Interactions between the sugar and the enzyme benefit from this movement. As reactants get closer to the transition state, interactions with the enzyme increase and become crucial for the stabilization of the TS during the rate-limiting step. Relevant structural features within the enzyme active site should reflect the specificity and the structure of the transition state for a particular enzyme. The specificity for a particular sugar residue that differentiates UDP-GlcNAc, UDP-Glc, UDP-GalNAc, and UDP-Gal is likely produced by a

sensitive array of hydrogen bonds, hydrophobic, and electrostatic interactions. Though the structure of the "sugar transition state pocket" is not experimentally known, one can hypothesize that this pocket will likely accommodate specific interactions with the proton-rich part of the half-chair sugar ring. Some amino acid residues located in the neighborhood of the *N*-acetyl group at C2 could also be responsible for the specificity of the enzyme distinguishing for example between UDP-GlcNAc and UDP-Glc substrates. In the case of A/B glycosyltransferases, (42) the difference for the donor specificity, UDP-Gal vs. UDP-GalNAc, has been shown to reside in the different nature of a single amino acid, e.g. methionine vs. leucine, interacting favorably with the *N*-acetyl group of the donor. In the same way, properly oriented amino acids should preferentially interact with the equatorially oriented hydroxyl group at the C4 atom of GlcNAc and not with the axially oriented OH4 of GalNAc. Indeed, the docking modeling of UDP-GlcNAc into Core2L GnT supports these assumptions, showing a specific hydrogen bond between the OH4 from GlcNAc and Ser-158 and a stacking interaction of the N-Acetyl group from GlcNAc with Leu-163. Such interactions would not be possible in a different type of sugar residue (i.e. Glc, Gal, GalNAc or Man).

Concerning the acceptor-binding site, it should reflect the differences appearing in the oligosaccharide-acceptor structures, specific for each *N*-acetylglucosaminyltransferase, and what contributes to the specificity of the enzyme. In the case of a general base mechanism, a catalytic base, presumably an aspartate or a glutamate residue, is likely to be positioned at a proper distance from the hydroxyl group of the oligosaccharide-acceptor where the sugar transfer will occur. In the homology models, a catalytic base (see Tables 10, 11, 12, and 13) is usually present in the neighborhood of the GlcNAc and oligosaccharide acceptor moieties. Inhibition studies of GlcNAc-T V revealed (47) that the α-D-mannopyranosyl residue to which GlcNAc-T V transfers is not tightly bound to the enzyme prior to the transfer of GlcNAc from the donor. This flexibility may allow the α-D-mannopyranosyl residue to adopt the optimal position for the nucleophilic attack. In the computed model of the GnT I-Transition state complex (Figure 10), the oligosaccharide-acceptor binds into a canal formed by a patch of hydrophobic residues (Phe-181, Tyr-184, Phe-289 and His-178). The key trimannosyl residues of the oligosaccharide-acceptor dock onto this region to stabilize the enzyme-transition state complex.

This example describes results on the catalytic mechanism and the homology modeling of GnTs and their complexes with ligands. These results contribute to the understanding of the reaction mechanism catalyzed by GnTs and to the essential requirements for a rational design of inhibitors. The results are consistent with the experimental data.

While the present invention has been described with reference to what are presently considered to be the preferred examples, it is to be understood that the invention is not limited to the disclosed examples. To the contrary, the invention is intended to cover various modifications and equivalent arrangements included within the spirit and scope of the appended claims.

All publications, patents and patent applications are herein incorporated by reference in their entirety to the same extent as if each individual publication, patent or patent application was specifically and individually indicated to be incorporated by reference in its entirety.

REFERENCES

(1) Beyer, T. A.; Sadler, J. E.; Rearick, J. I.; Paulson, J. C.; Hill, R. L. *Adv. Enzymol.* 1981, *52*, 23-175.

(2) Schachter, H. *Curr. Opin. Struct. Biol.* 1991, *1*, 755-765.

(3) Kleene, R.; Berger, E. G. *Biochim. Biophys. Acta* 1993, *1154*, 283-325.

(4) Montreuil, J.; Vliegenthart, J. F. G.; Schachter, H. *Glycoproteins*; Neuberger, A. and van Deenen, L. L. M., Ed.; Elsevier: Amsterdam, 1995; Vol. 29a.

(5) Montreuil, J.; Vliegenthart, J. F. G.; Schachter, H. *Glycoproteins and Disease*; Neuberger, A. and van Deenen, L. L. M., Ed.; Elsevier: Amsterdam, 1995; Vol. 30.

(6) Bendiak, B.; Schachter, H. *J. Biol. Chem.* 1987, *262*, 5784-5790.

(7) Raju, T. S.; Stanley, P. *J. Biol. Chem.* 1998, *273*, 14090-14098.

(8) Vrielink, A.; Ruger, W.; Driessen, H. P. C.; Freemont, P. S. *EMBO J.* 1994, *13*, 3413-3422.

(9) Campbell, J. A.; Davies, G. J.; Bulone, V.; Henrissat, B. *Biochem. J.* 1997, *326*, 929-942.

(10) Imberty, A.; Monier, C.; Bettler, E.; Morera, S.; Freemont, P.; Sippl, M.; Flockner, H.; Ruger, W.; Breton, C. *Glycobiology* 1999, *9*, 713-722.

(11) Charnock, S. J.; Davies, G. J. *Biochemistry* 1999, *38*, 6380-6385.

(12) Gastinel, L. N.; Cambillau, C.; Bourne, Y. *EMBO J.* 1999, *18*, 3546-3557.

(13) Coutinho, P. M.; Henrissat, B.; *http://afmb.cnrs-mrs.fr/~pedro/CAZY/db.html.*]

(14) Sinnott, M. L. *Chem. Rev.* 1990, *90*, 1171-1202.

(15) Legler, G. *Carbohydr. Res.* 1993, *250*, vii-xx.

(16) Davies, G.; Henrissat, B. *Structure* 1995, *3*, 853-859.

(17) Withers, S. G.; Aebersold, R. *Protein Sci.* 1995, *4*, 361-372.

(18) Davies, G.; Sinnott, M. L.; Withers, S. G. *Glycosyl transfer,* Chapter 3; In Comprehensive Biological Catalysis; Sinott, M. L., Ed.; Academic Press Limited: New York, 1997, pp 119-208.

(19) Zechel, D. L.; Withers, S. G. *Mechanisms of glycosyl transfer,* Chapter 5; In Comprehensive Natural Products Chemistry; Poulter, C. D., Ed.; Elsevier: New York, 1999, pp 279-314.

(20) Withers, S. G.; Namchuk, M.; Mosi, R. *Iminosugars as glycosidase inhibitors*; Stutz, A. E., Ed.; Wiley-VCH: Weinheim, 1999, pp 188-206.

(21) Heightman, T. D.; Vasella, A. T. *Angew. Chem. Int. Ed.* 1999, *38*, 750-770.

(22) Nishikawa, Y.; Pegg, W.; Paulsen, H.; Schachter, H. *J. Biol. Chem.* 1988, *263*, 8270-8281.

(23) Tvaroska, I.; André, I.; Carver, J. P. *J. Mol. Struct. (Theochem)* 1999, *469*, 103-114.

(24) Tvaroska, I.; André, I.; Carver, J. P. *J. Phys. Chem.B* 1999, *103*, 2560-2569.

(25) André, I.; Tvaroska, I.; Carver, J. P. *J. Phys. Chem.* 1999, *submitted*

(26) Jaguar 3.5, S., Inc., Portland, OR, 1998.

(27) Becke, A. D. *J. Chem. Phys.* 1993, *98*, 5648-5652.

(28) Khatra, B. S.; Herries, D. G.; Brew, K. *Eur. J. Biochem.* 1974, *44*, 537-560.

(29) Warshel, A.; Weiss, R. M. *J. Am. Chem. Soc.* 1980, *102*, 6218-6226.

(30) Sidhu, G.; Withers, S. G.; Nguyen, N. T.; McIntosh, L. P.; Ziser, L.; Brayer, G. D. *Biochemistry* 1999, *38*, 5346-5354.

(31) Brameld, K. A.; Goddard III, W. A. *J. Am. Chem. Soc.* 1998, *120*, 3571-3580.

(32) Fowler, P.; Bernet, B.; Vasella, A. *Helv. Chim. Acta* 1996, *79*, 269-287.

(33) Sulzenbacher, G.; Driguez, H.; Henrissat, B.; Schulein, M.; Davies, G. J. *Biochemistry* 1996, *35*, 15280-15287.

(34) Guthrie, J. P. *J. Am. Chem. Soc.* 1977, *99*, 3391-4000.

(35) Warshel, A. *Computer modeling of Chemical Reactions in Enzymes and Solutions*; John Wiley & Sons, Inc.: New York, 1997.

(36) Smith, B. J. *J. Am. Chem. Soc.* 1997, *119*, 2699-2706.

(37) Sinnott, M. L. *Adv. Phys. Org. Chem.* 1988, *24*, 113-224.

(38) Strynadka, N. C. J.; James, M. N. G. *J. Mol. Biol.* 1991, *220*, 401-424.

(39) Zhang, N.; Peng, K. C.; Chen, L.; Puett, D.; Pierce, M. *J. Biol. Chem.* 1997, *272*, 4225-4229.

(40) Murray, B. W.; Takayama, S.; Schultz, J.; Wong, C.-H. *Biochemistry* 1996, *35*, 11183-11195.

(41) Murray, B. W.; Wittmann, V.; Burkart, M. D.; Hung, S. C.; Wong, C. H. *Biochemistry* 1997, *36*, 823-831.

(42) Seto, N. O.; Compston, C. A.; Evans, S. V.; Bundle, D. R.; Narang, S. A.; Palcic, M. M. *Eur. J. Biochem.* 1999, *259*, 770-775.

(43) Lu, D.; Voth, G. A. *J. Am. Chem. Soc.* 1998, *120*, 4006-4014.

(44) Fuxreiter, M.; Warshel, A. *J. Am. Chem. Soc.* 1998, *120*, 183-194.

(45) Kapitonov, D.; Yu, R. K. *Glycobiology* 1999, *9*, 961-78.

(46) Hagen, F. K.; Hazes, B.; Raffo, R.; deSa, D.; Tabak, L. A. *J. Biol. Chem.* 1999, *274*, 6797-6803.

(47) Lu, P. P.; Hindsgaul, O.; Li, H.; Palcic, M. M. *Carbohydr. Res.* 1997, *303*, 283-291.

48) Taguchi, T.; Kitajima, K.; Inoue, S.; Inoue, Y.; Yang, J. M.; Schachter, H.; Brockhausen, I. *Biochem. Biophys. Res. Commun.* 1997, *230*, 533-6.

49) Unligil, U. M.; Zhou, S.; Yuwaraj, S.; Sarkar, M.; Schachter, H.; Rini, J. M. *X-ray Crystal Structure of Rabbit N-Acetylglucosaminyltransferase I, a Key Enzyme in the Biosynthesis of N-Linked Glycans*: Annual Conference of the Society for Glycobiology. San Francisco, CA, USA, 1999.

50) *Meeting on the Critical Assessment of Techniques for Protein Structure Prediction (CASP) at URL: http://moult.carb.nist.gov/casp/.*

51) Fischer, D.; Eisenberg, D. *Protein Sci.* 1996, *5*, 947-55.

52) Fischer, D. *Fold-Recognition server at URL: http://fold.doe-mbi.ucla.edu/Home.*

53) *Protein Data Bank at URL: http://www.rcsb.org/pdb/.*

54) Needleman, S. B.; Wunch, C. D. *J. Mol. Biol.* 1970, *48*, 443-453.

55) *Homology 95.0 User Guide*; Biosym/MSI: San Diego, 1995.

56) Goodsell, D. S.; Olson, A. J. *Proteins* 1990, *8*, 195-202.

TABLE 1

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REMARK Solvation parameters added by "addsol"
REMARK
ATOM      1  CB  ALA   106A    -17.148  -1.078  17.481  1.00  0.00    -0.159   16.15    4.00
ATOM      2  HB1 ALA   106A    -16.722  -0.081  17.603  1.00  0.00     0.053    0.00    0.00
ATOM      3  HB2 ALA   106A    -17.977  -1.206  18.176  1.00  0.00     0.053    0.00    0.00
ATOM      4  HB3 ALA   106A    -16.383  -1.826  17.686  1.00  0.00     0.053    0.00    0.00
ATOM      5  C   ALA   106A    -16.506  -1.033  15.073  1.00  0.00     0.396    9.82    4.00
ATOM      6  O   ALA   106A    -15.407  -1.538  15.276  1.00  0.00    -0.396    8.17  -17.40
ATOM      7  N   ALA   106A    -18.246  -2.612  15.849  1.00  0.00    -0.580    9.00  -17.40
ATOM      8  HN1 ALA   106A    -19.264  -2.530  15.721  1.00  0.00     0.249    0.00    0.00
ATOM      9  HN2 ALA   106A    -17.830  -3.050  15.015  1.00  0.00     0.249    0.00    0.00
ATOM     10  CA  ALA   106A    -17.654  -1.245  16.045  1.00  0.00     0.030    9.40    4.00
ATOM     11  HA  ALA   106A    -18.412  -0.482  15.869  1.00  0.00     0.053    0.00    0.00
ATOM     12  N   VAL   107     -16.765  -0.282  14.012  1.00  0.00    -0.650    9.00  -17.40
ATOM     13  HN  VAL   107     -17.706   0.118  13.890  1.00  0.00     0.440    0.00    0.00
ATOM     14  CA  VAL   107     -15.742  -0.016  13.021  1.00  0.00     0.158    9.40    4.00
ATOM     15  HA  VAL   107     -15.072  -0.874  12.966  1.00  0.00     0.053    0.00    0.00
ATOM     16  CB  VAL   107     -16.385   0.191  11.638  1.00  0.00    -0.053    9.40    4.00
ATOM     17  HB  VAL   107     -17.143   0.972  11.685  1.00  0.00     0.053    0.00    0.00
ATOM     18  CG1 VAL   107     -15.336   0.599  10.624  1.00  0.00    -0.159   16.15    4.00
ATOM     19  HG1 VAL   107     -15.806   0.741   9.651  1.00  0.00     0.053    0.00    0.00
ATOM     20  HG1 VAL   107     -14.867   1.530  10.940  1.00  0.00     0.053    0.00    0.00
ATOM     21  HG1 VAL   107     -14.578  -0.181  10.550  1.00  0.00     0.053    0.00    0.00
ATOM     22  CG2 VAL   107     -17.075  -1.098  11.206  1.00  0.00    -0.159   16.15    4.00
ATOM     23  HG2 VAL   107     -17.531  -0.955  10.226  1.00  0.00     0.053    0.00    0.00
ATOM     24  HG2 VAL   107     -16.341  -1.902  11.150  1.00  0.00     0.053    0.00    0.00
ATOM     25  HG2 VAL   107     -17.845  -1.358  11.931  1.00  0.00     0.053    0.00    0.00
ATOM     26  C   VAL   107     -14.964   1.229  13.437  1.00  0.00     0.396    9.82    4.00
ATOM     27  O   VAL   107     -15.559   2.286  13.678  1.00  0.00    -0.396    8.17  -17.40
ATOM     28  N   ILE   108     -13.641   1.098  13.523  1.00  0.00    -0.650    9.00  -17.40
ATOM     29  HN  ILE   108     -13.215   0.185  13.304  1.00  0.00     0.440    0.00    0.00
ATOM     30  CA  ILE   108     -12.772   2.209  13.918  1.00  0.00     0.158    9.40    4.00
ATOM     31  HA  ILE   108     -13.380   3.076  14.173  1.00  0.00     0.053    0.00    0.00
ATOM     32  CB  ILE   108     -11.894   1.841  15.128  1.00  0.00    -0.053    9.40    4.00
ATOM     33  HB  ILE   108     -11.260   0.989  14.880  1.00  0.00     0.053    0.00    0.00
ATOM     34  CG2 ILE   108     -11.002   3.039  15.511  1.00  0.00    -0.159   16.15    4.00
ATOM     35  HG2 ILE   108     -10.383   2.772  16.367  1.00  0.00     0.053    0.00    0.00
ATOM     36  HG2 ILE   108     -10.361   3.300  14.668  1.00  0.00     0.053    0.00    0.00
ATOM     37  HG2 ILE   108     -11.629   3.892  15.768  1.00  0.00     0.053    0.00    0.00
ATOM     38  CG1 ILE   108     -12.776   1.453  16.315  1.00  0.00    -0.106   12.77    4.00
ATOM     39  HG1 ILE   108     -13.473   0.649  16.081  1.00  0.00     0.053    0.00    0.00
ATOM     40  HG1 ILE   108     -13.387   2.279  16.678  1.00  0.00     0.053    0.00    0.00
ATOM     41  CD1 ILE   108     -11.971   0.967  17.524  1.00  0.00    -0.159   16.15    4.00
ATOM     42  HD1 ILE   108     -12.652   0.706  18.334  1.00  0.00     0.053    0.00    0.00
ATOM     43  HD1 ILE   108     -11.387   0.089  17.244  1.00  0.00     0.053    0.00    0.00
ATOM     44  HD1 ILE   108     -11.299   1.758  17.855  1.00  0.00     0.053    0.00    0.00
ATOM     45  C   ILE   108     -11.845   2.565  12.767  1.00  0.00     0.396    9.82    4.00
ATOM     46  O   ILE   108     -10.877   1.862  12.498  1.00  0.00    -0.396    8.17  -17.40
ATOM     47  N   PRO   109     -12.135   3.670  12.073  1.00  0.00    -0.422    9.00  -17.40
ATOM     48  CD  PRO   109     -13.304   4.556  12.253  1.00  0.00     0.105   12.77    4.00
ATOM     49  HD1 PRO   109     -13.420   4.849  13.296  1.00  0.00     0.053    0.00    0.00
ATOM     50  HD2 PRO   109     -14.225   4.062  11.944  1.00  0.00     0.053    0.00    0.00
ATOM     51  CA  PRO   109     -11.316   4.106  10.944  1.00  0.00     0.158    9.40    4.00
ATOM     52  HA  PRO   109     -11.017   3.286  10.290  1.00  0.00     0.053    0.00    0.00
ATOM     53  CB  PRO   109     -12.236   5.070  10.215  1.00  0.00    -0.106   12.77    4.00
ATOM     54  HB1 PRO   109     -12.913   4.543   9.543  1.00  0.00     0.053    0.00    0.00
ATOM     55  HB2 PRO   109     -11.671   5.783   9.615  1.00  0.00     0.053    0.00    0.00
ATOM     56  CG  PRO   109     -12.961   5.730  11.366  1.00  0.00    -0.106   12.77    4.00
ATOM     57  HG1 PRO   109     -13.850   6.257  11.022  1.00  0.00     0.053    0.00    0.00
ATOM     58  HG2 PRO   109     -12.322   6.453  11.872  1.00  0.00     0.053    0.00    0.00
ATOM     59  C   PRO   109     -10.025   4.780  11.370  1.00  0.00     0.396    9.82    4.00
ATOM     60  O   PRO   109      -9.933   5.391  12.450  1.00  0.00    -0.396    8.17  -17.40
ATOM     61  N   ILE   110      -9.010   4.618  10.532  1.00  0.00    -0.650    9.00  -17.40
ATOM     62  HN  ILE   110      -9.128   4.021   9.700  1.00  0.00     0.440    0.00    0.00
ATOM     63  CA  ILE   110      -7.740   5.266  10.768  1.00  0.00     0.158    9.40    4.00
ATOM     64  HA  ILE   110      -7.645   5.602  11.800  1.00  0.00     0.053    0.00    0.00
ATOM     65  CB  ILE   110      -6.542   4.379  10.376  1.00  0.00    -0.053    9.40    4.00
ATOM     66  HB  ILE   110      -6.559   4.187   9.303  1.00  0.00     0.053    0.00    0.00
ATOM     67  CG2 ILE   110      -5.217   5.093  10.742  1.00  0.00    -0.159   16.15    4.00
ATOM     68  HG2 ILE   110      -4.373   4.461  10.462  1.00  0.00     0.053    0.00    0.00
ATOM     69  HG2 ILE   110      -5.153   6.040  10.206  1.00  0.00     0.053    0.00    0.00
ATOM     70  HG2 ILE   110      -5.189   5.280  11.815  1.00  0.00     0.053    0.00    0.00
ATOM     71  CG1 ILE   110      -6.673   3.009  11.041  1.00  0.00    -0.106   12.77    4.00
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ATOM	72	HG1	ILE	110	-5.827	2.397	10.726	1.00	0.00	0.053	0.00	0.00
ATOM	73	HG1	ILE	110	-7.614	2.564	10.717	1.00	0.00	0.053	0.00	0.00
ATOM	74	CD1	ILE	110	-6.679	3.028	12.571	1.00	0.00	-0.159	16.15	4.00
ATOM	75	HD1	ILE	110	-6.775	2.009	12.947	1.00	0.00	0.053	0.00	0.00
ATOM	76	HD1	ILE	110	-5.746	3.461	12.933	1.00	0.00	0.053	0.00	0.00
ATOM	77	HD1	ILE	110	-7.518	3.626	12.924	1.00	0.00	0.053	0.00	0.00
ATOM	78	C	ILE	110	-7.821	6.417	9.778	1.00	0.00	0.396	9.82	4.00
ATOM	79	O	ILE	110	-7.960	6.185	8.568	1.00	0.00	-0.396	8.17	-17.40
ATOM	80	N	LEU	111	-7.772	7.644	10.288	1.00	0.00	-0.650	9.00	-17.40
ATOM	81	HN	LEU	111	-7.701	7.766	11.308	1.00	0.00	0.440	0.00	0.00
ATOM	82	CA	LEU	111	-7.817	8.815	9.429	1.00	0.00	0.158	9.40	4.00
ATOM	83	HA	LEU	111	-8.247	8.489	8.482	1.00	0.00	0.053	0.00	0.00
ATOM	84	CB	LEU	111	-8.659	9.929	10.051	1.00	0.00	-0.106	12.77	4.00
ATOM	85	HB1	LEU	111	-8.370	10.024	11.098	1.00	0.00	0.053	0.00	0.00
ATOM	86	HB2	LEU	111	-9.708	9.648	9.960	1.00	0.00	0.053	0.00	0.00
ATOM	87	CG	LEU	111	-8.502	11.311	9.410	1.00	0.00	-0.053	9.40	4.00
ATOM	88	HG	LEU	111	-7.462	11.633	9.457	1.00	0.00	0.053	0.00	0.00
ATOM	89	CD1	LEU	111	-8.934	11.268	7.944	1.00	0.00	-0.159	16.15	4.00
ATOM	90	HD1	LEU	111	-8.817	12.257	7.501	1.00	0.00	0.053	0.00	0.00
ATOM	91	HD1	LEU	111	-8.314	10.552	7.403	1.00	0.00	0.053	0.00	0.00
ATOM	92	HD1	LEU	111	-9.978	10.963	7.881	1.00	0.00	0.053	0.00	0.00
ATOM	93	CD2	LEU	111	-9.351	12.310	10.180	1.00	0.00	-0.159	16.15	4.00
ATOM	94	HD2	LEU	111	-9.246	13.298	9.731	1.00	0.00	0.053	0.00	0.00
ATOM	95	HD2	LEU	111	-10.396	12.003	10.143	1.00	0.00	0.053	0.00	0.00
ATOM	96	HD2	LEU	111	-9.019	12.345	11.217	1.00	0.00	0.053	0.00	0.00
ATOM	97	C	LEU	111	-6.380	9.295	9.273	1.00	0.00	0.396	9.82	4.00
ATOM	98	O	LEU	111	-5.758	9.752	10.230	1.00	0.00	-0.396	8.17	-17.40
ATOM	99	N	VAL	112	-5.854	9.151	8.068	1.00	0.00	-0.650	9.00	-17.40
ATOM	100	HN	VAL	112	-6.417	8.712	7.325	1.00	0.00	0.440	0.00	0.00
ATOM	101	CA	VAL	112	-4.503	9.594	7.762	1.00	0.00	0.158	9.40	4.00
ATOM	102	HA	VAL	112	-3.905	9.594	8.673	1.00	0.00	0.053	0.00	0.00
ATOM	103	CB	VAL	112	-3.834	8.632	6.751	1.00	0.00	-0.053	9.40	4.00
ATOM	104	HB	VAL	112	-4.445	8.521	5.855	1.00	0.00	0.053	0.00	0.00
ATOM	105	CG1	VAL	112	-2.476	9.150	6.329	1.00	0.00	-0.159	16.15	4.00
ATOM	106	HG1	VAL	112	-2.026	8.456	5.618	1.00	0.00	0.053	0.00	0.00
ATOM	107	HG1	VAL	112	-2.589	10.127	5.859	1.00	0.00	0.053	0.00	0.00
ATOM	108	HG1	VAL	112	-1.832	9.240	7.204	1.00	0.00	0.053	0.00	0.00
ATOM	109	CG2	VAL	112	-3.702	7.236	7.371	1.00	0.00	-0.159	16.15	4.00
ATOM	110	HG2	VAL	112	-3.230	6.562	6.655	1.00	0.00	0.053	0.00	0.00
ATOM	111	HG2	VAL	112	-3.090	7.294	8.271	1.00	0.00	0.053	0.00	0.00
ATOM	112	HG2	VAL	112	-4.691	6.857	7.628	1.00	0.00	0.053	0.00	0.00
ATOM	113	C	VAL	112	-4.549	11.016	7.179	1.00	0.00	0.396	9.82	4.00
ATOM	114	O	VAL	112	-5.245	11.273	6.188	1.00	0.00	-0.396	8.17	-17.40
ATOM	115	N	ILE	113	-3.802	11.924	7.806	1.00	0.00	-0.650	9.00	-17.40
ATOM	116	HN	ILE	113	-3.260	11.626	8.630	1.00	0.00	0.440	0.00	0.00
ATOM	117	CA	ILE	113	-3.713	13.318	7.384	1.00	0.00	0.158	9.40	4.00
ATOM	118	HA	ILE	113	-4.610	13.526	6.801	1.00	0.00	0.053	0.00	0.00
ATOM	119	CB	ILE	113	-3.687	14.304	8.604	1.00	0.00	-0.053	9.40	4.00
ATOM	120	HB	ILE	113	-2.859	14.067	9.272	1.00	0.00	0.053	0.00	0.00
ATOM	121	CG2	ILE	113	-3.520	15.752	8.126	1.00	0.00	-0.159	16.15	4.00
ATOM	122	HG2	ILE	113	-3.504	16.419	8.987	1.00	0.00	0.053	0.00	0.00
ATOM	123	HG2	ILE	113	-2.584	15.847	7.575	1.00	0.00	0.053	0.00	0.00
ATOM	124	HG2	ILE	113	-4.352	16.018	7.475	1.00	0.00	0.053	0.00	0.00
ATOM	125	CG1	ILE	113	-5.014	14.224	9.377	1.00	0.00	-0.106	12.77	4.00
ATOM	126	HG1	ILE	113	-5.892	14.359	8.746	1.00	0.00	0.053	0.00	0.00
ATOM	127	HG1	ILE	113	-5.105	14.976	10.160	1.00	0.00	0.053	0.00	0.00
ATOM	128	CD1	ILE	113	-5.223	12.918	10.063	1.00	0.00	-0.159	16.15	4.00
ATOM	129	HD1	ILE	113	-6.178	12.931	10.588	1.00	0.00	0.053	0.00	0.00
ATOM	130	HD1	ILE	113	-5.226	12.115	9.325	1.00	0.00	0.053	0.00	0.00
ATOM	131	HD1	ILE	113	-4.417	12.749	10.778	1.00	0.00	0.053	0.00	0.00
ATOM	132	C	ILE	113	-2.445	13.442	6.549	1.00	0.00	0.396	9.82	4.00
ATOM	133	O	ILE	113	-1.349	13.096	7.003	1.00	0.00	-0.396	8.17	-17.40
ATOM	134	N	ALA	114	-2.619	13.927	5.320	1.00	0.00	-0.650	9.00	-17.40
ATOM	135	HN	ALA	114	-3.564	14.220	5.035	1.00	0.00	0.440	0.00	0.00
ATOM	136	CA	ALA	114	-1.526	14.061	4.358	1.00	0.00	0.158	9.40	4.00
ATOM	137	HA	ALA	114	-0.556	13.990	4.851	1.00	0.00	0.053	0.00	0.00
ATOM	138	CB	ALA	114	-1.616	12.899	3.319	1.00	0.00	-0.159	16.15	4.00
ATOM	139	HB1	ALA	114	-0.803	12.992	2.598	1.00	0.00	0.053	0.00	0.00
ATOM	140	HB2	ALA	114	-1.535	11.942	3.835	1.00	0.00	0.053	0.00	0.00
ATOM	141	HB3	ALA	114	-2.571	12.950	2.797	1.00	0.00	0.053	0.00	0.00
ATOM	142	C	ALA	114	-1.585	15.410	3.638	1.00	0.00	0.396	9.82	4.00
ATOM	143	O	ALA	114	-2.595	16.112	3.705	1.00	0.00	-0.396	8.17	-17.40
ATOM	144	N	CYS	115	-0.504	15.768	2.938	1.00	0.00	-0.650	9.00	-17.40
ATOM	145	HN	CYS	115	0.311	15.139	2.908	1.00	0.00	0.440	0.00	0.00
ATOM	146	CA	CYS	115	-0.459	17.042	2.211	1.00	0.00	0.158	9.40	4.00
ATOM	147	HA	CYS	115	-1.428	17.348	1.819	1.00	0.00	0.053	0.00	0.00

ATOM	148	C	CYS	115	0.474	17.015	1.007	1.00	0.00	0.396	9.82	4.00
ATOM	149	O	CYS	115	0.035	16.810	-0.139	1.00	0.00	-0.396	8.17	-17.40
ATOM	150	CB	CYS	115	-0.048	18.162	3.182	1.00	0.00	-0.041	12.77	4.00
ATOM	151	HB1	CYS	115	0.803	17.788	3.751	1.00	0.00	0.053	0.00	0.00
ATOM	152	HB2	CYS	115	-0.910	18.359	3.818	1.00	0.00	0.053	0.00	0.00
ATOM	153	SG	CYS	115	0.470	19.793	2.539	1.00	0.00	-0.065	19.93	-6.40
ATOM	154	N	ASP	116P	1.766	17.200	1.268	1.00	0.00	-0.650	9.00	-17.40
ATOM	155	HN	ASP	116P	2.079	17.312	2.242	1.00	0.00	0.440	0.00	0.00
ATOM	156	CA	ASP	116P	2.737	17.245	0.189	1.00	0.00	0.158	9.40	4.00
ATOM	157	HA	ASP	116P	2.249	16.867	-0.709	1.00	0.00	0.053	0.00	0.00
ATOM	158	CB	ASP	116P	3.111	18.711	-0.106	1.00	0.00	-0.336	12.77	4.00
ATOM	159	HB1	ASP	116P	2.257	19.320	-0.403	1.00	0.00	0.053	0.00	0.00
ATOM	160	HB2	ASP	116P	3.836	18.814	-0.913	1.00	0.00	0.053	0.00	0.00
ATOM	161	CG	ASP	116P	3.729	19.429	1.093	1.00	0.00	0.297	9.82	4.00
ATOM	162	OD1	ASP	116P	3.864	20.668	1.027	1.00	0.00	-0.534	8.17	-18.95
ATOM	163	OD2	ASP	116P	4.093	18.779	2.096	1.00	0.00	-0.534	8.17	-18.95
ATOM	164	C	ASP	116P	4.003	16.435	0.371	1.00	0.00	0.396	9.82	4.00
ATOM	165	O	ASP	116P	5.038	16.772	-0.228	1.00	0.00	-0.396	8.17	-17.40
ATOM	166	N	ARG	117G	3.943	15.390	1.198	1.00	0.00	-0.650	9.00	-17.40
ATOM	167	HN	ARG	117G	3.065	15.189	1.697	1.00	0.00	0.440	0.00	0.00
ATOM	168	CA	ARG	117G	5.101	14.527	1.406	1.00	0.00	0.158	9.40	4.00
ATOM	169	HA	ARG	117G	5.955	14.953	0.879	1.00	0.00	0.053	0.00	0.00
ATOM	170	CB	ARG	117G	5.454	14.440	2.905	1.00	0.00	-0.106	12.77	4.00
ATOM	171	HB1	ARG	117G	6.128	13.617	3.144	1.00	0.00	0.053	0.00	0.00
ATOM	172	HB2	ARG	117G	4.585	14.294	3.547	1.00	0.00	0.053	0.00	0.00
ATOM	173	CG	ARG	117G	6.149	15.705	3.445	1.00	0.00	-0.106	12.77	4.00
ATOM	174	HG1	ARG	117G	5.526	16.597	3.384	1.00	0.00	0.053	0.00	0.00
ATOM	175	HG2	ARG	117G	7.065	15.953	2.910	1.00	0.00	0.053	0.00	0.00
ATOM	176	CD	ARG	117G	6.560	15.589	4.939	1.00	0.00	0.374	12.77	4.00
ATOM	177	HD1	ARG	117G	7.067	16.479	5.310	1.00	0.00	0.053	0.00	0.00
ATOM	178	HD2	ARG	117G	7.240	14.758	5.128	1.00	0.00	0.053	0.00	0.00
ATOM	179	NE	ARG	117G	5.422	15.381	5.826	1.00	0.00	-0.819	9.00	-24.67
ATOM	180	HE	ARG	117G	4.617	14.851	5.461	1.00	0.00	0.407	0.00	0.00
ATOM	181	CZ	ARG	117G	5.354	15.831	7.077	1.00	0.00	0.796	6.95	4.00
ATOM	182	NH1	ARG	117G	6.376	16.534	7.595	1.00	0.00	-0.746	9.00	-24.67
ATOM	183	HH1	ARG	117G	6.323	16.882	8.563	1.00	0.00	0.407	0.00	0.00
ATOM	184	HH1	ARG	117G	7.211	16.724	7.024	1.00	0.00	0.407	0.00	0.00
ATOM	185	NH2	ARG	117G	4.267	15.584	7.808	1.00	0.00	-0.746	9.00	-24.67
ATOM	186	HH2	ARG	117G	4.208	15.929	8.776	1.00	0.00	0.407	0.00	0.00
ATOM	187	HH2	ARG	117G	3.485	15.047	7.404	1.00	0.00	0.407	0.00	0.00
ATOM	188	C	ARG	117G	4.783	13.136	0.856	1.00	0.00	0.396	9.82	4.00
ATOM	189	O	ARG	117G	3.832	12.475	1.306	1.00	0.00	-0.396	8.17	-17.40
ATOM	190	N	SER	118	5.581	12.692	-0.111	1.00	0.00	-0.650	9.00	-17.40
ATOM	191	HN	SER	118	6.356	13.288	-0.433	1.00	0.00	0.440	0.00	0.00
ATOM	192	CA	SER	118	5.390	11.388	-0.728	1.00	0.00	0.158	9.40	4.00
ATOM	193	HA	SER	118	4.363	11.252	-1.068	1.00	0.00	0.053	0.00	0.00
ATOM	194	CB	SER	118	6.266	11.235	-1.983	1.00	0.00	0.007	12.77	4.00
ATOM	195	HB1	SER	118	5.990	11.965	-2.744	1.00	0.00	0.053	0.00	0.00
ATOM	196	HB2	SER	118	6.156	10.241	-2.418	1.00	0.00	0.053	0.00	0.00
ATOM	197	OG	SER	118	7.640	11.426	-1.672	1.00	0.00	-0.537	11.04	-17.40
ATOM	198	HG	SER	118	8.102	11.920	-2.449	1.00	0.00	0.424	0.00	0.00
ATOM	199	C	SER	118	5.696	10.269	0.236	1.00	0.00	0.396	9.82	4.00
ATOM	200	O	SER	118	5.278	9.133	0.007	1.00	0.00	-0.396	8.17	-17.40
ATOM	201	N	THR	119	6.421	10.588	1.304	1.00	0.00	-0.650	9.00	-17.40
ATOM	202	HN	THR	119	6.753	11.556	1.415	1.00	0.00	0.440	0.00	0.00
ATOM	203	CA	THR	119	6.756	9.602	2.318	1.00	0.00	0.158	9.40	4.00
ATOM	204	HA	THR	119	7.211	8.714	1.878	1.00	0.00	0.053	0.00	0.00
ATOM	205	CB	THR	119	7.826	10.147	3.300	1.00	0.00	0.060	9.40	4.00
ATOM	206	HB	THR	119	7.958	9.460	4.136	1.00	0.00	0.053	0.00	0.00
ATOM	207	OG1	THR	119	7.413	11.418	3.813	1.00	0.00	-0.537	11.04	-17.40
ATOM	208	HG1	THR	119	8.175	12.100	3.696	1.00	0.00	0.424	0.00	0.00
ATOM	209	CG2	THR	119	9.167	10.310	2.589	1.00	0.00	-0.159	16.15	4.00
ATOM	210	HG2	THR	119	9.907	10.693	3.291	1.00	0.00	0.053	0.00	0.00
ATOM	211	HG2	THR	119	9.495	9.343	2.206	1.00	0.00	0.053	0.00	0.00
ATOM	212	HG2	THR	119	9.056	11.009	1.760	1.00	0.00	0.053	0.00	0.00
ATOM	213	C	THR	119	5.508	9.142	3.092	1.00	0.00	0.396	9.82	4.00
ATOM	214	O	THR	119	5.593	8.372	4.060	1.00	0.00	-0.396	8.17	-17.40
ATOM	215	N	VAL	120	4.342	9.636	2.685	1.00	0.00	-0.650	9.00	-17.40
ATOM	216	HN	VAL	120	4.310	10.347	1.941	1.00	0.00	0.440	0.00	0.00
ATOM	217	CA	VAL	120	3.117	9.164	3.297	1.00	0.00	0.158	9.40	4.00
ATOM	218	HA	VAL	120	3.126	9.327	4.374	1.00	0.00	0.053	0.00	0.00
ATOM	219	CB	VAL	120	1.871	9.876	2.703	1.00	0.00	-0.053	9.40	4.00
ATOM	220	HB	VAL	120	1.914	10.944	2.914	1.00	0.00	0.053	0.00	0.00
ATOM	221	CG1	VAL	120	1.823	9.673	1.187	1.00	0.00	-0.159	16.15	4.00
ATOM	222	HG1	VAL	120	0.945	10.176	0.780	1.00	0.00	0.053	0.00	0.00
ATOM	223	HG1	VAL	120	2.722	10.090	0.735	1.00	0.00	0.053	0.00	0.00

ATOM	224	HG1	VAL	120	1.766	8.607	0.964	1.00	0.00	0.053	0.00	0.00
ATOM	225	CG2	VAL	120	0.596	9.324	3.360	1.00	0.00	-0.159	16.15	4.00
ATOM	226	HG2	VAL	120	-0.276	9.825	2.940	1.00	0.00	0.053	0.00	0.00
ATOM	227	HG2	VAL	120	0.523	8.252	3.171	1.00	0.00	0.053	0.00	0.00
ATOM	228	HG2	VAL	120	0.634	9.501	4.435	1.00	0.00	0.053	0.00	0.00
ATOM	229	C	VAL	120	3.117	7.657	2.937	1.00	0.00	0.396	9.82	4.00
ATOM	230	O	VAL	120	2.421	6.852	3.557	1.00	0.00	-0.396	8.17	-17.40
ATOM	231	N	ARG	121G	3.929	7.294	1.935	1.00	0.00	-0.650	9.00	-17.40
ATOM	232	HN	ARG	121G	4.469	8.023	1.448	1.00	0.00	0.440	0.00	0.00
ATOM	233	CA	ARG	121G	4.080	5.898	1.503	1.00	0.00	0.158	9.40	4.00
ATOM	234	HA	ARG	121G	3.131	5.530	1.113	1.00	0.00	0.053	0.00	0.00
ATOM	235	CB	ARG	121G	5.142	5.783	0.382	1.00	0.00	-0.106	12.77	4.00
ATOM	236	HB1	ARG	121G	6.087	6.162	0.768	1.00	0.00	0.053	0.00	0.00
ATOM	237	HB2	ARG	121G	4.806	6.377	-0.467	1.00	0.00	0.053	0.00	0.00
ATOM	238	CG	ARG	121G	5.389	4.348	-0.123	1.00	0.00	-0.106	12.77	4.00
ATOM	239	HG1	ARG	121G	4.502	3.908	-0.580	1.00	0.00	0.053	0.00	0.00
ATOM	240	HG2	ARG	121G	5.689	3.669	0.674	1.00	0.00	0.053	0.00	0.00
ATOM	241	CD	ARG	121G	6.506	4.281	-1.192	1.00	0.00	0.374	12.77	4.00
ATOM	242	HD1	ARG	121G	6.758	3.261	-1.484	1.00	0.00	0.053	0.00	0.00
ATOM	243	HD2	ARG	121G	7.441	4.731	-0.862	1.00	0.00	0.053	0.00	0.00
ATOM	244	NE	ARG	121G	6.155	4.968	-2.430	1.00	0.00	-0.819	9.00	-24.67
ATOM	245	HE	ARG	121G	6.554	5.904	-2.586	1.00	0.00	0.407	0.00	0.00
ATOM	246	CZ	ARG	121G	5.358	4.474	-3.371	1.00	0.00	0.796	6.95	4.00
ATOM	247	NH1	ARG	121G	4.818	3.265	-3.225	1.00	0.00	-0.746	9.00	-24.67
ATOM	248	HH1	ARG	121G	4.200	2.885	-3.957	1.00	0.00	0.407	0.00	0.00
ATOM	249	HH1	ARG	121G	5.018	2.710	-2.381	1.00	0.00	0.407	0.00	0.00
ATOM	250	NH2	ARG	121G	5.101	5.191	-4.463	1.00	0.00	-0.746	9.00	-24.67
ATOM	251	HH2	ARG	121G	4.483	4.811	-5.195	1.00	0.00	0.407	0.00	0.00
ATOM	252	HH2	ARG	121G	5.519	6.125	-4.576	1.00	0.00	0.407	0.00	0.00
ATOM	253	C	ARG	121G	4.507	5.033	2.694	1.00	0.00	0.396	9.82	4.00
ATOM	254	O	ARG	121G	3.917	3.990	2.969	1.00	0.00	-0.396	8.17	-17.40
ATOM	255	N	ARG	122G	5.532	5.476	3.410	1.00	0.00	-0.650	9.00	-17.40
ATOM	256	HN	ARG	122G	5.989	6.360	3.148	1.00	0.00	0.440	0.00	0.00
ATOM	257	CA	ARG	122G	6.017	4.732	4.557	1.00	0.00	0.158	9.40	4.00
ATOM	258	HA	ARG	122G	6.354	3.739	4.258	1.00	0.00	0.053	0.00	0.00
ATOM	259	CB	ARG	122G	7.234	5.443	5.156	1.00	0.00	-0.106	12.77	4.00
ATOM	260	HB1	ARG	122G	6.938	6.463	5.402	1.00	0.00	0.053	0.00	0.00
ATOM	261	HB2	ARG	122G	8.027	5.435	4.409	1.00	0.00	0.053	0.00	0.00
ATOM	262	CG	ARG	122G	7.804	4.827	6.418	1.00	0.00	-0.106	12.77	4.00
ATOM	263	HG1	ARG	122G	8.079	3.788	6.233	1.00	0.00	0.053	0.00	0.00
ATOM	264	HG2	ARG	122G	7.062	4.860	7.216	1.00	0.00	0.053	0.00	0.00
ATOM	265	CD	ARG	122G	9.047	5.601	6.861	1.00	0.00	0.374	12.77	4.00
ATOM	266	HD1	ARG	122G	8.840	6.670	6.912	1.00	0.00	0.053	0.00	0.00
ATOM	267	HD2	ARG	122G	9.868	5.448	6.161	1.00	0.00	0.053	0.00	0.00
ATOM	268	NE	ARG	122G	9.490	5.161	8.184	1.00	0.00	-0.819	9.00	-24.67
ATOM	269	HE	ARG	122G	8.889	4.495	8.692	1.00	0.00	0.407	0.00	0.00
ATOM	270	CZ	ARG	122G	10.614	5.558	8.780	1.00	0.00	0.796	6.95	4.00
ATOM	271	NH1	ARG	122G	11.429	6.408	8.175	1.00	0.00	-0.746	9.00	-24.67
ATOM	272	HH1	ARG	122G	12.296	6.710	8.641	1.00	0.00	0.407	0.00	0.00
ATOM	273	HH1	ARG	122G	11.196	6.766	7.238	1.00	0.00	0.407	0.00	0.00
ATOM	274	NH2	ARG	122G	10.914	5.111	9.994	1.00	0.00	-0.746	9.00	-24.67
ATOM	275	HH2	ARG	122G	11.782	5.417	10.455	1.00	0.00	0.407	0.00	0.00
ATOM	276	HH2	ARG	122G	10.278	4.458	10.474	1.00	0.00	0.407	0.00	0.00
ATOM	277	C	ARG	122G	4.920	4.568	5.594	1.00	0.00	0.396	9.82	4.00
ATOM	278	O	ARG	122G	4.780	3.495	6.191	1.00	0.00	-0.396	8.17	-17.40
ATOM	279	N	CYSH	123S	4.141	5.628	5.811	1.00	0.00	-0.65	9.00	-17.40
ATOM	280	HN	CYSH	123S	4.313	6.497	5.286	1.00	0.00	0.44	0.00	0.00
ATOM	281	CA	CYSH	123S	3.053	5.582	6.773	1.00	0.00	0.15	9.40	4.00
ATOM	282	HA	CYSH	123S	3.446	5.330	7.758	1.00	0.00	0.05	0.00	0.00
ATOM	283	CB	CYSH	123S	2.374	6.958	6.867	1.00	0.00	-0.04	12.77	4.00
ATOM	284	HB1	CYSH	123S	2.053	7.247	5.866	1.00	0.00	0.05	0.00	0.00
ATOM	285	HB2	CYSH	123S	3.100	7.668	7.261	1.00	0.00	0.05	0.00	0.00
ATOM	286	SG	CYSH	123S	0.913	7.019	7.945	1.00	0.00	-0.25	19.93	-6.40
ATOM	287	HG	CYSH	123S	0.595	8.296	8.196	1.00	0.00	0.19	0.00	0.00
ATOM	288	C	CYSH	123S	2.041	4.526	6.350	1.00	0.00	0.39	9.82	4.00
ATOM	289	O	CYSH	123S	1.714	3.631	7.136	1.00	0.00	-0.39	8.17	-17.40
ATOM	290	N	LEU	124	1.573	4.609	5.102	1.00	0.00	-0.650	9.00	-17.40
ATOM	291	HN	LEU	124	1.922	5.348	4.475	1.00	0.00	0.440	0.00	0.00
ATOM	292	CA	LEU	124	0.575	3.667	4.616	1.00	0.00	0.158	9.40	4.00
ATOM	293	HA	LEU	124	-0.315	3.628	5.243	1.00	0.00	0.053	0.00	0.00
ATOM	294	CB	LEU	124	0.013	4.109	3.245	1.00	0.00	-0.106	12.77	4.00
ATOM	295	HB1	LEU	124	-0.630	3.307	2.883	1.00	0.00	0.053	0.00	0.00
ATOM	296	HB2	LEU	124	0.862	4.269	2.581	1.00	0.00	0.053	0.00	0.00
ATOM	297	CG	LEU	124	-0.836	5.409	3.190	1.00	0.00	-0.053	9.40	4.00
ATOM	298	HG	LEU	124	-0.242	6.257	3.529	1.00	0.00	0.053	0.00	0.00
ATOM	299	CD1	LEU	124	-1.300	5.672	1.758	1.00	0.00	-0.159	16.15	4.00

ATOM	300	HD1	LEU	124	-1.894	6.585	1.730	1.00	0.00	0.053	0.00	0.00
ATOM	301	HD1	LEU	124	-0.431	5.784	1.109	1.00	0.00	0.053	0.00	0.00
ATOM	302	HD1	LEU	124	-1.905	4.834	1.412	1.00	0.00	0.053	0.00	0.00
ATOM	303	CD2	LEU	124	-2.062	5.280	4.106	1.00	0.00	-0.159	16.15	4.00
ATOM	304	HD2	LEU	124	-2.649	6.197	4.059	1.00	0.00	0.053	0.00	0.00
ATOM	305	HD2	LEU	124	-2.674	4.439	3.778	1.00	0.00	0.053	0.00	0.00
ATOM	306	HD2	LEU	124	-1.733	5.111	5.131	1.00	0.00	0.053	0.00	0.00
ATOM	307	C	LEU	124	1.093	2.232	4.545	1.00	0.00	0.396	9.82	4.00
ATOM	308	O	LEU	124	0.364	1.306	4.891	1.00	0.00	-0.396	8.17	-17.40
ATOM	309	N	ASP	125P	2.342	2.028	4.124	1.00	0.00	-0.650	9.00	-17.40
ATOM	310	HN	ASP	125P	2.940	2.820	3.852	1.00	0.00	0.440	0.00	0.00
ATOM	311	CA	ASP	125P	2.845	0.656	4.056	1.00	0.00	0.158	9.40	4.00
ATOM	312	HA	ASP	125P	2.300	0.058	3.324	1.00	0.00	0.053	0.00	0.00
ATOM	313	CB	ASP	125P	4.306	0.599	3.585	1.00	0.00	-0.336	12.77	4.00
ATOM	314	HB1	ASP	125P	4.748	-0.390	3.701	1.00	0.00	0.053	0.00	0.00
ATOM	315	HB2	ASP	125P	4.953	1.283	4.134	1.00	0.00	0.053	0.00	0.00
ATOM	316	CG	ASP	125P	4.466	0.961	2.110	1.00	0.00	0.297	9.82	4.00
ATOM	317	OD1	ASP	125P	3.486	0.881	1.331	1.00	0.00	-0.534	8.17	-18.95
ATOM	318	OD2	ASP	125P	5.596	1.314	1.724	1.00	0.00	-0.534	8.17	-18.95
ATOM	319	C	ASP	125P	2.722	-0.064	5.397	1.00	0.00	0.396	9.82	4.00
ATOM	320	O	ASP	125P	2.187	-1.171	5.449	1.00	0.00	-0.396	8.17	-17.40
ATOM	321	N	LYS	126S	3.175	0.578	6.474	1.00	0.00	-0.650	9.00	-17.40
ATOM	322	HN	LYS	126S	3.568	1.524	6.368	1.00	0.00	0.440	0.00	0.00
ATOM	323	CA	LYS	126S	3.125	-0.035	7.806	1.00	0.00	0.158	9.40	4.00
ATOM	324	HA	LYS	126S	3.619	-1.005	7.754	1.00	0.00	0.053	0.00	0.00
ATOM	325	CB	LYS	126S	3.918	0.808	8.802	1.00	0.00	-0.106	12.77	4.00
ATOM	326	HB1	LYS	126S	3.717	0.430	9.804	1.00	0.00	0.053	0.00	0.00
ATOM	327	HB2	LYS	126S	3.591	1.843	8.708	1.00	0.00	0.053	0.00	0.00
ATOM	328	CG	LYS	126S	5.425	0.781	8.594	1.00	0.00	-0.106	12.77	4.00
ATOM	329	HG1	LYS	126S	5.915	1.455	9.296	1.00	0.00	0.053	0.00	0.00
ATOM	330	HG2	LYS	126S	5.671	1.093	7.579	1.00	0.00	0.053	0.00	0.00
ATOM	331	CD	LYS	126S	5.965	-0.632	8.815	1.00	0.00	-0.106	12.77	4.00
ATOM	332	HD1	LYS	126S	5.570	-1.337	8.083	1.00	0.00	0.053	0.00	0.00
ATOM	333	HD2	LYS	126S	5.704	-1.017	9.800	1.00	0.00	0.053	0.00	0.00
ATOM	334	CE	LYS	126S	7.486	-0.684	8.706	1.00	0.00	0.099	12.77	4.00
ATOM	335	HE1	LYS	126S	7.899	-1.672	8.907	1.00	0.00	0.053	0.00	0.00
ATOM	336	HE2	LYS	126S	7.991	-0.012	9.400	1.00	0.00	0.053	0.00	0.00
ATOM	337	NZ	LYS	126S	7.996	-0.310	7.351	1.00	0.00	-0.045	13.25	-39.20
ATOM	338	HZ1	LYS	126S	9.024	-0.364	7.343	1.00	0.00	0.280	0.00	0.00
ATOM	339	HZ2	LYS	126S	7.613	-0.958	6.648	1.00	0.00	0.280	0.00	0.00
ATOM	340	HZ3	LYS	126S	7.702	0.651	7.126	1.00	0.00	0.280	0.00	0.00
ATOM	341	C	LYS	126S	1.713	-0.265	8.347	1.00	0.00	0.396	9.82	4.00
ATOM	342	O	LYS	126S	1.438	-1.311	8.938	1.00	0.00	-0.396	8.17	-17.40
ATOM	343	N	LEU	127	0.817	0.703	8.150	1.00	0.00	-0.650	9.00	-17.40
ATOM	344	HN	LEU	127	1.099	1.562	7.657	1.00	0.00	0.440	0.00	0.00
ATOM	345	CA	LEU	127	-0.562	0.564	8.622	1.00	0.00	0.158	9.40	4.00
ATOM	346	HA	LEU	127	-0.576	0.405	9.700	1.00	0.00	0.053	0.00	0.00
ATOM	347	CB	LEU	127	-1.382	1.816	8.290	1.00	0.00	-0.106	12.77	4.00
ATOM	348	HB1	LEU	127	-2.432	1.527	8.330	1.00	0.00	0.053	0.00	0.00
ATOM	349	HB2	LEU	127	-1.085	2.133	7.290	1.00	0.00	0.053	0.00	0.00
ATOM	350	CG	LEU	127	-1.261	3.054	9.168	1.00	0.00	-0.053	9.40	4.00
ATOM	351	HG	LEU	127	-0.208	3.266	9.356	1.00	0.00	0.053	0.00	0.00
ATOM	352	CD1	LEU	127	-1.904	4.254	8.457	1.00	0.00	-0.159	16.15	4.00
ATOM	353	HD1	LEU	127	-1.816	5.139	9.086	1.00	0.00	0.053	0.00	0.00
ATOM	354	HD1	LEU	127	-1.395	4.430	7.509	1.00	0.00	0.053	0.00	0.00
ATOM	355	HD1	LEU	127	-2.957	4.044	8.269	1.00	0.00	0.053	0.00	0.00
ATOM	356	CD2	LEU	127	-1.950	2.806	10.483	1.00	0.00	-0.159	16.15	4.00
ATOM	357	HD2	LEU	127	-1.863	3.692	11.112	1.00	0.00	0.053	0.00	0.00
ATOM	358	HD2	LEU	127	-3.003	2.587	10.306	1.00	0.00	0.053	0.00	0.00
ATOM	359	HD2	LEU	127	-1.482	1.958	10.984	1.00	0.00	0.053	0.00	0.00
ATOM	360	C	LEU	127	-1.230	-0.620	7.946	1.00	0.00	0.396	9.82	4.00
ATOM	361	O	LEU	127	-1.886	-1.433	8.583	1.00	0.00	-0.396	8.17	-17.40
ATOM	362	N	LEU	128	-1.076	-0.678	6.631	1.00	0.00	-0.650	9.00	-17.40
ATOM	363	HN	LEU	128	-0.515	0.048	6.164	1.00	0.00	0.440	0.00	0.00
ATOM	364	CA	LEU	128	-1.668	-1.726	5.828	1.00	0.00	0.158	9.40	4.00
ATOM	365	HA	LEU	128	-2.732	-1.823	6.040	1.00	0.00	0.053	0.00	0.00
ATOM	366	CB	LEU	128	-1.530	-1.363	4.340	1.00	0.00	-0.106	12.77	4.00
ATOM	367	HB1	LEU	128	-1.697	-2.265	3.752	1.00	0.00	0.053	0.00	0.00
ATOM	368	HB2	LEU	128	-0.523	-0.977	4.175	1.00	0.00	0.053	0.00	0.00
ATOM	369	CG	LEU	128	-2.513	-0.306	3.848	1.00	0.00	-0.053	9.40	4.00
ATOM	370	HG	LEU	128	-2.493	0.571	4.494	1.00	0.00	0.053	0.00	0.00
ATOM	371	CD1	LEU	128	-2.157	0.149	2.405	1.00	0.00	-0.159	16.15	4.00
ATOM	372	HD1	LEU	128	-2.871	0.903	2.074	1.00	0.00	0.053	0.00	0.00
ATOM	373	HD1	LEU	128	-1.152	0.571	2.394	1.00	0.00	0.053	0.00	0.00
ATOM	374	HD1	LEU	128	-2.197	-0.708	1.733	1.00	0.00	0.053	0.00	0.00
ATOM	375	CD2	LEU	128	-3.914	-0.930	3.875	1.00	0.00	-0.159	16.15	4.00

ATOM	376	HD2	LEU	128	-4.644	-0.199	3.528	1.00	0.00	0.053	0.00	0.00
ATOM	377	HD2	LEU	128	-3.936	-1.803	3.222	1.00	0.00	0.053	0.00	0.00
ATOM	378	HD2	LEU	128	-4.158	-1.231	4.893	1.00	0.00	0.053	0.00	0.00
ATOM	379	C	LEU	128	-1.009	-3.061	6.112	1.00	0.00	0.396	9.82	4.00
ATOM	380	O	LEU	128	-1.651	-4.103	6.040	1.00	0.00	-0.396	8.17	-17.40
ATOM	381	N	HIS	129S	0.279	-3.032	6.438	1.00	0.00	-0.650	9.00	-17.40
ATOM	382	HN	HIS	129S	0.775	-2.131	6.488	1.00	0.00	0.440	0.00	0.00
ATOM	383	CA	HIS	129S	0.989	-4.268	6.724	1.00	0.00	0.158	9.40	4.00
ATOM	384	HA	HIS	129S	0.843	-4.998	5.927	1.00	0.00	0.053	0.00	0.00
ATOM	385	CB	HIS	129S	2.490	-4.008	6.821	1.00	0.00	-0.106	12.77	4.00
ATOM	386	HB1	HIS	129S	2.757	-3.280	7.587	1.00	0.00	0.053	0.00	0.00
ATOM	387	HB2	HIS	129S	2.926	-3.622	5.899	1.00	0.00	0.053	0.00	0.00
ATOM	388	CG	HIS	129S	3.290	-5.231	7.149	1.00	0.00	-0.050	7.26	0.60
ATOM	389	CD2	HIS	129S	3.763	-5.694	8.332	1.00	0.00	-0.177	10.80	0.60
ATOM	390	HD2	HIS	129S	3.681	-5.199	9.300	1.00	0.00	0.127	0.00	0.00
ATOM	391	ND1	HIS	129S	3.626	-6.178	6.205	1.00	0.00	0.207	9.25	-17.40
ATOM	392	HD1	HIS	129S	3.409	-6.120	5.199	1.00	0.00	0.393	0.00	0.00
ATOM	393	CE1	HIS	129S	4.270	-7.172	6.792	1.00	0.00	-0.227	10.80	0.60
ATOM	394	HE1	HIS	129S	4.657	-8.062	6.295	1.00	0.00	0.127	0.00	0.00
ATOM	395	NE2	HIS	129S	4.365	-6.904	8.082	1.00	0.00	0.207	9.25	-17.40
ATOM	396	HE2	HIS	129S	4.817	-7.504	8.786	1.00	0.00	0.393	0.00	0.00
ATOM	397	C	HIS	129S	0.499	-4.895	8.026	1.00	0.00	0.396	9.82	4.00
ATOM	398	O	HIS	129S	0.314	-6.103	8.113	1.00	0.00	-0.396	8.17	-17.40
ATOM	399	N	TYR	130	0.274	-4.058	9.030	1.00	0.00	-0.650	9.00	-17.40
ATOM	400	HN	TYR	130	0.410	-3.048	8.881	1.00	0.00	0.440	0.00	0.00
ATOM	401	CA	TYR	130	-0.160	-4.528	10.335	1.00	0.00	0.158	9.40	4.00
ATOM	402	HA	TYR	130	0.261	-5.521	10.489	1.00	0.00	0.053	0.00	0.00
ATOM	403	CB	TYR	130	0.428	-3.609	11.409	1.00	0.00	-0.106	12.77	4.00
ATOM	404	HB1	TYR	130	0.014	-3.798	12.399	1.00	0.00	0.053	0.00	0.00
ATOM	405	HB2	TYR	130	0.247	-2.553	11.206	1.00	0.00	0.053	0.00	0.00
ATOM	406	CG	TYR	130	1.925	-3.755	11.549	1.00	0.00	0.000	7.26	0.60
ATOM	407	CD1	TYR	130	2.754	-2.635	11.637	1.00	0.00	-0.127	10.80	0.60
ATOM	408	HD1	TYR	130	2.313	-1.638	11.616	1.00	0.00	0.127	0.00	0.00
ATOM	409	CE1	TYR	130	4.137	-2.772	11.751	1.00	0.00	-0.127	10.80	0.60
ATOM	410	HE1	TYR	130	4.773	-1.889	11.814	1.00	0.00	0.127	0.00	0.00
ATOM	411	CD2	TYR	130	2.512	-5.017	11.582	1.00	0.00	-0.127	10.80	0.60
ATOM	412	HD2	TYR	130	1.880	-5.903	11.516	1.00	0.00	0.127	0.00	0.00
ATOM	413	CE2	TYR	130	3.888	-5.166	11.697	1.00	0.00	-0.127	10.80	0.60
ATOM	414	HE2	TYR	130	4.330	-6.161	11.719	1.00	0.00	0.127	0.00	0.00
ATOM	415	CZ	TYR	130	4.696	-4.042	11.783	1.00	0.00	0.026	7.26	0.60
ATOM	416	OH	TYR	130	6.063	-4.202	11.934	1.00	0.00	-0.451	10.94	-17.40
ATOM	417	HH	TYR	130	6.290	-4.291	12.934	1.00	0.00	0.424	0.00	0.00
ATOM	418	C	TYR	130	-1.668	-4.647	10.541	1.00	0.00	0.396	9.82	4.00
ATOM	419	O	TYR	130	-2.106	-5.329	11.453	1.00	0.00	-0.396	8.17	-17.40
ATOM	420	N	ARG	131G	-2.456	-3.981	9.710	1.00	0.00	-0.650	9.00	-17.40
ATOM	421	HN	ARG	131G	-2.035	-3.433	8.946	1.00	0.00	0.440	0.00	0.00
ATOM	422	CA	ARG	131G	-3.913	-4.008	9.856	1.00	0.00	0.158	9.40	4.00
ATOM	423	HA	ARG	131G	-4.240	-3.479	10.751	1.00	0.00	0.053	0.00	0.00
ATOM	424	CB	ARG	131G	-4.565	-3.274	8.670	1.00	0.00	-0.106	12.77	4.00
ATOM	425	HB1	ARG	131G	-4.361	-3.759	7.715	1.00	0.00	0.053	0.00	0.00
ATOM	426	HB2	ARG	131G	-4.214	-2.246	8.570	1.00	0.00	0.053	0.00	0.00
ATOM	427	CG	ARG	131G	-6.069	-3.197	8.793	1.00	0.00	-0.106	12.77	4.00
ATOM	428	HG1	ARG	131G	-6.406	-2.929	9.794	1.00	0.00	0.053	0.00	0.00
ATOM	429	HG2	ARG	131G	-6.568	-4.137	8.560	1.00	0.00	0.053	0.00	0.00
ATOM	430	CD	ARG	131G	-6.696	-2.166	7.866	1.00	0.00	0.374	12.77	4.00
ATOM	431	HD1	ARG	131G	-6.267	-1.170	7.986	1.00	0.00	0.053	0.00	0.00
ATOM	432	HD2	ARG	131G	-7.768	-2.048	8.024	1.00	0.00	0.053	0.00	0.00
ATOM	433	NE	ARG	131G	-6.537	-2.499	6.455	1.00	0.00	-0.819	9.00	-24.67
ATOM	434	HE	ARG	131G	-5.853	-3.225	6.196	1.00	0.00	0.407	0.00	0.00
ATOM	435	CZ	ARG	131G	-7.231	-1.911	5.487	1.00	0.00	0.796	6.95	4.00
ATOM	436	NH1	ARG	131G	-8.125	-0.979	5.800	1.00	0.00	-0.746	9.00	-24.67
ATOM	437	HH1	ARG	131G	-8.668	-0.516	5.057	1.00	0.00	0.407	0.00	0.00
ATOM	438	HH1	ARG	131G	-8.274	-0.719	6.785	1.00	0.00	0.407	0.00	0.00
ATOM	439	NH2	ARG	131G	-7.040	-2.253	4.218	1.00	0.00	-0.746	9.00	-24.67
ATOM	440	HH2	ARG	131G	-7.582	-1.792	3.473	1.00	0.00	0.407	0.00	0.00
ATOM	441	HH2	ARG	131G	-6.349	-2.978	3.978	1.00	0.00	0.407	0.00	0.00
ATOM	442	C	ARG	131G	-4.449	-5.442	9.960	1.00	0.00	0.396	9.82	4.00
ATOM	443	O	ARG	131G	-4.204	-6.262	9.084	1.00	0.00	-0.396	8.17	-17.40
ATOM	444	N	PRO	132	-5.162	-5.774	11.054	1.00	0.00	-0.422	9.00	-17.40
ATOM	445	CD	PRO	132	-5.111	-5.140	12.382	1.00	0.00	0.105	12.77	4.00
ATOM	446	HD1	PRO	132	-5.405	-4.091	12.332	1.00	0.00	0.053	0.00	0.00
ATOM	447	HD2	PRO	132	-4.105	-5.180	12.801	1.00	0.00	0.053	0.00	0.00
ATOM	448	CA	PRO	132	-5.679	-7.150	11.160	1.00	0.00	0.158	9.40	4.00
ATOM	449	HA	PRO	132	-4.945	-7.820	10.713	1.00	0.00	0.053	0.00	0.00
ATOM	450	CB	PRO	132	-5.780	-7.361	12.670	1.00	0.00	-0.106	12.77	4.00
ATOM	451	HB1	PRO	132	-4.843	-7.740	13.078	1.00	0.00	0.053	0.00	0.00

ATOM	452	HB2	PRO	132	-6.563	-8.077	12.916	1.00	0.00	0.053	0.00	0.00
ATOM	453	CG	PRO	132	-6.099	-5.976	13.177	1.00	0.00	-0.106	12.77	4.00
ATOM	454	HG1	PRO	132	-5.945	-5.897	14.253	1.00	0.00	0.053	0.00	0.00
ATOM	455	HG2	PRO	132	-7.135	-5.704	12.977	1.00	0.00	0.053	0.00	0.00
ATOM	456	C	PRO	132	-7.012	-7.409	10.461	1.00	0.00	0.396	9.82	4.00
ATOM	457	O	PRO	132	-7.433	-8.553	10.307	1.00	0.00	-0.396	8.17	-17.40
ATOM	458	N	SER	133	-7.676	-6.338	10.041	1.00	0.00	-0.650	9.00	-17.40
ATOM	459	HN	SER	133	-7.263	-5.404	10.179	1.00	0.00	0.440	0.00	0.00
ATOM	460	CA	SER	133	-8.967	-6.453	9.393	1.00	0.00	0.158	9.40	4.00
ATOM	461	HA	SER	133	-8.961	-7.269	8.671	1.00	0.00	0.053	0.00	0.00
ATOM	462	CB	SER	133	-10.045	-6.720	10.441	1.00	0.00	0.007	12.77	4.00
ATOM	463	HB1	SER	133	-9.905	-6.092	11.321	1.00	0.00	0.053	0.00	0.00
ATOM	464	HB2	SER	133	-10.027	-7.758	10.771	1.00	0.00	0.053	0.00	0.00
ATOM	465	OG	SER	133	-11.342	-6.455	9.926	1.00	0.00	-0.537	11.04	-17.40
ATOM	466	HG	SER	133	-11.474	-5.437	9.835	1.00	0.00	0.424	0.00	0.00
ATOM	467	C	SER	133	-9.309	-5.178	8.665	1.00	0.00	0.396	9.82	4.00
ATOM	468	O	SER	133	-9.390	-4.121	9.291	1.00	0.00	-0.396	8.17	-17.40
ATOM	469	N	ALA	134	-9.540	-5.286	7.356	1.00	0.00	-0.650	9.00	-17.40
ATOM	470	HN	ALA	134	-9.464	-6.209	6.905	1.00	0.00	0.440	0.00	0.00
ATOM	471	CA	ALA	134	-9.895	-4.130	6.554	1.00	0.00	0.158	9.40	4.00
ATOM	472	HA	ALA	134	-9.159	-3.337	6.691	1.00	0.00	0.053	0.00	0.00
ATOM	473	CB	ALA	134	-9.911	-4.507	5.077	1.00	0.00	-0.159	16.15	4.00
ATOM	474	HB1	ALA	134	-10.178	-3.634	4.481	1.00	0.00	0.053	0.00	0.00
ATOM	475	HB2	ALA	134	-8.923	-4.859	4.780	1.00	0.00	0.053	0.00	0.00
ATOM	476	HB3	ALA	134	-10.643	-5.297	4.911	1.00	0.00	0.053	0.00	0.00
ATOM	477	C	ALA	134	-11.265	-3.605	6.967	1.00	0.00	0.396	9.82	4.00
ATOM	478	O	ALA	134	-11.490	-2.396	6.998	1.00	0.00	-0.396	8.17	-17.40
ATOM	479	N	GLU	135	-12.182	-4.517	7.287	1.00	0.00	-0.650	9.00	-17.40
ATOM	480	HN	GLU	135	-11.938	-5.517	7.253	1.00	0.00	0.440	0.00	0.00
ATOM	481	CA	GLU	135	-13.525	-4.115	7.684	1.00	0.00	0.158	9.40	4.00
ATOM	482	HA	GLU	135	-13.996	-3.439	6.970	1.00	0.00	0.053	0.00	0.00
ATOM	483	CB	GLU	135	-14.479	-5.321	7.735	1.00	0.00	-0.106	12.77	4.00
ATOM	484	HB1	GLU	135	-15.124	-5.277	6.857	1.00	0.00	0.053	0.00	0.00
ATOM	485	HB2	GLU	135	-15.064	-5.249	8.651	1.00	0.00	0.053	0.00	0.00
ATOM	486	CG	GLU	135	-13.803	-6.693	7.734	1.00	0.00	-0.106	12.77	4.00
ATOM	487	HG1	GLU	135	-14.487	-7.498	8.001	1.00	0.00	0.053	0.00	0.00
ATOM	488	HG2	GLU	135	-12.974	-6.753	8.439	1.00	0.00	0.053	0.00	0.00
ATOM	489	CD	GLU	135	-13.229	-7.061	6.377	1.00	0.00	0.399	9.82	4.00
ATOM	490	OE1	GLU	135	-14.006	-7.070	5.398	1.00	0.00	-0.396	8.17	-18.95
ATOM	491	OE2	GLU	135	-12.008	-7.341	6.285	1.00	0.00	-0.427	8.17	-18.95
ATOM	492	HE2	GLU	135	-11.779	-7.566	5.306	1.00	0.00	0.424	0.00	0.00
ATOM	493	C	GLU	135	-13.558	-3.390	9.021	1.00	0.00	0.396	9.82	4.00
ATOM	494	O	GLU	135	-14.308	-2.436	9.186	1.00	0.00	-0.396	8.17	-17.40
ATOM	495	N	LEU	136	-12.747	-3.836	9.974	1.00	0.00	-0.650	9.00	-17.40
ATOM	496	HN	LEU	136	-12.131	-4.640	9.785	1.00	0.00	0.440	0.00	0.00
ATOM	497	CA	LEU	136	-12.720	-3.198	11.284	1.00	0.00	0.158	9.40	4.00
ATOM	498	HA	LEU	136	-13.714	-2.976	11.671	1.00	0.00	0.053	0.00	0.00
ATOM	499	CB	LEU	136	-12.092	-4.133	12.316	1.00	0.00	-0.106	12.77	4.00
ATOM	500	HB1	LEU	136	-11.976	-3.666	13.294	1.00	0.00	0.053	0.00	0.00
ATOM	501	HB2	LEU	136	-11.097	-4.473	12.028	1.00	0.00	0.053	0.00	0.00
ATOM	502	CG	LEU	136	-12.920	-5.403	12.550	1.00	0.00	-0.053	9.40	4.00
ATOM	503	HG	LEU	136	-12.902	-6.021	11.652	1.00	0.00	0.053	0.00	0.00
ATOM	504	CD1	LEU	136	-12.332	-6.188	13.716	1.00	0.00	-0.159	16.15	4.00
ATOM	505	HD1	LEU	136	-12.921	-7.090	13.881	1.00	0.00	0.053	0.00	0.00
ATOM	506	HD1	LEU	136	-11.302	-6.463	13.486	1.00	0.00	0.053	0.00	0.00
ATOM	507	HD1	LEU	136	-12.350	-5.572	14.615	1.00	0.00	0.053	0.00	0.00
ATOM	508	CD2	LEU	136	-14.377	-5.019	12.849	1.00	0.00	-0.159	16.15	4.00
ATOM	509	HD2	LEU	136	-14.964	-5.922	13.015	1.00	0.00	0.053	0.00	0.00
ATOM	510	HD2	LEU	136	-14.412	-4.393	13.741	1.00	0.00	0.053	0.00	0.00
ATOM	511	HD2	LEU	136	-14.789	-4.468	12.003	1.00	0.00	0.053	0.00	0.00
ATOM	512	C	LEU	136	-11.974	-1.873	11.285	1.00	0.00	0.396	9.82	4.00
ATOM	513	O	LEU	136	-12.360	-0.937	12.003	1.00	0.00	-0.396	8.17	-17.40
ATOM	514	N	PHE	137	-10.911	-1.803	10.482	1.00	0.00	-0.650	9.00	-17.40
ATOM	515	HN	PHE	137	-10.660	-2.625	9.915	1.00	0.00	0.440	0.00	0.00
ATOM	516	CA	PHE	137	-10.093	-0.601	10.380	1.00	0.00	0.158	9.40	4.00
ATOM	517	HA	PHE	137	-10.543	0.168	11.007	1.00	0.00	0.053	0.00	0.00
ATOM	518	CB	PHE	137	-8.681	-0.861	10.920	1.00	0.00	-0.106	12.77	4.00
ATOM	519	HB1	PHE	137	-8.017	0.000	10.841	1.00	0.00	0.053	0.00	0.00
ATOM	520	HB2	PHE	137	-8.158	-1.667	10.406	1.00	0.00	0.053	0.00	0.00
ATOM	521	CG	PHE	137	-8.652	-1.240	12.365	1.00	0.00	0.000	7.26	0.60
ATOM	522	CD1	PHE	137	-8.659	-2.573	12.743	1.00	0.00	-0.127	10.80	0.60
ATOM	523	HD1	PHE	137	-8.659	-3.350	11.978	1.00	0.00	0.127	0.00	0.00
ATOM	524	CD2	PHE	137	-8.650	-0.254	13.355	1.00	0.00	-0.127	10.80	0.60
ATOM	525	HD2	PHE	137	-8.644	0.798	13.070	1.00	0.00	0.127	0.00	0.00
ATOM	526	CE1	PHE	137	-8.665	-2.931	14.089	1.00	0.00	-0.127	10.80	0.60
ATOM	527	HE1	PHE	137	-8.671	-3.983	14.374	1.00	0.00	0.127	0.00	0.00

ATOM	528	CE2	PHE	137	-8.655	-0.606	14.706	1.00	0.00	-0.127	10.80	0.60
ATOM	529	HE2	PHE	137	-8.652	0.168	15.473	1.00	0.00	0.127	0.00	0.00
ATOM	530	CZ	PHE	137	-8.663	-1.945	15.068	1.00	0.00	-0.127	10.80	0.60
ATOM	531	HZ	PHE	137	-8.667	-2.224	16.121	1.00	0.00	0.127	0.00	0.00
ATOM	532	C	PHE	137	-9.959	-0.021	8.976	1.00	0.00	0.396	9.82	4.00
ATOM	533	O	PHE	137	-8.897	-0.115	8.359	1.00	0.00	-0.396	8.17	-17.40
ATOM	534	N	PRO	138	-11.023	0.606	8.460	1.00	0.00	-0.422	9.00	-17.40
ATOM	535	CD	PRO	138	-12.373	0.786	9.018	1.00	0.00	0.105	12.77	4.00
ATOM	536	HD1	PRO	138	-12.332	1.052	10.074	1.00	0.00	0.053	0.00	0.00
ATOM	537	HD2	PRO	138	-12.962	-0.126	8.931	1.00	0.00	0.053	0.00	0.00
ATOM	538	CA	PRO	138	-10.925	1.185	7.120	1.00	0.00	0.158	9.40	4.00
ATOM	539	HA	PRO	138	-10.529	0.405	6.469	1.00	0.00	0.053	0.00	0.00
ATOM	540	CB	PRO	138	-12.361	1.606	6.813	1.00	0.00	-0.106	12.77	4.00
ATOM	541	HB1	PRO	138	-12.906	0.807	6.309	1.00	0.00	0.053	0.00	0.00
ATOM	542	HB2	PRO	138	-12.384	2.482	6.166	1.00	0.00	0.053	0.00	0.00
ATOM	543	CG	PRO	138	-12.921	1.897	8.173	1.00	0.00	-0.106	12.77	4.00
ATOM	544	HG1	PRO	138	-14.010	1.892	8.156	1.00	0.00	0.053	0.00	0.00
ATOM	545	HG2	PRO	138	-12.595	2.874	8.529	1.00	0.00	0.053	0.00	0.00
ATOM	546	C	PRO	138	-9.984	2.372	7.224	1.00	0.00	0.396	9.82	4.00
ATOM	547	O	PRO	138	-10.013	3.101	8.209	1.00	0.00	-0.396	8.17	-17.40
ATOM	548	N	ILE	139	-9.152	2.555	6.210	1.00	0.00	-0.650	9.00	-17.40
ATOM	549	HN	ILE	139	-9.190	1.906	5.411	1.00	0.00	0.440	0.00	0.00
ATOM	550	CA	ILE	139	-8.184	3.643	6.187	1.00	0.00	0.158	9.40	4.00
ATOM	551	HA	ILE	139	-8.067	4.046	7.193	1.00	0.00	0.053	0.00	0.00
ATOM	552	CB	ILE	139	-6.803	3.121	5.713	1.00	0.00	-0.053	9.40	4.00
ATOM	553	HB	ILE	139	-6.905	2.523	4.807	1.00	0.00	0.053	0.00	0.00
ATOM	554	CG2	ILE	139	-5.838	4.309	5.405	1.00	0.00	-0.159	16.15	4.00
ATOM	555	HG2	ILE	139	-4.875	3.919	5.074	1.00	0.00	0.053	0.00	0.00
ATOM	556	HG2	ILE	139	-6.266	4.931	4.619	1.00	0.00	0.053	0.00	0.00
ATOM	557	HG2	ILE	139	-5.697	4.906	6.305	1.00	0.00	0.053	0.00	0.00
ATOM	558	CG1	ILE	139	-6.225	2.184	6.782	1.00	0.00	-0.106	12.77	4.00
ATOM	559	HG1	ILE	139	-6.971	1.518	7.214	1.00	0.00	0.053	0.00	0.00
ATOM	560	HG1	ILE	139	-5.783	2.717	7.623	1.00	0.00	0.053	0.00	0.00
ATOM	561	CD1	ILE	139	-5.138	1.288	6.254	1.00	0.00	-0.159	16.15	4.00
ATOM	562	HD1	ILE	139	-4.770	0.649	7.057	1.00	0.00	0.053	0.00	0.00
ATOM	563	HD1	ILE	139	-5.535	0.667	5.451	1.00	0.00	0.053	0.00	0.00
ATOM	564	HD1	ILE	139	-4.319	1.896	5.870	1.00	0.00	0.053	0.00	0.00
ATOM	565	C	ILE	139	-8.676	4.738	5.256	1.00	0.00	0.396	9.82	4.00
ATOM	566	O	ILE	139	-8.926	4.509	4.069	1.00	0.00	-0.396	8.17	-17.40
ATOM	567	N	ILE	140	-8.835	5.930	5.805	1.00	0.00	-0.650	9.00	-17.40
ATOM	568	HN	ILE	140	-8.630	6.056	6.806	1.00	0.00	0.440	0.00	0.00
ATOM	569	CA	ILE	140	-9.292	7.063	5.024	1.00	0.00	0.158	9.40	4.00
ATOM	570	HA	ILE	140	-9.516	6.664	4.034	1.00	0.00	0.053	0.00	0.00
ATOM	571	CB	ILE	140	-10.554	7.708	5.676	1.00	0.00	-0.053	9.40	4.00
ATOM	572	HB	ILE	140	-10.397	7.869	6.742	1.00	0.00	0.053	0.00	0.00
ATOM	573	CG2	ILE	140	-10.863	9.043	5.037	1.00	0.00	-0.159	16.15	4.00
ATOM	574	HG2	ILE	140	-11.746	9.475	5.506	1.00	0.00	0.053	0.00	0.00
ATOM	575	HG2	ILE	140	-10.015	9.715	5.170	1.00	0.00	0.053	0.00	0.00
ATOM	576	HG2	ILE	140	-11.050	8.902	3.972	1.00	0.00	0.053	0.00	0.00
ATOM	577	CG1	ILE	140	-11.779	6.797	5.488	1.00	0.00	-0.106	12.77	4.00
ATOM	578	HG1	ILE	140	-11.837	6.516	4.436	1.00	0.00	0.053	0.00	0.00
ATOM	579	HG1	ILE	140	-12.667	7.353	5.787	1.00	0.00	0.053	0.00	0.00
ATOM	580	CD1	ILE	140	-11.744	5.537	6.290	1.00	0.00	-0.159	16.15	4.00
ATOM	581	HD1	ILE	140	-12.646	4.956	6.095	1.00	0.00	0.053	0.00	0.00
ATOM	582	HD1	ILE	140	-10.868	4.951	6.009	1.00	0.00	0.053	0.00	0.00
ATOM	583	HD1	ILE	140	-11.692	5.782	7.350	1.00	0.00	0.053	0.00	0.00
ATOM	584	C	ILE	140	-8.134	8.051	5.021	1.00	0.00	0.396	9.82	4.00
ATOM	585	O	ILE	140	-7.722	8.535	6.076	1.00	0.00	-0.396	8.17	-17.40
ATOM	586	N	VAL	141	-7.583	8.315	3.841	1.00	0.00	-0.650	9.00	-17.40
ATOM	587	HN	VAL	141	-7.947	7.843	3.001	1.00	0.00	0.440	0.00	0.00
ATOM	588	CA	VAL	141	-6.476	9.255	3.704	1.00	0.00	0.158	9.40	4.00
ATOM	589	HA	VAL	141	-5.980	9.347	4.670	1.00	0.00	0.053	0.00	0.00
ATOM	590	CB	VAL	141	-5.456	8.780	2.633	1.00	0.00	-0.053	9.40	4.00
ATOM	591	HB	VAL	141	-5.894	8.853	1.637	1.00	0.00	0.053	0.00	0.00
ATOM	592	CG1	VAL	141	-4.182	9.658	2.682	1.00	0.00	-0.159	16.15	4.00
ATOM	593	HG1	VAL	141	-3.474	9.315	1.926	1.00	0.00	0.053	0.00	0.00
ATOM	594	HG1	VAL	141	-4.448	10.696	2.485	1.00	0.00	0.053	0.00	0.00
ATOM	595	HG1	VAL	141	-3.724	9.581	3.668	1.00	0.00	0.053	0.00	0.00
ATOM	596	CG2	VAL	141	-5.109	7.307	2.852	1.00	0.00	-0.159	16.15	4.00
ATOM	597	HG2	VAL	141	-4.393	6.985	2.095	1.00	0.00	0.053	0.00	0.00
ATOM	598	HG2	VAL	141	-4.671	7.179	3.842	1.00	0.00	0.053	0.00	0.00
ATOM	599	HG2	VAL	141	-6.014	6.704	2.774	1.00	0.00	0.053	0.00	0.00
ATOM	600	C	VAL	141	-7.038	10.601	3.262	1.00	0.00	0.396	9.82	4.00
ATOM	601	O	VAL	141	-7.539	10.729	2.137	1.00	0.00	-0.396	8.17	-17.40
ATOM	602	N	SER	142	-6.984	11.600	4.137	1.00	0.00	-0.650	9.00	-17.40
ATOM	603	HN	SER	142	-6.594	11.436	5.076	1.00	0.00	0.440	0.00	0.00

ATOM	604	CA	SER	142	-7.475	12.931	3.775	1.00	0.00	0.158	9.40	4.00
ATOM	605	HA	SER	142	-8.200	12.773	2.976	1.00	0.00	0.053	0.00	0.00
ATOM	606	CB	SER	142	-8.148	13.608	4.978	1.00	0.00	0.007	12.77	4.00
ATOM	607	HB1	SER	142	-7.418	13.920	5.725	1.00	0.00	0.053	0.00	0.00
ATOM	608	HB2	SER	142	-8.851	12.940	5.475	1.00	0.00	0.053	0.00	0.00
ATOM	609	OG	SER	142	-8.877	14.772	4.590	1.00	0.00	-0.537	11.04	-17.40
ATOM	610	HG	SER	142	-8.260	15.595	4.639	1.00	0.00	0.424	0.00	0.00
ATOM	611	C	SER	142	-6.252	13.715	3.317	1.00	0.00	0.396	9.82	4.00
ATOM	612	O	SER	142	-5.303	13.911	4.079	1.00	0.00	-0.396	8.17	-17.40
ATOM	613	N	GLN	143	-6.261	14.140	2.061	1.00	0.00	-0.650	9.00	-17.40
ATOM	614	HN	GLN	143	-7.071	13.938	1.458	1.00	0.00	0.440	0.00	0.00
ATOM	615	CA	GLN	143	-5.134	14.889	1.528	1.00	0.00	0.158	9.40	4.00
ATOM	616	HA	GLN	143	-4.285	14.863	2.211	1.00	0.00	0.053	0.00	0.00
ATOM	617	CB	GLN	143	-4.669	14.296	0.191	1.00	0.00	-0.106	12.77	4.00
ATOM	618	HB1	GLN	143	-5.280	14.628	-0.647	1.00	0.00	0.053	0.00	0.00
ATOM	619	HB2	GLN	143	-4.705	13.206	0.183	1.00	0.00	0.053	0.00	0.00
ATOM	620	CG	GLN	143	-3.231	14.679	-0.148	1.00	0.00	-0.106	12.77	4.00
ATOM	621	HG1	GLN	143	-2.485	14.008	0.279	1.00	0.00	0.053	0.00	0.00
ATOM	622	HG2	GLN	143	-2.947	15.672	0.199	1.00	0.00	0.053	0.00	0.00
ATOM	623	CD	GLN	143	-2.937	14.689	-1.637	1.00	0.00	0.396	9.82	4.00
ATOM	624	OE1	GLN	143	-3.668	14.114	-2.440	1.00	0.00	-0.396	8.17	-17.40
ATOM	625	NE2	GLN	143	-1.846	15.347	-2.008	1.00	0.00	-0.879	13.25	-17.40
ATOM	626	HE2	GLN	143	-1.261	15.815	-1.301	1.00	0.00	0.440	0.00	0.00
ATOM	627	HE2	GLN	143	-1.583	15.389	-3.004	1.00	0.00	0.440	0.00	0.00
ATOM	628	C	GLN	143	-5.500	16.345	1.302	1.00	0.00	0.396	9.82	4.00
ATOM	629	O	GLN	143	-6.510	16.653	0.666	1.00	0.00	-0.396	8.17	-17.40
ATOM	630	N	ASP	144P	-4.671	17.236	1.827	1.00	0.00	-0.650	9.00	-17.40
ATOM	631	HN	ASP	144P	-3.863	16.891	2.366	1.00	0.00	0.440	0.00	0.00
ATOM	632	CA	ASP	144P	-4.839	18.682	1.683	1.00	0.00	0.158	9.40	4.00
ATOM	633	HA	ASP	144P	-5.833	18.921	1.305	1.00	0.00	0.053	0.00	0.00
ATOM	634	CB	ASP	144P	-4.588	19.322	3.061	1.00	0.00	-0.336	12.77	4.00
ATOM	635	HB1	ASP	144P	-3.586	19.142	3.452	1.00	0.00	0.053	0.00	0.00
ATOM	636	HB2	ASP	144P	-5.261	18.964	3.840	1.00	0.00	0.053	0.00	0.00
ATOM	637	CG	ASP	144P	-4.746	20.830	3.072	1.00	0.00	0.297	9.82	4.00
ATOM	638	OD1	ASP	144P	-5.409	21.398	2.188	1.00	0.00	-0.534	8.17	-18.95
ATOM	639	OD2	ASP	144P	-4.214	21.461	4.011	1.00	0.00	-0.534	8.17	-18.95
ATOM	640	C	ASP	144P	-3.738	19.087	0.679	1.00	0.00	0.396	9.82	4.00
ATOM	641	O	ASP	144P	-3.009	18.221	0.187	1.00	0.00	-0.396	8.17	-17.40
ATOM	642	N	CYS	145	-3.655	20.371	0.343	1.00	0.00	-0.650	9.00	-17.40
ATOM	643	HN	CYS	145	-4.370	21.025	0.690	1.00	0.00	0.440	0.00	0.00
ATOM	644	CA	CYS	145	-2.577	20.882	-0.506	1.00	0.00	0.158	9.40	4.00
ATOM	645	HA	CYS	145	-2.598	21.967	-0.408	1.00	0.00	0.053	0.00	0.00
ATOM	646	C	CYS	145	-2.535	20.626	-2.013	1.00	0.00	0.396	9.82	4.00
ATOM	647	O	CYS	145	-1.862	21.357	-2.720	1.00	0.00	-0.396	8.17	-17.40
ATOM	648	CB	CYS	145	-1.248	20.432	0.106	1.00	0.00	-0.041	12.77	4.00
ATOM	649	HB1	CYS	145	-0.410	20.986	-0.317	1.00	0.00	0.053	0.00	0.00
ATOM	650	HB2	CYS	145	-1.069	19.372	-0.075	1.00	0.00	0.053	0.00	0.00
ATOM	651	SG	CYS	145	-1.231	20.697	1.915	1.00	0.00	-0.065	19.93	-6.40
ATOM	652	N	GLY	146	-3.205	19.593	-2.506	1.00	0.00	-0.650	9.00	-17.40
ATOM	653	HN	GLY	146	-3.736	18.973	-1.879	1.00	0.00	0.440	0.00	0.00
ATOM	654	CA	GLY	146	-3.185	19.340	-3.942	1.00	0.00	0.105	9.40	4.00
ATOM	655	HA1	GLY	146	-3.506	20.255	-4.439	1.00	0.00	0.053	0.00	0.00
ATOM	656	HA2	GLY	146	-3.872	18.517	-4.138	1.00	0.00	0.053	0.00	0.00
ATOM	657	C	GLY	146	-1.852	18.949	-4.579	1.00	0.00	0.396	9.82	4.00
ATOM	658	O	GLY	146	-1.664	19.142	-5.779	1.00	0.00	-0.396	8.17	-17.40
ATOM	659	N	HIS	147S	-0.926	18.396	-3.796	1.00	0.00	-0.650	9.00	-17.40
ATOM	660	HN	HIS	147S	-1.141	18.252	-2.799	1.00	0.00	0.440	0.00	0.00
ATOM	661	CA	HIS	147S	0.390	17.983	-4.302	1.00	0.00	0.158	9.40	4.00
ATOM	662	HA	HIS	147S	0.797	18.822	-4.866	1.00	0.00	0.053	0.00	0.00
ATOM	663	CB	HIS	147S	1.282	17.627	-3.105	1.00	0.00	-0.106	12.77	4.00
ATOM	664	HB1	HIS	147S	0.898	16.711	-2.655	1.00	0.00	0.053	0.00	0.00
ATOM	665	HB2	HIS	147S	1.243	18.452	-2.394	1.00	0.00	0.053	0.00	0.00
ATOM	666	CG	HIS	147S	2.721	17.393	-3.448	1.00	0.00	-0.050	7.26	0.60
ATOM	667	CD2	HIS	147S	3.744	18.260	-3.636	1.00	0.00	-0.177	10.80	0.60
ATOM	668	HD2	HIS	147S	3.682	19.347	-3.612	1.00	0.00	0.127	0.00	0.00
ATOM	669	ND1	HIS	147S	3.263	16.131	-3.573	1.00	0.00	0.207	9.25	-17.40
ATOM	670	HD1	HIS	147S	2.740	15.247	-3.487	1.00	0.00	0.393	0.00	0.00
ATOM	671	CE1	HIS	147S	4.557	16.230	-3.821	1.00	0.00	-0.227	10.80	0.60
ATOM	672	HE1	HIS	147S	5.244	15.396	-3.967	1.00	0.00	0.127	0.00	0.00
ATOM	673	NE2	HIS	147S	4.875	17.513	-3.863	1.00	0.00	0.207	9.25	-17.40
ATOM	674	HE2	HIS	147S	5.817	17.890	-4.038	1.00	0.00	0.393	0.00	0.00
ATOM	675	C	HIS	147S	0.170	16.762	-5.193	1.00	0.00	0.396	9.82	4.00
ATOM	676	O	HIS	147S	-0.197	15.698	-4.695	1.00	0.00	-0.396	8.17	-17.40
ATOM	677	N	GLU	148	0.398	16.918	-6.500	1.00	0.00	-0.650	9.00	-17.40
ATOM	678	HN	GLU	148	0.746	17.827	-6.837	1.00	0.00	0.440	0.00	0.00
ATOM	679	CA	GLU	148	0.171	15.842	-7.478	1.00	0.00	0.158	9.40	4.00

ATOM	680	HA	GLU	148	-0.897	15.627	-7.496	1.00	0.00	0.053	0.00	0.00
ATOM	681	CB	GLU	148	0.540	16.321	-8.892	1.00	0.00	-0.106	12.77	4.00
ATOM	682	HB1	GLU	148	1.601	16.568	-8.902	1.00	0.00	0.053	0.00	0.00
ATOM	683	HB2	GLU	148	-0.063	17.199	-9.122	1.00	0.00	0.053	0.00	0.00
ATOM	684	CG	GLU	148	0.297	15.290	-10.003	1.00	0.00	-0.106	12.77	4.00
ATOM	685	HG1	GLU	148	0.951	14.422	-9.921	1.00	0.00	0.053	0.00	0.00
ATOM	686	HG2	GLU	148	0.461	15.699	-11.000	1.00	0.00	0.053	0.00	0.00
ATOM	687	CD	GLU	148	-1.126	14.748	-9.999	1.00	0.00	0.399	9.82	4.00
ATOM	688	OE1	GLU	148	-2.051	15.519	-9.657	1.00	0.00	-0.396	8.17	-18.95
ATOM	689	OE2	GLU	148	-1.325	13.556	-10.349	1.00	0.00	-0.427	8.17	-18.95
ATOM	690	HE2	GLU	148	-2.332	13.347	-10.304	1.00	0.00	0.424	0.00	0.00
ATOM	691	C	GLU	148	0.885	14.523	-7.208	1.00	0.00	0.396	9.82	4.00
ATOM	692	O	GLU	148	0.268	13.455	-7.277	1.00	0.00	-0.396	8.17	-17.40
ATOM	693	N	GLU	149	2.178	14.586	-6.917	1.00	0.00	-0.650	9.00	-17.40
ATOM	694	HN	GLU	149	2.653	15.498	-6.871	1.00	0.00	0.440	0.00	0.00
ATOM	695	CA	GLU	149	2.920	13.364	-6.664	1.00	0.00	0.158	9.40	4.00
ATOM	696	HA	GLU	149	2.841	12.671	-7.502	1.00	0.00	0.053	0.00	0.00
ATOM	697	CB	GLU	149	4.410	13.648	-6.496	1.00	0.00	-0.106	12.77	4.00
ATOM	698	HB1	GLU	149	4.617	14.366	-5.703	1.00	0.00	0.053	0.00	0.00
ATOM	699	HB2	GLU	149	4.867	14.058	-7.397	1.00	0.00	0.053	0.00	0.00
ATOM	700	CG	GLU	149	5.208	12.413	-6.154	1.00	0.00	-0.106	12.77	4.00
ATOM	701	HG1	GLU	149	5.104	11.631	-6.908	1.00	0.00	0.053	0.00	0.00
ATOM	702	HG2	GLU	149	4.901	11.971	-5.206	1.00	0.00	0.053	0.00	0.00
ATOM	703	CD	GLU	149	6.690	12.701	-6.034	1.00	0.00	0.399	9.82	4.00
ATOM	704	OE1	GLU	149	7.412	11.901	-5.395	1.00	0.00	-0.396	8.17	-18.95
ATOM	705	OE2	GLU	149	7.132	13.729	-6.589	1.00	0.00	-0.427	8.17	-18.95
ATOM	706	HE2	GLU	149	8.147	13.794	-6.433	1.00	0.00	0.424	0.00	0.00
ATOM	707	C	GLU	149	2.402	12.647	-5.428	1.00	0.00	0.396	9.82	4.00
ATOM	708	O	GLU	149	2.257	11.430	-5.432	1.00	0.00	-0.396	8.17	-17.40
ATOM	709	N	THR	150	2.119	13.394	-4.367	1.00	0.00	-0.650	9.00	-17.40
ATOM	710	HN	THR	150	2.258	14.414	-4.393	1.00	0.00	0.440	0.00	0.00
ATOM	711	CA	THR	150	1.609	12.749	-3.169	1.00	0.00	0.158	9.40	4.00
ATOM	712	HA	THR	150	2.308	11.970	-2.866	1.00	0.00	0.053	0.00	0.00
ATOM	713	CB	THR	150	1.492	13.738	-2.003	1.00	0.00	0.060	9.40	4.00
ATOM	714	HB	THR	150	0.818	14.547	-2.283	1.00	0.00	0.053	0.00	0.00
ATOM	715	OG1	THR	150	2.797	14.274	-1.677	1.00	0.00	-0.537	11.04	-17.40
ATOM	716	HG1	THR	150	3.466	14.024	-2.420	1.00	0.00	0.424	0.00	0.00
ATOM	717	CG2	THR	150	0.938	13.010	-0.774	1.00	0.00	-0.159	16.15	4.00
ATOM	718	HG2	THR	150	0.853	13.710	0.055	1.00	0.00	0.053	0.00	0.00
ATOM	719	HG2	THR	150	-0.045	12.601	-1.006	1.00	0.00	0.053	0.00	0.00
ATOM	720	HG2	THR	150	1.611	12.198	-0.498	1.00	0.00	0.053	0.00	0.00
ATOM	721	C	THR	150	0.232	12.133	-3.486	1.00	0.00	0.396	9.82	4.00
ATOM	722	O	THR	150	-0.128	11.083	-2.939	1.00	0.00	-0.396	8.17	-17.40
ATOM	723	N	ALA	151	-0.528	12.785	-4.369	1.00	0.00	-0.650	9.00	-17.40
ATOM	724	HN	ALA	151	-0.178	13.658	-4.788	1.00	0.00	0.440	0.00	0.00
ATOM	725	CA	ALA	151	-1.847	12.284	-4.755	1.00	0.00	0.158	9.40	4.00
ATOM	726	HA	ALA	151	-2.471	12.117	-3.877	1.00	0.00	0.053	0.00	0.00
ATOM	727	CB	ALA	151	-2.570	13.315	-5.634	1.00	0.00	-0.159	16.15	4.00
ATOM	728	HB1	ALA	151	-3.550	12.930	-5.915	1.00	0.00	0.053	0.00	0.00
ATOM	729	HB2	ALA	151	-2.690	14.245	-5.080	1.00	0.00	0.053	0.00	0.00
ATOM	730	HB3	ALA	151	-1.982	13.502	-6.533	1.00	0.00	0.053	0.00	0.00
ATOM	731	C	ALA	151	-1.727	10.961	-5.508	1.00	0.00	0.396	9.82	4.00
ATOM	732	O	ALA	151	-2.497	10.018	-5.265	1.00	0.00	-0.396	8.17	-17.40
ATOM	733	N	GLN	152	-0.764	10.888	-6.426	1.00	0.00	-0.650	9.00	-17.40
ATOM	734	HN	GLN	152	-0.147	11.698	-6.582	1.00	0.00	0.440	0.00	0.00
ATOM	735	CA	GLN	152	-0.571	9.665	-7.219	1.00	0.00	0.158	9.40	4.00
ATOM	736	HA	GLN	152	-1.501	9.393	-7.717	1.00	0.00	0.053	0.00	0.00
ATOM	737	CB	GLN	152	0.472	9.904	-8.325	1.00	0.00	-0.106	12.77	4.00
ATOM	738	HB1	GLN	152	0.564	9.053	-9.001	1.00	0.00	0.053	0.00	0.00
ATOM	739	HB2	GLN	152	1.469	10.087	-7.925	1.00	0.00	0.053	0.00	0.00
ATOM	740	CG	GLN	152	0.130	11.116	-9.201	1.00	0.00	-0.106	12.77	4.00
ATOM	741	HG1	GLN	152	0.010	11.985	-8.554	1.00	0.00	0.053	0.00	0.00
ATOM	742	HG2	GLN	152	-0.797	10.904	-9.733	1.00	0.00	0.053	0.00	0.00
ATOM	743	CD	GLN	152	1.194	11.450	-10.237	1.00	0.00	0.396	9.82	4.00
ATOM	744	OE1	GLN	152	2.395	11.221	-10.024	1.00	0.00	-0.396	8.17	-17.40
ATOM	745	NE2	GLN	152	0.761	12.029	-11.357	1.00	0.00	-0.879	13.25	-17.40
ATOM	746	HE2	GLN	152	-0.245	12.200	-11.493	1.00	0.00	0.440	0.00	0.00
ATOM	747	HE2	GLN	152	1.433	12.305	-12.087	1.00	0.00	0.440	0.00	0.00
ATOM	748	C	GLN	152	-0.141	8.518	-6.311	1.00	0.00	0.396	9.82	4.00
ATOM	749	O	GLN	152	-0.603	7.386	-6.458	1.00	0.00	-0.396	8.17	-17.40
ATOM	750	N	VAL	153	0.752	8.812	-5.375	1.00	0.00	-0.650	9.00	-17.40
ATOM	751	HN	VAL	153	1.126	9.769	-5.320	1.00	0.00	0.440	0.00	0.00
ATOM	752	CA	VAL	153	1.214	7.813	-4.426	1.00	0.00	0.158	9.40	4.00
ATOM	753	HA	VAL	153	1.734	7.002	-4.937	1.00	0.00	0.053	0.00	0.00
ATOM	754	CB	VAL	153	2.187	8.436	-3.416	1.00	0.00	-0.053	9.40	4.00
ATOM	755	HB	VAL	153	1.756	9.337	-2.981	1.00	0.00	0.053	0.00	0.00

ATOM	756	CG1	VAL	153	2.493	7.438	-2.276	1.00	0.00	-0.159	16.15	4.00
ATOM	757	HG1	VAL	153	3.184	7.895	-1.569	1.00	0.00	0.053	0.00	0.00
ATOM	758	HG1	VAL	153	1.567	7.177	-1.763	1.00	0.00	0.053	0.00	0.00
ATOM	759	HG1	VAL	153	2.943	6.536	-2.693	1.00	0.00	0.053	0.00	0.00
ATOM	760	CG2	VAL	153	3.465	8.855	-4.146	1.00	0.00	-0.159	16.15	4.00
ATOM	761	HG2	VAL	153	4.161	9.298	-3.435	1.00	0.00	0.053	0.00	0.00
ATOM	762	HG2	VAL	153	3.924	7.980	-4.607	1.00	0.00	0.053	0.00	0.00
ATOM	763	HG2	VAL	153	3.220	9.584	-4.918	1.00	0.00	0.053	0.00	0.00
ATOM	764	C	VAL	153	0.041	7.210	-3.656	1.00	0.00	0.396	9.82	4.00
ATOM	765	O	VAL	153	-0.055	5.980	-3.508	1.00	0.00	-0.396	8.17	-17.40
ATOM	766	N	ILE	154	-0.854	8.075	-3.184	1.00	0.00	-0.650	9.00	-17.40
ATOM	767	HN	ILE	154	-0.723	9.080	-3.364	1.00	0.00	0.440	0.00	0.00
ATOM	768	CA	ILE	154	-2.011	7.635	-2.421	1.00	0.00	0.158	9.40	4.00
ATOM	769	HA	ILE	154	-1.657	7.020	-1.594	1.00	0.00	0.053	0.00	0.00
ATOM	770	CB	ILE	154	-2.786	8.834	-1.809	1.00	0.00	-0.053	9.40	4.00
ATOM	771	HB	ILE	154	-3.097	9.521	-2.596	1.00	0.00	0.053	0.00	0.00
ATOM	772	CG2	ILE	154	-4.026	8.339	-1.072	1.00	0.00	-0.159	16.15	4.00
ATOM	773	HG2	ILE	154	-4.560	9.188	-0.648	1.00	0.00	0.053	0.00	0.00
ATOM	774	HG2	ILE	154	-4.677	7.812	-1.770	1.00	0.00	0.053	0.00	0.00
ATOM	775	HG2	ILE	154	-3.727	7.661	-0.272	1.00	0.00	0.053	0.00	0.00
ATOM	776	CG1	ILE	154	-1.887	9.587	-0.816	1.00	0.00	-0.106	12.77	4.00
ATOM	777	HG1	ILE	154	-0.922	9.757	-1.294	1.00	0.00	0.053	0.00	0.00
ATOM	778	HG1	ILE	154	-1.773	8.969	0.073	1.00	0.00	0.053	0.00	0.00
ATOM	779	CD1	ILE	154	-2.428	10.962	-0.360	1.00	0.00	-0.159	16.15	4.00
ATOM	780	HD1	ILE	154	-1.725	11.416	0.337	1.00	0.00	0.053	0.00	0.00
ATOM	781	HD1	ILE	154	-2.548	11.611	-1.228	1.00	0.00	0.053	0.00	0.00
ATOM	782	HD1	ILE	154	-3.392	10.829	0.129	1.00	0.00	0.053	0.00	0.00
ATOM	783	C	ILE	154	-2.907	6.831	-3.345	1.00	0.00	0.396	9.82	4.00
ATOM	784	O	ILE	154	-3.307	5.733	-2.994	1.00	0.00	-0.396	8.17	-17.40
ATOM	785	N	ALA	155	-3.191	7.371	-4.532	1.00	0.00	-0.650	9.00	-17.40
ATOM	786	HN	ALA	155	-2.803	8.298	-4.758	1.00	0.00	0.440	0.00	0.00
ATOM	787	CA	ALA	155	-4.035	6.698	-5.533	1.00	0.00	0.158	9.40	4.00
ATOM	788	HA	ALA	155	-5.065	6.576	-5.200	1.00	0.00	0.053	0.00	0.00
ATOM	789	CB	ALA	155	-4.103	7.551	-6.821	1.00	0.00	-0.159	16.15	4.00
ATOM	790	HB1	ALA	155	-4.728	7.047	-7.558	1.00	0.00	0.053	0.00	0.00
ATOM	791	HB2	ALA	155	-4.529	8.527	-6.589	1.00	0.00	0.053	0.00	0.00
ATOM	792	HB3	ALA	155	-3.099	7.680	-7.226	1.00	0.00	0.053	0.00	0.00
ATOM	793	C	ALA	155	-3.530	5.288	-5.881	1.00	0.00	0.396	9.82	4.00
ATOM	794	O	ALA	155	-4.325	4.381	-6.150	1.00	0.00	-0.396	8.17	-17.40
ATOM	795	N	SER	156	-2.210	5.110	-5.888	1.00	0.00	-0.650	9.00	-17.40
ATOM	796	HN	SER	156	-1.592	5.901	-5.655	1.00	0.00	0.440	0.00	0.00
ATOM	797	CA	SER	156	-1.621	3.818	-6.219	1.00	0.00	0.158	9.40	4.00
ATOM	798	HA	SER	156	-1.944	3.540	-7.223	1.00	0.00	0.053	0.00	0.00
ATOM	799	CB	SER	156	-0.088	3.917	-6.282	1.00	0.00	0.007	12.77	4.00
ATOM	800	HB1	SER	156	0.256	4.860	-6.706	1.00	0.00	0.053	0.00	0.00
ATOM	801	HB2	SER	156	0.360	3.132	-6.892	1.00	0.00	0.053	0.00	0.00
ATOM	802	OG	SER	156	0.523	3.816	-5.002	1.00	0.00	-0.537	11.04	-17.40
ATOM	803	HG	SER	156	0.601	4.753	-4.584	1.00	0.00	0.424	0.00	0.00
ATOM	804	C	SER	156	-2.024	2.687	-5.268	1.00	0.00	0.396	9.82	4.00
ATOM	805	O	SER	156	-1.841	1.504	-5.599	1.00	0.00	-0.396	8.17	-17.40
ATOM	806	N	TYR	157	-2.557	3.026	-4.093	1.00	0.00	-0.650	9.00	-17.40
ATOM	807	HN	TYR	157	-2.659	4.019	-3.840	1.00	0.00	0.440	0.00	0.00
ATOM	808	CA	TYR	157	-2.995	1.986	-3.167	1.00	0.00	0.158	9.40	4.00
ATOM	809	HA	TYR	157	-2.283	1.160	-3.144	1.00	0.00	0.053	0.00	0.00
ATOM	810	CB	TYR	157	-3.048	2.502	-1.725	1.00	0.00	-0.106	12.77	4.00
ATOM	811	HB1	TYR	157	-3.593	1.817	-1.075	1.00	0.00	0.053	0.00	0.00
ATOM	812	HB2	TYR	157	-3.543	3.471	-1.665	1.00	0.00	0.053	0.00	0.00
ATOM	813	CG	TYR	157	-1.671	2.666	-1.147	1.00	0.00	0.000	7.26	0.60
ATOM	814	CD1	TYR	157	-0.894	3.777	-1.454	1.00	0.00	-0.127	10.80	0.60
ATOM	815	HD1	TYR	157	-1.310	4.559	-2.089	1.00	0.00	0.127	0.00	0.00
ATOM	816	CE1	TYR	157	0.411	3.914	-0.966	1.00	0.00	-0.127	10.80	0.60
ATOM	817	HE1	TYR	157	1.001	4.795	-1.216	1.00	0.00	0.127	0.00	0.00
ATOM	818	CD2	TYR	157	-1.116	1.674	-0.332	1.00	0.00	-0.127	10.80	0.60
ATOM	819	HD2	TYR	157	-1.708	0.795	-0.077	1.00	0.00	0.127	0.00	0.00
ATOM	820	CE2	TYR	157	0.187	1.792	0.159	1.00	0.00	-0.127	10.80	0.60
ATOM	821	HE2	TYR	157	0.609	1.010	0.790	1.00	0.00	0.127	0.00	0.00
ATOM	822	CZ	TYR	157	0.944	2.921	-0.165	1.00	0.00	0.026	7.26	0.60
ATOM	823	OH	TYR	157	2.238	3.024	0.313	1.00	0.00	-0.451	10.94	-17.40
ATOM	824	HH	TYR	157	2.631	3.937	0.046	1.00	0.00	0.424	0.00	0.00
ATOM	825	C	TYR	157	-4.349	1.427	-3.579	1.00	0.00	0.396	9.82	4.00
ATOM	826	O	TYR	157	-4.793	0.400	-3.067	1.00	0.00	-0.396	8.17	-17.40
ATOM	827	N	GLY	158	-4.992	2.094	-4.531	1.00	0.00	-0.650	9.00	-17.40
ATOM	828	HN	GLY	158	-4.577	2.947	-4.933	1.00	0.00	0.440	0.00	0.00
ATOM	829	CA	GLY	158	-6.277	1.619	-5.003	1.00	0.00	0.105	9.40	4.00
ATOM	830	HA1	GLY	158	-6.213	0.651	-5.501	1.00	0.00	0.053	0.00	0.00
ATOM	831	HA2	GLY	158	-6.739	2.295	-5.722	1.00	0.00	0.053	0.00	0.00

ATOM	832	C	GLY	158	-7.286	1.446	-3.886	1.00	0.00	0.396	9.82	4.00
ATOM	833	O	GLY	158	-7.398	2.310	-3.012	1.00	0.00	-0.396	8.17	-17.40
ATOM	834	N	SER	159	-8.008	0.327	-3.906	1.00	0.00	-0.650	9.00	-17.40
ATOM	835	HN	SER	159	-7.833	-0.364	-4.649	1.00	0.00	0.440	0.00	0.00
ATOM	836	CA	SER	159	-9.043	0.047	-2.905	1.00	0.00	0.158	9.40	4.00
ATOM	837	HA	SER	159	-9.730	0.892	-2.893	1.00	0.00	0.053	0.00	0.00
ATOM	838	CB	SER	159	-9.866	-1.184	-3.302	1.00	0.00	0.007	12.77	4.00
ATOM	839	HB1	SER	159	-10.182	-1.136	-4.344	1.00	0.00	0.053	0.00	0.00
ATOM	840	HB2	SER	159	-10.766	-1.278	-2.695	1.00	0.00	0.053	0.00	0.00
ATOM	841	OG	SER	159	-9.121	-2.387	-3.142	1.00	0.00	-0.537	11.04	-17.40
ATOM	842	HG	SER	159	-9.761	-3.159	-2.911	1.00	0.00	0.424	0.00	0.00
ATOM	843	C	SER	159	-8.566	-0.156	-1.473	1.00	0.00	0.396	9.82	4.00
ATOM	844	O	SER	159	-9.391	-0.219	-0.564	1.00	0.00	-0.396	8.17	-17.40
ATOM	845	N	ALA	160	-7.260	-0.269	-1.254	1.00	0.00	-0.650	9.00	-17.40
ATOM	846	HN	ALA	160	-6.597	-0.222	-2.041	1.00	0.00	0.440	0.00	0.00
ATOM	847	CA	ALA	160	-6.770	-0.460	0.107	1.00	0.00	0.158	9.40	4.00
ATOM	848	HA	ALA	160	-7.243	-1.337	0.547	1.00	0.00	0.053	0.00	0.00
ATOM	849	CB	ALA	160	-5.261	-0.725	0.108	1.00	0.00	-0.159	16.15	4.00
ATOM	850	HB1	ALA	160	-4.916	-0.864	1.132	1.00	0.00	0.053	0.00	0.00
ATOM	851	HB2	ALA	160	-5.049	-1.623	-0.471	1.00	0.00	0.053	0.00	0.00
ATOM	852	HB3	ALA	160	-4.742	0.124	-0.336	1.00	0.00	0.053	0.00	0.00
ATOM	853	C	ALA	160	-7.105	0.773	0.953	1.00	0.00	0.396	9.82	4.00
ATOM	854	O	ALA	160	-7.188	0.685	2.185	1.00	0.00	-0.396	8.17	-17.40
ATOM	855	N	VAL	161	-7.304	1.921	0.305	1.00	0.00	-0.650	9.00	-17.40
ATOM	856	HN	VAL	161	-7.207	1.960	-0.719	1.00	0.00	0.440	0.00	0.00
ATOM	857	CA	VAL	161	-7.660	3.122	1.056	1.00	0.00	0.158	9.40	4.00
ATOM	858	HA	VAL	161	-8.029	2.889	2.055	1.00	0.00	0.053	0.00	0.00
ATOM	859	CB	VAL	161	-6.442	4.058	1.247	1.00	0.00	-0.053	9.40	4.00
ATOM	860	HB	VAL	161	-6.736	4.946	1.805	1.00	0.00	0.053	0.00	0.00
ATOM	861	CG1	VAL	161	-5.349	3.341	2.011	1.00	0.00	-0.159	16.15	4.00
ATOM	862	HG1	VAL	161	-4.497	4.008	2.139	1.00	0.00	0.053	0.00	0.00
ATOM	863	HG1	VAL	161	-5.725	3.040	2.988	1.00	0.00	0.053	0.00	0.00
ATOM	864	HG1	VAL	161	-5.036	2.456	1.455	1.00	0.00	0.053	0.00	0.00
ATOM	865	CG2	VAL	161	-5.930	4.532	-0.132	1.00	0.00	-0.159	16.15	4.00
ATOM	866	HG2	VAL	161	-5.072	5.190	0.003	1.00	0.00	0.053	0.00	0.00
ATOM	867	HG2	VAL	161	-5.632	3.667	-0.727	1.00	0.00	0.053	0.00	0.00
ATOM	868	HG2	VAL	161	-6.723	5.071	-0.649	1.00	0.00	0.053	0.00	0.00
ATOM	869	C	VAL	161	-8.746	3.926	0.370	1.00	0.00	0.396	9.82	4.00
ATOM	870	O	VAL	161	-9.109	3.651	-0.783	1.00	0.00	-0.396	8.17	-17.40
ATOM	871	N	THR	162	-9.273	4.913	1.096	1.00	0.00	-0.650	9.00	-17.40
ATOM	872	HN	THR	162	-8.955	5.035	2.068	1.00	0.00	0.440	0.00	0.00
ATOM	873	CA	THR	162	-10.273	5.818	0.572	1.00	0.00	0.158	9.40	4.00
ATOM	874	HA	THR	162	-10.582	5.525	-0.431	1.00	0.00	0.053	0.00	0.00
ATOM	875	CB	THR	162	-11.545	5.881	1.468	1.00	0.00	0.060	9.40	4.00
ATOM	876	HB	THR	162	-11.269	6.107	2.498	1.00	0.00	0.053	0.00	0.00
ATOM	877	OG1	THR	162	-12.230	4.616	1.429	1.00	0.00	-0.537	11.04	-17.40
ATOM	878	HG1	THR	162	-13.247	4.776	1.404	1.00	0.00	0.424	0.00	0.00
ATOM	879	CG2	THR	162	-12.508	6.985	0.956	1.00	0.00	-0.159	16.15	4.00
ATOM	880	HG2	THR	162	-13.393	7.018	1.591	1.00	0.00	0.053	0.00	0.00
ATOM	881	HG2	THR	162	-12.003	7.950	0.985	1.00	0.00	0.053	0.00	0.00
ATOM	882	HG2	THR	162	-12.804	6.762	-0.068	1.00	0.00	0.053	0.00	0.00
ATOM	883	C	THR	162	-9.544	7.165	0.579	1.00	0.00	0.396	9.82	4.00
ATOM	884	O	THR	162	-9.136	7.655	1.636	1.00	0.00	-0.396	8.17	-17.40
ATOM	885	N	HIS	163S	-9.375	7.749	-0.604	1.00	0.00	-0.650	9.00	-17.40
ATOM	886	HN	HIS	163S	-9.765	7.294	-1.442	1.00	0.00	0.440	0.00	0.00
ATOM	887	CA	HIS	163S	-8.659	9.006	-0.759	1.00	0.00	0.158	9.40	4.00
ATOM	888	HA	HIS	163S	-8.021	9.196	0.103	1.00	0.00	0.053	0.00	0.00
ATOM	889	CB	HIS	163S	-7.777	8.910	-2.016	1.00	0.00	-0.106	12.77	4.00
ATOM	890	HB1	HIS	163S	-8.429	8.845	-2.887	1.00	0.00	0.053	0.00	0.00
ATOM	891	HB2	HIS	163S	-7.158	8.016	-1.932	1.00	0.00	0.053	0.00	0.00
ATOM	892	CG	HIS	163S	-6.861	10.075	-2.223	1.00	0.00	-0.050	7.26	0.60
ATOM	893	CD2	HIS	163S	-6.486	11.080	-1.395	1.00	0.00	-0.177	10.80	0.60
ATOM	894	HD2	HIS	163S	-6.822	11.232	-0.370	1.00	0.00	0.127	0.00	0.00
ATOM	895	ND1	HIS	163S	-6.183	10.284	-3.409	1.00	0.00	0.207	9.25	-17.40
ATOM	896	HD1	HIS	163S	-6.250	9.687	-4.246	1.00	0.00	0.393	0.00	0.00
ATOM	897	CE1	HIS	163S	-5.434	11.370	-3.302	1.00	0.00	-0.227	10.80	0.60
ATOM	898	HE1	HIS	163S	-4.789	11.780	-4.080	1.00	0.00	0.127	0.00	0.00
ATOM	899	NE2	HIS	163S	-5.601	11.872	-2.091	1.00	0.00	0.207	9.25	-17.40
ATOM	900	HE2	HIS	163S	-5.142	12.719	-1.727	1.00	0.00	0.393	0.00	0.00
ATOM	901	C	HIS	163S	-9.636	10.171	-0.896	1.00	0.00	0.396	9.82	4.00
ATOM	902	O	HIS	163S	-10.426	10.191	-1.846	1.00	0.00	-0.396	8.17	-17.40
ATOM	903	N	ILE	164	-9.625	11.102	0.063	1.00	0.00	-0.650	9.00	-17.40
ATOM	904	HN	ILE	164	-8.993	10.983	0.868	1.00	0.00	0.440	0.00	0.00
ATOM	905	CA	ILE	164	-10.485	12.285	0.002	1.00	0.00	0.158	9.40	4.00
ATOM	906	HA	ILE	164	-11.073	12.230	-0.913	1.00	0.00	0.053	0.00	0.00
ATOM	907	CB	ILE	164	-11.521	12.349	1.186	1.00	0.00	-0.053	9.40	4.00

ATOM	908	HB	ILE	164	-12.091	13.273	1.100	1.00	0.00	0.053	0.00	0.00
ATOM	909	CG2	ILE	164	-12.448	11.146	1.087	1.00	0.00	-0.159	16.15	4.00
ATOM	910	HG2	ILE	164	-13.171	11.176	1.901	1.00	0.00	0.053	0.00	0.00
ATOM	911	HG2	ILE	164	-12.974	11.169	0.132	1.00	0.00	0.053	0.00	0.00
ATOM	912	HG2	ILE	164	-11.862	10.229	1.156	1.00	0.00	0.053	0.00	0.00
ATOM	913	CG1	ILE	164	-10.807	12.397	2.542	1.00	0.00	-0.106	12.77	4.00
ATOM	914	HG1	ILE	164	-10.101	13.228	2.528	1.00	0.00	0.053	0.00	0.00
ATOM	915	HG1	ILE	164	-10.283	11.451	2.687	1.00	0.00	0.053	0.00	0.00
ATOM	916	CD1	ILE	164	-11.739	12.599	3.736	1.00	0.00	-0.159	16.15	4.00
ATOM	917	HD1	ILE	164	-11.153	12.621	4.655	1.00	0.00	0.053	0.00	0.00
ATOM	918	HD1	ILE	164	-12.274	13.541	3.624	1.00	0.00	0.053	0.00	0.00
ATOM	919	HD1	ILE	164	-12.454	11.778	3.781	1.00	0.00	0.053	0.00	0.00
ATOM	920	C	ILE	164	-9.592	13.522	-0.001	1.00	0.00	0.396	9.82	4.00
ATOM	921	O	ILE	164	-8.460	13.513	0.536	1.00	0.00	-0.396	8.17	-17.40
ATOM	922	N	ARG	165G	-10.093	14.586	-0.616	1.00	0.00	-0.650	9.00	-17.40
ATOM	923	HN	ARG	165G	-11.049	14.549	-0.996	1.00	0.00	0.440	0.00	0.00
ATOM	924	CA	ARG	165G	-9.310	15.801	-0.761	1.00	0.00	0.158	9.40	4.00
ATOM	925	HA	ARG	165G	-8.359	15.658	-0.247	1.00	0.00	0.053	0.00	0.00
ATOM	926	CB	ARG	165G	-9.009	16.010	-2.246	1.00	0.00	-0.106	12.77	4.00
ATOM	927	HB1	ARG	165G	-8.288	16.810	-2.415	1.00	0.00	0.053	0.00	0.00
ATOM	928	HB2	ARG	165G	-9.899	16.271	-2.818	1.00	0.00	0.053	0.00	0.00
ATOM	929	CG	ARG	165G	-8.431	14.769	-2.898	1.00	0.00	-0.106	12.77	4.00
ATOM	930	HG1	ARG	165G	-9.118	13.924	-2.861	1.00	0.00	0.053	0.00	0.00
ATOM	931	HG2	ARG	165G	-7.509	14.440	-2.418	1.00	0.00	0.053	0.00	0.00
ATOM	932	CD	ARG	165G	-8.098	14.990	-4.363	1.00	0.00	0.374	12.77	4.00
ATOM	933	HD1	ARG	165G	-7.201	15.599	-4.480	1.00	0.00	0.053	0.00	0.00
ATOM	934	HD2	ARG	165G	-8.909	15.498	-4.883	1.00	0.00	0.053	0.00	0.00
ATOM	935	NE	ARG	165G	-7.860	13.721	-5.054	1.00	0.00	-0.819	9.00	-24.67
ATOM	936	HE	ARG	165G	-8.424	12.907	-4.770	1.00	0.00	0.407	0.00	0.00
ATOM	937	CZ	ARG	165G	-6.963	13.544	-6.026	1.00	0.00	0.796	6.95	4.00
ATOM	938	NH1	ARG	165G	-6.202	14.555	-6.433	1.00	0.00	-0.746	9.00	-24.67
ATOM	939	HH1	ARG	165G	-5.511	14.410	-7.184	1.00	0.00	0.407	0.00	0.00
ATOM	940	HH1	ARG	165G	-6.302	15.483	-5.998	1.00	0.00	0.407	0.00	0.00
ATOM	941	NH2	ARG	165G	-6.827	12.352	-6.598	1.00	0.00	-0.746	9.00	-24.67
ATOM	942	HH2	ARG	165G	-6.134	12.216	-7.349	1.00	0.00	0.407	0.00	0.00
ATOM	943	HH2	ARG	165G	-7.414	11.563	-6.291	1.00	0.00	0.407	0.00	0.00
ATOM	944	C	ARG	165G	-9.960	17.033	-0.186	1.00	0.00	0.396	9.82	4.00
ATOM	945	O	ARG	165G	-11.082	17.395	-0.562	1.00	0.00	-0.396	8.17	-17.40
ATOM	946	N	GLN	166	-9.244	17.672	0.735	1.00	0.00	-0.650	9.00	-17.40
ATOM	947	HN	GLN	166	-8.322	17.294	0.998	1.00	0.00	0.440	0.00	0.00
ATOM	948	CA	GLN	166	-9.715	18.883	1.383	1.00	0.00	0.158	9.40	4.00
ATOM	949	HA	GLN	166	-10.586	18.683	2.007	1.00	0.00	0.053	0.00	0.00
ATOM	950	CB	GLN	166	-8.588	19.437	2.263	1.00	0.00	-0.106	12.77	4.00
ATOM	951	HB1	GLN	166	-7.898	19.988	1.624	1.00	0.00	0.053	0.00	0.00
ATOM	952	HB2	GLN	166	-8.084	18.596	2.739	1.00	0.00	0.053	0.00	0.00
ATOM	953	CG	GLN	166	-9.043	20.376	3.360	1.00	0.00	-0.106	12.77	4.00
ATOM	954	HG1	GLN	166	-8.295	20.469	4.147	1.00	0.00	0.053	0.00	0.00
ATOM	955	HG2	GLN	166	-9.963	20.030	3.830	1.00	0.00	0.053	0.00	0.00
ATOM	956	CD	GLN	166	-9.308	21.767	2.832	1.00	0.00	0.396	9.82	4.00
ATOM	957	OE1	GLN	166	-10.463	22.202	2.684	1.00	0.00	-0.396	8.17	-17.40
ATOM	958	NE2	GLN	166	-8.231	22.478	2.527	1.00	0.00	-0.879	13.25	-17.40
ATOM	959	HE2	GLN	166	-7.292	22.076	2.666	1.00	0.00	0.440	0.00	0.00
ATOM	960	HE2	GLN	166	-8.332	23.431	2.150	1.00	0.00	0.440	0.00	0.00
ATOM	961	C	GLN	166	-10.054	19.791	0.188	1.00	0.00	0.396	9.82	4.00
ATOM	962	O	GLN	166	-9.222	20.026	-0.679	1.00	0.00	-0.396	8.17	-17.40
ATOM	963	N	PRO	167	-11.292	20.298	0.127	1.00	0.00	-0.422	9.00	-17.40
ATOM	964	CD	PRO	167	-12.390	20.081	1.089	1.00	0.00	0.105	12.77	4.00
ATOM	965	HD1	PRO	167	-12.094	20.372	2.096	1.00	0.00	0.053	0.00	0.00
ATOM	966	HD2	PRO	167	-12.684	19.032	1.120	1.00	0.00	0.053	0.00	0.00
ATOM	967	CA	PRO	167	-11.721	21.150	-0.988	1.00	0.00	0.158	9.40	4.00
ATOM	968	HA	PRO	167	-11.343	20.681	-1.897	1.00	0.00	0.053	0.00	0.00
ATOM	969	CB	PRO	167	-13.240	21.006	-0.947	1.00	0.00	-0.106	12.77	4.00
ATOM	970	HB1	PRO	167	-13.568	20.095	-1.449	1.00	0.00	0.053	0.00	0.00
ATOM	971	HB2	PRO	167	-13.733	21.844	-1.438	1.00	0.00	0.053	0.00	0.00
ATOM	972	CG	PRO	167	-13.502	20.972	0.538	1.00	0.00	-0.106	12.77	4.00
ATOM	973	HG1	PRO	167	-14.488	20.558	0.749	1.00	0.00	0.053	0.00	0.00
ATOM	974	HG2	PRO	167	-13.458	21.974	0.963	1.00	0.00	0.053	0.00	0.00
ATOM	975	C	PRO	167	-11.297	22.606	-1.090	1.00	0.00	0.396	9.82	4.00
ATOM	976	O	PRO	167	-11.373	23.181	-2.176	1.00	0.00	-0.396	8.17	-17.40
ATOM	977	N	ASP	168P	-10.836	23.207	0.001	1.00	0.00	-0.650	9.00	-17.40
ATOM	978	HN	ASP	168P	-10.731	22.670	0.874	1.00	0.00	0.440	0.00	0.00
ATOM	979	CA	ASP	168P	-10.476	24.624	-0.026	1.00	0.00	0.158	9.40	4.00
ATOM	980	HA	ASP	168P	-10.814	25.137	-0.927	1.00	0.00	0.053	0.00	0.00
ATOM	981	CB	ASP	168P	-11.169	25.325	1.147	1.00	0.00	-0.336	12.77	4.00
ATOM	982	HB1	ASP	168P	-10.700	25.098	2.104	1.00	0.00	0.053	0.00	0.00
ATOM	983	HB2	ASP	168P	-12.216	25.039	1.245	1.00	0.00	0.053	0.00	0.00

ATOM	984	CG	ASP	168P	-11.153	26.828	1.015	1.00	0.00	0.297	9.82	4.00
ATOM	985	OD1	ASP	168P	-10.592	27.312	0.018	1.00	0.00	-0.534	8.17	-18.95
ATOM	986	OD2	ASP	168P	-11.699	27.521	1.904	1.00	0.00	-0.534	8.17	-18.95
ATOM	987	C	ASP	168P	-8.975	24.865	0.035	1.00	0.00	0.396	9.82	4.00
ATOM	988	O	ASP	168P	-8.380	24.809	1.104	1.00	0.00	-0.396	8.17	-17.40
ATOM	989	N	LEU	169	-8.359	25.140	-1.108	1.00	0.00	-0.650	9.00	-17.40
ATOM	990	HN	LEU	169	-8.903	25.196	-1.981	1.00	0.00	0.440	0.00	0.00
ATOM	991	CA	LEU	169	-6.920	25.362	-1.139	1.00	0.00	0.158	9.40	4.00
ATOM	992	HA	LEU	169	-6.480	24.861	-0.277	1.00	0.00	0.053	0.00	0.00
ATOM	993	CB	LEU	169	-6.319	24.682	-2.373	1.00	0.00	-0.106	12.77	4.00
ATOM	994	HB1	LEU	169	-5.242	24.849	-2.410	1.00	0.00	0.053	0.00	0.00
ATOM	995	HB2	LEU	169	-6.765	25.085	-3.282	1.00	0.00	0.053	0.00	0.00
ATOM	996	CG	LEU	169	-6.581	23.165	-2.327	1.00	0.00	-0.053	9.40	4.00
ATOM	997	HG	LEU	169	-7.643	22.948	-2.436	1.00	0.00	0.053	0.00	0.00
ATOM	998	CD1	LEU	169	-5.842	22.450	-3.447	1.00	0.00	-0.159	16.15	4.00
ATOM	999	HD1	LEU	169	-6.044	21.380	-3.392	1.00	0.00	0.053	0.00	0.00
ATOM	1000	HD1	LEU	169	-6.180	22.833	-4.410	1.00	0.00	0.053	0.00	0.00
ATOM	1001	HD1	LEU	169	-4.770	22.622	-3.345	1.00	0.00	0.053	0.00	0.00
ATOM	1002	CD2	LEU	169	-6.133	22.623	-0.963	1.00	0.00	-0.159	16.15	4.00
ATOM	1003	HD2	LEU	169	-6.314	21.549	-0.921	1.00	0.00	0.053	0.00	0.00
ATOM	1004	HD2	LEU	169	-5.069	22.816	-0.826	1.00	0.00	0.053	0.00	0.00
ATOM	1005	HD2	LEU	169	-6.696	23.117	-0.172	1.00	0.00	0.053	0.00	0.00
ATOM	1006	C	LEU	169	-6.498	26.826	-1.084	1.00	0.00	0.396	9.82	4.00
ATOM	1007	O	LEU	169	-5.325	27.146	-1.275	1.00	0.00	-0.396	8.17	-17.40
ATOM	1008	N	SER	170	-7.443	27.710	-0.796	1.00	0.00	-0.650	9.00	-17.40
ATOM	1009	HN	SER	170	-8.403	27.388	-0.610	1.00	0.00	0.440	0.00	0.00
ATOM	1010	CA	SER	170	-7.135	29.133	-0.741	1.00	0.00	0.158	9.40	4.00
ATOM	1011	HA	SER	170	-6.692	29.487	-1.672	1.00	0.00	0.053	0.00	0.00
ATOM	1012	CB	SER	170	-8.418	29.934	-0.502	1.00	0.00	0.007	12.77	4.00
ATOM	1013	HB1	SER	170	-9.184	29.624	-1.213	1.00	0.00	0.053	0.00	0.00
ATOM	1014	HB2	SER	170	-8.218	30.997	-0.632	1.00	0.00	0.053	0.00	0.00
ATOM	1015	OG	SER	170	-8.888	29.706	0.817	1.00	0.00	-0.537	11.04	-17.40
ATOM	1016	HG	SER	170	-9.157	30.602	1.245	1.00	0.00	0.424	0.00	0.00
ATOM	1017	C	SER	170	-6.148	29.456	0.374	1.00	0.00	0.396	9.82	4.00
ATOM	1018	O	SER	170	-5.988	28.686	1.318	1.00	0.00	-0.396	8.17	-17.40
ATOM	1019	N	ASN	171	-5.475	30.598	0.262	1.00	0.00	-0.650	9.00	-17.40
ATOM	1020	HN	ASN	171	-5.604	31.187	-0.572	1.00	0.00	0.440	0.00	0.00
ATOM	1021	CA	ASN	171	-4.556	31.021	1.310	1.00	0.00	0.158	9.40	4.00
ATOM	1022	HA	ASN	171	-3.983	30.134	1.583	1.00	0.00	0.053	0.00	0.00
ATOM	1023	CB	ASN	171	-3.624	32.138	0.837	1.00	0.00	-0.106	12.77	4.00
ATOM	1024	HB1	ASN	171	-3.157	32.671	1.665	1.00	0.00	0.053	0.00	0.00
ATOM	1025	HB2	ASN	171	-4.142	32.890	0.242	1.00	0.00	0.053	0.00	0.00
ATOM	1026	CG	ASN	171	-2.491	31.622	-0.025	1.00	0.00	0.396	9.82	4.00
ATOM	1027	OD1	ASN	171	-1.953	30.530	0.210	1.00	0.00	-0.396	8.17	-17.40
ATOM	1028	ND2	ASN	171	-2.107	32.408	-1.021	1.00	0.00	-0.879	13.25	-17.40
ATOM	1029	HD2	ASN	171	-2.583	33.307	-1.181	1.00	0.00	0.440	0.00	0.00
ATOM	1030	HD2	ASN	171	-1.332	32.119	-1.636	1.00	0.00	0.440	0.00	0.00
ATOM	1031	C	ASN	171	-5.421	31.530	2.442	1.00	0.00	0.396	9.82	4.00
ATOM	1032	O	ASN	171	-6.560	31.971	2.234	1.00	0.00	-0.396	8.17	-17.40
ATOM	1033	N	ILE	172	-4.883	31.483	3.648	1.00	0.00	-0.650	9.00	-17.40
ATOM	1034	HN	ILE	172	-3.917	31.143	3.766	1.00	0.00	0.440	0.00	0.00
ATOM	1035	CA	ILE	172	-5.643	31.906	4.800	1.00	0.00	0.158	9.40	4.00
ATOM	1036	HA	ILE	172	-6.697	32.048	4.565	1.00	0.00	0.053	0.00	0.00
ATOM	1037	CB	ILE	172	-5.617	30.799	5.879	1.00	0.00	-0.053	9.40	4.00
ATOM	1038	HB	ILE	172	-4.592	30.578	6.180	1.00	0.00	0.053	0.00	0.00
ATOM	1039	CG2	ILE	172	-6.390	31.232	7.110	1.00	0.00	-0.159	16.15	4.00
ATOM	1040	HG2	ILE	172	-6.359	30.438	7.856	1.00	0.00	0.053	0.00	0.00
ATOM	1041	HG2	ILE	172	-5.941	32.135	7.522	1.00	0.00	0.053	0.00	0.00
ATOM	1042	HG2	ILE	172	-7.425	31.433	6.837	1.00	0.00	0.053	0.00	0.00
ATOM	1043	CG1	ILE	172	-6.237	29.522	5.301	1.00	0.00	-0.106	12.77	4.00
ATOM	1044	HG1	ILE	172	-5.613	29.180	4.475	1.00	0.00	0.053	0.00	0.00
ATOM	1045	HG1	ILE	172	-7.241	29.756	4.949	1.00	0.00	0.053	0.00	0.00
ATOM	1046	CD1	ILE	172	-6.348	28.389	6.295	1.00	0.00	-0.159	16.15	4.00
ATOM	1047	HD1	ILE	172	-6.796	27.521	5.809	1.00	0.00	0.053	0.00	0.00
ATOM	1048	HD1	ILE	172	-5.355	28.127	6.661	1.00	0.00	0.053	0.00	0.00
ATOM	1049	HD1	ILE	172	-6.973	28.699	7.132	1.00	0.00	0.053	0.00	0.00
ATOM	1050	C	ILE	172	-5.138	33.226	5.366	1.00	0.00	0.396	9.82	4.00
ATOM	1051	O	ILE	172	-3.928	33.433	5.492	1.00	0.00	-0.396	8.17	-17.40
ATOM	1052	N	ALA	173	-6.074	34.121	5.680	1.00	0.00	-0.650	9.00	-17.40
ATOM	1053	HN	ALA	173	-7.064	33.888	5.518	1.00	0.00	0.440	0.00	0.00
ATOM	1054	CA	ALA	173	-5.733	35.423	6.247	1.00	0.00	0.158	9.40	4.00
ATOM	1055	HA	ALA	173	-4.862	35.813	5.719	1.00	0.00	0.053	0.00	0.00
ATOM	1056	CB	ALA	173	-6.900	36.401	6.073	1.00	0.00	-0.159	16.15	4.00
ATOM	1057	HB1	ALA	173	-6.631	37.367	6.500	1.00	0.00	0.053	0.00	0.00
ATOM	1058	HB2	ALA	173	-7.118	36.521	5.012	1.00	0.00	0.053	0.00	0.00
ATOM	1059	HB3	ALA	173	-7.780	36.010	6.583	1.00	0.00	0.053	0.00	0.00

ATOM	1060	C	ALA	173	-5.418	35.239	7.730	1.00	0.00	0.396	9.82	4.00
ATOM	1061	O	ALA	173	-6.314	35.005	8.537	1.00	0.00	-0.396	8.17	-17.40
ATOM	1062	N	VAL	174	-4.144	35.360	8.084	1.00	0.00	-0.650	9.00	-17.40
ATOM	1063	HN	VAL	174	-3.440	35.574	7.363	1.00	0.00	0.440	0.00	0.00
ATOM	1064	CA	VAL	174	-3.719	35.197	9.463	1.00	0.00	0.158	9.40	4.00
ATOM	1065	HA	VAL	174	-4.308	34.454	10.001	1.00	0.00	0.053	0.00	0.00
ATOM	1066	CB	VAL	174	-2.251	34.687	9.506	1.00	0.00	-0.053	9.40	4.00
ATOM	1067	HB	VAL	174	-1.938	34.530	10.538	1.00	0.00	0.053	0.00	0.00
ATOM	1068	CG1	VAL	174	-2.131	33.361	8.746	1.00	0.00	-0.159	16.15	4.00
ATOM	1069	HG1	VAL	174	-1.098	33.012	8.782	1.00	0.00	0.053	0.00	0.00
ATOM	1070	HG1	VAL	174	-2.781	32.617	9.207	1.00	0.00	0.053	0.00	0.00
ATOM	1071	HG1	VAL	174	-2.427	33.508	7.707	1.00	0.00	0.053	0.00	0.00
ATOM	1072	CG2	VAL	174	-1.323	35.736	8.872	1.00	0.00	-0.159	16.15	4.00
ATOM	1073	HG2	VAL	174	-0.294	35.377	8.902	1.00	0.00	0.053	0.00	0.00
ATOM	1074	HG2	VAL	174	-1.617	35.904	7.836	1.00	0.00	0.053	0.00	0.00
ATOM	1075	HG2	VAL	174	-1.398	36.671	9.427	1.00	0.00	0.053	0.00	0.00
ATOM	1076	C	VAL	174	-3.829	36.495	10.276	1.00	0.00	0.396	9.82	4.00
ATOM	1077	O	VAL	174	-3.933	37.586	9.726	1.00	0.00	-0.396	8.17	-17.40
ATOM	1078	N	GLN	175	-3.838	36.362	11.599	1.00	0.00	-0.650	9.00	-17.40
ATOM	1079	HN	GLN	175	-3.807	35.421	12.017	1.00	0.00	0.440	0.00	0.00
ATOM	1080	CA	GLN	175	-3.890	37.528	12.457	1.00	0.00	0.158	9.40	4.00
ATOM	1081	HA	GLN	175	-4.675	38.180	12.074	1.00	0.00	0.053	0.00	0.00
ATOM	1082	CB	GLN	175	-4.268	37.105	13.879	1.00	0.00	-0.106	12.77	4.00
ATOM	1083	HB1	GLN	175	-4.052	37.881	14.613	1.00	0.00	0.053	0.00	0.00
ATOM	1084	HB2	GLN	175	-3.729	36.214	14.203	1.00	0.00	0.053	0.00	0.00
ATOM	1085	CG	GLN	175	-5.753	36.784	14.013	1.00	0.00	-0.106	12.77	4.00
ATOM	1086	HG1	GLN	175	-5.977	36.337	14.981	1.00	0.00	0.053	0.00	0.00
ATOM	1087	HG2	GLN	175	-6.079	36.082	13.245	1.00	0.00	0.053	0.00	0.00
ATOM	1088	CD	GLN	175	-6.605	38.035	13.879	1.00	0.00	0.396	9.82	4.00
ATOM	1089	OE1	GLN	175	-6.458	38.968	14.659	1.00	0.00	-0.396	8.17	-17.40
ATOM	1090	NE2	GLN	175	-7.493	38.062	12.884	1.00	0.00	-0.879	13.25	-17.40
ATOM	1091	HE2	GLN	175	-7.582	37.253	12.251	1.00	0.00	0.440	0.00	0.00
ATOM	1092	HE2	GLN	175	-8.089	38.890	12.748	1.00	0.00	0.440	0.00	0.00
ATOM	1093	C	GLN	175	-2.520	38.206	12.393	1.00	0.00	0.396	9.82	4.00
ATOM	1094	O	GLN	175	-1.539	37.589	11.953	1.00	0.00	-0.396	8.17	-17.40
ATOM	1095	N	PRO	176	-2.428	39.476	12.828	1.00	0.00	-0.422	9.00	-17.40
ATOM	1096	CD	PRO	176	-3.486	40.256	13.488	1.00	0.00	0.105	12.77	4.00
ATOM	1097	HD1	PRO	176	-3.544	40.029	14.552	1.00	0.00	0.053	0.00	0.00
ATOM	1098	HD2	PRO	176	-4.464	40.046	13.056	1.00	0.00	0.053	0.00	0.00
ATOM	1099	CA	PRO	176	-1.171	40.242	12.802	1.00	0.00	0.158	9.40	4.00
ATOM	1100	HA	PRO	176	-0.905	40.404	11.757	1.00	0.00	0.053	0.00	0.00
ATOM	1101	CB	PRO	176	-1.551	41.569	13.464	1.00	0.00	-0.106	12.77	4.00
ATOM	1102	HB1	PRO	176	-1.011	42.400	13.011	1.00	0.00	0.053	0.00	0.00
ATOM	1103	HB2	PRO	176	-1.315	41.556	14.528	1.00	0.00	0.053	0.00	0.00
ATOM	1104	CG	PRO	176	-3.029	41.668	13.223	1.00	0.00	-0.106	12.77	4.00
ATOM	1105	HG1	PRO	176	-3.244	41.988	12.203	1.00	0.00	0.053	0.00	0.00
ATOM	1106	HG2	PRO	176	-3.494	42.386	13.897	1.00	0.00	0.053	0.00	0.00
ATOM	1107	C	PRO	176	0.041	39.606	13.467	1.00	0.00	0.396	9.82	4.00
ATOM	1108	O	PRO	176	1.171	39.912	13.113	1.00	0.00	-0.396	8.17	-17.40
ATOM	1109	N	ASP	177P	-0.183	38.727	14.435	1.00	0.00	-0.650	9.00	-17.40
ATOM	1110	HN	ASP	177P	-1.150	38.495	14.700	1.00	0.00	0.440	0.00	0.00
ATOM	1111	CA	ASP	177P	0.926	38.088	15.124	1.00	0.00	0.158	9.40	4.00
ATOM	1112	HA	ASP	177P	1.773	38.773	15.121	1.00	0.00	0.053	0.00	0.00
ATOM	1113	CB	ASP	177P	0.540	37.847	16.597	1.00	0.00	-0.336	12.77	4.00
ATOM	1114	HB1	ASP	177P	0.315	38.764	17.141	1.00	0.00	0.053	0.00	0.00
ATOM	1115	HB2	ASP	177P	1.322	37.354	17.174	1.00	0.00	0.053	0.00	0.00
ATOM	1116	CG	ASP	177P	-0.706	36.961	16.764	1.00	0.00	0.297	9.82	4.00
ATOM	1117	OD1	ASP	177P	-1.616	36.976	15.890	1.00	0.00	-0.534	8.17	-18.95
ATOM	1118	OD2	ASP	177P	-0.789	36.255	17.799	1.00	0.00	-0.534	8.17	-18.95
ATOM	1119	C	ASP	177P	1.382	36.774	14.479	1.00	0.00	0.396	9.82	4.00
ATOM	1120	O	ASP	177P	2.361	36.173	14.918	1.00	0.00	-0.396	8.17	-17.40
ATOM	1121	N	HIS	178S	0.713	36.358	13.405	1.00	0.00	-0.650	9.00	-17.40
ATOM	1122	HN	HIS	178S	-0.024	36.953	13.001	1.00	0.00	0.440	0.00	0.00
ATOM	1123	CA	HIS	178S	1.014	35.062	12.791	1.00	0.00	0.158	9.40	4.00
ATOM	1124	HA	HIS	178S	1.804	34.605	13.387	1.00	0.00	0.053	0.00	0.00
ATOM	1125	CB	HIS	178S	-0.218	34.167	12.927	1.00	0.00	-0.106	12.77	4.00
ATOM	1126	HB1	HIS	178S	-0.023	33.231	12.402	1.00	0.00	0.053	0.00	0.00
ATOM	1127	HB2	HIS	178S	-1.069	34.683	12.483	1.00	0.00	0.053	0.00	0.00
ATOM	1128	CG	HIS	178S	-0.573	33.832	14.347	1.00	0.00	-0.050	7.26	0.60
ATOM	1129	CD2	HIS	178S	0.199	33.688	15.450	1.00	0.00	-0.177	10.80	0.60
ATOM	1130	HD2	HIS	178S	1.275	33.847	15.512	1.00	0.00	0.127	0.00	0.00
ATOM	1131	ND1	HIS	178S	-1.861	33.535	14.740	1.00	0.00	0.207	9.25	-17.40
ATOM	1132	HD1	HIS	178S	-2.689	33.556	14.129	1.00	0.00	0.393	0.00	0.00
ATOM	1133	CE1	HIS	178S	-1.866	33.219	16.023	1.00	0.00	-0.227	10.80	0.60
ATOM	1134	HE1	HIS	178S	-2.741	32.936	16.607	1.00	0.00	0.127	0.00	0.00
ATOM	1135	NE2	HIS	178S	-0.629	33.304	16.476	1.00	0.00	0.207	9.25	-17.40

ATOM	1136	HE2	HIS	178S	-0.332	33.112	17.443	1.00	0.00	0.393	0.00	0.00
ATOM	1137	C	HIS	178S	1.499	34.998	11.347	1.00	0.00	0.396	9.82	4.00
ATOM	1138	O	HIS	178S	1.307	33.986	10.675	1.00	0.00	-0.396	8.17	-17.40
ATOM	1139	N	ARG	179G	2.150	36.048	10.875	1.00	0.00	-0.650	9.00	-17.40
ATOM	1140	HN	ARG	179G	2.309	36.862	11.484	1.00	0.00	0.440	0.00	0.00
ATOM	1141	CA	ARG	179G	2.649	36.069	9.495	1.00	0.00	0.158	9.40	4.00
ATOM	1142	HA	ARG	179G	1.838	36.125	8.768	1.00	0.00	0.053	0.00	0.00
ATOM	1143	CB	ARG	179G	3.523	37.309	9.274	1.00	0.00	-0.106	12.77	4.00
ATOM	1144	HB1	ARG	179G	4.558	36.985	9.168	1.00	0.00	0.053	0.00	0.00
ATOM	1145	HB2	ARG	179G	3.414	37.965	10.137	1.00	0.00	0.053	0.00	0.00
ATOM	1146	CG	ARG	179G	3.154	38.110	8.029	1.00	0.00	-0.106	12.77	4.00
ATOM	1147	HG1	ARG	179G	3.136	37.499	7.126	1.00	0.00	0.053	0.00	0.00
ATOM	1148	HG2	ARG	179G	3.851	38.923	7.830	1.00	0.00	0.053	0.00	0.00
ATOM	1149	CD	ARG	179G	1.761	38.759	8.131	1.00	0.00	0.374	12.77	4.00
ATOM	1150	HD1	ARG	179G	0.986	38.053	8.431	1.00	0.00	0.053	0.00	0.00
ATOM	1151	HD2	ARG	179G	1.423	39.188	7.187	1.00	0.00	0.053	0.00	0.00
ATOM	1152	NE	ARG	179G	1.711	39.851	9.110	1.00	0.00	-0.819	9.00	-24.67
ATOM	1153	HE	ARG	179G	2.547	40.019	9.686	1.00	0.00	0.407	0.00	0.00
ATOM	1154	CZ	ARG	179G	0.652	40.640	9.302	1.00	0.00	0.796	6.95	4.00
ATOM	1155	NH1	ARG	179G	-0.453	40.463	8.586	1.00	0.00	-0.746	9.00	-24.67
ATOM	1156	HH1	ARG	179G	-1.268	41.074	8.737	1.00	0.00	0.407	0.00	0.00
ATOM	1157	HH1	ARG	179G	-0.494	39.714	7.879	1.00	0.00	0.407	0.00	0.00
ATOM	1158	NH2	ARG	179G	0.700	41.617	10.202	1.00	0.00	-0.746	9.00	-24.67
ATOM	1159	HH2	ARG	179G	-0.119	42.223	10.347	1.00	0.00	0.407	0.00	0.00
ATOM	1160	HH2	ARG	179G	1.556	41.767	10.754	1.00	0.00	0.407	0.00	0.00
ATOM	1161	C	ARG	179G	3.459	34.813	9.159	1.00	0.00	0.396	9.82	4.00
ATOM	1162	O	ARG	179G	3.307	34.225	8.086	1.00	0.00	-0.396	8.17	-17.40
ATOM	1163	N	LYS	180S	4.311	34.405	10.086	1.00	0.00	-0.650	9.00	-17.40
ATOM	1164	HN	LYS	180S	4.378	34.926	10.971	1.00	0.00	0.440	0.00	0.00
ATOM	1165	CA	LYS	180S	5.155	33.235	9.882	1.00	0.00	0.158	9.40	4.00
ATOM	1166	HA	LYS	180S	5.464	33.216	8.837	1.00	0.00	0.053	0.00	0.00
ATOM	1167	CB	LYS	180S	6.416	33.362	10.750	1.00	0.00	-0.106	12.77	4.00
ATOM	1168	HB1	LYS	180S	7.182	32.632	10.489	1.00	0.00	0.053	0.00	0.00
ATOM	1169	HB2	LYS	180S	6.212	33.218	11.811	1.00	0.00	0.053	0.00	0.00
ATOM	1170	CG	LYS	180S	7.080	34.732	10.629	1.00	0.00	-0.106	12.77	4.00
ATOM	1171	HG1	LYS	180S	6.546	35.524	11.154	1.00	0.00	0.053	0.00	0.00
ATOM	1172	HG2	LYS	180S	7.169	35.085	9.602	1.00	0.00	0.053	0.00	0.00
ATOM	1173	CD	LYS	180S	8.496	34.776	11.185	1.00	0.00	-0.106	12.77	4.00
ATOM	1174	HD1	LYS	180S	8.950	35.761	11.087	1.00	0.00	0.053	0.00	0.00
ATOM	1175	HD2	LYS	180S	9.163	34.078	10.679	1.00	0.00	0.053	0.00	0.00
ATOM	1176	CE	LYS	180S	8.550	34.426	12.655	1.00	0.00	0.099	12.77	4.00
ATOM	1177	HE1	LYS	180S	7.859	35.056	13.216	1.00	0.00	0.053	0.00	0.00
ATOM	1178	HE2	LYS	180S	9.558	34.579	13.040	1.00	0.00	0.053	0.00	0.00
ATOM	1179	NZ	LYS	180S	8.171	33.002	12.856	1.00	0.00	-0.045	13.25	-39.20
ATOM	1180	HZ1	LYS	180S	8.210	32.773	13.859	1.00	0.00	0.280	0.00	0.00
ATOM	1181	HZ2	LYS	180S	7.214	32.848	12.507	1.00	0.00	0.280	0.00	0.00
ATOM	1182	HZ3	LYS	180S	8.825	32.396	12.340	1.00	0.00	0.280	0.00	0.00
ATOM	1183	C	LYS	180S	4.477	31.896	10.185	1.00	0.00	0.396	9.82	4.00
ATOM	1184	O	LYS	180S	5.102	30.850	10.068	1.00	0.00	-0.396	8.17	-17.40
ATOM	1185	N	PHE	181	3.197	31.904	10.529	1.00	0.00	-0.650	9.00	-17.40
ATOM	1186	HN	PHE	181	2.662	32.784	10.536	1.00	0.00	0.440	0.00	0.00
ATOM	1187	CA	PHE	181	2.558	30.649	10.896	1.00	0.00	0.158	9.40	4.00
ATOM	1188	HA	PHE	181	3.295	29.855	10.772	1.00	0.00	0.053	0.00	0.00
ATOM	1189	CB	PHE	181	2.205	30.680	12.387	1.00	0.00	-0.106	12.77	4.00
ATOM	1190	HB1	PHE	181	1.815	29.734	12.763	1.00	0.00	0.053	0.00	0.00
ATOM	1191	HB2	PHE	181	1.445	31.419	12.640	1.00	0.00	0.053	0.00	0.00
ATOM	1192	CG	PHE	181	3.377	31.003	13.279	1.00	0.00	0.000	7.26	0.60
ATOM	1193	CD1	PHE	181	3.570	32.292	13.762	1.00	0.00	-0.127	10.80	0.60
ATOM	1194	HD1	PHE	181	2.846	33.070	13.520	1.00	0.00	0.127	0.00	0.00
ATOM	1195	CD2	PHE	181	4.313	30.023	13.603	1.00	0.00	-0.127	10.80	0.60
ATOM	1196	HD2	PHE	181	4.176	29.005	13.235	1.00	0.00	0.127	0.00	0.00
ATOM	1197	CE1	PHE	181	4.675	32.602	14.550	1.00	0.00	-0.127	10.80	0.60
ATOM	1198	HE1	PHE	181	4.811	33.617	14.920	1.00	0.00	0.127	0.00	0.00
ATOM	1199	CE2	PHE	181	5.422	30.327	14.391	1.00	0.00	-0.127	10.80	0.60
ATOM	1200	HE2	PHE	181	6.147	29.551	14.636	1.00	0.00	0.127	0.00	0.00
ATOM	1201	CZ	PHE	181	5.600	31.622	14.863	1.00	0.00	-0.127	10.80	0.60
ATOM	1202	HZ	PHE	181	6.466	31.864	15.478	1.00	0.00	0.127	0.00	0.00
ATOM	1203	C	PHE	181	1.334	30.235	10.096	1.00	0.00	0.396	9.82	4.00
ATOM	1204	O	PHE	181	0.460	29.562	10.625	1.00	0.00	-0.396	8.17	-17.40
ATOM	1205	N	GLN	182	1.264	30.615	8.822	1.00	0.00	-0.650	9.00	-17.40
ATOM	1206	HN	GLN	182	2.021	31.169	8.399	1.00	0.00	0.440	0.00	0.00
ATOM	1207	CA	GLN	182	0.104	30.235	8.040	1.00	0.00	0.158	9.40	4.00
ATOM	1208	HA	GLN	182	-0.821	30.603	8.483	1.00	0.00	0.053	0.00	0.00
ATOM	1209	CB	GLN	182	0.146	30.857	6.644	1.00	0.00	-0.106	12.77	4.00
ATOM	1210	HB1	GLN	182	0.969	30.447	6.058	1.00	0.00	0.053	0.00	0.00
ATOM	1211	HB2	GLN	182	0.280	31.937	6.701	1.00	0.00	0.053	0.00	0.00

ATOM	1212	CG	GLN	182	-1.142	30.587	5.890	1.00	0.00	-0.106	12.77	4.00
ATOM	1213	HG1	GLN	182	-2.034	30.729	6.499	1.00	0.00	0.053	0.00	0.00
ATOM	1214	HG2	GLN	182	-1.210	29.568	5.507	1.00	0.00	0.053	0.00	0.00
ATOM	1215	CD	GLN	182	-1.326	31.478	4.695	1.00	0.00	0.396	9.82	4.00
ATOM	1216	OE1	GLN	182	-2.264	31.298	3.924	1.00	0.00	-0.396	8.17	-17.40
ATOM	1217	NE2	GLN	182	-0.437	32.452	4.530	1.00	0.00	-0.879	13.25	-17.40
ATOM	1218	HE2	GLN	182	0.334	32.564	5.203	1.00	0.00	0.440	0.00	0.00
ATOM	1219	HE2	GLN	182	-0.519	33.094	3.728	1.00	0.00	0.440	0.00	0.00
ATOM	1220	C	GLN	182	-0.029	28.718	7.922	1.00	0.00	0.396	9.82	4.00
ATOM	1221	O	GLN	182	-1.139	28.206	7.789	1.00	0.00	-0.396	8.17	-17.40
ATOM	1222	N	GLY	183	1.094	27.998	7.955	1.00	0.00	-0.650	9.00	-17.40
ATOM	1223	HN	GLY	183	2.006	28.466	8.045	1.00	0.00	0.440	0.00	0.00
ATOM	1224	CA	GLY	183	1.022	26.551	7.863	1.00	0.00	0.105	9.40	4.00
ATOM	1225	HA1	GLY	183	2.007	26.099	7.978	1.00	0.00	0.053	0.00	0.00
ATOM	1226	HA2	GLY	183	0.624	26.237	6.898	1.00	0.00	0.053	0.00	0.00
ATOM	1227	C	GLY	183	0.120	25.976	8.945	1.00	0.00	0.396	9.82	4.00
ATOM	1228	O	GLY	183	-0.668	25.063	8.687	1.00	0.00	-0.396	8.17	-17.40
ATOM	1229	N	TYR	184	0.231	26.505	10.165	1.00	0.00	-0.650	9.00	-17.40
ATOM	1230	HN	TYR	184	0.909	27.262	10.329	1.00	0.00	0.440	0.00	0.00
ATOM	1231	CA	TYR	184	-0.599	26.023	11.276	1.00	0.00	0.158	9.40	4.00
ATOM	1232	HA	TYR	184	-0.501	24.950	11.442	1.00	0.00	0.053	0.00	0.00
ATOM	1233	CB	TYR	184	-0.156	26.659	12.593	1.00	0.00	-0.106	12.77	4.00
ATOM	1234	HB1	TYR	184	-0.796	26.364	13.424	1.00	0.00	0.053	0.00	0.00
ATOM	1235	HB2	TYR	184	-0.177	27.747	12.548	1.00	0.00	0.053	0.00	0.00
ATOM	1236	CG	TYR	184	1.251	26.265	12.965	1.00	0.00	0.000	7.26	0.60
ATOM	1237	CD1	TYR	184	2.330	27.088	12.651	1.00	0.00	-0.127	10.80	0.60
ATOM	1238	HD1	TYR	184	2.145	28.054	12.181	1.00	0.00	0.127	0.00	0.00
ATOM	1239	CE1	TYR	184	3.638	26.703	12.924	1.00	0.00	-0.127	10.80	0.60
ATOM	1240	HE1	TYR	184	4.468	27.364	12.675	1.00	0.00	0.127	0.00	0.00
ATOM	1241	CD2	TYR	184	1.510	25.040	13.566	1.00	0.00	-0.127	10.80	0.60
ATOM	1242	HD2	TYR	184	0.679	24.385	13.828	1.00	0.00	0.127	0.00	0.00
ATOM	1243	CE2	TYR	184	2.823	24.632	13.841	1.00	0.00	-0.127	10.80	0.60
ATOM	1244	HE2	TYR	184	3.012	23.664	14.306	1.00	0.00	0.127	0.00	0.00
ATOM	1245	CZ	TYR	184	3.879	25.471	13.516	1.00	0.00	0.026	7.26	0.60
ATOM	1246	OH	TYR	184	5.174	25.084	13.777	1.00	0.00	-0.451	10.94	-17.40
ATOM	1247	HH	TYR	184	5.224	24.663	14.715	1.00	0.00	0.424	0.00	0.00
ATOM	1248	C	TYR	184	-2.093	26.280	11.056	1.00	0.00	0.396	9.82	4.00
ATOM	1249	O	TYR	184	-2.936	25.521	11.555	1.00	0.00	-0.396	8.17	-17.40
ATOM	1250	N	TYR	185	-2.419	27.352	10.330	1.00	0.00	-0.650	9.00	-17.40
ATOM	1251	HN	TYR	185	-1.673	27.957	9.958	1.00	0.00	0.440	0.00	0.00
ATOM	1252	CA	TYR	185	-3.812	27.679	10.055	1.00	0.00	0.158	9.40	4.00
ATOM	1253	HA	TYR	185	-4.342	27.653	11.007	1.00	0.00	0.053	0.00	0.00
ATOM	1254	CB	TYR	185	-3.942	29.069	9.406	1.00	0.00	-0.106	12.77	4.00
ATOM	1255	HB1	TYR	185	-4.892	29.105	8.874	1.00	0.00	0.053	0.00	0.00
ATOM	1256	HB2	TYR	185	-3.107	29.199	8.717	1.00	0.00	0.053	0.00	0.00
ATOM	1257	CG	TYR	185	-3.919	30.246	10.375	1.00	0.00	0.000	7.26	0.60
ATOM	1258	CD1	TYR	185	-2.776	30.545	11.133	1.00	0.00	-0.127	10.80	0.60
ATOM	1259	HD1	TYR	185	-1.891	29.914	11.043	1.00	0.00	0.127	0.00	0.00
ATOM	1260	CE1	TYR	185	-2.755	31.638	12.000	1.00	0.00	-0.127	10.80	0.60
ATOM	1261	HE1	TYR	185	-1.860	31.859	12.581	1.00	0.00	0.127	0.00	0.00
ATOM	1262	CD2	TYR	185	-5.040	31.072	10.516	1.00	0.00	-0.127	10.80	0.60
ATOM	1263	HD2	TYR	185	-5.940	30.855	9.941	1.00	0.00	0.127	0.00	0.00
ATOM	1264	CE2	TYR	185	-5.025	32.167	11.378	1.00	0.00	-0.127	10.80	0.60
ATOM	1265	HE2	TYR	185	-5.904	32.803	11.471	1.00	0.00	0.127	0.00	0.00
ATOM	1266	CZ	TYR	185	-3.881	32.441	12.117	1.00	0.00	0.026	7.26	0.60
ATOM	1267	OH	TYR	185	-3.887	33.503	12.996	1.00	0.00	-0.451	10.94	-17.40
ATOM	1268	HH	TYR	185	-3.140	34.165	12.740	1.00	0.00	0.424	0.00	0.00
ATOM	1269	C	TYR	185	-4.340	26.623	9.086	1.00	0.00	0.396	9.82	4.00
ATOM	1270	O	TYR	185	-5.488	26.166	9.196	1.00	0.00	-0.396	8.17	-17.40
ATOM	1271	N	LYS	186S	-3.495	26.242	8.129	1.00	0.00	-0.650	9.00	-17.40
ATOM	1272	HN	LYS	186S	-2.554	26.660	8.089	1.00	0.00	0.440	0.00	0.00
ATOM	1273	CA	LYS	186S	-3.875	25.248	7.141	1.00	0.00	0.158	9.40	4.00
ATOM	1274	HA	LYS	186S	-4.802	25.533	6.644	1.00	0.00	0.053	0.00	0.00
ATOM	1275	CB	LYS	186S	-2.814	25.197	6.026	1.00	0.00	-0.106	12.77	4.00
ATOM	1276	HB1	LYS	186S	-3.021	24.388	5.324	1.00	0.00	0.053	0.00	0.00
ATOM	1277	HB2	LYS	186S	-1.818	25.032	6.439	1.00	0.00	0.053	0.00	0.00
ATOM	1278	CG	LYS	186S	-2.783	26.514	5.232	1.00	0.00	-0.106	12.77	4.00
ATOM	1279	HG1	LYS	186S	-2.438	27.306	5.895	1.00	0.00	0.053	0.00	0.00
ATOM	1280	HG2	LYS	186S	-3.791	26.724	4.876	1.00	0.00	0.053	0.00	0.00
ATOM	1281	CD	LYS	186S	-1.865	26.488	4.028	1.00	0.00	-0.106	12.77	4.00
ATOM	1282	HD1	LYS	186S	-2.089	25.613	3.417	1.00	0.00	0.053	0.00	0.00
ATOM	1283	HD2	LYS	186S	-0.828	26.439	4.361	1.00	0.00	0.053	0.00	0.00
ATOM	1284	CE	LYS	186S	-2.074	27.757	3.197	1.00	0.00	0.099	12.77	4.00
ATOM	1285	HE1	LYS	186S	-1.892	28.672	3.759	1.00	0.00	0.053	0.00	0.00
ATOM	1286	HE2	LYS	186S	-3.086	27.851	2.805	1.00	0.00	0.053	0.00	0.00
ATOM	1287	NZ	LYS	186S	-1.181	27.834	2.012	1.00	0.00	-0.045	13.25	-39.20

ATOM	1288	HZ1	LYS	186S	-1.368	28.705	1.496	1.00	0.00	0.280	0.00	0.00
ATOM	1289	HZ2	LYS	186S	-0.198	27.822	2.320	1.00	0.00	0.280	0.00	0.00
ATOM	1290	HZ3	LYS	186S	-1.356	27.026	1.396	1.00	0.00	0.280	0.00	0.00
ATOM	1291	C	LYS	186S	-4.085	23.889	7.798	1.00	0.00	0.396	9.82	4.00
ATOM	1292	O	LYS	186S	-5.029	23.162	7.441	1.00	0.00	-0.396	8.17	-17.40
ATOM	1293	N	ILE	187	-3.246	23.555	8.788	1.00	0.00	-0.650	9.00	-17.40
ATOM	1294	HN	ILE	187	-2.494	24.204	9.061	1.00	0.00	0.440	0.00	0.00
ATOM	1295	CA	ILE	187	-3.389	22.275	9.484	1.00	0.00	0.158	9.40	4.00
ATOM	1296	HA	ILE	187	-3.351	21.458	8.762	1.00	0.00	0.053	0.00	0.00
ATOM	1297	CB	ILE	187	-2.242	22.027	10.521	1.00	0.00	-0.053	9.40	4.00
ATOM	1298	HB	ILE	187	-2.157	22.882	11.191	1.00	0.00	0.053	0.00	0.00
ATOM	1299	CG2	ILE	187	-2.546	20.781	11.341	1.00	0.00	-0.159	16.15	4.00
ATOM	1300	HG2	ILE	187	-1.744	20.614	12.060	1.00	0.00	0.053	0.00	0.00
ATOM	1301	HG2	ILE	187	-3.488	20.916	11.872	1.00	0.00	0.053	0.00	0.00
ATOM	1302	HG2	ILE	187	-2.623	19.919	10.678	1.00	0.00	0.053	0.00	0.00
ATOM	1303	CG1	ILE	187	-0.900	21.861	9.797	1.00	0.00	-0.106	12.77	4.00
ATOM	1304	HG1	ILE	187	-0.750	22.728	9.154	1.00	0.00	0.053	0.00	0.00
ATOM	1305	HG1	ILE	187	-0.943	20.946	9.205	1.00	0.00	0.053	0.00	0.00
ATOM	1306	CD1	ILE	187	0.315	21.756	10.720	1.00	0.00	-0.159	16.15	4.00
ATOM	1307	HD1	ILE	187	1.218	21.641	10.121	1.00	0.00	0.053	0.00	0.00
ATOM	1308	HD1	ILE	187	0.392	22.660	11.323	1.00	0.00	0.053	0.00	0.00
ATOM	1309	HD1	ILE	187	0.201	20.891	11.374	1.00	0.00	0.053	0.00	0.00
ATOM	1310	C	ILE	187	-4.729	22.236	10.221	1.00	0.00	0.396	9.82	4.00
ATOM	1311	O	ILE	187	-5.483	21.258	10.116	1.00	0.00	-0.396	8.17	-17.40
ATOM	1312	N	ALA	188	-5.047	23.298	10.958	1.00	0.00	-0.650	9.00	-17.40
ATOM	1313	HN	ALA	188	-4.408	24.104	11.010	1.00	0.00	0.440	0.00	0.00
ATOM	1314	CA	ALA	188	-6.308	23.309	11.690	1.00	0.00	0.158	9.40	4.00
ATOM	1315	HA	ALA	188	-6.362	22.478	12.394	1.00	0.00	0.053	0.00	0.00
ATOM	1316	CB	ALA	188	-6.406	24.571	12.531	1.00	0.00	-0.159	16.15	4.00
ATOM	1317	HB1	ALA	188	-7.350	24.573	13.075	1.00	0.00	0.053	0.00	0.00
ATOM	1318	HB2	ALA	188	-5.578	24.601	13.240	1.00	0.00	0.053	0.00	0.00
ATOM	1319	HB3	ALA	188	-6.359	25.445	11.882	1.00	0.00	0.053	0.00	0.00
ATOM	1320	C	ALA	188	-7.498	23.192	10.742	1.00	0.00	0.396	9.82	4.00
ATOM	1321	O	ALA	188	-8.394	22.359	10.950	1.00	0.00	-0.396	8.17	-17.40
ATOM	1322	N	ARG	189G	-7.511	24.015	9.691	1.00	0.00	-0.650	9.00	-17.40
ATOM	1323	HN	ARG	189G	-6.749	24.697	9.569	1.00	0.00	0.440	0.00	0.00
ATOM	1324	CA	ARG	189G	-8.596	23.959	8.709	1.00	0.00	0.158	9.40	4.00
ATOM	1325	HA	ARG	189G	-9.537	24.250	9.173	1.00	0.00	0.053	0.00	0.00
ATOM	1326	CB	ARG	189G	-8.351	24.916	7.534	1.00	0.00	-0.106	12.77	4.00
ATOM	1327	HB1	ARG	189G	-7.335	24.844	7.144	1.00	0.00	0.053	0.00	0.00
ATOM	1328	HB2	ARG	189G	-8.501	25.959	7.809	1.00	0.00	0.053	0.00	0.00
ATOM	1329	CG	ARG	189G	-9.290	24.641	6.348	1.00	0.00	-0.106	12.77	4.00
ATOM	1330	HG1	ARG	189G	-10.334	24.653	6.658	1.00	0.00	0.053	0.00	0.00
ATOM	1331	HG2	ARG	189G	-9.091	23.666	5.902	1.00	0.00	0.053	0.00	0.00
ATOM	1332	CD	ARG	189G	-9.123	25.693	5.250	1.00	0.00	0.374	12.77	4.00
ATOM	1333	HD1	ARG	189G	-9.155	26.705	5.653	1.00	0.00	0.053	0.00	0.00
ATOM	1334	HD2	ARG	189G	-9.910	25.620	4.499	1.00	0.00	0.053	0.00	0.00
ATOM	1335	NE	ARG	189G	-7.848	25.548	4.553	1.00	0.00	-0.819	9.00	-24.67
ATOM	1336	HE	ARG	189G	-7.272	24.719	4.762	1.00	0.00	0.407	0.00	0.00
ATOM	1337	CZ	ARG	189G	-7.388	26.421	3.666	1.00	0.00	0.796	6.95	4.00
ATOM	1338	NH1	ARG	189G	-8.107	27.500	3.377	1.00	0.00	-0.746	9.00	-24.67
ATOM	1339	HH1	ARG	189G	-7.757	28.182	2.689	1.00	0.00	0.407	0.00	0.00
ATOM	1340	HH1	ARG	189G	-9.014	27.653	3.840	1.00	0.00	0.407	0.00	0.00
ATOM	1341	NH2	ARG	189G	-6.224	26.213	3.068	1.00	0.00	-0.746	9.00	-24.67
ATOM	1342	HH2	ARG	189G	-5.869	26.892	2.380	1.00	0.00	0.407	0.00	0.00
ATOM	1343	HH2	ARG	189G	-5.673	25.371	3.291	1.00	0.00	0.407	0.00	0.00
ATOM	1344	C	ARG	189G	-8.736	22.540	8.161	1.00	0.00	0.396	9.82	4.00
ATOM	1345	O	ARG	189G	-9.855	22.035	8.035	1.00	0.00	-0.396	8.17	-17.40
ATOM	1346	N	HIS	190S	-7.615	21.889	7.830	1.00	0.00	-0.650	9.00	-17.40
ATOM	1347	HN	HIS	190S	-6.700	22.348	7.940	1.00	0.00	0.440	0.00	0.00
ATOM	1348	CA	HIS	190S	-7.690	20.519	7.309	1.00	0.00	0.158	9.40	4.00
ATOM	1349	HA	HIS	190S	-8.325	20.459	6.425	1.00	0.00	0.053	0.00	0.00
ATOM	1350	CB	HIS	190S	-6.326	19.994	6.848	1.00	0.00	-0.106	12.77	4.00
ATOM	1351	HB1	HIS	190S	-5.620	19.848	7.666	1.00	0.00	0.053	0.00	0.00
ATOM	1352	HB2	HIS	190S	-5.821	20.659	6.147	1.00	0.00	0.053	0.00	0.00
ATOM	1353	CG	HIS	190S	-6.404	18.668	6.150	1.00	0.00	-0.050	7.26	0.60
ATOM	1354	CD2	HIS	190S	-7.456	18.007	5.602	1.00	0.00	-0.177	10.80	0.60
ATOM	1355	HD2	HIS	190S	-8.496	18.331	5.607	1.00	0.00	0.127	0.00	0.00
ATOM	1356	ND1	HIS	190S	-5.295	17.887	5.903	1.00	0.00	0.207	9.25	-17.40
ATOM	1357	HD1	HIS	190S	-4.332	18.112	6.193	1.00	0.00	0.393	0.00	0.00
ATOM	1358	CE1	HIS	190S	-5.657	16.804	5.236	1.00	0.00	-0.227	10.80	0.60
ATOM	1359	HE1	HIS	190S	-4.991	16.006	4.905	1.00	0.00	0.127	0.00	0.00
ATOM	1360	NE2	HIS	190S	-6.965	16.853	5.039	1.00	0.00	0.207	9.25	-17.40
ATOM	1361	HE2	HIS	190S	-7.523	16.142	4.544	1.00	0.00	0.393	0.00	0.00
ATOM	1362	C	HIS	190S	-8.264	19.553	8.345	1.00	0.00	0.396	9.82	4.00
ATOM	1363	O	HIS	190S	-9.140	18.744	8.017	1.00	0.00	-0.396	8.17	-17.40

ATOM	1364	N	TYR	191	-7.771	19.609	9.584	1.00	0.00	-0.650	9.00	-17.40
ATOM	1365	HN	TYR	191	-7.011	20.269	9.803	1.00	0.00	0.440	0.00	0.00
ATOM	1366	CA	TYR	191	-8.303	18.736	10.635	1.00	0.00	0.158	9.40	4.00
ATOM	1367	HA	TYR	191	-8.098	17.688	10.411	1.00	0.00	0.053	0.00	0.00
ATOM	1368	CB	TYR	191	-7.663	19.042	11.995	1.00	0.00	-0.106	12.77	4.00
ATOM	1369	HB1	TYR	191	-8.346	18.891	12.830	1.00	0.00	0.053	0.00	0.00
ATOM	1370	HB2	TYR	191	-7.314	20.071	12.079	1.00	0.00	0.053	0.00	0.00
ATOM	1371	CG	TYR	191	-6.469	18.183	12.286	1.00	0.00	0.000	7.26	0.60
ATOM	1372	CD1	TYR	191	-5.311	18.285	11.512	1.00	0.00	-0.127	10.80	0.60
ATOM	1373	HD1	TYR	191	-5.275	19.001	10.691	1.00	0.00	0.127	0.00	0.00
ATOM	1374	CE1	TYR	191	-4.206	17.490	11.771	1.00	0.00	-0.127	10.80	0.60
ATOM	1375	HE1	TYR	191	-3.308	17.578	11.158	1.00	0.00	0.127	0.00	0.00
ATOM	1376	CD2	TYR	191	-6.495	17.261	13.335	1.00	0.00	-0.127	10.80	0.60
ATOM	1377	HD2	TYR	191	-7.392	17.169	13.947	1.00	0.00	0.127	0.00	0.00
ATOM	1378	CE2	TYR	191	-5.396	16.460	13.609	1.00	0.00	-0.127	10.80	0.60
ATOM	1379	HE2	TYR	191	-5.427	15.746	14.432	1.00	0.00	0.127	0.00	0.00
ATOM	1380	CZ	TYR	191	-4.254	16.574	12.825	1.00	0.00	0.026	7.26	0.60
ATOM	1381	OH	TYR	191	-3.164	15.771	13.087	1.00	0.00	-0.451	10.94	-17.40
ATOM	1382	HH	TYR	191	-3.457	14.970	13.665	1.00	0.00	0.424	0.00	0.00
ATOM	1383	C	TYR	191	-9.809	18.902	10.768	1.00	0.00	0.396	9.82	4.00
ATOM	1384	O	TYR	191	-10.550	17.916	10.865	1.00	0.00	-0.396	8.17	-17.40
ATOM	1385	N	ARG	192G	-10.274	20.149	10.767	1.00	0.00	-0.650	9.00	-17.40
ATOM	1386	HN	ARG	192G	-9.627	20.944	10.670	1.00	0.00	0.440	0.00	0.00
ATOM	1387	CA	ARG	192G	-11.705	20.378	10.904	1.00	0.00	0.158	9.40	4.00
ATOM	1388	HA	ARG	192G	-12.066	19.985	11.854	1.00	0.00	0.053	0.00	0.00
ATOM	1389	CB	ARG	192G	-12.019	21.869	10.893	1.00	0.00	-0.106	12.77	4.00
ATOM	1390	HB1	ARG	192G	-11.918	22.316	9.904	1.00	0.00	0.053	0.00	0.00
ATOM	1391	HB2	ARG	192G	-11.365	22.445	11.548	1.00	0.00	0.053	0.00	0.00
ATOM	1392	CG	ARG	192G	-13.433	22.178	11.344	1.00	0.00	-0.106	12.77	4.00
ATOM	1393	HG1	ARG	192G	-13.591	21.897	12.385	1.00	0.00	0.053	0.00	0.00
ATOM	1394	HG2	ARG	192G	-14.170	21.640	10.747	1.00	0.00	0.053	0.00	0.00
ATOM	1395	CD	ARG	192G	-13.746	23.656	11.223	1.00	0.00	0.374	12.77	4.00
ATOM	1396	HD1	ARG	192G	-14.547	23.844	10.509	1.00	0.00	0.053	0.00	0.00
ATOM	1397	HD2	ARG	192G	-12.881	24.228	10.888	1.00	0.00	0.053	0.00	0.00
ATOM	1398	NE	ARG	192G	-14.169	24.231	12.501	1.00	0.00	-0.819	9.00	-24.67
ATOM	1399	HE	ARG	192G	-13.914	23.729	13.364	1.00	0.00	0.407	0.00	0.00
ATOM	1400	CZ	ARG	192G	-14.863	25.362	12.618	1.00	0.00	0.796	6.95	4.00
ATOM	1401	NH1	ARG	192G	-15.220	26.034	11.527	1.00	0.00	-0.746	9.00	-24.67
ATOM	1402	HH1	ARG	192G	-15.756	26.908	11.613	1.00	0.00	0.407	0.00	0.00
ATOM	1403	HH1	ARG	192G	-14.959	25.679	10.595	1.00	0.00	0.407	0.00	0.00
ATOM	1404	NH2	ARG	192G	-15.186	25.829	13.823	1.00	0.00	-0.746	9.00	-24.67
ATOM	1405	HH2	ARG	192G	-15.722	26.703	13.909	1.00	0.00	0.407	0.00	0.00
ATOM	1406	HH2	ARG	192G	-14.899	25.315	14.668	1.00	0.00	0.407	0.00	0.00
ATOM	1407	C	ARG	192G	-12.469	19.687	9.777	1.00	0.00	0.396	9.82	4.00
ATOM	1408	O	ARG	192G	-13.436	18.976	10.018	1.00	0.00	-0.396	8.17	-17.40
ATOM	1409	N	TRP	193	-12.027	19.887	8.541	1.00	0.00	-0.650	9.00	-17.40
ATOM	1410	HN	TRP	193	-11.204	20.485	8.383	1.00	0.00	0.440	0.00	0.00
ATOM	1411	CA	TRP	193	-12.695	19.268	7.411	1.00	0.00	0.158	9.40	4.00
ATOM	1412	HA	TRP	193	-13.758	19.501	7.369	1.00	0.00	0.053	0.00	0.00
ATOM	1413	CB	TRP	193	-12.122	19.792	6.078	1.00	0.00	-0.106	12.77	4.00
ATOM	1414	HB1	TRP	193	-11.075	19.519	5.944	1.00	0.00	0.053	0.00	0.00
ATOM	1415	HB2	TRP	193	-12.172	20.878	6.006	1.00	0.00	0.053	0.00	0.00
ATOM	1416	CG	TRP	193	-12.871	19.242	4.874	1.00	0.00	0.000	7.26	0.60
ATOM	1417	CD2	TRP	193	-12.535	18.074	4.114	1.00	0.00	0.000	6.80	0.60
ATOM	1418	CE2	TRP	193	-13.549	17.898	3.134	1.00	0.00	-0.050	6.80	0.60
ATOM	1419	CD1	TRP	193	-14.043	19.714	4.339	1.00	0.00	-0.177	10.80	0.60
ATOM	1420	HD1	TRP	193	-14.575	20.598	4.690	1.00	0.00	0.127	0.00	0.00
ATOM	1421	NE1	TRP	193	-14.453	18.913	3.295	1.00	0.00	-0.292	9.00	-17.40
ATOM	1422	HE1	TRP	193	-15.301	19.055	2.728	1.00	0.00	0.393	0.00	0.00
ATOM	1423	CE3	TRP	193	-11.479	17.156	4.166	1.00	0.00	-0.127	10.80	0.60
ATOM	1424	HE3	TRP	193	-10.688	17.259	4.909	1.00	0.00	0.127	0.00	0.00
ATOM	1425	CZ2	TRP	193	-13.532	16.841	2.211	1.00	0.00	-0.127	10.80	0.60
ATOM	1426	HZ2	TRP	193	-14.321	16.726	1.468	1.00	0.00	0.127	0.00	0.00
ATOM	1427	CZ3	TRP	193	-11.459	16.101	3.243	1.00	0.00	-0.127	10.80	0.60
ATOM	1428	HZ3	TRP	193	-10.641	15.380	3.269	1.00	0.00	0.127	0.00	0.00
ATOM	1429	CH2	TRP	193	-12.483	15.956	2.278	1.00	0.00	-0.127	10.80	0.60
ATOM	1430	HH2	TRP	193	-12.439	15.125	1.573	1.00	0.00	0.127	0.00	0.00
ATOM	1431	C	TRP	193	-12.600	17.739	7.430	1.00	0.00	0.396	9.82	4.00
ATOM	1432	O	TRP	193	-13.615	17.049	7.230	1.00	0.00	-0.396	8.17	-17.40
ATOM	1433	N	ALA	194	-11.398	17.208	7.681	1.00	0.00	-0.650	9.00	-17.40
ATOM	1434	HN	ALA	194	-10.601	17.832	7.872	1.00	0.00	0.440	0.00	0.00
ATOM	1435	CA	ALA	194	-11.190	15.755	7.690	1.00	0.00	0.158	9.40	4.00
ATOM	1436	HA	ALA	194	-11.494	15.299	6.747	1.00	0.00	0.053	0.00	0.00
ATOM	1437	CB	ALA	194	-9.701	15.422	7.849	1.00	0.00	-0.159	16.15	4.00
ATOM	1438	HB1	ALA	194	-9.568	14.340	7.853	1.00	0.00	0.053	0.00	0.00
ATOM	1439	HB2	ALA	194	-9.141	15.852	7.019	1.00	0.00	0.053	0.00	0.00

ATOM	1440	HB3	ALA	194	-9.333	15.836	8.788	1.00	0.00	0.053	0.00	0.00
ATOM	1441	C	ALA	194	-11.986	15.083	8.790	1.00	0.00	0.396	9.82	4.00
ATOM	1442	O	ALA	194	-12.639	14.068	8.552	1.00	0.00	-0.396	8.17	-17.40
ATOM	1443	N	LEU	195	-11.936	15.638	9.998	1.00	0.00	-0.650	9.00	-17.40
ATOM	1444	HN	LEU	195	-11.369	16.482	10.162	1.00	0.00	0.440	0.00	0.00
ATOM	1445	CA	LEU	195	-12.695	15.034	11.086	1.00	0.00	0.158	9.40	4.00
ATOM	1446	HA	LEU	195	-12.448	13.978	11.203	1.00	0.00	0.053	0.00	0.00
ATOM	1447	CB	LEU	195	-12.295	15.669	12.422	1.00	0.00	-0.106	12.77	4.00
ATOM	1448	HB1	LEU	195	-12.965	15.377	13.230	1.00	0.00	0.053	0.00	0.00
ATOM	1449	HB2	LEU	195	-12.310	16.758	12.378	1.00	0.00	0.053	0.00	0.00
ATOM	1450	CG	LEU	195	-10.874	15.261	12.853	1.00	0.00	-0.053	9.40	4.00
ATOM	1451	HG	LEU	195	-10.173	15.397	12.029	1.00	0.00	0.053	0.00	0.00
ATOM	1452	CD1	LEU	195	-10.420	16.097	14.007	1.00	0.00	-0.159	16.15	4.00
ATOM	1453	HD1	LEU	195	-9.414	15.796	14.300	1.00	0.00	0.053	0.00	0.00
ATOM	1454	HD1	LEU	195	-10.414	17.147	13.715	1.00	0.00	0.053	0.00	0.00
ATOM	1455	HD1	LEU	195	-11.099	15.957	14.847	1.00	0.00	0.053	0.00	0.00
ATOM	1456	CD2	LEU	195	-10.849	13.777	13.218	1.00	0.00	-0.159	16.15	4.00
ATOM	1457	HD2	LEU	195	-9.841	13.494	13.522	1.00	0.00	0.053	0.00	0.00
ATOM	1458	HD2	LEU	195	-11.541	13.592	14.039	1.00	0.00	0.053	0.00	0.00
ATOM	1459	HD2	LEU	195	-11.146	13.184	12.353	1.00	0.00	0.053	0.00	0.00
ATOM	1460	C	LEU	195	-14.208	15.131	10.833	1.00	0.00	0.396	9.82	4.00
ATOM	1461	O	LEU	195	-14.958	14.225	11.191	1.00	0.00	-0.396	8.17	-17.40
ATOM	1462	N	GLY	196	-14.644	16.219	10.206	1.00	0.00	-0.650	9.00	-17.40
ATOM	1463	HN	GLY	196	-13.975	16.955	9.939	1.00	0.00	0.440	0.00	0.00
ATOM	1464	CA	GLY	196	-16.055	16.381	9.893	1.00	0.00	0.105	9.40	4.00
ATOM	1465	HA1	GLY	196	-16.226	17.375	9.481	1.00	0.00	0.053	0.00	0.00
ATOM	1466	HA2	GLY	196	-16.647	16.259	10.800	1.00	0.00	0.053	0.00	0.00
ATOM	1467	C	GLY	196	-16.475	15.334	8.873	1.00	0.00	0.396	9.82	4.00
ATOM	1468	O	GLY	196	-17.610	14.865	8.884	1.00	0.00	-0.396	8.17	-17.40
ATOM	1469	N	GLN	197	-15.571	14.965	7.972	1.00	0.00	-0.650	9.00	-17.40
ATOM	1470	HN	GLN	197	-14.638	15.403	7.973	1.00	0.00	0.440	0.00	0.00
ATOM	1471	CA	GLN	197	-15.890	13.943	6.981	1.00	0.00	0.158	9.40	4.00
ATOM	1472	HA	GLN	197	-16.796	14.223	6.443	1.00	0.00	0.053	0.00	0.00
ATOM	1473	CB	GLN	197	-14.749	13.812	5.955	1.00	0.00	-0.106	12.77	4.00
ATOM	1474	HB1	GLN	197	-14.887	12.878	5.410	1.00	0.00	0.053	0.00	0.00
ATOM	1475	HB2	GLN	197	-13.803	13.806	6.497	1.00	0.00	0.053	0.00	0.00
ATOM	1476	CG	GLN	197	-14.681	14.942	4.922	1.00	0.00	-0.106	12.77	4.00
ATOM	1477	HG1	GLN	197	-13.827	14.852	4.250	1.00	0.00	0.053	0.00	0.00
ATOM	1478	HG2	GLN	197	-14.598	15.928	5.377	1.00	0.00	0.053	0.00	0.00
ATOM	1479	CD	GLN	197	-15.913	15.000	4.023	1.00	0.00	0.396	9.82	4.00
ATOM	1480	OE1	GLN	197	-16.246	14.024	3.350	1.00	0.00	-0.396	8.17	-17.40
ATOM	1481	NE2	GLN	197	-16.594	16.147	4.011	1.00	0.00	-0.879	13.25	-17.40
ATOM	1482	HE2	GLN	197	-16.279	16.938	4.590	1.00	0.00	0.440	0.00	0.00
ATOM	1483	HE2	GLN	197	-17.434	16.241	3.422	1.00	0.00	0.440	0.00	0.00
ATOM	1484	C	GLN	197	-16.113	12.594	7.683	1.00	0.00	0.396	9.82	4.00
ATOM	1485	O	GLN	197	-17.068	11.870	7.387	1.00	0.00	-0.396	8.17	-17.40
ATOM	1486	N	ILE	198	-15.213	12.269	8.607	1.00	0.00	-0.650	9.00	-17.40
ATOM	1487	HN	ILE	198	-14.443	12.926	8.797	1.00	0.00	0.440	0.00	0.00
ATOM	1488	CA	ILE	198	-15.267	11.022	9.363	1.00	0.00	0.158	9.40	4.00
ATOM	1489	HA	ILE	198	-15.221	10.136	8.729	1.00	0.00	0.053	0.00	0.00
ATOM	1490	CB	ILE	198	-14.068	10.937	10.370	1.00	0.00	-0.053	9.40	4.00
ATOM	1491	HB	ILE	198	-13.945	11.893	10.878	1.00	0.00	0.053	0.00	0.00
ATOM	1492	CG2	ILE	198	-14.338	9.861	11.395	1.00	0.00	-0.159	16.15	4.00
ATOM	1493	HG2	ILE	198	-13.502	9.805	12.092	1.00	0.00	0.053	0.00	0.00
ATOM	1494	HG2	ILE	198	-15.251	10.099	11.940	1.00	0.00	0.053	0.00	0.00
ATOM	1495	HG2	ILE	198	-14.455	8.901	10.892	1.00	0.00	0.053	0.00	0.00
ATOM	1496	CG1	ILE	198	-12.745	10.685	9.639	1.00	0.00	-0.106	12.77	4.00
ATOM	1497	HG1	ILE	198	-11.931	10.806	10.354	1.00	0.00	0.053	0.00	0.00
ATOM	1498	HG1	ILE	198	-12.658	11.410	8.830	1.00	0.00	0.053	0.00	0.00
ATOM	1499	CD1	ILE	198	-12.613	9.297	9.026	1.00	0.00	-0.159	16.15	4.00
ATOM	1500	HD1	ILE	198	-11.646	9.208	8.530	1.00	0.00	0.053	0.00	0.00
ATOM	1501	HD1	ILE	198	-12.688	8.544	9.810	1.00	0.00	0.053	0.00	0.00
ATOM	1502	HD1	ILE	198	-13.409	9.143	8.298	1.00	0.00	0.053	0.00	0.00
ATOM	1503	C	ILE	198	-16.549	10.875	10.187	1.00	0.00	0.396	9.82	4.00
ATOM	1504	O	ILE	198	-17.201	9.817	10.190	1.00	0.00	-0.396	8.17	-17.40
ATOM	1505	N	PHE	199	-16.901	11.936	10.903	1.00	0.00	-0.650	9.00	-17.40
ATOM	1506	HN	PHE	199	-16.348	12.802	10.836	1.00	0.00	0.440	0.00	0.00
ATOM	1507	CA	PHE	199	-18.062	11.886	11.783	1.00	0.00	0.158	9.40	4.00
ATOM	1508	HA	PHE	199	-18.210	10.844	12.066	1.00	0.00	0.053	0.00	0.00
ATOM	1509	CB	PHE	199	-17.737	12.622	13.089	1.00	0.00	-0.106	12.77	4.00
ATOM	1510	HB1	PHE	199	-18.551	12.611	13.813	1.00	0.00	0.053	0.00	0.00
ATOM	1511	HB2	PHE	199	-17.499	13.676	12.951	1.00	0.00	0.053	0.00	0.00
ATOM	1512	CG	PHE	199	-16.550	12.051	13.831	1.00	0.00	0.000	7.26	0.60
ATOM	1513	CD1	PHE	199	-15.377	12.777	13.949	1.00	0.00	-0.127	10.80	0.60
ATOM	1514	HD1	PHE	199	-15.307	13.760	13.485	1.00	0.00	0.127	0.00	0.00
ATOM	1515	CD2	PHE	199	-16.614	10.787	14.426	1.00	0.00	-0.127	10.80	0.60

ATOM	1516	HD2	PHE	199	-17.528	10.199	14.341	1.00	0.00	0.127	0.00	0.00
ATOM	1517	CE1	PHE	199	-14.280	12.272	14.652	1.00	0.00	-0.127	10.80	0.60
ATOM	1518	HE1	PHE	199	-13.368	12.863	14.735	1.00	0.00	0.127	0.00	0.00
ATOM	1519	CE2	PHE	199	-15.514	10.262	15.134	1.00	0.00	-0.127	10.80	0.60
ATOM	1520	HE2	PHE	199	-15.576	9.273	15.589	1.00	0.00	0.127	0.00	0.00
ATOM	1521	CZ	PHE	199	-14.349	11.011	15.248	1.00	0.00	-0.127	10.80	0.60
ATOM	1522	HZ	PHE	199	-13.495	10.616	15.799	1.00	0.00	0.127	0.00	0.00
ATOM	1523	C	PHE	199	-19.399	12.375	11.236	1.00	0.00	0.396	9.82	4.00
ATOM	1524	O	PHE	199	-20.447	12.015	11.776	1.00	0.00	-0.396	8.17	-17.40
ATOM	1525	N	HIS	200S	-19.381	13.177	10.173	1.00	0.00	-0.650	9.00	-17.40
ATOM	1526	HN	HIS	200S	-18.480	13.443	9.751	1.00	0.00	0.440	0.00	0.00
ATOM	1527	CA	HIS	200S	-20.627	13.683	9.598	1.00	0.00	0.158	9.40	4.00
ATOM	1528	HA	HIS	200S	-21.476	13.558	10.269	1.00	0.00	0.053	0.00	0.00
ATOM	1529	CB	HIS	200S	-20.539	15.186	9.317	1.00	0.00	-0.106	12.77	4.00
ATOM	1530	HB1	HIS	200S	-21.467	15.501	8.840	1.00	0.00	0.053	0.00	0.00
ATOM	1531	HB2	HIS	200S	-19.690	15.363	8.656	1.00	0.00	0.053	0.00	0.00
ATOM	1532	CG	HIS	200S	-20.347	16.023	10.542	1.00	0.00	-0.050	7.26	0.60
ATOM	1533	CD2	HIS	200S	-19.545	17.089	10.775	1.00	0.00	-0.177	10.80	0.60
ATOM	1534	HD2	HIS	200S	-18.861	17.552	10.064	1.00	0.00	0.127	0.00	0.00
ATOM	1535	ND1	HIS	200S	-21.034	15.792	11.718	1.00	0.00	0.207	9.25	-17.40
ATOM	1536	HD1	HIS	200S	-21.728	15.046	11.865	1.00	0.00	0.393	0.00	0.00
ATOM	1537	CE1	HIS	200S	-20.659	16.679	12.624	1.00	0.00	-0.227	10.80	0.60
ATOM	1538	HE1	HIS	200S	-21.030	16.742	13.646	1.00	0.00	0.127	0.00	0.00
ATOM	1539	NE2	HIS	200S	-19.756	17.477	12.078	1.00	0.00	0.207	9.25	-17.40
ATOM	1540	HE2	HIS	200S	-19.286	18.261	12.552	1.00	0.00	0.393	0.00	0.00
ATOM	1541	C	HIS	200S	-20.998	12.980	8.309	1.00	0.00	0.396	9.82	4.00
ATOM	1542	O	HIS	200S	-22.166	12.703	8.063	1.00	0.00	-0.396	8.17	-17.40
ATOM	1543	N	ASN	201	-20.008	12.702	7.474	1.00	0.00	-0.650	9.00	-17.40
ATOM	1544	HN	ASN	201	-19.041	12.954	7.724	1.00	0.00	0.440	0.00	0.00
ATOM	1545	CA	ASN	201	-20.277	12.045	6.212	1.00	0.00	0.158	9.40	4.00
ATOM	1546	HA	ASN	201	-21.274	12.290	5.848	1.00	0.00	0.053	0.00	0.00
ATOM	1547	CB	ASN	201	-19.311	12.564	5.156	1.00	0.00	-0.106	12.77	4.00
ATOM	1548	HB1	ASN	201	-19.530	12.150	4.171	1.00	0.00	0.053	0.00	0.00
ATOM	1549	HB2	ASN	201	-18.279	12.303	5.392	1.00	0.00	0.053	0.00	0.00
ATOM	1550	CG	ASN	201	-19.375	14.069	5.033	1.00	0.00	0.396	9.82	4.00
ATOM	1551	OD1	ASN	201	-20.168	14.612	4.256	1.00	0.00	-0.396	8.17	-17.40
ATOM	1552	ND2	ASN	201	-18.563	14.760	5.827	1.00	0.00	-0.879	13.25	-17.40
ATOM	1553	HD2	ASN	201	-17.917	14.265	6.459	1.00	0.00	0.440	0.00	0.00
ATOM	1554	HD2	ASN	201	-18.579	15.789	5.809	1.00	0.00	0.440	0.00	0.00
ATOM	1555	C	ASN	201	-20.192	10.543	6.354	1.00	0.00	0.396	9.82	4.00
ATOM	1556	O	ASN	201	-21.192	9.852	6.124	1.00	0.00	-0.396	8.17	-17.40
ATOM	1557	N	PHE	202	-19.026	10.022	6.739	1.00	0.00	-0.650	9.00	-17.40
ATOM	1558	HN	PHE	202	-18.216	10.634	6.914	1.00	0.00	0.440	0.00	0.00
ATOM	1559	CA	PHE	202	-18.906	8.581	6.910	1.00	0.00	0.158	9.40	4.00
ATOM	1560	HA	PHE	202	-19.282	8.065	6.026	1.00	0.00	0.053	0.00	0.00
ATOM	1561	CB	PHE	202	-17.439	8.151	7.047	1.00	0.00	-0.106	12.77	4.00
ATOM	1562	HB1	PHE	202	-17.315	7.099	7.305	1.00	0.00	0.053	0.00	0.00
ATOM	1563	HB2	PHE	202	-16.894	8.697	7.816	1.00	0.00	0.053	0.00	0.00
ATOM	1564	CG	PHE	202	-16.632	8.343	5.783	1.00	0.00	0.000	7.26	0.60
ATOM	1565	CD1	PHE	202	-15.910	9.511	5.569	1.00	0.00	-0.127	10.80	0.60
ATOM	1566	HD1	PHE	202	-15.916	10.292	6.329	1.00	0.00	0.127	0.00	0.00
ATOM	1567	CD2	PHE	202	-16.609	7.355	4.801	1.00	0.00	-0.127	10.80	0.60
ATOM	1568	HD2	PHE	202	-17.169	6.432	4.952	1.00	0.00	0.127	0.00	0.00
ATOM	1569	CE1	PHE	202	-15.173	9.701	4.390	1.00	0.00	-0.127	10.80	0.60
ATOM	1570	HE1	PHE	202	-14.615	10.624	4.237	1.00	0.00	0.127	0.00	0.00
ATOM	1571	CE2	PHE	202	-15.873	7.534	3.620	1.00	0.00	-0.127	10.80	0.60
ATOM	1572	HE2	PHE	202	-15.862	6.752	2.860	1.00	0.00	0.127	0.00	0.00
ATOM	1573	CZ	PHE	202	-15.156	8.710	3.419	1.00	0.00	-0.127	10.80	0.60
ATOM	1574	HZ	PHE	202	-14.583	8.851	2.502	1.00	0.00	0.127	0.00	0.00
ATOM	1575	C	PHE	202	-19.710	8.127	8.123	1.00	0.00	0.396	9.82	4.00
ATOM	1576	O	PHE	202	-20.163	6.977	8.178	1.00	0.00	-0.396	8.17	-17.40
ATOM	1577	N	ASN	203	-19.874	9.028	9.090	1.00	0.00	-0.650	9.00	-17.40
ATOM	1578	HN	ASN	203	-19.429	9.951	8.984	1.00	0.00	0.440	0.00	0.00
ATOM	1579	CA	ASN	203	-20.661	8.761	10.299	1.00	0.00	0.158	9.40	4.00
ATOM	1580	HA	ASN	203	-20.675	9.668	10.902	1.00	0.00	0.053	0.00	0.00
ATOM	1581	CB	ASN	203	-22.116	8.473	9.888	1.00	0.00	-0.106	12.77	4.00
ATOM	1582	HB1	ASN	203	-22.247	7.482	9.451	1.00	0.00	0.053	0.00	0.00
ATOM	1583	HB2	ASN	203	-22.496	9.175	9.146	1.00	0.00	0.053	0.00	0.00
ATOM	1584	CG	ASN	203	-23.090	8.541	11.057	1.00	0.00	0.396	9.82	4.00
ATOM	1585	OD1	ASN	203	-24.155	7.916	11.018	1.00	0.00	-0.396	8.17	-17.40
ATOM	1586	ND2	ASN	203	-22.743	9.309	12.096	1.00	0.00	-0.879	13.25	-17.40
ATOM	1587	HD2	ASN	203	-21.844	9.812	12.086	1.00	0.00	0.440	0.00	0.00
ATOM	1588	HD2	ASN	203	-23.374	9.396	12.905	1.00	0.00	0.440	0.00	0.00
ATOM	1589	C	ASN	203	-20.117	7.625	11.184	1.00	0.00	0.396	9.82	4.00
ATOM	1590	O	ASN	203	-20.870	6.768	11.660	1.00	0.00	-0.396	8.17	-17.40
ATOM	1591	N	TYR	204	-18.807	7.631	11.406	1.00	0.00	-0.650	9.00	-17.40

ATOM	1592	HN	TYR	204	-18.234	8.370	10.974	1.00	0.00	0.440	0.00	0.00
ATOM	1593	CA	TYR	204	-18.149	6.630	12.238	1.00	0.00	0.158	9.40	4.00
ATOM	1594	HA	TYR	204	-18.629	5.667	12.062	1.00	0.00	0.053	0.00	0.00
ATOM	1595	CB	TYR	204	-16.669	6.523	11.862	1.00	0.00	-0.106	12.77	4.00
ATOM	1596	HB1	TYR	204	-16.159	5.953	12.639	1.00	0.00	0.053	0.00	0.00
ATOM	1597	HB2	TYR	204	-16.259	7.531	11.793	1.00	0.00	0.053	0.00	0.00
ATOM	1598	CG	TYR	204	-16.409	5.832	10.541	1.00	0.00	0.000	7.26	0.60
ATOM	1599	CD1	TYR	204	-15.745	6.487	9.499	1.00	0.00	-0.127	10.80	0.60
ATOM	1600	HD1	TYR	204	-15.440	7.525	9.626	1.00	0.00	0.127	0.00	0.00
ATOM	1601	CE1	TYR	204	-15.465	5.828	8.294	1.00	0.00	-0.127	10.80	0.60
ATOM	1602	HE1	TYR	204	-14.944	6.349	7.491	1.00	0.00	0.127	0.00	0.00
ATOM	1603	CD2	TYR	204	-16.792	4.505	10.344	1.00	0.00	-0.127	10.80	0.60
ATOM	1604	HD2	TYR	204	-17.312	3.974	11.141	1.00	0.00	0.127	0.00	0.00
ATOM	1605	CE2	TYR	204	-16.519	3.843	9.140	1.00	0.00	-0.127	10.80	0.60
ATOM	1606	HE2	TYR	204	-16.830	2.807	9.004	1.00	0.00	0.127	0.00	0.00
ATOM	1607	CZ	TYR	204	-15.857	4.501	8.130	1.00	0.00	0.026	7.26	0.60
ATOM	1608	OH	TYR	204	-15.548	3.809	6.983	1.00	0.00	-0.451	10.94	-17.40
ATOM	1609	HH	TYR	204	-15.959	4.289	6.170	1.00	0.00	0.424	0.00	0.00
ATOM	1610	C	TYR	204	-18.298	7.044	13.696	1.00	0.00	0.396	9.82	4.00
ATOM	1611	O	TYR	204	-18.378	8.233	14.000	1.00	0.00	-0.396	8.17	-17.40
ATOM	1612	N	PRO	205	-18.300	6.068	14.620	1.00	0.00	-0.422	9.00	-17.40
ATOM	1613	CD	PRO	205	-18.114	4.621	14.383	1.00	0.00	0.105	12.77	4.00
ATOM	1614	HD1	PRO	205	-17.200	4.427	13.821	1.00	0.00	0.053	0.00	0.00
ATOM	1615	HD2	PRO	205	-18.945	4.204	13.815	1.00	0.00	0.053	0.00	0.00
ATOM	1616	CA	PRO	205	-18.451	6.338	16.049	1.00	0.00	0.158	9.40	4.00
ATOM	1617	HA	PRO	205	-19.201	7.118	16.171	1.00	0.00	0.053	0.00	0.00
ATOM	1618	CB	PRO	205	-18.920	5.000	16.583	1.00	0.00	-0.106	12.77	4.00
ATOM	1619	HB1	PRO	205	-19.981	4.841	16.390	1.00	0.00	0.053	0.00	0.00
ATOM	1620	HB2	PRO	205	-18.770	4.924	17.660	1.00	0.00	0.053	0.00	0.00
ATOM	1621	CG	PRO	205	-18.046	4.053	15.811	1.00	0.00	-0.106	12.77	4.00
ATOM	1622	HG1	PRO	205	-18.426	3.032	15.864	1.00	0.00	0.053	0.00	0.00
ATOM	1623	HG2	PRO	205	-17.028	4.047	16.201	1.00	0.00	0.053	0.00	0.00
ATOM	1624	C	PRO	205	-17.179	6.810	16.739	1.00	0.00	0.396	9.82	4.00
ATOM	1625	O	PRO	205	-17.216	7.255	17.886	1.00	0.00	-0.396	8.17	-17.40
ATOM	1626	N	ALA	206	-16.059	6.705	16.029	1.00	0.00	-0.650	9.00	-17.40
ATOM	1627	HN	ALA	206	-16.110	6.340	15.067	1.00	0.00	0.440	0.00	0.00
ATOM	1628	CA	ALA	206	-14.762	7.090	16.569	1.00	0.00	0.158	9.40	4.00
ATOM	1629	HA	ALA	206	-14.844	8.098	16.974	1.00	0.00	0.053	0.00	0.00
ATOM	1630	CB	ALA	206	-14.365	6.119	17.681	1.00	0.00	-0.159	16.15	4.00
ATOM	1631	HB1	ALA	206	-13.394	6.406	18.085	1.00	0.00	0.053	0.00	0.00
ATOM	1632	HB2	ALA	206	-15.112	6.149	18.474	1.00	0.00	0.053	0.00	0.00
ATOM	1633	HB3	ALA	206	-14.304	5.108	17.277	1.00	0.00	0.053	0.00	0.00
ATOM	1634	C	ALA	206	-13.739	7.050	15.438	1.00	0.00	0.396	9.82	4.00
ATOM	1635	O	ALA	206	-14.068	6.651	14.311	1.00	0.00	-0.396	8.17	-17.40
ATOM	1636	N	ALA	207	-12.509	7.480	15.722	1.00	0.00	-0.650	9.00	-17.40
ATOM	1637	HN	ALA	207	-12.304	7.833	16.667	1.00	0.00	0.440	0.00	0.00
ATOM	1638	CA	ALA	207	-11.442	7.461	14.718	1.00	0.00	0.158	9.40	4.00
ATOM	1639	HA	ALA	207	-11.420	6.542	14.132	1.00	0.00	0.053	0.00	0.00
ATOM	1640	CB	ALA	207	-11.669	8.581	13.708	1.00	0.00	-0.159	16.15	4.00
ATOM	1641	HB1	ALA	207	-10.874	8.565	12.962	1.00	0.00	0.053	0.00	0.00
ATOM	1642	HB2	ALA	207	-12.631	8.437	13.216	1.00	0.00	0.053	0.00	0.00
ATOM	1643	HB3	ALA	207	-11.664	9.541	14.223	1.00	0.00	0.053	0.00	0.00
ATOM	1644	C	ALA	207	-10.042	7.593	15.324	1.00	0.00	0.396	9.82	4.00
ATOM	1645	O	ALA	207	-9.849	8.232	16.369	1.00	0.00	-0.396	8.17	-17.40
ATOM	1646	N	VAL	208	-9.062	6.973	14.676	1.00	0.00	-0.650	9.00	-17.40
ATOM	1647	HN	VAL	208	-9.283	6.402	13.847	1.00	0.00	0.440	0.00	0.00
ATOM	1648	CA	VAL	208	-7.680	7.087	15.118	1.00	0.00	0.158	9.40	4.00
ATOM	1649	HA	VAL	208	-7.748	7.519	16.116	1.00	0.00	0.053	0.00	0.00
ATOM	1650	CB	VAL	208	-6.951	5.709	15.173	1.00	0.00	-0.053	9.40	4.00
ATOM	1651	HB	VAL	208	-7.041	5.192	14.217	1.00	0.00	0.053	0.00	0.00
ATOM	1652	CG1	VAL	208	-5.449	5.905	15.484	1.00	0.00	-0.159	16.15	4.00
ATOM	1653	HG1	VAL	208	-4.954	4.934	15.519	1.00	0.00	0.053	0.00	0.00
ATOM	1654	HG1	VAL	208	-4.993	6.516	14.705	1.00	0.00	0.053	0.00	0.00
ATOM	1655	HG1	VAL	208	-5.338	6.402	16.447	1.00	0.00	0.053	0.00	0.00
ATOM	1656	CG2	VAL	208	-7.569	4.837	16.278	1.00	0.00	-0.159	16.15	4.00
ATOM	1657	HG2	VAL	208	-7.056	3.875	16.312	1.00	0.00	0.053	0.00	0.00
ATOM	1658	HG2	VAL	208	-7.463	5.339	17.239	1.00	0.00	0.053	0.00	0.00
ATOM	1659	HG2	VAL	208	-8.626	4.677	16.066	1.00	0.00	0.053	0.00	0.00
ATOM	1660	C	VAL	208	-7.023	8.005	14.086	1.00	0.00	0.396	9.82	4.00
ATOM	1661	O	VAL	208	-6.944	7.678	12.895	1.00	0.00	-0.396	8.17	-17.40
ATOM	1662	N	VAL	209	-6.573	9.161	14.561	1.00	0.00	-0.650	9.00	-17.40
ATOM	1663	HN	VAL	209	-6.686	9.355	15.566	1.00	0.00	0.440	0.00	0.00
ATOM	1664	CA	VAL	209	-5.924	10.171	13.726	1.00	0.00	0.158	9.40	4.00
ATOM	1665	HA	VAL	209	-6.351	10.147	12.723	1.00	0.00	0.053	0.00	0.00
ATOM	1666	CB	VAL	209	-6.101	11.597	14.334	1.00	0.00	-0.053	9.40	4.00
ATOM	1667	HB	VAL	209	-5.550	11.668	15.271	1.00	0.00	0.053	0.00	0.00

ATOM	1668	CG1	VAL	209	-5.572	12.638	13.364	1.00	0.00	-0.159	16.15	4.00
ATOM	1669	HG1	VAL	209	-5.697	13.632	13.793	1.00	0.00	0.053	0.00	0.00
ATOM	1670	HG1	VAL	209	-4.514	12.455	13.175	1.00	0.00	0.053	0.00	0.00
ATOM	1671	HG1	VAL	209	-6.123	12.575	12.426	1.00	0.00	0.053	0.00	0.00
ATOM	1672	CG2	VAL	209	-7.567	11.869	14.664	1.00	0.00	-0.159	16.15	4.00
ATOM	1673	HG2	VAL	209	-7.665	12.868	15.086	1.00	0.00	0.053	0.00	0.00
ATOM	1674	HG2	VAL	209	-8.163	11.799	13.754	1.00	0.00	0.053	0.00	0.00
ATOM	1675	HG2	VAL	209	-7.919	11.133	15.387	1.00	0.00	0.053	0.00	0.00
ATOM	1676	C	VAL	209	-4.418	9.882	13.643	1.00	0.00	0.396	9.82	4.00
ATOM	1677	O	VAL	209	-3.726	9.828	14.668	1.00	0.00	-0.396	8.17	-17.40
ATOM	1678	N	VAL	210	-3.918	9.748	12.419	1.00	0.00	-0.650	9.00	-17.40
ATOM	1679	HN	VAL	210	-4.547	9.856	11.611	1.00	0.00	0.440	0.00	0.00
ATOM	1680	CA	VAL	210	-2.504	9.452	12.177	1.00	0.00	0.158	9.40	4.00
ATOM	1681	HA	VAL	210	-1.907	9.566	13.082	1.00	0.00	0.053	0.00	0.00
ATOM	1682	CB	VAL	210	-2.329	8.005	11.668	1.00	0.00	-0.053	9.40	4.00
ATOM	1683	HB	VAL	210	-2.855	7.884	10.721	1.00	0.00	0.053	0.00	0.00
ATOM	1684	CG1	VAL	210	-0.851	7.712	11.464	1.00	0.00	-0.159	16.15	4.00
ATOM	1685	HG1	VAL	210	-0.728	6.690	11.104	1.00	0.00	0.053	0.00	0.00
ATOM	1686	HG1	VAL	210	-0.440	8.406	10.730	1.00	0.00	0.053	0.00	0.00
ATOM	1687	HG1	VAL	210	-0.322	7.829	12.410	1.00	0.00	0.053	0.00	0.00
ATOM	1688	CG2	VAL	210	-2.961	7.015	12.663	1.00	0.00	-0.159	16.15	4.00
ATOM	1689	HG2	VAL	210	-2.832	5.997	12.295	1.00	0.00	0.053	0.00	0.00
ATOM	1690	HG2	VAL	210	-2.474	7.114	13.633	1.00	0.00	0.053	0.00	0.00
ATOM	1691	HG2	VAL	210	-4.024	7.231	12.766	1.00	0.00	0.053	0.00	0.00
ATOM	1692	C	VAL	210	-1.905	10.379	11.124	1.00	0.00	0.396	9.82	4.00
ATOM	1693	O	VAL	210	-2.327	10.357	9.971	1.00	0.00	-0.396	8.17	-17.40
ATOM	1694	N	GLU	211	-0.925	11.191	11.505	1.00	0.00	-0.650	9.00	-17.40
ATOM	1695	HN	GLU	211	-0.595	11.193	12.481	1.00	0.00	0.440	0.00	0.00
ATOM	1696	CA	GLU	211	-0.326	12.076	10.520	1.00	0.00	0.158	9.40	4.00
ATOM	1697	HA	GLU	211	-1.107	12.559	9.933	1.00	0.00	0.053	0.00	0.00
ATOM	1698	CB	GLU	211	0.404	13.225	11.220	1.00	0.00	-0.106	12.77	4.00
ATOM	1699	HB1	GLU	211	0.929	13.831	10.482	1.00	0.00	0.053	0.00	0.00
ATOM	1700	HB2	GLU	211	1.124	12.824	11.932	1.00	0.00	0.053	0.00	0.00
ATOM	1701	CG	GLU	211	-0.605	14.102	11.965	1.00	0.00	-0.106	12.77	4.00
ATOM	1702	HG1	GLU	211	-1.101	13.490	12.718	1.00	0.00	0.053	0.00	0.00
ATOM	1703	HG2	GLU	211	-1.328	14.482	11.243	1.00	0.00	0.053	0.00	0.00
ATOM	1704	CD	GLU	211	0.012	15.286	12.667	1.00	0.00	0.399	9.82	4.00
ATOM	1705	OE1	GLU	211	1.175	15.180	13.104	1.00	0.00	-0.396	8.17	-18.95
ATOM	1706	OE2	GLU	211	-0.681	16.324	12.799	1.00	0.00	-0.427	8.17	-18.95
ATOM	1707	HE2	GLU	211	-0.139	17.036	13.309	1.00	0.00	0.424	0.00	0.00
ATOM	1708	C	GLU	211	0.583	11.270	9.579	1.00	0.00	0.396	9.82	4.00
ATOM	1709	O	GLU	211	1.101	10.209	9.955	1.00	0.00	-0.396	8.17	-17.40
ATOM	1710	N	ASP	212P	0.749	11.778	8.360	1.00	0.00	-0.650	9.00	-17.40
ATOM	1711	HN	ASP	212P	0.304	12.681	8.143	1.00	0.00	0.440	0.00	0.00
ATOM	1712	CA	ASP	212P	1.528	11.122	7.312	1.00	0.00	0.158	9.40	4.00
ATOM	1713	HA	ASP	212P	1.043	10.171	7.090	1.00	0.00	0.053	0.00	0.00
ATOM	1714	CB	ASP	212P	1.457	11.959	6.028	1.00	0.00	-0.336	12.77	4.00
ATOM	1715	HB1	ASP	212P	0.430	12.140	5.709	1.00	0.00	0.053	0.00	0.00
ATOM	1716	HB2	ASP	212P	1.960	11.475	5.191	1.00	0.00	0.053	0.00	0.00
ATOM	1717	CG	ASP	212P	2.108	13.326	6.193	1.00	0.00	0.297	9.82	4.00
ATOM	1718	OD1	ASP	212P	1.842	13.976	7.210	1.00	0.00	-0.534	8.17	-18.95
ATOM	1719	OD2	ASP	212P	2.876	13.758	5.318	1.00	0.00	-0.534	8.17	-18.95
ATOM	1720	C	ASP	212P	2.989	10.804	7.615	1.00	0.00	0.396	9.82	4.00
ATOM	1721	O	ASP	212P	3.608	10.009	6.888	1.00	0.00	-0.396	8.17	-17.40
ATOM	1722	N	ASP	213P	3.552	11.406	8.663	1.00	0.00	-0.650	9.00	-17.40
ATOM	1723	HN	ASP	213P	3.000	12.056	9.240	1.00	0.00	0.440	0.00	0.00
ATOM	1724	CA	ASP	213P	4.947	11.144	8.993	1.00	0.00	0.158	9.40	4.00
ATOM	1725	HA	ASP	213P	5.412	10.641	8.145	1.00	0.00	0.053	0.00	0.00
ATOM	1726	CB	ASP	213P	5.727	12.470	9.124	1.00	0.00	-0.336	12.77	4.00
ATOM	1727	HB1	ASP	213P	5.731	13.064	8.210	1.00	0.00	0.053	0.00	0.00
ATOM	1728	HB2	ASP	213P	6.777	12.333	9.379	1.00	0.00	0.053	0.00	0.00
ATOM	1729	CG	ASP	213P	5.173	13.400	10.202	1.00	0.00	0.297	9.82	4.00
ATOM	1730	OD1	ASP	213P	4.080	13.123	10.751	1.00	0.00	-0.534	8.17	-18.95
ATOM	1731	OD2	ASP	213P	5.837	14.431	10.497	1.00	0.00	-0.534	8.17	-18.95
ATOM	1732	C	ASP	213P	5.139	10.253	10.229	1.00	0.00	0.396	9.82	4.00
ATOM	1733	O	ASP	213P	6.180	10.289	10.892	1.00	0.00	-0.396	8.17	-17.40
ATOM	1734	N	LEU	214	4.135	9.433	10.524	1.00	0.00	-0.650	9.00	-17.40
ATOM	1735	HN	LEU	214	3.283	9.441	9.944	1.00	0.00	0.440	0.00	0.00
ATOM	1736	CA	LEU	214	4.225	8.520	11.662	1.00	0.00	0.158	9.40	4.00
ATOM	1737	HA	LEU	214	5.134	8.706	12.233	1.00	0.00	0.053	0.00	0.00
ATOM	1738	CB	LEU	214	3.028	8.678	12.613	1.00	0.00	-0.106	12.77	4.00
ATOM	1739	HB1	LEU	214	3.237	8.080	13.500	1.00	0.00	0.053	0.00	0.00
ATOM	1740	HB2	LEU	214	2.145	8.315	12.086	1.00	0.00	0.053	0.00	0.00
ATOM	1741	CG	LEU	214	2.682	10.085	13.114	1.00	0.00	-0.053	9.40	4.00
ATOM	1742	HG	LEU	214	2.413	10.705	12.258	1.00	0.00	0.053	0.00	0.00
ATOM	1743	CD1	LEU	214	1.500	9.985	14.087	1.00	0.00	-0.159	16.15	4.00

ATOM	1744	HD1	LEU	214	1.243	10.979	14.451	1.00	0.00	0.053	0.00	0.00
ATOM	1745	HD1	LEU	214	0.640	9.554	13.572	1.00	0.00	0.053	0.00	0.00
ATOM	1746	HD1	LEU	214	1.774	9.349	14.929	1.00	0.00	0.053	0.00	0.00
ATOM	1747	CD2	LEU	214	3.899	10.708	13.793	1.00	0.00	-0.159	16.15	4.00
ATOM	1748	HD2	LEU	214	3.646	11.707	14.146	1.00	0.00	0.053	0.00	0.00
ATOM	1749	HD2	LEU	214	4.200	10.089	14.638	1.00	0.00	0.053	0.00	0.00
ATOM	1750	HD2	LEU	214	4.720	10.772	13.079	1.00	0.00	0.053	0.00	0.00
ATOM	1751	C	LEU	214	4.246	7.077	11.190	1.00	0.00	0.396	9.82	4.00
ATOM	1752	O	LEU	214	3.483	6.681	10.289	1.00	0.00	-0.396	8.17	-17.40
ATOM	1753	N	GLU	215	5.125	6.286	11.782	1.00	0.00	-0.650	9.00	-17.40
ATOM	1754	HN	GLU	215	5.787	6.679	12.466	1.00	0.00	0.440	0.00	0.00
ATOM	1755	CA	GLU	215	5.164	4.866	11.475	1.00	0.00	0.158	9.40	4.00
ATOM	1756	HA	GLU	215	4.584	4.763	10.557	1.00	0.00	0.053	0.00	0.00
ATOM	1757	CB	GLU	215	6.592	4.376	11.328	1.00	0.00	-0.106	12.77	4.00
ATOM	1758	HB1	GLU	215	7.178	4.543	12.231	1.00	0.00	0.053	0.00	0.00
ATOM	1759	HB2	GLU	215	7.117	4.879	10.516	1.00	0.00	0.053	0.00	0.00
ATOM	1760	CG	GLU	215	6.658	2.901	11.037	1.00	0.00	-0.106	12.77	4.00
ATOM	1761	HG1	GLU	215	6.021	2.608	10.202	1.00	0.00	0.053	0.00	0.00
ATOM	1762	HG2	GLU	215	6.344	2.290	11.884	1.00	0.00	0.053	0.00	0.00
ATOM	1763	CD	GLU	215	8.060	2.436	10.680	1.00	0.00	0.399	9.82	4.00
ATOM	1764	OE1	GLU	215	8.764	3.177	9.955	1.00	0.00	-0.396	8.17	-18.95
ATOM	1765	OE2	GLU	215	8.441	1.325	11.116	1.00	0.00	-0.427	8.17	-18.95
ATOM	1766	HE2	GLU	215	9.398	1.135	10.785	1.00	0.00	0.424	0.00	0.00
ATOM	1767	C	GLU	215	4.523	4.186	12.686	1.00	0.00	0.396	9.82	4.00
ATOM	1768	O	GLU	215	4.885	4.496	13.824	1.00	0.00	-0.396	8.17	-17.40
ATOM	1769	N	VAL	216	3.578	3.278	12.456	1.00	0.00	-0.650	9.00	-17.40
ATOM	1770	HN	VAL	216	3.308	3.062	11.485	1.00	0.00	0.440	0.00	0.00
ATOM	1771	CA	VAL	216	2.914	2.578	13.561	1.00	0.00	0.158	9.40	4.00
ATOM	1772	HA	VAL	216	2.839	3.179	14.466	1.00	0.00	0.053	0.00	0.00
ATOM	1773	CB	VAL	216	1.447	2.213	13.192	1.00	0.00	-0.053	9.40	4.00
ATOM	1774	HB	VAL	216	0.953	1.719	14.029	1.00	0.00	0.053	0.00	0.00
ATOM	1775	CG1	VAL	216	0.648	3.481	12.836	1.00	0.00	-0.159	16.15	4.00
ATOM	1776	HG1	VAL	216	-0.375	3.206	12.580	1.00	0.00	0.053	0.00	0.00
ATOM	1777	HG1	VAL	216	0.639	4.157	13.690	1.00	0.00	0.053	0.00	0.00
ATOM	1778	HG1	VAL	216	1.113	3.977	11.984	1.00	0.00	0.053	0.00	0.00
ATOM	1779	CG2	VAL	216	1.436	1.234	12.015	1.00	0.00	-0.159	16.15	4.00
ATOM	1780	HG2	VAL	216	0.406	0.981	11.761	1.00	0.00	0.053	0.00	0.00
ATOM	1781	HG2	VAL	216	1.919	1.694	11.153	1.00	0.00	0.053	0.00	0.00
ATOM	1782	HG2	VAL	216	1.974	0.327	12.291	1.00	0.00	0.053	0.00	0.00
ATOM	1783	C	VAL	216	3.637	1.289	13.981	1.00	0.00	0.396	9.82	4.00
ATOM	1784	O	VAL	216	4.296	0.638	13.168	1.00	0.00	-0.396	8.17	-17.40
ATOM	1785	N	ALA	217	3.524	0.933	15.264	1.00	0.00	-0.650	9.00	-17.40
ATOM	1786	HN	ALA	217	2.993	1.543	15.901	1.00	0.00	0.440	0.00	0.00
ATOM	1787	CA	ALA	217	4.125	-0.291	15.801	1.00	0.00	0.158	9.40	4.00
ATOM	1788	HA	ALA	217	5.129	-0.406	15.393	1.00	0.00	0.053	0.00	0.00
ATOM	1789	CB	ALA	217	4.205	-0.193	17.325	1.00	0.00	-0.159	16.15	4.00
ATOM	1790	HB1	ALA	217	4.651	-1.103	17.725	1.00	0.00	0.053	0.00	0.00
ATOM	1791	HB2	ALA	217	4.817	0.664	17.602	1.00	0.00	0.053	0.00	0.00
ATOM	1792	HB3	ALA	217	3.202	-0.070	17.735	1.00	0.00	0.053	0.00	0.00
ATOM	1793	C	ALA	217	3.261	-1.496	15.401	1.00	0.00	0.396	9.82	4.00
ATOM	1794	O	ALA	217	2.107	-1.331	15.024	1.00	0.00	-0.396	8.17	-17.40
ATOM	1795	N	PRO	218	3.800	-2.727	15.515	1.00	0.00	-0.422	9.00	-17.40
ATOM	1796	CD	PRO	218	5.177	-3.030	15.961	1.00	0.00	0.105	12.77	4.00
ATOM	1797	HD1	PRO	218	5.249	-3.019	17.048	1.00	0.00	0.053	0.00	0.00
ATOM	1798	HD2	PRO	218	5.885	-2.297	15.573	1.00	0.00	0.053	0.00	0.00
ATOM	1799	CA	PRO	218	3.080	-3.962	15.163	1.00	0.00	0.158	9.40	4.00
ATOM	1800	HA	PRO	218	2.826	-4.031	14.105	1.00	0.00	0.053	0.00	0.00
ATOM	1801	CB	PRO	218	4.076	-5.071	15.555	1.00	0.00	-0.106	12.77	4.00
ATOM	1802	HB1	PRO	218	3.972	-5.938	14.902	1.00	0.00	0.053	0.00	0.00
ATOM	1803	HB2	PRO	218	3.909	-5.401	16.580	1.00	0.00	0.053	0.00	0.00
ATOM	1804	CG	PRO	218	5.421	-4.406	15.393	1.00	0.00	-0.106	12.77	4.00
ATOM	1805	HG1	PRO	218	5.720	-4.370	14.345	1.00	0.00	0.053	0.00	0.00
ATOM	1806	HG2	PRO	218	6.195	-4.943	15.939	1.00	0.00	0.053	0.00	0.00
ATOM	1807	C	PRO	218	1.753	-4.126	15.903	1.00	0.00	0.396	9.82	4.00
ATOM	1808	O	PRO	218	0.795	-4.708	15.372	1.00	0.00	-0.396	8.17	-17.40
ATOM	1809	N	ASP	219P	1.707	-3.654	17.143	1.00	0.00	-0.650	9.00	-17.40
ATOM	1810	HN	ASP	219P	2.535	-3.195	17.548	1.00	0.00	0.440	0.00	0.00
ATOM	1811	CA	ASP	219P	0.495	-3.781	17.929	1.00	0.00	0.158	9.40	4.00
ATOM	1812	HA	ASP	219P	-0.186	-4.535	17.536	1.00	0.00	0.053	0.00	0.00
ATOM	1813	CB	ASP	219P	0.812	-4.288	19.357	1.00	0.00	-0.336	12.77	4.00
ATOM	1814	HB1	ASP	219P	1.157	-5.321	19.386	1.00	0.00	0.053	0.00	0.00
ATOM	1815	HB2	ASP	219P	-0.044	-4.256	20.031	1.00	0.00	0.053	0.00	0.00
ATOM	1816	CG	ASP	219P	1.901	-3.486	20.061	1.00	0.00	0.297	9.82	4.00
ATOM	1817	OD1	ASP	219P	2.355	-2.441	19.545	1.00	0.00	-0.534	8.17	-18.95
ATOM	1818	OD2	ASP	219P	2.301	-3.916	21.166	1.00	0.00	-0.534	8.17	-18.95
ATOM	1819	C	ASP	219P	-0.307	-2.487	17.993	1.00	0.00	0.396	9.82	4.00

ATOM	1820	O	ASP	219P	-1.042	-2.244	18.941	1.00	0.00	-0.396	8.17	-17.40
ATOM	1821	N	PHE	220	-0.177	-1.671	16.960	1.00	0.00	-0.650	9.00	-17.40
ATOM	1822	HN	PHE	220	0.450	-1.937	16.188	1.00	0.00	0.440	0.00	0.00
ATOM	1823	CA	PHE	220	-0.896	-0.405	16.881	1.00	0.00	0.158	9.40	4.00
ATOM	1824	HA	PHE	220	-0.632	0.267	17.697	1.00	0.00	0.053	0.00	0.00
ATOM	1825	CB	PHE	220	-0.505	0.308	15.580	1.00	0.00	-0.106	12.77	4.00
ATOM	1826	HB1	PHE	220	-0.671	-0.378	14.750	1.00	0.00	0.053	0.00	0.00
ATOM	1827	HB2	PHE	220	0.547	0.584	15.644	1.00	0.00	0.053	0.00	0.00
ATOM	1828	CG	PHE	220	-1.294	1.566	15.301	1.00	0.00	0.000	7.26	0.60
ATOM	1829	CD1	PHE	220	-0.921	2.787	15.873	1.00	0.00	-0.127	10.80	0.60
ATOM	1830	HD1	PHE	220	-0.062	2.826	16.543	1.00	0.00	0.127	0.00	0.00
ATOM	1831	CD2	PHE	220	-2.396	1.530	14.448	1.00	0.00	-0.127	10.80	0.60
ATOM	1832	HD2	PHE	220	-2.697	0.584	13.998	1.00	0.00	0.127	0.00	0.00
ATOM	1833	CE1	PHE	220	-1.632	3.955	15.598	1.00	0.00	-0.127	10.80	0.60
ATOM	1834	HE1	PHE	220	-1.326	4.897	16.052	1.00	0.00	0.127	0.00	0.00
ATOM	1835	CE2	PHE	220	-3.119	2.692	14.162	1.00	0.00	-0.127	10.80	0.60
ATOM	1836	HE2	PHE	220	-3.978	2.651	13.492	1.00	0.00	0.127	0.00	0.00
ATOM	1837	CZ	PHE	220	-2.730	3.918	14.745	1.00	0.00	-0.127	10.80	0.60
ATOM	1838	HZ	PHE	220	-3.286	4.829	14.528	1.00	0.00	0.127	0.00	0.00
ATOM	1839	C	PHE	220	-2.413	-0.600	16.942	1.00	0.00	0.396	9.82	4.00
ATOM	1840	O	PHE	220	-3.085	0.021	17.761	1.00	0.00	-0.396	8.17	-17.40
ATOM	1841	N	PHE	221	-2.955	-1.452	16.071	1.00	0.00	-0.650	9.00	-17.40
ATOM	1842	HN	PHE	221	-2.346	-1.952	15.407	1.00	0.00	0.440	0.00	0.00
ATOM	1843	CA	PHE	221	-4.393	-1.688	16.042	1.00	0.00	0.158	9.40	4.00
ATOM	1844	HA	PHE	221	-4.964	-0.760	16.015	1.00	0.00	0.053	0.00	0.00
ATOM	1845	CB	PHE	221	-4.774	-2.465	14.780	1.00	0.00	-0.106	12.77	4.00
ATOM	1846	HB1	PHE	221	-5.860	-2.536	14.736	1.00	0.00	0.053	0.00	0.00
ATOM	1847	HB2	PHE	221	-4.326	-3.457	14.839	1.00	0.00	0.053	0.00	0.00
ATOM	1848	CG	PHE	221	-4.305	-1.827	13.501	1.00	0.00	0.000	7.26	0.60
ATOM	1849	CD1	PHE	221	-3.001	-2.040	13.035	1.00	0.00	-0.127	10.80	0.60
ATOM	1850	HD1	PHE	221	-2.313	-2.653	13.617	1.00	0.00	0.127	0.00	0.00
ATOM	1851	CD2	PHE	221	-5.170	-1.039	12.750	1.00	0.00	-0.127	10.80	0.60
ATOM	1852	HD2	PHE	221	-6.184	-0.863	13.109	1.00	0.00	0.127	0.00	0.00
ATOM	1853	CE1	PHE	221	-2.567	-1.468	11.817	1.00	0.00	-0.127	10.80	0.60
ATOM	1854	HE1	PHE	221	-1.549	-1.638	11.464	1.00	0.00	0.127	0.00	0.00
ATOM	1855	CE2	PHE	221	-4.758	-0.466	11.536	1.00	0.00	-0.127	10.80	0.60
ATOM	1856	HE2	PHE	221	-5.449	0.145	10.956	1.00	0.00	0.127	0.00	0.00
ATOM	1857	CZ	PHE	221	-3.445	-0.686	11.070	1.00	0.00	-0.127	10.80	0.60
ATOM	1858	HZ	PHE	221	-3.118	-0.245	10.128	1.00	0.00	0.127	0.00	0.00
ATOM	1859	C	PHE	221	-4.880	-2.463	17.269	1.00	0.00	0.396	9.82	4.00
ATOM	1860	O	PHE	221	-5.933	-2.160	17.828	1.00	0.00	-0.396	8.17	-17.40
ATOM	1861	N	GLU	222	-4.119	-3.477	17.664	1.00	0.00	-0.650	9.00	-17.40
ATOM	1862	HN	GLU	222	-3.267	-3.696	17.127	1.00	0.00	0.440	0.00	0.00
ATOM	1863	CA	GLU	222	-4.443	-4.290	18.826	1.00	0.00	0.158	9.40	4.00
ATOM	1864	HA	GLU	222	-5.363	-4.823	18.591	1.00	0.00	0.053	0.00	0.00
ATOM	1865	CB	GLU	222	-3.281	-5.276	19.077	1.00	0.00	-0.106	12.77	4.00
ATOM	1866	HB1	GLU	222	-2.363	-4.694	19.165	1.00	0.00	0.053	0.00	0.00
ATOM	1867	HB2	GLU	222	-3.233	-5.958	18.228	1.00	0.00	0.053	0.00	0.00
ATOM	1868	CG	GLU	222	-3.384	-6.123	20.315	1.00	0.00	-0.106	12.77	4.00
ATOM	1869	HG1	GLU	222	-3.658	-5.560	21.207	1.00	0.00	0.053	0.00	0.00
ATOM	1870	HG2	GLU	222	-2.455	-6.630	20.575	1.00	0.00	0.053	0.00	0.00
ATOM	1871	CD	GLU	222	-4.418	-7.224	20.212	1.00	0.00	0.399	9.82	4.00
ATOM	1872	OE1	GLU	222	-4.788	-7.594	19.078	1.00	0.00	-0.396	8.17	-18.95
ATOM	1873	OE2	GLU	222	-4.838	-7.747	21.271	1.00	0.00	-0.427	8.17	-18.95
ATOM	1874	HE2	GLU	222	-5.507	-8.496	21.042	1.00	0.00	0.424	0.00	0.00
ATOM	1875	C	GLU	222	-4.622	-3.332	19.999	1.00	0.00	0.396	9.82	4.00
ATOM	1876	O	GLU	222	-5.595	-3.403	20.743	1.00	0.00	-0.396	8.17	-17.40
ATOM	1877	N	TYR	223	-3.693	-2.394	20.123	1.00	0.00	-0.650	9.00	-17.40
ATOM	1878	HN	TYR	223	-2.926	-2.355	19.436	1.00	0.00	0.440	0.00	0.00
ATOM	1879	CA	TYR	223	-3.725	-1.419	21.201	1.00	0.00	0.158	9.40	4.00
ATOM	1880	HA	TYR	223	-3.626	-1.888	22.179	1.00	0.00	0.053	0.00	0.00
ATOM	1881	CB	TYR	223	-2.538	-0.481	21.034	1.00	0.00	-0.106	12.77	4.00
ATOM	1882	HB1	TYR	223	-2.548	-0.099	20.013	1.00	0.00	0.053	0.00	0.00
ATOM	1883	HB2	TYR	223	-1.627	-1.049	21.225	1.00	0.00	0.053	0.00	0.00
ATOM	1884	CG	TYR	223	-2.528	0.711	21.960	1.00	0.00	0.000	7.26	0.60
ATOM	1885	CD1	TYR	223	-2.537	0.542	23.339	1.00	0.00	-0.127	10.80	0.60
ATOM	1886	HD1	TYR	223	-2.627	-0.460	23.757	1.00	0.00	0.127	0.00	0.00
ATOM	1887	CE1	TYR	223	-2.431	1.648	24.203	1.00	0.00	-0.127	10.80	0.60
ATOM	1888	HE1	TYR	223	-2.436	1.501	25.283	1.00	0.00	0.127	0.00	0.00
ATOM	1889	CD2	TYR	223	-2.427	2.010	21.451	1.00	0.00	-0.127	10.80	0.60
ATOM	1890	HD2	TYR	223	-2.428	2.162	20.371	1.00	0.00	0.127	0.00	0.00
ATOM	1891	CE2	TYR	223	-2.324	3.122	22.303	1.00	0.00	-0.127	10.80	0.60
ATOM	1892	HE2	TYR	223	-2.248	4.128	21.890	1.00	0.00	0.127	0.00	0.00
ATOM	1893	CZ	TYR	223	-2.320	2.924	23.673	1.00	0.00	0.026	7.26	0.60
ATOM	1894	OH	TYR	223	-2.161	3.986	24.528	1.00	0.00	-0.451	10.94	-17.40
ATOM	1895	HH	TYR	223	-1.370	4.565	24.213	1.00	0.00	0.424	0.00	0.00

ATOM	1896	C	TYR	223	-5.038	-0.626	21.220	1.00	0.00	0.396	9.82	4.00
ATOM	1897	O	TYR	223	-5.712	-0.518	22.255	1.00	0.00	-0.396	8.17	-17.40
ATOM	1898	N	PHE	224	-5.414	-0.087	20.069	1.00	0.00	-0.650	9.00	-17.40
ATOM	1899	HN	PHE	224	-4.837	-0.220	19.226	1.00	0.00	0.440	0.00	0.00
ATOM	1900	CA	PHE	224	-6.635	0.689	19.996	1.00	0.00	0.158	9.40	4.00
ATOM	1901	HA	PHE	224	-6.634	1.402	20.820	1.00	0.00	0.053	0.00	0.00
ATOM	1902	CB	PHE	224	-6.621	1.563	18.729	1.00	0.00	-0.106	12.77	4.00
ATOM	1903	HB1	PHE	224	-7.594	1.995	18.498	1.00	0.00	0.053	0.00	0.00
ATOM	1904	HB2	PHE	224	-6.323	1.014	17.835	1.00	0.00	0.053	0.00	0.00
ATOM	1905	CG	PHE	224	-5.671	2.728	18.827	1.00	0.00	0.000	7.26	0.60
ATOM	1906	CD1	PHE	224	-4.466	2.740	18.126	1.00	0.00	-0.127	10.80	0.60
ATOM	1907	HD1	PHE	224	-4.225	1.917	17.453	1.00	0.00	0.127	0.00	0.00
ATOM	1908	CD2	PHE	224	-5.965	3.794	19.682	1.00	0.00	-0.127	10.80	0.60
ATOM	1909	HD2	PHE	224	-6.906	3.796	20.232	1.00	0.00	0.127	0.00	0.00
ATOM	1910	CE1	PHE	224	-3.557	3.803	18.278	1.00	0.00	-0.127	10.80	0.60
ATOM	1911	HE1	PHE	224	-2.616	3.801	17.727	1.00	0.00	0.127	0.00	0.00
ATOM	1912	CE2	PHE	224	-5.077	4.851	19.842	1.00	0.00	-0.127	10.80	0.60
ATOM	1913	HE2	PHE	224	-5.321	5.673	20.514	1.00	0.00	0.127	0.00	0.00
ATOM	1914	CZ	PHE	224	-3.862	4.857	19.134	1.00	0.00	-0.127	10.80	0.60
ATOM	1915	HZ	PHE	224	-3.162	5.683	19.255	1.00	0.00	0.127	0.00	0.00
ATOM	1916	C	PHE	224	-7.926	-0.135	20.099	1.00	0.00	0.396	9.82	4.00
ATOM	1917	O	PHE	224	-8.909	0.370	20.642	1.00	0.00	-0.396	8.17	-17.40
ATOM	1918	N	GLN	225	-7.955	-1.373	19.597	1.00	0.00	-0.650	9.00	-17.40
ATOM	1919	HN	GLN	225	-7.130	-1.768	19.123	1.00	0.00	0.440	0.00	0.00
ATOM	1920	CA	GLN	225	-9.193	-2.160	19.737	1.00	0.00	0.158	9.40	4.00
ATOM	1921	HA	GLN	225	-10.033	-1.547	19.411	1.00	0.00	0.053	0.00	0.00
ATOM	1922	CB	GLN	225	-9.187	-3.411	18.842	1.00	0.00	-0.106	12.77	4.00
ATOM	1923	HB1	GLN	225	-8.364	-4.050	19.163	1.00	0.00	0.053	0.00	0.00
ATOM	1924	HB2	GLN	225	-9.047	-3.085	17.811	1.00	0.00	0.053	0.00	0.00
ATOM	1925	CG	GLN	225	-10.496	-4.284	18.881	1.00	0.00	-0.106	12.77	4.00
ATOM	1926	HG1	GLN	225	-10.598	-4.692	19.886	1.00	0.00	0.053	0.00	0.00
ATOM	1927	HG2	GLN	225	-10.391	-5.081	18.146	1.00	0.00	0.053	0.00	0.00
ATOM	1928	CD	GLN	225	-11.819	-3.523	18.553	1.00	0.00	0.396	9.82	4.00
ATOM	1929	OE1	GLN	225	-12.479	-2.948	19.449	1.00	0.00	-0.396	8.17	-17.40
ATOM	1930	NE2	GLN	225	-12.202	-3.522	17.268	1.00	0.00	-0.879	13.25	-17.40
ATOM	1931	HE2	GLN	225	-11.631	-4.006	16.560	1.00	0.00	0.440	0.00	0.00
ATOM	1932	HE2	GLN	225	-13.066	-3.036	16.988	1.00	0.00	0.440	0.00	0.00
ATOM	1933	C	GLN	225	-9.360	-2.553	21.211	1.00	0.00	0.396	9.82	4.00
ATOM	1934	O	GLN	225	-10.465	-2.742	21.683	1.00	0.00	-0.396	8.17	-17.40
ATOM	1935	N	ALA	226	-8.264	-2.670	21.953	1.00	0.00	-0.650	9.00	-17.40
ATOM	1936	HN	ALA	226	-7.335	-2.513	21.535	1.00	0.00	0.440	0.00	0.00
ATOM	1937	CA	ALA	226	-8.385	-3.023	23.369	1.00	0.00	0.158	9.40	4.00
ATOM	1938	HA	ALA	226	-9.142	-3.782	23.564	1.00	0.00	0.053	0.00	0.00
ATOM	1939	CB	ALA	226	-7.088	-3.661	23.872	1.00	0.00	-0.159	16.15	4.00
ATOM	1940	HB1	ALA	226	-7.193	-3.917	24.926	1.00	0.00	0.053	0.00	0.00
ATOM	1941	HB2	ALA	226	-6.880	-4.563	23.297	1.00	0.00	0.053	0.00	0.00
ATOM	1942	HB3	ALA	226	-6.265	-2.956	23.751	1.00	0.00	0.053	0.00	0.00
ATOM	1943	C	ALA	226	-8.766	-1.836	24.266	1.00	0.00	0.396	9.82	4.00
ATOM	1944	O	ALA	226	-9.464	-2.017	25.272	1.00	0.00	-0.396	8.17	-17.40
ATOM	1945	N	THR	227	-8.324	-0.627	23.915	1.00	0.00	-0.650	9.00	-17.40
ATOM	1946	HN	THR	227	-7.771	-0.519	23.052	1.00	0.00	0.440	0.00	0.00
ATOM	1947	CA	THR	227	-8.610	0.541	24.732	1.00	0.00	0.158	9.40	4.00
ATOM	1948	HA	THR	227	-8.723	0.212	25.765	1.00	0.00	0.053	0.00	0.00
ATOM	1949	CB	THR	227	-7.401	1.545	24.747	1.00	0.00	0.060	9.40	4.00
ATOM	1950	HB	THR	227	-7.667	2.443	25.303	1.00	0.00	0.053	0.00	0.00
ATOM	1951	OG1	THR	227	-7.068	1.954	23.402	1.00	0.00	-0.537	11.04	-17.40
ATOM	1952	HG1	THR	227	-6.713	2.921	23.414	1.00	0.00	0.424	0.00	0.00
ATOM	1953	CG2	THR	227	-6.174	0.888	25.419	1.00	0.00	-0.159	16.15	4.00
ATOM	1954	HG2	THR	227	-5.341	1.591	25.424	1.00	0.00	0.053	0.00	0.00
ATOM	1955	HG2	THR	227	-6.423	0.613	26.444	1.00	0.00	0.053	0.00	0.00
ATOM	1956	HG2	THR	227	-5.889	-0.005	24.863	1.00	0.00	0.053	0.00	0.00
ATOM	1957	C	THR	227	-9.883	1.301	24.351	1.00	0.00	0.396	9.82	4.00
ATOM	1958	O	THR	227	-10.380	2.118	25.137	1.00	0.00	-0.396	8.17	-17.40
ATOM	1959	N	TYR	228	-10.416	1.035	23.163	1.00	0.00	-0.650	9.00	-17.40
ATOM	1960	HN	TYR	228	-9.964	0.350	22.539	1.00	0.00	0.440	0.00	0.00
ATOM	1961	CA	TYR	228	-11.642	1.710	22.737	1.00	0.00	0.158	9.40	4.00
ATOM	1962	HA	TYR	228	-11.482	2.781	22.618	1.00	0.00	0.053	0.00	0.00
ATOM	1963	CB	TYR	228	-12.064	1.177	21.366	1.00	0.00	-0.106	12.77	4.00
ATOM	1964	HB1	TYR	228	-12.104	0.089	21.420	1.00	0.00	0.053	0.00	0.00
ATOM	1965	HB2	TYR	228	-11.324	1.498	20.632	1.00	0.00	0.053	0.00	0.00
ATOM	1966	CG	TYR	228	-13.411	1.660	20.896	1.00	0.00	0.000	7.26	0.60
ATOM	1967	CD1	TYR	228	-13.645	3.012	20.653	1.00	0.00	-0.127	10.80	0.60
ATOM	1968	HD1	TYR	228	-12.838	3.730	20.801	1.00	0.00	0.127	0.00	0.00
ATOM	1969	CE1	TYR	228	-14.895	3.463	20.222	1.00	0.00	-0.127	10.80	0.60
ATOM	1970	HE1	TYR	228	-15.064	4.524	20.038	1.00	0.00	0.127	0.00	0.00
ATOM	1971	CD2	TYR	228	-14.461	0.758	20.695	1.00	0.00	-0.127	10.80	0.60

ATOM	1972	HD2	TYR	228	-14.298	-0.303	20.881	1.00	0.00	0.127	0.00	0.00
ATOM	1973	CE2	TYR	228	-15.712	1.193	20.261	1.00	0.00	-0.127	10.80	0.60
ATOM	1974	HE2	TYR	228	-16.519	0.477	20.104	1.00	0.00	0.127	0.00	0.00
ATOM	1975	CZ	TYR	228	-15.920	2.545	20.030	1.00	0.00	0.026	7.26	0.60
ATOM	1976	OH	TYR	228	-17.152	2.981	19.616	1.00	0.00	-0.451	10.94	-17.40
ATOM	1977	HH	TYR	228	-17.152	4.009	19.561	1.00	0.00	0.424	0.00	0.00
ATOM	1978	C	TYR	228	-12.777	1.517	23.771	1.00	0.00	0.396	9.82	4.00
ATOM	1979	O	TYR	228	-13.457	2.466	24.152	1.00	0.00	-0.396	8.17	-17.40
ATOM	1980	N	PRO	229	-12.991	0.282	24.244	1.00	0.00	-0.422	9.00	-17.40
ATOM	1981	CD	PRO	229	-12.395	-1.014	23.869	1.00	0.00	0.105	12.77	4.00
ATOM	1982	HD1	PRO	229	-11.321	-0.922	23.702	1.00	0.00	0.053	0.00	0.00
ATOM	1983	HD2	PRO	229	-12.838	-1.403	22.952	1.00	0.00	0.053	0.00	0.00
ATOM	1984	CA	PRO	229	-14.071	0.123	25.224	1.00	0.00	0.158	9.40	4.00
ATOM	1985	HA	PRO	229	-14.997	0.479	24.773	1.00	0.00	0.053	0.00	0.00
ATOM	1986	CB	PRO	229	-14.130	-1.392	25.448	1.00	0.00	-0.106	12.77	4.00
ATOM	1987	HB1	PRO	229	-14.894	-1.849	24.819	1.00	0.00	0.053	0.00	0.00
ATOM	1988	HB2	PRO	229	-14.366	-1.623	26.486	1.00	0.00	0.053	0.00	0.00
ATOM	1989	CG	PRO	229	-12.714	-1.873	25.065	1.00	0.00	-0.106	12.77	4.00
ATOM	1990	HG1	PRO	229	-12.709	-2.935	24.821	1.00	0.00	0.053	0.00	0.00
ATOM	1991	HG2	PRO	229	-12.009	-1.719	25.882	1.00	0.00	0.053	0.00	0.00
ATOM	1992	C	PRO	229	-13.857	0.901	26.526	1.00	0.00	0.396	9.82	4.00
ATOM	1993	O	PRO	229	-14.828	1.275	27.185	1.00	0.00	-0.396	8.17	-17.40
ATOM	1994	N	LEU	230	-12.596	1.151	26.889	1.00	0.00	-0.650	9.00	-17.40
ATOM	1995	HN	LEU	230	-11.824	0.813	26.296	1.00	0.00	0.440	0.00	0.00
ATOM	1996	CA	LEU	230	-12.288	1.892	28.108	1.00	0.00	0.158	9.40	4.00
ATOM	1997	HA	LEU	230	-12.875	1.476	28.926	1.00	0.00	0.053	0.00	0.00
ATOM	1998	CB	LEU	230	-10.801	1.781	28.441	1.00	0.00	-0.106	12.77	4.00
ATOM	1999	HB1	LEU	230	-10.391	2.789	28.372	1.00	0.00	0.053	0.00	0.00
ATOM	2000	HB2	LEU	230	-10.367	1.108	27.701	1.00	0.00	0.053	0.00	0.00
ATOM	2001	CG	LEU	230	-10.327	1.251	29.786	1.00	0.00	-0.053	9.40	4.00
ATOM	2002	HG	LEU	230	-10.382	0.163	29.731	1.00	0.00	0.053	0.00	0.00
ATOM	2003	CD1	LEU	230	-8.900	1.742	29.971	1.00	0.00	-0.159	16.15	4.00
ATOM	2004	HD1	LEU	230	-8.513	1.386	30.926	1.00	0.00	0.053	0.00	0.00
ATOM	2005	HD1	LEU	230	-8.276	1.360	29.162	1.00	0.00	0.053	0.00	0.00
ATOM	2006	HD1	LEU	230	-8.885	2.831	29.957	1.00	0.00	0.053	0.00	0.00
ATOM	2007	CD2	LEU	230	-11.204	1.733	30.936	1.00	0.00	-0.159	16.15	4.00
ATOM	2008	HD2	LEU	230	-10.826	1.329	31.875	1.00	0.00	0.053	0.00	0.00
ATOM	2009	HD2	LEU	230	-11.185	2.822	30.976	1.00	0.00	0.053	0.00	0.00
ATOM	2010	HD2	LEU	230	-12.227	1.393	30.780	1.00	0.00	0.053	0.00	0.00
ATOM	2011	C	LEU	230	-12.649	3.367	27.890	1.00	0.00	0.396	9.82	4.00
ATOM	2012	O	LEU	230	-13.219	4.023	28.764	1.00	0.00	-0.396	8.17	-17.40
ATOM	2013	N	LEU	231	-12.317	3.872	26.711	1.00	0.00	-0.650	9.00	-17.40
ATOM	2014	HN	LEU	231	-11.841	3.272	26.021	1.00	0.00	0.440	0.00	0.00
ATOM	2015	CA	LEU	231	-12.611	5.259	26.369	1.00	0.00	0.158	9.40	4.00
ATOM	2016	HA	LEU	231	-12.149	5.909	27.112	1.00	0.00	0.053	0.00	0.00
ATOM	2017	CB	LEU	231	-12.037	5.596	24.988	1.00	0.00	-0.106	12.77	4.00
ATOM	2018	HB1	LEU	231	-12.544	4.975	24.249	1.00	0.00	0.053	0.00	0.00
ATOM	2019	HB2	LEU	231	-10.968	5.382	25.004	1.00	0.00	0.053	0.00	0.00
ATOM	2020	CG	LEU	231	-12.205	7.049	24.554	1.00	0.00	-0.053	9.40	4.00
ATOM	2021	HG	LEU	231	-13.261	7.267	24.400	1.00	0.00	0.053	0.00	0.00
ATOM	2022	CD1	LEU	231	-11.652	7.978	25.634	1.00	0.00	-0.159	16.15	4.00
ATOM	2023	HD1	LEU	231	-11.774	9.014	25.319	1.00	0.00	0.053	0.00	0.00
ATOM	2024	HD1	LEU	231	-12.193	7.815	26.566	1.00	0.00	0.053	0.00	0.00
ATOM	2025	HD1	LEU	231	-10.593	7.767	25.787	1.00	0.00	0.053	0.00	0.00
ATOM	2026	CD2	LEU	231	-11.504	7.275	23.211	1.00	0.00	-0.159	16.15	4.00
ATOM	2027	HD2	LEU	231	-11.627	8.314	22.906	1.00	0.00	0.053	0.00	0.00
ATOM	2028	HD2	LEU	231	-10.442	7.050	23.312	1.00	0.00	0.053	0.00	0.00
ATOM	2029	HD2	LEU	231	-11.942	6.621	22.457	1.00	0.00	0.053	0.00	0.00
ATOM	2030	C	LEU	231	-14.127	5.455	26.367	1.00	0.00	0.396	9.82	4.00
ATOM	2031	O	LEU	231	-14.638	6.487	26.815	1.00	0.00	-0.396	8.17	-17.40
ATOM	2032	N	LYS	232S	-14.848	4.454	25.883	1.00	0.00	-0.650	9.00	-17.40
ATOM	2033	HN	LYS	232S	-14.380	3.603	25.538	1.00	0.00	0.440	0.00	0.00
ATOM	2034	CA	LYS	232S	-16.304	4.555	25.837	1.00	0.00	0.158	9.40	4.00
ATOM	2035	HA	LYS	232S	-16.652	5.491	25.401	1.00	0.00	0.053	0.00	0.00
ATOM	2036	CB	LYS	232S	-16.897	3.465	24.940	1.00	0.00	-0.106	12.77	4.00
ATOM	2037	HB1	LYS	232S	-17.739	2.937	25.387	1.00	0.00	0.053	0.00	0.00
ATOM	2038	HB2	LYS	232S	-16.188	2.681	24.672	1.00	0.00	0.053	0.00	0.00
ATOM	2039	CG	LYS	232S	-17.425	3.984	23.608	1.00	0.00	-0.106	12.77	4.00
ATOM	2040	HG1	LYS	232S	-16.635	4.017	22.857	1.00	0.00	0.053	0.00	0.00
ATOM	2041	HG2	LYS	232S	-17.828	4.991	23.709	1.00	0.00	0.053	0.00	0.00
ATOM	2042	CD	LYS	232S	-18.536	3.093	23.071	1.00	0.00	-0.106	12.77	4.00
ATOM	2043	HD1	LYS	232S	-18.931	3.457	22.123	1.00	0.00	0.053	0.00	0.00
ATOM	2044	HD2	LYS	232S	-19.379	3.029	23.758	1.00	0.00	0.053	0.00	0.00
ATOM	2045	CE	LYS	232S	-18.056	1.654	22.826	1.00	0.00	0.099	12.77	4.00
ATOM	2046	HE1	LYS	232S	-17.671	1.185	23.731	1.00	0.00	0.053	0.00	0.00
ATOM	2047	HE2	LYS	232S	-17.254	1.603	22.088	1.00	0.00	0.053	0.00	0.00

ATOM	2048	NZ	LYS	232S	-19.158	0.760	22.319	1.00	0.00	-0.045	13.25	-39.20
ATOM	2049	HZ1	LYS	232S	-18.789	-0.190	22.170	1.00	0.00	0.280	0.00	0.00
ATOM	2050	HZ2	LYS	232S	-19.920	0.727	23.011	1.00	0.00	0.280	0.00	0.00
ATOM	2051	HZ3	LYS	232S	-19.519	1.130	21.428	1.00	0.00	0.280	0.00	0.00
ATOM	2052	C	LYS	232S	-16.951	4.475	27.217	1.00	0.00	0.396	9.82	4.00
ATOM	2053	O	LYS	232S	-18.001	5.080	27.447	1.00	0.00	-0.396	8.17	-17.40
ATOM	2054	N	ALA	233	-16.312	3.750	28.133	1.00	0.00	-0.650	9.00	-17.40
ATOM	2055	HN	ALA	233	-15.411	3.313	27.888	1.00	0.00	0.440	0.00	0.00
ATOM	2056	CA	ALA	233	-16.854	3.557	29.474	1.00	0.00	0.158	9.40	4.00
ATOM	2057	HA	ALA	233	-17.940	3.607	29.399	1.00	0.00	0.053	0.00	0.00
ATOM	2058	CB	ALA	233	-16.515	2.142	29.963	1.00	0.00	-0.159	16.15	4.00
ATOM	2059	HB1	ALA	233	-16.919	1.996	30.964	1.00	0.00	0.053	0.00	0.00
ATOM	2060	HB2	ALA	233	-16.951	1.408	29.285	1.00	0.00	0.053	0.00	0.00
ATOM	2061	HB3	ALA	233	-15.432	2.014	29.986	1.00	0.00	0.053	0.00	0.00
ATOM	2062	C	ALA	233	-16.448	4.555	30.542	1.00	0.00	0.396	9.82	4.00
ATOM	2063	O	ALA	233	-17.122	4.675	31.569	1.00	0.00	-0.396	8.17	-17.40
ATOM	2064	N	ASP	234P	-15.355	5.269	30.328	1.00	0.00	-0.650	9.00	-17.40
ATOM	2065	HN	ASP	234P	-14.832	5.156	29.447	1.00	0.00	0.440	0.00	0.00
ATOM	2066	CA	ASP	234P	-14.889	6.210	31.329	1.00	0.00	0.158	9.40	4.00
ATOM	2067	HA	ASP	234P	-15.551	6.207	32.194	1.00	0.00	0.053	0.00	0.00
ATOM	2068	CB	ASP	234P	-13.499	5.762	31.788	1.00	0.00	-0.336	12.77	4.00
ATOM	2069	HB1	ASP	234P	-12.747	5.830	31.001	1.00	0.00	0.053	0.00	0.00
ATOM	2070	HB2	ASP	234P	-13.475	4.726	32.128	1.00	0.00	0.053	0.00	0.00
ATOM	2071	CG	ASP	234P	-12.966	6.579	32.932	1.00	0.00	0.297	9.82	4.00
ATOM	2072	OD1	ASP	234P	-13.626	7.560	33.356	1.00	0.00	-0.534	8.17	-18.95
ATOM	2073	OD2	ASP	234P	-11.861	6.238	33.408	1.00	0.00	-0.534	8.17	-18.95
ATOM	2074	C	ASP	234P	-14.849	7.633	30.754	1.00	0.00	0.396	9.82	4.00
ATOM	2075	O	ASP	234P	-13.932	7.979	30.019	1.00	0.00	-0.396	8.17	-17.40
ATOM	2076	N	PRO	235	-15.863	8.462	31.076	1.00	0.00	-0.422	9.00	-17.40
ATOM	2077	CD	PRO	235	-17.026	8.088	31.906	1.00	0.00	0.105	12.77	4.00
ATOM	2078	HD1	PRO	235	-16.727	7.463	32.748	1.00	0.00	0.053	0.00	0.00
ATOM	2079	HD2	PRO	235	-17.762	7.530	31.328	1.00	0.00	0.053	0.00	0.00
ATOM	2080	CA	PRO	235	-15.985	9.852	30.612	1.00	0.00	0.158	9.40	4.00
ATOM	2081	HA	PRO	235	-15.923	9.856	29.523	1.00	0.00	0.053	0.00	0.00
ATOM	2082	CB	PRO	235	-17.387	10.251	31.078	1.00	0.00	-0.106	12.77	4.00
ATOM	2083	HB1	PRO	235	-18.138	9.995	30.331	1.00	0.00	0.053	0.00	0.00
ATOM	2084	HB2	PRO	235	-17.452	11.323	31.259	1.00	0.00	0.053	0.00	0.00
ATOM	2085	CG	PRO	235	-17.552	9.446	32.353	1.00	0.00	-0.106	12.77	4.00
ATOM	2086	HG1	PRO	235	-18.593	9.409	32.674	1.00	0.00	0.053	0.00	0.00
ATOM	2087	HG2	PRO	235	-16.975	9.871	33.174	1.00	0.00	0.053	0.00	0.00
ATOM	2088	C	PRO	235	-14.902	10.788	31.141	1.00	0.00	0.396	9.82	4.00
ATOM	2089	O	PRO	235	-14.799	11.940	30.696	1.00	0.00	-0.396	8.17	-17.40
ATOM	2090	N	SER	236	-14.105	10.311	32.095	1.00	0.00	-0.650	9.00	-17.40
ATOM	2091	HN	SER	236	-14.250	9.358	32.459	1.00	0.00	0.440	0.00	0.00
ATOM	2092	CA	SER	236	-13.020	11.141	32.626	1.00	0.00	0.158	9.40	4.00
ATOM	2093	HA	SER	236	-13.393	12.164	32.668	1.00	0.00	0.053	0.00	0.00
ATOM	2094	CB	SER	236	-12.632	10.686	34.050	1.00	0.00	0.007	12.77	4.00
ATOM	2095	HB1	SER	236	-13.505	10.572	34.691	1.00	0.00	0.053	0.00	0.00
ATOM	2096	HB2	SER	236	-11.968	11.400	34.537	1.00	0.00	0.053	0.00	0.00
ATOM	2097	OG	SER	236	-11.963	9.442	34.040	1.00	0.00	-0.537	11.04	-17.40
ATOM	2098	HG	SER	236	-12.655	8.679	34.026	1.00	0.00	0.424	0.00	0.00
ATOM	2099	C	SER	236	-11.831	11.003	31.653	1.00	0.00	0.396	9.82	4.00
ATOM	2100	O	SER	236	-10.817	11.691	31.766	1.00	0.00	-0.396	8.17	-17.40
ATOM	2101	N	LEU	237	-11.975	10.096	30.694	1.00	0.00	-0.650	9.00	-17.40
ATOM	2102	HN	LEU	237	-12.827	9.518	30.676	1.00	0.00	0.440	0.00	0.00
ATOM	2103	CA	LEU	237	-10.956	9.891	29.658	1.00	0.00	0.158	9.40	4.00
ATOM	2104	HA	LEU	237	-10.044	10.372	30.010	1.00	0.00	0.053	0.00	0.00
ATOM	2105	CB	LEU	237	-10.773	8.403	29.366	1.00	0.00	-0.106	12.77	4.00
ATOM	2106	HB1	LEU	237	-10.259	8.337	28.407	1.00	0.00	0.053	0.00	0.00
ATOM	2107	HB2	LEU	237	-11.772	7.969	29.330	1.00	0.00	0.053	0.00	0.00
ATOM	2108	CG	LEU	237	-9.979	7.494	30.306	1.00	0.00	-0.053	9.40	4.00
ATOM	2109	HG	LEU	237	-10.427	7.538	31.298	1.00	0.00	0.053	0.00	0.00
ATOM	2110	CD1	LEU	237	-10.031	6.061	29.766	1.00	0.00	-0.159	16.15	4.00
ATOM	2111	HD1	LEU	237	-9.468	5.402	30.427	1.00	0.00	0.053	0.00	0.00
ATOM	2112	HD1	LEU	237	-11.067	5.727	29.718	1.00	0.00	0.053	0.00	0.00
ATOM	2113	HD1	LEU	237	-9.594	6.032	28.768	1.00	0.00	0.053	0.00	0.00
ATOM	2114	CD2	LEU	237	-8.537	8.009	30.421	1.00	0.00	-0.159	16.15	4.00
ATOM	2115	HD2	LEU	237	-7.971	7.361	31.090	1.00	0.00	0.053	0.00	0.00
ATOM	2116	HD2	LEU	237	-8.070	8.007	29.436	1.00	0.00	0.053	0.00	0.00
ATOM	2117	HD2	LEU	237	-8.543	9.024	30.818	1.00	0.00	0.053	0.00	0.00
ATOM	2118	C	LEU	237	-11.483	10.536	28.385	1.00	0.00	0.396	9.82	4.00
ATOM	2119	O	LEU	237	-12.657	10.350	28.035	1.00	0.00	-0.396	8.17	-17.40
ATOM	2120	N	TRP	238	-10.647	11.291	27.670	1.00	0.00	-0.650	9.00	-17.40
ATOM	2121	HN	TRP	238	-9.681	11.454	27.987	1.00	0.00	0.440	0.00	0.00
ATOM	2122	CA	TRP	238	-11.134	11.879	26.428	1.00	0.00	0.158	9.40	4.00
ATOM	2123	HA	TRP	238	-12.167	11.615	26.203	1.00	0.00	0.053	0.00	0.00

ATOM	2124	CB	TRP	238	-11.227	13.409	26.560	1.00	0.00	-0.106	12.77	4.00
ATOM	2125	HB1	TRP	238	-11.649	13.629	27.540	1.00	0.00	0.053	0.00	0.00
ATOM	2126	HB2	TRP	238	-11.873	13.769	25.759	1.00	0.00	0.053	0.00	0.00
ATOM	2127	CG	TRP	238	-9.950	14.186	26.461	1.00	0.00	0.000	7.26	0.60
ATOM	2128	CD2	TRP	238	-9.818	15.532	25.987	1.00	0.00	0.000	6.80	0.60
ATOM	2129	CE2	TRP	238	-8.458	15.893	26.116	1.00	0.00	-0.050	6.80	0.60
ATOM	2130	CD1	TRP	238	-8.700	13.790	26.847	1.00	0.00	-0.177	10.80	0.60
ATOM	2131	HD1	TRP	238	-8.453	12.811	27.258	1.00	0.00	0.127	0.00	0.00
ATOM	2132	NE1	TRP	238	-7.794	14.814	26.639	1.00	0.00	-0.292	9.00	-17.40
ATOM	2133	HE1	TRP	238	-6.785	14.772	26.843	1.00	0.00	0.393	0.00	0.00
ATOM	2134	CE3	TRP	238	-10.723	16.469	25.469	1.00	0.00	-0.127	10.80	0.60
ATOM	2135	HE3	TRP	238	-11.779	16.221	25.361	1.00	0.00	0.127	0.00	0.00
ATOM	2136	CZ2	TRP	238	-7.978	17.155	25.742	1.00	0.00	-0.127	10.80	0.60
ATOM	2137	HZ2	TRP	238	-6.925	17.415	25.851	1.00	0.00	0.127	0.00	0.00
ATOM	2138	CZ3	TRP	238	-10.245	17.723	25.094	1.00	0.00	-0.127	10.80	0.60
ATOM	2139	HZ3	TRP	238	-10.936	18.460	24.687	1.00	0.00	0.127	0.00	0.00
ATOM	2140	CH2	TRP	238	-8.885	18.052	25.232	1.00	0.00	-0.127	10.80	0.60
ATOM	2141	HH2	TRP	238	-8.542	19.041	24.927	1.00	0.00	0.127	0.00	0.00
ATOM	2142	C	TRP	238	-10.325	11.449	25.196	1.00	0.00	0.396	9.82	4.00
ATOM	2143	O	TRP	238	-10.612	11.864	24.069	1.00	0.00	-0.396	8.17	-17.40
ATOM	2144	N	CYS	239	-9.332	10.588	25.409	1.00	0.00	-0.650	9.00	-17.40
ATOM	2145	HN	CYS	239	-9.126	10.276	26.369	1.00	0.00	0.440	0.00	0.00
ATOM	2146	CA	CYS	239	-8.531	10.080	24.298	1.00	0.00	0.158	9.40	4.00
ATOM	2147	HA	CYS	239	-9.208	9.728	23.520	1.00	0.00	0.053	0.00	0.00
ATOM	2148	C	CYS	239	-7.614	8.927	24.666	1.00	0.00	0.396	9.82	4.00
ATOM	2149	O	CYS	239	-7.362	8.670	25.840	1.00	0.00	-0.396	8.17	-17.40
ATOM	2150	CB	CYS	239	-7.707	11.227	23.693	1.00	0.00	-0.041	12.77	4.00
ATOM	2151	HB1	CYS	239	-8.043	12.145	24.174	1.00	0.00	0.053	0.00	0.00
ATOM	2152	HB2	CYS	239	-7.909	11.230	22.622	1.00	0.00	0.053	0.00	0.00
ATOM	2153	SG	CYS	239	-5.882	11.228	23.850	1.00	0.00	-0.065	19.93	-6.40
ATOM	2154	N	VAL	240	-7.156	8.205	23.649	1.00	0.00	-0.650	9.00	-17.40
ATOM	2155	HN	VAL	240	-7.491	8.414	22.698	1.00	0.00	0.440	0.00	0.00
ATOM	2156	CA	VAL	240	-6.195	7.127	23.835	1.00	0.00	0.158	9.40	4.00
ATOM	2157	HA	VAL	240	-5.818	7.109	24.857	1.00	0.00	0.053	0.00	0.00
ATOM	2158	CB	VAL	240	-6.787	5.728	23.542	1.00	0.00	-0.053	9.40	4.00
ATOM	2159	HB	VAL	240	-7.201	5.700	22.534	1.00	0.00	0.053	0.00	0.00
ATOM	2160	CG1	VAL	240	-5.671	4.637	23.660	1.00	0.00	-0.159	16.15	4.00
ATOM	2161	HG1	VAL	240	-6.097	3.655	23.452	1.00	0.00	0.053	0.00	0.00
ATOM	2162	HG1	VAL	240	-4.878	4.847	22.941	1.00	0.00	0.053	0.00	0.00
ATOM	2163	HG1	VAL	240	-5.258	4.646	24.668	1.00	0.00	0.053	0.00	0.00
ATOM	2164	CG2	VAL	240	-7.906	5.427	24.549	1.00	0.00	-0.159	16.15	4.00
ATOM	2165	HG2	VAL	240	-8.324	4.441	24.344	1.00	0.00	0.053	0.00	0.00
ATOM	2166	HG2	VAL	240	-7.500	5.445	25.560	1.00	0.00	0.053	0.00	0.00
ATOM	2167	HG2	VAL	240	-8.689	6.179	24.458	1.00	0.00	0.053	0.00	0.00
ATOM	2168	C	VAL	240	-5.098	7.465	22.831	1.00	0.00	0.396	9.82	4.00
ATOM	2169	O	VAL	240	-5.346	7.555	21.619	1.00	0.00	-0.396	8.17	-17.40
ATOM	2170	N	SER	241	-3.886	7.666	23.338	1.00	0.00	-0.650	9.00	-17.40
ATOM	2171	HN	SER	241	-3.737	7.559	24.351	1.00	0.00	0.440	0.00	0.00
ATOM	2172	CA	SER	241	-2.763	8.035	22.486	1.00	0.00	0.158	9.40	4.00
ATOM	2173	HA	SER	241	-3.051	8.200	21.448	1.00	0.00	0.053	0.00	0.00
ATOM	2174	CB	SER	241	-2.174	9.372	22.968	1.00	0.00	0.007	12.77	4.00
ATOM	2175	HB1	SER	241	-1.908	9.325	24.024	1.00	0.00	0.053	0.00	0.00
ATOM	2176	HB2	SER	241	-2.889	10.184	22.839	1.00	0.00	0.053	0.00	0.00
ATOM	2177	OG	SER	241	-1.002	9.705	22.240	1.00	0.00	-0.537	11.04	-17.40
ATOM	2178	HG	SER	241	-0.490	10.449	22.734	1.00	0.00	0.424	0.00	0.00
ATOM	2179	C	SER	241	-1.667	6.970	22.446	1.00	0.00	0.396	9.82	4.00
ATOM	2180	O	SER	241	-1.415	6.272	23.431	1.00	0.00	-0.396	8.17	-17.40
ATOM	2181	N	ALA	242	-1.035	6.839	21.286	1.00	0.00	-0.650	9.00	-17.40
ATOM	2182	HN	ALA	242	-1.322	7.435	20.496	1.00	0.00	0.440	0.00	0.00
ATOM	2183	CA	ALA	242	0.049	5.886	21.084	1.00	0.00	0.158	9.40	4.00
ATOM	2184	HA	ALA	242	-0.148	4.950	21.608	1.00	0.00	0.053	0.00	0.00
ATOM	2185	CB	ALA	242	0.200	5.606	19.596	1.00	0.00	-0.159	16.15	4.00
ATOM	2186	HB1	ALA	242	1.010	4.893	19.440	1.00	0.00	0.053	0.00	0.00
ATOM	2187	HB2	ALA	242	-0.729	5.189	19.208	1.00	0.00	0.053	0.00	0.00
ATOM	2188	HB3	ALA	242	0.427	6.534	19.072	1.00	0.00	0.053	0.00	0.00
ATOM	2189	C	ALA	242	1.372	6.442	21.603	1.00	0.00	0.396	9.82	4.00
ATOM	2190	O	ALA	242	2.348	5.707	21.782	1.00	0.00	-0.396	8.17	-17.40
ATOM	2191	N	TRP	243	1.383	7.735	21.882	1.00	0.00	-0.650	9.00	-17.40
ATOM	2192	HN	TRP	243	0.498	8.260	21.839	1.00	0.00	0.440	0.00	0.00
ATOM	2193	CA	TRP	243	2.607	8.442	22.249	1.00	0.00	0.158	9.40	4.00
ATOM	2194	HA	TRP	243	3.428	7.891	21.790	1.00	0.00	0.053	0.00	0.00
ATOM	2195	CB	TRP	243	2.547	9.806	21.533	1.00	0.00	-0.106	12.77	4.00
ATOM	2196	HB1	TRP	243	1.857	10.441	22.088	1.00	0.00	0.053	0.00	0.00
ATOM	2197	HB2	TRP	243	2.191	9.631	20.517	1.00	0.00	0.053	0.00	0.00
ATOM	2198	CG	TRP	243	3.842	10.566	21.416	1.00	0.00	0.000	7.26	0.60
ATOM	2199	CD2	TRP	243	4.825	10.422	20.378	1.00	0.00	0.000	6.80	0.60

ATOM	2200	CE2	TRP	243	5.872	11.332	20.659	1.00	0.00	-0.050	6.80	0.60
ATOM	2201	CD1	TRP	243	4.317	11.529	22.265	1.00	0.00	-0.177	10.80	0.60
ATOM	2202	HD1	TRP	243	3.807	11.876	23.163	1.00	0.00	0.127	0.00	0.00
ATOM	2203	NE1	TRP	243	5.543	11.998	21.813	1.00	0.00	-0.292	9.00	-17.40
ATOM	2204	HE1	TRP	243	6.111	12.725	22.268	1.00	0.00	0.393	0.00	0.00
ATOM	2205	CE3	TRP	243	4.917	9.615	19.234	1.00	0.00	-0.127	10.80	0.60
ATOM	2206	HE3	TRP	243	4.127	8.904	18.990	1.00	0.00	0.127	0.00	0.00
ATOM	2207	CZ2	TRP	243	6.998	11.455	19.839	1.00	0.00	-0.127	10.80	0.60
ATOM	2208	HZ2	TRP	243	7.793	12.161	20.075	1.00	0.00	0.127	0.00	0.00
ATOM	2209	CZ3	TRP	243	6.043	9.741	18.412	1.00	0.00	-0.127	10.80	0.60
ATOM	2210	HZ3	TRP	243	6.127	9.123	17.517	1.00	0.00	0.127	0.00	0.00
ATOM	2211	CH2	TRP	243	7.067	10.654	18.725	1.00	0.00	-0.127	10.80	0.60
ATOM	2212	HH2	TRP	243	7.934	10.727	18.069	1.00	0.00	0.127	0.00	0.00
ATOM	2213	C	TRP	243	3.031	8.636	23.709	1.00	0.00	0.396	9.82	4.00
ATOM	2214	O	TRP	243	2.241	9.068	24.560	1.00	0.00	-0.396	8.17	-17.40
ATOM	2215	N	ASN	244	4.293	8.295	23.993	1.00	0.00	-0.650	9.00	-17.40
ATOM	2216	HN	ASN	244	4.879	7.863	23.264	1.00	0.00	0.440	0.00	0.00
ATOM	2217	CA	ASN	244	4.853	8.528	25.328	1.00	0.00	0.158	9.40	4.00
ATOM	2218	HA	ASN	244	4.068	8.770	26.044	1.00	0.00	0.053	0.00	0.00
ATOM	2219	CB	ASN	244	5.631	7.304	25.846	1.00	0.00	-0.106	12.77	4.00
ATOM	2220	HB1	ASN	244	6.383	6.965	25.134	1.00	0.00	0.053	0.00	0.00
ATOM	2221	HB2	ASN	244	4.976	6.454	26.039	1.00	0.00	0.053	0.00	0.00
ATOM	2222	CG	ASN	244	6.371	7.603	27.165	1.00	0.00	0.396	9.82	4.00
ATOM	2223	OD1	ASN	244	6.322	8.732	27.667	1.00	0.00	-0.396	8.17	-17.40
ATOM	2224	ND2	ASN	244	7.056	6.605	27.717	1.00	0.00	-0.879	13.25	-17.40
ATOM	2225	HD2	ASN	244	7.070	5.679	27.266	1.00	0.00	0.440	0.00	0.00
ATOM	2226	HD2	ASN	244	7.571	6.758	28.595	1.00	0.00	0.440	0.00	0.00
ATOM	2227	C	ASN	244	5.811	9.709	25.112	1.00	0.00	0.396	9.82	4.00
ATOM	2228	O	ASN	244	6.852	9.561	24.464	1.00	0.00	-0.396	8.17	-17.40
ATOM	2229	N	ASP	245P	5.462	10.886	25.621	1.00	0.00	-0.650	9.00	-17.40
ATOM	2230	HN	ASP	245P	4.590	10.966	26.164	1.00	0.00	0.440	0.00	0.00
ATOM	2231	CA	ASP	245P	6.302	12.073	25.419	1.00	0.00	0.158	9.40	4.00
ATOM	2232	HA	ASP	245P	6.322	12.290	24.351	1.00	0.00	0.053	0.00	0.00
ATOM	2233	CB	ASP	245P	5.640	13.286	26.072	1.00	0.00	-0.336	12.77	4.00
ATOM	2234	HB1	ASP	245P	6.340	14.109	26.212	1.00	0.00	0.053	0.00	0.00
ATOM	2235	HB2	ASP	245P	5.231	13.050	27.054	1.00	0.00	0.053	0.00	0.00
ATOM	2236	CG	ASP	245P	4.496	13.825	25.243	1.00	0.00	0.297	9.82	4.00
ATOM	2237	OD1	ASP	245P	4.764	14.540	24.250	1.00	0.00	-0.534	8.17	-18.95
ATOM	2238	OD2	ASP	245P	3.326	13.522	25.566	1.00	0.00	-0.534	8.17	-18.95
ATOM	2239	C	ASP	245P	7.759	11.953	25.881	1.00	0.00	0.396	9.82	4.00
ATOM	2240	O	ASP	245P	8.640	12.658	25.368	1.00	0.00	-0.396	8.17	-17.40
ATOM	2241	N	ASN	246	8.005	11.068	26.848	1.00	0.00	-0.650	9.00	-17.40
ATOM	2242	HN	ASN	246	7.218	10.532	27.242	1.00	0.00	0.440	0.00	0.00
ATOM	2243	CA	ASN	246	9.346	10.830	27.368	1.00	0.00	0.158	9.40	4.00
ATOM	2244	HA	ASN	246	10.031	11.553	26.927	1.00	0.00	0.053	0.00	0.00
ATOM	2245	CB	ASN	246	9.352	10.992	28.891	1.00	0.00	-0.106	12.77	4.00
ATOM	2246	HB1	ASN	246	10.307	10.715	29.336	1.00	0.00	0.053	0.00	0.00
ATOM	2247	HB2	ASN	246	8.597	10.375	29.379	1.00	0.00	0.053	0.00	0.00
ATOM	2248	CG	ASN	246	9.079	12.418	29.324	1.00	0.00	0.396	9.82	4.00
ATOM	2249	OD1	ASN	246	9.828	13.339	28.973	1.00	0.00	-0.396	8.17	-17.40
ATOM	2250	ND2	ASN	246	8.003	12.615	30.081	1.00	0.00	-0.879	13.25	-17.40
ATOM	2251	HD2	ASN	246	7.408	11.817	30.348	1.00	0.00	0.440	0.00	0.00
ATOM	2252	HD2	ASN	246	7.764	13.565	30.399	1.00	0.00	0.440	0.00	0.00
ATOM	2253	C	ASN	246	9.781	9.407	26.998	1.00	0.00	0.396	9.82	4.00
ATOM	2254	O	ASN	246	10.603	8.793	27.678	1.00	0.00	-0.396	8.17	-17.40
ATOM	2255	N	GLY	247	9.233	8.896	25.900	1.00	0.00	-0.650	9.00	-17.40
ATOM	2256	HN	GLY	247	8.583	9.468	25.341	1.00	0.00	0.440	0.00	0.00
ATOM	2257	CA	GLY	247	9.539	7.543	25.480	1.00	0.00	0.105	9.40	4.00
ATOM	2258	HA1	GLY	247	8.755	7.241	24.784	1.00	0.00	0.053	0.00	0.00
ATOM	2259	HA2	GLY	247	9.545	6.925	26.378	1.00	0.00	0.053	0.00	0.00
ATOM	2260	C	GLY	247	10.854	7.253	24.771	1.00	0.00	0.396	9.82	4.00
ATOM	2261	O	GLY	247	10.866	6.480	23.805	1.00	0.00	-0.396	8.17	-17.40
ATOM	2262	N	LYS	248S	11.950	7.859	25.225	1.00	0.00	-0.650	9.00	-17.40
ATOM	2263	HN	LYS	248S	11.871	8.516	26.014	1.00	0.00	0.440	0.00	0.00
ATOM	2264	CA	LYS	248S	13.261	7.613	24.629	1.00	0.00	0.158	9.40	4.00
ATOM	2265	HA	LYS	248S	13.151	7.684	23.547	1.00	0.00	0.053	0.00	0.00
ATOM	2266	CB	LYS	248S	14.268	8.657	25.116	1.00	0.00	-0.106	12.77	4.00
ATOM	2267	HB1	LYS	248S	15.222	8.466	24.625	1.00	0.00	0.053	0.00	0.00
ATOM	2268	HB2	LYS	248S	14.365	8.559	26.197	1.00	0.00	0.053	0.00	0.00
ATOM	2269	CG	LYS	248S	13.874	10.104	24.815	1.00	0.00	-0.106	12.77	4.00
ATOM	2270	HG1	LYS	248S	12.915	10.317	25.288	1.00	0.00	0.053	0.00	0.00
ATOM	2271	HG2	LYS	248S	13.791	10.232	23.735	1.00	0.00	0.053	0.00	0.00
ATOM	2272	CD	LYS	248S	14.945	11.036	25.369	1.00	0.00	-0.106	12.77	4.00
ATOM	2273	HD1	LYS	248S	15.927	10.871	24.925	1.00	0.00	0.053	0.00	0.00
ATOM	2274	HD2	LYS	248S	15.088	10.932	26.444	1.00	0.00	0.053	0.00	0.00
ATOM	2275	CE	LYS	248S	14.636	12.501	25.140	1.00	0.00	0.099	12.77	4.00

ATOM	2276	HE1	LYS	248S	13.672	12.743	25.587	1.00	0.00	0.053	0.00	0.00
ATOM	2277	HE2	LYS	248S	14.600	12.701	24.069	1.00	0.00	0.053	0.00	0.00
ATOM	2278	NZ	LYS	248S	15.711	13.346	25.774	1.00	0.00	-0.045	13.25	-39.20
ATOM	2279	HZ1	LYS	248S	15.501	14.342	25.618	1.00	0.00	0.280	0.00	0.00
ATOM	2280	HZ2	LYS	248S	15.745	13.156	26.786	1.00	0.00	0.280	0.00	0.00
ATOM	2281	HZ3	LYS	248S	16.622	13.117	25.351	1.00	0.00	0.280	0.00	0.00
ATOM	2282	C	LYS	248S	13.708	6.208	25.049	1.00	0.00	0.396	9.82	4.00
ATOM	2283	O	LYS	248S	13.255	5.698	26.075	1.00	0.00	-0.396	8.17	-17.40
ATOM	2284	N	GLU	249	14.601	5.588	24.280	1.00	0.00	-0.650	9.00	-17.40
ATOM	2285	HN	GLU	249	14.995	6.078	23.464	1.00	0.00	0.440	0.00	0.00
ATOM	2286	CA	GLU	249	15.030	4.221	24.576	1.00	0.00	0.158	9.40	4.00
ATOM	2287	HA	GLU	249	14.178	3.563	24.402	1.00	0.00	0.053	0.00	0.00
ATOM	2288	CB	GLU	249	16.104	3.755	23.577	1.00	0.00	-0.106	12.77	4.00
ATOM	2289	HB1	GLU	249	16.995	4.365	23.721	1.00	0.00	0.053	0.00	0.00
ATOM	2290	HB2	GLU	249	15.712	3.882	22.567	1.00	0.00	0.053	0.00	0.00
ATOM	2291	CG	GLU	249	16.516	2.266	23.742	1.00	0.00	-0.106	12.77	4.00
ATOM	2292	HG1	GLU	249	15.701	1.569	23.542	1.00	0.00	0.053	0.00	0.00
ATOM	2293	HG2	GLU	249	16.864	2.024	24.746	1.00	0.00	0.053	0.00	0.00
ATOM	2294	CD	GLU	249	17.659	1.842	22.798	1.00	0.00	0.399	9.82	4.00
ATOM	2295	OE1	GLU	249	17.425	1.664	21.581	1.00	0.00	-0.396	8.17	-18.95
ATOM	2296	OE2	GLU	249	18.804	1.697	23.276	1.00	0.00	-0.427	8.17	-18.95
ATOM	2297	HE2	GLU	249	19.457	1.424	22.527	1.00	0.00	0.424	0.00	0.00
ATOM	2298	C	GLU	249	15.519	3.940	25.993	1.00	0.00	0.396	9.82	4.00
ATOM	2299	O	GLU	249	15.109	2.958	26.593	1.00	0.00	-0.396	8.17	-17.40
ATOM	2300	N	GLN	250	16.398	4.776	26.531	1.00	0.00	-0.650	9.00	-17.40
ATOM	2301	HN	GLN	250	16.715	5.601	26.002	1.00	0.00	0.440	0.00	0.00
ATOM	2302	CA	GLN	250	16.913	4.524	27.871	1.00	0.00	0.158	9.40	4.00
ATOM	2303	HA	GLN	250	17.095	3.470	28.081	1.00	0.00	0.053	0.00	0.00
ATOM	2304	CB	GLN	250	18.293	5.177	28.048	1.00	0.00	-0.106	12.77	4.00
ATOM	2305	HB1	GLN	250	18.605	5.034	29.082	1.00	0.00	0.053	0.00	0.00
ATOM	2306	HB2	GLN	250	18.198	6.237	27.815	1.00	0.00	0.053	0.00	0.00
ATOM	2307	CG	GLN	250	19.398	4.607	27.152	1.00	0.00	-0.106	12.77	4.00
ATOM	2308	HG1	GLN	250	20.383	5.025	27.355	1.00	0.00	0.053	0.00	0.00
ATOM	2309	HG2	GLN	250	19.230	4.780	26.089	1.00	0.00	0.053	0.00	0.00
ATOM	2310	CD	GLN	250	19.574	3.093	27.285	1.00	0.00	0.396	9.82	4.00
ATOM	2311	OE1	GLN	250	19.674	2.550	28.396	1.00	0.00	-0.396	8.17	-17.40
ATOM	2312	NE2	GLN	250	19.625	2.406	26.148	1.00	0.00	-0.879	13.25	-17.40
ATOM	2313	HE2	GLN	250	19.537	2.895	25.246	1.00	0.00	0.440	0.00	0.00
ATOM	2314	HE2	GLN	250	19.751	1.384	26.169	1.00	0.00	0.440	0.00	0.00
ATOM	2315	C	GLN	250	15.979	4.990	28.990	1.00	0.00	0.396	9.82	4.00
ATOM	2316	O	GLN	250	16.310	4.860	30.172	1.00	0.00	-0.396	8.17	-17.40
ATOM	2317	N	MET	251	14.810	5.515	28.619	1.00	0.00	-0.650	9.00	-17.40
ATOM	2318	HN	MET	251	14.582	5.579	27.616	1.00	0.00	0.440	0.00	0.00
ATOM	2319	CA	MET	251	13.851	5.997	29.596	1.00	0.00	0.158	9.40	4.00
ATOM	2320	HA	MET	251	14.329	5.980	30.575	1.00	0.00	0.053	0.00	0.00
ATOM	2321	CB	MET	251	13.527	7.464	29.321	1.00	0.00	-0.106	12.77	4.00
ATOM	2322	HB1	MET	251	12.678	7.806	29.913	1.00	0.00	0.053	0.00	0.00
ATOM	2323	HB2	MET	251	13.276	7.631	28.273	1.00	0.00	0.053	0.00	0.00
ATOM	2324	CG	MET	251	14.722	8.385	29.658	1.00	0.00	-0.041	12.77	4.00
ATOM	2325	HG1	MET	251	15.568	8.089	29.038	1.00	0.00	0.053	0.00	0.00
ATOM	2326	HG2	MET	251	14.960	8.264	30.714	1.00	0.00	0.053	0.00	0.00
ATOM	2327	SD	MET	251	14.415	10.108	29.367	1.00	0.00	-0.130	16.39	-6.40
ATOM	2328	CE	MET	251	13.476	10.468	30.775	1.00	0.00	-0.094	16.15	4.00
ATOM	2329	HE1	MET	251	13.190	11.519	30.762	1.00	0.00	0.053	0.00	0.00
ATOM	2330	HE2	MET	251	12.579	9.848	30.782	1.00	0.00	0.053	0.00	0.00
ATOM	2331	HE3	MET	251	14.066	10.262	31.668	1.00	0.00	0.053	0.00	0.00
ATOM	2332	C	MET	251	12.566	5.184	29.706	1.00	0.00	0.396	9.82	4.00
ATOM	2333	O	MET	251	11.623	5.608	30.378	1.00	0.00	-0.396	8.17	-17.40
ATOM	2334	N	VAL	252	12.518	4.036	29.034	1.00	0.00	-0.650	9.00	-17.40
ATOM	2335	HN	VAL	252	13.323	3.754	28.457	1.00	0.00	0.440	0.00	0.00
ATOM	2336	CA	VAL	252	11.346	3.167	29.098	1.00	0.00	0.158	9.40	4.00
ATOM	2337	HA	VAL	252	10.677	3.561	29.862	1.00	0.00	0.053	0.00	0.00
ATOM	2338	CB	VAL	252	10.556	3.105	27.742	1.00	0.00	-0.053	9.40	4.00
ATOM	2339	HB	VAL	252	9.651	2.508	27.857	1.00	0.00	0.053	0.00	0.00
ATOM	2340	CG1	VAL	252	10.159	4.509	27.295	1.00	0.00	-0.159	16.15	4.00
ATOM	2341	HG1	VAL	252	9.612	4.450	26.354	1.00	0.00	0.053	0.00	0.00
ATOM	2342	HG1	VAL	252	9.525	4.967	28.054	1.00	0.00	0.053	0.00	0.00
ATOM	2343	HG1	VAL	252	11.055	5.113	27.156	1.00	0.00	0.053	0.00	0.00
ATOM	2344	CG2	VAL	252	11.403	2.430	26.653	1.00	0.00	-0.159	16.15	4.00
ATOM	2345	HG2	VAL	252	10.838	2.396	25.721	1.00	0.00	0.053	0.00	0.00
ATOM	2346	HG2	VAL	252	12.320	2.998	26.501	1.00	0.00	0.053	0.00	0.00
ATOM	2347	HG2	VAL	252	11.652	1.415	26.962	1.00	0.00	0.053	0.00	0.00
ATOM	2348	C	VAL	252	11.823	1.760	29.461	1.00	0.00	0.396	9.82	4.00
ATOM	2349	O	VAL	252	12.972	1.388	29.156	1.00	0.00	-0.396	8.17	-17.40
ATOM	2350	N	ASP	253P	10.942	0.996	30.111	1.00	0.00	-0.650	9.00	-17.40
ATOM	2351	HN	ASP	253P	10.019	1.398	30.327	1.00	0.00	0.440	0.00	0.00

ATOM	2352	CA	ASP	253P	11.211	-0.386	30.536	1.00	0.00	0.158	9.40	4.00
ATOM	2353	HA	ASP	253P	12.275	-0.511	30.736	1.00	0.00	0.053	0.00	0.00
ATOM	2354	CB	ASP	253P	10.422	-0.693	31.816	1.00	0.00	-0.336	12.77	4.00
ATOM	2355	HB1	ASP	253P	9.345	-0.739	31.650	1.00	0.00	0.053	0.00	0.00
ATOM	2356	HB2	ASP	253P	10.570	0.054	32.595	1.00	0.00	0.053	0.00	0.00
ATOM	2357	CG	ASP	253P	10.804	-2.027	32.442	1.00	0.00	0.297	9.82	4.00
ATOM	2358	OD1	ASP	253P	11.407	-2.881	31.753	1.00	0.00	-0.534	8.17	-18.95
ATOM	2359	OD2	ASP	253P	10.487	-2.230	33.635	1.00	0.00	-0.534	8.17	-18.95
ATOM	2360	C	ASP	253P	10.790	-1.363	29.429	1.00	0.00	0.396	9.82	4.00
ATOM	2361	O	ASP	253P	9.592	-1.666	29.263	1.00	0.00	-0.396	8.17	-17.40
ATOM	2362	N	SER	254	11.773	-1.870	28.688	1.00	0.00	-0.650	9.00	-17.40
ATOM	2363	HN	SER	254	12.746	-1.604	28.894	1.00	0.00	0.440	0.00	0.00
ATOM	2364	CA	SER	254	11.505	-2.794	27.589	1.00	0.00	0.158	9.40	4.00
ATOM	2365	HA	SER	254	10.800	-2.318	26.906	1.00	0.00	0.053	0.00	0.00
ATOM	2366	CB	SER	254	12.791	-3.050	26.796	1.00	0.00	0.007	12.77	4.00
ATOM	2367	HB1	SER	254	13.130	-2.140	26.301	1.00	0.00	0.053	0.00	0.00
ATOM	2368	HB2	SER	254	12.631	-3.809	26.030	1.00	0.00	0.053	0.00	0.00
ATOM	2369	OG	SER	254	13.828	-3.498	27.647	1.00	0.00	-0.537	11.04	-17.40
ATOM	2370	HG	SER	254	13.772	-3.001	28.547	1.00	0.00	0.424	0.00	0.00
ATOM	2371	C	SER	254	10.903	-4.125	28.021	1.00	0.00	0.396	9.82	4.00
ATOM	2372	O	SER	254	10.421	-4.887	27.182	1.00	0.00	-0.396	8.17	-17.40
ATOM	2373	N	SER	255	10.930	-4.405	29.323	1.00	0.00	-0.650	9.00	-17.40
ATOM	2374	HN	SER	255	11.344	-3.725	29.977	1.00	0.00	0.440	0.00	0.00
ATOM	2375	CA	SER	255	10.382	-5.660	29.842	1.00	0.00	0.158	9.40	4.00
ATOM	2376	HA	SER	255	10.462	-6.442	29.087	1.00	0.00	0.053	0.00	0.00
ATOM	2377	CB	SER	255	11.165	-6.152	31.069	1.00	0.00	0.007	12.77	4.00
ATOM	2378	HB1	SER	255	12.241	-6.034	30.941	1.00	0.00	0.053	0.00	0.00
ATOM	2379	HB2	SER	255	10.985	-7.207	31.272	1.00	0.00	0.053	0.00	0.00
ATOM	2380	OG	SER	255	10.811	-5.441	32.247	1.00	0.00	-0.537	11.04	-17.40
ATOM	2381	HG	SER	255	11.211	-4.492	32.209	1.00	0.00	0.424	0.00	0.00
ATOM	2382	C	SER	255	8.912	-5.476	30.209	1.00	0.00	0.396	9.82	4.00
ATOM	2383	O	SER	255	8.248	-6.420	30.659	1.00	0.00	-0.396	8.17	-17.40
ATOM	2384	N	LYS	256S	8.402	-4.257	30.022	1.00	0.00	-0.650	9.00	-17.40
ATOM	2385	HN	LYS	256S	9.013	-3.501	29.680	1.00	0.00	0.440	0.00	0.00
ATOM	2386	CA	LYS	256S	6.985	-3.969	30.293	1.00	0.00	0.158	9.40	4.00
ATOM	2387	HA	LYS	256S	6.446	-4.891	30.510	1.00	0.00	0.053	0.00	0.00
ATOM	2388	CB	LYS	256S	6.843	-3.047	31.504	1.00	0.00	-0.106	12.77	4.00
ATOM	2389	HB1	LYS	256S	5.804	-2.720	31.562	1.00	0.00	0.053	0.00	0.00
ATOM	2390	HB2	LYS	256S	7.508	-2.195	31.362	1.00	0.00	0.053	0.00	0.00
ATOM	2391	CG	LYS	256S	7.202	-3.696	32.864	1.00	0.00	-0.106	12.77	4.00
ATOM	2392	HG1	LYS	256S	7.191	-2.978	33.684	1.00	0.00	0.053	0.00	0.00
ATOM	2393	HG2	LYS	256S	8.195	-4.144	32.862	1.00	0.00	0.053	0.00	0.00
ATOM	2394	CD	LYS	256S	6.221	-4.819	33.259	1.00	0.00	-0.106	12.77	4.00
ATOM	2395	HD1	LYS	256S	6.527	-5.311	34.182	1.00	0.00	0.053	0.00	0.00
ATOM	2396	HD2	LYS	256S	6.159	-5.585	32.486	1.00	0.00	0.053	0.00	0.00
ATOM	2397	CE	LYS	256S	4.799	-4.274	33.480	1.00	0.00	0.099	12.77	4.00
ATOM	2398	HE1	LYS	256S	4.404	-3.795	32.583	1.00	0.00	0.053	0.00	0.00
ATOM	2399	HE2	LYS	256S	4.768	-3.531	34.277	1.00	0.00	0.053	0.00	0.00
ATOM	2400	NZ	LYS	256S	3.842	-5.356	33.855	1.00	0.00	-0.045	13.25	-39.20
ATOM	2401	HZ1	LYS	256S	2.904	-4.952	33.994	1.00	0.00	0.280	0.00	0.00
ATOM	2402	HZ2	LYS	256S	3.805	-6.058	33.102	1.00	0.00	0.280	0.00	0.00
ATOM	2403	HZ3	LYS	256S	4.155	-5.804	34.727	1.00	0.00	0.280	0.00	0.00
ATOM	2404	C	LYS	256S	6.337	-3.299	29.078	1.00	0.00	0.396	9.82	4.00
ATOM	2405	O	LYS	256S	5.740	-2.239	29.201	1.00	0.00	-0.396	8.17	-17.40
ATOM	2406	N	PRO	257	6.415	-3.920	27.889	1.00	0.00	-0.422	9.00	-17.40
ATOM	2407	CD	PRO	257	6.890	-5.261	27.482	1.00	0.00	0.105	12.77	4.00
ATOM	2408	HD1	PRO	257	6.549	-6.027	28.178	1.00	0.00	0.053	0.00	0.00
ATOM	2409	HD2	PRO	257	7.978	-5.300	27.451	1.00	0.00	0.053	0.00	0.00
ATOM	2410	CA	PRO	257	5.780	-3.209	26.777	1.00	0.00	0.158	9.40	4.00
ATOM	2411	HA	PRO	257	6.170	-2.191	26.753	1.00	0.00	0.053	0.00	0.00
ATOM	2412	CB	PRO	257	6.259	-3.987	25.560	1.00	0.00	-0.106	12.77	4.00
ATOM	2413	HB1	PRO	257	7.247	-3.656	25.240	1.00	0.00	0.053	0.00	0.00
ATOM	2414	HB2	PRO	257	5.581	-3.859	24.715	1.00	0.00	0.053	0.00	0.00
ATOM	2415	CG	PRO	257	6.269	-5.434	26.089	1.00	0.00	-0.106	12.77	4.00
ATOM	2416	HG1	PRO	257	6.863	-6.086	25.449	1.00	0.00	0.053	0.00	0.00
ATOM	2417	HG2	PRO	257	5.261	-5.847	26.133	1.00	0.00	0.053	0.00	0.00
ATOM	2418	C	PRO	257	4.254	-3.119	26.876	1.00	0.00	0.396	9.82	4.00
ATOM	2419	O	PRO	257	3.606	-2.371	26.114	1.00	0.00	-0.396	8.17	-17.40
ATOM	2420	N	GLU	258	3.675	-3.848	27.829	1.00	0.00	-0.650	9.00	-17.40
ATOM	2421	HN	GLU	258	4.259	-4.414	28.460	1.00	0.00	0.440	0.00	0.00
ATOM	2422	CA	GLU	258	2.226	-3.856	27.992	1.00	0.00	0.158	9.40	4.00
ATOM	2423	HA	GLU	258	1.704	-3.685	27.050	1.00	0.00	0.053	0.00	0.00
ATOM	2424	CB	GLU	258	1.753	-5.235	28.507	1.00	0.00	-0.106	12.77	4.00
ATOM	2425	HB1	GLU	258	2.284	-6.005	27.948	1.00	0.00	0.053	0.00	0.00
ATOM	2426	HB2	GLU	258	0.678	-5.308	28.340	1.00	0.00	0.053	0.00	0.00
ATOM	2427	CG	GLU	258	2.006	-5.497	30.010	1.00	0.00	-0.106	12.77	4.00

ATOM	2428	HG1	GLU	258	1.236	-6.178	30.372	1.00	0.00	0.053	0.00	0.00
ATOM	2429	HG2	GLU	258	1.954	-4.544	30.536	1.00	0.00	0.053	0.00	0.00
ATOM	2430	CD	GLU	258	3.374	-6.129	30.323	1.00	0.00	0.399	9.82	4.00
ATOM	2431	OE1	GLU	258	4.344	-5.931	29.558	1.00	0.00	-0.396	8.17	-18.95
ATOM	2432	OE2	GLU	258	3.485	-6.813	31.360	1.00	0.00	-0.427	8.17	-18.95
ATOM	2433	HE2	GLU	258	4.454	-7.150	31.447	1.00	0.00	0.424	0.00	0.00
ATOM	2434	C	GLU	258	1.748	-2.773	28.959	1.00	0.00	0.396	9.82	4.00
ATOM	2435	O	GLU	258	0.563	-2.454	29.007	1.00	0.00	-0.396	8.17	-17.40
ATOM	2436	N	LEU	259	2.673	-2.199	29.717	1.00	0.00	-0.650	9.00	-17.40
ATOM	2437	HN	LEU	259	3.661	-2.461	29.599	1.00	0.00	0.440	0.00	0.00
ATOM	2438	CA	LEU	259	2.306	-1.196	30.720	1.00	0.00	0.158	9.40	4.00
ATOM	2439	HA	LEU	259	1.564	-1.637	31.386	1.00	0.00	0.053	0.00	0.00
ATOM	2440	CB	LEU	259	3.517	-0.860	31.581	1.00	0.00	-0.106	12.77	4.00
ATOM	2441	HB1	LEU	259	4.256	-0.364	30.952	1.00	0.00	0.053	0.00	0.00
ATOM	2442	HB2	LEU	259	3.917	-1.789	31.985	1.00	0.00	0.053	0.00	0.00
ATOM	2443	CG	LEU	259	3.215	0.066	32.759	1.00	0.00	-0.053	9.40	4.00
ATOM	2444	HG	LEU	259	2.875	1.035	32.395	1.00	0.00	0.053	0.00	0.00
ATOM	2445	CD1	LEU	259	2.127	-0.539	33.634	1.00	0.00	-0.159	16.15	4.00
ATOM	2446	HD1	LEU	259	1.919	0.128	34.470	1.00	0.00	0.053	0.00	0.00
ATOM	2447	HD1	LEU	259	1.220	-0.675	33.045	1.00	0.00	0.053	0.00	0.00
ATOM	2448	HD1	LEU	259	2.461	-1.504	34.014	1.00	0.00	0.053	0.00	0.00
ATOM	2449	CD2	LEU	259	4.491	0.289	33.530	1.00	0.00	-0.159	16.15	4.00
ATOM	2450	HD2	LEU	259	4.294	0.948	34.375	1.00	0.00	0.053	0.00	0.00
ATOM	2451	HD2	LEU	259	4.867	-0.666	33.895	1.00	0.00	0.053	0.00	0.00
ATOM	2452	HD2	LEU	259	5.234	0.746	32.878	1.00	0.00	0.053	0.00	0.00
ATOM	2453	C	LEU	259	1.706	0.088	30.157	1.00	0.00	0.396	9.82	4.00
ATOM	2454	O	LEU	259	2.291	0.725	29.282	1.00	0.00	-0.396	8.17	-17.40
ATOM	2455	N	LEU	260	0.528	0.463	30.652	1.00	0.00	-0.650	9.00	-17.40
ATOM	2456	HN	LEU	260	0.071	-0.123	31.365	1.00	0.00	0.440	0.00	0.00
ATOM	2457	CA	LEU	260	-0.132	1.690	30.204	1.00	0.00	0.158	9.40	4.00
ATOM	2458	HA	LEU	260	0.476	2.185	29.447	1.00	0.00	0.053	0.00	0.00
ATOM	2459	CB	LEU	260	-1.506	1.394	29.575	1.00	0.00	-0.106	12.77	4.00
ATOM	2460	HB1	LEU	260	-1.901	2.326	29.171	1.00	0.00	0.053	0.00	0.00
ATOM	2461	HB2	LEU	260	-2.158	1.002	30.355	1.00	0.00	0.053	0.00	0.00
ATOM	2462	CG	LEU	260	-1.492	0.380	28.444	1.00	0.00	-0.053	9.40	4.00
ATOM	2463	HG	LEU	260	-1.066	-0.558	28.800	1.00	0.00	0.053	0.00	0.00
ATOM	2464	CD1	LEU	260	-2.931	0.135	27.954	1.00	0.00	-0.159	16.15	4.00
ATOM	2465	HD1	LEU	260	-2.920	-0.592	27.142	1.00	0.00	0.053	0.00	0.00
ATOM	2466	HD1	LEU	260	-3.535	-0.247	28.776	1.00	0.00	0.053	0.00	0.00
ATOM	2467	HD1	LEU	260	-3.357	1.071	27.595	1.00	0.00	0.053	0.00	0.00
ATOM	2468	CD2	LEU	260	-0.608	0.909	27.308	1.00	0.00	-0.159	16.15	4.00
ATOM	2469	HD2	LEU	260	-0.592	0.186	26.492	1.00	0.00	0.053	0.00	0.00
ATOM	2470	HD2	LEU	260	-1.008	1.856	26.946	1.00	0.00	0.053	0.00	0.00
ATOM	2471	HD2	LEU	260	0.406	1.060	27.677	1.00	0.00	0.053	0.00	0.00
ATOM	2472	C	LEU	260	-0.325	2.638	31.383	1.00	0.00	0.396	9.82	4.00
ATOM	2473	O	LEU	260	-0.217	2.222	32.547	1.00	0.00	-0.396	8.17	-17.40
ATOM	2474	N	TYR	261	-0.619	3.904	31.061	1.00	0.00	-0.650	9.00	-17.40
ATOM	2475	HN	TYR	261	-0.710	4.142	30.063	1.00	0.00	0.440	0.00	0.00
ATOM	2476	CA	TYR	261	-0.817	4.967	32.044	1.00	0.00	0.158	9.40	4.00
ATOM	2477	HA	TYR	261	-1.092	4.583	33.026	1.00	0.00	0.053	0.00	0.00
ATOM	2478	CB	TYR	261	0.445	5.833	32.161	1.00	0.00	-0.106	12.77	4.00
ATOM	2479	HB1	TYR	261	0.248	6.597	32.913	1.00	0.00	0.053	0.00	0.00
ATOM	2480	HB2	TYR	261	0.629	6.276	31.182	1.00	0.00	0.053	0.00	0.00
ATOM	2481	CG	TYR	261	1.735	5.144	32.573	1.00	0.00	0.000	7.26	0.60
ATOM	2482	CD1	TYR	261	2.511	4.445	31.654	1.00	0.00	-0.127	10.80	0.60
ATOM	2483	HD1	TYR	261	2.165	4.341	30.625	1.00	0.00	0.127	0.00	0.00
ATOM	2484	CE1	TYR	261	3.737	3.870	32.037	1.00	0.00	-0.127	10.80	0.60
ATOM	2485	HE1	TYR	261	4.344	3.328	31.311	1.00	0.00	0.127	0.00	0.00
ATOM	2486	CD2	TYR	261	2.202	5.250	33.882	1.00	0.00	-0.127	10.80	0.60
ATOM	2487	HD2	TYR	261	1.604	5.789	34.617	1.00	0.00	0.127	0.00	0.00
ATOM	2488	CE2	TYR	261	3.397	4.691	34.270	1.00	0.00	-0.127	10.80	0.60
ATOM	2489	HE2	TYR	261	3.738	4.792	35.300	1.00	0.00	0.127	0.00	0.00
ATOM	2490	CZ	TYR	261	4.162	4.002	33.352	1.00	0.00	0.026	7.26	0.60
ATOM	2491	OH	TYR	261	5.337	3.425	33.776	1.00	0.00	-0.451	10.94	-17.40
ATOM	2492	HH	TYR	261	5.223	3.082	34.741	1.00	0.00	0.424	0.00	0.00
ATOM	2493	C	TYR	261	-1.925	5.941	31.641	1.00	0.00	0.396	9.82	4.00
ATOM	2494	O	TYR	261	-2.400	5.940	30.503	1.00	0.00	-0.396	8.17	-17.40
ATOM	2495	N	ARG	262G	-2.298	6.799	32.590	1.00	0.00	-0.650	9.00	-17.40
ATOM	2496	HN	ARG	262G	-1.904	6.692	33.535	1.00	0.00	0.440	0.00	0.00
ATOM	2497	CA	ARG	262G	-3.240	7.882	32.343	1.00	0.00	0.158	9.40	4.00
ATOM	2498	HA	ARG	262G	-3.779	7.731	31.408	1.00	0.00	0.053	0.00	0.00
ATOM	2499	CB	ARG	262G	-4.244	8.052	33.510	1.00	0.00	-0.106	12.77	4.00
ATOM	2500	HB1	ARG	262G	-4.715	9.029	33.409	1.00	0.00	0.053	0.00	0.00
ATOM	2501	HB2	ARG	262G	-3.688	7.982	34.445	1.00	0.00	0.053	0.00	0.00
ATOM	2502	CG	ARG	262G	-5.377	7.001	33.571	1.00	0.00	-0.106	12.77	4.00
ATOM	2503	HG1	ARG	262G	-4.977	5.993	33.688	1.00	0.00	0.053	0.00	0.00

ATOM	2504	HG2	ARG	262G	-5.977	7.012	32.661	1.00	0.00	0.053	0.00	0.00
ATOM	2505	CD	ARG	262G	-6.332	7.268	34.766	1.00	0.00	0.374	12.77	4.00
ATOM	2506	HD1	ARG	262G	-5.802	7.478	35.695	1.00	0.00	0.053	0.00	0.00
ATOM	2507	HD2	ARG	262G	-6.987	6.424	34.984	1.00	0.00	0.053	0.00	0.00
ATOM	2508	NE	ARG	262G	-7.220	8.415	34.545	1.00	0.00	-0.819	9.00	-24.67
ATOM	2509	HE	ARG	262G	-6.838	9.357	34.707	1.00	0.00	0.407	0.00	0.00
ATOM	2510	CZ	ARG	262G	-8.491	8.316	34.147	1.00	0.00	0.796	6.95	4.00
ATOM	2511	NH1	ARG	262G	-9.038	7.124	33.922	1.00	0.00	-0.746	9.00	-24.67
ATOM	2512	HH1	ARG	262G	-10.019	7.057	33.615	1.00	0.00	0.407	0.00	0.00
ATOM	2513	HH1	ARG	262G	-8.480	6.268	34.054	1.00	0.00	0.407	0.00	0.00
ATOM	2514	NH2	ARG	262G	-9.224	9.411	33.971	1.00	0.00	-0.746	9.00	-24.67
ATOM	2515	HH2	ARG	262G	-10.203	9.330	33.664	1.00	0.00	0.407	0.00	0.00
ATOM	2516	HH2	ARG	262G	-8.812	10.339	34.141	1.00	0.00	0.407	0.00	0.00
ATOM	2517	C	ARG	262G	-2.318	9.119	32.290	1.00	0.00	0.396	9.82	4.00
ATOM	2518	O	ARG	262G	-1.275	9.140	32.968	1.00	0.00	-0.396	8.17	-17.40
ATOM	2519	N	THR	263	-2.665	10.114	31.466	1.00	0.00	-0.650	9.00	-17.40
ATOM	2520	HN	THR	263	-3.487	9.990	30.858	1.00	0.00	0.440	0.00	0.00
ATOM	2521	CA	THR	263	-1.912	11.385	31.395	1.00	0.00	0.158	9.40	4.00
ATOM	2522	HA	THR	263	-1.366	11.577	32.319	1.00	0.00	0.053	0.00	0.00
ATOM	2523	CB	THR	263	-0.856	11.436	30.258	1.00	0.00	0.060	9.40	4.00
ATOM	2524	HB	THR	263	-0.091	10.671	30.396	1.00	0.00	0.053	0.00	0.00
ATOM	2525	OG1	THR	263	-0.248	12.740	30.256	1.00	0.00	-0.537	11.04	-17.40
ATOM	2526	HG1	THR	263	0.777	12.641	30.257	1.00	0.00	0.424	0.00	0.00
ATOM	2527	CG2	THR	263	-1.497	11.208	28.906	1.00	0.00	-0.159	16.15	4.00
ATOM	2528	HG2	THR	263	-0.733	11.249	28.129	1.00	0.00	0.053	0.00	0.00
ATOM	2529	HG2	THR	263	-1.976	10.229	28.891	1.00	0.00	0.053	0.00	0.00
ATOM	2530	HG2	THR	263	-2.243	11.980	28.722	1.00	0.00	0.053	0.00	0.00
ATOM	2531	C	THR	263	-2.845	12.576	31.157	1.00	0.00	0.396	9.82	4.00
ATOM	2532	O	THR	263	-3.781	12.498	30.348	1.00	0.00	-0.396	8.17	-17.40
ATOM	2533	N	ASP	264P	-2.577	13.678	31.861	1.00	0.00	-0.650	9.00	-17.40
ATOM	2534	HN	ASP	264P	-1.789	13.659	32.524	1.00	0.00	0.440	0.00	0.00
ATOM	2535	CA	ASP	264P	-3.355	14.914	31.731	1.00	0.00	0.158	9.40	4.00
ATOM	2536	HA	ASP	264P	-4.408	14.655	31.623	1.00	0.00	0.053	0.00	0.00
ATOM	2537	CB	ASP	264P	-3.162	15.796	32.978	1.00	0.00	-0.336	12.77	4.00
ATOM	2538	HB1	ASP	264P	-3.551	16.805	32.844	1.00	0.00	0.053	0.00	0.00
ATOM	2539	HB2	ASP	264P	-2.113	15.912	33.253	1.00	0.00	0.053	0.00	0.00
ATOM	2540	CG	ASP	264P	-3.857	15.238	34.203	1.00	0.00	0.297	9.82	4.00
ATOM	2541	OD1	ASP	264P	-3.262	15.286	35.307	1.00	0.00	-0.534	8.17	-18.95
ATOM	2542	OD2	ASP	264P	-5.012	14.774	34.066	1.00	0.00	-0.534	8.17	-18.95
ATOM	2543	C	ASP	264P	-2.871	15.671	30.500	1.00	0.00	0.396	9.82	4.00
ATOM	2544	O	ASP	264P	-3.581	16.531	29.953	1.00	0.00	-0.396	8.17	-17.40
ATOM	2545	N	PHE	265	-1.663	15.335	30.058	1.00	0.00	-0.650	9.00	-17.40
ATOM	2546	HN	PHE	265	-1.142	14.598	30.555	1.00	0.00	0.440	0.00	0.00
ATOM	2547	CA	PHE	265	-1.044	15.969	28.894	1.00	0.00	0.158	9.40	4.00
ATOM	2548	HA	PHE	265	-1.354	17.009	28.797	1.00	0.00	0.053	0.00	0.00
ATOM	2549	CB	PHE	265	0.495	15.978	29.053	1.00	0.00	-0.106	12.77	4.00
ATOM	2550	HB1	PHE	265	0.863	14.966	28.880	1.00	0.00	0.053	0.00	0.00
ATOM	2551	HB2	PHE	265	0.733	16.305	30.065	1.00	0.00	0.053	0.00	0.00
ATOM	2552	CG	PHE	265	1.214	16.907	28.082	1.00	0.00	0.000	7.26	0.60
ATOM	2553	CD1	PHE	265	1.598	18.185	28.468	1.00	0.00	-0.127	10.80	0.60
ATOM	2554	HD1	PHE	265	1.393	18.521	29.484	1.00	0.00	0.127	0.00	0.00
ATOM	2555	CD2	PHE	265	1.492	16.499	26.772	1.00	0.00	-0.127	10.80	0.60
ATOM	2556	HD2	PHE	265	1.202	15.499	26.448	1.00	0.00	0.127	0.00	0.00
ATOM	2557	CE1	PHE	265	2.241	19.046	27.578	1.00	0.00	-0.127	10.80	0.60
ATOM	2558	HE1	PHE	265	2.533	20.046	27.898	1.00	0.00	0.127	0.00	0.00
ATOM	2559	CE2	PHE	265	2.133	17.351	25.876	1.00	0.00	-0.127	10.80	0.60
ATOM	2560	HE2	PHE	265	2.338	17.015	24.859	1.00	0.00	0.127	0.00	0.00
ATOM	2561	CZ	PHE	265	2.509	18.620	26.272	1.00	0.00	-0.127	10.80	0.60
ATOM	2562	HZ	PHE	265	3.011	19.286	25.571	1.00	0.00	0.127	0.00	0.00
ATOM	2563	C	PHE	265	-1.431	15.244	27.588	1.00	0.00	0.396	9.82	4.00
ATOM	2564	O	PHE	265	-1.010	14.090	27.334	1.00	0.00	-0.396	8.17	-17.40
ATOM	2565	N	PHE	266	-2.237	15.927	26.766	1.00	0.00	-0.650	9.00	-17.40
ATOM	2566	HN	PHE	266	-2.554	16.864	27.052	1.00	0.00	0.440	0.00	0.00
ATOM	2567	CA	PHE	266	-2.688	15.396	25.473	1.00	0.00	0.158	9.40	4.00
ATOM	2568	HA	PHE	266	-3.193	14.443	25.632	1.00	0.00	0.053	0.00	0.00
ATOM	2569	CB	PHE	266	-3.664	16.378	24.813	1.00	0.00	-0.106	12.77	4.00
ATOM	2570	HB1	PHE	266	-3.267	17.389	24.721	1.00	0.00	0.053	0.00	0.00
ATOM	2571	HB2	PHE	266	-4.602	16.488	25.355	1.00	0.00	0.053	0.00	0.00
ATOM	2572	CG	PHE	266	-4.061	15.982	23.416	1.00	0.00	0.000	7.26	0.60
ATOM	2573	CD1	PHE	266	-4.788	14.812	23.195	1.00	0.00	-0.127	10.80	0.60
ATOM	2574	HD1	PHE	266	-5.095	14.204	24.046	1.00	0.00	0.127	0.00	0.00
ATOM	2575	CD2	PHE	266	-3.677	16.746	22.324	1.00	0.00	-0.127	10.80	0.60
ATOM	2576	HD2	PHE	266	-3.111	17.664	22.480	1.00	0.00	0.127	0.00	0.00
ATOM	2577	CE1	PHE	266	-5.128	14.406	21.907	1.00	0.00	-0.127	10.80	0.60
ATOM	2578	HE1	PHE	266	-5.695	13.488	21.752	1.00	0.00	0.127	0.00	0.00
ATOM	2579	CE2	PHE	266	-4.009	16.349	21.024	1.00	0.00	-0.127	10.80	0.60

ATOM	2580	HE2	PHE	266	-3.696	16.954	20.173	1.00	0.00	0.127	0.00	0.00
ATOM	2581	CZ	PHE	266	-4.738	15.182	20.816	1.00	0.00	-0.127	10.80	0.60
ATOM	2582	HZ	PHE	266	-5.003	14.875	19.804	1.00	0.00	0.127	0.00	0.00
ATOM	2583	C	PHE	266	-1.468	15.189	24.556	1.00	0.00	0.396	9.82	4.00
ATOM	2584	O	PHE	266	-0.809	16.171	24.150	1.00	0.00	-0.396	8.17	-17.40
ATOM	2585	N	PRO	267	-1.155	13.928	24.193	1.00	0.00	-0.422	9.00	-17.40
ATOM	2586	CD	PRO	267	-1.655	12.666	24.769	1.00	0.00	0.105	12.77	4.00
ATOM	2587	HD1	PRO	267	-2.328	12.151	24.083	1.00	0.00	0.053	0.00	0.00
ATOM	2588	HD2	PRO	267	-2.204	12.838	25.694	1.00	0.00	0.053	0.00	0.00
ATOM	2589	CA	PRO	267	0.015	13.667	23.324	1.00	0.00	0.158	9.40	4.00
ATOM	2590	HA	PRO	267	0.776	14.408	23.567	1.00	0.00	0.053	0.00	0.00
ATOM	2591	CB	PRO	267	0.433	12.239	23.704	1.00	0.00	-0.106	12.77	4.00
ATOM	2592	HB1	PRO	267	1.509	12.298	23.866	1.00	0.00	0.053	0.00	0.00
ATOM	2593	HB2	PRO	267	0.152	11.629	22.845	1.00	0.00	0.053	0.00	0.00
ATOM	2594	CG	PRO	267	-0.376	11.918	24.989	1.00	0.00	-0.106	12.77	4.00
ATOM	2595	HG1	PRO	267	0.149	12.259	25.881	1.00	0.00	0.053	0.00	0.00
ATOM	2596	HG2	PRO	267	-0.542	10.845	25.092	1.00	0.00	0.053	0.00	0.00
ATOM	2597	C	PRO	267	-0.202	13.744	21.812	1.00	0.00	0.396	9.82	4.00
ATOM	2598	O	PRO	267	0.730	14.023	21.069	1.00	0.00	-0.396	8.17	-17.40
ATOM	2599	N	GLY	268	-1.421	13.473	21.363	1.00	0.00	-0.650	9.00	-17.40
ATOM	2600	HN	GLY	268	-2.180	13.260	22.025	1.00	0.00	0.440	0.00	0.00
ATOM	2601	CA	GLY	268	-1.680	13.478	19.933	1.00	0.00	0.105	9.40	4.00
ATOM	2602	HA1	GLY	268	-1.359	14.457	19.579	1.00	0.00	0.053	0.00	0.00
ATOM	2603	HA2	GLY	268	-2.753	13.317	19.827	1.00	0.00	0.053	0.00	0.00
ATOM	2604	C	GLY	268	-0.852	12.341	19.362	1.00	0.00	0.396	9.82	4.00
ATOM	2605	O	GLY	268	-0.775	11.251	19.957	1.00	0.00	-0.396	8.17	-17.40
ATOM	2606	N	LEU	269	-0.229	12.594	18.215	1.00	0.00	-0.650	9.00	-17.40
ATOM	2607	HN	LEU	269	-0.364	13.518	17.780	1.00	0.00	0.440	0.00	0.00
ATOM	2608	CA	LEU	269	0.639	11.631	17.536	1.00	0.00	0.158	9.40	4.00
ATOM	2609	HA	LEU	269	0.735	11.937	16.494	1.00	0.00	0.053	0.00	0.00
ATOM	2610	CB	LEU	269	2.055	11.736	18.134	1.00	0.00	-0.106	12.77	4.00
ATOM	2611	HB1	LEU	269	2.710	11.034	17.618	1.00	0.00	0.053	0.00	0.00
ATOM	2612	HB2	LEU	269	2.010	11.492	19.195	1.00	0.00	0.053	0.00	0.00
ATOM	2613	CG	LEU	269	2.575	13.180	17.945	1.00	0.00	-0.053	9.40	4.00
ATOM	2614	HG	LEU	269	1.839	13.915	18.270	1.00	0.00	0.053	0.00	0.00
ATOM	2615	CD1	LEU	269	3.852	13.426	18.748	1.00	0.00	-0.159	16.15	4.00
ATOM	2616	HD1	LEU	269	4.188	14.450	18.591	1.00	0.00	0.053	0.00	0.00
ATOM	2617	HD1	LEU	269	3.651	13.268	19.807	1.00	0.00	0.053	0.00	0.00
ATOM	2618	HD1	LEU	269	4.627	12.734	18.418	1.00	0.00	0.053	0.00	0.00
ATOM	2619	CD2	LEU	269	2.796	13.431	16.456	1.00	0.00	-0.159	16.15	4.00
ATOM	2620	HD2	LEU	269	3.163	14.446	16.308	1.00	0.00	0.053	0.00	0.00
ATOM	2621	HD2	LEU	269	3.528	12.721	16.072	1.00	0.00	0.053	0.00	0.00
ATOM	2622	HD2	LEU	269	1.854	13.304	15.922	1.00	0.00	0.053	0.00	0.00
ATOM	2623	C	LEU	269	0.132	10.181	17.544	1.00	0.00	0.396	9.82	4.00
ATOM	2624	O	LEU	269	0.760	9.291	18.104	1.00	0.00	-0.396	8.17	-17.40
ATOM	2625	N	GLY	270	-0.980	9.948	16.850	1.00	0.00	-0.650	9.00	-17.40
ATOM	2626	HN	GLY	270	-1.422	10.718	16.328	1.00	0.00	0.440	0.00	0.00
ATOM	2627	CA	GLY	270	-1.579	8.628	16.816	1.00	0.00	0.105	9.40	4.00
ATOM	2628	HA1	GLY	270	-0.740	7.942	16.941	1.00	0.00	0.053	0.00	0.00
ATOM	2629	HA2	GLY	270	-2.055	8.568	15.837	1.00	0.00	0.053	0.00	0.00
ATOM	2630	C	GLY	270	-2.557	8.622	17.978	1.00	0.00	0.396	9.82	4.00
ATOM	2631	O	GLY	270	-2.222	8.170	19.077	1.00	0.00	-0.396	8.17	-17.40
ATOM	2632	N	TRP	271	-3.765	9.131	17.753	1.00	0.00	-0.650	9.00	-17.40
ATOM	2633	HN	TRP	271	-4.013	9.484	16.817	1.00	0.00	0.440	0.00	0.00
ATOM	2634	CA	TRP	271	-4.739	9.186	18.843	1.00	0.00	0.158	9.40	4.00
ATOM	2635	HA	TRP	271	-4.468	8.425	19.575	1.00	0.00	0.053	0.00	0.00
ATOM	2636	CB	TRP	271	-4.672	10.528	19.575	1.00	0.00	-0.106	12.77	4.00
ATOM	2637	HB1	TRP	271	-3.666	10.646	19.979	1.00	0.00	0.053	0.00	0.00
ATOM	2638	HB2	TRP	271	-5.410	10.516	20.377	1.00	0.00	0.053	0.00	0.00
ATOM	2639	CG	TRP	271	-4.958	11.724	18.713	1.00	0.00	0.000	7.26	0.60
ATOM	2640	CD2	TRP	271	-6.109	12.576	18.778	1.00	0.00	0.000	6.80	0.60
ATOM	2641	CE2	TRP	271	-5.923	13.603	17.819	1.00	0.00	-0.050	6.80	0.60
ATOM	2642	CD1	TRP	271	-4.144	12.253	17.737	1.00	0.00	-0.177	10.80	0.60
ATOM	2643	HD1	TRP	271	-3.182	11.838	17.433	1.00	0.00	0.127	0.00	0.00
ATOM	2644	NE1	TRP	271	-4.719	13.378	17.203	1.00	0.00	-0.292	9.00	-17.40
ATOM	2645	HE1	TRP	271	-4.311	13.960	16.458	1.00	0.00	0.393	0.00	0.00
ATOM	2646	CE3	TRP	271	-7.278	12.577	19.556	1.00	0.00	-0.127	10.80	0.60
ATOM	2647	HE3	TRP	271	-7.450	11.798	20.299	1.00	0.00	0.127	0.00	0.00
ATOM	2648	CZ2	TRP	271	-6.865	14.625	17.616	1.00	0.00	-0.127	10.80	0.60
ATOM	2649	HZ2	TRP	271	-6.702	15.402	16.870	1.00	0.00	0.127	0.00	0.00
ATOM	2650	CZ3	TRP	271	-8.216	13.595	19.360	1.00	0.00	-0.127	10.80	0.60
ATOM	2651	HZ3	TRP	271	-9.126	13.610	19.959	1.00	0.00	0.127	0.00	0.00
ATOM	2652	CH2	TRP	271	-7.997	14.609	18.390	1.00	0.00	-0.127	10.80	0.60
ATOM	2653	HH2	TRP	271	-8.744	15.391	18.258	1.00	0.00	0.127	0.00	0.00
ATOM	2654	C	TRP	271	-6.170	8.934	18.444	1.00	0.00	0.396	9.82	4.00
ATOM	2655	O	TRP	271	-6.626	9.351	17.370	1.00	0.00	-0.396	8.17	-17.40

ATOM	2656	N	LEU	272	-6.869	8.255	19.344	1.00	0.00	-0.650	9.00	-17.40
ATOM	2657	HN	LEU	272	-6.392	7.966	20.210	1.00	0.00	0.440	0.00	0.00
ATOM	2658	CA	LEU	272	-8.264	7.895	19.180	1.00	0.00	0.158	9.40	4.00
ATOM	2659	HA	LEU	272	-8.574	7.890	18.135	1.00	0.00	0.053	0.00	0.00
ATOM	2660	CB	LEU	272	-8.473	6.479	19.737	1.00	0.00	-0.106	12.77	4.00
ATOM	2661	HB1	LEU	272	-8.012	6.451	20.724	1.00	0.00	0.053	0.00	0.00
ATOM	2662	HB2	LEU	272	-7.989	5.788	19.046	1.00	0.00	0.053	0.00	0.00
ATOM	2663	CG	LEU	272	-9.900	5.956	19.924	1.00	0.00	-0.053	9.40	4.00
ATOM	2664	HG	LEU	272	-10.527	6.735	20.356	1.00	0.00	0.053	0.00	0.00
ATOM	2665	CD1	LEU	272	-10.481	5.541	18.579	1.00	0.00	-0.159	16.15	4.00
ATOM	2666	HD1	LEU	272	-11.496	5.170	18.720	1.00	0.00	0.053	0.00	0.00
ATOM	2667	HD1	LEU	272	-10.498	6.400	17.909	1.00	0.00	0.053	0.00	0.00
ATOM	2668	HD1	LEU	272	-9.864	4.754	18.143	1.00	0.00	0.053	0.00	0.00
ATOM	2669	CD2	LEU	272	-9.875	4.774	20.891	1.00	0.00	-0.159	16.15	4.00
ATOM	2670	HD2	LEU	272	-10.887	4.395	21.029	1.00	0.00	0.053	0.00	0.00
ATOM	2671	HD2	LEU	272	-9.245	3.983	20.483	1.00	0.00	0.053	0.00	0.00
ATOM	2672	HD2	LEU	272	-9.474	5.098	21.851	1.00	0.00	0.053	0.00	0.00
ATOM	2673	C	LEU	272	-9.213	8.865	19.907	1.00	0.00	0.396	9.82	4.00
ATOM	2674	O	LEU	272	-8.983	9.236	21.060	1.00	0.00	-0.396	8.17	-17.40
ATOM	2675	N	LEU	273	-10.273	9.283	19.227	1.00	0.00	-0.650	9.00	-17.40
ATOM	2676	HN	LEU	273	-10.396	9.004	18.243	1.00	0.00	0.440	0.00	0.00
ATOM	2677	CA	LEU	273	-11.258	10.133	19.870	1.00	0.00	0.158	9.40	4.00
ATOM	2678	HA	LEU	273	-11.076	10.086	20.944	1.00	0.00	0.053	0.00	0.00
ATOM	2679	CB	LEU	273	-11.142	11.590	19.424	1.00	0.00	-0.106	12.77	4.00
ATOM	2680	HB1	LEU	273	-10.079	11.834	19.413	1.00	0.00	0.053	0.00	0.00
ATOM	2681	HB2	LEU	273	-11.690	12.188	20.151	1.00	0.00	0.053	0.00	0.00
ATOM	2682	CG	LEU	273	-11.676	12.015	18.055	1.00	0.00	-0.053	9.40	4.00
ATOM	2683	HG	LEU	273	-12.651	11.547	17.923	1.00	0.00	0.053	0.00	0.00
ATOM	2684	CD1	LEU	273	-11.786	13.541	18.057	1.00	0.00	-0.159	16.15	4.00
ATOM	2685	HD1	LEU	273	-12.165	13.879	17.092	1.00	0.00	0.053	0.00	0.00
ATOM	2686	HD1	LEU	273	-12.469	13.855	18.846	1.00	0.00	0.053	0.00	0.00
ATOM	2687	HD1	LEU	273	-10.802	13.976	18.233	1.00	0.00	0.053	0.00	0.00
ATOM	2688	CD2	LEU	273	-10.759	11.550	16.920	1.00	0.00	-0.159	16.15	4.00
ATOM	2689	HD2	LEU	273	-11.172	11.871	15.963	1.00	0.00	0.053	0.00	0.00
ATOM	2690	HD2	LEU	273	-9.768	11.984	17.051	1.00	0.00	0.053	0.00	0.00
ATOM	2691	HD2	LEU	273	-10.683	10.462	16.935	1.00	0.00	0.053	0.00	0.00
ATOM	2692	C	LEU	273	-12.634	9.586	19.512	1.00	0.00	0.396	9.82	4.00
ATOM	2693	O	LEU	273	-12.797	8.866	18.521	1.00	0.00	-0.396	8.17	-17.40
ATOM	2694	N	LEU	274	-13.616	9.893	20.351	1.00	0.00	-0.650	9.00	-17.40
ATOM	2695	HN	LEU	274	-13.411	10.445	21.195	1.00	0.00	0.440	0.00	0.00
ATOM	2696	CA	LEU	274	-14.977	9.457	20.089	1.00	0.00	0.158	9.40	4.00
ATOM	2697	HA	LEU	274	-14.959	8.553	19.479	1.00	0.00	0.053	0.00	0.00
ATOM	2698	CB	LEU	274	-15.713	9.180	21.391	1.00	0.00	-0.106	12.77	4.00
ATOM	2699	HB1	LEU	274	-16.749	8.938	21.155	1.00	0.00	0.053	0.00	0.00
ATOM	2700	HB2	LEU	274	-15.660	10.074	22.012	1.00	0.00	0.053	0.00	0.00
ATOM	2701	CG	LEU	274	-15.136	8.019	22.196	1.00	0.00	-0.053	9.40	4.00
ATOM	2702	HG	LEU	274	-14.107	8.267	22.455	1.00	0.00	0.053	0.00	0.00
ATOM	2703	CD1	LEU	274	-15.991	7.845	23.456	1.00	0.00	-0.159	16.15	4.00
ATOM	2704	HD1	LEU	274	-15.599	7.019	24.050	1.00	0.00	0.053	0.00	0.00
ATOM	2705	HD1	LEU	274	-15.962	8.761	24.044	1.00	0.00	0.053	0.00	0.00
ATOM	2706	HD1	LEU	274	-17.020	7.629	23.170	1.00	0.00	0.053	0.00	0.00
ATOM	2707	CD2	LEU	274	-15.108	6.750	21.375	1.00	0.00	-0.159	16.15	4.00
ATOM	2708	HD2	LEU	274	-14.692	5.938	21.973	1.00	0.00	0.053	0.00	0.00
ATOM	2709	HD2	LEU	274	-16.121	6.492	21.069	1.00	0.00	0.053	0.00	0.00
ATOM	2710	HD2	LEU	274	-14.489	6.902	20.490	1.00	0.00	0.053	0.00	0.00
ATOM	2711	C	LEU	274	-15.724	10.547	19.352	1.00	0.00	0.396	9.82	4.00
ATOM	2712	O	LEU	274	-15.391	11.724	19.453	1.00	0.00	-0.396	8.17	-17.40
ATOM	2713	N	ALA	275	-16.741	10.137	18.610	1.00	0.00	-0.650	9.00	-17.40
ATOM	2714	HN	ALA	275	-16.950	9.130	18.554	1.00	0.00	0.440	0.00	0.00
ATOM	2715	CA	ALA	275	-17.566	11.075	17.875	1.00	0.00	0.158	9.40	4.00
ATOM	2716	HA	ALA	275	-16.899	11.565	17.165	1.00	0.00	0.053	0.00	0.00
ATOM	2717	CB	ALA	275	-18.689	10.335	17.151	1.00	0.00	-0.159	16.15	4.00
ATOM	2718	HB1	ALA	275	-19.301	11.050	16.602	1.00	0.00	0.053	0.00	0.00
ATOM	2719	HB2	ALA	275	-18.260	9.615	16.454	1.00	0.00	0.053	0.00	0.00
ATOM	2720	HB3	ALA	275	-19.307	9.810	17.879	1.00	0.00	0.053	0.00	0.00
ATOM	2721	C	ALA	275	-18.131	12.033	18.913	1.00	0.00	0.396	9.82	4.00
ATOM	2722	O	ALA	275	-18.343	13.190	18.611	1.00	0.00	-0.396	8.17	-17.40
ATOM	2723	N	GLU	276	-18.340	11.553	20.145	1.00	0.00	-0.650	9.00	-17.40
ATOM	2724	HN	GLU	276	-18.126	10.566	20.349	1.00	0.00	0.440	0.00	0.00
ATOM	2725	CA	GLU	276	-18.868	12.413	21.207	1.00	0.00	0.158	9.40	4.00
ATOM	2726	HA	GLU	276	-19.847	12.815	20.949	1.00	0.00	0.053	0.00	0.00
ATOM	2727	CB	GLU	276	-19.062	11.630	22.515	1.00	0.00	-0.106	12.77	4.00
ATOM	2728	HB1	GLU	276	-19.113	12.351	23.330	1.00	0.00	0.053	0.00	0.00
ATOM	2729	HB2	GLU	276	-18.207	10.963	22.633	1.00	0.00	0.053	0.00	0.00
ATOM	2730	CG	GLU	276	-20.317	10.764	22.609	1.00	0.00	-0.106	12.77	4.00
ATOM	2731	HG1	GLU	276	-21.203	11.224	22.173	1.00	0.00	0.053	0.00	0.00

ATOM	2732	HG2	GLU	276	-20.605	10.516	23.630	1.00	0.00	0.053	0.00	0.00
ATOM	2733	CD	GLU	276	-20.191	9.418	21.903	1.00	0.00	0.399	9.82	4.00
ATOM	2734	OE1	GLU	276	-20.937	8.475	22.285	1.00	0.00	-0.396	8.17	-18.95
ATOM	2735	OE2	GLU	276	-19.356	9.290	20.975	1.00	0.00	-0.427	8.17	-18.95
ATOM	2736	HE2	GLU	276	-19.394	8.328	20.608	1.00	0.00	0.424	0.00	0.00
ATOM	2737	C	GLU	276	-17.943	13.609	21.481	1.00	0.00	0.396	9.82	4.00
ATOM	2738	O	GLU	276	-18.411	14.708	21.780	1.00	0.00	-0.396	8.17	-17.40
ATOM	2739	N	LEU	277	-16.631	13.399	21.397	1.00	0.00	-0.650	9.00	-17.40
ATOM	2740	HN	LEU	277	-16.277	12.459	21.164	1.00	0.00	0.440	0.00	0.00
ATOM	2741	CA	LEU	277	-15.689	14.490	21.632	1.00	0.00	0.158	9.40	4.00
ATOM	2742	HA	LEU	277	-15.941	15.040	22.538	1.00	0.00	0.053	0.00	0.00
ATOM	2743	CB	LEU	277	-14.251	13.977	21.846	1.00	0.00	-0.106	12.77	4.00
ATOM	2744	HB1	LEU	277	-13.901	13.357	21.020	1.00	0.00	0.053	0.00	0.00
ATOM	2745	HB2	LEU	277	-14.154	13.368	22.745	1.00	0.00	0.053	0.00	0.00
ATOM	2746	CG	LEU	277	-13.231	15.122	21.988	1.00	0.00	-0.053	9.40	4.00
ATOM	2747	HG	LEU	277	-13.255	15.743	21.092	1.00	0.00	0.053	0.00	0.00
ATOM	2748	CD1	LEU	277	-13.589	15.979	23.219	1.00	0.00	-0.159	16.15	4.00
ATOM	2749	HD1	LEU	277	-12.867	16.789	23.320	1.00	0.00	0.053	0.00	0.00
ATOM	2750	HD1	LEU	277	-14.588	16.396	23.093	1.00	0.00	0.053	0.00	0.00
ATOM	2751	HD1	LEU	277	-13.564	15.357	24.114	1.00	0.00	0.053	0.00	0.00
ATOM	2752	CD2	LEU	277	-11.807	14.564	22.116	1.00	0.00	-0.159	16.15	4.00
ATOM	2753	HD2	LEU	277	-11.100	15.388	22.215	1.00	0.00	0.053	0.00	0.00
ATOM	2754	HD2	LEU	277	-11.744	13.924	22.996	1.00	0.00	0.053	0.00	0.00
ATOM	2755	HD2	LEU	277	-11.562	13.982	21.227	1.00	0.00	0.053	0.00	0.00
ATOM	2756	C	LEU	277	-15.692	15.479	20.474	1.00	0.00	0.396	9.82	4.00
ATOM	2757	O	LEU	277	-15.628	16.702	20.686	1.00	0.00	-0.396	8.17	-17.40
ATOM	2758	N	TRP	278	-15.738	14.964	19.251	1.00	0.00	-0.650	9.00	-17.40
ATOM	2759	HN	TRP	278	-15.755	13.942	19.123	1.00	0.00	0.440	0.00	0.00
ATOM	2760	CA	TRP	278	-15.763	15.838	18.097	1.00	0.00	0.158	9.40	4.00
ATOM	2761	HA	TRP	278	-14.854	16.439	18.074	1.00	0.00	0.053	0.00	0.00
ATOM	2762	CB	TRP	278	-15.800	15.026	16.804	1.00	0.00	-0.106	12.77	4.00
ATOM	2763	HB1	TRP	278	-16.703	14.422	16.717	1.00	0.00	0.053	0.00	0.00
ATOM	2764	HB2	TRP	278	-14.960	14.335	16.722	1.00	0.00	0.053	0.00	0.00
ATOM	2765	CG	TRP	278	-15.753	15.892	15.584	1.00	0.00	0.000	7.26	0.60
ATOM	2766	CD2	TRP	278	-14.755	16.866	15.277	1.00	0.00	0.000	6.80	0.60
ATOM	2767	CE2	TRP	278	-15.145	17.502	14.076	1.00	0.00	-0.050	6.80	0.60
ATOM	2768	CD1	TRP	278	-16.685	15.964	14.578	1.00	0.00	-0.177	10.80	0.60
ATOM	2769	HD1	TRP	278	-17.578	15.343	14.508	1.00	0.00	0.127	0.00	0.00
ATOM	2770	NE1	TRP	278	-16.326	16.935	13.669	1.00	0.00	-0.292	9.00	-17.40
ATOM	2771	HE1	TRP	278	-16.856	17.192	12.824	1.00	0.00	0.393	0.00	0.00
ATOM	2772	CE3	TRP	278	-13.566	17.267	15.906	1.00	0.00	-0.127	10.80	0.60
ATOM	2773	HE3	TRP	278	-13.240	16.792	16.832	1.00	0.00	0.127	0.00	0.00
ATOM	2774	CZ2	TRP	278	-14.386	18.522	13.491	1.00	0.00	-0.127	10.80	0.60
ATOM	2775	HZ2	TRP	278	-14.700	19.002	12.564	1.00	0.00	0.127	0.00	0.00
ATOM	2776	CZ3	TRP	278	-12.813	18.278	15.327	1.00	0.00	-0.127	10.80	0.60
ATOM	2777	HZ3	TRP	278	-11.887	18.599	15.805	1.00	0.00	0.127	0.00	0.00
ATOM	2778	CH2	TRP	278	-13.225	18.894	14.134	1.00	0.00	-0.127	10.80	0.60
ATOM	2779	HH2	TRP	278	-12.611	19.686	13.705	1.00	0.00	0.127	0.00	0.00
ATOM	2780	C	TRP	278	-16.979	16.760	18.179	1.00	0.00	0.396	9.82	4.00
ATOM	2781	O	TRP	278	-16.921	17.912	17.751	1.00	0.00	-0.396	8.17	-17.40
ATOM	2782	N	ALA	279	-18.086	16.252	18.725	1.00	0.00	-0.650	9.00	-17.40
ATOM	2783	HN	ALA	279	-18.086	15.272	19.042	1.00	0.00	0.440	0.00	0.00
ATOM	2784	CA	ALA	279	-19.302	17.058	18.883	1.00	0.00	0.158	9.40	4.00
ATOM	2785	HA	ALA	279	-19.623	17.435	17.912	1.00	0.00	0.053	0.00	0.00
ATOM	2786	CB	ALA	279	-20.441	16.201	19.461	1.00	0.00	-0.159	16.15	4.00
ATOM	2787	HB1	ALA	279	-21.336	16.812	19.572	1.00	0.00	0.053	0.00	0.00
ATOM	2788	HB2	ALA	279	-20.650	15.371	18.786	1.00	0.00	0.053	0.00	0.00
ATOM	2789	HB3	ALA	279	-20.144	15.810	20.434	1.00	0.00	0.053	0.00	0.00
ATOM	2790	C	ALA	279	-19.023	18.243	19.816	1.00	0.00	0.396	9.82	4.00
ATOM	2791	O	ALA	279	-19.557	19.342	19.631	1.00	0.00	-0.396	8.17	-17.40
ATOM	2792	N	GLU	280	-18.165	18.011	20.804	1.00	0.00	-0.650	9.00	-17.40
ATOM	2793	HN	GLU	280	-17.744	17.074	20.885	1.00	0.00	0.440	0.00	0.00
ATOM	2794	CA	GLU	280	-17.797	19.026	21.773	1.00	0.00	0.158	9.40	4.00
ATOM	2795	HA	GLU	280	-18.653	19.594	22.135	1.00	0.00	0.053	0.00	0.00
ATOM	2796	CB	GLU	280	-17.154	18.339	22.983	1.00	0.00	-0.106	12.77	4.00
ATOM	2797	HB1	GLU	280	-16.114	18.119	22.738	1.00	0.00	0.053	0.00	0.00
ATOM	2798	HB2	GLU	280	-17.704	17.420	23.185	1.00	0.00	0.053	0.00	0.00
ATOM	2799	CG	GLU	280	-17.160	19.154	24.236	1.00	0.00	-0.106	12.77	4.00
ATOM	2800	HG1	GLU	280	-18.163	19.361	24.607	1.00	0.00	0.053	0.00	0.00
ATOM	2801	HG2	GLU	280	-16.685	20.128	24.115	1.00	0.00	0.053	0.00	0.00
ATOM	2802	CD	GLU	280	-16.428	18.483	25.389	1.00	0.00	0.399	9.82	4.00
ATOM	2803	OE1	GLU	280	-16.567	17.254	25.575	1.00	0.00	-0.396	8.17	-18.95
ATOM	2804	OE2	GLU	280	-15.733	19.205	26.129	1.00	0.00	-0.427	8.17	-18.95
ATOM	2805	HE2	GLU	280	-15.319	18.632	26.878	1.00	0.00	0.424	0.00	0.00
ATOM	2806	C	GLU	280	-16.808	20.066	21.205	1.00	0.00	0.396	9.82	4.00
ATOM	2807	O	GLU	280	-16.924	21.268	21.462	1.00	0.00	-0.396	8.17	-17.40

ATOM	2808	N	LEU	281	-15.848	19.596	20.418	1.00	0.00	-0.650	9.00	-17.40
ATOM	2809	HN	LEU	281	-15.847	18.594	20.176	1.00	0.00	0.440	0.00	0.00
ATOM	2810	CA	LEU	281	-14.795	20.451	19.884	1.00	0.00	0.158	9.40	4.00
ATOM	2811	HA	LEU	281	-14.547	21.183	20.652	1.00	0.00	0.053	0.00	0.00
ATOM	2812	CB	LEU	281	-13.532	19.606	19.655	1.00	0.00	-0.106	12.77	4.00
ATOM	2813	HB1	LEU	281	-12.729	20.274	19.341	1.00	0.00	0.053	0.00	0.00
ATOM	2814	HB2	LEU	281	-13.751	18.872	18.879	1.00	0.00	0.053	0.00	0.00
ATOM	2815	CG	LEU	281	-13.029	18.831	20.893	1.00	0.00	-0.053	9.40	4.00
ATOM	2816	HG	LEU	281	-13.787	18.113	21.205	1.00	0.00	0.053	0.00	0.00
ATOM	2817	CD1	LEU	281	-11.737	18.087	20.539	1.00	0.00	-0.159	16.15	4.00
ATOM	2818	HD1	LEU	281	-11.381	17.539	21.412	1.00	0.00	0.053	0.00	0.00
ATOM	2819	HD1	LEU	281	-11.931	17.386	19.726	1.00	0.00	0.053	0.00	0.00
ATOM	2820	HD1	LEU	281	-10.978	18.804	20.226	1.00	0.00	0.053	0.00	0.00
ATOM	2821	CD2	LEU	281	-12.803	19.793	22.071	1.00	0.00	-0.159	16.15	4.00
ATOM	2822	HD2	LEU	281	-12.448	19.232	22.936	1.00	0.00	0.053	0.00	0.00
ATOM	2823	HD2	LEU	281	-12.059	20.539	21.793	1.00	0.00	0.053	0.00	0.00
ATOM	2824	HD2	LEU	281	-13.740	20.289	22.320	1.00	0.00	0.053	0.00	0.00
ATOM	2825	C	LEU	281	-15.100	21.234	18.625	1.00	0.00	0.396	9.82	4.00
ATOM	2826	O	LEU	281	-14.793	22.427	18.534	1.00	0.00	-0.396	8.17	-17.40
ATOM	2827	N	GLU	282	-15.707	20.573	17.651	1.00	0.00	-0.650	9.00	-17.40
ATOM	2828	HN	GLU	282	-15.985	19.591	17.793	1.00	0.00	0.440	0.00	0.00
ATOM	2829	CA	GLU	282	-15.983	21.230	16.374	1.00	0.00	0.158	9.40	4.00
ATOM	2830	HA	GLU	282	-15.037	21.327	15.841	1.00	0.00	0.053	0.00	0.00
ATOM	2831	CB	GLU	282	-16.847	20.326	15.480	1.00	0.00	-0.106	12.77	4.00
ATOM	2832	HB1	GLU	282	-17.813	20.078	15.918	1.00	0.00	0.053	0.00	0.00
ATOM	2833	HB2	GLU	282	-16.381	19.366	15.254	1.00	0.00	0.053	0.00	0.00
ATOM	2834	CG	GLU	282	-17.172	20.949	14.111	1.00	0.00	-0.106	12.77	4.00
ATOM	2835	HG1	GLU	282	-16.287	21.337	13.606	1.00	0.00	0.053	0.00	0.00
ATOM	2836	HG2	GLU	282	-17.869	21.783	14.185	1.00	0.00	0.053	0.00	0.00
ATOM	2837	CD	GLU	282	-17.802	19.956	13.153	1.00	0.00	0.399	9.82	4.00
ATOM	2838	OE1	GLU	282	-17.146	19.593	12.148	1.00	0.00	-0.396	8.17	-18.95
ATOM	2839	OE2	GLU	282	-18.945	19.518	13.403	1.00	0.00	-0.427	8.17	-18.95
ATOM	2840	HE2	GLU	282	-19.223	18.847	12.672	1.00	0.00	0.424	0.00	0.00
ATOM	2841	C	GLU	282	-16.599	22.626	16.435	1.00	0.00	0.396	9.82	4.00
ATOM	2842	O	GLU	282	-16.173	23.517	15.706	1.00	0.00	-0.396	8.17	-17.40
ATOM	2843	N	PRO	283	-17.591	22.845	17.312	1.00	0.00	-0.422	9.00	-17.40
ATOM	2844	CD	PRO	283	-18.223	21.902	18.254	1.00	0.00	0.105	12.77	4.00
ATOM	2845	HD1	PRO	283	-17.657	21.832	19.183	1.00	0.00	0.053	0.00	0.00
ATOM	2846	HD2	PRO	283	-18.283	20.900	17.829	1.00	0.00	0.053	0.00	0.00
ATOM	2847	CA	PRO	283	-18.213	24.169	17.393	1.00	0.00	0.158	9.40	4.00
ATOM	2848	HA	PRO	283	-18.650	24.402	16.422	1.00	0.00	0.053	0.00	0.00
ATOM	2849	CB	PRO	283	-19.286	23.995	18.478	1.00	0.00	-0.106	12.77	4.00
ATOM	2850	HB1	PRO	283	-20.173	24.583	18.245	1.00	0.00	0.053	0.00	0.00
ATOM	2851	HB2	PRO	283	-18.912	24.318	19.449	1.00	0.00	0.053	0.00	0.00
ATOM	2852	CG	PRO	283	-19.582	22.513	18.462	1.00	0.00	-0.106	12.77	4.00
ATOM	2853	HG1	PRO	283	-20.271	22.258	17.657	1.00	0.00	0.053	0.00	0.00
ATOM	2854	HG2	PRO	283	-20.034	22.192	19.400	1.00	0.00	0.053	0.00	0.00
ATOM	2855	C	PRO	283	-17.242	25.292	17.748	1.00	0.00	0.396	9.82	4.00
ATOM	2856	O	PRO	283	-17.450	26.445	17.368	1.00	0.00	-0.396	8.17	-17.40
ATOM	2857	N	LYS	284S	-16.192	24.960	18.490	1.00	0.00	-0.650	9.00	-17.40
ATOM	2858	HN	LYS	284S	-16.050	23.977	18.763	1.00	0.00	0.440	0.00	0.00
ATOM	2859	CA	LYS	284S	-15.242	25.971	18.920	1.00	0.00	0.158	9.40	4.00
ATOM	2860	HA	LYS	284S	-15.530	26.976	18.612	1.00	0.00	0.053	0.00	0.00
ATOM	2861	CB	LYS	284S	-15.192	26.017	20.461	1.00	0.00	-0.106	12.77	4.00
ATOM	2862	HB1	LYS	284S	-16.116	26.470	20.819	1.00	0.00	0.053	0.00	0.00
ATOM	2863	HB2	LYS	284S	-14.330	26.615	20.757	1.00	0.00	0.053	0.00	0.00
ATOM	2864	CG	LYS	284S	-15.057	24.648	21.131	1.00	0.00	-0.106	12.77	4.00
ATOM	2865	HG1	LYS	284S	-14.229	24.067	20.724	1.00	0.00	0.053	0.00	0.00
ATOM	2866	HG2	LYS	284S	-15.951	24.037	21.009	1.00	0.00	0.053	0.00	0.00
ATOM	2867	CD	LYS	284S	-14.807	24.760	22.652	1.00	0.00	-0.106	12.77	4.00
ATOM	2868	HD1	LYS	284S	-15.610	25.308	23.144	1.00	0.00	0.053	0.00	0.00
ATOM	2869	HD2	LYS	284S	-13.873	25.282	22.860	1.00	0.00	0.053	0.00	0.00
ATOM	2870	CE	LYS	284S	-14.721	23.370	23.305	1.00	0.00	0.099	12.77	4.00
ATOM	2871	HE1	LYS	284S	-14.056	22.707	22.750	1.00	0.00	0.053	0.00	0.00
ATOM	2872	HE2	LYS	284S	-15.697	22.887	23.349	1.00	0.00	0.053	0.00	0.00
ATOM	2873	NZ	LYS	284S	-14.204	23.452	24.696	1.00	0.00	-0.045	13.25	-39.20
ATOM	2874	HZ1	LYS	284S	-14.159	22.506	25.102	1.00	0.00	0.280	0.00	0.00
ATOM	2875	HZ2	LYS	284S	-13.261	23.866	24.688	1.00	0.00	0.280	0.00	0.00
ATOM	2876	HZ3	LYS	284S	-14.832	24.039	25.262	1.00	0.00	0.280	0.00	0.00
ATOM	2877	C	LYS	284S	-13.851	25.742	18.360	1.00	0.00	0.396	9.82	4.00
ATOM	2878	O	LYS	284S	-12.887	26.309	18.880	1.00	0.00	-0.396	8.17	-17.40
ATOM	2879	N	TRP	285	-13.740	24.920	17.312	1.00	0.00	-0.650	9.00	-17.40
ATOM	2880	HN	TRP	285	-14.587	24.482	16.922	1.00	0.00	0.440	0.00	0.00
ATOM	2881	CA	TRP	285	-12.440	24.628	16.707	1.00	0.00	0.158	9.40	4.00
ATOM	2882	HA	TRP	285	-11.825	24.024	17.374	1.00	0.00	0.053	0.00	0.00
ATOM	2883	CB	TRP	285	-12.623	23.786	15.433	1.00	0.00	-0.106	12.77	4.00

ATOM	2884	HB1	TRP	285	-12.964	24.442	14.632	1.00	0.00	0.053	0.00	0.00
ATOM	2885	HB2	TRP	285	-13.364	23.012	15.635	1.00	0.00	0.053	0.00	0.00
ATOM	2886	CG	TRP	285	-11.363	23.106	14.966	1.00	0.00	0.000	7.26	0.60
ATOM	2887	CD2	TRP	285	-10.711	21.989	15.585	1.00	0.00	0.000	6.80	0.60
ATOM	2888	CE2	TRP	285	-9.589	21.667	14.791	1.00	0.00	-0.050	6.80	0.60
ATOM	2889	CD1	TRP	285	-10.621	23.414	13.847	1.00	0.00	-0.177	10.80	0.60
ATOM	2890	HD1	TRP	285	-10.843	24.223	13.151	1.00	0.00	0.127	0.00	0.00
ATOM	2891	NE1	TRP	285	-9.559	22.549	13.739	1.00	0.00	-0.292	9.00	-17.40
ATOM	2892	HE1	TRP	285	-8.853	22.560	12.989	1.00	0.00	0.393	0.00	0.00
ATOM	2893	CE3	TRP	285	-10.968	21.225	16.739	1.00	0.00	-0.127	10.80	0.60
ATOM	2894	HE3	TRP	285	-11.826	21.448	17.372	1.00	0.00	0.127	0.00	0.00
ATOM	2895	CZ2	TRP	285	-8.720	20.614	15.110	1.00	0.00	-0.127	10.80	0.60
ATOM	2896	HZ2	TRP	285	-7.858	20.383	14.483	1.00	0.00	0.127	0.00	0.00
ATOM	2897	CZ3	TRP	285	-10.100	20.171	17.059	1.00	0.00	-0.127	10.80	0.60
ATOM	2898	HZ3	TRP	285	-10.287	19.571	17.949	1.00	0.00	0.127	0.00	0.00
ATOM	2899	CH2	TRP	285	-8.994	19.879	16.247	1.00	0.00	-0.127	10.80	0.60
ATOM	2900	HH2	TRP	285	-8.336	19.053	16.519	1.00	0.00	0.127	0.00	0.00
ATOM	2901	C	TRP	285	-11.667	25.931	16.398	1.00	0.00	0.396	9.82	4.00
ATOM	2902	O	TRP	285	-12.179	26.840	15.748	1.00	0.00	-0.396	8.17	-17.40
ATOM	2903	N	PRO	286	-10.406	26.015	16.851	1.00	0.00	-0.422	9.00	-17.40
ATOM	2904	CD	PRO	286	-9.649	24.891	17.443	1.00	0.00	0.105	12.77	4.00
ATOM	2905	HD1	PRO	286	-9.757	23.985	16.845	1.00	0.00	0.053	0.00	0.00
ATOM	2906	HD2	PRO	286	-9.999	24.667	18.450	1.00	0.00	0.053	0.00	0.00
ATOM	2907	CA	PRO	286	-9.539	27.184	16.662	1.00	0.00	0.158	9.40	4.00
ATOM	2908	HA	PRO	286	-10.106	28.070	16.944	1.00	0.00	0.053	0.00	0.00
ATOM	2909	CB	PRO	286	-8.403	26.911	17.633	1.00	0.00	-0.106	12.77	4.00
ATOM	2910	HB1	PRO	286	-8.677	27.170	18.655	1.00	0.00	0.053	0.00	0.00
ATOM	2911	HB2	PRO	286	-7.512	27.487	17.381	1.00	0.00	0.053	0.00	0.00
ATOM	2912	CG	PRO	286	-8.207	25.412	17.439	1.00	0.00	-0.106	12.77	4.00
ATOM	2913	HG1	PRO	286	-7.611	24.982	18.245	1.00	0.00	0.053	0.00	0.00
ATOM	2914	HG2	PRO	286	-7.694	25.197	16.501	1.00	0.00	0.053	0.00	0.00
ATOM	2915	C	PRO	286	-9.026	27.413	15.241	1.00	0.00	0.396	9.82	4.00
ATOM	2916	O	PRO	286	-9.091	26.521	14.397	1.00	0.00	-0.396	8.17	-17.40
ATOM	2917	N	LYS	287S	-8.496	28.612	14.997	1.00	0.00	-0.650	9.00	-17.40
ATOM	2918	HN	LYS	287S	-8.474	29.314	15.750	1.00	0.00	0.440	0.00	0.00
ATOM	2919	CA	LYS	287S	-7.942	28.956	13.681	1.00	0.00	0.158	9.40	4.00
ATOM	2920	HA	LYS	287S	-8.551	28.550	12.873	1.00	0.00	0.053	0.00	0.00
ATOM	2921	CB	LYS	287S	-7.874	30.472	13.485	1.00	0.00	-0.106	12.77	4.00
ATOM	2922	HB1	LYS	287S	-7.557	30.665	12.460	1.00	0.00	0.053	0.00	0.00
ATOM	2923	HB2	LYS	287S	-7.151	30.871	14.196	1.00	0.00	0.053	0.00	0.00
ATOM	2924	CG	LYS	287S	-9.164	31.211	13.699	1.00	0.00	-0.106	12.77	4.00
ATOM	2925	HG1	LYS	287S	-9.025	32.279	13.536	1.00	0.00	0.053	0.00	0.00
ATOM	2926	HG2	LYS	287S	-9.526	31.063	14.716	1.00	0.00	0.053	0.00	0.00
ATOM	2927	CD	LYS	287S	-10.225	30.718	12.740	1.00	0.00	-0.106	12.77	4.00
ATOM	2928	HD1	LYS	287S	-10.404	29.650	12.869	1.00	0.00	0.053	0.00	0.00
ATOM	2929	HD2	LYS	287S	-9.924	30.883	11.705	1.00	0.00	0.053	0.00	0.00
ATOM	2930	CE	LYS	287S	-11.542	31.442	12.964	1.00	0.00	0.099	12.77	4.00
ATOM	2931	HE1	LYS	287S	-11.408	32.515	12.833	1.00	0.00	0.053	0.00	0.00
ATOM	2932	HE2	LYS	287S	-11.907	31.255	13.974	1.00	0.00	0.053	0.00	0.00
ATOM	2933	NZ	LYS	287S	-12.561	30.966	11.993	1.00	0.00	-0.045	13.25	-39.20
ATOM	2934	HZ1	LYS	287S	-13.448	31.463	12.154	1.00	0.00	0.280	0.00	0.00
ATOM	2935	HZ2	LYS	287S	-12.234	31.150	11.033	1.00	0.00	0.280	0.00	0.00
ATOM	2936	HZ3	LYS	287S	-12.707	29.954	12.117	1.00	0.00	0.280	0.00	0.00
ATOM	2937	C	LYS	287S	-6.524	28.402	13.508	1.00	0.00	0.396	9.82	4.00
ATOM	2938	O	LYS	287S	-6.046	28.287	12.366	1.00	0.00	-0.396	8.17	-17.40
ATOM	2939	N	ALA	288	-5.852	28.066	14.617	1.00	0.00	-0.650	9.00	-17.40
ATOM	2940	HN	ALA	288	-6.304	28.170	15.536	1.00	0.00	0.440	0.00	0.00
ATOM	2941	CA	ALA	288	-4.468	27.546	14.539	1.00	0.00	0.158	9.40	4.00
ATOM	2942	HA	ALA	288	-4.330	26.784	13.771	1.00	0.00	0.053	0.00	0.00
ATOM	2943	CB	ALA	288	-3.500	28.686	14.162	1.00	0.00	-0.159	16.15	4.00
ATOM	2944	HB1	ALA	288	-2.483	28.296	14.106	1.00	0.00	0.053	0.00	0.00
ATOM	2945	HB2	ALA	288	-3.783	29.099	13.194	1.00	0.00	0.053	0.00	0.00
ATOM	2946	HB3	ALA	288	-3.547	29.469	14.918	1.00	0.00	0.053	0.00	0.00
ATOM	2947	C	ALA	288	-3.986	26.896	15.831	1.00	0.00	0.396	9.82	4.00
ATOM	2948	O	ALA	288	-4.549	27.138	16.908	1.00	0.00	-0.396	8.17	-17.40
ATOM	2949	N	PHE	289	-2.902	26.123	15.720	1.00	0.00	-0.650	9.00	-17.40
ATOM	2950	HN	PHE	289	-2.470	26.018	14.790	1.00	0.00	0.440	0.00	0.00
ATOM	2951	CA	PHE	289	-2.294	25.416	16.852	1.00	0.00	0.158	9.40	4.00
ATOM	2952	HA	PHE	289	-1.516	24.738	16.499	1.00	0.00	0.053	0.00	0.00
ATOM	2953	CB	PHE	289	-1.628	26.420	17.793	1.00	0.00	-0.106	12.77	4.00
ATOM	2954	HB1	PHE	289	-0.983	25.949	18.535	1.00	0.00	0.053	0.00	0.00
ATOM	2955	HB2	PHE	289	-2.343	27.014	18.361	1.00	0.00	0.053	0.00	0.00
ATOM	2956	CG	PHE	289	-0.758	27.413	17.077	1.00	0.00	0.000	7.26	0.60
ATOM	2957	CD1	PHE	289	-1.173	28.730	16.908	1.00	0.00	-0.127	10.80	0.60
ATOM	2958	HD1	PHE	289	-2.128	29.049	17.323	1.00	0.00	0.127	0.00	0.00
ATOM	2959	CD2	PHE	289	0.469	27.016	16.541	1.00	0.00	-0.127	10.80	0.60

ATOM	2960	HD2	PHE	289	0.806	25.987	16.668	1.00	0.00	0.127	0.00	0.00
ATOM	2961	CE1	PHE	289	-0.381	29.652	16.212	1.00	0.00	-0.127	10.80	0.60
ATOM	2962	HE1	PHE	289	-0.716	30.681	16.087	1.00	0.00	0.127	0.00	0.00
ATOM	2963	CE2	PHE	289	1.261	27.918	15.849	1.00	0.00	-0.127	10.80	0.60
ATOM	2964	HE2	PHE	289	2.216	27.596	15.433	1.00	0.00	0.127	0.00	0.00
ATOM	2965	CZ	PHE	289	0.835	29.243	15.683	1.00	0.00	-0.127	10.80	0.60
ATOM	2966	HZ	PHE	289	1.458	29.952	15.138	1.00	0.00	0.127	0.00	0.00
ATOM	2967	C	PHE	289	-3.344	24.609	17.592	1.00	0.00	0.396	9.82	4.00
ATOM	2968	O	PHE	289	-3.559	24.779	18.808	1.00	0.00	-0.396	8.17	-17.40
ATOM	2969	N	TRP	290	-3.978	23.703	16.855	1.00	0.00	-0.650	9.00	-17.40
ATOM	2970	HN	TRP	290	-3.697	23.566	15.873	1.00	0.00	0.440	0.00	0.00
ATOM	2971	CA	TRP	290	-5.055	22.903	17.402	1.00	0.00	0.158	9.40	4.00
ATOM	2972	HA	TRP	290	-5.838	23.578	17.746	1.00	0.00	0.053	0.00	0.00
ATOM	2973	CB	TRP	290	-5.722	22.072	16.295	1.00	0.00	-0.106	12.77	4.00
ATOM	2974	HB1	TRP	290	-5.908	22.723	15.441	1.00	0.00	0.053	0.00	0.00
ATOM	2975	HB2	TRP	290	-6.659	21.672	16.682	1.00	0.00	0.053	0.00	0.00
ATOM	2976	CG	TRP	290	-4.909	20.939	15.827	1.00	0.00	0.000	7.26	0.60
ATOM	2977	CD2	TRP	290	-4.821	19.657	16.445	1.00	0.00	0.000	6.80	0.60
ATOM	2978	CE2	TRP	290	-3.800	18.942	15.783	1.00	0.00	-0.050	6.80	0.60
ATOM	2979	CD1	TRP	290	-3.979	20.950	14.829	1.00	0.00	-0.177	10.80	0.60
ATOM	2980	HD1	TRP	290	-3.797	21.787	14.155	1.00	0.00	0.127	0.00	0.00
ATOM	2981	NE1	TRP	290	-3.303	19.751	14.796	1.00	0.00	-0.292	9.00	-17.40
ATOM	2982	HE1	TRP	290	-2.549	19.503	14.139	1.00	0.00	0.393	0.00	0.00
ATOM	2983	CE3	TRP	290	-5.500	19.044	17.509	1.00	0.00	-0.127	10.80	0.60
ATOM	2984	HE3	TRP	290	-6.297	19.567	18.035	1.00	0.00	0.127	0.00	0.00
ATOM	2985	CZ2	TRP	290	-3.433	17.639	16.154	1.00	0.00	-0.127	10.80	0.60
ATOM	2986	HZ2	TRP	290	-2.642	17.102	15.628	1.00	0.00	0.127	0.00	0.00
ATOM	2987	CZ3	TRP	290	-5.133	17.753	17.878	1.00	0.00	-0.127	10.80	0.60
ATOM	2988	HZ3	TRP	290	-5.648	17.263	18.704	1.00	0.00	0.127	0.00	0.00
ATOM	2989	CH2	TRP	290	-4.104	17.068	17.199	1.00	0.00	-0.127	10.80	0.60
ATOM	2990	HH2	TRP	290	-3.837	16.059	17.515	1.00	0.00	0.127	0.00	0.00
ATOM	2991	C	TRP	290	-4.664	22.017	18.582	1.00	0.00	0.396	9.82	4.00
ATOM	2992	O	TRP	290	-5.436	21.909	19.538	1.00	0.00	-0.396	8.17	-17.40
ATOM	2993	N	ASP	291P	-3.473	21.414	18.547	1.00	0.00	-0.650	9.00	-17.40
ATOM	2994	HN	ASP	291P	-2.848	21.560	17.740	1.00	0.00	0.440	0.00	0.00
ATOM	2995	CA	ASP	291P	-3.049	20.547	19.646	1.00	0.00	0.158	9.40	4.00
ATOM	2996	HA	ASP	291P	-3.829	19.805	19.817	1.00	0.00	0.053	0.00	0.00
ATOM	2997	CB	ASP	291P	-1.822	19.690	19.241	1.00	0.00	-0.336	12.77	4.00
ATOM	2998	HB1	ASP	291P	-2.050	18.944	18.479	1.00	0.00	0.053	0.00	0.00
ATOM	2999	HB2	ASP	291P	-1.392	19.132	20.073	1.00	0.00	0.053	0.00	0.00
ATOM	3000	CG	ASP	291P	-0.681	20.510	18.673	1.00	0.00	0.297	9.82	4.00
ATOM	3001	OD1	ASP	291P	0.456	20.000	18.639	1.00	0.00	-0.534	8.17	-18.95
ATOM	3002	OD2	ASP	291P	-0.908	21.653	18.247	1.00	0.00	-0.534	8.17	-18.95
ATOM	3003	C	ASP	291P	-2.805	21.285	20.974	1.00	0.00	0.396	9.82	4.00
ATOM	3004	O	ASP	291P	-3.192	20.781	22.028	1.00	0.00	-0.396	8.17	-17.40
ATOM	3005	N	ASP	292P	-2.180	22.461	20.937	1.00	0.00	-0.650	9.00	-17.40
ATOM	3006	HN	ASP	292P	-1.852	22.833	20.034	1.00	0.00	0.440	0.00	0.00
ATOM	3007	CA	ASP	292P	-1.951	23.235	22.167	1.00	0.00	0.158	9.40	4.00
ATOM	3008	HA	ASP	292P	-1.505	22.602	22.935	1.00	0.00	0.053	0.00	0.00
ATOM	3009	CB	ASP	292P	-0.960	24.384	21.932	1.00	0.00	-0.336	12.77	4.00
ATOM	3010	HB1	ASP	292P	-1.069	25.178	22.670	1.00	0.00	0.053	0.00	0.00
ATOM	3011	HB2	ASP	292P	-1.091	24.846	20.953	1.00	0.00	0.053	0.00	0.00
ATOM	3012	CG	ASP	292P	0.485	23.918	22.004	1.00	0.00	0.297	9.82	4.00
ATOM	3013	OD1	ASP	292P	0.715	22.720	22.323	1.00	0.00	-0.534	8.17	-18.95
ATOM	3014	OD2	ASP	292P	1.392	24.733	21.758	1.00	0.00	-0.534	8.17	-18.95
ATOM	3015	C	ASP	292P	-3.265	23.788	22.696	1.00	0.00	0.396	9.82	4.00
ATOM	3016	O	ASP	292P	-3.420	24.012	23.913	1.00	0.00	-0.396	8.17	-17.40
ATOM	3017	N	TRP	293	-4.207	24.001	21.777	1.00	0.00	-0.650	9.00	-17.40
ATOM	3018	HN	TRP	293	-3.987	23.808	20.789	1.00	0.00	0.440	0.00	0.00
ATOM	3019	CA	TRP	293	-5.551	24.501	22.120	1.00	0.00	0.158	9.40	4.00
ATOM	3020	HA	TRP	293	-5.457	25.391	22.742	1.00	0.00	0.053	0.00	0.00
ATOM	3021	CB	TRP	293	-6.296	24.863	20.834	1.00	0.00	-0.106	12.77	4.00
ATOM	3022	HB1	TRP	293	-6.241	24.005	20.163	1.00	0.00	0.053	0.00	0.00
ATOM	3023	HB2	TRP	293	-5.805	25.733	20.397	1.00	0.00	0.053	0.00	0.00
ATOM	3024	CG	TRP	293	-7.737	25.206	20.986	1.00	0.00	0.000	7.26	0.60
ATOM	3025	CD2	TRP	293	-8.854	24.339	20.738	1.00	0.00	0.000	6.80	0.60
ATOM	3026	CE2	TRP	293	-10.028	25.094	20.971	1.00	0.00	-0.050	6.80	0.60
ATOM	3027	CD1	TRP	293	-8.263	26.413	21.353	1.00	0.00	-0.177	10.80	0.60
ATOM	3028	HD1	TRP	293	-7.677	27.294	21.615	1.00	0.00	0.127	0.00	0.00
ATOM	3029	NE1	TRP	293	-9.639	26.356	21.344	1.00	0.00	-0.292	9.00	-17.40
ATOM	3030	HE1	TRP	293	-10.272	27.133	21.579	1.00	0.00	0.393	0.00	0.00
ATOM	3031	CE3	TRP	293	-8.974	22.995	20.345	1.00	0.00	-0.127	10.80	0.60
ATOM	3032	HE3	TRP	293	-8.086	22.390	20.161	1.00	0.00	0.127	0.00	0.00
ATOM	3033	CZ2	TRP	293	-11.308	24.554	20.820	1.00	0.00	-0.127	10.80	0.60
ATOM	3034	HZ2	TRP	293	-12.199	25.153	21.003	1.00	0.00	0.127	0.00	0.00
ATOM	3035	CZ3	TRP	293	-10.245	22.449	20.194	1.00	0.00	-0.127	10.80	0.60

ATOM	3036	HZ3	TRP	293	-10.353	21.407	19.890	1.00	0.00	0.127	0.00	0.00
ATOM	3037	CH2	TRP	293	-11.400	23.235	20.431	1.00	0.00	-0.127	10.80	0.60
ATOM	3038	HH2	TRP	293	-12.384	22.785	20.302	1.00	0.00	0.127	0.00	0.00
ATOM	3039	C	TRP	293	-6.318	23.415	22.888	1.00	0.00	0.396	9.82	4.00
ATOM	3040	O	TRP	293	-7.058	23.699	23.840	1.00	0.00	-0.396	8.17	-17.40
ATOM	3041	N	MET	294	-6.155	22.166	22.478	1.00	0.00	-0.650	9.00	-17.40
ATOM	3042	HN	MET	294	-5.559	21.956	21.664	1.00	0.00	0.440	0.00	0.00
ATOM	3043	CA	MET	294	-6.835	21.087	23.200	1.00	0.00	0.158	9.40	4.00
ATOM	3044	HA	MET	294	-7.888	21.330	23.340	1.00	0.00	0.053	0.00	0.00
ATOM	3045	CB	MET	294	-6.777	19.782	22.399	1.00	0.00	-0.106	12.77	4.00
ATOM	3046	HB1	MET	294	-6.802	18.947	23.100	1.00	0.00	0.053	0.00	0.00
ATOM	3047	HB2	MET	294	-5.850	19.772	21.825	1.00	0.00	0.053	0.00	0.00
ATOM	3048	CG	MET	294	-7.941	19.600	21.412	1.00	0.00	-0.041	12.77	4.00
ATOM	3049	HG1	MET	294	-8.018	20.448	20.732	1.00	0.00	0.053	0.00	0.00
ATOM	3050	HG2	MET	294	-8.892	19.508	21.936	1.00	0.00	0.053	0.00	0.00
ATOM	3051	SD	MET	294	-7.725	18.134	20.424	1.00	0.00	-0.130	16.39	-6.40
ATOM	3052	CE	MET	294	-8.130	16.824	21.657	1.00	0.00	-0.094	16.15	4.00
ATOM	3053	HE1	MET	294	-8.040	15.843	21.189	1.00	0.00	0.053	0.00	0.00
ATOM	3054	HE2	MET	294	-7.439	16.889	22.497	1.00	0.00	0.053	0.00	0.00
ATOM	3055	HE3	MET	294	-9.150	16.963	22.014	1.00	0.00	0.053	0.00	0.00
ATOM	3056	C	MET	294	-6.195	20.881	24.574	1.00	0.00	0.396	9.82	4.00
ATOM	3057	O	MET	294	-6.825	20.326	25.480	1.00	0.00	-0.396	8.17	-17.40
ATOM	3058	N	ARG	295G	-4.950	21.329	24.733	1.00	0.00	-0.650	9.00	-17.40
ATOM	3059	HN	ARG	295G	-4.470	21.789	23.946	1.00	0.00	0.440	0.00	0.00
ATOM	3060	CA	ARG	295G	-4.263	21.176	26.002	1.00	0.00	0.158	9.40	4.00
ATOM	3061	HA	ARG	295G	-4.388	20.185	26.439	1.00	0.00	0.053	0.00	0.00
ATOM	3062	CB	ARG	295G	-2.744	21.266	25.810	1.00	0.00	-0.106	12.77	4.00
ATOM	3063	HB1	ARG	295G	-2.221	21.504	26.736	1.00	0.00	0.053	0.00	0.00
ATOM	3064	HB2	ARG	295G	-2.460	22.034	25.090	1.00	0.00	0.053	0.00	0.00
ATOM	3065	CG	ARG	295G	-2.140	19.952	25.299	1.00	0.00	-0.106	12.77	4.00
ATOM	3066	HG1	ARG	295G	-2.800	19.401	24.628	1.00	0.00	0.053	0.00	0.00
ATOM	3067	HG2	ARG	295G	-1.891	19.249	26.094	1.00	0.00	0.053	0.00	0.00
ATOM	3068	CD	ARG	295G	-0.838	20.143	24.512	1.00	0.00	0.374	12.77	4.00
ATOM	3069	HD1	ARG	295G	-0.034	20.468	25.172	1.00	0.00	0.053	0.00	0.00
ATOM	3070	HD2	ARG	295G	-0.967	20.894	23.733	1.00	0.00	0.053	0.00	0.00
ATOM	3071	NE	ARG	295G	-0.430	18.885	23.875	1.00	0.00	-0.819	9.00	-24.67
ATOM	3072	HE	ARG	295G	-0.793	18.003	24.265	1.00	0.00	0.407	0.00	0.00
ATOM	3073	CZ	ARG	295G	0.380	18.816	22.825	1.00	0.00	0.796	6.95	4.00
ATOM	3074	NH1	ARG	295G	0.875	19.927	22.284	1.00	0.00	-0.746	9.00	-24.67
ATOM	3075	HH1	ARG	295G	1.502	19.867	21.469	1.00	0.00	0.407	0.00	0.00
ATOM	3076	HH1	ARG	295G	0.630	20.845	22.679	1.00	0.00	0.407	0.00	0.00
ATOM	3077	NH2	ARG	295G	0.697	17.639	22.307	1.00	0.00	-0.746	9.00	-24.67
ATOM	3078	HH2	ARG	295G	1.325	17.587	21.492	1.00	0.00	0.407	0.00	0.00
ATOM	3079	HH2	ARG	295G	0.315	16.775	22.718	1.00	0.00	0.407	0.00	0.00
ATOM	3080	C	ARG	295G	-4.746	22.160	27.067	1.00	0.00	0.396	9.82	4.00
ATOM	3081	O	ARG	295G	-4.470	21.983	28.255	1.00	0.00	-0.396	8.17	-17.40
ATOM	3082	N	ARG	296G	-5.485	23.178	26.646	1.00	0.00	-0.650	9.00	-17.40
ATOM	3083	HN	ARG	296G	-5.682	23.276	25.639	1.00	0.00	0.440	0.00	0.00
ATOM	3084	CA	ARG	296G	-6.026	24.164	27.582	1.00	0.00	0.158	9.40	4.00
ATOM	3085	HA	ARG	296G	-5.251	24.530	28.255	1.00	0.00	0.053	0.00	0.00
ATOM	3086	CB	ARG	296G	-6.596	25.359	26.826	1.00	0.00	-0.106	12.77	4.00
ATOM	3087	HB1	ARG	296G	-7.008	26.122	27.485	1.00	0.00	0.053	0.00	0.00
ATOM	3088	HB2	ARG	296G	-7.404	25.087	26.146	1.00	0.00	0.053	0.00	0.00
ATOM	3089	CG	ARG	296G	-5.575	26.059	25.983	1.00	0.00	-0.106	12.77	4.00
ATOM	3090	HG1	ARG	296G	-5.186	25.362	25.240	1.00	0.00	0.053	0.00	0.00
ATOM	3091	HG2	ARG	296G	-4.763	26.408	26.621	1.00	0.00	0.053	0.00	0.00
ATOM	3092	CD	ARG	296G	-6.219	27.222	25.299	1.00	0.00	0.374	12.77	4.00
ATOM	3093	HD1	ARG	296G	-6.638	27.931	26.012	1.00	0.00	0.053	0.00	0.00
ATOM	3094	HD2	ARG	296G	-7.033	26.909	24.645	1.00	0.00	0.053	0.00	0.00
ATOM	3095	NE	ARG	296G	-5.276	27.956	24.477	1.00	0.00	-0.819	9.00	-24.67
ATOM	3096	HE	ARG	296G	-4.284	27.676	24.497	1.00	0.00	0.407	0.00	0.00
ATOM	3097	CZ	ARG	296G	-5.632	28.974	23.698	1.00	0.00	0.796	6.95	4.00
ATOM	3098	NH1	ARG	296G	-6.911	29.356	23.646	1.00	0.00	-0.746	9.00	-24.67
ATOM	3099	HH1	ARG	296G	-7.189	30.143	23.043	1.00	0.00	0.407	0.00	0.00
ATOM	3100	HH1	ARG	296G	-7.619	28.862	24.208	1.00	0.00	0.407	0.00	0.00
ATOM	3101	NH2	ARG	296G	-4.715	29.618	22.987	1.00	0.00	-0.746	9.00	-24.67
ATOM	3102	HH2	ARG	296G	-4.990	30.406	22.384	1.00	0.00	0.407	0.00	0.00
ATOM	3103	HH2	ARG	296G	-3.727	29.329	23.038	1.00	0.00	0.407	0.00	0.00
ATOM	3104	C	ARG	296G	-7.141	23.557	28.436	1.00	0.00	0.396	9.82	4.00
ATOM	3105	O	ARG	296G	-7.880	22.667	27.986	1.00	0.00	-0.396	8.17	-17.40
ATOM	3106	N	PRO	297	-7.305	24.059	29.670	1.00	0.00	-0.422	9.00	-17.40
ATOM	3107	CD	PRO	297	-6.485	25.036	30.414	1.00	0.00	0.105	12.77	4.00
ATOM	3108	HD1	PRO	297	-6.254	25.906	29.800	1.00	0.00	0.053	0.00	0.00
ATOM	3109	HD2	PRO	297	-5.539	24.596	30.732	1.00	0.00	0.053	0.00	0.00
ATOM	3110	CA	PRO	297	-8.367	23.477	30.501	1.00	0.00	0.158	9.40	4.00
ATOM	3111	HA	PRO	297	-8.203	22.400	30.554	1.00	0.00	0.053	0.00	0.00

ATOM	3112	CB	PRO	297	-8.107	24.085	31.892	1.00	0.00	-0.106	12.77	4.00
ATOM	3113	HB1	PRO	297	-7.495	23.339	32.401	1.00	0.00	0.053	0.00	0.00
ATOM	3114	HB2	PRO	297	-9.101	24.213	32.319	1.00	0.00	0.053	0.00	0.00
ATOM	3115	CG	PRO	297	-7.382	25.391	31.601	1.00	0.00	-0.106	12.77	4.00
ATOM	3116	HG1	PRO	297	-6.802	25.717	32.464	1.00	0.00	0.053	0.00	0.00
ATOM	3117	HG2	PRO	297	-8.087	26.184	31.353	1.00	0.00	0.053	0.00	0.00
ATOM	3118	C	PRO	297	-9.792	23.699	29.982	1.00	0.00	0.396	9.82	4.00
ATOM	3119	O	PRO	297	-10.681	22.870	30.227	1.00	0.00	-0.396	8.17	-17.40
ATOM	3120	N	GLU	298	-10.013	24.790	29.252	1.00	0.00	-0.650	9.00	-17.40
ATOM	3121	HN	GLU	298	-9.240	25.444	29.062	1.00	0.00	0.440	0.00	0.00
ATOM	3122	CA	GLU	298	-11.341	25.064	28.720	1.00	0.00	0.158	9.40	4.00
ATOM	3123	HA	GLU	298	-12.060	25.131	29.536	1.00	0.00	0.053	0.00	0.00
ATOM	3124	CB	GLU	298	-11.371	26.396	27.951	1.00	0.00	-0.106	12.77	4.00
ATOM	3125	HB1	GLU	298	-12.354	26.494	27.491	1.00	0.00	0.053	0.00	0.00
ATOM	3126	HB2	GLU	298	-10.586	26.362	27.194	1.00	0.00	0.053	0.00	0.00
ATOM	3127	CG	GLU	298	-11.138	27.656	28.780	1.00	0.00	-0.106	12.77	4.00
ATOM	3128	HG1	GLU	298	-11.752	27.701	29.679	1.00	0.00	0.053	0.00	0.00
ATOM	3129	HG2	GLU	298	-11.352	28.576	28.237	1.00	0.00	0.053	0.00	0.00
ATOM	3130	CD	GLU	298	-9.699	27.802	29.268	1.00	0.00	0.399	9.82	4.00
ATOM	3131	OE1	GLU	298	-8.803	27.167	28.681	1.00	0.00	-0.396	8.17	-18.95
ATOM	3132	OE2	GLU	298	-9.468	28.568	30.236	1.00	0.00	-0.427	8.17	-18.95
ATOM	3133	HE2	GLU	298	-8.458	28.570	30.439	1.00	0.00	0.424	0.00	0.00
ATOM	3134	C	GLU	298	-11.765	23.938	27.771	1.00	0.00	0.396	9.82	4.00
ATOM	3135	O	GLU	298	-12.947	23.729	27.537	1.00	0.00	-0.396	8.17	-17.40
ATOM	3136	N	GLN	299	-10.792	23.226	27.216	1.00	0.00	-0.650	9.00	-17.40
ATOM	3137	HN	GLN	299	-9.812	23.453	27.437	1.00	0.00	0.440	0.00	0.00
ATOM	3138	CA	GLN	299	-11.081	22.127	26.298	1.00	0.00	0.158	9.40	4.00
ATOM	3139	HA	GLN	299	-12.084	22.214	25.880	1.00	0.00	0.053	0.00	0.00
ATOM	3140	CB	GLN	299	-10.079	22.119	25.141	1.00	0.00	-0.106	12.77	4.00
ATOM	3141	HB1	GLN	299	-10.013	21.098	24.763	1.00	0.00	0.053	0.00	0.00
ATOM	3142	HB2	GLN	299	-9.118	22.455	25.530	1.00	0.00	0.053	0.00	0.00
ATOM	3143	CG	GLN	299	-10.417	23.017	23.945	1.00	0.00	-0.106	12.77	4.00
ATOM	3144	HG1	GLN	299	-11.321	22.717	23.415	1.00	0.00	0.053	0.00	0.00
ATOM	3145	HG2	GLN	299	-9.638	23.041	23.182	1.00	0.00	0.053	0.00	0.00
ATOM	3146	CD	GLN	299	-10.647	24.484	24.323	1.00	0.00	0.396	9.82	4.00
ATOM	3147	OE1	GLN	299	-11.778	24.895	24.584	1.00	0.00	-0.396	8.17	-17.40
ATOM	3148	NE2	GLN	299	-9.568	25.274	24.357	1.00	0.00	-0.879	13.25	-17.40
ATOM	3149	HE2	GLN	299	-8.640	24.888	24.131	1.00	0.00	0.440	0.00	0.00
ATOM	3150	HE2	GLN	299	-9.665	26.268	24.609	1.00	0.00	0.440	0.00	0.00
ATOM	3151	C	GLN	299	-10.991	20.785	27.001	1.00	0.00	0.396	9.82	4.00
ATOM	3152	O	GLN	299	-11.876	19.947	26.883	1.00	0.00	-0.396	8.17	-17.40
ATOM	3153	N	ARG	300G	-9.891	20.596	27.723	1.00	0.00	-0.650	9.00	-17.40
ATOM	3154	HN	ARG	300G	-9.207	21.363	27.794	1.00	0.00	0.440	0.00	0.00
ATOM	3155	CA	ARG	300G	-9.614	19.345	28.418	1.00	0.00	0.158	9.40	4.00
ATOM	3156	HA	ARG	300G	-9.620	18.472	27.764	1.00	0.00	0.053	0.00	0.00
ATOM	3157	CB	ARG	300G	-8.206	19.406	29.013	1.00	0.00	-0.106	12.77	4.00
ATOM	3158	HB1	ARG	300G	-8.217	20.106	29.847	1.00	0.00	0.053	0.00	0.00
ATOM	3159	HB2	ARG	300G	-7.520	19.745	28.236	1.00	0.00	0.053	0.00	0.00
ATOM	3160	CG	ARG	300G	-7.690	18.075	29.535	1.00	0.00	-0.106	12.77	4.00
ATOM	3161	HG1	ARG	300G	-7.842	17.289	28.795	1.00	0.00	0.053	0.00	0.00
ATOM	3162	HG2	ARG	300G	-8.214	17.793	30.448	1.00	0.00	0.053	0.00	0.00
ATOM	3163	CD	ARG	300G	-6.192	18.164	29.845	1.00	0.00	0.374	12.77	4.00
ATOM	3164	HD1	ARG	300G	-5.720	18.784	29.083	1.00	0.00	0.053	0.00	0.00
ATOM	3165	HD2	ARG	300G	-5.777	17.156	29.828	1.00	0.00	0.053	0.00	0.00
ATOM	3166	NE	ARG	300G	-5.887	18.751	31.151	1.00	0.00	-0.819	9.00	-24.67
ATOM	3167	HE	ARG	300G	-5.490	19.701	31.169	1.00	0.00	0.407	0.00	0.00
ATOM	3168	CZ	ARG	300G	-6.088	18.139	32.319	1.00	0.00	0.796	6.95	4.00
ATOM	3169	NH1	ARG	300G	-6.606	16.908	32.369	1.00	0.00	-0.746	9.00	-24.67
ATOM	3170	HH1	ARG	300G	-6.755	16.448	33.278	1.00	0.00	0.407	0.00	0.00
ATOM	3171	HH1	ARG	300G	-6.856	16.418	31.497	1.00	0.00	0.407	0.00	0.00
ATOM	3172	NH2	ARG	300G	-5.749	18.750	33.449	1.00	0.00	-0.746	9.00	-24.67
ATOM	3173	HH2	ARG	300G	-5.902	18.281	34.353	1.00	0.00	0.407	0.00	0.00
ATOM	3174	HH2	ARG	300G	-5.333	19.691	33.420	1.00	0.00	0.407	0.00	0.00
ATOM	3175	C	ARG	300G	-10.612	19.025	29.511	1.00	0.00	0.396	9.82	4.00
ATOM	3176	O	ARG	300G	-11.061	17.889	29.647	1.00	0.00	-0.396	8.17	-17.40
ATOM	3177	N	LYS	301S	-10.925	20.034	30.314	1.00	0.00	-0.650	9.00	-17.40
ATOM	3178	HN	LYS	301S	-10.500	20.957	30.144	1.00	0.00	0.440	0.00	0.00
ATOM	3179	CA	LYS	301S	-11.847	19.877	31.424	1.00	0.00	0.158	9.40	4.00
ATOM	3180	HA	LYS	301S	-11.889	20.776	32.038	1.00	0.00	0.053	0.00	0.00
ATOM	3181	CB	LYS	301S	-13.257	19.668	30.882	1.00	0.00	-0.106	12.77	4.00
ATOM	3182	HB1	LYS	301S	-13.987	19.441	31.659	1.00	0.00	0.053	0.00	0.00
ATOM	3183	HB2	LYS	301S	-13.326	18.845	30.169	1.00	0.00	0.053	0.00	0.00
ATOM	3184	CG	LYS	301S	-13.810	20.894	30.146	1.00	0.00	-0.106	12.77	4.00
ATOM	3185	HG1	LYS	301S	-13.086	21.314	29.447	1.00	0.00	0.053	0.00	0.00
ATOM	3186	HG2	LYS	301S	-14.084	21.695	30.832	1.00	0.00	0.053	0.00	0.00
ATOM	3187	CD	LYS	301S	-15.057	20.563	29.338	1.00	0.00	-0.106	12.77	4.00

ATOM	3188	HD1	LYS	301S	-15.869	20.192	29.963	1.00	0.00	0.053	0.00	0.00
ATOM	3189	HD2	LYS	301S	-14.871	19.796	28.586	1.00	0.00	0.053	0.00	0.00
ATOM	3190	CE	LYS	301S	-15.604	21.777	28.592	1.00	0.00	0.099	12.77	4.00
ATOM	3191	HE1	LYS	301S	-14.893	22.158	27.859	1.00	0.00	0.053	0.00	0.00
ATOM	3192	HE2	LYS	301S	-15.834	22.600	29.268	1.00	0.00	0.053	0.00	0.00
ATOM	3193	NZ	LYS	301S	-16.871	21.454	27.847	1.00	0.00	-0.045	13.25	-39.20
ATOM	3194	HZ1	LYS	301S	-17.206	22.296	27.358	1.00	0.00	0.280	0.00	0.00
ATOM	3195	HZ2	LYS	301S	-16.685	20.710	27.159	1.00	0.00	0.280	0.00	0.00
ATOM	3196	HZ3	LYS	301S	-17.589	21.134	28.512	1.00	0.00	0.280	0.00	0.00
ATOM	3197	C	LYS	301S	-11.431	18.712	32.342	1.00	0.00	0.396	9.82	4.00
ATOM	3198	O	LYS	301S	-12.215	17.819	32.634	1.00	0.00	-0.396	8.17	-17.40
ATOM	3199	N	GLY	302	-10.171	18.719	32.759	1.00	0.00	-0.650	9.00	-17.40
ATOM	3200	HN	GLY	302	-9.532	19.457	32.431	1.00	0.00	0.440	0.00	0.00
ATOM	3201	CA	GLY	302	-9.678	17.699	33.672	1.00	0.00	0.105	9.40	4.00
ATOM	3202	HA1	GLY	302	-10.336	17.696	34.540	1.00	0.00	0.053	0.00	0.00
ATOM	3203	HA2	GLY	302	-8.658	17.973	33.942	1.00	0.00	0.053	0.00	0.00
ATOM	3204	C	GLY	302	-9.614	16.263	33.188	1.00	0.00	0.396	9.82	4.00
ATOM	3205	O	GLY	302	-9.218	15.381	33.945	1.00	0.00	-0.396	8.17	-17.40
ATOM	3206	N	ARG	303G	-9.966	16.026	31.928	1.00	0.00	-0.650	9.00	-17.40
ATOM	3207	HN	ARG	303G	-10.247	16.814	31.328	1.00	0.00	0.440	0.00	0.00
ATOM	3208	CA	ARG	303G	-9.963	14.683	31.378	1.00	0.00	0.158	9.40	4.00
ATOM	3209	HA	ARG	303G	-10.342	13.947	32.087	1.00	0.00	0.053	0.00	0.00
ATOM	3210	CB	ARG	303G	-10.920	14.619	30.191	1.00	0.00	-0.106	12.77	4.00
ATOM	3211	HB1	ARG	303G	-10.860	13.673	29.652	1.00	0.00	0.053	0.00	0.00
ATOM	3212	HB2	ARG	303G	-10.728	15.398	29.453	1.00	0.00	0.053	0.00	0.00
ATOM	3213	CG	ARG	303G	-12.388	14.779	30.604	1.00	0.00	-0.106	12.77	4.00
ATOM	3214	HG1	ARG	303G	-12.549	15.676	31.201	1.00	0.00	0.053	0.00	0.00
ATOM	3215	HG2	ARG	303G	-12.739	13.936	31.199	1.00	0.00	0.053	0.00	0.00
ATOM	3216	CD	ARG	303G	-13.316	14.882	29.394	1.00	0.00	0.374	12.77	4.00
ATOM	3217	HD1	ARG	303G	-14.360	14.823	29.701	1.00	0.00	0.053	0.00	0.00
ATOM	3218	HD2	ARG	303G	-13.124	14.073	28.689	1.00	0.00	0.053	0.00	0.00
ATOM	3219	NE	ARG	303G	-13.119	16.146	28.697	1.00	0.00	-0.819	9.00	-24.67
ATOM	3220	HE	ARG	303G	-12.304	16.718	28.960	1.00	0.00	0.407	0.00	0.00
ATOM	3221	CZ	ARG	303G	-13.925	16.611	27.740	1.00	0.00	0.796	6.95	4.00
ATOM	3222	NH1	ARG	303G	-14.991	15.911	27.356	1.00	0.00	-0.746	9.00	-24.67
ATOM	3223	HH1	ARG	303G	-15.608	16.276	26.617	1.00	0.00	0.407	0.00	0.00
ATOM	3224	HH1	ARG	303G	-15.198	15.004	27.798	1.00	0.00	0.407	0.00	0.00
ATOM	3225	NH2	ARG	303G	-13.678	17.791	27.190	1.00	0.00	-0.746	9.00	-24.67
ATOM	3226	HH2	ARG	303G	-14.296	18.154	26.451	1.00	0.00	0.407	0.00	0.00
ATOM	3227	HH2	ARG	303G	-12.867	18.344	27.501	1.00	0.00	0.407	0.00	0.00
ATOM	3228	C	ARG	303G	-8.567	14.228	30.984	1.00	0.00	0.396	9.82	4.00
ATOM	3229	O	ARG	303G	-7.683	15.046	30.702	1.00	0.00	-0.396	8.17	-17.40
ATOM	3230	N	ALA	304	-8.382	12.917	30.969	1.00	0.00	-0.650	9.00	-17.40
ATOM	3231	HN	ALA	304	-9.177	12.300	31.188	1.00	0.00	0.440	0.00	0.00
ATOM	3232	CA	ALA	304	-7.094	12.317	30.654	1.00	0.00	0.158	9.40	4.00
ATOM	3233	HA	ALA	304	-6.379	13.119	30.470	1.00	0.00	0.053	0.00	0.00
ATOM	3234	CB	ALA	304	-6.607	11.510	31.864	1.00	0.00	-0.159	16.15	4.00
ATOM	3235	HB1	ALA	304	-5.642	11.057	31.635	1.00	0.00	0.053	0.00	0.00
ATOM	3236	HB2	ALA	304	-6.502	12.171	32.724	1.00	0.00	0.053	0.00	0.00
ATOM	3237	HB3	ALA	304	-7.329	10.727	32.094	1.00	0.00	0.053	0.00	0.00
ATOM	3238	C	ALA	304	-7.100	11.419	29.430	1.00	0.00	0.396	9.82	4.00
ATOM	3239	O	ALA	304	-8.152	11.084	28.868	1.00	0.00	-0.396	8.17	-17.40
ATOM	3240	N	CYS	305	-5.902	11.032	29.009	1.00	0.00	-0.650	9.00	-17.40
ATOM	3241	HN	CYS	305	-5.058	11.395	29.475	1.00	0.00	0.440	0.00	0.00
ATOM	3242	CA	CYS	305	-5.762	10.103	27.900	1.00	0.00	0.158	9.40	4.00
ATOM	3243	HA	CYS	305	-6.774	9.824	27.606	1.00	0.00	0.053	0.00	0.00
ATOM	3244	C	CYS	305	-4.968	8.927	28.431	1.00	0.00	0.396	9.82	4.00
ATOM	3245	O	CYS	305	-4.263	9.031	29.428	1.00	0.00	-0.396	8.17	-17.40
ATOM	3246	CB	CYS	305	-4.917	10.648	26.734	1.00	0.00	-0.041	12.77	4.00
ATOM	3247	HB1	CYS	305	-4.790	9.819	26.037	1.00	0.00	0.053	0.00	0.00
ATOM	3248	HB2	CYS	305	-3.972	10.975	27.169	1.00	0.00	0.053	0.00	0.00
ATOM	3249	SG	CYS	305	-5.457	12.044	25.699	1.00	0.00	-0.065	19.93	-6.40
ATOM	3250	N	VAL	306	-5.073	7.811	27.737	1.00	0.00	-0.650	9.00	-17.40
ATOM	3251	HN	VAL	306	-5.720	7.764	26.937	1.00	0.00	0.440	0.00	0.00
ATOM	3252	CA	VAL	306	-4.283	6.651	28.092	1.00	0.00	0.158	9.40	4.00
ATOM	3253	HA	VAL	306	-4.012	6.659	29.148	1.00	0.00	0.053	0.00	0.00
ATOM	3254	CB	VAL	306	-4.997	5.328	27.712	1.00	0.00	-0.053	9.40	4.00
ATOM	3255	HB	VAL	306	-5.387	5.392	26.696	1.00	0.00	0.053	0.00	0.00
ATOM	3256	CG1	VAL	306	-4.014	4.162	27.791	1.00	0.00	-0.159	16.15	4.00
ATOM	3257	HG1	VAL	306	-4.524	3.237	27.522	1.00	0.00	0.053	0.00	0.00
ATOM	3258	HG1	VAL	306	-3.188	4.334	27.100	1.00	0.00	0.053	0.00	0.00
ATOM	3259	HG1	VAL	306	-3.626	4.080	28.806	1.00	0.00	0.053	0.00	0.00
ATOM	3260	CG2	VAL	306	-6.159	5.075	28.671	1.00	0.00	-0.159	16.15	4.00
ATOM	3261	HG2	VAL	306	-6.658	4.144	28.400	1.00	0.00	0.053	0.00	0.00
ATOM	3262	HG2	VAL	306	-5.779	5.000	29.690	1.00	0.00	0.053	0.00	0.00
ATOM	3263	HG2	VAL	306	-6.869	5.899	28.607	1.00	0.00	0.053	0.00	0.00

ATOM	3264	C	VAL	306	-3.082	6.816	27.184	1.00	0.00	0.396	9.82	4.00
ATOM	3265	O	VAL	306	-3.229	7.262	26.042	1.00	0.00	-0.396	8.17	-17.40
ATOM	3266	N	ARG	307G	-1.897	6.515	27.698	1.00	0.00	-0.650	9.00	-17.40
ATOM	3267	HN	ARG	307G	-1.836	6.239	28.688	1.00	0.00	0.440	0.00	0.00
ATOM	3268	CA	ARG	307G	-0.673	6.563	26.897	1.00	0.00	0.158	9.40	4.00
ATOM	3269	HA	ARG	307G	-0.900	6.506	25.832	1.00	0.00	0.053	0.00	0.00
ATOM	3270	CB	ARG	307G	0.096	7.892	27.089	1.00	0.00	-0.106	12.77	4.00
ATOM	3271	HB1	ARG	307G	-0.596	8.705	26.873	1.00	0.00	0.053	0.00	0.00
ATOM	3272	HB2	ARG	307G	0.934	7.889	26.392	1.00	0.00	0.053	0.00	0.00
ATOM	3273	CG	ARG	307G	0.682	8.175	28.473	1.00	0.00	-0.106	12.77	4.00
ATOM	3274	HG1	ARG	307G	0.019	7.796	29.252	1.00	0.00	0.053	0.00	0.00
ATOM	3275	HG2	ARG	307G	0.811	9.247	28.620	1.00	0.00	0.053	0.00	0.00
ATOM	3276	CD	ARG	307G	2.041	7.500	28.625	1.00	0.00	0.374	12.77	4.00
ATOM	3277	HD1	ARG	307G	2.736	7.841	27.858	1.00	0.00	0.053	0.00	0.00
ATOM	3278	HD2	ARG	307G	1.952	6.417	28.537	1.00	0.00	0.053	0.00	0.00
ATOM	3279	NE	ARG	307G	2.635	7.798	29.934	1.00	0.00	-0.819	9.00	-24.67
ATOM	3280	HE	ARG	307G	2.131	8.436	30.566	1.00	0.00	0.407	0.00	0.00
ATOM	3281	CZ	ARG	307G	3.788	7.286	30.342	1.00	0.00	0.796	6.95	4.00
ATOM	3282	NH1	ARG	307G	4.463	6.459	29.540	1.00	0.00	-0.746	9.00	-24.67
ATOM	3283	HH1	ARG	307G	5.359	6.057	29.850	1.00	0.00	0.407	0.00	0.00
ATOM	3284	HH1	ARG	307G	4.087	6.222	28.610	1.00	0.00	0.407	0.00	0.00
ATOM	3285	NH2	ARG	307G	4.250	7.583	31.545	1.00	0.00	-0.746	9.00	-24.67
ATOM	3286	HH2	ARG	307G	5.145	7.186	31.865	1.00	0.00	0.407	0.00	0.00
ATOM	3287	HH2	ARG	307G	3.714	8.210	32.162	1.00	0.00	0.407	0.00	0.00
ATOM	3288	C	ARG	307G	0.120	5.332	27.378	1.00	0.00	0.396	9.82	4.00
ATOM	3289	O	ARG	307G	-0.068	4.868	28.503	1.00	0.00	-0.396	8.17	-17.40
ATOM	3290	N	PRO	308	0.998	4.784	26.525	1.00	0.00	-0.422	9.00	-17.40
ATOM	3291	CD	PRO	308	1.201	5.151	25.106	1.00	0.00	0.105	12.77	4.00
ATOM	3292	HD1	PRO	308	1.688	6.121	25.016	1.00	0.00	0.053	0.00	0.00
ATOM	3293	HD2	PRO	308	0.251	5.206	24.573	1.00	0.00	0.053	0.00	0.00
ATOM	3294	CA	PRO	308	1.785	3.601	26.880	1.00	0.00	0.158	9.40	4.00
ATOM	3295	HA	PRO	308	1.252	3.063	27.664	1.00	0.00	0.053	0.00	0.00
ATOM	3296	CB	PRO	308	1.851	2.852	25.563	1.00	0.00	-0.106	12.77	4.00
ATOM	3297	HB1	PRO	308	0.922	2.318	25.359	1.00	0.00	0.053	0.00	0.00
ATOM	3298	HB2	PRO	308	2.655	2.116	25.560	1.00	0.00	0.053	0.00	0.00
ATOM	3299	CG	PRO	308	2.099	3.997	24.578	1.00	0.00	-0.106	12.77	4.00
ATOM	3300	HG1	PRO	308	1.787	3.590	23.615	1.00	0.00	0.053	0.00	0.00
ATOM	3301	HG2	PRO	308	3.169	4.188	24.658	1.00	0.00	0.053	0.00	0.00
ATOM	3302	C	PRO	308	3.181	3.887	27.395	1.00	0.00	0.396	9.82	4.00
ATOM	3303	O	PRO	308	3.708	4.975	27.188	1.00	0.00	-0.396	8.17	-17.40
ATOM	3304	N	GLU	309	3.780	2.881	28.031	1.00	0.00	-0.650	9.00	-17.40
ATOM	3305	HN	GLU	309	3.253	2.010	28.189	1.00	0.00	0.440	0.00	0.00
ATOM	3306	CA	GLU	309	5.156	2.968	28.511	1.00	0.00	0.158	9.40	4.00
ATOM	3307	HA	GLU	309	5.231	3.849	29.147	1.00	0.00	0.053	0.00	0.00
ATOM	3308	CB	GLU	309	5.505	1.689	29.285	1.00	0.00	-0.106	12.77	4.00
ATOM	3309	HB1	GLU	309	5.222	0.838	28.664	1.00	0.00	0.053	0.00	0.00
ATOM	3310	HB2	GLU	309	4.940	1.701	30.217	1.00	0.00	0.053	0.00	0.00
ATOM	3311	CG	GLU	309	6.992	1.488	29.667	1.00	0.00	-0.106	12.77	4.00
ATOM	3312	HG1	GLU	309	7.682	1.739	28.862	1.00	0.00	0.053	0.00	0.00
ATOM	3313	HG2	GLU	309	7.232	0.461	29.942	1.00	0.00	0.053	0.00	0.00
ATOM	3314	CD	GLU	309	7.427	2.330	30.844	1.00	0.00	0.399	9.82	4.00
ATOM	3315	OE1	GLU	309	6.554	2.982	31.453	1.00	0.00	-0.396	8.17	-18.95
ATOM	3316	OE2	GLU	309	8.642	2.334	31.166	1.00	0.00	-0.427	8.17	-18.95
ATOM	3317	HE2	GLU	309	8.778	2.944	31.984	1.00	0.00	0.424	0.00	0.00
ATOM	3318	C	GLU	309	6.074	3.090	27.285	1.00	0.00	0.396	9.82	4.00
ATOM	3319	O	GLU	309	7.065	3.829	27.314	1.00	0.00	-0.396	8.17	-17.40
ATOM	3320	N	ILE	310	5.748	2.350	26.219	1.00	0.00	-0.650	9.00	-17.40
ATOM	3321	HN	ILE	310	4.904	1.760	26.267	1.00	0.00	0.440	0.00	0.00
ATOM	3322	CA	ILE	310	6.544	2.343	24.980	1.00	0.00	0.158	9.40	4.00
ATOM	3323	HA	ILE	310	7.358	3.052	25.126	1.00	0.00	0.053	0.00	0.00
ATOM	3324	CB	ILE	310	7.118	0.916	24.698	1.00	0.00	-0.053	9.40	4.00
ATOM	3325	HB	ILE	310	6.313	0.188	24.590	1.00	0.00	0.053	0.00	0.00
ATOM	3326	CG2	ILE	310	7.943	0.905	23.409	1.00	0.00	-0.159	16.15	4.00
ATOM	3327	HG2	ILE	310	8.331	-0.098	23.234	1.00	0.00	0.053	0.00	0.00
ATOM	3328	HG2	ILE	310	7.312	1.200	22.570	1.00	0.00	0.053	0.00	0.00
ATOM	3329	HG2	ILE	310	8.773	1.604	23.502	1.00	0.00	0.053	0.00	0.00
ATOM	3330	CG1	ILE	310	7.970	0.458	25.883	1.00	0.00	-0.106	12.77	4.00
ATOM	3331	HG1	ILE	310	7.331	0.402	26.764	1.00	0.00	0.053	0.00	0.00
ATOM	3332	HG1	ILE	310	8.768	1.184	26.034	1.00	0.00	0.053	0.00	0.00
ATOM	3333	CD1	ILE	310	8.632	-0.944	25.683	1.00	0.00	-0.159	16.15	4.00
ATOM	3334	HD1	ILE	310	9.219	-1.198	26.565	1.00	0.00	0.053	0.00	0.00
ATOM	3335	HD1	ILE	310	7.856	-1.695	25.534	1.00	0.00	0.053	0.00	0.00
ATOM	3336	HD1	ILE	310	9.283	-0.917	24.809	1.00	0.00	0.053	0.00	0.00
ATOM	3337	C	ILE	310	5.604	2.771	23.849	1.00	0.00	0.396	9.82	4.00
ATOM	3338	O	ILE	310	4.538	2.167	23.660	1.00	0.00	-0.396	8.17	-17.40
ATOM	3339	N	SER	311	5.997	3.802	23.102	1.00	0.00	-0.650	9.00	-17.40

ATOM	3340	HN	SER	311	6.923	4.219	23.272	1.00	0.00	0.440	0.00	0.00
ATOM	3341	CA	SER	311	5.145	4.360	22.041	1.00	0.00	0.158	9.40	4.00
ATOM	3342	HA	SER	311	4.230	4.729	22.505	1.00	0.00	0.053	0.00	0.00
ATOM	3343	CB	SER	311	5.818	5.584	21.403	1.00	0.00	0.007	12.77	4.00
ATOM	3344	HB1	SER	311	5.154	6.082	20.696	1.00	0.00	0.053	0.00	0.00
ATOM	3345	HB2	SER	311	6.721	5.306	20.859	1.00	0.00	0.053	0.00	0.00
ATOM	3346	OG	SER	311	6.190	6.540	22.378	1.00	0.00	-0.537	11.04	-17.40
ATOM	3347	HG	SER	311	6.936	7.142	22.002	1.00	0.00	0.424	0.00	0.00
ATOM	3348	C	SER	311	4.727	3.384	20.937	1.00	0.00	0.396	9.82	4.00
ATOM	3349	O	SER	311	5.477	2.475	20.563	1.00	0.00	-0.396	8.17	-17.40
ATOM	3350	N	ARG	312G	3.514	3.578	20.421	1.00	0.00	-0.650	9.00	-17.40
ATOM	3351	HN	ARG	312G	2.918	4.333	20.787	1.00	0.00	0.440	0.00	0.00
ATOM	3352	CA	ARG	312G	3.024	2.731	19.344	1.00	0.00	0.158	9.40	4.00
ATOM	3353	HA	ARG	312G	3.596	1.805	19.286	1.00	0.00	0.053	0.00	0.00
ATOM	3354	CB	ARG	312G	1.594	2.269	19.623	1.00	0.00	-0.106	12.77	4.00
ATOM	3355	HB1	ARG	312G	0.979	2.341	18.725	1.00	0.00	0.053	0.00	0.00
ATOM	3356	HB2	ARG	312G	1.131	2.880	20.397	1.00	0.00	0.053	0.00	0.00
ATOM	3357	CG	ARG	312G	1.572	0.796	20.100	1.00	0.00	-0.106	12.77	4.00
ATOM	3358	HG1	ARG	312G	2.014	0.155	19.337	1.00	0.00	0.053	0.00	0.00
ATOM	3359	HG2	ARG	312G	0.543	0.482	20.279	1.00	0.00	0.053	0.00	0.00
ATOM	3360	CD	ARG	312G	2.380	0.660	21.408	1.00	0.00	0.374	12.77	4.00
ATOM	3361	HD1	ARG	312G	1.917	1.200	22.234	1.00	0.00	0.053	0.00	0.00
ATOM	3362	HD2	ARG	312G	3.393	1.049	21.307	1.00	0.00	0.053	0.00	0.00
ATOM	3363	NE	ARG	312G	2.506	-0.732	21.835	1.00	0.00	-0.819	9.00	-24.67
ATOM	3364	HE	ARG	312G	2.293	-1.467	21.145	1.00	0.00	0.407	0.00	0.00
ATOM	3365	CZ	ARG	312G	2.878	-1.115	23.059	1.00	0.00	0.796	6.95	4.00
ATOM	3366	NH1	ARG	312G	3.163	-0.211	23.975	1.00	0.00	-0.746	9.00	-24.67
ATOM	3367	HH1	ARG	312G	3.449	-0.507	24.919	1.00	0.00	0.407	0.00	0.00
ATOM	3368	HH1	ARG	312G	3.098	0.791	23.746	1.00	0.00	0.407	0.00	0.00
ATOM	3369	NH2	ARG	312G	2.945	-2.405	23.371	1.00	0.00	-0.746	9.00	-24.67
ATOM	3370	HH2	ARG	312G	3.232	-2.691	24.317	1.00	0.00	0.407	0.00	0.00
ATOM	3371	HH2	ARG	312G	2.708	-3.118	22.666	1.00	0.00	0.407	0.00	0.00
ATOM	3372	C	ARG	312G	3.138	3.437	18.006	1.00	0.00	0.396	9.82	4.00
ATOM	3373	O	ARG	312G	2.646	2.960	16.984	1.00	0.00	-0.396	8.17	-17.40
ATOM	3374	N	THR	313	3.791	4.596	18.035	1.00	0.00	-0.650	9.00	-17.40
ATOM	3375	HN	THR	313	4.113	4.961	18.942	1.00	0.00	0.440	0.00	0.00
ATOM	3376	CA	THR	313	4.068	5.370	16.823	1.00	0.00	0.158	9.40	4.00
ATOM	3377	HA	THR	313	4.095	4.668	15.989	1.00	0.00	0.053	0.00	0.00
ATOM	3378	CB	THR	313	3.042	6.491	16.534	1.00	0.00	0.060	9.40	4.00
ATOM	3379	HB	THR	313	3.398	7.138	15.733	1.00	0.00	0.053	0.00	0.00
ATOM	3380	OG1	THR	313	2.888	7.307	17.698	1.00	0.00	-0.537	11.04	-17.40
ATOM	3381	HG1	THR	313	3.405	8.188	17.570	1.00	0.00	0.424	0.00	0.00
ATOM	3382	CG2	THR	313	1.703	5.895	16.111	1.00	0.00	-0.159	16.15	4.00
ATOM	3383	HG2	THR	313	0.993	6.698	15.912	1.00	0.00	0.053	0.00	0.00
ATOM	3384	HG2	THR	313	1.838	5.299	15.208	1.00	0.00	0.053	0.00	0.00
ATOM	3385	HG2	THR	313	1.318	5.261	16.910	1.00	0.00	0.053	0.00	0.00
ATOM	3386	C	THR	313	5.413	6.056	17.021	1.00	0.00	0.396	9.82	4.00
ATOM	3387	O	THR	313	5.884	6.212	18.151	1.00	0.00	-0.396	8.17	-17.40
ATOM	3388	N	MET	314	6.019	6.462	15.914	1.00	0.00	-0.650	9.00	-17.40
ATOM	3389	HN	MET	314	5.572	6.270	15.005	1.00	0.00	0.440	0.00	0.00
ATOM	3390	CA	MET	314	7.289	7.167	15.935	1.00	0.00	0.158	9.40	4.00
ATOM	3391	HA	MET	314	7.438	7.681	16.884	1.00	0.00	0.053	0.00	0.00
ATOM	3392	CB	MET	314	8.464	6.215	15.657	1.00	0.00	-0.106	12.77	4.00
ATOM	3393	HB1	MET	314	8.506	5.368	16.342	1.00	0.00	0.053	0.00	0.00
ATOM	3394	HB2	MET	314	9.438	6.696	15.734	1.00	0.00	0.053	0.00	0.00
ATOM	3395	CG	MET	314	8.428	5.598	14.256	1.00	0.00	-0.041	12.77	4.00
ATOM	3396	HG1	MET	314	8.216	6.391	13.539	1.00	0.00	0.053	0.00	0.00
ATOM	3397	HG2	MET	314	7.642	4.842	14.236	1.00	0.00	0.053	0.00	0.00
ATOM	3398	SD	MET	314	9.960	4.803	13.750	1.00	0.00	-0.130	16.39	-6.40
ATOM	3399	CE	MET	314	10.989	6.220	13.391	1.00	0.00	-0.094	16.15	4.00
ATOM	3400	HE1	MET	314	11.972	5.882	13.064	1.00	0.00	0.053	0.00	0.00
ATOM	3401	HE2	MET	314	10.528	6.813	12.601	1.00	0.00	0.053	0.00	0.00
ATOM	3402	HE3	MET	314	11.094	6.829	14.288	1.00	0.00	0.053	0.00	0.00
ATOM	3403	C	MET	314	7.154	8.135	14.781	1.00	0.00	0.396	9.82	4.00
ATOM	3404	O	MET	314	6.330	7.927	13.891	1.00	0.00	-0.396	8.17	-17.40
ATOM	3405	N	THR	315	7.938	9.200	14.794	1.00	0.00	-0.650	9.00	-17.40
ATOM	3406	HN	THR	315	8.584	9.356	15.581	1.00	0.00	0.440	0.00	0.00
ATOM	3407	CA	THR	315	7.885	10.146	13.697	1.00	0.00	0.158	9.40	4.00
ATOM	3408	HA	THR	315	7.132	9.887	12.952	1.00	0.00	0.053	0.00	0.00
ATOM	3409	CB	THR	315	7.405	11.578	14.148	1.00	0.00	0.060	9.40	4.00
ATOM	3410	HB	THR	315	6.467	11.541	14.702	1.00	0.00	0.053	0.00	0.00
ATOM	3411	OG1	THR	315	7.200	12.401	12.987	1.00	0.00	-0.537	11.04	-17.40
ATOM	3412	HG1	THR	315	7.706	13.290	13.102	1.00	0.00	0.424	0.00	0.00
ATOM	3413	CG2	THR	315	8.420	12.265	15.051	1.00	0.00	-0.159	16.15	4.00
ATOM	3414	HG2	THR	315	8.046	13.248	15.336	1.00	0.00	0.053	0.00	0.00
ATOM	3415	HG2	THR	315	8.577	11.662	15.946	1.00	0.00	0.053	0.00	0.00

ATOM	3416	HG2	THR	315	9.364	12.376	14.518	1.00	0.00	0.053	0.00	0.00
ATOM	3417	C	THR	315	9.205	10.248	12.941	1.00	0.00	0.396	9.82	4.00
ATOM	3418	O	THR	315	10.294	10.206	13.522	1.00	0.00	-0.396	8.17	-17.40
ATOM	3419	N	PHE	316	9.081	10.361	11.624	1.00	0.00	-0.650	9.00	-17.40
ATOM	3420	HN	PHE	316	8.137	10.348	11.210	1.00	0.00	0.440	0.00	0.00
ATOM	3421	CA	PHE	316	10.233	10.502	10.743	1.00	0.00	0.158	9.40	4.00
ATOM	3422	HA	PHE	316	11.143	10.512	11.342	1.00	0.00	0.053	0.00	0.00
ATOM	3423	CB	PHE	316	10.324	9.296	9.806	1.00	0.00	-0.106	12.77	4.00
ATOM	3424	HB1	PHE	316	10.536	8.411	10.406	1.00	0.00	0.053	0.00	0.00
ATOM	3425	HB2	PHE	316	11.127	9.476	9.092	1.00	0.00	0.053	0.00	0.00
ATOM	3426	CG	PHE	316	9.062	9.027	9.020	1.00	0.00	0.000	7.26	0.60
ATOM	3427	CD1	PHE	316	8.168	8.047	9.427	1.00	0.00	-0.127	10.80	0.60
ATOM	3428	HD1	PHE	316	8.375	7.469	10.328	1.00	0.00	0.127	0.00	0.00
ATOM	3429	CD2	PHE	316	8.781	9.757	7.865	1.00	0.00	-0.127	10.80	0.60
ATOM	3430	HD2	PHE	316	9.475	10.529	7.535	1.00	0.00	0.127	0.00	0.00
ATOM	3431	CE1	PHE	316	7.007	7.792	8.696	1.00	0.00	-0.127	10.80	0.60
ATOM	3432	HE1	PHE	316	6.312	7.019	9.026	1.00	0.00	0.127	0.00	0.00
ATOM	3433	CE2	PHE	316	7.622	9.511	7.125	1.00	0.00	-0.127	10.80	0.60
ATOM	3434	HE2	PHE	316	7.413	10.088	6.224	1.00	0.00	0.127	0.00	0.00
ATOM	3435	CZ	PHE	316	6.737	8.527	7.543	1.00	0.00	-0.127	10.80	0.60
ATOM	3436	HZ	PHE	316	5.831	8.329	6.970	1.00	0.00	0.127	0.00	0.00
ATOM	3437	C	PHE	316	10.111	11.828	9.955	1.00	0.00	0.396	9.82	4.00
ATOM	3438	O	PHE	316	10.933	12.134	9.093	1.00	0.00	-0.396	8.17	-17.40
ATOM	3439	N	GLY	317	9.095	12.623	10.296	1.00	0.00	-0.650	9.00	-17.40
ATOM	3440	HN	GLY	317	8.455	12.320	11.044	1.00	0.00	0.440	0.00	0.00
ATOM	3441	CA	GLY	317	8.861	13.910	9.641	1.00	0.00	0.105	9.40	4.00
ATOM	3442	HA1	GLY	317	7.853	14.233	9.902	1.00	0.00	0.053	0.00	0.00
ATOM	3443	HA2	GLY	317	8.961	13.755	8.566	1.00	0.00	0.053	0.00	0.00
ATOM	3444	C	GLY	317	9.796	15.061	10.005	1.00	0.00	0.396	9.82	4.00
ATOM	3445	O	GLY	317	9.382	16.088	10.594	1.00	0.00	-0.396	8.17	-17.40
ATOM	3446	N	ARG	318G	11.062	14.887	9.623	1.00	0.00	-0.650	9.00	-17.40
ATOM	3447	HN	ARG	318G	11.298	14.008	9.140	1.00	0.00	0.440	0.00	0.00
ATOM	3448	CA	ARG	318G	12.138	15.853	9.839	1.00	0.00	0.158	9.40	4.00
ATOM	3449	HA	ARG	318G	12.379	15.950	10.897	1.00	0.00	0.053	0.00	0.00
ATOM	3450	CB	ARG	318G	13.382	15.375	9.089	1.00	0.00	-0.106	12.77	4.00
ATOM	3451	HB1	ARG	318G	14.274	15.950	9.333	1.00	0.00	0.053	0.00	0.00
ATOM	3452	HB2	ARG	318G	13.277	15.438	8.006	1.00	0.00	0.053	0.00	0.00
ATOM	3453	CG	ARG	318G	13.733	13.931	9.383	1.00	0.00	-0.106	12.77	4.00
ATOM	3454	HG1	ARG	318G	12.928	13.255	9.092	1.00	0.00	0.053	0.00	0.00
ATOM	3455	HG2	ARG	318G	13.921	13.771	10.444	1.00	0.00	0.053	0.00	0.00
ATOM	3456	CD	ARG	318G	14.989	13.492	8.629	1.00	0.00	0.374	12.77	4.00
ATOM	3457	HD1	ARG	318G	15.637	14.341	8.411	1.00	0.00	0.053	0.00	0.00
ATOM	3458	HD2	ARG	318G	14.736	13.018	7.680	1.00	0.00	0.053	0.00	0.00
ATOM	3459	NE	ARG	318G	15.768	12.530	9.409	1.00	0.00	-0.819	9.00	-24.67
ATOM	3460	HE	ARG	318G	15.871	11.573	9.041	1.00	0.00	0.407	0.00	0.00
ATOM	3461	CZ	ARG	318G	16.349	12.827	10.567	1.00	0.00	0.796	6.95	4.00
ATOM	3462	NH1	ARG	318G	16.228	14.053	11.061	1.00	0.00	-0.746	9.00	-24.67
ATOM	3463	HH1	ARG	318G	16.674	14.293	11.957	1.00	0.00	0.407	0.00	0.00
ATOM	3464	HH1	ARG	318G	15.687	14.764	10.547	1.00	0.00	0.407	0.00	0.00
ATOM	3465	NH2	ARG	318G	17.049	11.912	11.228	1.00	0.00	-0.746	9.00	-24.67
ATOM	3466	HH2	ARG	318G	17.495	12.153	12.124	1.00	0.00	0.407	0.00	0.00
ATOM	3467	HH2	ARG	318G	17.145	10.961	10.844	1.00	0.00	0.407	0.00	0.00
ATOM	3468	C	ARG	318G	11.754	17.241	9.327	1.00	0.00	0.396	9.82	4.00
ATOM	3469	O	ARG	318G	11.783	18.238	10.066	1.00	0.00	-0.396	8.17	-17.40
ATOM	3470	N	LYS	319S	11.404	17.279	8.045	1.00	0.00	-0.650	9.00	-17.40
ATOM	3471	HN	LYS	319S	11.423	16.399	7.509	1.00	0.00	0.440	0.00	0.00
ATOM	3472	CA	LYS	319S	10.993	18.499	7.353	1.00	0.00	0.158	9.40	4.00
ATOM	3473	HA	LYS	319S	11.381	19.341	7.925	1.00	0.00	0.053	0.00	0.00
ATOM	3474	CB	LYS	319S	11.571	18.496	5.924	1.00	0.00	-0.106	12.77	4.00
ATOM	3475	HB1	LYS	319S	11.433	17.497	5.509	1.00	0.00	0.053	0.00	0.00
ATOM	3476	HB2	LYS	319S	12.629	18.749	5.989	1.00	0.00	0.053	0.00	0.00
ATOM	3477	CG	LYS	319S	10.933	19.481	4.946	1.00	0.00	-0.106	12.77	4.00
ATOM	3478	HG1	LYS	319S	9.843	19.454	4.977	1.00	0.00	0.053	0.00	0.00
ATOM	3479	HG2	LYS	319S	11.213	19.283	3.911	1.00	0.00	0.053	0.00	0.00
ATOM	3480	CD	LYS	319S	11.331	20.919	5.226	1.00	0.00	-0.106	12.77	4.00
ATOM	3481	HD1	LYS	319S	12.405	21.047	5.097	1.00	0.00	0.053	0.00	0.00
ATOM	3482	HD2	LYS	319S	11.069	21.193	6.248	1.00	0.00	0.053	0.00	0.00
ATOM	3483	CE	LYS	319S	10.614	21.862	4.274	1.00	0.00	0.099	12.77	4.00
ATOM	3484	HE1	LYS	319S	10.882	21.636	3.241	1.00	0.00	0.053	0.00	0.00
ATOM	3485	HE2	LYS	319S	10.887	22.895	4.485	1.00	0.00	0.053	0.00	0.00
ATOM	3486	NZ	LYS	319S	9.133	21.724	4.420	1.00	0.00	-0.045	13.25	-39.20
ATOM	3487	HZ1	LYS	319S	8.661	22.368	3.769	1.00	0.00	0.280	0.00	0.00
ATOM	3488	HZ2	LYS	319S	8.855	20.755	4.205	1.00	0.00	0.280	0.00	0.00
ATOM	3489	HZ3	LYS	319S	8.860	21.952	5.386	1.00	0.00	0.280	0.00	0.00
ATOM	3490	C	LYS	319S	9.467	18.503	7.312	1.00	0.00	0.396	9.82	4.00
ATOM	3491	O	LYS	319S	8.849	17.531	6.874	1.00	0.00	-0.396	8.17	-17.40

ATOM	3492	N	GLY	320	8.866	19.590	7.782	1.00	0.00	-0.650	9.00	-17.40
ATOM	3493	HN	GLY	320	9.434	20.366	8.149	1.00	0.00	0.440	0.00	0.00
ATOM	3494	CA	GLY	320	7.420	19.697	7.784	1.00	0.00	0.105	9.40	4.00
ATOM	3495	HA1	GLY	320	6.973	19.122	8.595	1.00	0.00	0.053	0.00	0.00
ATOM	3496	HA2	GLY	320	6.986	19.329	6.854	1.00	0.00	0.053	0.00	0.00
ATOM	3497	C	GLY	320	6.964	21.130	7.951	1.00	0.00	0.396	9.82	4.00
ATOM	3498	O	GLY	320	7.638	22.068	7.492	1.00	0.00	-0.396	8.17	-17.40
ATOM	3499	N	VAL	321	5.809	21.317	8.582	1.00	0.00	-0.650	9.00	-17.40
ATOM	3500	HN	VAL	321	5.263	20.505	8.905	1.00	0.00	0.440	0.00	0.00
ATOM	3501	CA	VAL	321	5.312	22.665	8.817	1.00	0.00	0.158	9.40	4.00
ATOM	3502	HA	VAL	321	5.337	23.172	7.852	1.00	0.00	0.053	0.00	0.00
ATOM	3503	CB	VAL	321	3.883	22.646	9.373	1.00	0.00	-0.053	9.40	4.00
ATOM	3504	HB	VAL	321	3.812	21.963	10.220	1.00	0.00	0.053	0.00	0.00
ATOM	3505	CG1	VAL	321	3.473	24.040	9.841	1.00	0.00	-0.159	16.15	4.00
ATOM	3506	HG1	VAL	321	2.456	24.007	10.232	1.00	0.00	0.053	0.00	0.00
ATOM	3507	HG1	VAL	321	4.152	24.375	10.624	1.00	0.00	0.053	0.00	0.00
ATOM	3508	HG1	VAL	321	3.516	24.733	9.001	1.00	0.00	0.053	0.00	0.00
ATOM	3509	CG2	VAL	321	2.942	22.152	8.294	1.00	0.00	-0.159	16.15	4.00
ATOM	3510	HG2	VAL	321	1.922	22.134	8.680	1.00	0.00	0.053	0.00	0.00
ATOM	3511	HG2	VAL	321	2.992	22.819	7.433	1.00	0.00	0.053	0.00	0.00
ATOM	3512	HG2	VAL	321	3.232	21.146	7.991	1.00	0.00	0.053	0.00	0.00
ATOM	3513	C	VAL	321	6.254	23.296	9.830	1.00	0.00	0.396	9.82	4.00
ATOM	3514	O	VAL	321	6.976	24.247	9.512	1.00	0.00	-0.396	8.17	-17.40
ATOM	3515	N	SER	322	6.255	22.759	11.047	1.00	0.00	-0.650	9.00	-17.40
ATOM	3516	HN	SER	322	5.622	21.974	11.259	1.00	0.00	0.440	0.00	0.00
ATOM	3517	CA	SER	322	7.144	23.272	12.083	1.00	0.00	0.158	9.40	4.00
ATOM	3518	HA	SER	322	6.929	24.329	12.235	1.00	0.00	0.053	0.00	0.00
ATOM	3519	CB	SER	322	6.973	22.510	13.406	1.00	0.00	0.007	12.77	4.00
ATOM	3520	HB1	SER	322	7.633	22.886	14.187	1.00	0.00	0.053	0.00	0.00
ATOM	3521	HB2	SER	322	7.190	21.447	13.301	1.00	0.00	0.053	0.00	0.00
ATOM	3522	OG	SER	322	5.654	22.604	13.912	1.00	0.00	-0.537	11.04	-17.40
ATOM	3523	HG	SER	322	5.398	23.595	14.023	1.00	0.00	0.424	0.00	0.00
ATOM	3524	C	SER	322	8.582	23.088	11.627	1.00	0.00	0.396	9.82	4.00
ATOM	3525	O	SER	322	8.883	22.248	10.771	1.00	0.00	-0.396	8.17	-17.40
ATOM	3526	N	HIS	323S	9.468	23.882	12.211	1.00	0.00	-0.650	9.00	-17.40
ATOM	3527	HN	HIS	323S	9.144	24.581	12.894	1.00	0.00	0.440	0.00	0.00
ATOM	3528	CA	HIS	323S	10.882	23.788	11.909	1.00	0.00	0.158	9.40	4.00
ATOM	3529	HA	HIS	323S	10.950	23.686	10.826	1.00	0.00	0.053	0.00	0.00
ATOM	3530	CB	HIS	323S	11.577	25.075	12.358	1.00	0.00	-0.106	12.77	4.00
ATOM	3531	HB1	HIS	323S	12.618	25.131	12.040	1.00	0.00	0.053	0.00	0.00
ATOM	3532	HB2	HIS	323S	11.592	25.195	13.441	1.00	0.00	0.053	0.00	0.00
ATOM	3533	CG	HIS	323S	10.923	26.313	11.822	1.00	0.00	-0.050	7.26	0.60
ATOM	3534	CD2	HIS	323S	10.432	27.410	12.448	1.00	0.00	-0.177	10.80	0.60
ATOM	3535	HD2	HIS	323S	10.458	27.609	13.519	1.00	0.00	0.127	0.00	0.00
ATOM	3536	ND1	HIS	323S	10.671	26.494	10.477	1.00	0.00	0.207	9.25	-17.40
ATOM	3537	HD1	HIS	323S	10.925	25.833	9.729	1.00	0.00	0.393	0.00	0.00
ATOM	3538	CE1	HIS	323S	10.052	27.649	10.299	1.00	0.00	-0.227	10.80	0.60
ATOM	3539	HE1	HIS	323S	9.727	28.056	9.342	1.00	0.00	0.127	0.00	0.00
ATOM	3540	NE2	HIS	323S	9.894	28.225	11.478	1.00	0.00	0.207	9.25	-17.40
ATOM	3541	HE2	HIS	323S	9.441	29.135	11.644	1.00	0.00	0.393	0.00	0.00
ATOM	3542	C	HIS	323S	11.392	22.543	12.658	1.00	0.00	0.396	9.82	4.00
ATOM	3543	O	HIS	323S	10.748	22.069	13.603	1.00	0.00	-0.396	8.17	-17.40
ATOM	3544	N	GLY	324	12.534	22.013	12.231	1.00	0.00	-0.650	9.00	-17.40
ATOM	3545	HN	GLY	324	13.053	22.467	11.467	1.00	0.00	0.440	0.00	0.00
ATOM	3546	CA	GLY	324	13.054	20.799	12.833	1.00	0.00	0.105	9.40	4.00
ATOM	3547	HA1	GLY	324	13.786	20.403	12.129	1.00	0.00	0.053	0.00	0.00
ATOM	3548	HA2	GLY	324	12.198	20.137	12.965	1.00	0.00	0.053	0.00	0.00
ATOM	3549	C	GLY	324	13.766	20.773	14.178	1.00	0.00	0.396	9.82	4.00
ATOM	3550	O	GLY	324	14.357	19.738	14.502	1.00	0.00	-0.396	8.17	-17.40
ATOM	3551	N	GLN	325	13.728	21.843	14.973	1.00	0.00	-0.650	9.00	-17.40
ATOM	3552	HN	GLN	325	13.209	22.688	14.693	1.00	0.00	0.440	0.00	0.00
ATOM	3553	CA	GLN	325	14.439	21.791	16.253	1.00	0.00	0.158	9.40	4.00
ATOM	3554	HA	GLN	325	15.457	21.450	16.067	1.00	0.00	0.053	0.00	0.00
ATOM	3555	CB	GLN	325	14.596	23.177	16.878	1.00	0.00	-0.106	12.77	4.00
ATOM	3556	HB1	GLN	325	13.635	23.616	17.146	1.00	0.00	0.053	0.00	0.00
ATOM	3557	HB2	GLN	325	15.084	23.878	16.201	1.00	0.00	0.053	0.00	0.00
ATOM	3558	CG	GLN	325	15.436	23.139	18.156	1.00	0.00	-0.106	12.77	4.00
ATOM	3559	HG1	GLN	325	16.217	22.379	18.140	1.00	0.00	0.053	0.00	0.00
ATOM	3560	HG2	GLN	325	14.853	22.930	19.053	1.00	0.00	0.053	0.00	0.00
ATOM	3561	CD	GLN	325	16.160	24.449	18.447	1.00	0.00	0.396	9.82	4.00
ATOM	3562	OE1	GLN	325	15.533	25.478	18.719	1.00	0.00	-0.396	8.17	-17.40
ATOM	3563	NE2	GLN	325	17.492	24.415	18.384	1.00	0.00	-0.879	13.25	-17.40
ATOM	3564	HE2	GLN	325	17.974	23.534	18.153	1.00	0.00	0.440	0.00	0.00
ATOM	3565	HE2	GLN	325	18.038	25.269	18.565	1.00	0.00	0.440	0.00	0.00
ATOM	3566	C	GLN	325	13.811	20.848	17.271	1.00	0.00	0.396	9.82	4.00
ATOM	3567	O	GLN	325	14.502	20.013	17.863	1.00	0.00	-0.396	8.17	-17.40

ATOM	3568	N	PHE	326	12.509	20.976	17.485	1.00	0.00	-0.650	9.00	-17.40
ATOM	3569	HN	PHE	326	11.976	21.696	16.977	1.00	0.00	0.440	0.00	0.00
ATOM	3570	CA	PHE	326	11.829	20.109	18.428	1.00	0.00	0.158	9.40	4.00
ATOM	3571	HA	PHE	326	12.285	20.212	19.412	1.00	0.00	0.053	0.00	0.00
ATOM	3572	CB	PHE	326	10.357	20.511	18.564	1.00	0.00	-0.106	12.77	4.00
ATOM	3573	HB1	PHE	326	9.765	20.309	17.670	1.00	0.00	0.053	0.00	0.00
ATOM	3574	HB2	PHE	326	10.211	21.572	18.767	1.00	0.00	0.053	0.00	0.00
ATOM	3575	CG	PHE	326	9.642	19.801	19.672	1.00	0.00	0.000	7.26	0.60
ATOM	3576	CD1	PHE	326	10.205	19.736	20.947	1.00	0.00	-0.127	10.80	0.60
ATOM	3577	HD1	PHE	326	11.155	20.233	21.140	1.00	0.00	0.127	0.00	0.00
ATOM	3578	CD2	PHE	326	8.427	19.169	19.443	1.00	0.00	-0.127	10.80	0.60
ATOM	3579	HD2	PHE	326	7.972	19.216	18.453	1.00	0.00	0.127	0.00	0.00
ATOM	3580	CE1	PHE	326	9.576	19.050	21.968	1.00	0.00	-0.127	10.80	0.60
ATOM	3581	HE1	PHE	326	10.028	19.005	22.958	1.00	0.00	0.127	0.00	0.00
ATOM	3582	CE2	PHE	326	7.788	18.480	20.459	1.00	0.00	-0.127	10.80	0.60
ATOM	3583	HE2	PHE	326	6.834	17.987	20.267	1.00	0.00	0.127	0.00	0.00
ATOM	3584	CZ	PHE	326	8.361	18.416	21.724	1.00	0.00	-0.127	10.80	0.60
ATOM	3585	HZ	PHE	326	7.859	17.870	22.523	1.00	0.00	0.127	0.00	0.00
ATOM	3586	C	PHE	326	11.946	18.659	17.964	1.00	0.00	0.396	9.82	4.00
ATOM	3587	O	PHE	326	12.147	17.757	18.786	1.00	0.00	-0.396	8.17	-17.40
ATOM	3588	N	PHE	327	11.847	18.437	16.653	1.00	0.00	-0.650	9.00	-17.40
ATOM	3589	HN	PHE	327	11.684	19.232	16.019	1.00	0.00	0.440	0.00	0.00
ATOM	3590	CA	PHE	327	11.964	17.086	16.092	1.00	0.00	0.158	9.40	4.00
ATOM	3591	HA	PHE	327	11.279	16.405	16.598	1.00	0.00	0.053	0.00	0.00
ATOM	3592	CB	PHE	327	11.633	17.061	14.584	1.00	0.00	-0.106	12.77	4.00
ATOM	3593	HB1	PHE	327	12.193	17.794	14.004	1.00	0.00	0.053	0.00	0.00
ATOM	3594	HB2	PHE	327	10.584	17.265	14.365	1.00	0.00	0.053	0.00	0.00
ATOM	3595	CG	PHE	327	11.923	15.726	13.923	1.00	0.00	0.000	7.26	0.60
ATOM	3596	CD1	PHE	327	10.920	14.762	13.796	1.00	0.00	-0.127	10.80	0.60
ATOM	3597	HD1	PHE	327	9.902	15.003	14.101	1.00	0.00	0.127	0.00	0.00
ATOM	3598	CD2	PHE	327	13.222	15.402	13.519	1.00	0.00	-0.127	10.80	0.60
ATOM	3599	HD2	PHE	327	14.011	16.148	13.606	1.00	0.00	0.127	0.00	0.00
ATOM	3600	CE1	PHE	327	11.202	13.488	13.282	1.00	0.00	-0.127	10.80	0.60
ATOM	3601	HE1	PHE	327	10.408	12.746	13.190	1.00	0.00	0.127	0.00	0.00
ATOM	3602	CE2	PHE	327	13.526	14.135	13.004	1.00	0.00	-0.127	10.80	0.60
ATOM	3603	HE2	PHE	327	14.544	13.898	12.696	1.00	0.00	0.127	0.00	0.00
ATOM	3604	CZ	PHE	327	12.512	13.171	12.886	1.00	0.00	-0.127	10.80	0.60
ATOM	3605	HZ	PHE	327	12.740	12.181	12.489	1.00	0.00	0.127	0.00	0.00
ATOM	3606	C	PHE	327	13.385	16.564	16.263	1.00	0.00	0.396	9.82	4.00
ATOM	3607	O	PHE	327	13.592	15.379	16.554	1.00	0.00	-0.396	8.17	-17.40
ATOM	3608	N	ASP	328P	14.358	17.453	16.073	1.00	0.00	-0.650	9.00	-17.40
ATOM	3609	HN	ASP	328P	14.106	18.430	15.866	1.00	0.00	0.440	0.00	0.00
ATOM	3610	CA	ASP	328P	15.766	17.090	16.148	1.00	0.00	0.158	9.40	4.00
ATOM	3611	HA	ASP	328P	15.907	16.173	15.575	1.00	0.00	0.053	0.00	0.00
ATOM	3612	CB	ASP	328P	16.637	18.167	15.483	1.00	0.00	-0.336	12.77	4.00
ATOM	3613	HB1	ASP	328P	17.620	18.261	15.943	1.00	0.00	0.053	0.00	0.00
ATOM	3614	HB2	ASP	328P	16.191	19.160	15.528	1.00	0.00	0.053	0.00	0.00
ATOM	3615	CG	ASP	328P	16.895	17.893	13.999	1.00	0.00	0.297	9.82	4.00
ATOM	3616	OD1	ASP	328P	16.766	16.723	13.555	1.00	0.00	-0.534	8.17	-18.95
ATOM	3617	OD2	ASP	328P	17.254	18.855	13.273	1.00	0.00	-0.534	8.17	-18.95
ATOM	3618	C	ASP	328P	16.306	16.834	17.545	1.00	0.00	0.396	9.82	4.00
ATOM	3619	O	ASP	328P	17.203	16.003	17.731	1.00	0.00	-0.396	8.17	-17.40
ATOM	3620	N	GLN	329	15.765	17.537	18.529	1.00	0.00	-0.650	9.00	-17.40
ATOM	3621	HN	GLN	329	14.994	18.192	18.333	1.00	0.00	0.440	0.00	0.00
ATOM	3622	CA	GLN	329	16.262	17.381	19.886	1.00	0.00	0.158	9.40	4.00
ATOM	3623	HA	GLN	329	17.258	16.943	19.836	1.00	0.00	0.053	0.00	0.00
ATOM	3624	CB	GLN	329	16.415	18.748	20.534	1.00	0.00	-0.106	12.77	4.00
ATOM	3625	HB1	GLN	329	16.656	18.690	21.595	1.00	0.00	0.053	0.00	0.00
ATOM	3626	HB2	GLN	329	15.511	19.353	20.468	1.00	0.00	0.053	0.00	0.00
ATOM	3627	CG	GLN	329	17.513	19.579	19.907	1.00	0.00	-0.106	12.77	4.00
ATOM	3628	HG1	GLN	329	17.257	19.882	18.891	1.00	0.00	0.053	0.00	0.00
ATOM	3629	HG2	GLN	329	18.452	19.029	19.852	1.00	0.00	0.053	0.00	0.00
ATOM	3630	CD	GLN	329	17.778	20.835	20.694	1.00	0.00	0.396	9.82	4.00
ATOM	3631	OE1	GLN	329	16.900	21.690	20.827	1.00	0.00	-0.396	8.17	-17.40
ATOM	3632	NE2	GLN	329	18.989	20.956	21.231	1.00	0.00	-0.879	13.25	-17.40
ATOM	3633	HE2	GLN	329	19.690	20.214	21.092	1.00	0.00	0.440	0.00	0.00
ATOM	3634	HE2	GLN	329	19.225	21.791	21.785	1.00	0.00	0.440	0.00	0.00
ATOM	3635	C	GLN	329	15.414	16.489	20.766	1.00	0.00	0.396	9.82	4.00
ATOM	3636	O	GLN	329	15.855	16.067	21.835	1.00	0.00	-0.396	8.17	-17.40
ATOM	3637	N	HIS	330S	14.212	16.172	20.308	1.00	0.00	-0.650	9.00	-17.40
ATOM	3638	HN	HIS	330S	13.897	16.513	19.388	1.00	0.00	0.440	0.00	0.00
ATOM	3639	CA	HIS	330S	13.346	15.339	21.118	1.00	0.00	0.158	9.40	4.00
ATOM	3640	HA	HIS	330S	13.973	14.821	21.843	1.00	0.00	0.053	0.00	0.00
ATOM	3641	CB	HIS	330S	12.387	16.225	21.908	1.00	0.00	-0.106	12.77	4.00
ATOM	3642	HB1	HIS	330S	11.748	16.843	21.277	1.00	0.00	0.053	0.00	0.00
ATOM	3643	HB2	HIS	330S	12.891	16.923	22.575	1.00	0.00	0.053	0.00	0.00

ATOM	3644	CG	HIS	330S	11.449	15.456	22.782	1.00	0.00	-0.050	7.26	0.60
ATOM	3645	CD2	HIS	330S	10.127	15.184	22.649	1.00	0.00	-0.177	10.80	0.60
ATOM	3646	HD2	HIS	330S	9.471	15.531	21.850	1.00	0.00	0.127	0.00	0.00
ATOM	3647	ND1	HIS	330S	11.861	14.815	23.934	1.00	0.00	0.207	9.25	-17.40
ATOM	3648	HD1	HIS	330S	12.818	14.828	24.314	1.00	0.00	0.393	0.00	0.00
ATOM	3649	CE1	HIS	330S	10.833	14.181	24.472	1.00	0.00	-0.227	10.80	0.60
ATOM	3650	HE1	HIS	330S	10.857	13.588	25.386	1.00	0.00	0.127	0.00	0.00
ATOM	3651	NE2	HIS	330S	9.769	14.388	23.711	1.00	0.00	0.207	9.25	-17.40
ATOM	3652	HE2	HIS	330S	8.825	14.013	23.886	1.00	0.00	0.393	0.00	0.00
ATOM	3653	C	HIS	330S	12.530	14.261	20.400	1.00	0.00	0.396	9.82	4.00
ATOM	3654	O	HIS	330S	12.694	13.069	20.667	1.00	0.00	-0.396	8.17	-17.40
ATOM	3655	N	LEU	331	11.657	14.687	19.490	1.00	0.00	-0.650	9.00	-17.40
ATOM	3656	HN	LEU	331	11.605	15.692	19.274	1.00	0.00	0.440	0.00	0.00
ATOM	3657	CA	LEU	331	10.777	13.769	18.795	1.00	0.00	0.158	9.40	4.00
ATOM	3658	HA	LEU	331	10.081	13.361	19.528	1.00	0.00	0.053	0.00	0.00
ATOM	3659	CB	LEU	331	9.901	14.529	17.798	1.00	0.00	-0.106	12.77	4.00
ATOM	3660	HB1	LEU	331	9.291	13.794	17.272	1.00	0.00	0.053	0.00	0.00
ATOM	3661	HB2	LEU	331	10.566	15.057	17.114	1.00	0.00	0.053	0.00	0.00
ATOM	3662	CG	LEU	331	8.928	15.581	18.359	1.00	0.00	-0.053	9.40	4.00
ATOM	3663	HG	LEU	331	9.512	16.310	18.920	1.00	0.00	0.053	0.00	0.00
ATOM	3664	CD1	LEU	331	8.225	16.232	17.188	1.00	0.00	-0.159	16.15	4.00
ATOM	3665	HD1	LEU	331	7.526	16.984	17.555	1.00	0.00	0.053	0.00	0.00
ATOM	3666	HD1	LEU	331	8.961	16.706	16.539	1.00	0.00	0.053	0.00	0.00
ATOM	3667	HD1	LEU	331	7.679	15.475	16.624	1.00	0.00	0.053	0.00	0.00
ATOM	3668	CD2	LEU	331	7.913	14.967	19.305	1.00	0.00	-0.159	16.15	4.00
ATOM	3669	HD2	LEU	331	7.246	15.744	19.677	1.00	0.00	0.053	0.00	0.00
ATOM	3670	HD2	LEU	331	7.331	14.213	18.775	1.00	0.00	0.053	0.00	0.00
ATOM	3671	HD2	LEU	331	8.431	14.501	20.143	1.00	0.00	0.053	0.00	0.00
ATOM	3672	C	LEU	331	11.420	12.582	18.100	1.00	0.00	0.396	9.82	4.00
ATOM	3673	O	LEU	331	10.867	11.480	18.147	1.00	0.00	-0.396	8.17	-17.40
ATOM	3674	N	LYS	332S	12.574	12.795	17.465	1.00	0.00	-0.650	9.00	-17.40
ATOM	3675	HN	LYS	332S	13.000	13.732	17.487	1.00	0.00	0.440	0.00	0.00
ATOM	3676	CA	LYS	332S	13.243	11.714	16.736	1.00	0.00	0.158	9.40	4.00
ATOM	3677	HA	LYS	332S	12.584	11.219	16.022	1.00	0.00	0.053	0.00	0.00
ATOM	3678	CB	LYS	332S	14.422	12.261	15.897	1.00	0.00	-0.106	12.77	4.00
ATOM	3679	HB1	LYS	332S	14.058	13.106	15.313	1.00	0.00	0.053	0.00	0.00
ATOM	3680	HB2	LYS	332S	14.772	11.461	15.243	1.00	0.00	0.053	0.00	0.00
ATOM	3681	CG	LYS	332S	15.646	12.757	16.724	1.00	0.00	-0.106	12.77	4.00
ATOM	3682	HG1	LYS	332S	16.079	11.977	17.350	1.00	0.00	0.053	0.00	0.00
ATOM	3683	HG2	LYS	332S	15.399	13.576	17.398	1.00	0.00	0.053	0.00	0.00
ATOM	3684	CD	LYS	332S	16.810	13.279	15.832	1.00	0.00	-0.106	12.77	4.00
ATOM	3685	HD1	LYS	332S	17.462	13.945	16.396	1.00	0.00	0.053	0.00	0.00
ATOM	3686	HD2	LYS	332S	16.424	13.830	14.974	1.00	0.00	0.053	0.00	0.00
ATOM	3687	CE	LYS	332S	17.652	12.125	15.310	1.00	0.00	0.099	12.77	4.00
ATOM	3688	HE1	LYS	332S	17.050	11.551	14.604	1.00	0.00	0.053	0.00	0.00
ATOM	3689	HE2	LYS	332S	17.945	11.503	16.156	1.00	0.00	0.053	0.00	0.00
ATOM	3690	NZ	LYS	332S	18.904	12.555	14.601	1.00	0.00	-0.045	13.25	-39.20
ATOM	3691	HZ1	LYS	332S	19.418	11.723	14.278	1.00	0.00	0.280	0.00	0.00
ATOM	3692	HZ2	LYS	332S	18.656	13.141	13.791	1.00	0.00	0.280	0.00	0.00
ATOM	3693	HZ3	LYS	332S	19.496	13.095	15.247	1.00	0.00	0.280	0.00	0.00
ATOM	3694	C	LYS	332S	13.764	10.621	17.659	1.00	0.00	0.396	9.82	4.00
ATOM	3695	O	LYS	332S	14.106	9.541	17.201	1.00	0.00	-0.396	8.17	-17.40
ATOM	3696	N	PHE	333	13.824	10.893	18.955	1.00	0.00	-0.650	9.00	-17.40
ATOM	3697	HN	PHE	333	13.492	11.801	19.309	1.00	0.00	0.440	0.00	0.00
ATOM	3698	CA	PHE	333	14.363	9.897	19.879	1.00	0.00	0.158	9.40	4.00
ATOM	3699	HA	PHE	333	15.045	9.255	19.322	1.00	0.00	0.053	0.00	0.00
ATOM	3700	CB	PHE	333	15.223	10.592	20.943	1.00	0.00	-0.106	12.77	4.00
ATOM	3701	HB1	PHE	333	15.616	9.900	21.687	1.00	0.00	0.053	0.00	0.00
ATOM	3702	HB2	PHE	333	14.674	11.350	21.501	1.00	0.00	0.053	0.00	0.00
ATOM	3703	CG	PHE	333	16.416	11.292	20.362	1.00	0.00	0.000	7.26	0.60
ATOM	3704	CD1	PHE	333	16.505	12.681	20.382	1.00	0.00	-0.127	10.80	0.60
ATOM	3705	HD1	PHE	333	15.729	13.262	20.880	1.00	0.00	0.127	0.00	0.00
ATOM	3706	CD2	PHE	333	17.420	10.556	19.726	1.00	0.00	-0.127	10.80	0.60
ATOM	3707	HD2	PHE	333	17.361	9.467	19.711	1.00	0.00	0.127	0.00	0.00
ATOM	3708	CE1	PHE	333	17.577	13.340	19.770	1.00	0.00	-0.127	10.80	0.60
ATOM	3709	HE1	PHE	333	17.634	14.428	19.792	1.00	0.00	0.127	0.00	0.00
ATOM	3710	CE2	PHE	333	18.498	11.197	19.109	1.00	0.00	-0.127	10.80	0.60
ATOM	3711	HE2	PHE	333	19.275	10.613	18.615	1.00	0.00	0.127	0.00	0.00
ATOM	3712	CZ	PHE	333	18.571	12.600	19.131	1.00	0.00	-0.127	10.80	0.60
ATOM	3713	HZ	PHE	333	19.404	13.109	18.648	1.00	0.00	0.127	0.00	0.00
ATOM	3714	C	PHE	333	13.335	8.995	20.540	1.00	0.00	0.396	9.82	4.00
ATOM	3715	O	PHE	333	13.700	8.057	21.252	1.00	0.00	-0.396	8.17	-17.40
ATOM	3716	N	ILE	334	12.055	9.262	20.286	1.00	0.00	-0.650	9.00	-17.40
ATOM	3717	HN	ILE	334	11.815	10.052	19.670	1.00	0.00	0.440	0.00	0.00
ATOM	3718	CA	ILE	334	10.988	8.457	20.862	1.00	0.00	0.158	9.40	4.00
ATOM	3719	HA	ILE	334	11.190	8.351	21.928	1.00	0.00	0.053	0.00	0.00

ATOM	3720	CB	ILE	334	9.624	9.176	20.700	1.00	0.00	-0.053	9.40	4.00
ATOM	3721	HB	ILE	334	9.401	9.368	19.650	1.00	0.00	0.053	0.00	0.00
ATOM	3722	CG2	ILE	334	8.493	8.340	21.264	1.00	0.00	-0.159	16.15	4.00
ATOM	3723	HG2	ILE	334	7.549	8.870	21.135	1.00	0.00	0.053	0.00	0.00
ATOM	3724	HG2	ILE	334	8.447	7.386	20.737	1.00	0.00	0.053	0.00	0.00
ATOM	3725	HG2	ILE	334	8.667	8.160	22.325	1.00	0.00	0.053	0.00	0.00
ATOM	3726	CG1	ILE	334	9.691	10.528	21.417	1.00	0.00	-0.106	12.77	4.00
ATOM	3727	HG1	ILE	334	8.694	10.970	21.404	1.00	0.00	0.053	0.00	0.00
ATOM	3728	HG1	ILE	334	10.400	11.161	20.884	1.00	0.00	0.053	0.00	0.00
ATOM	3729	CD1	ILE	334	10.142	10.456	22.871	1.00	0.00	-0.159	16.15	4.00
ATOM	3730	HD1	ILE	334	10.159	11.459	23.296	1.00	0.00	0.053	0.00	0.00
ATOM	3731	HD1	ILE	334	9.448	9.833	23.436	1.00	0.00	0.053	0.00	0.00
ATOM	3732	HD1	ILE	334	11.141	10.023	22.921	1.00	0.00	0.053	0.00	0.00
ATOM	3733	C	ILE	334	11.000	7.101	20.162	1.00	0.00	0.396	9.82	4.00
ATOM	3734	O	ILE	334	10.825	7.015	18.941	1.00	0.00	-0.396	8.17	-17.40
ATOM	3735	N	LYS	335S	11.215	6.048	20.946	1.00	0.00	-0.650	9.00	-17.40
ATOM	3736	HN	LYS	335S	11.325	6.199	21.959	1.00	0.00	0.440	0.00	0.00
ATOM	3737	CA	LYS	335S	11.301	4.687	20.426	1.00	0.00	0.158	9.40	4.00
ATOM	3738	HA	LYS	335S	11.908	4.718	19.521	1.00	0.00	0.053	0.00	0.00
ATOM	3739	CB	LYS	335S	12.043	3.800	21.433	1.00	0.00	-0.106	12.77	4.00
ATOM	3740	HB1	LYS	335S	11.533	3.711	22.392	1.00	0.00	0.053	0.00	0.00
ATOM	3741	HB2	LYS	335S	13.043	4.158	21.674	1.00	0.00	0.053	0.00	0.00
ATOM	3742	CG	LYS	335S	12.240	2.362	20.951	1.00	0.00	-0.106	12.77	4.00
ATOM	3743	HG1	LYS	335S	12.912	2.294	20.095	1.00	0.00	0.053	0.00	0.00
ATOM	3744	HG2	LYS	335S	11.307	1.891	20.640	1.00	0.00	0.053	0.00	0.00
ATOM	3745	CD	LYS	335S	12.833	1.456	22.029	1.00	0.00	-0.106	12.77	4.00
ATOM	3746	HD1	LYS	335S	12.154	1.362	22.876	1.00	0.00	0.053	0.00	0.00
ATOM	3747	HD2	LYS	335S	13.777	1.855	22.398	1.00	0.00	0.053	0.00	0.00
ATOM	3748	CE	LYS	335S	13.098	0.052	21.480	1.00	0.00	0.099	12.77	4.00
ATOM	3749	HE1	LYS	335S	12.172	-0.454	21.206	1.00	0.00	0.053	0.00	0.00
ATOM	3750	HE2	LYS	335S	13.605	-0.577	22.211	1.00	0.00	0.053	0.00	0.00
ATOM	3751	NZ	LYS	335S	13.960	0.090	20.255	1.00	0.00	-0.045	13.25	-39.20
ATOM	3752	HZ1	LYS	335S	14.116	-0.869	19.915	1.00	0.00	0.280	0.00	0.00
ATOM	3753	HZ2	LYS	335S	13.491	0.641	19.522	1.00	0.00	0.280	0.00	0.00
ATOM	3754	HZ3	LYS	335S	14.865	0.524	20.485	1.00	0.00	0.280	0.00	0.00
ATOM	3755	C	LYS	335S	9.986	3.992	20.045	1.00	0.00	0.396	9.82	4.00
ATOM	3756	O	LYS	335S	8.993	4.029	20.783	1.00	0.00	-0.396	8.17	-17.40
ATOM	3757	N	LEU	336	9.998	3.333	18.891	1.00	0.00	-0.650	9.00	-17.40
ATOM	3758	HN	LEU	336	10.848	3.344	18.310	1.00	0.00	0.440	0.00	0.00
ATOM	3759	CA	LEU	336	8.826	2.593	18.433	1.00	0.00	0.158	9.40	4.00
ATOM	3760	HA	LEU	336	7.907	3.109	18.712	1.00	0.00	0.053	0.00	0.00
ATOM	3761	CB	LEU	336	8.850	2.448	16.903	1.00	0.00	-0.106	12.77	4.00
ATOM	3762	HB1	LEU	336	9.711	1.832	16.642	1.00	0.00	0.053	0.00	0.00
ATOM	3763	HB2	LEU	336	8.936	3.447	16.476	1.00	0.00	0.053	0.00	0.00
ATOM	3764	CG	LEU	336	7.618	1.790	16.250	1.00	0.00	-0.053	9.40	4.00
ATOM	3765	HG	LEU	336	7.510	0.773	16.629	1.00	0.00	0.053	0.00	0.00
ATOM	3766	CD1	LEU	336	6.381	2.597	16.592	1.00	0.00	-0.159	16.15	4.00
ATOM	3767	HD1	LEU	336	5.507	2.135	16.132	1.00	0.00	0.053	0.00	0.00
ATOM	3768	HD1	LEU	336	6.251	2.622	17.674	1.00	0.00	0.053	0.00	0.00
ATOM	3769	HD1	LEU	336	6.494	3.613	16.216	1.00	0.00	0.053	0.00	0.00
ATOM	3770	CD2	LEU	336	7.781	1.735	14.723	1.00	0.00	-0.159	16.15	4.00
ATOM	3771	HD2	LEU	336	6.901	1.267	14.280	1.00	0.00	0.053	0.00	0.00
ATOM	3772	HD2	LEU	336	7.889	2.746	14.332	1.00	0.00	0.053	0.00	0.00
ATOM	3773	HD2	LEU	336	8.667	1.151	14.472	1.00	0.00	0.053	0.00	0.00
ATOM	3774	C	LEU	336	8.790	1.202	19.048	1.00	0.00	0.396	9.82	4.00
ATOM	3775	O	LEU	336	9.768	0.445	18.954	1.00	0.00	-0.396	8.17	-17.40
ATOM	3776	N	ASN	337	7.674	0.845	19.676	1.00	0.00	-0.650	9.00	-17.40
ATOM	3777	HN	ASN	337	6.899	1.517	19.771	1.00	0.00	0.440	0.00	0.00
ATOM	3778	CA	ASN	337	7.546	-0.494	20.228	1.00	0.00	0.158	9.40	4.00
ATOM	3779	HA	ASN	337	8.322	-0.676	20.970	1.00	0.00	0.053	0.00	0.00
ATOM	3780	CB	ASN	337	6.190	-0.674	20.913	1.00	0.00	-0.106	12.77	4.00
ATOM	3781	HB1	ASN	337	5.362	-0.540	20.216	1.00	0.00	0.053	0.00	0.00
ATOM	3782	HB2	ASN	337	6.044	0.043	21.720	1.00	0.00	0.053	0.00	0.00
ATOM	3783	CG	ASN	337	6.043	-2.045	21.512	1.00	0.00	0.396	9.82	4.00
ATOM	3784	OD1	ASN	337	6.814	-2.433	22.392	1.00	0.00	-0.396	8.17	-17.40
ATOM	3785	ND2	ASN	337	5.064	-2.798	21.040	1.00	0.00	-0.879	13.25	-17.40
ATOM	3786	HD2	ASN	337	4.442	-2.433	20.304	1.00	0.00	0.440	0.00	0.00
ATOM	3787	HD2	ASN	337	4.922	-3.749	21.408	1.00	0.00	0.440	0.00	0.00
ATOM	3788	C	ASN	337	7.677	-1.546	19.121	1.00	0.00	0.396	9.82	4.00
ATOM	3789	O	ASN	337	7.123	-1.387	18.026	1.00	0.00	-0.396	8.17	-17.40
ATOM	3790	N	GLN	338	8.401	-2.622	19.417	1.00	0.00	-0.650	9.00	-17.40
ATOM	3791	HN	GLN	338	8.827	-2.695	20.351	1.00	0.00	0.440	0.00	0.00
ATOM	3792	CA	GLN	338	8.609	-3.700	18.458	1.00	0.00	0.158	9.40	4.00
ATOM	3793	HA	GLN	338	8.149	-3.497	17.490	1.00	0.00	0.053	0.00	0.00
ATOM	3794	CB	GLN	338	10.105	-3.885	18.188	1.00	0.00	-0.106	12.77	4.00
ATOM	3795	HB1	GLN	338	10.230	-4.740	17.524	1.00	0.00	0.053	0.00	0.00

ATOM	3796	HB2	GLN	338	10.606	-4.061	19.139	1.00	0.00	0.053	0.00	0.00
ATOM	3797	CG	GLN	338	10.774	-2.681	17.526	1.00	0.00	-0.106	12.77	4.00
ATOM	3798	HG1	GLN	338	11.845	-2.822	17.383	1.00	0.00	0.053	0.00	0.00
ATOM	3799	HG2	GLN	338	10.664	-1.767	18.110	1.00	0.00	0.053	0.00	0.00
ATOM	3800	CD	GLN	338	10.200	-2.376	16.150	1.00	0.00	0.396	9.82	4.00
ATOM	3801	OE1	GLN	338	10.590	-1.397	15.503	1.00	0.00	-0.396	8.17	-17.40
ATOM	3802	NE2	GLN	338	9.272	-3.215	15.694	1.00	0.00	-0.879	13.25	-17.40
ATOM	3803	HE2	GLN	338	8.977	-4.018	16.267	1.00	0.00	0.440	0.00	0.00
ATOM	3804	HE2	GLN	338	8.848	-3.060	14.767	1.00	0.00	0.440	0.00	0.00
ATOM	3805	C	GLN	338	8.028	-5.029	18.931	1.00	0.00	0.396	9.82	4.00
ATOM	3806	O	GLN	338	7.795	-5.922	18.128	1.00	0.00	-0.396	8.17	-17.40
ATOM	3807	N	GLN	339	7.805	-5.166	20.235	1.00	0.00	-0.650	9.00	-17.40
ATOM	3808	HN	GLN	339	8.011	-4.385	20.874	1.00	0.00	0.440	0.00	0.00
ATOM	3809	CA	GLN	339	7.269	-6.417	20.766	1.00	0.00	0.158	9.40	4.00
ATOM	3810	HA	GLN	339	7.557	-7.250	20.125	1.00	0.00	0.053	0.00	0.00
ATOM	3811	CB	GLN	339	7.841	-6.712	22.158	1.00	0.00	-0.106	12.77	4.00
ATOM	3812	HB1	GLN	339	7.588	-5.934	22.879	1.00	0.00	0.053	0.00	0.00
ATOM	3813	HB2	GLN	339	8.928	-6.787	22.148	1.00	0.00	0.053	0.00	0.00
ATOM	3814	CG	GLN	339	7.316	-8.026	22.729	1.00	0.00	-0.106	12.77	4.00
ATOM	3815	HG1	GLN	339	7.538	-8.895	22.110	1.00	0.00	0.053	0.00	0.00
ATOM	3816	HG2	GLN	339	6.234	-8.047	22.860	1.00	0.00	0.053	0.00	0.00
ATOM	3817	CD	GLN	339	7.880	-8.369	24.096	1.00	0.00	0.396	9.82	4.00
ATOM	3818	OE1	GLN	339	7.400	-9.302	24.753	1.00	0.00	-0.396	8.17	-17.40
ATOM	3819	NE2	GLN	339	8.903	-7.628	24.533	1.00	0.00	-0.879	13.25	-17.40
ATOM	3820	HE2	GLN	339	9.269	-6.861	23.950	1.00	0.00	0.440	0.00	0.00
ATOM	3821	HE2	GLN	339	9.325	-7.823	25.452	1.00	0.00	0.440	0.00	0.00
ATOM	3822	C	GLN	339	5.749	-6.350	20.830	1.00	0.00	0.396	9.82	4.00
ATOM	3823	O	GLN	339	5.180	-5.503	21.522	1.00	0.00	-0.396	8.17	-17.40
ATOM	3824	N	PHE	340	5.105	-7.238	20.079	1.00	0.00	-0.650	9.00	-17.40
ATOM	3825	HN	PHE	340	5.649	-7.918	19.529	1.00	0.00	0.440	0.00	0.00
ATOM	3826	CA	PHE	340	3.651	-7.275	20.013	1.00	0.00	0.158	9.40	4.00
ATOM	3827	HA	PHE	340	3.230	-6.304	19.749	1.00	0.00	0.053	0.00	0.00
ATOM	3828	CB	PHE	340	3.183	-8.262	18.931	1.00	0.00	-0.106	12.77	4.00
ATOM	3829	HB1	PHE	340	3.428	-9.299	19.158	1.00	0.00	0.053	0.00	0.00
ATOM	3830	HB2	PHE	340	3.622	-8.069	17.952	1.00	0.00	0.053	0.00	0.00
ATOM	3831	CG	PHE	340	1.698	-8.243	18.712	1.00	0.00	0.000	7.26	0.60
ATOM	3832	CD1	PHE	340	1.146	-7.481	17.688	1.00	0.00	-0.127	10.80	0.60
ATOM	3833	HD1	PHE	340	1.804	-6.950	17.000	1.00	0.00	0.127	0.00	0.00
ATOM	3834	CD2	PHE	340	0.847	-8.923	19.579	1.00	0.00	-0.127	10.80	0.60
ATOM	3835	HD2	PHE	340	1.266	-9.530	20.381	1.00	0.00	0.127	0.00	0.00
ATOM	3836	CE1	PHE	340	-0.233	-7.385	17.527	1.00	0.00	-0.127	10.80	0.60
ATOM	3837	HE1	PHE	340	-0.649	-6.783	16.719	1.00	0.00	0.127	0.00	0.00
ATOM	3838	CE2	PHE	340	-0.542	-8.834	19.431	1.00	0.00	-0.127	10.80	0.60
ATOM	3839	HE2	PHE	340	-1.200	-9.367	20.117	1.00	0.00	0.127	0.00	0.00
ATOM	3840	CZ	PHE	340	-1.080	-8.063	18.406	1.00	0.00	-0.127	10.80	0.60
ATOM	3841	HZ	PHE	340	-2.161	-7.988	18.289	1.00	0.00	0.127	0.00	0.00
ATOM	3842	C	PHE	340	3.030	-7.680	21.347	1.00	0.00	0.396	9.82	4.00
ATOM	3843	O	PHE	340	3.331	-8.741	21.878	1.00	0.00	-0.396	8.17	-17.40
ATOM	3844	N	VAL	341	2.166	-6.827	21.883	1.00	0.00	-0.650	9.00	-17.40
ATOM	3845	HN	VAL	341	1.971	-5.936	21.404	1.00	0.00	0.440	0.00	0.00
ATOM	3846	CA	VAL	341	1.487	-7.129	23.138	1.00	0.00	0.158	9.40	4.00
ATOM	3847	HA	VAL	341	1.967	-8.017	23.549	1.00	0.00	0.053	0.00	0.00
ATOM	3848	CB	VAL	341	1.576	-5.947	24.116	1.00	0.00	-0.053	9.40	4.00
ATOM	3849	HB	VAL	341	1.211	-5.041	23.631	1.00	0.00	0.053	0.00	0.00
ATOM	3850	CG1	VAL	341	0.729	-6.234	25.345	1.00	0.00	-0.159	16.15	4.00
ATOM	3851	HG1	VAL	341	0.794	-5.393	26.036	1.00	0.00	0.053	0.00	0.00
ATOM	3852	HG1	VAL	341	-0.309	-6.377	25.046	1.00	0.00	0.053	0.00	0.00
ATOM	3853	HG1	VAL	341	1.093	-7.136	25.835	1.00	0.00	0.053	0.00	0.00
ATOM	3854	CG2	VAL	341	3.035	-5.703	24.518	1.00	0.00	-0.159	16.15	4.00
ATOM	3855	HG2	VAL	341	3.085	-4.863	25.211	1.00	0.00	0.053	0.00	0.00
ATOM	3856	HG2	VAL	341	3.433	-6.595	24.999	1.00	0.00	0.053	0.00	0.00
ATOM	3857	HG2	VAL	341	3.624	-5.476	23.629	1.00	0.00	0.053	0.00	0.00
ATOM	3858	C	VAL	341	0.012	-7.378	22.794	1.00	0.00	0.396	9.82	4.00
ATOM	3859	O	VAL	341	-0.620	-6.554	22.117	1.00	0.00	-0.396	8.17	-17.40
ATOM	3860	N	PRO	342	-0.547	-8.521	23.228	1.00	0.00	-0.422	9.00	-17.40
ATOM	3861	CD	PRO	342	0.078	-9.643	23.967	1.00	0.00	0.105	12.77	4.00
ATOM	3862	HD1	PRO	342	0.559	-9.293	24.880	1.00	0.00	0.053	0.00	0.00
ATOM	3863	HD2	PRO	342	0.836	-10.139	23.361	1.00	0.00	0.053	0.00	0.00
ATOM	3864	CA	PRO	342	-1.958	-8.806	22.925	1.00	0.00	0.158	9.40	4.00
ATOM	3865	HA	PRO	342	-2.200	-8.489	21.910	1.00	0.00	0.053	0.00	0.00
ATOM	3866	CB	PRO	342	-2.044	-10.329	23.092	1.00	0.00	-0.106	12.77	4.00
ATOM	3867	HB1	PRO	342	-1.705	-10.845	22.193	1.00	0.00	0.053	0.00	0.00
ATOM	3868	HB2	PRO	342	-3.067	-10.648	23.290	1.00	0.00	0.053	0.00	0.00
ATOM	3869	CG	PRO	342	-1.135	-10.575	24.265	1.00	0.00	-0.106	12.77	4.00
ATOM	3870	HG1	PRO	342	-0.839	-11.622	24.320	1.00	0.00	0.053	0.00	0.00
ATOM	3871	HG2	PRO	342	-1.625	-10.317	25.203	1.00	0.00	0.053	0.00	0.00

ATOM	3872	C	PRO	342	-2.878	-8.058	23.902	1.00	0.00	0.396	9.82	4.00
ATOM	3873	O	PRO	342	-3.560	-8.677	24.725	1.00	0.00	-0.396	8.17	-17.40
ATOM	3874	N	PHE	343	-2.892	-6.730	23.809	1.00	0.00	-0.650	9.00	-17.40
ATOM	3875	HN	PHE	343	-2.307	-6.266	23.098	1.00	0.00	0.440	0.00	0.00
ATOM	3876	CA	PHE	343	-3.722	-5.917	24.697	1.00	0.00	0.158	9.40	4.00
ATOM	3877	HA	PHE	343	-3.292	-5.953	25.698	1.00	0.00	0.053	0.00	0.00
ATOM	3878	CB	PHE	343	-3.718	-4.443	24.283	1.00	0.00	-0.106	12.77	4.00
ATOM	3879	HB1	PHE	343	-4.465	-3.918	24.878	1.00	0.00	0.053	0.00	0.00
ATOM	3880	HB2	PHE	343	-3.962	-4.384	23.222	1.00	0.00	0.053	0.00	0.00
ATOM	3881	CG	PHE	343	-2.392	-3.743	24.489	1.00	0.00	0.000	7.26	0.60
ATOM	3882	CD1	PHE	343	-1.545	-3.501	23.414	1.00	0.00	-0.127	10.80	0.60
ATOM	3883	HD1	PHE	343	-1.801	-3.890	22.428	1.00	0.00	0.127	0.00	0.00
ATOM	3884	CD2	PHE	343	-2.042	-3.250	25.740	1.00	0.00	-0.127	10.80	0.60
ATOM	3885	HD2	PHE	343	-2.692	-3.440	26.593	1.00	0.00	0.127	0.00	0.00
ATOM	3886	CE1	PHE	343	-0.371	-2.766	23.581	1.00	0.00	-0.127	10.80	0.60
ATOM	3887	HE1	PHE	343	0.283	-2.579	22.729	1.00	0.00	0.127	0.00	0.00
ATOM	3888	CE2	PHE	343	-0.874	-2.517	25.919	1.00	0.00	-0.127	10.80	0.60
ATOM	3889	HE2	PHE	343	-0.615	-2.135	26.907	1.00	0.00	0.127	0.00	0.00
ATOM	3890	CZ	PHE	343	-0.038	-2.271	24.839	1.00	0.00	-0.127	10.80	0.60
ATOM	3891	HZ	PHE	343	0.875	-1.692	24.975	1.00	0.00	0.127	0.00	0.00
ATOM	3892	C	PHE	343	-5.157	-6.382	24.794	1.00	0.00	0.396	9.82	4.00
ATOM	3893	O	PHE	343	-5.749	-6.270	25.866	1.00	0.00	-0.396	8.17	-17.40
ATOM	3894	N	THR	344	-5.731	-6.889	23.699	1.00	0.00	-0.650	9.00	-17.40
ATOM	3895	HN	THR	344	-5.205	-6.943	22.815	1.00	0.00	0.440	0.00	0.00
ATOM	3896	CA	THR	344	-7.123	-7.370	23.767	1.00	0.00	0.158	9.40	4.00
ATOM	3897	HA	THR	344	-7.815	-6.608	24.125	1.00	0.00	0.053	0.00	0.00
ATOM	3898	CB	THR	344	-7.717	-7.720	22.359	1.00	0.00	0.060	9.40	4.00
ATOM	3899	HB	THR	344	-8.760	-8.020	22.450	1.00	0.00	0.053	0.00	0.00
ATOM	3900	OG1	THR	344	-7.002	-8.809	21.770	1.00	0.00	-0.537	11.04	-17.40
ATOM	3901	HG1	THR	344	-7.569	-9.226	21.019	1.00	0.00	0.424	0.00	0.00
ATOM	3902	CG2	THR	344	-7.641	-6.508	21.432	1.00	0.00	-0.159	16.15	4.00
ATOM	3903	HG2	THR	344	-8.057	-6.767	20.458	1.00	0.00	0.053	0.00	0.00
ATOM	3904	HG2	THR	344	-8.210	-5.684	21.862	1.00	0.00	0.053	0.00	0.00
ATOM	3905	HG2	THR	344	-6.600	-6.205	21.312	1.00	0.00	0.053	0.00	0.00
ATOM	3906	C	THR	344	-7.292	-8.574	24.710	1.00	0.00	0.396	9.82	4.00
ATOM	3907	O	THR	344	-8.417	-8.904	25.103	1.00	0.00	-0.396	8.17	-17.40
ATOM	3908	N	GLN	345	-6.187	-9.212	25.101	1.00	0.00	-0.650	9.00	-17.40
ATOM	3909	HN	GLN	345	-5.269	-8.899	24.753	1.00	0.00	0.440	0.00	0.00
ATOM	3910	CA	GLN	345	-6.262	-10.356	26.022	1.00	0.00	0.158	9.40	4.00
ATOM	3911	HA	GLN	345	-7.256	-10.801	26.051	1.00	0.00	0.053	0.00	0.00
ATOM	3912	CB	GLN	345	-5.293	-11.469	25.600	1.00	0.00	-0.106	12.77	4.00
ATOM	3913	HB1	GLN	345	-5.374	-12.273	26.331	1.00	0.00	0.053	0.00	0.00
ATOM	3914	HB2	GLN	345	-4.288	-11.045	25.589	1.00	0.00	0.053	0.00	0.00
ATOM	3915	CG	GLN	345	-5.522	-12.109	24.207	1.00	0.00	-0.106	12.77	4.00
ATOM	3916	HG1	GLN	345	-5.513	-11.358	23.416	1.00	0.00	0.053	0.00	0.00
ATOM	3917	HG2	GLN	345	-6.481	-12.623	24.157	1.00	0.00	0.053	0.00	0.00
ATOM	3918	CD	GLN	345	-4.432	-13.137	23.875	1.00	0.00	0.396	9.82	4.00
ATOM	3919	OE1	GLN	345	-3.378	-13.155	24.511	1.00	0.00	-0.396	8.17	-17.40
ATOM	3920	NE2	GLN	345	-4.680	-13.984	22.867	1.00	0.00	-0.879	13.25	-17.40
ATOM	3921	HE2	GLN	345	-5.575	-13.934	22.361	1.00	0.00	0.440	0.00	0.00
ATOM	3922	HE2	GLN	345	-3.974	-14.684	22.598	1.00	0.00	0.440	0.00	0.00
ATOM	3923	C	GLN	345	-5.917	-9.965	27.476	1.00	0.00	0.396	9.82	4.00
ATOM	3924	O	GLN	345	-5.904	-10.814	28.360	1.00	0.00	-0.396	8.17	-17.40
ATOM	3925	N	LEU	346	-5.628	-8.694	27.725	1.00	0.00	-0.650	9.00	-17.40
ATOM	3926	HN	LEU	346	-5.670	-8.009	26.957	1.00	0.00	0.440	0.00	0.00
ATOM	3927	CA	LEU	346	-5.248	-8.240	29.072	1.00	0.00	0.158	9.40	4.00
ATOM	3928	HA	LEU	346	-4.931	-9.108	29.650	1.00	0.00	0.053	0.00	0.00
ATOM	3929	CB	LEU	346	-4.096	-7.244	28.965	1.00	0.00	-0.106	12.77	4.00
ATOM	3930	HB1	LEU	346	-3.621	-7.019	29.920	1.00	0.00	0.053	0.00	0.00
ATOM	3931	HB2	LEU	346	-4.390	-6.274	28.562	1.00	0.00	0.053	0.00	0.00
ATOM	3932	CG	LEU	346	-2.958	-7.716	28.061	1.00	0.00	-0.053	9.40	4.00
ATOM	3933	HG	LEU	346	-3.326	-7.899	27.051	1.00	0.00	0.053	0.00	0.00
ATOM	3934	CD1	LEU	346	-1.855	-6.653	27.992	1.00	0.00	-0.159	16.15	4.00
ATOM	3935	HD1	LEU	346	-1.051	-7.003	27.344	1.00	0.00	0.053	0.00	0.00
ATOM	3936	HD1	LEU	346	-2.266	-5.727	27.590	1.00	0.00	0.053	0.00	0.00
ATOM	3937	HD1	LEU	346	-1.461	-6.471	28.992	1.00	0.00	0.053	0.00	0.00
ATOM	3938	CD2	LEU	346	-2.405	-9.008	28.618	1.00	0.00	-0.159	16.15	4.00
ATOM	3939	HD2	LEU	346	-1.591	-9.358	27.983	1.00	0.00	0.053	0.00	0.00
ATOM	3940	HD2	LEU	346	-2.030	-8.838	29.627	1.00	0.00	0.053	0.00	0.00
ATOM	3941	HD2	LEU	346	-3.193	-9.759	28.645	1.00	0.00	0.053	0.00	0.00
ATOM	3942	C	LEU	346	-6.368	-7.560	29.834	1.00	0.00	0.396	9.82	4.00
ATOM	3943	O	LEU	346	-7.310	-7.048	29.235	1.00	0.00	-0.396	8.17	-17.40
ATOM	3944	N	ASP	347P	-6.243	-7.505	31.157	1.00	0.00	-0.650	9.00	-17.40
ATOM	3945	HN	ASP	347P	-5.424	-7.936	31.610	1.00	0.00	0.440	0.00	0.00
ATOM	3946	CA	ASP	347P	-7.252	-6.841	31.971	1.00	0.00	0.158	9.40	4.00
ATOM	3947	HA	ASP	347P	-8.193	-6.923	31.427	1.00	0.00	0.053	0.00	0.00

ATOM	3948	CB	ASP	347P	-7.352	-7.510	33.346	1.00	0.00	-0.336	12.77	4.00
ATOM	3949	HB1	ASP	347P	-6.427	-7.435	33.919	1.00	0.00	0.053	0.00	0.00
ATOM	3950	HB2	ASP	347P	-7.580	-8.573	33.281	1.00	0.00	0.053	0.00	0.00
ATOM	3951	CG	ASP	347P	-8.439	-6.899	34.220	1.00	0.00	0.297	9.82	4.00
ATOM	3952	OD1	ASP	347P	-8.914	-5.785	33.900	1.00	0.00	-0.534	8.17	-18.95
ATOM	3953	OD2	ASP	347P	-8.814	-7.542	35.238	1.00	0.00	-0.534	8.17	-18.95
ATOM	3954	C	ASP	347P	-6.797	-5.382	32.128	1.00	0.00	0.396	9.82	4.00
ATOM	3955	O	ASP	347P	-5.851	-5.100	32.859	1.00	0.00	-0.396	8.17	-17.40
ATOM	3956	N	LEU	348	-7.446	-4.456	31.425	1.00	0.00	-0.650	9.00	-17.40
ATOM	3957	HN	LEU	348	-8.226	-4.733	30.813	1.00	0.00	0.440	0.00	0.00
ATOM	3958	CA	LEU	348	-7.062	-3.056	31.513	1.00	0.00	0.158	9.40	4.00
ATOM	3959	HA	LEU	348	-6.044	-2.915	31.878	1.00	0.00	0.053	0.00	0.00
ATOM	3960	CB	LEU	348	-7.092	-2.417	30.112	1.00	0.00	-0.106	12.77	4.00
ATOM	3961	HB1	LEU	348	-6.747	-1.383	30.099	1.00	0.00	0.053	0.00	0.00
ATOM	3962	HB2	LEU	348	-8.087	-2.392	29.668	1.00	0.00	0.053	0.00	0.00
ATOM	3963	CG	LEU	348	-6.212	-3.148	29.089	1.00	0.00	-0.053	9.40	4.00
ATOM	3964	HG	LEU	348	-6.559	-4.172	28.955	1.00	0.00	0.053	0.00	0.00
ATOM	3965	CD1	LEU	348	-6.265	-2.421	27.714	1.00	0.00	-0.159	16.15	4.00
ATOM	3966	HD1	LEU	348	-5.636	-2.950	26.998	1.00	0.00	0.053	0.00	0.00
ATOM	3967	HD1	LEU	348	-7.292	-2.403	27.351	1.00	0.00	0.053	0.00	0.00
ATOM	3968	HD1	LEU	348	-5.903	-1.399	27.828	1.00	0.00	0.053	0.00	0.00
ATOM	3969	CD2	LEU	348	-4.788	-3.231	29.631	1.00	0.00	-0.159	16.15	4.00
ATOM	3970	HD2	LEU	348	-4.154	-3.749	28.911	1.00	0.00	0.053	0.00	0.00
ATOM	3971	HD2	LEU	348	-4.402	-2.225	29.796	1.00	0.00	0.053	0.00	0.00
ATOM	3972	HD2	LEU	348	-4.788	-3.778	30.573	1.00	0.00	0.053	0.00	0.00
ATOM	3973	C	LEU	348	-7.954	-2.250	32.454	1.00	0.00	0.396	9.82	4.00
ATOM	3974	O	LEU	348	-8.040	-1.030	32.329	1.00	0.00	-0.396	8.17	-17.40
ATOM	3975	N	SER	349	-8.613	-2.918	33.395	1.00	0.00	-0.650	9.00	-17.40
ATOM	3976	HN	SER	349	-8.502	-3.938	33.475	1.00	0.00	0.440	0.00	0.00
ATOM	3977	CA	SER	349	-9.497	-2.202	34.319	1.00	0.00	0.158	9.40	4.00
ATOM	3978	HA	SER	349	-10.212	-1.568	33.795	1.00	0.00	0.053	0.00	0.00
ATOM	3979	CB	SER	349	-10.348	-3.186	35.134	1.00	0.00	0.007	12.77	4.00
ATOM	3980	HB1	SER	349	-10.967	-3.802	34.482	1.00	0.00	0.053	0.00	0.00
ATOM	3981	HB2	SER	349	-11.010	-2.658	35.820	1.00	0.00	0.053	0.00	0.00
ATOM	3982	OG	SER	349	-9.534	-4.050	35.900	1.00	0.00	-0.537	11.04	-17.40
ATOM	3983	HG	SER	349	-9.929	-4.146	36.846	1.00	0.00	0.424	0.00	0.00
ATOM	3984	C	SER	349	-8.722	-1.295	35.269	1.00	0.00	0.396	9.82	4.00
ATOM	3985	O	SER	349	-9.303	-0.426	35.921	1.00	0.00	-0.396	8.17	-17.40
ATOM	3986	N	TYR	350	-7.416	-1.506	35.363	1.00	0.00	-0.650	9.00	-17.40
ATOM	3987	HN	TYR	350	-6.979	-2.258	34.811	1.00	0.00	0.440	0.00	0.00
ATOM	3988	CA	TYR	350	-6.591	-0.680	36.243	1.00	0.00	0.158	9.40	4.00
ATOM	3989	HA	TYR	350	-6.990	-0.650	37.256	1.00	0.00	0.053	0.00	0.00
ATOM	3990	CB	TYR	350	-5.181	-1.292	36.378	1.00	0.00	-0.106	12.77	4.00
ATOM	3991	HB1	TYR	350	-5.296	-2.341	36.649	1.00	0.00	0.053	0.00	0.00
ATOM	3992	HB2	TYR	350	-4.650	-0.743	37.156	1.00	0.00	0.053	0.00	0.00
ATOM	3993	CG	TYR	350	-4.316	-1.246	35.132	1.00	0.00	0.000	7.26	0.60
ATOM	3994	CD1	TYR	350	-3.343	-0.252	34.962	1.00	0.00	-0.127	10.80	0.60
ATOM	3995	HD1	TYR	350	-3.240	0.528	35.715	1.00	0.00	0.127	0.00	0.00
ATOM	3996	CE1	TYR	350	-2.503	-0.240	33.850	1.00	0.00	-0.127	10.80	0.60
ATOM	3997	HE1	TYR	350	-1.747	0.538	33.744	1.00	0.00	0.127	0.00	0.00
ATOM	3998	CD2	TYR	350	-4.431	-2.223	34.140	1.00	0.00	-0.127	10.80	0.60
ATOM	3999	HD2	TYR	350	-5.181	-3.007	34.245	1.00	0.00	0.127	0.00	0.00
ATOM	4000	CE2	TYR	350	-3.594	-2.213	33.005	1.00	0.00	-0.127	10.80	0.60
ATOM	4001	HE2	TYR	350	-3.703	-2.977	32.235	1.00	0.00	0.127	0.00	0.00
ATOM	4002	CZ	TYR	350	-2.632	-1.226	32.874	1.00	0.00	0.026	7.26	0.60
ATOM	4003	OH	TYR	350	-1.776	-1.247	31.788	1.00	0.00	-0.451	10.94	-17.40
ATOM	4004	HH	TYR	350	-1.577	-0.281	31.487	1.00	0.00	0.424	0.00	0.00
ATOM	4005	C	TYR	350	-6.508	0.773	35.743	1.00	0.00	0.396	9.82	4.00
ATOM	4006	O	TYR	350	-6.112	1.667	36.501	1.00	0.00	-0.396	8.17	-17.40
ATOM	4007	N	LEU	351	-6.889	1.005	34.479	1.00	0.00	-0.650	9.00	-17.40
ATOM	4008	HN	LEU	351	-7.210	0.217	33.897	1.00	0.00	0.440	0.00	0.00
ATOM	4009	CA	LEU	351	-6.859	2.347	33.909	1.00	0.00	0.158	9.40	4.00
ATOM	4010	HA	LEU	351	-6.003	2.877	34.328	1.00	0.00	0.053	0.00	0.00
ATOM	4011	CB	LEU	351	-6.638	2.276	32.390	1.00	0.00	-0.106	12.77	4.00
ATOM	4012	HB1	LEU	351	-6.818	3.269	31.980	1.00	0.00	0.053	0.00	0.00
ATOM	4013	HB2	LEU	351	-7.343	1.550	31.984	1.00	0.00	0.053	0.00	0.00
ATOM	4014	CG	LEU	351	-5.242	1.849	31.924	1.00	0.00	-0.053	9.40	4.00
ATOM	4015	HG	LEU	351	-4.959	0.924	32.428	1.00	0.00	0.053	0.00	0.00
ATOM	4016	CD1	LEU	351	-5.260	1.622	30.405	1.00	0.00	-0.159	16.15	4.00
ATOM	4017	HD1	LEU	351	-4.268	1.318	30.070	1.00	0.00	0.053	0.00	0.00
ATOM	4018	HD1	LEU	351	-5.979	0.840	30.162	1.00	0.00	0.053	0.00	0.00
ATOM	4019	HD1	LEU	351	-5.544	2.546	29.902	1.00	0.00	0.053	0.00	0.00
ATOM	4020	CD2	LEU	351	-4.216	2.940	32.294	1.00	0.00	-0.159	16.15	4.00
ATOM	4021	HD2	LEU	351	-3.223	2.634	31.961	1.00	0.00	0.053	0.00	0.00
ATOM	4022	HD2	LEU	351	-4.489	3.876	31.807	1.00	0.00	0.053	0.00	0.00
ATOM	4023	HD2	LEU	351	-4.209	3.081	33.374	1.00	0.00	0.053	0.00	0.00

ATOM	4024	C	LEU	351	-8.108	3.184	34.194	1.00	0.00	0.396	9.82	4.00
ATOM	4025	O	LEU	351	-8.130	4.389	33.921	1.00	0.00	-0.396	8.17	-17.40
ATOM	4026	N	GLN	352	-9.156	2.555	34.709	1.00	0.00	-0.650	9.00	-17.40
ATOM	4027	HN	GLN	352	-9.111	1.540	34.879	1.00	0.00	0.440	0.00	0.00
ATOM	4028	CA	GLN	352	-10.371	3.293	35.035	1.00	0.00	0.158	9.40	4.00
ATOM	4029	HA	GLN	352	-10.659	3.851	34.144	1.00	0.00	0.053	0.00	0.00
ATOM	4030	CB	GLN	352	-11.488	2.340	35.450	1.00	0.00	-0.106	12.77	4.00
ATOM	4031	HB1	GLN	352	-12.335	2.935	35.790	1.00	0.00	0.053	0.00	0.00
ATOM	4032	HB2	GLN	352	-11.114	1.706	36.255	1.00	0.00	0.053	0.00	0.00
ATOM	4033	CG	GLN	352	-11.983	1.429	34.342	1.00	0.00	-0.106	12.77	4.00
ATOM	4034	HG1	GLN	352	-11.162	1.003	33.764	1.00	0.00	0.053	0.00	0.00
ATOM	4035	HG2	GLN	352	-12.624	1.955	33.635	1.00	0.00	0.053	0.00	0.00
ATOM	4036	CD	GLN	352	-12.792	0.260	34.882	1.00	0.00	0.396	9.82	4.00
ATOM	4037	OE1	GLN	352	-13.401	-0.495	34.118	1.00	0.00	-0.396	8.17	-17.40
ATOM	4038	NE2	GLN	352	-12.798	0.100	36.206	1.00	0.00	-0.879	13.25	-17.40
ATOM	4039	HE2	GLN	352	-12.275	0.754	36.806	1.00	0.00	0.440	0.00	0.00
ATOM	4040	HE2	GLN	352	-13.325	-0.677	36.628	1.00	0.00	0.440	0.00	0.00
ATOM	4041	C	GLN	352	-10.039	4.222	36.195	1.00	0.00	0.396	9.82	4.00
ATOM	4042	O	GLN	352	-9.312	3.853	37.127	1.00	0.00	-0.396	8.17	-17.40
ATOM	4043	N	GLN	353	-10.588	5.427	36.130	1.00	0.00	-0.650	9.00	-17.40
ATOM	4044	HN	GLN	353	-11.208	5.640	35.336	1.00	0.00	0.440	0.00	0.00
ATOM	4045	CA	GLN	353	-10.356	6.462	37.126	1.00	0.00	0.158	9.40	4.00
ATOM	4046	HA	GLN	353	-9.350	6.851	36.965	1.00	0.00	0.053	0.00	0.00
ATOM	4047	CB	GLN	353	-11.308	7.612	36.836	1.00	0.00	-0.106	12.77	4.00
ATOM	4048	HB1	GLN	353	-12.302	7.192	36.683	1.00	0.00	0.053	0.00	0.00
ATOM	4049	HB2	GLN	353	-10.955	8.119	35.938	1.00	0.00	0.053	0.00	0.00
ATOM	4050	CG	GLN	353	-11.430	8.643	37.897	1.00	0.00	-0.106	12.77	4.00
ATOM	4051	HG1	GLN	353	-10.457	9.078	38.127	1.00	0.00	0.053	0.00	0.00
ATOM	4052	HG2	GLN	353	-11.833	8.210	38.812	1.00	0.00	0.053	0.00	0.00
ATOM	4053	CD	GLN	353	-12.354	9.761	37.458	1.00	0.00	0.396	9.82	4.00
ATOM	4054	OE1	GLN	353	-13.495	9.519	37.030	1.00	0.00	-0.396	8.17	-17.40
ATOM	4055	NE2	GLN	353	-11.865	10.983	37.540	1.00	0.00	-0.879	13.25	-17.40
ATOM	4056	HE2	GLN	353	-10.912	11.133	37.902	1.00	0.00	0.440	0.00	0.00
ATOM	4057	HE2	GLN	353	-12.435	11.787	37.242	1.00	0.00	0.440	0.00	0.00
ATOM	4058	C	GLN	353	-10.435	6.058	38.596	1.00	0.00	0.396	9.82	4.00
ATOM	4059	O	GLN	353	-9.514	6.349	39.367	1.00	0.00	-0.396	8.17	-17.40
ATOM	4060	N	GLU	354	-11.510	5.380	38.991	1.00	0.00	-0.650	9.00	-17.40
ATOM	4061	HN	GLU	354	-12.235	5.125	38.306	1.00	0.00	0.440	0.00	0.00
ATOM	4062	CA	GLU	354	-11.666	4.994	40.394	1.00	0.00	0.158	9.40	4.00
ATOM	4063	HA	GLU	354	-11.575	5.890	41.007	1.00	0.00	0.053	0.00	0.00
ATOM	4064	CB	GLU	354	-13.090	4.474	40.681	1.00	0.00	-0.106	12.77	4.00
ATOM	4065	HB1	GLU	354	-13.796	5.214	40.306	1.00	0.00	0.053	0.00	0.00
ATOM	4066	HB2	GLU	354	-13.187	4.349	41.759	1.00	0.00	0.053	0.00	0.00
ATOM	4067	CG	GLU	354	-13.467	3.135	40.042	1.00	0.00	-0.106	12.77	4.00
ATOM	4068	HG1	GLU	354	-14.303	2.640	40.535	1.00	0.00	0.053	0.00	0.00
ATOM	4069	HG2	GLU	354	-12.655	2.407	40.052	1.00	0.00	0.053	0.00	0.00
ATOM	4070	CD	GLU	354	-13.877	3.257	38.584	1.00	0.00	0.399	9.82	4.00
ATOM	4071	OE1	GLU	354	-14.440	2.275	38.044	1.00	0.00	-0.396	8.17	-18.95
ATOM	4072	OE2	GLU	354	-13.634	4.326	37.980	1.00	0.00	-0.427	8.17	-18.95
ATOM	4073	HE2	GLU	354	-13.964	4.254	37.007	1.00	0.00	0.424	0.00	0.00
ATOM	4074	C	GLU	354	-10.634	3.991	40.891	1.00	0.00	0.396	9.82	4.00
ATOM	4075	O	GLU	354	-10.442	3.844	42.101	1.00	0.00	-0.396	8.17	-17.40
ATOM	4076	N	ALA	355	-9.964	3.290	39.980	1.00	0.00	-0.650	9.00	-17.40
ATOM	4077	HN	ALA	355	-10.172	3.409	38.978	1.00	0.00	0.440	0.00	0.00
ATOM	4078	CA	ALA	355	-8.929	2.348	40.408	1.00	0.00	0.158	9.40	4.00
ATOM	4079	HA	ALA	355	-9.148	2.029	41.427	1.00	0.00	0.053	0.00	0.00
ATOM	4080	CB	ALA	355	-8.920	1.110	39.492	1.00	0.00	-0.159	16.15	4.00
ATOM	4081	HB1	ALA	355	-8.145	0.418	39.822	1.00	0.00	0.053	0.00	0.00
ATOM	4082	HB2	ALA	355	-9.890	0.616	39.538	1.00	0.00	0.053	0.00	0.00
ATOM	4083	HB3	ALA	355	-8.717	1.417	38.466	1.00	0.00	0.053	0.00	0.00
ATOM	4084	C	ALA	355	-7.559	3.062	40.352	1.00	0.00	0.396	9.82	4.00
ATOM	4085	O	ALA	355	-6.799	3.077	41.330	1.00	0.00	-0.396	8.17	-17.40
ATOM	4086	N	TYR	356	-7.267	3.663	39.203	1.00	0.00	-0.650	9.00	-17.40
ATOM	4087	HN	TYR	356	-7.956	3.632	38.438	1.00	0.00	0.440	0.00	0.00
ATOM	4088	CA	TYR	356	-6.005	4.366	38.984	1.00	0.00	0.158	9.40	4.00
ATOM	4089	HA	TYR	356	-5.196	3.635	39.012	1.00	0.00	0.053	0.00	0.00
ATOM	4090	CB	TYR	356	-6.007	4.999	37.588	1.00	0.00	-0.106	12.77	4.00
ATOM	4091	HB1	TYR	356	-6.530	5.953	37.646	1.00	0.00	0.053	0.00	0.00
ATOM	4092	HB2	TYR	356	-6.520	4.320	36.906	1.00	0.00	0.053	0.00	0.00
ATOM	4093	CG	TYR	356	-4.639	5.264	37.022	1.00	0.00	0.000	7.26	0.60
ATOM	4094	CD1	TYR	356	-3.935	4.255	36.360	1.00	0.00	-0.127	10.80	0.60
ATOM	4095	HD1	TYR	356	-4.379	3.263	36.270	1.00	0.00	0.127	0.00	0.00
ATOM	4096	CE1	TYR	356	-2.679	4.490	35.814	1.00	0.00	-0.127	10.80	0.60
ATOM	4097	HE1	TYR	356	-2.145	3.691	35.298	1.00	0.00	0.127	0.00	0.00
ATOM	4098	CD2	TYR	356	-4.045	6.525	37.130	1.00	0.00	-0.127	10.80	0.60
ATOM	4099	HD2	TYR	356	-4.574	7.325	37.646	1.00	0.00	0.127	0.00	0.00

ATOM	4100	CE2	TYR	356	-2.789	6.772	36.589	1.00	0.00	-0.127	10.80	0.60
ATOM	4101	HE2	TYR	356	-2.336	7.759	36.677	1.00	0.00	0.127	0.00	0.00
ATOM	4102	CZ	TYR	356	-2.113	5.743	35.931	1.00	0.00	0.026	7.26	0.60
ATOM	4103	OH	TYR	356	-0.880	5.958	35.375	1.00	0.00	-0.451	10.94	-17.40
ATOM	4104	HH	TYR	356	-0.418	6.742	35.856	1.00	0.00	0.424	0.00	0.00
ATOM	4105	C	TYR	356	-5.696	5.447	40.033	1.00	0.00	0.396	9.82	4.00
ATOM	4106	O	TYR	356	-4.605	5.459	40.598	1.00	0.00	-0.396	8.17	-17.40
ATOM	4107	N	ASP	357P	-6.645	6.343	40.293	1.00	0.00	-0.650	9.00	-17.40
ATOM	4108	HN	ASP	357P	-7.550	6.277	39.805	1.00	0.00	0.440	0.00	0.00
ATOM	4109	CA	ASP	357P	-6.425	7.424	41.262	1.00	0.00	0.158	9.40	4.00
ATOM	4110	HA	ASP	357P	-5.506	7.942	40.988	1.00	0.00	0.053	0.00	0.00
ATOM	4111	CB	ASP	357P	-7.538	8.476	41.144	1.00	0.00	-0.336	12.77	4.00
ATOM	4112	HB1	ASP	357P	-7.500	9.215	41.944	1.00	0.00	0.053	0.00	0.00
ATOM	4113	HB2	ASP	357P	-8.534	8.036	41.182	1.00	0.00	0.053	0.00	0.00
ATOM	4114	CG	ASP	357P	-7.467	9.258	39.837	1.00	0.00	0.297	9.82	4.00
ATOM	4115	OD1	ASP	357P	-6.645	8.900	38.962	1.00	0.00	-0.534	8.17	-18.95
ATOM	4116	OD2	ASP	357P	-8.236	10.235	39.677	1.00	0.00	-0.534	8.17	-18.95
ATOM	4117	C	ASP	357P	-6.279	6.969	42.717	1.00	0.00	0.396	9.82	4.00
ATOM	4118	O	ASP	357P	-5.941	7.762	43.595	1.00	0.00	-0.396	8.17	-17.40
ATOM	4119	N	ARG	358G	-6.540	5.699	42.983	1.00	0.00	-0.650	9.00	-17.40
ATOM	4120	HN	ARG	358G	-6.860	5.073	42.230	1.00	0.00	0.440	0.00	0.00
ATOM	4121	CA	ARG	358G	-6.377	5.182	44.330	1.00	0.00	0.158	9.40	4.00
ATOM	4122	HA	ARG	358G	-6.354	6.044	44.996	1.00	0.00	0.053	0.00	0.00
ATOM	4123	CB	ARG	358G	-7.543	4.248	44.686	1.00	0.00	-0.106	12.77	4.00
ATOM	4124	HB1	ARG	358G	-7.564	3.433	43.962	1.00	0.00	0.053	0.00	0.00
ATOM	4125	HB2	ARG	358G	-8.468	4.821	44.643	1.00	0.00	0.053	0.00	0.00
ATOM	4126	CG	ARG	358G	-7.441	3.637	46.068	1.00	0.00	-0.106	12.77	4.00
ATOM	4127	HG1	ARG	358G	-8.371	3.749	46.624	1.00	0.00	0.053	0.00	0.00
ATOM	4128	HG2	ARG	358G	-6.652	4.107	46.655	1.00	0.00	0.053	0.00	0.00
ATOM	4129	CD	ARG	358G	-7.129	2.145	45.998	1.00	0.00	0.374	12.77	4.00
ATOM	4130	HD1	ARG	358G	-6.592	1.775	46.872	1.00	0.00	0.053	0.00	0.00
ATOM	4131	HD2	ARG	358G	-6.510	1.873	45.142	1.00	0.00	0.053	0.00	0.00
ATOM	4132	NE	ARG	358G	-8.326	1.307	45.893	1.00	0.00	-0.819	9.00	-24.67
ATOM	4133	HE	ARG	358G	-9.241	1.778	45.885	1.00	0.00	0.407	0.00	0.00
ATOM	4134	CZ	ARG	358G	-8.312	-0.024	45.807	1.00	0.00	0.796	6.95	4.00
ATOM	4135	NH1	ARG	358G	-7.159	-0.688	45.802	1.00	0.00	-0.746	9.00	-24.67
ATOM	4136	HH1	ARG	358G	-7.156	-1.715	45.735	1.00	0.00	0.407	0.00	0.00
ATOM	4137	HH1	ARG	358G	-6.268	-0.174	45.864	1.00	0.00	0.407	0.00	0.00
ATOM	4138	NH2	ARG	358G	-9.455	-0.699	45.751	1.00	0.00	-0.746	9.00	-24.67
ATOM	4139	HH2	ARG	358G	-9.443	-1.726	45.684	1.00	0.00	0.407	0.00	0.00
ATOM	4140	HH2	ARG	358G	-10.352	-0.194	45.774	1.00	0.00	0.407	0.00	0.00
ATOM	4141	C	ARG	358G	-5.061	4.409	44.348	1.00	0.00	0.396	9.82	4.00
ATOM	4142	O	ARG	358G	-4.143	4.715	45.126	1.00	0.00	-0.396	8.17	-17.40
ATOM	4143	N	ASP	359P	-4.963	3.431	43.447	1.00	0.00	-0.650	9.00	-17.40
ATOM	4144	HN	ASP	359P	-5.744	3.278	42.793	1.00	0.00	0.440	0.00	0.00
ATOM	4145	CA	ASP	359P	-3.793	2.572	43.353	1.00	0.00	0.158	9.40	4.00
ATOM	4146	HA	ASP	359P	-3.585	2.179	44.348	1.00	0.00	0.053	0.00	0.00
ATOM	4147	CB	ASP	359P	-4.130	1.367	42.478	1.00	0.00	-0.336	12.77	4.00
ATOM	4148	HB1	ASP	359P	-3.271	0.713	42.323	1.00	0.00	0.053	0.00	0.00
ATOM	4149	HB2	ASP	359P	-4.478	1.658	41.487	1.00	0.00	0.053	0.00	0.00
ATOM	4150	CG	ASP	359P	-5.225	0.502	43.081	1.00	0.00	0.297	9.82	4.00
ATOM	4151	OD1	ASP	359P	-5.704	0.839	44.189	1.00	0.00	-0.534	8.17	-18.95
ATOM	4152	OD2	ASP	359P	-5.603	-0.517	42.454	1.00	0.00	-0.534	8.17	-18.95
ATOM	4153	C	ASP	359P	-2.505	3.239	42.856	1.00	0.00	0.396	9.82	4.00
ATOM	4154	O	ASP	359P	-1.500	3.234	43.563	1.00	0.00	-0.396	8.17	-17.40
ATOM	4155	N	PHE	360	-2.528	3.823	41.660	1.00	0.00	-0.650	9.00	-17.40
ATOM	4156	HN	PHE	360	-3.398	3.838	41.110	1.00	0.00	0.440	0.00	0.00
ATOM	4157	CA	PHE	360	-1.318	4.441	41.130	1.00	0.00	0.158	9.40	4.00
ATOM	4158	HA	PHE	360	-0.497	3.735	40.998	1.00	0.00	0.053	0.00	0.00
ATOM	4159	CB	PHE	360	-1.537	5.003	39.726	1.00	0.00	-0.106	12.77	4.00
ATOM	4160	HB1	PHE	360	-2.168	5.891	39.717	1.00	0.00	0.053	0.00	0.00
ATOM	4161	HB2	PHE	360	-2.016	4.292	39.053	1.00	0.00	0.053	0.00	0.00
ATOM	4162	CG	PHE	360	-0.253	5.407	39.047	1.00	0.00	0.000	7.26	0.60
ATOM	4163	CD1	PHE	360	0.640	4.437	38.596	1.00	0.00	-0.127	10.80	0.60
ATOM	4164	HD1	PHE	360	0.376	3.382	38.680	1.00	0.00	0.127	0.00	0.00
ATOM	4165	CD2	PHE	360	0.093	6.748	38.928	1.00	0.00	-0.127	10.80	0.60
ATOM	4166	HD2	PHE	360	-0.601	7.512	39.275	1.00	0.00	0.127	0.00	0.00
ATOM	4167	CE1	PHE	360	1.870	4.797	38.037	1.00	0.00	-0.127	10.80	0.60
ATOM	4168	HE1	PHE	360	2.561	4.029	37.690	1.00	0.00	0.127	0.00	0.00
ATOM	4169	CE2	PHE	360	1.318	7.134	38.370	1.00	0.00	-0.127	10.80	0.60
ATOM	4170	HE2	PHE	360	1.570	8.190	38.285	1.00	0.00	0.127	0.00	0.00
ATOM	4171	CZ	PHE	360	2.211	6.167	37.925	1.00	0.00	-0.127	10.80	0.60
ATOM	4172	HZ	PHE	360	3.167	6.460	37.492	1.00	0.00	0.127	0.00	0.00
ATOM	4173	C	PHE	360	-0.766	5.546	42.026	1.00	0.00	0.396	9.82	4.00
ATOM	4174	O	PHE	360	0.426	5.587	42.289	1.00	0.00	-0.396	8.17	-17.40
ATOM	4175	N	LEU	361	-1.630	6.444	42.484	1.00	0.00	-0.650	9.00	-17.40

ATOM	4176	HN	LEU	361	-2.619	6.369	42.207	1.00	0.00	0.440	0.00	0.00
ATOM	4177	CA	LEU	361	-1.221	7.542	43.373	1.00	0.00	0.158	9.40	4.00
ATOM	4178	HA	LEU	361	-0.443	8.156	42.920	1.00	0.00	0.053	0.00	0.00
ATOM	4179	CB	LEU	361	-2.413	8.473	43.653	1.00	0.00	-0.106	12.77	4.00
ATOM	4180	HB1	LEU	361	-2.186	9.032	44.560	1.00	0.00	0.053	0.00	0.00
ATOM	4181	HB2	LEU	361	-3.295	7.846	43.783	1.00	0.00	0.053	0.00	0.00
ATOM	4182	CG	LEU	361	-2.768	9.507	42.582	1.00	0.00	-0.053	9.40	4.00
ATOM	4183	HG	LEU	361	-3.651	10.052	42.915	1.00	0.00	0.053	0.00	0.00
ATOM	4184	CD1	LEU	361	-1.579	10.451	42.419	1.00	0.00	-0.159	16.15	4.00
ATOM	4185	HD1	LEU	361	-1.809	11.198	41.659	1.00	0.00	0.053	0.00	0.00
ATOM	4186	HD1	LEU	361	-1.376	10.948	43.367	1.00	0.00	0.053	0.00	0.00
ATOM	4187	HD1	LEU	361	-0.701	9.881	42.113	1.00	0.00	0.053	0.00	0.00
ATOM	4188	CD2	LEU	361	-3.087	8.829	41.257	1.00	0.00	-0.159	16.15	4.00
ATOM	4189	HD2	LEU	361	-3.336	9.584	40.512	1.00	0.00	0.053	0.00	0.00
ATOM	4190	HD2	LEU	361	-2.219	8.260	40.921	1.00	0.00	0.053	0.00	0.00
ATOM	4191	HD2	LEU	361	-3.933	8.155	41.387	1.00	0.00	0.053	0.00	0.00
ATOM	4192	C	LEU	361	-0.670	7.018	44.698	1.00	0.00	0.396	9.82	4.00
ATOM	4193	O	LEU	361	0.283	7.569	45.256	1.00	0.00	-0.396	8.17	-17.40
ATOM	4194	N	ALA	362	-1.268	5.952	45.209	1.00	0.00	-0.650	9.00	-17.40
ATOM	4195	HN	ALA	362	-2.073	5.532	44.722	1.00	0.00	0.440	0.00	0.00
ATOM	4196	CA	ALA	362	-0.790	5.368	46.461	1.00	0.00	0.158	9.40	4.00
ATOM	4197	HA	ALA	362	-0.770	6.170	47.198	1.00	0.00	0.053	0.00	0.00
ATOM	4198	CB	ALA	362	-1.741	4.251	46.938	1.00	0.00	-0.159	16.15	4.00
ATOM	4199	HB1	ALA	362	-1.367	3.829	47.871	1.00	0.00	0.053	0.00	0.00
ATOM	4200	HB2	ALA	362	-2.736	4.664	47.099	1.00	0.00	0.053	0.00	0.00
ATOM	4201	HB3	ALA	362	-1.791	3.468	46.181	1.00	0.00	0.053	0.00	0.00
ATOM	4202	C	ALA	362	0.607	4.811	46.188	1.00	0.00	0.396	9.82	4.00
ATOM	4203	O	ALA	362	1.522	4.960	46.991	1.00	0.00	-0.396	8.17	-17.40
ATOM	4204	N	ARG	363G	0.765	4.201	45.020	1.00	0.00	-0.650	9.00	-17.40
ATOM	4205	HN	ARG	363G	-0.043	4.123	44.386	1.00	0.00	0.440	0.00	0.00
ATOM	4206	CA	ARG	363G	2.042	3.637	44.603	1.00	0.00	0.158	9.40	4.00
ATOM	4207	HA	ARG	363G	2.344	2.847	45.291	1.00	0.00	0.053	0.00	0.00
ATOM	4208	CB	ARG	363G	1.894	3.044	43.195	1.00	0.00	-0.106	12.77	4.00
ATOM	4209	HB1	ARG	363G	1.839	3.804	42.416	1.00	0.00	0.053	0.00	0.00
ATOM	4210	HB2	ARG	363G	0.994	2.438	43.080	1.00	0.00	0.053	0.00	0.00
ATOM	4211	CG	ARG	363G	3.037	2.151	42.812	1.00	0.00	-0.106	12.77	4.00
ATOM	4212	HG1	ARG	363G	2.901	1.126	43.157	1.00	0.00	0.053	0.00	0.00
ATOM	4213	HG2	ARG	363G	3.987	2.488	43.225	1.00	0.00	0.053	0.00	0.00
ATOM	4214	CD	ARG	363G	3.235	2.068	41.298	1.00	0.00	0.374	12.77	4.00
ATOM	4215	HD1	ARG	363G	3.480	3.058	40.915	1.00	0.00	0.053	0.00	0.00
ATOM	4216	HD2	ARG	363G	2.314	1.711	40.836	1.00	0.00	0.053	0.00	0.00
ATOM	4217	NE	ARG	363G	4.324	1.142	41.009	1.00	0.00	-0.819	9.00	-24.67
ATOM	4218	HE	ARG	363G	5.238	1.543	40.759	1.00	0.00	0.407	0.00	0.00
ATOM	4219	CZ	ARG	363G	4.221	-0.187	41.045	1.00	0.00	0.796	6.95	4.00
ATOM	4220	NH1	ARG	363G	3.066	-0.764	41.347	1.00	0.00	-0.746	9.00	-24.67
ATOM	4221	HH1	ARG	363G	2.994	-1.791	41.372	1.00	0.00	0.407	0.00	0.00
ATOM	4222	HH1	ARG	363G	2.240	-0.185	41.556	1.00	0.00	0.407	0.00	0.00
ATOM	4223	NH2	ARG	363G	5.287	-0.939	40.800	1.00	0.00	-0.746	9.00	-24.67
ATOM	4224	HH2	ARG	363G	5.210	-1.965	40.827	1.00	0.00	0.407	0.00	0.00
ATOM	4225	HH2	ARG	363G	6.191	-0.495	40.582	1.00	0.00	0.407	0.00	0.00
ATOM	4226	C	ARG	363G	3.126	4.733	44.594	1.00	0.00	0.396	9.82	4.00
ATOM	4227	O	ARG	363G	4.204	4.574	45.169	1.00	0.00	-0.396	8.17	-17.40
ATOM	4228	N	VAL	364	2.801	5.853	43.956	1.00	0.00	-0.650	9.00	-17.40
ATOM	4229	HN	VAL	364	1.864	5.915	43.531	1.00	0.00	0.440	0.00	0.00
ATOM	4230	CA	VAL	364	3.698	7.004	43.822	1.00	0.00	0.158	9.40	4.00
ATOM	4231	HA	VAL	364	4.650	6.756	43.352	1.00	0.00	0.053	0.00	0.00
ATOM	4232	CB	VAL	364	3.061	8.072	42.898	1.00	0.00	-0.053	9.40	4.00
ATOM	4233	HB	VAL	364	2.041	8.301	43.206	1.00	0.00	0.053	0.00	0.00
ATOM	4234	CG1	VAL	364	3.873	9.396	42.928	1.00	0.00	-0.159	16.15	4.00
ATOM	4235	HG1	VAL	364	3.402	10.126	42.270	1.00	0.00	0.053	0.00	0.00
ATOM	4236	HG1	VAL	364	3.895	9.785	43.945	1.00	0.00	0.053	0.00	0.00
ATOM	4237	HG1	VAL	364	4.891	9.206	42.589	1.00	0.00	0.053	0.00	0.00
ATOM	4238	CG2	VAL	364	2.974	7.533	41.510	1.00	0.00	-0.159	16.15	4.00
ATOM	4239	HG2	VAL	364	2.526	8.281	40.856	1.00	0.00	0.053	0.00	0.00
ATOM	4240	HG2	VAL	364	3.973	7.289	41.151	1.00	0.00	0.053	0.00	0.00
ATOM	4241	HG2	VAL	364	2.358	6.633	41.507	1.00	0.00	0.053	0.00	0.00
ATOM	4242	C	VAL	364	4.061	7.646	45.159	1.00	0.00	0.396	9.82	4.00
ATOM	4243	O	VAL	364	5.244	7.876	45.446	1.00	0.00	-0.396	8.17	-17.40
ATOM	4244	N	TYR	365	3.056	7.951	45.974	1.00	0.00	-0.650	9.00	-17.40
ATOM	4245	HN	TYR	365	2.083	7.746	45.702	1.00	0.00	0.440	0.00	0.00
ATOM	4246	CA	TYR	365	3.346	8.575	47.250	1.00	0.00	0.158	9.40	4.00
ATOM	4247	HA	TYR	365	4.178	9.265	47.112	1.00	0.00	0.053	0.00	0.00
ATOM	4248	CB	TYR	365	2.184	9.481	47.669	1.00	0.00	-0.106	12.77	4.00
ATOM	4249	HB1	TYR	365	2.301	9.814	48.700	1.00	0.00	0.053	0.00	0.00
ATOM	4250	HB2	TYR	365	1.232	8.955	47.592	1.00	0.00	0.053	0.00	0.00
ATOM	4251	CG	TYR	365	2.110	10.710	46.787	1.00	0.00	0.000	7.26	0.60

ATOM	4252	CD1	TYR	365	1.295	10.743	45.653	1.00	0.00	-0.127	10.80	0.60
ATOM	4253	HD1	TYR	365	0.638	9.899	45.440	1.00	0.00	0.127	0.00	0.00
ATOM	4254	CE1	TYR	365	1.308	11.841	44.785	1.00	0.00	-0.127	10.80	0.60
ATOM	4255	HE1	TYR	365	0.665	11.855	43.904	1.00	0.00	0.127	0.00	0.00
ATOM	4256	CD2	TYR	365	2.933	11.802	47.035	1.00	0.00	-0.127	10.80	0.60
ATOM	4257	HD2	TYR	365	3.571	11.799	47.918	1.00	0.00	0.127	0.00	0.00
ATOM	4258	CE2	TYR	365	2.960	12.902	46.177	1.00	0.00	-0.127	10.80	0.60
ATOM	4259	HE2	TYR	365	3.616	13.745	46.389	1.00	0.00	0.127	0.00	0.00
ATOM	4260	CZ	TYR	365	2.153	12.917	45.060	1.00	0.00	0.026	7.26	0.60
ATOM	4261	OH	TYR	365	2.218	14.004	44.214	1.00	0.00	-0.451	10.94	-17.40
ATOM	4262	HH	TYR	365	2.999	14.612	44.496	1.00	0.00	0.424	0.00	0.00
ATOM	4263	C	TYR	365	3.733	7.599	48.349	1.00	0.00	0.396	9.82	4.00
ATOM	4264	O	TYR	365	4.034	8.009	49.478	1.00	0.00	-0.396	8.17	-17.40
ATOM	4265	N	GLY	366	3.737	6.316	48.010	1.00	0.00	-0.650	9.00	-17.40
ATOM	4266	HN	GLY	366	3.439	6.044	47.062	1.00	0.00	0.440	0.00	0.00
ATOM	4267	CA	GLY	366	4.152	5.286	48.947	1.00	0.00	0.105	9.40	4.00
ATOM	4268	HA1	GLY	366	3.534	4.405	48.772	1.00	0.00	0.053	0.00	0.00
ATOM	4269	HA2	GLY	366	4.004	5.671	49.955	1.00	0.00	0.053	0.00	0.00
ATOM	4270	C	GLY	366	5.627	4.981	48.687	1.00	0.00	0.396	9.82	4.00
ATOM	4271	O	GLY	366	6.329	4.425	49.532	1.00	0.00	-0.396	8.17	-17.40
ATOM	4272	N	ALA	367	6.102	5.364	47.504	1.00	0.00	-0.650	9.00	-17.40
ATOM	4273	HN	ALA	367	5.471	5.831	46.837	1.00	0.00	0.440	0.00	0.00
ATOM	4274	CA	ALA	367	7.491	5.139	47.129	1.00	0.00	0.158	9.40	4.00
ATOM	4275	HA	ALA	367	7.787	4.111	47.340	1.00	0.00	0.053	0.00	0.00
ATOM	4276	CB	ALA	367	7.671	5.366	45.622	1.00	0.00	-0.159	16.15	4.00
ATOM	4277	HB1	ALA	367	8.712	5.195	45.350	1.00	0.00	0.053	0.00	0.00
ATOM	4278	HB2	ALA	367	7.034	4.673	45.071	1.00	0.00	0.053	0.00	0.00
ATOM	4279	HB3	ALA	367	7.393	6.390	45.372	1.00	0.00	0.053	0.00	0.00
ATOM	4280	C	ALA	367	8.417	6.067	47.903	1.00	0.00	0.396	9.82	4.00
ATOM	4281	O	ALA	367	8.072	7.219	48.187	1.00	0.00	-0.396	8.17	-17.40
ATOM	4282	N	PRO	368	9.620	5.586	48.239	1.00	0.00	-0.422	9.00	-17.40
ATOM	4283	CD	PRO	368	10.241	4.281	47.948	1.00	0.00	0.105	12.77	4.00
ATOM	4284	HD1	PRO	368	10.031	3.959	46.927	1.00	0.00	0.053	0.00	0.00
ATOM	4285	HD2	PRO	368	9.869	3.505	48.618	1.00	0.00	0.053	0.00	0.00
ATOM	4286	CA	PRO	368	10.541	6.441	48.976	1.00	0.00	0.158	9.40	4.00
ATOM	4287	HA	PRO	368	10.086	6.838	49.883	1.00	0.00	0.053	0.00	0.00
ATOM	4288	CB	PRO	368	11.682	5.488	49.320	1.00	0.00	-0.106	12.77	4.00
ATOM	4289	HB1	PRO	368	11.484	4.959	50.252	1.00	0.00	0.053	0.00	0.00
ATOM	4290	HB2	PRO	368	12.622	6.026	49.436	1.00	0.00	0.053	0.00	0.00
ATOM	4291	CG	PRO	368	11.710	4.578	48.169	1.00	0.00	-0.106	12.77	4.00
ATOM	4292	HG1	PRO	368	12.281	3.677	48.392	1.00	0.00	0.053	0.00	0.00
ATOM	4293	HG2	PRO	368	12.167	5.053	47.301	1.00	0.00	0.053	0.00	0.00
ATOM	4294	C	PRO	368	10.994	7.635	48.144	1.00	0.00	0.396	9.82	4.00
ATOM	4295	O	PRO	368	11.062	7.574	46.917	1.00	0.00	-0.396	8.17	-17.40
ATOM	4296	N	GLN	369	11.305	8.724	48.832	1.00	0.00	-0.650	9.00	-17.40
ATOM	4297	HN	GLN	369	11.218	8.703	49.858	1.00	0.00	0.440	0.00	0.00
ATOM	4298	CA	GLN	369	11.764	9.949	48.193	1.00	0.00	0.158	9.40	4.00
ATOM	4299	HA	GLN	369	11.325	9.998	47.196	1.00	0.00	0.053	0.00	0.00
ATOM	4300	CB	GLN	369	11.330	11.140	49.035	1.00	0.00	-0.106	12.77	4.00
ATOM	4301	HB1	GLN	369	12.043	11.259	49.850	1.00	0.00	0.053	0.00	0.00
ATOM	4302	HB2	GLN	369	10.332	10.937	49.424	1.00	0.00	0.053	0.00	0.00
ATOM	4303	CG	GLN	369	11.271	12.448	48.284	1.00	0.00	-0.106	12.77	4.00
ATOM	4304	HG1	GLN	369	10.707	12.363	47.355	1.00	0.00	0.053	0.00	0.00
ATOM	4305	HG2	GLN	369	12.262	12.812	48.016	1.00	0.00	0.053	0.00	0.00
ATOM	4306	CD	GLN	369	10.607	13.547	49.099	1.00	0.00	0.396	9.82	4.00
ATOM	4307	OE1	GLN	369	9.521	13.351	49.669	1.00	0.00	-0.396	8.17	-17.40
ATOM	4308	NE2	GLN	369	11.247	14.712	49.153	1.00	0.00	-0.879	13.25	-17.40
ATOM	4309	HE2	GLN	369	12.146	14.828	48.664	1.00	0.00	0.440	0.00	0.00
ATOM	4310	HE2	GLN	369	10.843	15.497	49.683	1.00	0.00	0.440	0.00	0.00
ATOM	4311	C	GLN	369	13.289	9.903	48.110	1.00	0.00	0.396	9.82	4.00
ATOM	4312	O	GLN	369	13.945	9.482	49.057	1.00	0.00	-0.396	8.17	-17.40
ATOM	4313	N	LEU	370	13.854	10.314	46.980	1.00	0.00	-0.650	9.00	-17.40
ATOM	4314	HN	LEU	370	13.261	10.636	46.202	1.00	0.00	0.440	0.00	0.00
ATOM	4315	CA	LEU	370	15.305	10.313	46.829	1.00	0.00	0.158	9.40	4.00
ATOM	4316	HA	LEU	370	15.775	10.181	47.803	1.00	0.00	0.053	0.00	0.00
ATOM	4317	CB	LEU	370	15.756	9.136	45.936	1.00	0.00	-0.106	12.77	4.00
ATOM	4318	HB1	LEU	370	15.453	9.366	44.914	1.00	0.00	0.053	0.00	0.00
ATOM	4319	HB2	LEU	370	15.261	8.237	46.305	1.00	0.00	0.053	0.00	0.00
ATOM	4320	CG	LEU	370	17.256	8.814	45.882	1.00	0.00	-0.053	9.40	4.00
ATOM	4321	HG	LEU	370	17.788	9.691	45.515	1.00	0.00	0.053	0.00	0.00
ATOM	4322	CD1	LEU	370	17.733	8.456	47.296	1.00	0.00	-0.159	16.15	4.00
ATOM	4323	HD1	LEU	370	18.797	8.224	47.273	1.00	0.00	0.053	0.00	0.00
ATOM	4324	HD1	LEU	370	17.559	9.300	47.963	1.00	0.00	0.053	0.00	0.00
ATOM	4325	HD1	LEU	370	17.180	7.588	47.657	1.00	0.00	0.053	0.00	0.00
ATOM	4326	CD2	LEU	370	17.544	7.661	44.918	1.00	0.00	-0.159	16.15	4.00
ATOM	4327	HD2	LEU	370	18.614	7.458	44.903	1.00	0.00	0.053	0.00	0.00

ATOM	4328	HD2	LEU	370	17.010	6.769	45.247	1.00	0.00	0.053	0.00	0.00
ATOM	4329	HD2	LEU	370	17.212	7.933	43.916	1.00	0.00	0.053	0.00	0.00
ATOM	4330	C	LEU	370	15.761	11.643	46.223	1.00	0.00	0.396	9.82	4.00
ATOM	4331	O	LEU	370	15.113	12.183	45.317	1.00	0.00	-0.396	8.17	-17.40
ATOM	4332	N	GLN	371	16.867	12.177	46.739	1.00	0.00	-0.650	9.00	-17.40
ATOM	4333	HN	GLN	371	17.348	11.688	47.507	1.00	0.00	0.440	0.00	0.00
ATOM	4334	CA	GLN	371	17.415	13.437	46.243	1.00	0.00	0.158	9.40	4.00
ATOM	4335	HA	GLN	371	16.683	14.227	46.410	1.00	0.00	0.053	0.00	0.00
ATOM	4336	CB	GLN	371	18.704	13.769	46.990	1.00	0.00	-0.106	12.77	4.00
ATOM	4337	HB1	GLN	371	19.321	14.515	46.490	1.00	0.00	0.053	0.00	0.00
ATOM	4338	HB2	GLN	371	19.362	12.911	47.133	1.00	0.00	0.053	0.00	0.00
ATOM	4339	CG	GLN	371	18.479	14.319	48.375	1.00	0.00	-0.106	12.77	4.00
ATOM	4340	HG1	GLN	371	17.507	14.038	48.782	1.00	0.00	0.053	0.00	0.00
ATOM	4341	HG2	GLN	371	18.519	15.407	48.402	1.00	0.00	0.053	0.00	0.00
ATOM	4342	CD	GLN	371	19.514	13.830	49.368	1.00	0.00	0.396	9.82	4.00
ATOM	4343	OE1	GLN	371	20.712	13.784	49.065	1.00	0.00	-0.396	8.17	-17.40
ATOM	4344	NE2	GLN	371	19.059	13.468	50.569	1.00	0.00	-0.879	13.25	-17.40
ATOM	4345	HE2	GLN	371	18.051	13.523	50.776	1.00	0.00	0.440	0.00	0.00
ATOM	4346	HE2	GLN	371	19.715	13.133	51.289	1.00	0.00	0.440	0.00	0.00
ATOM	4347	C	GLN	371	17.702	13.294	44.759	1.00	0.00	0.396	9.82	4.00
ATOM	4348	O	GLN	371	18.278	12.299	44.337	1.00	0.00	-0.396	8.17	-17.40
ATOM	4349	N	VAL	372	17.313	14.285	43.964	1.00	0.00	-0.650	9.00	-17.40
ATOM	4350	HN	VAL	372	16.847	15.112	44.363	1.00	0.00	0.440	0.00	0.00
ATOM	4351	CA	VAL	372	17.544	14.203	42.524	1.00	0.00	0.158	9.40	4.00
ATOM	4352	HA	VAL	372	16.905	13.471	42.028	1.00	0.00	0.053	0.00	0.00
ATOM	4353	CB	VAL	372	17.170	15.545	41.825	1.00	0.00	-0.053	9.40	4.00
ATOM	4354	HB	VAL	372	16.146	15.831	42.065	1.00	0.00	0.053	0.00	0.00
ATOM	4355	CG1	VAL	372	18.098	16.665	42.280	1.00	0.00	-0.159	16.15	4.00
ATOM	4356	HG1	VAL	372	17.820	17.593	41.780	1.00	0.00	0.053	0.00	0.00
ATOM	4357	HG1	VAL	372	18.011	16.793	43.359	1.00	0.00	0.053	0.00	0.00
ATOM	4358	HG1	VAL	372	19.127	16.410	42.026	1.00	0.00	0.053	0.00	0.00
ATOM	4359	CG2	VAL	372	17.207	15.373	40.308	1.00	0.00	-0.159	16.15	4.00
ATOM	4360	HG2	VAL	372	16.944	16.315	39.828	1.00	0.00	0.053	0.00	0.00
ATOM	4361	HG2	VAL	372	18.209	15.076	40.000	1.00	0.00	0.053	0.00	0.00
ATOM	4362	HG2	VAL	372	16.493	14.604	40.011	1.00	0.00	0.053	0.00	0.00
ATOM	4363	C	VAL	372	18.987	13.803	42.164	1.00	0.00	0.396	9.82	4.00
ATOM	4364	O	VAL	372	19.217	12.958	41.291	1.00	0.00	-0.396	8.17	-17.40
ATOM	4365	N	GLU	373	19.954	14.385	42.862	1.00	0.00	-0.650	9.00	-17.40
ATOM	4366	HN	GLU	373	19.702	15.055	43.602	1.00	0.00	0.440	0.00	0.00
ATOM	4367	CA	GLU	373	21.363	14.103	42.612	1.00	0.00	0.158	9.40	4.00
ATOM	4368	HA	GLU	373	21.651	14.351	41.590	1.00	0.00	0.053	0.00	0.00
ATOM	4369	CB	GLU	373	22.221	14.977	43.536	1.00	0.00	-0.106	12.77	4.00
ATOM	4370	HB1	GLU	373	22.078	14.624	44.557	1.00	0.00	0.053	0.00	0.00
ATOM	4371	HB2	GLU	373	21.885	16.008	43.428	1.00	0.00	0.053	0.00	0.00
ATOM	4372	CG	GLU	373	23.717	14.965	43.265	1.00	0.00	-0.106	12.77	4.00
ATOM	4373	HG1	GLU	373	24.156	13.969	43.331	1.00	0.00	0.053	0.00	0.00
ATOM	4374	HG2	GLU	373	24.283	15.582	43.962	1.00	0.00	0.053	0.00	0.00
ATOM	4375	CD	GLU	373	24.078	15.479	41.878	1.00	0.00	0.399	9.82	4.00
ATOM	4376	OE1	GLU	373	23.253	16.206	41.271	1.00	0.00	-0.396	8.17	-18.95
ATOM	4377	OE2	GLU	373	25.195	15.162	41.403	1.00	0.00	-0.427	8.17	-18.95
ATOM	4378	HE2	GLU	373	25.305	15.586	40.471	1.00	0.00	0.424	0.00	0.00
ATOM	4379	C	GLU	373	21.694	12.621	42.823	1.00	0.00	0.396	9.82	4.00
ATOM	4380	O	GLU	373	22.504	12.052	42.102	1.00	0.00	-0.396	8.17	-17.40
ATOM	4381	N	LYS	374S	21.075	12.003	43.827	1.00	0.00	-0.650	9.00	-17.40
ATOM	4382	HN	LYS	374S	20.417	12.524	44.424	1.00	0.00	0.440	0.00	0.00
ATOM	4383	CA	LYS	374S	21.325	10.599	44.081	1.00	0.00	0.158	9.40	4.00
ATOM	4384	HA	LYS	374S	22.393	10.406	44.178	1.00	0.00	0.053	0.00	0.00
ATOM	4385	CB	LYS	374S	20.704	10.195	45.419	1.00	0.00	-0.106	12.77	4.00
ATOM	4386	HB1	LYS	374S	20.708	9.118	45.587	1.00	0.00	0.053	0.00	0.00
ATOM	4387	HB2	LYS	374S	19.662	10.500	45.519	1.00	0.00	0.053	0.00	0.00
ATOM	4388	CG	LYS	374S	21.423	10.798	46.623	1.00	0.00	-0.106	12.77	4.00
ATOM	4389	HG1	LYS	374S	21.406	11.886	46.576	1.00	0.00	0.053	0.00	0.00
ATOM	4390	HG2	LYS	374S	22.463	10.474	46.652	1.00	0.00	0.053	0.00	0.00
ATOM	4391	CD	LYS	374S	20.758	10.370	47.913	1.00	0.00	-0.106	12.77	4.00
ATOM	4392	HD1	LYS	374S	20.735	9.284	48.011	1.00	0.00	0.053	0.00	0.00
ATOM	4393	HD2	LYS	374S	19.727	10.721	47.969	1.00	0.00	0.053	0.00	0.00
ATOM	4394	CE	LYS	374S	21.486	10.916	49.123	1.00	0.00	0.099	12.77	4.00
ATOM	4395	HE1	LYS	374S	21.540	12.003	49.075	1.00	0.00	0.053	0.00	0.00
ATOM	4396	HE2	LYS	374S	22.500	10.520	49.166	1.00	0.00	0.053	0.00	0.00
ATOM	4397	NZ	LYS	374S	20.767	10.528	50.387	1.00	0.00	-0.045	13.25	-39.20
ATOM	4398	HZ1	LYS	374S	21.273	10.906	51.200	1.00	0.00	0.280	0.00	0.00
ATOM	4399	HZ2	LYS	374S	19.810	10.910	50.370	1.00	0.00	0.280	0.00	0.00
ATOM	4400	HZ3	LYS	374S	20.724	9.501	50.456	1.00	0.00	0.280	0.00	0.00
ATOM	4401	C	LYS	374S	20.789	9.734	42.937	1.00	0.00	0.396	9.82	4.00
ATOM	4402	O	LYS	374S	21.387	8.701	42.586	1.00	0.00	-0.396	8.17	-17.40
ATOM	4403	N	VAL	375	19.680	10.162	42.336	1.00	0.00	-0.650	9.00	-17.40

ATOM	4404	HN	VAL	375	19.236	11.034	42.658	1.00	0.00	0.440	0.00	0.00
ATOM	4405	CA	VAL	375	19.078	9.420	41.229	1.00	0.00	0.158	9.40	4.00
ATOM	4406	HA	VAL	375	18.978	8.371	41.509	1.00	0.00	0.053	0.00	0.00
ATOM	4407	CB	VAL	375	17.671	9.982	40.848	1.00	0.00	-0.053	9.40	4.00
ATOM	4408	HB	VAL	375	17.743	11.046	40.626	1.00	0.00	0.053	0.00	0.00
ATOM	4409	CG1	VAL	375	17.136	9.255	39.621	1.00	0.00	-0.159	16.15	4.00
ATOM	4410	HG1	VAL	375	16.154	9.652	39.361	1.00	0.00	0.053	0.00	0.00
ATOM	4411	HG1	VAL	375	17.819	9.401	38.784	1.00	0.00	0.053	0.00	0.00
ATOM	4412	HG1	VAL	375	17.050	8.190	39.837	1.00	0.00	0.053	0.00	0.00
ATOM	4413	CG2	VAL	375	16.702	9.842	42.006	1.00	0.00	-0.159	16.15	4.00
ATOM	4414	HG2	VAL	375	15.729	10.240	41.716	1.00	0.00	0.053	0.00	0.00
ATOM	4415	HG2	VAL	375	16.599	8.789	42.269	1.00	0.00	0.053	0.00	0.00
ATOM	4416	HG2	VAL	375	17.079	10.395	42.865	1.00	0.00	0.053	0.00	0.00
ATOM	4417	C	VAL	375	19.973	9.538	39.995	1.00	0.00	0.396	9.82	4.00
ATOM	4418	O	VAL	375	20.294	8.547	39.345	1.00	0.00	-0.396	8.17	-17.40
ATOM	4419	N	ARG	376G	20.355	10.775	39.685	1.00	0.00	-0.650	9.00	-17.40
ATOM	4420	HN	ARG	376G	20.045	11.548	40.290	1.00	0.00	0.440	0.00	0.00
ATOM	4421	CA	ARG	376G	21.188	11.089	38.534	1.00	0.00	0.158	9.40	4.00
ATOM	4422	HA	ARG	376G	20.688	10.895	37.584	1.00	0.00	0.053	0.00	0.00
ATOM	4423	CB	ARG	376G	21.509	12.597	38.512	1.00	0.00	-0.106	12.77	4.00
ATOM	4424	HB1	ARG	376G	22.408	12.848	39.073	1.00	0.00	0.053	0.00	0.00
ATOM	4425	HB2	ARG	376G	20.713	13.207	38.938	1.00	0.00	0.053	0.00	0.00
ATOM	4426	CG	ARG	376G	21.736	13.138	37.100	1.00	0.00	-0.106	12.77	4.00
ATOM	4427	HG1	ARG	376G	20.785	13.512	36.720	1.00	0.00	0.053	0.00	0.00
ATOM	4428	HG2	ARG	376G	22.104	12.323	36.477	1.00	0.00	0.053	0.00	0.00
ATOM	4429	CD	ARG	376G	22.754	14.285	37.017	1.00	0.00	0.374	12.77	4.00
ATOM	4430	HD1	ARG	376G	23.105	14.355	35.987	1.00	0.00	0.053	0.00	0.00
ATOM	4431	HD2	ARG	376G	23.580	14.057	37.690	1.00	0.00	0.053	0.00	0.00
ATOM	4432	NE	ARG	376G	22.223	15.593	37.394	1.00	0.00	-0.819	9.00	-24.67
ATOM	4433	HE	ARG	376G	21.336	15.624	37.918	1.00	0.00	0.407	0.00	0.00
ATOM	4434	CZ	ARG	376G	22.821	16.749	37.098	1.00	0.00	0.796	6.95	4.00
ATOM	4435	NH1	ARG	376G	23.963	16.750	36.420	1.00	0.00	-0.746	9.00	-24.67
ATOM	4436	HH1	ARG	376G	24.425	17.641	36.191	1.00	0.00	0.407	0.00	0.00
ATOM	4437	HH1	ARG	376G	24.386	15.859	36.123	1.00	0.00	0.407	0.00	0.00
ATOM	4438	NH2	ARG	376G	22.290	17.906	37.484	1.00	0.00	-0.746	9.00	-24.67
ATOM	4439	HH2	ARG	376G	22.760	18.792	37.250	1.00	0.00	0.407	0.00	0.00
ATOM	4440	HH2	ARG	376G	21.408	17.915	38.017	1.00	0.00	0.407	0.00	0.00
ATOM	4441	C	ARG	376G	22.487	10.275	38.499	1.00	0.00	0.396	9.82	4.00
ATOM	4442	O	ARG	376G	22.866	9.747	37.452	1.00	0.00	-0.396	8.17	-17.40
ATOM	4443	N	THR	377	23.157	10.149	39.641	1.00	0.00	-0.650	9.00	-17.40
ATOM	4444	HN	THR	377	22.783	10.577	40.500	1.00	0.00	0.440	0.00	0.00
ATOM	4445	CA	THR	377	24.417	9.410	39.691	1.00	0.00	0.158	9.40	4.00
ATOM	4446	HA	THR	377	24.970	9.443	38.752	1.00	0.00	0.053	0.00	0.00
ATOM	4447	CB	THR	377	25.356	9.986	40.736	1.00	0.00	0.060	9.40	4.00
ATOM	4448	HB	THR	377	26.311	9.462	40.707	1.00	0.00	0.053	0.00	0.00
ATOM	4449	OG1	THR	377	24.775	9.815	42.034	1.00	0.00	-0.537	11.04	-17.40
ATOM	4450	HG1	THR	377	24.519	10.735	42.420	1.00	0.00	0.424	0.00	0.00
ATOM	4451	CG2	THR	377	25.593	11.462	40.464	1.00	0.00	-0.159	16.15	4.00
ATOM	4452	HG2	THR	377	26.267	11.867	41.218	1.00	0.00	0.053	0.00	0.00
ATOM	4453	HG2	THR	377	26.038	11.583	39.476	1.00	0.00	0.053	0.00	0.00
ATOM	4454	HG2	THR	377	24.643	11.996	40.502	1.00	0.00	0.053	0.00	0.00
ATOM	4455	C	THR	377	24.232	7.942	40.002	1.00	0.00	0.396	9.82	4.00
ATOM	4456	O	THR	377	25.204	7.211	40.168	1.00	0.00	-0.396	8.17	-17.40
ATOM	4457	N	ASN	378	22.983	7.511	40.103	1.00	0.00	-0.650	9.00	-17.40
ATOM	4458	HN	ASN	378	22.206	8.178	39.990	1.00	0.00	0.440	0.00	0.00
ATOM	4459	CA	ASN	378	22.691	6.110	40.370	1.00	0.00	0.158	9.40	4.00
ATOM	4460	HA	ASN	378	21.627	5.875	40.318	1.00	0.00	0.053	0.00	0.00
ATOM	4461	CB	ASN	378	23.343	5.243	39.283	1.00	0.00	-0.106	12.77	4.00
ATOM	4462	HB1	ASN	378	24.249	4.744	39.625	1.00	0.00	0.053	0.00	0.00
ATOM	4463	HB2	ASN	378	23.633	5.815	38.401	1.00	0.00	0.053	0.00	0.00
ATOM	4464	CG	ASN	378	22.428	4.140	38.779	1.00	0.00	0.396	9.82	4.00
ATOM	4465	OD1	ASN	378	21.252	4.068	39.145	1.00	0.00	-0.396	8.17	-17.40
ATOM	4466	ND2	ASN	378	22.966	3.276	37.924	1.00	0.00	-0.879	13.25	-17.40
ATOM	4467	HD2	ASN	378	23.952	3.373	37.645	1.00	0.00	0.440	0.00	0.00
ATOM	4468	HD2	ASN	378	22.396	2.508	37.540	1.00	0.00	0.440	0.00	0.00
ATOM	4469	C	ASN	378	23.144	5.653	41.763	1.00	0.00	0.396	9.82	4.00
ATOM	4470	O	ASN	378	23.641	4.534	41.931	1.00	0.00	-0.396	8.17	-17.40
ATOM	4471	N	ASP	379P	22.984	6.513	42.764	1.00	0.00	-0.650	9.00	-17.40
ATOM	4472	HN	ASP	379P	22.605	7.453	42.579	1.00	0.00	0.440	0.00	0.00
ATOM	4473	CA	ASP	379P	23.344	6.126	44.123	1.00	0.00	0.158	9.40	4.00
ATOM	4474	HA	ASP	379P	24.197	5.453	44.034	1.00	0.00	0.053	0.00	0.00
ATOM	4475	CB	ASP	379P	23.711	7.358	44.956	1.00	0.00	-0.336	12.77	4.00
ATOM	4476	HB1	ASP	379P	22.846	7.987	45.167	1.00	0.00	0.053	0.00	0.00
ATOM	4477	HB2	ASP	379P	24.441	7.994	44.455	1.00	0.00	0.053	0.00	0.00
ATOM	4478	CG	ASP	379P	24.316	6.986	46.307	1.00	0.00	0.297	9.82	4.00
ATOM	4479	OD1	ASP	379P	24.511	5.780	46.570	1.00	0.00	-0.534	8.17	-18.95

ATOM	4480	OD2	ASP	379P	24.604	7.900	47.104	1.00	0.00	-0.534	8.17	-18.95
ATOM	4481	C	ASP	379P	22.109	5.431	44.716	1.00	0.00	0.396	9.82	4.00
ATOM	4482	O	ASP	379P	20.999	5.566	44.177	1.00	0.00	-0.396	8.17	-17.40
ATOM	4483	N	ARG	380G	22.295	4.666	45.794	1.00	0.00	-0.650	9.00	-17.40
ATOM	4484	HN	ARG	380G	23.243	4.558	46.180	1.00	0.00	0.440	0.00	0.00
ATOM	4485	CA	ARG	380G	21.180	3.980	46.434	1.00	0.00	0.158	9.40	4.00
ATOM	4486	HA	ARG	380G	21.492	3.310	47.235	1.00	0.00	0.053	0.00	0.00
ATOM	4487	CB	ARG	380G	20.257	5.009	47.088	1.00	0.00	-0.106	12.77	4.00
ATOM	4488	HB1	ARG	380G	19.383	4.484	47.475	1.00	0.00	0.053	0.00	0.00
ATOM	4489	HB2	ARG	380G	19.966	5.735	46.329	1.00	0.00	0.053	0.00	0.00
ATOM	4490	CG	ARG	380G	20.880	5.783	48.250	1.00	0.00	-0.106	12.77	4.00
ATOM	4491	HG1	ARG	380G	20.249	6.613	48.569	1.00	0.00	0.053	0.00	0.00
ATOM	4492	HG2	ARG	380G	21.849	6.203	47.984	1.00	0.00	0.053	0.00	0.00
ATOM	4493	CD	ARG	380G	21.099	4.896	49.470	1.00	0.00	0.374	12.77	4.00
ATOM	4494	HD1	ARG	380G	21.609	5.419	50.278	1.00	0.00	0.053	0.00	0.00
ATOM	4495	HD2	ARG	380G	21.704	4.018	49.242	1.00	0.00	0.053	0.00	0.00
ATOM	4496	NE	ARG	380G	19.842	4.397	50.030	1.00	0.00	-0.819	9.00	-24.67
ATOM	4497	HE	ARG	380G	19.657	3.385	49.976	1.00	0.00	0.407	0.00	0.00
ATOM	4498	CZ	ARG	380G	18.921	5.169	50.605	1.00	0.00	0.796	6.95	4.00
ATOM	4499	NH1	ARG	380G	19.120	6.478	50.698	1.00	0.00	-0.746	9.00	-24.67
ATOM	4500	HH1	ARG	380G	18.409	7.076	51.142	1.00	0.00	0.407	0.00	0.00
ATOM	4501	HH1	ARG	380G	19.985	6.895	50.326	1.00	0.00	0.407	0.00	0.00
ATOM	4502	NH2	ARG	380G	17.796	4.638	51.075	1.00	0.00	-0.746	9.00	-24.67
ATOM	4503	HH2	ARG	380G	17.088	5.240	51.518	1.00	0.00	0.407	0.00	0.00
ATOM	4504	HH2	ARG	380G	17.632	3.624	50.995	1.00	0.00	0.407	0.00	0.00
ATOM	4505	C	ARG	380G	20.369	3.110	45.463	1.00	0.00	0.396	9.82	4.00
ATOM	4506	O	ARG	380G	19.137	3.164	45.440	1.00	0.00	-0.396	8.17	-17.40
ATOM	4507	N	LYS	381S	21.051	2.283	44.683	1.00	0.00	-0.650	9.00	-17.40
ATOM	4508	HN	LYS	381S	22.076	2.232	44.761	1.00	0.00	0.440	0.00	0.00
ATOM	4509	CA	LYS	381S	20.356	1.448	43.718	1.00	0.00	0.158	9.40	4.00
ATOM	4510	HA	LYS	381S	19.782	2.101	43.061	1.00	0.00	0.053	0.00	0.00
ATOM	4511	CB	LYS	381S	21.379	0.760	42.814	1.00	0.00	-0.106	12.77	4.00
ATOM	4512	HB1	LYS	381S	20.912	0.032	42.150	1.00	0.00	0.053	0.00	0.00
ATOM	4513	HB2	LYS	381S	22.135	0.225	43.387	1.00	0.00	0.053	0.00	0.00
ATOM	4514	CG	LYS	381S	22.113	1.749	41.934	1.00	0.00	-0.106	12.77	4.00
ATOM	4515	HG1	LYS	381S	22.364	2.673	42.453	1.00	0.00	0.053	0.00	0.00
ATOM	4516	HG2	LYS	381S	21.536	2.046	41.058	1.00	0.00	0.053	0.00	0.00
ATOM	4517	CD	LYS	381S	23.431	1.202	41.398	1.00	0.00	-0.106	12.77	4.00
ATOM	4518	HD1	LYS	381S	24.080	0.829	42.190	1.00	0.00	0.053	0.00	0.00
ATOM	4519	HD2	LYS	381S	24.006	1.955	40.859	1.00	0.00	0.053	0.00	0.00
ATOM	4520	CE	LYS	381S	23.231	0.053	40.437	1.00	0.00	0.099	12.77	4.00
ATOM	4521	HE1	LYS	381S	22.556	0.352	39.635	1.00	0.00	0.053	0.00	0.00
ATOM	4522	HE2	LYS	381S	22.801	-0.800	40.962	1.00	0.00	0.053	0.00	0.00
ATOM	4523	NZ	LYS	381S	24.545	-0.351	39.843	1.00	0.00	-0.045	13.25	-39.20
ATOM	4524	HZ1	LYS	381S	24.400	-1.134	39.189	1.00	0.00	0.280	0.00	0.00
ATOM	4525	HZ2	LYS	381S	24.953	0.447	39.336	1.00	0.00	0.280	0.00	0.00
ATOM	4526	HZ3	LYS	381S	25.186	-0.644	40.594	1.00	0.00	0.280	0.00	0.00
ATOM	4527	C	LYS	381S	19.380	0.428	44.299	1.00	0.00	0.396	9.82	4.00
ATOM	4528	O	LYS	381S	18.582	-0.145	43.561	1.00	0.00	-0.396	8.17	-17.40
ATOM	4529	N	GLU	382	19.410	0.201	45.611	1.00	0.00	-0.650	9.00	-17.40
ATOM	4530	HN	GLU	382	20.078	0.700	46.215	1.00	0.00	0.440	0.00	0.00
ATOM	4531	CA	GLU	382	18.480	-0.766	46.175	1.00	0.00	0.158	9.40	4.00
ATOM	4532	HA	GLU	382	18.545	-1.698	45.615	1.00	0.00	0.053	0.00	0.00
ATOM	4533	CB	GLU	382	18.808	-1.102	47.643	1.00	0.00	-0.106	12.77	4.00
ATOM	4534	HB1	GLU	382	19.859	-1.381	47.702	1.00	0.00	0.053	0.00	0.00
ATOM	4535	HB2	GLU	382	18.171	-1.930	47.953	1.00	0.00	0.053	0.00	0.00
ATOM	4536	CG	GLU	382	18.582	0.039	48.617	1.00	0.00	-0.106	12.77	4.00
ATOM	4537	HG1	GLU	382	18.378	-0.312	49.628	1.00	0.00	0.053	0.00	0.00
ATOM	4538	HG2	GLU	382	17.736	0.666	48.333	1.00	0.00	0.053	0.00	0.00
ATOM	4539	CD	GLU	382	19.775	0.953	48.717	1.00	0.00	0.399	9.82	4.00
ATOM	4540	OE1	GLU	382	20.592	0.968	47.761	1.00	0.00	-0.396	8.17	-18.95
ATOM	4541	OE2	GLU	382	19.891	1.659	49.746	1.00	0.00	-0.427	8.17	-18.95
ATOM	4542	HE2	GLU	382	20.742	2.233	49.674	1.00	0.00	0.424	0.00	0.00
ATOM	4543	C	GLU	382	17.064	-0.215	46.085	1.00	0.00	0.396	9.82	4.00
ATOM	4544	O	GLU	382	16.102	-0.948	46.309	1.00	0.00	-0.396	8.17	-17.40
ATOM	4545	N	LEU	383	16.936	1.075	45.767	1.00	0.00	-0.650	9.00	-17.40
ATOM	4546	HN	LEU	383	17.780	1.641	45.603	1.00	0.00	0.440	0.00	0.00
ATOM	4547	CA	LEU	383	15.617	1.699	45.647	1.00	0.00	0.158	9.40	4.00
ATOM	4548	HA	LEU	383	14.934	1.110	46.260	1.00	0.00	0.053	0.00	0.00
ATOM	4549	CB	LEU	383	15.648	3.152	46.164	1.00	0.00	-0.106	12.77	4.00
ATOM	4550	HB1	LEU	383	14.634	3.551	46.116	1.00	0.00	0.053	0.00	0.00
ATOM	4551	HB2	LEU	383	16.319	3.725	45.525	1.00	0.00	0.053	0.00	0.00
ATOM	4552	CG	LEU	383	16.137	3.312	47.605	1.00	0.00	-0.053	9.40	4.00
ATOM	4553	HG	LEU	383	17.118	2.858	47.740	1.00	0.00	0.053	0.00	0.00
ATOM	4554	CD1	LEU	383	16.250	4.789	47.990	1.00	0.00	-0.159	16.15	4.00
ATOM	4555	HD1	LEU	383	16.599	4.871	49.019	1.00	0.00	0.053	0.00	0.00

ATOM	4556	HD1	LEU	383	16.957	5.285	47.325	1.00	0.00	0.053	0.00	0.00
ATOM	4557	HD1	LEU	383	15.273	5.264	47.899	1.00	0.00	0.053	0.00	0.00
ATOM	4558	CD2	LEU	383	15.169	2.568	48.541	1.00	0.00	-0.159	16.15	4.00
ATOM	4559	HD2	LEU	383	15.506	2.674	49.572	1.00	0.00	0.053	0.00	0.00
ATOM	4560	HD2	LEU	383	14.169	2.990	48.441	1.00	0.00	0.053	0.00	0.00
ATOM	4561	HD2	LEU	383	15.144	1.511	48.274	1.00	0.00	0.053	0.00	0.00
ATOM	4562	C	LEU	383	15.242	1.654	44.167	1.00	0.00	0.396	9.82	4.00
ATOM	4563	O	LEU	383	15.532	2.589	43.413	1.00	0.00	-0.396	8.17	-17.40
ATOM	4564	N	GLY	384	14.632	0.538	43.764	1.00	0.00	-0.650	9.00	-17.40
ATOM	4565	HN	GLY	384	14.446	-0.205	44.452	1.00	0.00	0.440	0.00	0.00
ATOM	4566	CA	GLY	384	14.221	0.339	42.385	1.00	0.00	0.105	9.40	4.00
ATOM	4567	HA1	GLY	384	13.898	-0.696	42.276	1.00	0.00	0.053	0.00	0.00
ATOM	4568	HA2	GLY	384	15.077	0.548	41.745	1.00	0.00	0.053	0.00	0.00
ATOM	4569	C	GLY	384	13.075	1.221	41.907	1.00	0.00	0.396	9.82	4.00
ATOM	4570	O	GLY	384	12.772	1.247	40.705	1.00	0.00	-0.396	8.17	-17.40
ATOM	4571	N	GLU	385	12.435	1.941	42.826	1.00	0.00	-0.650	9.00	-17.40
ATOM	4572	HN	GLU	385	12.725	1.873	43.812	1.00	0.00	0.440	0.00	0.00
ATOM	4573	CA	GLU	385	11.319	2.834	42.462	1.00	0.00	0.158	9.40	4.00
ATOM	4574	HA	GLU	385	11.482	3.193	41.446	1.00	0.00	0.053	0.00	0.00
ATOM	4575	CB	GLU	385	9.974	2.085	42.498	1.00	0.00	-0.106	12.77	4.00
ATOM	4576	HB1	GLU	385	9.813	1.716	43.511	1.00	0.00	0.053	0.00	0.00
ATOM	4577	HB2	GLU	385	10.024	1.255	41.792	1.00	0.00	0.053	0.00	0.00
ATOM	4578	CG	GLU	385	8.762	2.949	42.118	1.00	0.00	-0.106	12.77	4.00
ATOM	4579	HG1	GLU	385	8.969	3.631	41.294	1.00	0.00	0.053	0.00	0.00
ATOM	4580	HG2	GLU	385	8.411	3.573	42.940	1.00	0.00	0.053	0.00	0.00
ATOM	4581	CD	GLU	385	7.551	2.118	41.678	1.00	0.00	0.399	9.82	4.00
ATOM	4582	OE1	GLU	385	7.681	0.883	41.577	1.00	0.00	-0.396	8.17	-18.95
ATOM	4583	OE2	GLU	385	6.470	2.692	41.432	1.00	0.00	-0.427	8.17	-18.95
ATOM	4584	HE2	GLU	385	5.766	1.994	41.152	1.00	0.00	0.424	0.00	0.00
ATOM	4585	C	GLU	385	11.296	3.995	43.439	1.00	0.00	0.396	9.82	4.00
ATOM	4586	O	GLU	385	11.085	3.814	44.646	1.00	0.00	-0.396	8.17	-17.40
ATOM	4587	N	VAL	386	11.519	5.195	42.924	1.00	0.00	-0.650	9.00	-17.40
ATOM	4588	HN	VAL	386	11.675	5.304	41.912	1.00	0.00	0.440	0.00	0.00
ATOM	4589	CA	VAL	386	11.541	6.355	43.797	1.00	0.00	0.158	9.40	4.00
ATOM	4590	HA	VAL	386	11.158	6.051	44.771	1.00	0.00	0.053	0.00	0.00
ATOM	4591	CB	VAL	386	12.957	6.868	43.990	1.00	0.00	-0.053	9.40	4.00
ATOM	4592	HB	VAL	386	12.960	7.705	44.688	1.00	0.00	0.053	0.00	0.00
ATOM	4593	CG1	VAL	386	13.844	5.761	44.546	1.00	0.00	-0.159	16.15	4.00
ATOM	4594	HG1	VAL	386	14.857	6.139	44.680	1.00	0.00	0.053	0.00	0.00
ATOM	4595	HG1	VAL	386	13.450	5.427	45.506	1.00	0.00	0.053	0.00	0.00
ATOM	4596	HG1	VAL	386	13.859	4.922	43.849	1.00	0.00	0.053	0.00	0.00
ATOM	4597	CG2	VAL	386	13.500	7.407	42.657	1.00	0.00	-0.159	16.15	4.00
ATOM	4598	HG2	VAL	386	14.516	7.774	42.800	1.00	0.00	0.053	0.00	0.00
ATOM	4599	HG2	VAL	386	13.503	6.607	41.916	1.00	0.00	0.053	0.00	0.00
ATOM	4600	HG2	VAL	386	12.865	8.221	42.308	1.00	0.00	0.053	0.00	0.00
ATOM	4601	C	VAL	386	10.712	7.523	43.335	1.00	0.00	0.396	9.82	4.00
ATOM	4602	O	VAL	386	10.185	7.552	42.216	1.00	0.00	-0.396	8.17	-17.40
ATOM	4603	N	ARG	387G	10.623	8.501	44.220	1.00	0.00	-0.650	9.00	-17.40
ATOM	4604	HN	ARG	387G	11.084	8.380	45.133	1.00	0.00	0.440	0.00	0.00
ATOM	4605	CA	ARG	387G	9.910	9.728	43.967	1.00	0.00	0.158	9.40	4.00
ATOM	4606	HA	ARG	387G	9.530	9.648	42.948	1.00	0.00	0.053	0.00	0.00
ATOM	4607	CB	ARG	387G	8.792	9.896	45.003	1.00	0.00	-0.106	12.77	4.00
ATOM	4608	HB1	ARG	387G	9.258	10.049	45.976	1.00	0.00	0.053	0.00	0.00
ATOM	4609	HB2	ARG	387G	8.191	8.986	44.996	1.00	0.00	0.053	0.00	0.00
ATOM	4610	CG	ARG	387G	7.845	11.053	44.780	1.00	0.00	-0.106	12.77	4.00
ATOM	4611	HG1	ARG	387G	7.681	11.201	43.712	1.00	0.00	0.053	0.00	0.00
ATOM	4612	HG2	ARG	387G	8.264	11.965	45.203	1.00	0.00	0.053	0.00	0.00
ATOM	4613	CD	ARG	387G	6.492	10.765	45.457	1.00	0.00	0.374	12.77	4.00
ATOM	4614	HD1	ARG	387G	5.863	10.113	44.850	1.00	0.00	0.053	0.00	0.00
ATOM	4615	HD2	ARG	387G	5.923	11.677	45.634	1.00	0.00	0.053	0.00	0.00
ATOM	4616	NE	ARG	387G	6.659	10.107	46.756	1.00	0.00	-0.819	9.00	-24.67
ATOM	4617	HE	ARG	387G	6.577	9.080	46.787	1.00	0.00	0.407	0.00	0.00
ATOM	4618	CZ	ARG	387G	6.909	10.743	47.899	1.00	0.00	0.796	6.95	4.00
ATOM	4619	NH1	ARG	387G	7.014	12.061	47.913	1.00	0.00	-0.746	9.00	-24.67
ATOM	4620	HH1	ARG	387G	7.207	12.552	48.797	1.00	0.00	0.407	0.00	0.00
ATOM	4621	HH1	ARG	387G	6.902	12.595	47.039	1.00	0.00	0.407	0.00	0.00
ATOM	4622	NH2	ARG	387G	7.069	10.058	49.025	1.00	0.00	-0.746	9.00	-24.67
ATOM	4623	HH2	ARG	387G	7.262	10.554	49.906	1.00	0.00	0.407	0.00	0.00
ATOM	4624	HH2	ARG	387G	6.999	9.030	49.017	1.00	0.00	0.407	0.00	0.00
ATOM	4625	C	ARG	387G	10.927	10.841	44.129	1.00	0.00	0.396	9.82	4.00
ATOM	4626	O	ARG	387G	11.649	10.876	45.116	1.00	0.00	-0.396	8.17	-17.40
ATOM	4627	N	VAL	388	11.032	11.701	43.122	1.00	0.00	-0.650	9.00	-17.40
ATOM	4628	HN	VAL	388	10.474	11.537	42.271	1.00	0.00	0.440	0.00	0.00
ATOM	4629	CA	VAL	388	11.907	12.870	43.173	1.00	0.00	0.158	9.40	4.00
ATOM	4630	HA	VAL	388	12.586	12.838	44.024	1.00	0.00	0.053	0.00	0.00
ATOM	4631	CB	VAL	388	12.732	13.053	41.879	1.00	0.00	-0.053	9.40	4.00

ATOM	4632	HB	VAL	388	12.084	12.966	41.006	1.00	0.00	0.053	0.00	0.00
ATOM	4633	CG1	VAL	388	13.403	14.450	41.868	1.00	0.00	-0.159	16.15	4.00
ATOM	4634	HG1	VAL	388	13.981	14.568	40.952	1.00	0.00	0.053	0.00	0.00
ATOM	4635	HG1	VAL	388	12.635	15.222	41.914	1.00	0.00	0.053	0.00	0.00
ATOM	4636	HG1	VAL	388	14.064	14.542	42.729	1.00	0.00	0.053	0.00	0.00
ATOM	4637	CG2	VAL	388	13.812	11.975	41.801	1.00	0.00	-0.159	16.15	4.00
ATOM	4638	HG2	VAL	388	14.392	12.106	40.887	1.00	0.00	0.053	0.00	0.00
ATOM	4639	HG2	VAL	388	14.471	12.057	42.664	1.00	0.00	0.053	0.00	0.00
ATOM	4640	HG2	VAL	388	13.343	10.990	41.795	1.00	0.00	0.053	0.00	0.00
ATOM	4641	C	VAL	388	10.842	13.954	43.284	1.00	0.00	0.396	9.82	4.00
ATOM	4642	O	VAL	388	10.032	14.146	42.366	1.00	0.00	-0.396	8.17	-17.40
ATOM	4643	N	GLN	389	10.811	14.636	44.422	1.00	0.00	-0.650	9.00	-17.40
ATOM	4644	HN	GLN	389	11.512	14.448	45.152	1.00	0.00	0.440	0.00	0.00
ATOM	4645	CA	GLN	389	9.782	15.654	44.642	1.00	0.00	0.158	9.40	4.00
ATOM	4646	HA	GLN	389	8.863	15.467	44.086	1.00	0.00	0.053	0.00	0.00
ATOM	4647	CB	GLN	389	9.365	15.639	46.117	1.00	0.00	-0.106	12.77	4.00
ATOM	4648	HB1	GLN	389	10.264	15.746	46.724	1.00	0.00	0.053	0.00	0.00
ATOM	4649	HB2	GLN	389	8.872	14.688	46.319	1.00	0.00	0.053	0.00	0.00
ATOM	4650	CG	GLN	389	8.399	16.751	46.531	1.00	0.00	-0.106	12.77	4.00
ATOM	4651	HG1	GLN	389	7.521	16.798	45.886	1.00	0.00	0.053	0.00	0.00
ATOM	4652	HG2	GLN	389	8.862	17.736	46.494	1.00	0.00	0.053	0.00	0.00
ATOM	4653	CD	GLN	389	7.879	16.568	47.960	1.00	0.00	0.396	9.82	4.00
ATOM	4654	OE1	GLN	389	7.020	15.722	48.217	1.00	0.00	-0.396	8.17	-17.40
ATOM	4655	NE2	GLN	389	8.410	17.356	48.894	1.00	0.00	-0.879	13.25	-17.40
ATOM	4656	HE2	GLN	389	9.125	18.050	48.636	1.00	0.00	0.440	0.00	0.00
ATOM	4657	HE2	GLN	389	8.104	17.270	49.874	1.00	0.00	0.440	0.00	0.00
ATOM	4658	C	GLN	389	10.218	17.047	44.237	1.00	0.00	0.396	9.82	4.00
ATOM	4659	O	GLN	389	11.326	17.470	44.561	1.00	0.00	-0.396	8.17	-17.40
ATOM	4660	N	TYR	390	9.360	17.745	43.493	1.00	0.00	-0.650	9.00	-17.40
ATOM	4661	HN	TYR	390	8.474	17.307	43.200	1.00	0.00	0.440	0.00	0.00
ATOM	4662	CA	TYR	390	9.650	19.118	43.084	1.00	0.00	0.158	9.40	4.00
ATOM	4663	HA	TYR	390	10.666	19.302	43.431	1.00	0.00	0.053	0.00	0.00
ATOM	4664	CB	TYR	390	9.560	19.282	41.555	1.00	0.00	-0.106	12.77	4.00
ATOM	4665	HB1	TYR	390	10.225	18.549	41.098	1.00	0.00	0.053	0.00	0.00
ATOM	4666	HB2	TYR	390	9.869	20.297	41.306	1.00	0.00	0.053	0.00	0.00
ATOM	4667	CG	TYR	390	8.179	19.072	40.953	1.00	0.00	0.000	7.26	0.60
ATOM	4668	CD1	TYR	390	7.216	20.104	40.964	1.00	0.00	-0.127	10.80	0.60
ATOM	4669	HD1	TYR	390	7.449	21.045	41.461	1.00	0.00	0.127	0.00	0.00
ATOM	4670	CE1	TYR	390	5.970	19.946	40.352	1.00	0.00	-0.127	10.80	0.60
ATOM	4671	HE1	TYR	390	5.241	20.756	40.369	1.00	0.00	0.127	0.00	0.00
ATOM	4672	CD2	TYR	390	7.852	17.872	40.324	1.00	0.00	-0.127	10.80	0.60
ATOM	4673	HD2	TYR	390	8.576	17.058	40.312	1.00	0.00	0.127	0.00	0.00
ATOM	4674	CE2	TYR	390	6.599	17.694	39.703	1.00	0.00	-0.127	10.80	0.60
ATOM	4675	HE2	TYR	390	6.358	16.749	39.215	1.00	0.00	0.127	0.00	0.00
ATOM	4676	CZ	TYR	390	5.668	18.734	39.716	1.00	0.00	0.026	7.26	0.60
ATOM	4677	OH	TYR	390	4.460	18.569	39.061	1.00	0.00	-0.451	10.94	-17.40
ATOM	4678	HH	TYR	390	4.044	19.491	38.869	1.00	0.00	0.424	0.00	0.00
ATOM	4679	C	TYR	390	8.595	19.966	43.792	1.00	0.00	0.396	9.82	4.00
ATOM	4680	O	TYR	390	7.483	19.495	44.058	1.00	0.00	-0.396	8.17	-17.40
ATOM	4681	N	THR	391	8.932	21.203	44.116	1.00	0.00	-0.650	9.00	-17.40
ATOM	4682	HN	THR	391	9.862	21.569	43.870	1.00	0.00	0.440	0.00	0.00
ATOM	4683	CA	THR	391	7.976	22.041	44.822	1.00	0.00	0.158	9.40	4.00
ATOM	4684	HA	THR	391	7.068	21.460	44.986	1.00	0.00	0.053	0.00	0.00
ATOM	4685	CB	THR	391	8.522	22.430	46.210	1.00	0.00	0.060	9.40	4.00
ATOM	4686	HB	THR	391	7.878	23.179	46.670	1.00	0.00	0.053	0.00	0.00
ATOM	4687	OG1	THR	391	9.841	22.964	46.061	1.00	0.00	-0.537	11.04	-17.40
ATOM	4688	HG1	THR	391	10.520	22.332	46.508	1.00	0.00	0.424	0.00	0.00
ATOM	4689	CG2	THR	391	8.575	21.211	47.112	1.00	0.00	-0.159	16.15	4.00
ATOM	4690	HG2	THR	391	8.962	21.498	48.089	1.00	0.00	0.053	0.00	0.00
ATOM	4691	HG2	THR	391	7.572	20.798	47.225	1.00	0.00	0.053	0.00	0.00
ATOM	4692	HG2	THR	391	9.228	20.459	46.669	1.00	0.00	0.053	0.00	0.00
ATOM	4693	C	THR	391	7.586	23.304	44.082	1.00	0.00	0.396	9.82	4.00
ATOM	4694	O	THR	391	6.542	23.880	44.348	1.00	0.00	-0.396	8.17	-17.40
ATOM	4695	N	GLY	392	8.421	23.752	43.161	1.00	0.00	-0.650	9.00	-17.40
ATOM	4696	HN	GLY	392	9.300	23.253	42.964	1.00	0.00	0.440	0.00	0.00
ATOM	4697	CA	GLY	392	8.078	24.956	42.434	1.00	0.00	0.105	9.40	4.00
ATOM	4698	HA1	GLY	392	8.658	25.800	42.805	1.00	0.00	0.053	0.00	0.00
ATOM	4699	HA2	GLY	392	7.018	25.182	42.554	1.00	0.00	0.053	0.00	0.00
ATOM	4700	C	GLY	392	8.368	24.782	40.968	1.00	0.00	0.396	9.82	4.00
ATOM	4701	O	GLY	392	8.803	23.719	40.542	1.00	0.00	-0.396	8.17	-17.40
ATOM	4702	N	ARG	393G	8.131	25.829	40.196	1.00	0.00	-0.650	9.00	-17.40
ATOM	4703	HN	ARG	393G	7.761	26.692	40.618	1.00	0.00	0.440	0.00	0.00
ATOM	4704	CA	ARG	393G	8.380	25.788	38.764	1.00	0.00	0.158	9.40	4.00
ATOM	4705	HA	ARG	393G	7.863	24.954	38.289	1.00	0.00	0.053	0.00	0.00
ATOM	4706	CB	ARG	393G	7.820	27.057	38.108	1.00	0.00	-0.106	12.77	4.00
ATOM	4707	HB1	ARG	393G	6.731	27.008	38.142	1.00	0.00	0.053	0.00	0.00

ATOM	4708	HB2	ARG	393G	8.170	27.092	37.076	1.00	0.00	0.053	0.00	0.00
ATOM	4709	CG	ARG	393G	8.249	28.363	38.790	1.00	0.00	-0.106	12.77	4.00
ATOM	4710	HG1	ARG	393G	9.310	28.565	38.644	1.00	0.00	0.053	0.00	0.00
ATOM	4711	HG2	ARG	393G	8.073	28.334	39.865	1.00	0.00	0.053	0.00	0.00
ATOM	4712	CD	ARG	393G	7.482	29.569	38.241	1.00	0.00	0.374	12.77	4.00
ATOM	4713	HD1	ARG	393G	7.335	29.524	37.162	1.00	0.00	0.053	0.00	0.00
ATOM	4714	HD2	ARG	393G	7.985	30.516	38.432	1.00	0.00	0.053	0.00	0.00
ATOM	4715	NE	ARG	393G	6.144	29.706	38.819	1.00	0.00	-0.819	9.00	-24.67
ATOM	4716	HE	ARG	393G	5.980	29.319	39.759	1.00	0.00	0.407	0.00	0.00
ATOM	4717	CZ	ARG	393G	5.125	30.302	38.200	1.00	0.00	0.796	6.95	4.00
ATOM	4718	NH1	ARG	393G	5.306	30.805	36.988	1.00	0.00	-0.746	9.00	-24.67
ATOM	4719	HH1	ARG	393G	4.525	31.267	36.500	1.00	0.00	0.407	0.00	0.00
ATOM	4720	HH1	ARG	393G	6.227	30.733	36.533	1.00	0.00	0.407	0.00	0.00
ATOM	4721	NH2	ARG	393G	3.929	30.394	38.782	1.00	0.00	-0.746	9.00	-24.67
ATOM	4722	HH2	ARG	393G	3.151	30.857	38.290	1.00	0.00	0.407	0.00	0.00
ATOM	4723	HH2	ARG	393G	3.782	30.001	39.723	1.00	0.00	0.407	0.00	0.00
ATOM	4724	C	ARG	393G	9.868	25.632	38.454	1.00	0.00	0.396	9.82	4.00
ATOM	4725	O	ARG	393G	10.243	24.902	37.544	1.00	0.00	-0.396	8.17	-17.40
ATOM	4726	N	ASP	394P	10.715	26.312	39.215	1.00	0.00	-0.650	9.00	-17.40
ATOM	4727	HN	ASP	394P	10.349	26.909	39.970	1.00	0.00	0.440	0.00	0.00
ATOM	4728	CA	ASP	394P	12.158	26.228	39.001	1.00	0.00	0.158	9.40	4.00
ATOM	4729	HA	ASP	394P	12.442	26.445	37.971	1.00	0.00	0.053	0.00	0.00
ATOM	4730	CB	ASP	394P	12.883	27.277	39.851	1.00	0.00	-0.336	12.77	4.00
ATOM	4731	HB1	ASP	394P	13.966	27.213	39.755	1.00	0.00	0.053	0.00	0.00
ATOM	4732	HB2	ASP	394P	12.662	27.175	40.913	1.00	0.00	0.053	0.00	0.00
ATOM	4733	CG	ASP	394P	12.503	28.694	39.469	1.00	0.00	0.297	9.82	4.00
ATOM	4734	OD1	ASP	394P	12.436	28.973	38.249	1.00	0.00	-0.534	8.17	-18.95
ATOM	4735	OD2	ASP	394P	12.274	29.526	40.379	1.00	0.00	-0.534	8.17	-18.95
ATOM	4736	C	ASP	394P	12.720	24.838	39.313	1.00	0.00	0.396	9.82	4.00
ATOM	4737	O	ASP	394P	13.574	24.331	38.573	1.00	0.00	-0.396	8.17	-17.40
ATOM	4738	N	SER	395	12.260	24.231	40.409	1.00	0.00	-0.650	9.00	-17.40
ATOM	4739	HN	SER	395	11.569	24.708	41.006	1.00	0.00	0.440	0.00	0.00
ATOM	4740	CA	SER	395	12.727	22.900	40.767	1.00	0.00	0.158	9.40	4.00
ATOM	4741	HA	SER	395	13.816	22.888	40.773	1.00	0.00	0.053	0.00	0.00
ATOM	4742	CB	SER	395	12.289	22.512	42.194	1.00	0.00	0.007	12.77	4.00
ATOM	4743	HB1	SER	395	12.743	23.133	42.965	1.00	0.00	0.053	0.00	0.00
ATOM	4744	HB2	SER	395	12.544	21.485	42.456	1.00	0.00	0.053	0.00	0.00
ATOM	4745	OG	SER	395	10.883	22.619	42.397	1.00	0.00	-0.537	11.04	-17.40
ATOM	4746	HG	SER	395	10.616	23.613	42.440	1.00	0.00	0.424	0.00	0.00
ATOM	4747	C	SER	395	12.208	21.884	39.740	1.00	0.00	0.396	9.82	4.00
ATOM	4748	O	SER	395	12.932	20.954	39.351	1.00	0.00	-0.396	8.17	-17.40
ATOM	4749	N	PHE	396	10.964	22.054	39.290	1.00	0.00	-0.650	9.00	-17.40
ATOM	4750	HN	PHE	396	10.380	22.827	39.640	1.00	0.00	0.440	0.00	0.00
ATOM	4751	CA	PHE	396	10.444	21.123	38.291	1.00	0.00	0.158	9.40	4.00
ATOM	4752	HA	PHE	396	10.405	20.111	38.696	1.00	0.00	0.053	0.00	0.00
ATOM	4753	CB	PHE	396	9.024	21.482	37.830	1.00	0.00	-0.106	12.77	4.00
ATOM	4754	HB1	PHE	396	8.918	22.533	37.564	1.00	0.00	0.053	0.00	0.00
ATOM	4755	HB2	PHE	396	8.270	21.289	38.593	1.00	0.00	0.053	0.00	0.00
ATOM	4756	CG	PHE	396	8.589	20.703	36.614	1.00	0.00	0.000	7.26	0.60
ATOM	4757	CD1	PHE	396	8.242	19.354	36.720	1.00	0.00	-0.127	10.80	0.60
ATOM	4758	HD1	PHE	396	8.192	18.888	37.704	1.00	0.00	0.127	0.00	0.00
ATOM	4759	CD2	PHE	396	8.635	21.282	35.345	1.00	0.00	-0.127	10.80	0.60
ATOM	4760	HD2	PHE	396	8.894	22.335	35.243	1.00	0.00	0.127	0.00	0.00
ATOM	4761	CE1	PHE	396	7.959	18.595	35.588	1.00	0.00	-0.127	10.80	0.60
ATOM	4762	HE1	PHE	396	7.692	17.542	35.688	1.00	0.00	0.127	0.00	0.00
ATOM	4763	CE2	PHE	396	8.354	20.530	34.209	1.00	0.00	-0.127	10.80	0.60
ATOM	4764	HE2	PHE	396	8.397	20.994	33.224	1.00	0.00	0.127	0.00	0.00
ATOM	4765	CZ	PHE	396	8.017	19.181	34.330	1.00	0.00	-0.127	10.80	0.60
ATOM	4766	HZ	PHE	396	7.800	18.589	33.440	1.00	0.00	0.127	0.00	0.00
ATOM	4767	C	PHE	396	11.335	21.114	37.058	1.00	0.00	0.396	9.82	4.00
ATOM	4768	O	PHE	396	11.832	20.067	36.649	1.00	0.00	-0.396	8.17	-17.40
ATOM	4769	N	LYS	397S	11.539	22.278	36.451	1.00	0.00	-0.650	9.00	-17.40
ATOM	4770	HN	LYS	397S	11.119	23.138	36.830	1.00	0.00	0.440	0.00	0.00
ATOM	4771	CA	LYS	397S	12.359	22.333	35.245	1.00	0.00	0.158	9.40	4.00
ATOM	4772	HA	LYS	397S	11.994	21.699	34.437	1.00	0.00	0.053	0.00	0.00
ATOM	4773	CB	LYS	397S	12.317	23.733	34.614	1.00	0.00	-0.106	12.77	4.00
ATOM	4774	HB1	LYS	397S	13.281	24.049	34.216	1.00	0.00	0.053	0.00	0.00
ATOM	4775	HB2	LYS	397S	12.018	24.508	35.319	1.00	0.00	0.053	0.00	0.00
ATOM	4776	CG	LYS	397S	11.326	23.833	33.437	1.00	0.00	-0.106	12.77	4.00
ATOM	4777	HG1	LYS	397S	10.289	23.721	33.756	1.00	0.00	0.053	0.00	0.00
ATOM	4778	HG2	LYS	397S	11.499	23.066	32.682	1.00	0.00	0.053	0.00	0.00
ATOM	4779	CD	LYS	397S	11.413	25.167	32.721	1.00	0.00	-0.106	12.77	4.00
ATOM	4780	HD1	LYS	397S	12.429	25.388	32.395	1.00	0.00	0.053	0.00	0.00
ATOM	4781	HD2	LYS	397S	11.097	25.992	33.359	1.00	0.00	0.053	0.00	0.00
ATOM	4782	CE	LYS	397S	10.528	25.204	31.474	1.00	0.00	0.099	12.77	4.00
ATOM	4783	HE1	LYS	397S	10.468	26.235	31.127	1.00	0.00	0.053	0.00	0.00

ATOM	4784	HE2	LYS	397S	9.539	24.832	31.744	1.00	0.00	0.053	0.00	0.00
ATOM	4785	NZ	LYS	397S	11.032	24.371	30.339	1.00	0.00	-0.045	13.25	-39.20
ATOM	4786	HZ1	LYS	397S	10.384	24.448	29.541	1.00	0.00	0.280	0.00	0.00
ATOM	4787	HZ2	LYS	397S	11.965	24.703	30.056	1.00	0.00	0.280	0.00	0.00
ATOM	4788	HZ3	LYS	397S	11.093	23.386	30.636	1.00	0.00	0.280	0.00	0.00
ATOM	4789	C	LYS	397S	13.803	21.896	35.464	1.00	0.00	0.396	9.82	4.00
ATOM	4790	O	LYS	397S	14.410	21.302	34.577	1.00	0.00	-0.396	8.17	-17.40
ATOM	4791	N	ALA	398	14.355	22.178	36.639	1.00	0.00	-0.650	9.00	-17.40
ATOM	4792	HN	ALA	398	13.810	22.681	37.354	1.00	0.00	0.440	0.00	0.00
ATOM	4793	CA	ALA	398	15.736	21.775	36.921	1.00	0.00	0.158	9.40	4.00
ATOM	4794	HA	ALA	398	16.397	22.102	36.119	1.00	0.00	0.053	0.00	0.00
ATOM	4795	CB	ALA	398	16.221	22.427	38.194	1.00	0.00	-0.159	16.15	4.00
ATOM	4796	HB1	ALA	398	17.247	22.119	38.392	1.00	0.00	0.053	0.00	0.00
ATOM	4797	HB2	ALA	398	16.181	23.510	38.085	1.00	0.00	0.053	0.00	0.00
ATOM	4798	HB3	ALA	398	15.584	22.121	39.024	1.00	0.00	0.053	0.00	0.00
ATOM	4799	C	ALA	398	15.832	20.252	37.041	1.00	0.00	0.396	9.82	4.00
ATOM	4800	O	ALA	398	16.681	19.627	36.412	1.00	0.00	-0.396	8.17	-17.40
ATOM	4801	N	PHE	399	14.954	19.658	37.846	1.00	0.00	-0.650	9.00	-17.40
ATOM	4802	HN	PHE	399	14.258	20.228	38.347	1.00	0.00	0.440	0.00	0.00
ATOM	4803	CA	PHE	399	14.963	18.210	38.029	1.00	0.00	0.158	9.40	4.00
ATOM	4804	HA	PHE	399	15.946	17.870	38.355	1.00	0.00	0.053	0.00	0.00
ATOM	4805	CB	PHE	399	13.982	17.806	39.132	1.00	0.00	-0.106	12.77	4.00
ATOM	4806	HB1	PHE	399	13.999	16.720	39.226	1.00	0.00	0.053	0.00	0.00
ATOM	4807	HB2	PHE	399	12.986	18.149	38.849	1.00	0.00	0.053	0.00	0.00
ATOM	4808	CG	PHE	399	14.305	18.391	40.484	1.00	0.00	0.000	7.26	0.60
ATOM	4809	CD1	PHE	399	13.472	18.153	41.565	1.00	0.00	-0.127	10.80	0.60
ATOM	4810	HD1	PHE	399	12.582	17.538	41.430	1.00	0.00	0.127	0.00	0.00
ATOM	4811	CD2	PHE	399	15.441	19.181	40.673	1.00	0.00	-0.127	10.80	0.60
ATOM	4812	HD2	PHE	399	16.105	19.376	39.831	1.00	0.00	0.127	0.00	0.00
ATOM	4813	CE1	PHE	399	13.754	18.690	42.833	1.00	0.00	-0.127	10.80	0.60
ATOM	4814	HE1	PHE	399	13.089	18.492	43.674	1.00	0.00	0.127	0.00	0.00
ATOM	4815	CE2	PHE	399	15.735	19.720	41.917	1.00	0.00	-0.127	10.80	0.60
ATOM	4816	HE2	PHE	399	16.625	20.334	42.047	1.00	0.00	0.127	0.00	0.00
ATOM	4817	CZ	PHE	399	14.889	19.476	43.005	1.00	0.00	-0.127	10.80	0.60
ATOM	4818	HZ	PHE	399	15.118	19.899	43.982	1.00	0.00	0.127	0.00	0.00
ATOM	4819	C	PHE	399	14.619	17.497	36.714	1.00	0.00	0.396	9.82	4.00
ATOM	4820	O	PHE	399	15.227	16.474	36.387	1.00	0.00	-0.396	8.17	-17.40
ATOM	4821	N	ALA	400	13.656	18.040	35.966	1.00	0.00	-0.650	9.00	-17.40
ATOM	4822	HN	ALA	400	13.181	18.888	36.304	1.00	0.00	0.440	0.00	0.00
ATOM	4823	CA	ALA	400	13.253	17.468	34.680	1.00	0.00	0.158	9.40	4.00
ATOM	4824	HA	ALA	400	12.856	16.464	34.833	1.00	0.00	0.053	0.00	0.00
ATOM	4825	CB	ALA	400	12.158	18.330	34.037	1.00	0.00	-0.159	16.15	4.00
ATOM	4826	HB1	ALA	400	11.866	17.894	33.081	1.00	0.00	0.053	0.00	0.00
ATOM	4827	HB2	ALA	400	11.291	18.369	34.697	1.00	0.00	0.053	0.00	0.00
ATOM	4828	HB3	ALA	400	12.537	19.339	33.875	1.00	0.00	0.053	0.00	0.00
ATOM	4829	C	ALA	400	14.461	17.396	33.748	1.00	0.00	0.396	9.82	4.00
ATOM	4830	O	ALA	400	14.760	16.355	33.164	1.00	0.00	-0.396	8.17	-17.40
ATOM	4831	N	LYS	401S	15.141	18.529	33.616	1.00	0.00	-0.650	9.00	-17.40
ATOM	4832	HN	LYS	401S	14.820	19.359	34.134	1.00	0.00	0.440	0.00	0.00
ATOM	4833	CA	LYS	401S	16.318	18.647	32.772	1.00	0.00	0.158	9.40	4.00
ATOM	4834	HA	LYS	401S	16.078	18.348	31.751	1.00	0.00	0.053	0.00	0.00
ATOM	4835	CB	LYS	401S	16.755	20.121	32.746	1.00	0.00	-0.106	12.77	4.00
ATOM	4836	HB1	LYS	401S	17.064	20.396	33.754	1.00	0.00	0.053	0.00	0.00
ATOM	4837	HB2	LYS	401S	15.902	20.717	32.422	1.00	0.00	0.053	0.00	0.00
ATOM	4838	CG	LYS	401S	17.911	20.454	31.818	1.00	0.00	-0.106	12.77	4.00
ATOM	4839	HG1	LYS	401S	17.794	19.909	30.880	1.00	0.00	0.053	0.00	0.00
ATOM	4840	HG2	LYS	401S	18.851	20.167	32.289	1.00	0.00	0.053	0.00	0.00
ATOM	4841	CD	LYS	401S	17.923	21.958	31.534	1.00	0.00	-0.106	12.77	4.00
ATOM	4842	HD1	LYS	401S	17.695	22.540	32.426	1.00	0.00	0.053	0.00	0.00
ATOM	4843	HD2	LYS	401S	17.188	22.233	30.777	1.00	0.00	0.053	0.00	0.00
ATOM	4844	CE	LYS	401S	19.282	22.428	31.028	1.00	0.00	0.099	12.77	4.00
ATOM	4845	HE1	LYS	401S	19.259	23.480	30.744	1.00	0.00	0.053	0.00	0.00
ATOM	4846	HE2	LYS	401S	19.599	21.860	30.153	1.00	0.00	0.053	0.00	0.00
ATOM	4847	NZ	LYS	401S	20.344	22.268	32.078	1.00	0.00	-0.045	13.25	-39.20
ATOM	4848	HZ1	LYS	401S	21.247	22.593	31.705	1.00	0.00	0.280	0.00	0.00
ATOM	4849	HZ2	LYS	401S	20.094	22.825	32.907	1.00	0.00	0.280	0.00	0.00
ATOM	4850	HZ3	LYS	401S	20.419	21.275	32.342	1.00	0.00	0.280	0.00	0.00
ATOM	4851	C	LYS	401S	17.442	17.743	33.303	1.00	0.00	0.396	9.82	4.00
ATOM	4852	O	LYS	401S	18.121	17.060	32.542	1.00	0.00	-0.396	8.17	-17.40
ATOM	4853	N	ALA	402	17.622	17.711	34.613	1.00	0.00	-0.650	9.00	-17.40
ATOM	4854	HN	ALA	402	17.021	18.277	35.228	1.00	0.00	0.440	0.00	0.00
ATOM	4855	CA	ALA	402	18.665	16.879	35.185	1.00	0.00	0.158	9.40	4.00
ATOM	4856	HA	ALA	402	19.660	17.134	34.822	1.00	0.00	0.053	0.00	0.00
ATOM	4857	CB	ALA	402	18.727	17.098	36.685	1.00	0.00	-0.159	16.15	4.00
ATOM	4858	HB1	ALA	402	19.510	16.472	37.112	1.00	0.00	0.053	0.00	0.00
ATOM	4859	HB2	ALA	402	18.946	18.145	36.891	1.00	0.00	0.053	0.00	0.00

ATOM	4860	HB3	ALA	402	17.768	16.833	37.131	1.00	0.00	0.053	0.00	0.00
ATOM	4861	C	ALA	402	18.480	15.384	34.874	1.00	0.00	0.396	9.82	4.00
ATOM	4862	O	ALA	402	19.461	14.647	34.746	1.00	0.00	-0.396	8.17	-17.40
ATOM	4863	N	LEU	403	17.239	14.933	34.732	1.00	0.00	-0.650	9.00	-17.40
ATOM	4864	HN	LEU	403	16.442	15.581	34.812	1.00	0.00	0.440	0.00	0.00
ATOM	4865	CA	LEU	403	17.003	13.514	34.461	1.00	0.00	0.158	9.40	4.00
ATOM	4866	HA	LEU	403	17.914	12.967	34.703	1.00	0.00	0.053	0.00	0.00
ATOM	4867	CB	LEU	403	15.935	12.977	35.418	1.00	0.00	-0.106	12.77	4.00
ATOM	4868	HB1	LEU	403	15.794	11.898	35.351	1.00	0.00	0.053	0.00	0.00
ATOM	4869	HB2	LEU	403	14.946	13.404	35.250	1.00	0.00	0.053	0.00	0.00
ATOM	4870	CG	LEU	403	16.244	13.250	36.895	1.00	0.00	-0.053	9.40	4.00
ATOM	4871	HG	LEU	403	16.466	14.307	37.040	1.00	0.00	0.053	0.00	0.00
ATOM	4872	CD1	LEU	403	15.056	12.878	37.748	1.00	0.00	-0.159	16.15	4.00
ATOM	4873	HD1	LEU	403	15.284	13.075	38.795	1.00	0.00	0.053	0.00	0.00
ATOM	4874	HD1	LEU	403	14.192	13.470	37.447	1.00	0.00	0.053	0.00	0.00
ATOM	4875	HD1	LEU	403	14.832	11.819	37.618	1.00	0.00	0.053	0.00	0.00
ATOM	4876	CD2	LEU	403	17.486	12.482	37.325	1.00	0.00	-0.159	16.15	4.00
ATOM	4877	HD2	LEU	403	17.693	12.685	38.375	1.00	0.00	0.053	0.00	0.00
ATOM	4878	HD2	LEU	403	17.318	11.413	37.188	1.00	0.00	0.053	0.00	0.00
ATOM	4879	HD2	LEU	403	18.336	12.796	36.719	1.00	0.00	0.053	0.00	0.00
ATOM	4880	C	LEU	403	16.640	13.178	33.008	1.00	0.00	0.396	9.82	4.00
ATOM	4881	O	LEU	403	16.375	12.018	32.687	1.00	0.00	-0.396	8.17	-17.40
ATOM	4882	N	GLY	404	16.632	14.187	32.138	1.00	0.00	-0.650	9.00	-17.40
ATOM	4883	HN	GLY	404	16.826	15.143	32.468	1.00	0.00	0.440	0.00	0.00
ATOM	4884	CA	GLY	404	16.353	13.958	30.729	1.00	0.00	0.105	9.40	4.00
ATOM	4885	HA1	GLY	404	16.786	12.992	30.467	1.00	0.00	0.053	0.00	0.00
ATOM	4886	HA2	GLY	404	16.817	14.771	30.172	1.00	0.00	0.053	0.00	0.00
ATOM	4887	C	GLY	404	14.906	13.907	30.269	1.00	0.00	0.396	9.82	4.00
ATOM	4888	O	GLY	404	14.614	13.380	29.189	1.00	0.00	-0.396	8.17	-17.40
ATOM	4889	N	VAL	405	14.004	14.458	31.079	1.00	0.00	-0.650	9.00	-17.40
ATOM	4890	HN	VAL	405	14.325	14.875	31.964	1.00	0.00	0.440	0.00	0.00
ATOM	4891	CA	VAL	405	12.576	14.495	30.765	1.00	0.00	0.158	9.40	4.00
ATOM	4892	HA	VAL	405	12.332	13.622	30.158	1.00	0.00	0.053	0.00	0.00
ATOM	4893	CB	VAL	405	11.723	14.509	32.064	1.00	0.00	-0.053	9.40	4.00
ATOM	4894	HB	VAL	405	12.067	15.303	32.725	1.00	0.00	0.053	0.00	0.00
ATOM	4895	CG1	VAL	405	10.258	14.749	31.720	1.00	0.00	-0.159	16.15	4.00
ATOM	4896	HG1	VAL	405	9.666	14.757	32.635	1.00	0.00	0.053	0.00	0.00
ATOM	4897	HG1	VAL	405	10.155	15.708	31.212	1.00	0.00	0.053	0.00	0.00
ATOM	4898	HG1	VAL	405	9.902	13.953	31.065	1.00	0.00	0.053	0.00	0.00
ATOM	4899	CG2	VAL	405	11.890	13.204	32.817	1.00	0.00	-0.159	16.15	4.00
ATOM	4900	HG2	VAL	405	11.286	13.227	33.724	1.00	0.00	0.053	0.00	0.00
ATOM	4901	HG2	VAL	405	11.564	12.376	32.187	1.00	0.00	0.053	0.00	0.00
ATOM	4902	HG2	VAL	405	12.938	13.068	33.081	1.00	0.00	0.053	0.00	0.00
ATOM	4903	C	VAL	405	12.283	15.779	29.994	1.00	0.00	0.396	9.82	4.00
ATOM	4904	O	VAL	405	12.974	16.789	30.189	1.00	0.00	-0.396	8.17	-17.40
ATOM	4905	N	MET	406	11.282	15.752	29.115	1.00	0.00	-0.650	9.00	-17.40
ATOM	4906	HN	MET	406	10.753	14.881	28.961	1.00	0.00	0.440	0.00	0.00
ATOM	4907	CA	MET	406	10.935	16.960	28.370	1.00	0.00	0.158	9.40	4.00
ATOM	4908	HA	MET	406	11.792	17.337	27.813	1.00	0.00	0.053	0.00	0.00
ATOM	4909	CB	MET	406	9.789	16.709	27.373	1.00	0.00	-0.106	12.77	4.00
ATOM	4910	HB1	MET	406	8.943	17.334	27.660	1.00	0.00	0.053	0.00	0.00
ATOM	4911	HB2	MET	406	9.520	15.653	27.420	1.00	0.00	0.053	0.00	0.00
ATOM	4912	CG	MET	406	10.137	17.038	25.904	1.00	0.00	-0.041	12.77	4.00
ATOM	4913	HG1	MET	406	9.202	17.183	25.362	1.00	0.00	0.053	0.00	0.00
ATOM	4914	HG2	MET	406	10.698	16.197	25.496	1.00	0.00	0.053	0.00	0.00
ATOM	4915	SD	MET	406	11.159	18.553	25.639	1.00	0.00	-0.130	16.39	-6.40
ATOM	4916	CE	MET	406	9.938	19.798	25.460	1.00	0.00	-0.094	16.15	4.00
ATOM	4917	HE1	MET	406	10.421	20.760	25.294	1.00	0.00	0.053	0.00	0.00
ATOM	4918	HE2	MET	406	9.299	19.561	24.608	1.00	0.00	0.053	0.00	0.00
ATOM	4919	HE3	MET	406	9.332	19.846	26.365	1.00	0.00	0.053	0.00	0.00
ATOM	4920	C	MET	406	10.498	17.924	29.460	1.00	0.00	0.396	9.82	4.00
ATOM	4921	O	MET	406	9.661	17.582	30.292	1.00	0.00	-0.396	8.17	-17.40
ATOM	4922	N	ASP	407P	11.075	19.123	29.461	1.00	0.00	-0.650	9.00	-17.40
ATOM	4923	HN	ASP	407P	11.738	19.366	28.711	1.00	0.00	0.440	0.00	0.00
ATOM	4924	CA	ASP	407P	10.786	20.094	30.500	1.00	0.00	0.158	9.40	4.00
ATOM	4925	HA	ASP	407P	10.340	19.549	31.332	1.00	0.00	0.053	0.00	0.00
ATOM	4926	CB	ASP	407P	12.109	20.657	31.034	1.00	0.00	-0.336	12.77	4.00
ATOM	4927	HB1	ASP	407P	12.762	19.887	31.445	1.00	0.00	0.053	0.00	0.00
ATOM	4928	HB2	ASP	407P	11.969	21.385	31.832	1.00	0.00	0.053	0.00	0.00
ATOM	4929	CG	ASP	407P	12.924	21.365	29.967	1.00	0.00	0.297	9.82	4.00
ATOM	4930	OD1	ASP	407P	12.695	21.142	28.764	1.00	0.00	-0.534	8.17	-18.95
ATOM	4931	OD2	ASP	407P	13.827	22.139	30.341	1.00	0.00	-0.534	8.17	-18.95
ATOM	4932	C	ASP	407P	9.834	21.246	30.197	1.00	0.00	0.396	9.82	4.00
ATOM	4933	O	ASP	407P	9.622	22.097	31.064	1.00	0.00	-0.396	8.17	-17.40
ATOM	4934	N	ASP	408P	9.247	21.291	29.004	1.00	0.00	-0.650	9.00	-17.40
ATOM	4935	HN	ASP	408P	9.434	20.560	28.302	1.00	0.00	0.440	0.00	0.00

ATOM	4936	CA	ASP	408P	8.332	22.392	28.703	1.00	0.00	0.158	9.40	4.00
ATOM	4937	HA	ASP	408P	8.741	23.309	29.126	1.00	0.00	0.053	0.00	0.00
ATOM	4938	CB	ASP	408P	8.215	22.605	27.179	1.00	0.00	-0.336	12.77	4.00
ATOM	4939	HB1	ASP	408P	9.179	22.695	26.679	1.00	0.00	0.053	0.00	0.00
ATOM	4940	HB2	ASP	408P	7.665	23.506	26.908	1.00	0.00	0.053	0.00	0.00
ATOM	4941	CG	ASP	408P	7.494	21.463	26.459	1.00	0.00	0.297	9.82	4.00
ATOM	4942	OD1	ASP	408P	7.611	20.296	26.894	1.00	0.00	-0.534	8.17	-18.95
ATOM	4943	OD2	ASP	408P	6.827	21.733	25.432	1.00	0.00	-0.534	8.17	-18.95
ATOM	4944	C	ASP	408P	6.979	22.081	29.323	1.00	0.00	0.396	9.82	4.00
ATOM	4945	O	ASP	408P	6.744	20.944	29.753	1.00	0.00	-0.396	8.17	-17.40
ATOM	4946	N	LEU	409	6.113	23.088	29.422	1.00	0.00	-0.650	9.00	-17.40
ATOM	4947	HN	LEU	409	6.387	24.023	29.089	1.00	0.00	0.440	0.00	0.00
ATOM	4948	CA	LEU	409	4.783	22.894	29.993	1.00	0.00	0.158	9.40	4.00
ATOM	4949	HA	LEU	409	4.532	21.839	30.113	1.00	0.00	0.053	0.00	0.00
ATOM	4950	CB	LEU	409	4.713	23.527	31.385	1.00	0.00	-0.106	12.77	4.00
ATOM	4951	HB1	LEU	409	3.690	23.424	31.749	1.00	0.00	0.053	0.00	0.00
ATOM	4952	HB2	LEU	409	4.989	24.577	31.291	1.00	0.00	0.053	0.00	0.00
ATOM	4953	CG	LEU	409	5.633	22.910	32.440	1.00	0.00	-0.053	9.40	4.00
ATOM	4954	HG	LEU	409	6.098	22.008	32.041	1.00	0.00	0.053	0.00	0.00
ATOM	4955	CD1	LEU	409	6.718	23.905	32.822	1.00	0.00	-0.159	16.15	4.00
ATOM	4956	HD1	LEU	409	7.370	23.460	33.573	1.00	0.00	0.053	0.00	0.00
ATOM	4957	HD1	LEU	409	7.303	24.161	31.939	1.00	0.00	0.053	0.00	0.00
ATOM	4958	HD1	LEU	409	6.258	24.806	33.227	1.00	0.00	0.053	0.00	0.00
ATOM	4959	CD2	LEU	409	4.812	22.504	33.650	1.00	0.00	-0.159	16.15	4.00
ATOM	4960	HD2	LEU	409	5.466	22.064	34.402	1.00	0.00	0.053	0.00	0.00
ATOM	4961	HD2	LEU	409	4.318	23.382	34.066	1.00	0.00	0.053	0.00	0.00
ATOM	4962	HD2	LEU	409	4.060	21.773	33.351	1.00	0.00	0.053	0.00	0.00
ATOM	4963	C	LEU	409	3.678	23.506	29.121	1.00	0.00	0.396	9.82	4.00
ATOM	4964	O	LEU	409	3.859	24.596	28.566	1.00	0.00	-0.396	8.17	-17.40
ATOM	4965	N	LYS	410S	2.534	22.827	28.991	1.00	0.00	-0.650	9.00	-17.40
ATOM	4966	HN	LYS	410S	2.428	21.905	29.438	1.00	0.00	0.440	0.00	0.00
ATOM	4967	CA	LYS	410S	1.428	23.395	28.211	1.00	0.00	0.158	9.40	4.00
ATOM	4968	HA	LYS	410S	1.779	24.325	27.765	1.00	0.00	0.053	0.00	0.00
ATOM	4969	CB	LYS	410S	1.010	22.459	27.068	1.00	0.00	-0.106	12.77	4.00
ATOM	4970	HB1	LYS	410S	0.173	22.916	26.540	1.00	0.00	0.053	0.00	0.00
ATOM	4971	HB2	LYS	410S	0.715	21.502	27.500	1.00	0.00	0.053	0.00	0.00
ATOM	4972	CG	LYS	410S	2.116	22.183	26.036	1.00	0.00	-0.106	12.77	4.00
ATOM	4973	HG1	LYS	410S	1.820	21.423	25.312	1.00	0.00	0.053	0.00	0.00
ATOM	4974	HG2	LYS	410S	3.034	21.829	26.504	1.00	0.00	0.053	0.00	0.00
ATOM	4975	CD	LYS	410S	2.480	23.428	25.242	1.00	0.00	-0.106	12.77	4.00
ATOM	4976	HD1	LYS	410S	3.026	24.146	25.852	1.00	0.00	0.053	0.00	0.00
ATOM	4977	HD2	LYS	410S	1.592	23.934	24.862	1.00	0.00	0.053	0.00	0.00
ATOM	4978	CE	LYS	410S	3.363	23.089	24.036	1.00	0.00	0.099	12.77	4.00
ATOM	4979	HE1	LYS	410S	2.905	22.330	23.401	1.00	0.00	0.053	0.00	0.00
ATOM	4980	HE2	LYS	410S	4.336	22.705	24.343	1.00	0.00	0.053	0.00	0.00
ATOM	4981	NZ	LYS	410S	3.615	24.299	23.171	1.00	0.00	-0.045	13.25	-39.20
ATOM	4982	HZ1	LYS	410S	4.209	24.033	22.373	1.00	0.00	0.280	0.00	0.00
ATOM	4983	HZ2	LYS	410S	2.717	24.665	22.822	1.00	0.00	0.280	0.00	0.00
ATOM	4984	HZ3	LYS	410S	4.089	25.025	23.726	1.00	0.00	0.280	0.00	0.00
ATOM	4985	C	LYS	410S	0.266	23.647	29.168	1.00	0.00	0.396	9.82	4.00
ATOM	4986	O	LYS	410S	-0.254	22.722	29.794	1.00	0.00	-0.396	8.17	-17.40
ATOM	4987	N	SER	411	-0.153	24.904	29.276	1.00	0.00	-0.650	9.00	-17.40
ATOM	4988	HN	SER	411	0.275	25.630	28.685	1.00	0.00	0.440	0.00	0.00
ATOM	4989	CA	SER	411	-1.208	25.276	30.215	1.00	0.00	0.158	9.40	4.00
ATOM	4990	HA	SER	411	-1.316	26.360	30.247	1.00	0.00	0.053	0.00	0.00
ATOM	4991	CB	SER	411	-2.575	24.744	29.766	1.00	0.00	0.007	12.77	4.00
ATOM	4992	HB1	SER	411	-3.293	24.834	30.581	1.00	0.00	0.053	0.00	0.00
ATOM	4993	HB2	SER	411	-2.488	23.695	29.481	1.00	0.00	0.053	0.00	0.00
ATOM	4994	OG	SER	411	-3.042	25.493	28.648	1.00	0.00	-0.537	11.04	-17.40
ATOM	4995	HG	SER	411	-2.644	26.442	28.680	1.00	0.00	0.424	0.00	0.00
ATOM	4996	C	SER	411	-0.865	24.773	31.618	1.00	0.00	0.396	9.82	4.00
ATOM	4997	O	SER	411	-1.746	24.405	32.403	1.00	0.00	-0.396	8.17	-17.40
ATOM	4998	N	GLY	412	0.431	24.757	31.928	1.00	0.00	-0.650	9.00	-17.40
ATOM	4999	HN	GLY	412	1.128	25.045	31.227	1.00	0.00	0.440	0.00	0.00
ATOM	5000	CA	GLY	412	0.868	24.334	33.253	1.00	0.00	0.105	9.40	4.00
ATOM	5001	HA1	GLY	412	0.102	24.635	33.968	1.00	0.00	0.053	0.00	0.00
ATOM	5002	HA2	GLY	412	1.817	24.826	33.463	1.00	0.00	0.053	0.00	0.00
ATOM	5003	C	GLY	412	1.091	22.835	33.445	1.00	0.00	0.396	9.82	4.00
ATOM	5004	O	GLY	412	1.614	22.421	34.468	1.00	0.00	-0.396	8.17	-17.40
ATOM	5005	N	VAL	413	0.706	22.027	32.460	1.00	0.00	-0.650	9.00	-17.40
ATOM	5006	HN	VAL	413	0.296	22.439	31.610	1.00	0.00	0.440	0.00	0.00
ATOM	5007	CA	VAL	413	0.845	20.565	32.543	1.00	0.00	0.158	9.40	4.00
ATOM	5008	HA	VAL	413	0.832	20.183	33.564	1.00	0.00	0.053	0.00	0.00
ATOM	5009	CB	VAL	413	-0.312	19.865	31.794	1.00	0.00	-0.053	9.40	4.00
ATOM	5010	HB	VAL	413	-0.274	20.090	30.728	1.00	0.00	0.053	0.00	0.00
ATOM	5011	CG1	VAL	413	-0.225	18.316	31.967	1.00	0.00	-0.159	16.15	4.00

ATOM	5012	HG1	VAL	413	-1.048	17.843	31.432	1.00	0.00	0.053	0.00	0.00
ATOM	5013	HG1	VAL	413	0.722	17.957	31.564	1.00	0.00	0.053	0.00	0.00
ATOM	5014	HG1	VAL	413	-0.287	18.064	33.025	1.00	0.00	0.053	0.00	0.00
ATOM	5015	CG2	VAL	413	-1.647	20.411	32.298	1.00	0.00	-0.159	16.15	4.00
ATOM	5016	HG2	VAL	413	-2.463	19.918	31.770	1.00	0.00	0.053	0.00	0.00
ATOM	5017	HG2	VAL	413	-1.737	20.220	33.367	1.00	0.00	0.053	0.00	0.00
ATOM	5018	HG2	VAL	413	-1.693	21.484	32.116	1.00	0.00	0.053	0.00	0.00
ATOM	5019	C	VAL	413	2.141	20.042	31.940	1.00	0.00	0.396	9.82	4.00
ATOM	5020	O	VAL	413	2.458	20.348	30.792	1.00	0.00	-0.396	8.17	-17.40
ATOM	5021	N	PRO	414	2.911	19.246	32.701	1.00	0.00	-0.422	9.00	-17.40
ATOM	5022	CD	PRO	414	2.848	19.043	34.162	1.00	0.00	0.105	12.77	4.00
ATOM	5023	HD1	PRO	414	1.844	18.758	34.479	1.00	0.00	0.053	0.00	0.00
ATOM	5024	HD2	PRO	414	3.118	19.951	34.700	1.00	0.00	0.053	0.00	0.00
ATOM	5025	CA	PRO	414	4.164	18.709	32.153	1.00	0.00	0.158	9.40	4.00
ATOM	5026	HA	PRO	414	4.734	19.453	31.597	1.00	0.00	0.053	0.00	0.00
ATOM	5027	CB	PRO	414	4.937	18.288	33.402	1.00	0.00	-0.106	12.77	4.00
ATOM	5028	HB1	PRO	414	5.563	19.100	33.769	1.00	0.00	0.053	0.00	0.00
ATOM	5029	HB2	PRO	414	5.584	17.436	33.194	1.00	0.00	0.053	0.00	0.00
ATOM	5030	CG	PRO	414	3.845	17.939	34.373	1.00	0.00	-0.106	12.77	4.00
ATOM	5031	HG1	PRO	414	4.220	17.917	35.396	1.00	0.00	0.053	0.00	0.00
ATOM	5032	HG2	PRO	414	3.421	16.958	34.154	1.00	0.00	0.053	0.00	0.00
ATOM	5033	C	PRO	414	3.936	17.545	31.187	1.00	0.00	0.396	9.82	4.00
ATOM	5034	O	PRO	414	2.876	16.910	31.184	1.00	0.00	-0.396	8.17	-17.40
ATOM	5035	N	ARG	415G	4.941	17.277	30.367	1.00	0.00	-0.650	9.00	-17.40
ATOM	5036	HN	ARG	415G	5.792	17.853	30.431	1.00	0.00	0.440	0.00	0.00
ATOM	5037	CA	ARG	415G	4.903	16.210	29.381	1.00	0.00	0.158	9.40	4.00
ATOM	5038	HA	ARG	415G	4.109	16.396	28.657	1.00	0.00	0.053	0.00	0.00
ATOM	5039	CB	ARG	415G	6.252	16.161	28.659	1.00	0.00	-0.106	12.77	4.00
ATOM	5040	HB1	ARG	415G	6.262	15.284	28.010	1.00	0.00	0.053	0.00	0.00
ATOM	5041	HB2	ARG	415G	7.039	16.091	29.409	1.00	0.00	0.053	0.00	0.00
ATOM	5042	CG	ARG	415G	6.539	17.371	27.801	1.00	0.00	-0.106	12.77	4.00
ATOM	5043	HG1	ARG	415G	7.611	17.563	27.762	1.00	0.00	0.053	0.00	0.00
ATOM	5044	HG2	ARG	415G	6.042	18.251	28.208	1.00	0.00	0.053	0.00	0.00
ATOM	5045	CD	ARG	415G	6.037	17.146	26.382	1.00	0.00	0.374	12.77	4.00
ATOM	5046	HD1	ARG	415G	4.999	16.812	26.365	1.00	0.00	0.053	0.00	0.00
ATOM	5047	HD2	ARG	415G	6.621	16.389	25.858	1.00	0.00	0.053	0.00	0.00
ATOM	5048	NE	ARG	415G	6.104	18.361	25.583	1.00	0.00	-0.819	9.00	-24.67
ATOM	5049	HE	ARG	415G	6.546	19.191	26.001	1.00	0.00	0.407	0.00	0.00
ATOM	5050	CZ	ARG	415G	5.628	18.463	24.345	1.00	0.00	0.796	6.95	4.00
ATOM	5051	NH1	ARG	415G	5.051	17.409	23.767	1.00	0.00	-0.746	9.00	-24.67
ATOM	5052	HH1	ARG	415G	4.681	17.485	22.808	1.00	0.00	0.407	0.00	0.00
ATOM	5053	HH1	ARG	415G	4.974	16.518	24.279	1.00	0.00	0.407	0.00	0.00
ATOM	5054	NH2	ARG	415G	5.721	19.615	23.692	1.00	0.00	-0.746	9.00	-24.67
ATOM	5055	HH2	ARG	415G	5.352	19.694	22.733	1.00	0.00	0.407	0.00	0.00
ATOM	5056	HH2	ARG	415G	6.161	20.429	24.144	1.00	0.00	0.407	0.00	0.00
ATOM	5057	C	ARG	415G	4.641	14.874	30.065	1.00	0.00	0.396	9.82	4.00
ATOM	5058	O	ARG	415G	5.398	14.487	30.954	1.00	0.00	-0.396	8.17	-17.40
ATOM	5059	N	ALA	416	3.577	14.187	29.651	1.00	0.00	-0.650	9.00	-17.40
ATOM	5060	HN	ALA	416	3.004	14.589	28.895	1.00	0.00	0.440	0.00	0.00
ATOM	5061	CA	ALA	416	3.171	12.886	30.210	1.00	0.00	0.158	9.40	4.00
ATOM	5062	HA	ALA	416	2.309	12.445	29.707	1.00	0.00	0.053	0.00	0.00
ATOM	5063	CB	ALA	416	4.295	11.838	30.014	1.00	0.00	-0.159	16.15	4.00
ATOM	5064	HB1	ALA	416	3.978	10.882	30.432	1.00	0.00	0.053	0.00	0.00
ATOM	5065	HB2	ALA	416	4.499	11.718	28.950	1.00	0.00	0.053	0.00	0.00
ATOM	5066	HB3	ALA	416	5.199	12.174	30.521	1.00	0.00	0.053	0.00	0.00
ATOM	5067	C	ALA	416	2.779	12.951	31.691	1.00	0.00	0.396	9.82	4.00
ATOM	5068	O	ALA	416	2.675	11.919	32.375	1.00	0.00	-0.396	8.17	-17.40
ATOM	5069	N	GLY	417	2.554	14.157	32.192	1.00	0.00	-0.650	9.00	-17.40
ATOM	5070	HN	GLY	417	2.639	14.991	31.594	1.00	0.00	0.440	0.00	0.00
ATOM	5071	CA	GLY	417	2.185	14.293	33.593	1.00	0.00	0.105	9.40	4.00
ATOM	5072	HA1	GLY	417	2.314	15.337	33.878	1.00	0.00	0.053	0.00	0.00
ATOM	5073	HA2	GLY	417	2.839	13.648	34.180	1.00	0.00	0.053	0.00	0.00
ATOM	5074	C	GLY	417	0.756	13.907	33.918	1.00	0.00	0.396	9.82	4.00
ATOM	5075	O	GLY	417	-0.144	14.019	33.082	1.00	0.00	-0.396	8.17	-17.40
ATOM	5076	N	TYR	418	0.560	13.433	35.142	1.00	0.00	-0.650	9.00	-17.40
ATOM	5077	HN	TYR	418	1.374	13.328	35.763	1.00	0.00	0.440	0.00	0.00
ATOM	5078	CA	TYR	418	-0.754	13.053	35.650	1.00	0.00	0.158	9.40	4.00
ATOM	5079	HA	TYR	418	-1.453	13.586	35.006	1.00	0.00	0.053	0.00	0.00
ATOM	5080	CB	TYR	418	-0.960	11.539	35.611	1.00	0.00	-0.106	12.77	4.00
ATOM	5081	HB1	TYR	418	-0.313	11.038	36.332	1.00	0.00	0.053	0.00	0.00
ATOM	5082	HB2	TYR	418	-0.732	11.139	34.622	1.00	0.00	0.053	0.00	0.00
ATOM	5083	CG	TYR	418	-2.378	11.182	35.937	1.00	0.00	0.000	7.26	0.60
ATOM	5084	CD1	TYR	418	-3.413	11.539	35.076	1.00	0.00	-0.127	10.80	0.60
ATOM	5085	HD1	TYR	418	-3.182	12.053	34.143	1.00	0.00	0.127	0.00	0.00
ATOM	5086	CE1	TYR	418	-4.738	11.249	35.389	1.00	0.00	-0.127	10.80	0.60
ATOM	5087	HE1	TYR	418	-5.538	11.529	34.704	1.00	0.00	0.127	0.00	0.00

ATOM	5088	CD2	TYR	418	-2.701	10.531	37.127	1.00	0.00	-0.127	10.80	0.60
ATOM	5089	HD2	TYR	418	-1.904	10.243	37.813	1.00	0.00	0.127	0.00	0.00
ATOM	5090	CE2	TYR	418	-4.023	10.242	37.455	1.00	0.00	-0.127	10.80	0.60
ATOM	5091	HE2	TYR	418	-4.261	9.739	38.392	1.00	0.00	0.127	0.00	0.00
ATOM	5092	CZ	TYR	418	-5.030	10.601	36.577	1.00	0.00	0.026	7.26	0.60
ATOM	5093	OH	TYR	418	-6.327	10.294	36.871	1.00	0.00	-0.451	10.94	-17.40
ATOM	5094	HH	TYR	418	-6.872	11.162	36.969	1.00	0.00	0.424	0.00	0.00
ATOM	5095	C	TYR	418	-0.747	13.534	37.105	1.00	0.00	0.396	9.82	4.00
ATOM	5096	O	TYR	418	0.068	13.076	37.893	1.00	0.00	-0.396	8.17	-17.40
ATOM	5097	N	ARG	419G	-1.663	14.446	37.449	1.00	0.00	-0.650	9.00	-17.40
ATOM	5098	HN	ARG	419G	-2.360	14.731	36.747	1.00	0.00	0.440	0.00	0.00
ATOM	5099	CA	ARG	419G	-1.719	15.058	38.780	1.00	0.00	0.158	9.40	4.00
ATOM	5100	HA	ARG	419G	-2.459	15.856	38.726	1.00	0.00	0.053	0.00	0.00
ATOM	5101	CB	ARG	419G	-2.165	14.066	39.854	1.00	0.00	-0.106	12.77	4.00
ATOM	5102	HB1	ARG	419G	-2.204	14.502	40.852	1.00	0.00	0.053	0.00	0.00
ATOM	5103	HB2	ARG	419G	-1.506	13.201	39.939	1.00	0.00	0.053	0.00	0.00
ATOM	5104	CG	ARG	419G	-3.568	13.491	39.602	1.00	0.00	-0.106	12.77	4.00
ATOM	5105	HG1	ARG	419G	-3.567	12.766	38.787	1.00	0.00	0.053	0.00	0.00
ATOM	5106	HG2	ARG	419G	-4.282	14.270	39.337	1.00	0.00	0.053	0.00	0.00
ATOM	5107	CD	ARG	419G	-4.116	12.781	40.832	1.00	0.00	0.374	12.77	4.00
ATOM	5108	HD1	ARG	419G	-3.445	11.990	41.168	1.00	0.00	0.053	0.00	0.00
ATOM	5109	HD2	ARG	419G	-5.084	12.323	40.630	1.00	0.00	0.053	0.00	0.00
ATOM	5110	NE	ARG	419G	-4.295	13.708	41.950	1.00	0.00	-0.819	9.00	-24.67
ATOM	5111	HE	ARG	419G	-3.565	13.732	42.676	1.00	0.00	0.407	0.00	0.00
ATOM	5112	CZ	ARG	419G	-5.341	14.524	42.091	1.00	0.00	0.796	6.95	4.00
ATOM	5113	NH1	ARG	419G	-6.315	14.527	41.187	1.00	0.00	-0.746	9.00	-24.67
ATOM	5114	HH1	ARG	419G	-7.120	15.158	41.300	1.00	0.00	0.407	0.00	0.00
ATOM	5115	HH1	ARG	419G	-6.264	13.897	40.373	1.00	0.00	0.407	0.00	0.00
ATOM	5116	NH2	ARG	419G	-5.408	15.351	43.133	1.00	0.00	-0.746	9.00	-24.67
ATOM	5117	HH2	ARG	419G	-6.216	15.980	43.240	1.00	0.00	0.407	0.00	0.00
ATOM	5118	HH2	ARG	419G	-4.651	15.361	43.832	1.00	0.00	0.407	0.00	0.00
ATOM	5119	C	ARG	419G	-0.321	15.591	39.076	1.00	0.00	0.396	9.82	4.00
ATOM	5120	O	ARG	419G	0.163	15.547	40.218	1.00	0.00	-0.396	8.17	-17.40
ATOM	5121	N	GLY	420	0.321	16.074	38.014	1.00	0.00	-0.650	9.00	-17.40
ATOM	5122	HN	GLY	420	-0.147	16.029	37.097	1.00	0.00	0.440	0.00	0.00
ATOM	5123	CA	GLY	420	1.657	16.665	38.083	1.00	0.00	0.105	9.40	4.00
ATOM	5124	HA1	GLY	420	1.723	17.239	39.007	1.00	0.00	0.053	0.00	0.00
ATOM	5125	HA2	GLY	420	1.784	17.309	37.213	1.00	0.00	0.053	0.00	0.00
ATOM	5126	C	GLY	420	2.817	15.674	38.084	1.00	0.00	0.396	9.82	4.00
ATOM	5127	O	GLY	420	3.974	16.056	38.000	1.00	0.00	-0.396	8.17	-17.40
ATOM	5128	N	ILE	421	2.500	14.394	38.163	1.00	0.00	-0.650	9.00	-17.40
ATOM	5129	HN	ILE	421	1.506	14.123	38.185	1.00	0.00	0.440	0.00	0.00
ATOM	5130	CA	ILE	421	3.523	13.354	38.220	1.00	0.00	0.158	9.40	4.00
ATOM	5131	HA	ILE	421	4.380	13.747	38.766	1.00	0.00	0.053	0.00	0.00
ATOM	5132	CB	ILE	421	2.975	12.124	38.970	1.00	0.00	-0.053	9.40	4.00
ATOM	5133	HB	ILE	421	2.125	11.694	38.438	1.00	0.00	0.053	0.00	0.00
ATOM	5134	CG2	ILE	421	4.045	11.052	39.099	1.00	0.00	-0.159	16.15	4.00
ATOM	5135	HG2	ILE	421	3.637	10.192	39.631	1.00	0.00	0.053	0.00	0.00
ATOM	5136	HG2	ILE	421	4.371	10.742	38.106	1.00	0.00	0.053	0.00	0.00
ATOM	5137	HG2	ILE	421	4.895	11.451	39.652	1.00	0.00	0.053	0.00	0.00
ATOM	5138	CG1	ILE	421	2.435	12.548	40.333	1.00	0.00	-0.106	12.77	4.00
ATOM	5139	HG1	ILE	421	1.944	13.521	40.307	1.00	0.00	0.053	0.00	0.00
ATOM	5140	HG1	ILE	421	3.215	12.623	41.090	1.00	0.00	0.053	0.00	0.00
ATOM	5141	CD1	ILE	421	1.399	11.567	40.890	1.00	0.00	-0.159	16.15	4.00
ATOM	5142	HD1	ILE	421	1.049	11.918	41.860	1.00	0.00	0.053	0.00	0.00
ATOM	5143	HD1	ILE	421	0.555	11.500	40.203	1.00	0.00	0.053	0.00	0.00
ATOM	5144	HD1	ILE	421	1.853	10.582	41.003	1.00	0.00	0.053	0.00	0.00
ATOM	5145	C	ILE	421	4.017	12.887	36.864	1.00	0.00	0.396	9.82	4.00
ATOM	5146	O	ILE	421	3.222	12.457	36.017	1.00	0.00	-0.396	8.17	-17.40
ATOM	5147	N	VAL	422	5.330	12.973	36.659	1.00	0.00	-0.650	9.00	-17.40
ATOM	5148	HN	VAL	422	5.926	13.379	37.394	1.00	0.00	0.440	0.00	0.00
ATOM	5149	CA	VAL	422	5.945	12.508	35.424	1.00	0.00	0.158	9.40	4.00
ATOM	5150	HA	VAL	422	5.120	12.356	34.727	1.00	0.00	0.053	0.00	0.00
ATOM	5151	CB	VAL	422	6.937	13.537	34.868	1.00	0.00	-0.053	9.40	4.00
ATOM	5152	HB	VAL	422	7.732	13.718	35.590	1.00	0.00	0.053	0.00	0.00
ATOM	5153	CG1	VAL	422	7.562	13.016	33.559	1.00	0.00	-0.159	16.15	4.00
ATOM	5154	HG1	VAL	422	8.264	13.754	33.172	1.00	0.00	0.053	0.00	0.00
ATOM	5155	HG1	VAL	422	8.087	12.081	33.753	1.00	0.00	0.053	0.00	0.00
ATOM	5156	HG1	VAL	422	6.775	12.843	32.824	1.00	0.00	0.053	0.00	0.00
ATOM	5157	CG2	VAL	422	6.202	14.844	34.614	1.00	0.00	-0.159	16.15	4.00
ATOM	5158	HG2	VAL	422	6.899	15.582	34.218	1.00	0.00	0.053	0.00	0.00
ATOM	5159	HG2	VAL	422	5.402	14.677	33.892	1.00	0.00	0.053	0.00	0.00
ATOM	5160	HG2	VAL	422	5.777	15.210	35.548	1.00	0.00	0.053	0.00	0.00
ATOM	5161	C	VAL	422	6.669	11.208	35.791	1.00	0.00	0.396	9.82	4.00
ATOM	5162	O	VAL	422	7.576	11.199	36.650	1.00	0.00	-0.396	8.17	-17.40
ATOM	5163	N	THR	423	6.248	10.111	35.156	1.00	0.00	-0.650	9.00	-17.40

ATOM	5164	HN	THR	423	5.498	10.202	34.455	1.00	0.00	0.440	0.00	0.00
ATOM	5165	CA	THR	423	6.814	8.774	35.418	1.00	0.00	0.158	9.40	4.00
ATOM	5166	HA	THR	423	7.456	8.781	36.298	1.00	0.00	0.053	0.00	0.00
ATOM	5167	CB	THR	423	5.675	7.758	35.713	1.00	0.00	0.060	9.40	4.00
ATOM	5168	HB	THR	423	4.954	7.723	34.896	1.00	0.00	0.053	0.00	0.00
ATOM	5169	OG1	THR	423	4.989	8.166	36.907	1.00	0.00	-0.537	11.04	-17.40
ATOM	5170	HG1	THR	423	5.100	9.181	37.037	1.00	0.00	0.424	0.00	0.00
ATOM	5171	CG2	THR	423	6.230	6.338	35.904	1.00	0.00	-0.159	16.15	4.00
ATOM	5172	HG2	THR	423	5.409	5.650	36.108	1.00	0.00	0.053	0.00	0.00
ATOM	5173	HG2	THR	423	6.747	6.024	34.997	1.00	0.00	0.053	0.00	0.00
ATOM	5174	HG2	THR	423	6.927	6.329	36.741	1.00	0.00	0.053	0.00	0.00
ATOM	5175	C	THR	423	7.653	8.286	34.240	1.00	0.00	0.396	9.82	4.00
ATOM	5176	O	THR	423	7.216	8.364	33.090	1.00	0.00	-0.396	8.17	-17.40
ATOM	5177	N	PHE	424	8.849	7.778	34.539	1.00	0.00	-0.650	9.00	-17.40
ATOM	5178	HN	PHE	424	9.129	7.702	35.527	1.00	0.00	0.440	0.00	0.00
ATOM	5179	CA	PHE	424	9.770	7.326	33.502	1.00	0.00	0.158	9.40	4.00
ATOM	5180	HA	PHE	424	9.232	6.783	32.724	1.00	0.00	0.053	0.00	0.00
ATOM	5181	CB	PHE	424	10.453	8.560	32.886	1.00	0.00	-0.106	12.77	4.00
ATOM	5182	HB1	PHE	424	9.767	9.217	32.351	1.00	0.00	0.053	0.00	0.00
ATOM	5183	HB2	PHE	424	11.230	8.314	32.162	1.00	0.00	0.053	0.00	0.00
ATOM	5184	CG	PHE	424	11.137	9.454	33.910	1.00	0.00	0.000	7.26	0.60
ATOM	5185	CD1	PHE	424	12.518	9.381	34.124	1.00	0.00	-0.127	10.80	0.60
ATOM	5186	HD1	PHE	424	13.116	8.673	33.550	1.00	0.00	0.127	0.00	0.00
ATOM	5187	CD2	PHE	424	10.397	10.367	34.658	1.00	0.00	-0.127	10.80	0.60
ATOM	5188	HD2	PHE	424	9.320	10.437	34.504	1.00	0.00	0.127	0.00	0.00
ATOM	5189	CE1	PHE	424	13.146	10.219	35.080	1.00	0.00	-0.127	10.80	0.60
ATOM	5190	HE1	PHE	424	14.222	10.154	35.236	1.00	0.00	0.127	0.00	0.00
ATOM	5191	CE2	PHE	424	11.017	11.199	35.608	1.00	0.00	-0.127	10.80	0.60
ATOM	5192	HE2	PHE	424	10.421	11.907	36.183	1.00	0.00	0.127	0.00	0.00
ATOM	5193	CZ	PHE	424	12.397	11.116	35.813	1.00	0.00	-0.127	10.80	0.60
ATOM	5194	HZ	PHE	424	12.879	11.758	36.549	1.00	0.00	0.127	0.00	0.00
ATOM	5195	C	PHE	424	10.822	6.404	34.090	1.00	0.00	0.396	9.82	4.00
ATOM	5196	O	PHE	424	10.856	6.196	35.307	1.00	0.00	-0.396	8.17	-17.40
ATOM	5197	N	LEU	425	11.664	5.834	33.232	1.00	0.00	-0.650	9.00	-17.40
ATOM	5198	HN	LEU	425	11.542	5.991	32.221	1.00	0.00	0.440	0.00	0.00
ATOM	5199	CA	LEU	425	12.761	4.987	33.703	1.00	0.00	0.158	9.40	4.00
ATOM	5200	HA	LEU	425	12.533	4.722	34.735	1.00	0.00	0.053	0.00	0.00
ATOM	5201	CB	LEU	425	12.891	3.701	32.861	1.00	0.00	-0.106	12.77	4.00
ATOM	5202	HB1	LEU	425	13.620	3.884	32.071	1.00	0.00	0.053	0.00	0.00
ATOM	5203	HB2	LEU	425	11.913	3.471	32.438	1.00	0.00	0.053	0.00	0.00
ATOM	5204	CG	LEU	425	13.358	2.461	33.642	1.00	0.00	-0.053	9.40	4.00
ATOM	5205	HG	LEU	425	14.264	2.697	34.199	1.00	0.00	0.053	0.00	0.00
ATOM	5206	CD1	LEU	425	12.266	2.026	34.618	1.00	0.00	-0.159	16.15	4.00
ATOM	5207	HD1	LEU	425	12.600	1.147	35.169	1.00	0.00	0.053	0.00	0.00
ATOM	5208	HD1	LEU	425	12.059	2.836	35.317	1.00	0.00	0.053	0.00	0.00
ATOM	5209	HD1	LEU	425	11.358	1.783	34.064	1.00	0.00	0.053	0.00	0.00
ATOM	5210	CD2	LEU	425	13.685	1.323	32.695	1.00	0.00	-0.159	16.15	4.00
ATOM	5211	HD2	LEU	425	14.013	0.455	33.268	1.00	0.00	0.053	0.00	0.00
ATOM	5212	HD2	LEU	425	12.797	1.062	32.119	1.00	0.00	0.053	0.00	0.00
ATOM	5213	HD2	LEU	425	14.480	1.631	32.016	1.00	0.00	0.053	0.00	0.00
ATOM	5214	C	LEU	425	14.049	5.825	33.592	1.00	0.00	0.396	9.82	4.00
ATOM	5215	O	LEU	425	14.235	6.601	32.629	1.00	0.00	-0.396	8.17	-17.40
ATOM	5216	N	PHE	426	14.914	5.708	34.593	1.00	0.00	-0.650	9.00	-17.40
ATOM	5217	HN	PHE	426	14.686	5.095	35.389	1.00	0.00	0.440	0.00	0.00
ATOM	5218	CA	PHE	426	16.184	6.434	34.584	1.00	0.00	0.158	9.40	4.00
ATOM	5219	HA	PHE	426	16.366	6.764	33.561	1.00	0.00	0.053	0.00	0.00
ATOM	5220	CB	PHE	426	16.156	7.650	35.517	1.00	0.00	-0.106	12.77	4.00
ATOM	5221	HB1	PHE	426	16.154	7.382	36.573	1.00	0.00	0.053	0.00	0.00
ATOM	5222	HB2	PHE	426	15.277	8.280	35.376	1.00	0.00	0.053	0.00	0.00
ATOM	5223	CG	PHE	426	17.335	8.562	35.338	1.00	0.00	0.000	7.26	0.60
ATOM	5224	CD1	PHE	426	17.350	9.514	34.317	1.00	0.00	-0.127	10.80	0.60
ATOM	5225	HD1	PHE	426	16.477	9.626	33.673	1.00	0.00	0.127	0.00	0.00
ATOM	5226	CD2	PHE	426	18.461	8.431	36.153	1.00	0.00	-0.127	10.80	0.60
ATOM	5227	HD2	PHE	426	18.460	7.693	36.956	1.00	0.00	0.127	0.00	0.00
ATOM	5228	CE1	PHE	426	18.470	10.325	34.110	1.00	0.00	-0.127	10.80	0.60
ATOM	5229	HE1	PHE	426	18.467	11.066	33.311	1.00	0.00	0.127	0.00	0.00
ATOM	5230	CE2	PHE	426	19.588	9.231	35.954	1.00	0.00	-0.127	10.80	0.60
ATOM	5231	HE2	PHE	426	20.460	9.112	36.596	1.00	0.00	0.127	0.00	0.00
ATOM	5232	CZ	PHE	426	19.597	10.181	34.934	1.00	0.00	-0.127	10.80	0.60
ATOM	5233	HZ	PHE	426	20.474	10.808	34.777	1.00	0.00	0.127	0.00	0.00
ATOM	5234	C	PHE	426	17.265	5.474	35.056	1.00	0.00	0.396	9.82	4.00
ATOM	5235	O	PHE	426	17.297	5.083	36.226	1.00	0.00	-0.396	8.17	-17.40
ATOM	5236	N	ARG	427G	18.140	5.096	34.135	1.00	0.00	-0.650	9.00	-17.40
ATOM	5237	HN	ARG	427G	18.050	5.470	33.179	1.00	0.00	0.440	0.00	0.00
ATOM	5238	CA	ARG	427G	19.218	4.174	34.428	1.00	0.00	0.158	9.40	4.00
ATOM	5239	HA	ARG	427G	19.726	3.864	33.514	1.00	0.00	0.053	0.00	0.00

ATOM	5240	CB	ARG	427G	20.283	4.875	35.277	1.00	0.00	-0.106	12.77	4.00
ATOM	5241	HB1	ARG	427G	21.160	4.241	35.407	1.00	0.00	0.053	0.00	0.00
ATOM	5242	HB2	ARG	427G	19.897	5.118	36.267	1.00	0.00	0.053	0.00	0.00
ATOM	5243	CG	ARG	427G	20.736	6.166	34.626	1.00	0.00	-0.106	12.77	4.00
ATOM	5244	HG1	ARG	427G	19.920	6.886	34.686	1.00	0.00	0.053	0.00	0.00
ATOM	5245	HG2	ARG	427G	20.985	5.957	33.585	1.00	0.00	0.053	0.00	0.00
ATOM	5246	CD	ARG	427G	21.956	6.788	35.281	1.00	0.00	0.374	12.77	4.00
ATOM	5247	HD1	ARG	427G	21.834	6.931	36.354	1.00	0.00	0.053	0.00	0.00
ATOM	5248	HD2	ARG	427G	22.200	7.769	34.876	1.00	0.00	0.053	0.00	0.00
ATOM	5249	NE	ARG	427G	23.162	5.979	35.121	1.00	0.00	-0.819	9.00	-24.67
ATOM	5250	HE	ARG	427G	23.077	5.054	34.674	1.00	0.00	0.407	0.00	0.00
ATOM	5251	CZ	ARG	427G	24.363	6.379	35.524	1.00	0.00	0.796	6.95	4.00
ATOM	5252	NH1	ARG	427G	24.492	7.562	36.098	1.00	0.00	-0.746	9.00	-24.67
ATOM	5253	HH1	ARG	427G	25.418	7.882	36.414	1.00	0.00	0.407	0.00	0.00
ATOM	5254	HH1	ARG	427G	23.666	8.163	36.229	1.00	0.00	0.407	0.00	0.00
ATOM	5255	NH2	ARG	427G	25.426	5.604	35.360	1.00	0.00	-0.746	9.00	-24.67
ATOM	5256	HH2	ARG	427G	26.351	5.925	35.677	1.00	0.00	0.407	0.00	0.00
ATOM	5257	HH2	ARG	427G	25.326	4.680	34.916	1.00	0.00	0.407	0.00	0.00
ATOM	5258	C	ARG	427G	18.692	2.922	35.119	1.00	0.00	0.396	9.82	4.00
ATOM	5259	O	ARG	427G	19.262	2.457	36.094	1.00	0.00	-0.396	8.17	-17.40
ATOM	5260	N	GLY	428	17.579	2.401	34.604	1.00	0.00	-0.650	9.00	-17.40
ATOM	5261	HN	GLY	428	17.133	2.870	33.802	1.00	0.00	0.440	0.00	0.00
ATOM	5262	CA	GLY	428	16.973	1.192	35.136	1.00	0.00	0.105	9.40	4.00
ATOM	5263	HA1	GLY	428	17.777	0.513	35.418	1.00	0.00	0.053	0.00	0.00
ATOM	5264	HA2	GLY	428	16.351	0.759	34.352	1.00	0.00	0.053	0.00	0.00
ATOM	5265	C	GLY	428	16.087	1.360	36.360	1.00	0.00	0.396	9.82	4.00
ATOM	5266	O	GLY	428	15.515	0.390	36.859	1.00	0.00	-0.396	8.17	-17.40
ATOM	5267	N	ARG	429G	15.947	2.591	36.835	1.00	0.00	-0.650	9.00	-17.40
ATOM	5268	HN	ARG	429G	16.414	3.376	36.360	1.00	0.00	0.440	0.00	0.00
ATOM	5269	CA	ARG	429G	15.137	2.844	38.023	1.00	0.00	0.158	9.40	4.00
ATOM	5270	HA	ARG	429G	14.910	1.911	38.539	1.00	0.00	0.053	0.00	0.00
ATOM	5271	CB	ARG	429G	15.905	3.752	38.992	1.00	0.00	-0.106	12.77	4.00
ATOM	5272	HB1	ARG	429G	15.848	4.773	38.615	1.00	0.00	0.053	0.00	0.00
ATOM	5273	HB2	ARG	429G	16.938	3.408	39.029	1.00	0.00	0.053	0.00	0.00
ATOM	5274	CG	ARG	429G	15.378	3.767	40.428	1.00	0.00	-0.106	12.77	4.00
ATOM	5275	HG1	ARG	429G	15.778	2.924	40.992	1.00	0.00	0.053	0.00	0.00
ATOM	5276	HG2	ARG	429G	14.290	3.700	40.438	1.00	0.00	0.053	0.00	0.00
ATOM	5277	CD	ARG	429G	15.787	5.060	41.139	1.00	0.00	0.374	12.77	4.00
ATOM	5278	HD1	ARG	429G	15.504	4.974	42.188	1.00	0.00	0.053	0.00	0.00
ATOM	5279	HD2	ARG	429G	15.262	5.889	40.664	1.00	0.00	0.053	0.00	0.00
ATOM	5280	NE	ARG	429G	17.227	5.363	41.092	1.00	0.00	-0.819	9.00	-24.67
ATOM	5281	HE	ARG	429G	17.583	5.855	40.260	1.00	0.00	0.407	0.00	0.00
ATOM	5282	CZ	ARG	429G	18.105	5.048	42.045	1.00	0.00	0.796	6.95	4.00
ATOM	5283	NH1	ARG	429G	17.710	4.406	43.134	1.00	0.00	-0.746	9.00	-24.67
ATOM	5284	HH1	ARG	429G	18.393	4.165	43.866	1.00	0.00	0.407	0.00	0.00
ATOM	5285	HH1	ARG	429G	16.719	4.147	43.248	1.00	0.00	0.407	0.00	0.00
ATOM	5286	NH2	ARG	429G	19.380	5.398	41.922	1.00	0.00	-0.746	9.00	-24.67
ATOM	5287	HH2	ARG	429G	20.054	5.152	42.660	1.00	0.00	0.407	0.00	0.00
ATOM	5288	HH2	ARG	429G	19.694	5.914	41.088	1.00	0.00	0.407	0.00	0.00
ATOM	5289	C	ARG	429G	13.820	3.512	37.643	1.00	0.00	0.396	9.82	4.00
ATOM	5290	O	ARG	429G	13.793	4.400	36.788	1.00	0.00	-0.396	8.17	-17.40
ATOM	5291	N	ARG	430G	12.733	3.077	38.264	1.00	0.00	-0.650	9.00	-17.40
ATOM	5292	HN	ARG	430G	12.807	2.303	38.939	1.00	0.00	0.440	0.00	0.00
ATOM	5293	CA	ARG	430G	11.433	3.681	38.002	1.00	0.00	0.158	9.40	4.00
ATOM	5294	HA	ARG	430G	11.393	3.860	36.927	1.00	0.00	0.053	0.00	0.00
ATOM	5295	CB	ARG	430G	10.295	2.754	38.437	1.00	0.00	-0.106	12.77	4.00
ATOM	5296	HB1	ARG	430G	10.392	2.414	39.468	1.00	0.00	0.053	0.00	0.00
ATOM	5297	HB2	ARG	430G	10.228	1.848	37.833	1.00	0.00	0.053	0.00	0.00
ATOM	5298	CG	ARG	430G	8.935	3.406	38.348	1.00	0.00	-0.106	12.77	4.00
ATOM	5299	HG1	ARG	430G	8.871	4.257	39.025	1.00	0.00	0.053	0.00	0.00
ATOM	5300	HG2	ARG	430G	8.150	2.697	38.615	1.00	0.00	0.053	0.00	0.00
ATOM	5301	CD	ARG	430G	8.667	3.904	36.925	1.00	0.00	0.374	12.77	4.00
ATOM	5302	HD1	ARG	430G	9.468	4.558	36.582	1.00	0.00	0.053	0.00	0.00
ATOM	5303	HD2	ARG	430G	7.733	4.464	36.876	1.00	0.00	0.053	0.00	0.00
ATOM	5304	NE	ARG	430G	8.570	2.791	35.992	1.00	0.00	-0.819	9.00	-24.67
ATOM	5305	HE	ARG	430G	8.490	1.842	36.385	1.00	0.00	0.407	0.00	0.00
ATOM	5306	CZ	ARG	430G	8.577	2.912	34.670	1.00	0.00	0.796	6.95	4.00
ATOM	5307	NH1	ARG	430G	8.674	4.120	34.111	1.00	0.00	-0.746	9.00	-24.67
ATOM	5308	HH1	ARG	430G	8.679	4.213	33.085	1.00	0.00	0.407	0.00	0.00
ATOM	5309	HH1	ARG	430G	8.743	4.958	34.705	1.00	0.00	0.407	0.00	0.00
ATOM	5310	NH2	ARG	430G	8.511	1.814	33.908	1.00	0.00	-0.746	9.00	-24.67
ATOM	5311	HH2	ARG	430G	8.515	1.898	32.881	1.00	0.00	0.407	0.00	0.00
ATOM	5312	HH2	ARG	430G	8.455	0.884	34.348	1.00	0.00	0.407	0.00	0.00
ATOM	5313	C	ARG	430G	11.394	4.970	38.813	1.00	0.00	0.396	9.82	4.00
ATOM	5314	O	ARG	430G	11.573	4.958	40.045	1.00	0.00	-0.396	8.17	-17.40
ATOM	5315	N	VAL	431	11.178	6.082	38.128	1.00	0.00	-0.650	9.00	-17.40

ATOM	5316	HN	VAL	431	11.025	6.037	37.110	1.00	0.00	0.440	0.00	0.00
ATOM	5317	CA	VAL	431	11.155	7.370	38.811	1.00	0.00	0.158	9.40	4.00
ATOM	5318	HA	VAL	431	11.255	7.288	39.893	1.00	0.00	0.053	0.00	0.00
ATOM	5319	CB	VAL	431	12.335	8.254	38.343	1.00	0.00	-0.053	9.40	4.00
ATOM	5320	HB	VAL	431	12.315	8.384	37.261	1.00	0.00	0.053	0.00	0.00
ATOM	5321	CG1	VAL	431	12.267	9.638	38.991	1.00	0.00	-0.159	16.15	4.00
ATOM	5322	HG1	VAL	431	13.106	10.242	38.647	1.00	0.00	0.053	0.00	0.00
ATOM	5323	HG1	VAL	431	11.332	10.124	38.713	1.00	0.00	0.053	0.00	0.00
ATOM	5324	HG1	VAL	431	12.313	9.534	40.075	1.00	0.00	0.053	0.00	0.00
ATOM	5325	CG2	VAL	431	13.661	7.566	38.693	1.00	0.00	-0.159	16.15	4.00
ATOM	5326	HG2	VAL	431	14.492	8.189	38.363	1.00	0.00	0.053	0.00	0.00
ATOM	5327	HG2	VAL	431	13.722	7.420	39.771	1.00	0.00	0.053	0.00	0.00
ATOM	5328	HG2	VAL	431	13.712	6.598	38.193	1.00	0.00	0.053	0.00	0.00
ATOM	5329	C	VAL	431	9.871	8.149	38.587	1.00	0.00	0.396	9.82	4.00
ATOM	5330	O	VAL	431	9.358	8.212	37.454	1.00	0.00	-0.396	8.17	-17.40
ATOM	5331	N	HIS	432S	9.355	8.724	39.673	1.00	0.00	-0.650	9.00	-17.40
ATOM	5332	HN	HIS	432S	9.807	8.561	40.584	1.00	0.00	0.440	0.00	0.00
ATOM	5333	CA	HIS	432S	8.173	9.574	39.616	1.00	0.00	0.158	9.40	4.00
ATOM	5334	HA	HIS	432S	7.799	9.559	38.592	1.00	0.00	0.053	0.00	0.00
ATOM	5335	CB	HIS	432S	7.088	9.086	40.584	1.00	0.00	-0.106	12.77	4.00
ATOM	5336	HB1	HIS	432S	6.213	9.726	40.471	1.00	0.00	0.053	0.00	0.00
ATOM	5337	HB2	HIS	432S	7.479	9.148	41.599	1.00	0.00	0.053	0.00	0.00
ATOM	5338	CG	HIS	432S	6.655	7.677	40.348	1.00	0.00	-0.050	7.26	0.60
ATOM	5339	CD2	HIS	432S	6.893	6.542	41.051	1.00	0.00	-0.177	10.80	0.60
ATOM	5340	HD2	HIS	432S	7.451	6.463	41.984	1.00	0.00	0.127	0.00	0.00
ATOM	5341	ND1	HIS	432S	5.917	7.299	39.248	1.00	0.00	0.207	9.25	-17.40
ATOM	5342	HD1	HIS	432S	5.574	7.934	38.513	1.00	0.00	0.393	0.00	0.00
ATOM	5343	CE1	HIS	432S	5.717	5.993	39.284	1.00	0.00	-0.227	10.80	0.60
ATOM	5344	HE1	HIS	432S	5.165	5.413	38.544	1.00	0.00	0.127	0.00	0.00
ATOM	5345	NE2	HIS	432S	6.298	5.509	40.366	1.00	0.00	0.207	9.25	-17.40
ATOM	5346	HE2	HIS	432S	6.304	4.519	40.650	1.00	0.00	0.393	0.00	0.00
ATOM	5347	C	HIS	432S	8.593	10.994	40.030	1.00	0.00	0.396	9.82	4.00
ATOM	5348	O	HIS	432S	8.753	11.280	41.226	1.00	0.00	-0.396	8.17	-17.40
ATOM	5349	N	LEU	433	8.805	11.873	39.056	1.00	0.00	-0.650	9.00	-17.40
ATOM	5350	HN	LEU	433	8.732	11.569	38.074	1.00	0.00	0.440	0.00	0.00
ATOM	5351	CA	LEU	433	9.139	13.263	39.356	1.00	0.00	0.158	9.40	4.00
ATOM	5352	HA	LEU	433	9.877	13.343	40.154	1.00	0.00	0.053	0.00	0.00
ATOM	5353	CB	LEU	433	9.644	13.996	38.101	1.00	0.00	-0.106	12.77	4.00
ATOM	5354	HB1	LEU	433	8.868	13.909	37.339	1.00	0.00	0.053	0.00	0.00
ATOM	5355	HB2	LEU	433	10.566	13.507	37.788	1.00	0.00	0.053	0.00	0.00
ATOM	5356	CG	LEU	433	9.967	15.495	38.222	1.00	0.00	-0.053	9.40	4.00
ATOM	5357	HG	LEU	433	9.098	16.044	38.584	1.00	0.00	0.053	0.00	0.00
ATOM	5358	CD1	LEU	433	11.116	15.715	39.195	1.00	0.00	-0.159	16.15	4.00
ATOM	5359	HD1	LEU	433	11.331	16.781	39.268	1.00	0.00	0.053	0.00	0.00
ATOM	5360	HD1	LEU	433	10.839	15.332	40.177	1.00	0.00	0.053	0.00	0.00
ATOM	5361	HD1	LEU	433	12.001	15.189	38.837	1.00	0.00	0.053	0.00	0.00
ATOM	5362	CD2	LEU	433	10.344	16.050	36.840	1.00	0.00	-0.159	16.15	4.00
ATOM	5363	HD2	LEU	433	10.573	17.112	36.924	1.00	0.00	0.053	0.00	0.00
ATOM	5364	HD2	LEU	433	11.217	15.519	36.460	1.00	0.00	0.053	0.00	0.00
ATOM	5365	HD2	LEU	433	9.509	15.912	36.152	1.00	0.00	0.053	0.00	0.00
ATOM	5366	C	LEU	433	7.759	13.764	39.756	1.00	0.00	0.396	9.82	4.00
ATOM	5367	O	LEU	433	6.883	13.927	38.898	1.00	0.00	-0.396	8.17	-17.40
ATOM	5368	N	ALA	434	7.558	14.005	41.052	1.00	0.00	-0.650	9.00	-17.40
ATOM	5369	HN	ALA	434	8.336	13.906	41.718	1.00	0.00	0.440	0.00	0.00
ATOM	5370	CA	ALA	434	6.239	14.408	41.530	1.00	0.00	0.158	9.40	4.00
ATOM	5371	HA	ALA	434	5.631	14.650	40.658	1.00	0.00	0.053	0.00	0.00
ATOM	5372	CB	ALA	434	5.569	13.223	42.231	1.00	0.00	-0.159	16.15	4.00
ATOM	5373	HB1	ALA	434	4.583	13.521	42.589	1.00	0.00	0.053	0.00	0.00
ATOM	5374	HB2	ALA	434	5.464	12.396	41.528	1.00	0.00	0.053	0.00	0.00
ATOM	5375	HB3	ALA	434	6.181	12.906	43.075	1.00	0.00	0.053	0.00	0.00
ATOM	5376	C	ALA	434	6.182	15.607	42.447	1.00	0.00	0.396	9.82	4.00
ATOM	5377	O	ALA	434	7.173	15.971	43.089	1.00	0.00	-0.396	8.17	-17.40
ATOM	5378	N	PRO	435	4.999	16.232	42.534	1.00	0.00	-0.422	9.00	-17.40
ATOM	5379	CD	PRO	435	3.769	16.013	41.742	1.00	0.00	0.105	12.77	4.00
ATOM	5380	HD1	PRO	435	3.426	14.981	41.822	1.00	0.00	0.053	0.00	0.00
ATOM	5381	HD2	PRO	435	3.937	16.224	40.686	1.00	0.00	0.053	0.00	0.00
ATOM	5382	CA	PRO	435	4.854	17.399	43.406	1.00	0.00	0.158	9.40	4.00
ATOM	5383	HA	PRO	435	5.824	17.894	43.395	1.00	0.00	0.053	0.00	0.00
ATOM	5384	CB	PRO	435	3.687	18.149	42.774	1.00	0.00	-0.106	12.77	4.00
ATOM	5385	HB1	PRO	435	4.008	18.741	41.917	1.00	0.00	0.053	0.00	0.00
ATOM	5386	HB2	PRO	435	3.218	18.831	43.483	1.00	0.00	0.053	0.00	0.00
ATOM	5387	CG	PRO	435	2.775	17.003	42.379	1.00	0.00	-0.106	12.77	4.00
ATOM	5388	HG1	PRO	435	2.007	17.329	41.677	1.00	0.00	0.053	0.00	0.00
ATOM	5389	HG2	PRO	435	2.267	16.581	43.246	1.00	0.00	0.053	0.00	0.00
ATOM	5390	C	PRO	435	4.483	16.844	44.772	1.00	0.00	0.396	9.82	4.00
ATOM	5391	O	PRO	435	4.271	15.629	44.910	1.00	0.00	-0.396	8.17	-17.40

ATOM	5392	N	PRO	436	4.390	17.718	45.797	1.00	0.00	-0.422	9.00	-17.40
ATOM	5393	CD	PRO	436	4.674	19.162	45.816	1.00	0.00	0.105	12.77	4:00
ATOM	5394	HD1	PRO	436	3.798	19.743	45.525	1.00	0.00	0.053	0.00	0.00
ATOM	5395	HD2	PRO	436	5.479	19.418	45.128	1.00	0.00	0.053	0.00	0.00
ATOM	5396	CA	PRO	436	4.024	17.245	47.139	1.00	0.00	0.158	9.40	4.00
ATOM	5397	HA	PRO	436	4.733	16.461	47.405	1.00	0.00	0.053	0.00	0.00
ATOM	5398	CB	PRO	436	4.098	18.506	47.996	1.00	0.00	-0.106	12.77	4.00
ATOM	5399	HB1	PRO	436	4.459	18.149	48.960	1.00	0.00	0.053	0.00	0.00
ATOM	5400	HB2	PRO	436	3.073	18.876	48.010	1.00	0.00	0.053	0.00	0.00
ATOM	5401	CG	PRO	436	5.060	19.385	47.265	1.00	0.00	-0.106	12.77	4.00
ATOM	5402	HG1	PRO	436	6.091	19.093	47.464	1.00	0.00	0.053	0.00	0.00
ATOM	5403	HG2	PRO	436	4.947	20.427	47.563	1.00	0.00	0.053	0.00	0.00
ATOM	5404	C	PRO	436	2.603	16.714	47.051	1.00	0.00	0.396	9.82	4.00
ATOM	5405	O	PRO	436	1.823	17.140	46.198	1.00	0.00	-0.396	8.17	-17.40
ATOM	5406	N	GLN	437	2.272	15.793	47.945	1.00	0.00	-0.650	9.00	-17.40
ATOM	5407	HN	GLN	437	2.969	15.516	48.650	1.00	0.00	0.440	0.00	0.00
ATOM	5408	CA	GLN	437	0.962	15.156	47.971	1.00	0.00	0.158	9.40	4.00
ATOM	5409	HA	GLN	437	0.821	14.631	47.026	1.00	0.00	0.053	0.00	0.00
ATOM	5410	CB	GLN	437	0.966	14.095	49.076	1.00	0.00	-0.106	12.77	4.00
ATOM	5411	HB1	GLN	437	1.097	14.603	50.031	1.00	0.00	0.053	0.00	0.00
ATOM	5412	HB2	GLN	437	1.792	13.410	48.883	1.00	0.00	0.053	0.00	0.00
ATOM	5413	CG	GLN	437	-0.284	13.267	49.179	1.00	0.00	-0.106	12.77	4.00
ATOM	5414	HG1	GLN	437	-0.773	13.157	48.211	1.00	0.00	0.053	0.00	0.00
ATOM	5415	HG2	GLN	437	-1.008	13.716	49.858	1.00	0.00	0.053	0.00	0.00
ATOM	5416	CD	GLN	437	0.011	11.873	49.694	1.00	0.00	0.396	9.82	4.00
ATOM	5417	OE1	GLN	437	0.901	11.687	50.537	1.00	0.00	-0.396	8.17	-17.40
ATOM	5418	NE2	GLN	437	-0.733	10.884	49.197	1.00	0.00	-0.879	13.25	-17.40
ATOM	5419	HE2	GLN	437	-1.461	11.088	48.497	1.00	0.00	0.440	0.00	0.00
ATOM	5420	HE2	GLN	437	-0.579	9.915	49.512	1.00	0.00	0.440	0.00	0.00
ATOM	5421	C	GLN	437	-0.222	16.113	48.143	1.00	0.00	0.396	9.82	4.00
ATOM	5422	O	GLN	437	-1.382	15.706	48.037	1.00	0.00	-0.396	8.17	-17.40
ATOM	5423	N	THR	438	0.072	17.381	48.394	1.00	0.00	-0.650	9.00	-17.40
ATOM	5424	HN	THR	438	1.059	17.665	48.467	1.00	0.00	0.440	0.00	0.00
ATOM	5425	CA	THR	438	-0.973	18.380	48.568	1.00	0.00	0.158	9.40	4.00
ATOM	5426	HA	THR	438	-1.874	17.959	49.015	1.00	0.00	0.053	0.00	0.00
ATOM	5427	CB	THR	438	-0.513	19.488	49.522	1.00	0.00	0.060	9.40	4.00
ATOM	5428	HB	THR	438	-1.232	20.307	49.528	1.00	0.00	0.053	0.00	0.00
ATOM	5429	OG1	THR	438	0.751	19.992	49.083	1.00	0.00	-0.537	11.04	-17.40
ATOM	5430	HG1	THR	438	1.397	20.044	49.883	1.00	0.00	0.424	0.00	0.00
ATOM	5431	CG2	THR	438	-0.382	18.945	50.948	1.00	0.00	-0.159	16.15	4.00
ATOM	5432	HG2	THR	438	-0.054	19.744	51.613	1.00	0.00	0.053	0.00	0.00
ATOM	5433	HG2	THR	438	-1.347	18.566	51.283	1.00	0.00	0.053	0.00	0.00
ATOM	5434	HG2	THR	438	0.349	18.137	50.964	1.00	0.00	0.053	0.00	0.00
ATOM	5435	C	THR	438	-1.398	19.013	47.235	1.00	0.00	0.396	9.82	4.00
ATOM	5436	O	THR	438	-2.264	19.894	47.205	1.00	0.00	-0.396	8.17	-17.40
ATOM	5437	N	TRP	439	-0.783	18.560	46.143	1.00	0.00	-0.650	9.00	-17.40
ATOM	5438	HN	TRP	439	-0.056	17.837	46.249	1.00	0.00	0.440	0.00	0.00
ATOM	5439	CA	TRP	439	-1.099	19.048	44.797	1.00	0.00	0.158	9.40	4.00
ATOM	5440	HA	TRP	439	-0.653	20.036	44.687	1.00	0.00	0.053	0.00	0.00
ATOM	5441	CB	TRP	439	-0.576	18.072	43.744	1.00	0.00	-0.106	12.77	4.00
ATOM	5442	HB1	TRP	439	-1.122	17.134	43.849	1.00	0.00	0.053	0.00	0.00
ATOM	5443	HB2	TRP	439	0.488	17.920	43.921	1.00	0.00	0.053	0.00	0.00
ATOM	5444	CG	TRP	439	-0.735	18.527	42.324	1.00	0.00	0.000	7.26	0.60
ATOM	5445	CD2	TRP	439	-1.829	18.243	41.440	1.00	0.00	0.000	6.80	0.60
ATOM	5446	CE2	TRP	439	-1.537	18.859	40.199	1.00	0.00	-0.050	6.80	0.60
ATOM	5447	CD1	TRP	439	0.147	19.285	41.605	1.00	0.00	-0.177	10.80	0.60
ATOM	5448	HD1	TRP	439	1.090	19.674	41.988	1.00	0.00	0.127	0.00	0.00
ATOM	5449	NE1	TRP	439	-0.326	19.487	40.328	1.00	0.00	-0.292	9.00	-17.40
ATOM	5450	HE1	TRP	439	0.152	20.022	39.590	1.00	0.00	0.393	0.00	0.00
ATOM	5451	CE3	TRP	439	-3.025	17.527	41.573	1.00	0.00	-0.127	10.80	0.60
ATOM	5452	HE3	TRP	439	-3.280	17.041	42.515	1.00	0.00	0.127	0.00	0.00
ATOM	5453	CZ2	TRP	439	-2.399	18.781	39.095	1.00	0.00	-0.127	10.80	0.60
ATOM	5454	HZ2	TRP	439	-2.151	19.264	38.150	1.00	0.00	0.127	0.00	0.00
ATOM	5455	CZ3	TRP	439	-3.886	17.447	40.472	1.00	0.00	-0.127	10.80	0.60
ATOM	5456	HZ3	TRP	439	-4.819	16.891	40.560	1.00	0.00	0.127	0.00	0.00
ATOM	5457	CH2	TRP	439	-3.564	18.074	39.248	1.00	0.00	-0.127	10.80	0.60
ATOM	5458	HH2	TRP	439	-4.254	17.994	38.408	1.00	0.00	0.127	0.00	0.00
ATOM	5459	C	TRP	439	-2.609	19.114	44.669	1.00	0.00	0.396	9.82	4.00
ATOM	5460	O	TRP	439	-3.312	18.194	45.080	1.00	0.00	-0.396	8.17	-17.40
ATOM	5461	N	ASP	440P	-3.102	20.175	44.054	1.00	0.00	-0.650	9.00	-17.40
ATOM	5462	HN	ASP	440P	-2.461	20.892	43.685	1.00	0.00	0.440	0.00	0.00
ATOM	5463	CA	ASP	440P	-4.530	20.341	43.893	1.00	0.00	0.158	9.40	4.00
ATOM	5464	HA	ASP	440P	-5.044	19.381	43.838	1.00	0.00	0.053	0.00	0.00
ATOM	5465	CB	ASP	440P	-5.091	21.098	45.092	1.00	0.00	-0.336	12.77	4.00
ATOM	5466	HB1	ASP	440P	-4.857	22.162	45.056	1.00	0.00	0.053	0.00	0.00
ATOM	5467	HB2	ASP	440P	-4.696	20.726	46.037	1.00	0.00	0.053	0.00	0.00

ATOM	5468	CG	ASP	440P	-6.599	20.992	45.185	1.00	0.00	0.297	9.82	4.00
ATOM	5469	OD1	ASP	440P	-7.198	21.763	45.967	1.00	0.00	-0.534	8.17	-18.95
ATOM	5470	OD2	ASP	440P	-7.183	20.130	44.483	1.00	0.00	-0.534	8.17	-18.95
ATOM	5471	C	ASP	440P	-4.870	21.107	42.616	1.00	0.00	0.396	9.82	4.00
ATOM	5472	O	ASP	440P	-5.526	22.153	42.671	1.00	0.00	-0.396	8.17	-17.40
ATOM	5473	N	GLY	441	-4.419	20.607	41.471	1.00	0.00	-0.650	9.00	-17.40
ATOM	5474	HN	GLY	441	-3.856	19.744	41.469	1.00	0.00	0.440	0.00	0.00
ATOM	5475	CA	GLY	441	-4.723	21.283	40.221	1.00	0.00	0.105	9.40	4.00
ATOM	5476	HA1	GLY	441	-5.493	22.029	40.413	1.00	0.00	0.053	0.00	0.00
ATOM	5477	HA2	GLY	441	-5.079	20.540	39.507	1.00	0.00	0.053	0.00	0.00
ATOM	5478	C	GLY	441	-3.536	21.994	39.595	1.00	0.00	0.396	9.82	4.00
ATOM	5479	O	GLY	441	-2.619	22.453	40.282	1.00	0.00	-0.396	8.17	-17.40
ATOM	5480	N	TYR	442	-3.565	22.105	38.273	1.00	0.00	-0.650	9.00	-17.40
ATOM	5481	HN	TYR	442	-4.373	21.733	37.753	1.00	0.00	0.440	0.00	0.00
ATOM	5482	CA	TYR	442	-2.482	22.739	37.544	1.00	0.00	0.158	9.40	4.00
ATOM	5483	HA	TYR	442	-1.490	22.488	37.921	1.00	0.00	0.053	0.00	0.00
ATOM	5484	CB	TYR	442	-2.489	22.256	36.094	1.00	0.00	-0.106	12.77	4.00
ATOM	5485	HB1	TYR	442	-1.769	22.779	35.465	1.00	0.00	0.053	0.00	0.00
ATOM	5486	HB2	TYR	442	-3.454	22.384	35.604	1.00	0.00	0.053	0.00	0.00
ATOM	5487	CG	TYR	442	-2.159	20.800	35.957	1.00	0.00	0.000	7.26	0.60
ATOM	5488	CD1	TYR	442	-3.157	19.858	35.705	1.00	0.00	-0.127	10.80	0.60
ATOM	5489	HD1	TYR	442	-4.194	20.181	35.618	1.00	0.00	0.127	0.00	0.00
ATOM	5490	CE1	TYR	442	-2.841	18.505	35.563	1.00	0.00	-0.127	10.80	0.60
ATOM	5491	HE1	TYR	442	-3.626	17.776	35.361	1.00	0.00	0.127	0.00	0.00
ATOM	5492	CD2	TYR	442	-0.838	20.357	36.069	1.00	0.00	-0.127	10.80	0.60
ATOM	5493	HD2	TYR	442	-0.046	21.079	36.269	1.00	0.00	0.127	0.00	0.00
ATOM	5494	CE2	TYR	442	-0.517	19.018	35.930	1.00	0.00	-0.127	10.80	0.60
ATOM	5495	HE2	TYR	442	0.519	18.692	36.016	1.00	0.00	0.127	0.00	0.00
ATOM	5496	CZ	TYR	442	-1.518	18.092	35.680	1.00	0.00	0.026	7.26	0.60
ATOM	5497	OH	TYR	442	-1.207	16.747	35.580	1.00	0.00	-0.451	10.94	-17.40
ATOM	5498	HH	TYR	442	-2.073	16.201	35.467	1.00	0.00	0.424	0.00	0.00
ATOM	5499	C	TYR	442	-2.533	24.261	37.567	1.00	0.00	0.396	9.82	4.00
ATOM	5500	O	TYR	442	-3.583	24.858	37.802	1.00	0.00	-0.396	8.17	-17.40
ATOM	5501	N	ASP	443P	-1.390	24.882	37.302	1.00	0.00	-0.650	9.00	-17.40
ATOM	5502	HN	ASP	443P	-0.547	24.318	37.116	1.00	0.00	0.440	0.00	0.00
ATOM	5503	CA	ASP	443P	-1.289	26.342	37.266	1.00	0.00	0.158	9.40	4.00
ATOM	5504	HA	ASP	443P	-2.283	26.755	37.432	1.00	0.00	0.053	0.00	0.00
ATOM	5505	CB	ASP	443P	-0.337	26.813	38.362	1.00	0.00	-0.336	12.77	4.00
ATOM	5506	HB1	ASP	443P	0.692	26.502	38.184	1.00	0.00	0.053	0.00	0.00
ATOM	5507	HB2	ASP	443P	-0.605	26.426	39.345	1.00	0.00	0.053	0.00	0.00
ATOM	5508	CG	ASP	443P	-0.305	28.316	38.496	1.00	0.00	0.297	9.82	4.00
ATOM	5509	OD1	ASP	443P	-0.836	28.997	37.594	1.00	0.00	-0.534	8.17	-18.95
ATOM	5510	OD2	ASP	443P	0.253	28.816	39.496	1.00	0.00	-0.534	8.17	-18.95
ATOM	5511	C	ASP	443P	-0.757	26.748	35.896	1.00	0.00	0.396	9.82	4.00
ATOM	5512	O	ASP	443P	0.424	26.548	35.601	1.00	0.00	-0.396	8.17	-17.40
ATOM	5513	N	PRO	444	-1.617	27.340	35.052	1.00	0.00	-0.422	9.00	-17.40
ATOM	5514	CD	PRO	444	-2.992	27.767	35.376	1.00	0.00	0.105	12.77	4.00
ATOM	5515	HD1	PRO	444	-3.067	28.107	36.408	1.00	0.00	0.053	0.00	0.00
ATOM	5516	HD2	PRO	444	-3.701	26.949	35.246	1.00	0.00	0.053	0.00	0.00
ATOM	5517	CA	PRO	444	-1.240	27.777	33.702	1.00	0.00	0.158	9.40	4.00
ATOM	5518	HA	PRO	444	-0.908	26.963	33.057	1.00	0.00	0.053	0.00	0.00
ATOM	5519	CB	PRO	444	-2.547	28.347	33.153	1.00	0.00	-0.106	12.77	4.00
ATOM	5520	HB1	PRO	444	-3.140	27.572	32.666	1.00	0.00	0.053	0.00	0.00
ATOM	5521	HB2	PRO	444	-2.357	29.129	32.418	1.00	0.00	0.053	0.00	0.00
ATOM	5522	CG	PRO	444	-3.223	28.884	34.389	1.00	0.00	-0.106	12.77	4.00
ATOM	5523	HG1	PRO	444	-4.282	29.071	34.214	1.00	0.00	0.053	0.00	0.00
ATOM	5524	HG2	PRO	444	-2.774	29.823	34.712	1.00	0.00	0.053	0.00	0.00
ATOM	5525	C	PRO	444	-0.099	28.787	33.685	1.00	0.00	0.396	9.82	4.00
ATOM	5526	O	PRO	444	0.531	29.007	32.648	1.00	0.00	-0.396	8.17	-17.40
ATOM	5527	N	SER	445	0.184	29.385	34.838	1.00	0.00	-0.650	9.00	-17.40
ATOM	5528	HN	SER	445	-0.363	29.147	35.677	1.00	0.00	0.440	0.00	0.00
ATOM	5529	CA	SER	445	1.257	30.373	34.938	1.00	0.00	0.158	9.40	4.00
ATOM	5530	HA	SER	445	1.241	31.064	34.095	1.00	0.00	0.053	0.00	0.00
ATOM	5531	CB	SER	445	1.079	31.276	36.183	1.00	0.00	0.007	12.77	4.00
ATOM	5532	HB1	SER	445	0.117	31.789	36.199	1.00	0.00	0.053	0.00	0.00
ATOM	5533	HB2	SER	445	1.836	32.057	36.250	1.00	0.00	0.053	0.00	0.00
ATOM	5534	OG	SER	445	1.155	30.556	37.398	1.00	0.00	-0.537	11.04	-17.40
ATOM	5535	HG	SER	445	0.679	31.086	38.142	1.00	0.00	0.424	0.00	0.00
ATOM	5536	C	SER	445	2.629	29.706	34.957	1.00	0.00	0.396	9.82	4.00
ATOM	5537	O	SER	445	3.651	30.395	34.871	1.00	0.00	-0.396	8.17	-17.40
ATOM	5538	N	TRP	446	2.652	28.375	35.081	1.00	0.00	-0.650	9.00	-17.40
ATOM	5539	HN	TRP	446	1.764	27.863	35.190	1.00	0.00	0.440	0.00	0.00
ATOM	5540	CA	TRP	446	3.919	27.625	35.065	1.00	0.00	0.158	9.40	4.00
ATOM	5541	HA	TRP	446	4.705	28.165	35.592	1.00	0.00	0.053	0.00	0.00
ATOM	5542	CB	TRP	446	3.758	26.223	35.685	1.00	0.00	-0.106	12.77	4.00
ATOM	5543	HB1	TRP	446	4.536	25.583	35.270	1.00	0.00	0.053	0.00	0.00

ATOM	5544	HB2	TRP	446	2.766	25.854	35.422	1.00	0.00	0.053	0.00	0.00
ATOM	5545	CG	TRP	446	3.877	26.139	37.215	1.00	0.00	0.000	7.26	0.60
ATOM	5546	CD2	TRP	446	4.572	25.126	37.977	1.00	0.00	0.000	6.80	0.60
ATOM	5547	CE2	TRP	446	4.352	25.403	39.347	1.00	0.00	-0.050	6.80	0.60
ATOM	5548	CD1	TRP	446	3.286	26.964	38.138	1.00	0.00	-0.177	10.80	0.60
ATOM	5549	HD1	TRP	446	2.681	27.838	37.896	1.00	0.00	0.127	0.00	0.00
ATOM	5550	NE1	TRP	446	3.568	26.525	39.421	1.00	0.00	-0.292	9.00	-17.40
ATOM	5551	HE1	TRP	446	3.241	26.969	40.290	1.00	0.00	0.393	0.00	0.00
ATOM	5552	CE3	TRP	446	5.354	24.017	37.631	1.00	0.00	-0.127	10.80	0.60
ATOM	5553	HE3	TRP	446	5.543	23.776	36.584	1.00	0.00	0.127	0.00	0.00
ATOM	5554	CZ2	TRP	446	4.889	24.604	40.374	1.00	0.00	-0.127	10.80	0.60
ATOM	5555	HZ2	TRP	446	4.706	24.834	41.423	1.00	0.00	0.127	0.00	0.00
ATOM	5556	CZ3	TRP	446	5.887	23.225	38.648	1.00	0.00	-0.127	10.80	0.60
ATOM	5557	HZ3	TRP	446	6.497	22.359	38.389	1.00	0.00	0.127	0.00	0.00
ATOM	5558	CH2	TRP	446	5.650	23.525	40.004	1.00	0.00	-0.127	10.80	0.60
ATOM	5559	HH2	TRP	446	6.080	22.886	40.775	1.00	0.00	0.127	0.00	0.00
ATOM	5560	C	TRP	446	4.207	27.501	33.578	1.00	0.00	0.396	9.82	4.00
ATOM	5561	O	TRP	446	3.542	26.744	32.881	1.00	0.00	-0.396	8.17	-17.40
ATOM	5562	N	THR	447	5.180	28.267	33.087	1.00	0.00	-0.650	9.00	-17.40
ATOM	5563	HN	THR	447	5.710	28.881	33.721	1.00	0.00	0.440	0.00	0.00
ATOM	5564	CA	THR	447	5.506	28.250	31.668	1.00	0.00	-0.072	9.40	4.00
ATOM	5565	HA	THR	447	4.944	27.476	31.144	1.00	0.00	0.053	0.00	0.00
ATOM	5566	CB	THR	447	5.173	29.608	31.001	1.00	0.00	0.060	9.40	4.00
ATOM	5567	HB	THR	447	5.477	29.586	29.954	1.00	0.00	0.053	0.00	0.00
ATOM	5568	OG1	THR	447	5.874	30.663	31.678	1.00	0.00	-0.537	11.04	-17.40
ATOM	5569	HG1	THR	447	6.755	30.863	31.183	1.00	0.00	0.424	0.00	0.00
ATOM	5570	CG2	THR	447	3.664	29.893	31.083	1.00	0.00	-0.159	16.15	4.00
ATOM	5571	HG2	THR	447	3.448	30.850	30.609	1.00	0.00	0.053	0.00	0.00
ATOM	5572	HG2	THR	447	3.116	29.102	30.569	1.00	0.00	0.053	0.00	0.00
ATOM	5573	HG2	THR	447	3.356	29.927	32.128	1.00	0.00	0.053	0.00	0.00
ATOM	5574	C	THR	447	6.968	27.930	31.406	1.00	0.00	0.297	9.82	4.00
ATOM	5575	O	THR	447	7.719	27.750	32.375	1.00	0.00	-0.534	8.17	-17.40
ATOM	5576	OT2	THR	447	7.336	27.863	30.218	1.00	0.00	-0.534	0.00	0.00
ATOM	2812	MN	MN2	448	5.281	16.167	11.610	1.00	0.00	0.500	0.00	0.00

TABLE 2

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REMARK Solvation parameters added by "addsol"
REMARK
ATOM      1  N   GLU   325       5.889   2.827 -27.227  0.00  0.00    -0.247    9.00  -17.40
ATOM      2  HN1 GLU   325       5.803   2.916 -28.250  0.00  0.00     0.280    0.00    0.00
ATOM      3  HN2 GLU   325       6.121   3.745 -26.821  0.00  0.00     0.280    0.00    0.00
ATOM      4  HN3 GLU   325       6.636   2.155 -27.003  0.00  0.00     0.280    0.00    0.00
ATOM      5  CA  GLU   325       4.664   2.368 -26.689  0.00  0.00     0.354    9.40    4.00
ATOM      6  HA  GLU   325       3.856   3.064 -26.913  0.00  0.00     0.053    0.00    0.00
ATOM      7  C   GLU   325       4.925   2.286 -25.234  0.00  0.00     0.396    9.82    4.00
ATOM      8  O   GLU   325       5.847   2.890 -24.693  0.00  0.00    -0.396    8.17  -17.40
ATOM      9  CB  GLU   325       4.255   0.957 -27.143  0.00  0.00    -0.106   12.77    4.00
ATOM     10  HB1 GLU   325       3.368   0.660 -26.583  0.00  0.00     0.053    0.00    0.00
ATOM     11  HB2 GLU   325       5.082   0.277 -26.939  0.00  0.00     0.053    0.00    0.00
ATOM     12  CG  GLU   325       3.923   0.853 -28.631  0.00  0.00    -0.336   12.77    4.00
ATOM     13  HG1 GLU   325       4.763   1.263 -29.192  0.00  0.00     0.053    0.00    0.00
ATOM     14  HG2 GLU   325       3.015   1.427 -28.813  0.00  0.00     0.053    0.00    0.00
ATOM     15  CD  GLU   325       3.713  -0.619 -28.963  0.00  0.00     0.297    9.82    4.00
ATOM     16  OE1 GLU   325       3.260  -1.374 -28.061  0.00  0.00    -0.534    8.17  -18.95
ATOM     17  OE2 GLU   325       4.008  -1.007 -30.125  0.00  0.00    -0.534    8.17  -18.95
ATOM     18  N   ILE   326       4.038   1.575 -24.556  0.00  0.00    -0.650    9.00  -17.40
ATOM     19  HN  ILE   326       3.197   1.255 -25.057  0.00  0.00     0.439    0.00    0.00
ATOM     20  CA  ILE   326       4.164   1.223 -23.189  0.00  0.00     0.158    9.40    4.00
ATOM     21  HA  ILE   326       5.187   0.942 -22.938  0.00  0.00     0.053    0.00    0.00
ATOM     22  C   ILE   326       3.228   0.096 -23.112  0.00  0.00     0.396    9.82    4.00
ATOM     23  O   ILE   326       2.183   0.110 -23.756  0.00  0.00    -0.396    8.17  -17.40
ATOM     24  CB  ILE   326       3.636   2.222 -22.208  0.00  0.00    -0.053    9.40    4.00
ATOM     25  HB  ILE   326       3.492   1.749 -21.237  0.00  0.00     0.053    0.00    0.00
ATOM     26  CG1 ILE   326       2.197   2.583 -22.610  0.00  0.00    -0.106   12.77    4.00
ATOM     27 HG11ILE   326       1.715   1.683 -22.992  0.00  0.00     0.053    0.00    0.00
ATOM     28 HG12ILE   326       2.243   3.353 -23.380  0.00  0.00     0.053    0.00    0.00
ATOM     29  CG2 ILE   326       4.628   3.381 -22.057  0.00  0.00    -0.159   16.15    4.00
ATOM     30 HG21ILE   326       4.237   4.104 -21.341  0.00  0.00     0.053    0.00    0.00
ATOM     31 HG22ILE   326       5.584   2.998 -21.700  0.00  0.00     0.053    0.00    0.00
ATOM     32 HG23ILE   326       4.770   3.867 -23.022  0.00  0.00     0.053    0.00    0.00
ATOM     33  CD1 ILE   326       1.331   3.119 -21.480  0.00  0.00    -0.159   16.15    4.00
ATOM     34 HD11ILE   326       0.335   3.345 -21.861  0.00  0.00     0.053    0.00    0.00
ATOM     35 HD12ILE   326       1.257   2.370 -20.692  0.00  0.00     0.053    0.00    0.00
ATOM     36 HD13ILE   326       1.780   4.027 -21.077  0.00  0.00     0.053    0.00    0.00
ATOM     37  N   MET   327       3.548  -0.944 -22.358  0.00  0.00    -0.650    9.00  -17.40
ATOM     38  HN  MET   327       4.434  -1.035 -21.841  0.00  0.00     0.439    0.00    0.00
ATOM     39  CA  MET   327       2.518  -1.916 -22.353  0.00  0.00     0.158    9.40    4.00
ATOM     40  HA  MET   327       1.755  -1.687 -23.097  0.00  0.00     0.053    0.00    0.00
ATOM     41  C   MET   327       1.991  -1.822 -20.960  0.00  0.00     0.396    9.82    4.00
ATOM     42  O   MET   327       2.750  -1.601 -20.017  0.00  0.00    -0.396    8.17  -17.40
ATOM     43  CB  MET   327       3.047  -3.329 -22.608  0.00  0.00    -0.106   12.77    4.00
ATOM     44  HB1 MET   327       3.130  -3.826 -21.642  0.00  0.00     0.053    0.00    0.00
ATOM     45  HB2 MET   327       4.020  -3.232 -23.090  0.00  0.00     0.053    0.00    0.00
ATOM     46  CG  MET   327       2.213  -4.249 -23.498  0.00  0.00    -0.041   12.77    4.00
ATOM     47  HG1 MET   327       1.143  -4.083 -23.372  0.00  0.00     0.053    0.00    0.00
ATOM     48  HG2 MET   327       2.393  -5.302 -23.284  0.00  0.00     0.053    0.00    0.00
ATOM     49  SD  MET   327       2.574  -4.007 -25.264  0.00  0.00    -0.130   16.39   -6.40
ATOM     50  CE  MET   327       1.965  -5.631 -25.803  0.00  0.00    -0.094   16.15    4.00
ATOM     51  HE1 MET   327       2.084  -5.724 -26.883  0.00  0.00     0.053    0.00    0.00
ATOM     52  HE2 MET   327       2.535  -6.416 -25.306  0.00  0.00     0.053    0.00    0.00
ATOM     53  HE3 MET   327       0.911  -5.729 -25.544  0.00  0.00     0.053    0.00    0.00
ATOM     54  N   LYS   328       0.661  -1.911 -20.804  0.00  0.00    -0.650    9.00  -17.40
ATOM     55  HN  LYS   328       0.059  -2.026 -21.632  0.00  0.00     0.439    0.00    0.00
ATOM     56  CA  LYS   328       0.068  -1.848 -19.505  0.00  0.00     0.158    9.40    4.00
ATOM     57  HA  LYS   328       0.740  -1.223 -18.917  0.00  0.00     0.053    0.00    0.00
ATOM     58  C   LYS   328       0.009  -3.259 -19.038  0.00  0.00     0.396    9.82    4.00
ATOM     59  O   LYS   328      -0.599  -4.113 -19.684  0.00  0.00    -0.396    8.17  -17.40
ATOM     60  CB  LYS   328      -1.375  -1.325 -19.551  0.00  0.00    -0.106   12.77    4.00
ATOM     61  HB1 LYS   328      -1.955  -1.989 -20.191  0.00  0.00     0.053    0.00    0.00
ATOM     62  HB2 LYS   328      -1.356  -0.314 -19.958  0.00  0.00     0.053    0.00    0.00
ATOM     63  CG  LYS   328      -2.086  -1.259 -18.199  0.00  0.00    -0.106   12.77    4.00
ATOM     64  HG1 LYS   328      -1.521  -0.685 -17.464  0.00  0.00     0.053    0.00    0.00
ATOM     65  HG2 LYS   328      -2.244  -2.248 -17.768  0.00  0.00     0.053    0.00    0.00
ATOM     66  CD  LYS   328      -3.465  -0.601 -18.302  0.00  0.00    -0.106   12.77    4.00
ATOM     67  HD1 LYS   328      -3.981  -1.021 -19.165  0.00  0.00     0.053    0.00    0.00
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ATOM	68	HD2	LYS	328	-3.324	0.473	-18.425	0.00	0.00	0.053	0.00	0.00
ATOM	69	CE	LYS	328	-4.356	-0.816	-17.077	0.00	0.00	0.099	12.77	4.00
ATOM	70	HE1	LYS	328	-3.858	-1.464	-16.356	0.00	0.00	0.053	0.00	0.00
ATOM	71	HE2	LYS	328	-5.297	-1.280	-17.371	0.00	0.00	0.053	0.00	0.00
ATOM	72	NZ	LYS	328	-4.651	0.478	-16.424	0.00	0.00	-0.045	13.25	-39.20
ATOM	73	HZ1	LYS	328	-5.251	0.319	-15.602	0.00	0.00	0.280	0.00	0.00
ATOM	74	HZ2	LYS	328	-3.770	0.921	-16.126	0.00	0.00	0.280	0.00	0.00
ATOM	75	HZ3	LYS	328	-5.137	1.096	-17.089	0.00	0.00	0.280	0.00	0.00
ATOM	76	N	LYS	329	0.672	-3.552	-17.908	0.00	0.00	-0.650	9.00	-17.40
ATOM	77	HN	LYS	329	1.198	-2.826	-17.401	0.00	0.00	0.439	0.00	0.00
ATOM	78	CA	LYS	329	0.629	-4.896	-17.427	0.00	0.00	0.158	9.40	4.00
ATOM	79	HA	LYS	329	0.361	-5.514	-18.284	0.00	0.00	0.053	0.00	0.00
ATOM	80	C	LYS	329	-0.409	-4.917	-16.355	0.00	0.00	0.396	9.82	4.00
ATOM	81	O	LYS	329	-0.296	-4.213	-15.354	0.00	0.00	-0.396	8.17	-17.40
ATOM	82	CB	LYS	329	1.963	-5.362	-16.824	0.00	0.00	-0.106	12.77	4.00
ATOM	83	HB1	LYS	329	1.907	-6.378	-16.434	0.00	0.00	0.053	0.00	0.00
ATOM	84	HB2	LYS	329	2.286	-4.730	-15.997	0.00	0.00	0.053	0.00	0.00
ATOM	85	CG	LYS	329	3.100	-5.351	-17.851	0.00	0.00	-0.106	12.77	4.00
ATOM	86	HG1	LYS	329	3.128	-4.366	-18.317	0.00	0.00	0.053	0.00	0.00
ATOM	87	HG2	LYS	329	2.896	-6.123	-18.593	0.00	0.00	0.053	0.00	0.00
ATOM	88	CD	LYS	329	4.486	-5.625	-17.273	0.00	0.00	-0.106	12.77	4.00
ATOM	89	HD1	LYS	329	5.029	-6.265	-17.969	0.00	0.00	0.053	0.00	0.00
ATOM	90	HD2	LYS	329	4.365	-6.123	-16.311	0.00	0.00	0.053	0.00	0.00
ATOM	91	CE	LYS	329	5.323	-4.366	-17.046	0.00	0.00	0.099	12.77	4.00
ATOM	92	HE1	LYS	329	5.269	-3.719	-17.922	0.00	0.00	0.053	0.00	0.00
ATOM	93	HE2	LYS	329	6.364	-4.637	-16.870	0.00	0.00	0.053	0.00	0.00
ATOM	94	NZ	LYS	329	4.815	-3.625	-15.871	0.00	0.00	-0.045	13.25	-39.20
ATOM	95	HZ1	LYS	329	5.384	-2.779	-15.726	0.00	0.00	0.280	0.00	0.00
ATOM	96	HZ2	LYS	329	3.834	-3.355	-16.033	0.00	0.00	0.280	0.00	0.00
ATOM	97	HZ3	LYS	329	4.872	-4.225	-15.035	0.00	0.00	0.280	0.00	0.00
ATOM	98	N	VAL	330	-1.468	-5.726	-16.549	0.00	0.00	-0.650	9.00	-17.40
ATOM	99	HN	VAL	330	-1.528	-6.305	-17.398	0.00	0.00	0.439	0.00	0.00
ATOM	100	CA	VAL	330	-2.511	-5.777	-15.569	0.00	0.00	0.158	9.40	4.00
ATOM	101	HA	VAL	330	-2.417	-4.885	-14.949	0.00	0.00	0.053	0.00	0.00
ATOM	102	C	VAL	330	-2.310	-7.022	-14.772	0.00	0.00	0.396	9.82	4.00
ATOM	103	O	VAL	330	-2.198	-8.117	-15.321	0.00	0.00	-0.396	8.17	-17.40
ATOM	104	CB	VAL	330	-3.891	-5.844	-16.166	0.00	0.00	-0.053	9.40	4.00
ATOM	105	HB	VAL	330	-3.944	-6.698	-16.841	0.00	0.00	0.053	0.00	0.00
ATOM	106	CG1	VAL	330	-4.919	-6.005	-15.032	0.00	0.00	-0.159	16.15	4.00
ATOM	107	HG11	VAL	330	-5.922	-6.055	-15.455	0.00	0.00	0.053	0.00	0.00
ATOM	108	HG12	VAL	330	-4.712	-6.922	-14.481	0.00	0.00	0.053	0.00	0.00
ATOM	109	HG13	VAL	330	-4.852	-5.152	-14.356	0.00	0.00	0.053	0.00	0.00
ATOM	110	CG2	VAL	330	-4.117	-4.588	-17.024	0.00	0.00	-0.159	16.15	4.00
ATOM	111	HG21	VAL	330	-5.114	-4.622	-17.464	0.00	0.00	0.053	0.00	0.00
ATOM	112	HG22	VAL	330	-4.026	-3.699	-16.399	0.00	0.00	0.053	0.00	0.00
ATOM	113	HG23	VAL	330	-3.371	-4.551	-17.818	0.00	0.00	0.053	0.00	0.00
ATOM	114	N	VAL	331	-2.242	-6.874	-13.436	0.00	0.00	-0.650	9.00	-17.40
ATOM	115	HN	VAL	331	-2.311	-5.934	-13.021	0.00	0.00	0.439	0.00	0.00
ATOM	116	CA	VAL	331	-2.074	-8.013	-12.589	0.00	0.00	0.158	9.40	4.00
ATOM	117	HA	VAL	331	-1.580	-8.769	-13.199	0.00	0.00	0.053	0.00	0.00
ATOM	118	C	VAL	331	-3.446	-8.416	-12.169	0.00	0.00	0.396	9.82	4.00
ATOM	119	O	VAL	331	-4.267	-7.577	-11.798	0.00	0.00	-0.396	8.17	-17.40
ATOM	120	CB	VAL	331	-1.278	-7.731	-11.349	0.00	0.00	-0.053	9.40	4.00
ATOM	121	HB	VAL	331	-1.751	-6.909	-10.812	0.00	0.00	0.053	0.00	0.00
ATOM	122	CG1	VAL	331	-1.261	-8.999	-10.479	0.00	0.00	-0.159	16.15	4.00
ATOM	123	HG11	VAL	331	-0.686	-8.811	-9.573	0.00	0.00	0.053	0.00	0.00
ATOM	124	HG12	VAL	331	-2.282	-9.270	-10.211	0.00	0.00	0.053	0.00	0.00
ATOM	125	HG13	VAL	331	-0.803	-9.816	-11.036	0.00	0.00	0.053	0.00	0.00
ATOM	126	CG2	VAL	331	0.122	-7.250	-11.768	0.00	0.00	-0.159	16.15	4.00
ATOM	127	HG21	VAL	331	0.716	-7.040	-10.878	0.00	0.00	0.053	0.00	0.00
ATOM	128	HG22	VAL	331	0.612	-8.026	-12.357	0.00	0.00	0.053	0.00	0.00
ATOM	129	HG23	VAL	331	0.031	-6.343	-12.366	0.00	0.00	0.053	0.00	0.00
ATOM	130	N	GLY	332	-3.739	-9.727	-12.240	0.00	0.00	-0.650	9.00	-17.40
ATOM	131	HN	GLY	332	-3.024	-10.407	-12.534	0.00	0.00	0.439	0.00	0.00
ATOM	132	CA	GLY	332	-5.059	-10.163	-11.901	0.00	0.00	0.105	9.40	4.00
ATOM	133	HA1	GLY	332	-5.574	-10.451	-12.817	0.00	0.00	0.053	0.00	0.00
ATOM	134	HA2	GLY	332	-5.581	-9.339	-11.414	0.00	0.00	0.053	0.00	0.00
ATOM	135	C	GLY	332	-4.950	-11.326	-10.979	0.00	0.00	0.396	9.82	4.00
ATOM	136	O	GLY	332	-3.976	-12.080	-11.005	0.00	0.00	-0.396	8.17	-17.40
ATOM	137	N	ASN	333	-5.985	-11.495	-10.136	0.00	0.00	-0.650	9.00	-17.40
ATOM	138	HN	ASN	333	-6.781	-10.842	-10.180	0.00	0.00	0.439	0.00	0.00
ATOM	139	CA	ASN	333	-6.008	-12.557	-9.181	0.00	0.00	0.158	9.40	4.00
ATOM	140	HA	ASN	333	-5.416	-13.372	-9.597	0.00	0.00	0.053	0.00	0.00
ATOM	141	C	ASN	333	-7.441	-12.948	-8.996	0.00	0.00	0.396	9.82	4.00
ATOM	142	O	ASN	333	-7.893	-13.943	-9.558	0.00	0.00	-0.396	8.17	-17.40
ATOM	143	CB	ASN	333	-5.475	-12.126	-7.804	0.00	0.00	-0.106	12.77	4.00

ATOM	144	HB1	ASN	333	-6.218	-11.476	-7.341	0.00	0.00	0.053	0.00	0.00
ATOM	145	HB2	ASN	333	-4.536	-11.594	-7.955	0.00	0.00	0.053	0.00	0.00
ATOM	146	CG	ASN	333	-5.257	-13.378	-6.968	0.00	0.00	0.396	9.82	4.00
ATOM	147	OD1	ASN	333	-5.849	-14.424	-7.227	0.00	0.00	-0.396	8.17	-17.40
ATOM	148	ND2	ASN	333	-4.380	-13.272	-5.935	0.00	0.00	-0.879	13.25	-17.40
ATOM	149	HD21	ASN	333	-3.905	-12.376	-5.753	0.00	0.00	0.439	0.00	0.00
ATOM	150	HD22	ASN	333	-4.190	-14.087	-5.335	0.00	0.00	0.439	0.00	0.00
ATOM	151	N	ARG	334	-8.201	-12.153	-8.213	0.00	0.00	-0.650	9.00	-17.40
ATOM	152	HN	ARG	334	-7.794	-11.295	-7.814	0.00	0.00	0.439	0.00	0.00
ATOM	153	CA	ARG	334	-9.567	-12.486	-7.928	0.00	0.00	0.158	9.40	4.00
ATOM	154	HA	ARG	334	-9.632	-13.566	-7.794	0.00	0.00	0.053	0.00	0.00
ATOM	155	C	ARG	334	-10.403	-12.045	-9.082	0.00	0.00	0.396	9.82	4.00
ATOM	156	O	ARG	334	-10.533	-10.852	-9.351	0.00	0.00	-0.396	8.17	-17.40
ATOM	157	CB	ARG	334	-10.110	-11.768	-6.685	0.00	0.00	-0.106	12.77	4.00
ATOM	158	HB1	ARG	334	-11.116	-12.084	-6.409	0.00	0.00	0.053	0.00	0.00
ATOM	159	HB2	ARG	334	-10.169	-10.686	-6.803	0.00	0.00	0.053	0.00	0.00
ATOM	160	CG	ARG	334	-9.258	-11.993	-5.435	0.00	0.00	-0.106	12.77	4.00
ATOM	161	HG1	ARG	334	-8.220	-11.685	-5.560	0.00	0.00	0.053	0.00	0.00
ATOM	162	HG2	ARG	334	-9.215	-13.037	-5.125	0.00	0.00	0.053	0.00	0.00
ATOM	163	CD	ARG	334	-9.764	-11.227	-4.212	0.00	0.00	0.374	12.77	4.00
ATOM	164	HD1	ARG	334	-9.005	-11.318	-3.435	0.00	0.00	0.053	0.00	0.00
ATOM	165	HD2	ARG	334	-10.705	-11.686	-3.908	0.00	0.00	0.053	0.00	0.00
ATOM	166	NE	ARG	334	-9.956	-9.807	-4.626	0.00	0.00	-0.819	9.00	-24.67
ATOM	167	HE	ARG	334	-10.900	-9.470	-4.862	0.00	0.00	0.407	0.00	0.00
ATOM	168	CZ	ARG	334	-8.896	-8.948	-4.696	0.00	0.00	0.796	6.95	4.00
ATOM	169	NH1	ARG	334	-7.633	-9.391	-4.426	0.00	0.00	-0.746	9.00	-24.67
ATOM	170	HH11	ARG	334	-6.836	-8.740	-4.480	0.00	0.00	0.407	0.00	0.00
ATOM	171	HH12	ARG	334	-7.477	-10.376	-4.168	0.00	0.00	0.407	0.00	0.00
ATOM	172	NH2	ARG	334	-9.102	-7.645	-5.049	0.00	0.00	-0.746	9.00	-24.67
ATOM	173	HH21	ARG	334	-8.306	-6.994	-5.103	0.00	0.00	0.407	0.00	0.00
ATOM	174	HH22	ARG	334	-10.054	-7.313	-5.261	0.00	0.00	0.407	0.00	0.00
ATOM	175	N	SER	335	-10.989	-13.015	-9.805	0.00	0.00	-0.650	9.00	-17.40
ATOM	176	HN	SER	335	-10.837	-14.004	-9.561	0.00	0.00	0.439	0.00	0.00
ATOM	177	CA	SER	335	-11.824	-12.671	-10.913	0.00	0.00	0.158	9.40	4.00
ATOM	178	HA	SER	335	-11.235	-12.037	-11.576	0.00	0.00	0.053	0.00	0.00
ATOM	179	C	SER	335	-13.001	-11.949	-10.368	0.00	0.00	0.396	9.82	4.00
ATOM	180	O	SER	335	-13.358	-10.879	-10.859	0.00	0.00	-0.396	8.17	-17.40
ATOM	181	CB	SER	335	-12.348	-13.901	-11.672	0.00	0.00	0.007	12.77	4.00
ATOM	182	HB1	SER	335	-12.935	-14.532	-11.005	0.00	0.00	0.053	0.00	0.00
ATOM	183	HB2	SER	335	-11.515	-14.484	-12.064	0.00	0.00	0.053	0.00	0.00
ATOM	184	OG	SER	335	-13.170	-13.494	-12.756	0.00	0.00	-0.537	11.04	-17.40
ATOM	185	HG	SER	335	-13.091	-12.475	-12.884	0.00	0.00	0.424	0.00	0.00
ATOM	186	N	GLY	336	-13.600	-12.511	-9.297	0.00	0.00	-0.650	9.00	-17.40
ATOM	187	HN	GLY	336	-13.203	-13.366	-8.882	0.00	0.00	0.439	0.00	0.00
ATOM	188	CA	GLY	336	-14.779	-11.932	-8.732	0.00	0.00	0.105	9.40	4.00
ATOM	189	HA1	GLY	336	-14.470	-10.957	-8.356	0.00	0.00	0.053	0.00	0.00
ATOM	190	HA2	GLY	336	-15.088	-12.619	-7.944	0.00	0.00	0.053	0.00	0.00
ATOM	191	C	GLY	336	-15.752	-11.848	-9.853	0.00	0.00	0.396	9.82	4.00
ATOM	192	O	GLY	336	-16.373	-12.840	-10.236	0.00	0.00	-0.396	8.17	-17.40
ATOM	193	N	CYS	337	-15.913	-10.631	-10.396	0.00	0.00	-0.650	9.00	-17.40
ATOM	194	HN	CYS	337	-15.427	-9.827	-9.974	0.00	0.00	0.439	0.00	0.00
ATOM	195	CA	CYS	337	-16.737	-10.418	-11.540	0.00	0.00	0.158	9.40	4.00
ATOM	196	HA	CYS	337	-16.389	-11.120	-12.297	0.00	0.00	0.053	0.00	0.00
ATOM	197	C	CYS	337	-16.530	-8.990	-11.939	0.00	0.00	0.396	9.82	4.00
ATOM	198	O	CYS	337	-15.627	-8.716	-12.729	0.00	0.00	-0.396	8.17	-17.40
ATOM	199	CB	CYS	337	-18.236	-10.745	-11.345	0.00	0.00	-0.041	12.77	4.00
ATOM	200	HB1	CYS	337	-18.690	-10.145	-10.556	0.00	0.00	0.053	0.00	0.00
ATOM	201	HB2	CYS	337	-18.398	-11.788	-11.074	0.00	0.00	0.053	0.00	0.00
ATOM	202	SG	CYS	337	-19.208	-10.442	-12.853	0.00	0.00	-0.255	19.93	-6.40
ATOM	203	HG	CYS	337	-19.237	-9.127	-13.110	0.00	0.00	0.190	0.00	0.00
ATOM	204	N	PRO	338	-17.314	-8.066	-11.440	0.00	0.00	-0.422	9.00	-17.40
ATOM	205	CA	PRO	338	-17.193	-6.706	-11.888	0.00	0.00	0.158	9.40	4.00
ATOM	206	HA	PRO	338	-17.424	-6.630	-12.950	0.00	0.00	0.053	0.00	0.00
ATOM	207	CD	PRO	338	-17.724	-8.098	-10.038	0.00	0.00	0.105	12.77	4.00
ATOM	208	HD1	PRO	338	-16.889	-8.538	-9.492	0.00	0.00	0.053	0.00	0.00
ATOM	209	HD2	PRO	338	-18.622	-8.714	-10.003	0.00	0.00	0.053	0.00	0.00
ATOM	210	C	PRO	338	-15.802	-6.203	-11.673	0.00	0.00	0.396	9.82	4.00
ATOM	211	O	PRO	338	-15.308	-5.431	-12.492	0.00	0.00	-0.396	8.17	-17.40
ATOM	212	CB	PRO	338	-18.133	-5.912	-10.991	0.00	0.00	-0.106	12.77	4.00
ATOM	213	HB1	PRO	338	-19.156	-5.940	-11.366	0.00	0.00	0.053	0.00	0.00
ATOM	214	HB2	PRO	338	-17.833	-4.866	-10.930	0.00	0.00	0.053	0.00	0.00
ATOM	215	CG	PRO	338	-17.989	-6.637	-9.643	0.00	0.00	-0.106	12.77	4.00
ATOM	216	HG1	PRO	338	-18.899	-6.540	-9.050	0.00	0.00	0.053	0.00	0.00
ATOM	217	HG2	PRO	338	-17.164	-6.222	-9.064	0.00	0.00	0.053	0.00	0.00
ATOM	218	N	THR	339	-15.145	-6.630	-10.580	0.00	0.00	-0.650	9.00	-17.40
ATOM	219	HN	THR	339	-15.539	-7.380	-9.994	0.00	0.00	0.439	0.00	0.00

ATOM	220	CA	THR	339	-13.892	-6.029	-10.243	0.00	0.00	0.158	9.40	4.00
ATOM	221	HA	THR	339	-13.989	-4.959	-10.059	0.00	0.00	0.053	0.00	0.00
ATOM	222	C	THR	339	-12.881	-6.191	-11.334	0.00	0.00	0.396	9.82	4.00
ATOM	223	O	THR	339	-12.377	-5.197	-11.853	0.00	0.00	-0.396	8.17	-17.40
ATOM	224	CB	THR	339	-13.334	-6.570	-8.956	0.00	0.00	0.060	9.40	4.00
ATOM	225	HB	THR	339	-14.012	-6.335	-8.136	0.00	0.00	0.053	0.00	0.00
ATOM	226	OG1	THR	339	-12.095	-5.945	-8.652	0.00	0.00	-0.537	11.04	-17.40
ATOM	227	HG1	THR	339	-11.368	-6.293	-9.293	0.00	0.00	0.424	0.00	0.00
ATOM	228	CG2	THR	339	-13.175	-8.096	-9.064	0.00	0.00	-0.159	16.15	4.00
ATOM	229	HG21	THR	339	-12.770	-8.487	-8.130	0.00	0.00	0.053	0.00	0.00
ATOM	230	HG22	THR	339	-14.147	-8.550	-9.257	0.00	0.00	0.053	0.00	0.00
ATOM	231	HG23	THR	339	-12.495	-8.334	-9.882	0.00	0.00	0.053	0.00	0.00
ATOM	232	N	VAL	340	-12.555	-7.430	-11.737	0.00	0.00	-0.650	9.00	-17.40
ATOM	233	HN	VAL	340	-12.998	-8.260	-11.318	0.00	0.00	0.439	0.00	0.00
ATOM	234	CA	VAL	340	-11.570	-7.559	-12.770	0.00	0.00	0.158	9.40	4.00
ATOM	235	HA	VAL	340	-10.686	-7.001	-12.462	0.00	0.00	0.053	0.00	0.00
ATOM	236	C	VAL	340	-12.145	-6.997	-14.025	0.00	0.00	0.396	9.82	4.00
ATOM	237	O	VAL	340	-11.651	-6.018	-14.582	0.00	0.00	-0.396	8.17	-17.40
ATOM	238	CB	VAL	340	-11.288	-9.002	-13.089	0.00	0.00	-0.053	9.40	4.00
ATOM	239	HB	VAL	340	-12.220	-9.507	-13.342	0.00	0.00	0.053	0.00	0.00
ATOM	240	CG1	VAL	340	-10.323	-9.083	-14.279	0.00	0.00	-0.159	16.15	4.00
ATOM	241	HG11	VAL	340	-10.118	-10.128	-14.511	0.00	0.00	0.053	0.00	0.00
ATOM	242	HG12	VAL	340	-10.774	-8.601	-15.146	0.00	0.00	0.053	0.00	0.00
ATOM	243	HG13	VAL	340	-9.391	-8.578	-14.026	0.00	0.00	0.053	0.00	0.00
ATOM	244	CG2	VAL	340	-10.783	-9.715	-11.832	0.00	0.00	-0.159	16.15	4.00
ATOM	245	HG21	VAL	340	-10.579	-10.760	-12.064	0.00	0.00	0.053	0.00	0.00
ATOM	246	HG22	VAL	340	-9.868	-9.235	-11.484	0.00	0.00	0.053	0.00	0.00
ATOM	247	HG23	VAL	340	-11.542	-9.658	-11.052	0.00	0.00	0.053	0.00	0.00
ATOM	248	N	GLY	341	-13.265	-7.598	-14.463	0.00	0.00	-0.650	9.00	-17.40
ATOM	249	HN	GLY	341	-13.745	-8.291	-13.871	0.00	0.00	0.439	0.00	0.00
ATOM	250	CA	GLY	341	-13.787	-7.273	-15.752	0.00	0.00	0.105	9.40	4.00
ATOM	251	HA1	GLY	341	-14.618	-7.907	-16.062	0.00	0.00	0.053	0.00	0.00
ATOM	252	HA2	GLY	341	-13.056	-7.358	-16.556	0.00	0.00	0.053	0.00	0.00
ATOM	253	C	GLY	341	-14.308	-5.883	-15.855	0.00	0.00	0.396	9.82	4.00
ATOM	254	O	GLY	341	-13.731	-5.065	-16.570	0.00	0.00	-0.396	8.17	-17.40
ATOM	255	N	ASP	342	-15.382	-5.553	-15.109	0.00	0.00	-0.650	9.00	-17.40
ATOM	256	HN	ASP	342	-15.758	-6.179	-14.383	0.00	0.00	0.439	0.00	0.00
ATOM	257	CA	ASP	342	-15.966	-4.278	-15.390	0.00	0.00	0.158	9.40	4.00
ATOM	258	HA	ASP	342	-15.892	-4.075	-16.458	0.00	0.00	0.053	0.00	0.00
ATOM	259	C	ASP	342	-15.243	-3.230	-14.633	0.00	0.00	0.396	9.82	4.00
ATOM	260	O	ASP	342	-15.832	-2.286	-14.108	0.00	0.00	-0.396	8.17	-17.40
ATOM	261	CB	ASP	342	-17.499	-4.187	-15.169	0.00	0.00	-0.336	12.77	4.00
ATOM	262	HB1	ASP	342	-17.978	-4.952	-15.780	0.00	0.00	0.053	0.00	0.00
ATOM	263	HB2	ASP	342	-17.829	-3.192	-15.469	0.00	0.00	0.053	0.00	0.00
ATOM	264	CG	ASP	342	-17.941	-4.404	-13.729	0.00	0.00	0.297	9.82	4.00
ATOM	265	OD1	ASP	342	-17.289	-3.882	-12.788	0.00	0.00	-0.534	8.17	-18.95
ATOM	266	OD2	ASP	342	-18.974	-5.106	-13.562	0.00	0.00	-0.534	8.17	-18.95
ATOM	267	N	ARG	343	-13.911	-3.375	-14.583	0.00	0.00	-0.650	9.00	-17.40
ATOM	268	HN	ARG	343	-13.465	-4.208	-14.992	0.00	0.00	0.439	0.00	0.00
ATOM	269	CA	ARG	343	-13.119	-2.373	-13.963	0.00	0.00	0.158	9.40	4.00
ATOM	270	HA	ARG	343	-13.772	-1.888	-13.237	0.00	0.00	0.053	0.00	0.00
ATOM	271	C	ARG	343	-12.690	-1.459	-15.063	0.00	0.00	0.396	9.82	4.00
ATOM	272	O	ARG	343	-12.634	-0.246	-14.879	0.00	0.00	-0.396	8.17	-17.40
ATOM	273	CB	ARG	343	-11.844	-2.932	-13.305	0.00	0.00	-0.106	12.77	4.00
ATOM	274	HB1	ARG	343	-11.084	-3.239	-14.024	0.00	0.00	0.053	0.00	0.00
ATOM	275	HB2	ARG	343	-12.025	-3.811	-12.687	0.00	0.00	0.053	0.00	0.00
ATOM	276	CG	ARG	343	-11.145	-1.930	-12.384	0.00	0.00	-0.106	12.77	4.00
ATOM	277	HG1	ARG	343	-11.110	-0.967	-12.893	0.00	0.00	0.053	0.00	0.00
ATOM	278	HG2	ARG	343	-10.138	-2.297	-12.183	0.00	0.00	0.053	0.00	0.00
ATOM	279	CD	ARG	343	-11.836	-1.714	-11.032	0.00	0.00	0.374	12.77	4.00
ATOM	280	HD1	ARG	343	-11.189	-1.108	-10.398	0.00	0.00	0.053	0.00	0.00
ATOM	281	HD2	ARG	343	-12.013	-2.684	-10.567	0.00	0.00	0.053	0.00	0.00
ATOM	282	NE	ARG	343	-13.133	-1.011	-11.259	0.00	0.00	-0.819	9.00	-24.67
ATOM	283	HE	ARG	343	-13.146	0.015	-11.347	0.00	0.00	0.407	0.00	0.00
ATOM	284	CZ	ARG	343	-14.302	-1.711	-11.351	0.00	0.00	0.796	6.95	4.00
ATOM	285	NH1	ARG	343	-14.297	-3.070	-11.230	0.00	0.00	-0.746	9.00	-24.67
ATOM	286	HH11	ARG	343	-15.180	-3.596	-11.300	0.00	0.00	0.407	0.00	0.00
ATOM	287	HH12	ARG	343	-13.411	-3.569	-11.069	0.00	0.00	0.407	0.00	0.00
ATOM	288	NH2	ARG	343	-15.476	-1.049	-11.567	0.00	0.00	-0.746	9.00	-24.67
ATOM	289	HH21	ARG	343	-16.359	-1.575	-11.637	0.00	0.00	0.407	0.00	0.00
ATOM	290	HH22	ARG	343	-15.479	-0.023	-11.660	0.00	0.00	0.407	0.00	0.00
ATOM	291	N	ILE	344	-12.440	-2.035	-16.262	0.00	0.00	-0.650	9.00	-17.40
ATOM	292	HN	ILE	344	-12.563	-3.053	-16.354	0.00	0.00	0.439	0.00	0.00
ATOM	293	CA	ILE	344	-12.012	-1.290	-17.408	0.00	0.00	0.158	9.40	4.00
ATOM	294	HA	ILE	344	-12.459	-0.296	-17.388	0.00	0.00	0.053	0.00	0.00
ATOM	295	C	ILE	344	-12.441	-2.003	-18.669	0.00	0.00	0.396	9.82	4.00

ATOM	296	O	ILE	344	-12.607	-3.217	-18.642	0.00	0.00	-0.396	8.17	-17.40
ATOM	297	CB	ILE	344	-10.506	-1.134	-17.348	0.00	0.00	-0.053	9.40	4.00
ATOM	298	HB	ILE	344	-10.200	-0.636	-18.268	0.00	0.00	0.053	0.00	0.00
ATOM	299	CG1	ILE	344	-9.803	-2.485	-17.271	0.00	0.00	-0.106	12.77	4.00
ATOM	300	HG11	ILE	344	-10.151	-3.205	-18.011	0.00	0.00	0.053	0.00	0.00
ATOM	301	HG12	ILE	344	-9.924	-2.990	-16.313	0.00	0.00	0.053	0.00	0.00
ATOM	302	CG2	ILE	344	-10.192	-0.287	-16.110	0.00	0.00	-0.159	16.15	4.00
ATOM	303	HG21	ILE	344	-9.114	-0.149	-16.027	0.00	0.00	0.053	0.00	0.00
ATOM	304	HG22	ILE	344	-10.676	0.685	-16.202	0.00	0.00	0.053	0.00	0.00
ATOM	305	HG23	ILE	344	-10.562	-0.794	-15.219	0.00	0.00	0.053	0.00	0.00
ATOM	306	CD1	ILE	344	-8.293	-2.407	-17.483	0.00	0.00	-0.159	16.15	4.00
ATOM	307	HD11	ILE	344	-7.864	-3.407	-17.414	0.00	0.00	0.053	0.00	0.00
ATOM	308	HD12	ILE	344	-8.085	-1.990	-18.468	0.00	0.00	0.053	0.00	0.00
ATOM	309	HD13	ILE	344	-7.851	-1.769	-16.718	0.00	0.00	0.053	0.00	0.00
ATOM	310	N	VAL	345	-12.690	-1.280	-19.800	0.00	0.00	-0.650	9.00	-17.40
ATOM	311	HN	VAL	345	-12.586	-0.255	-19.808	0.00	0.00	0.439	0.00	0.00
ATOM	312	CA	VAL	345	-13.105	-1.998	-20.988	0.00	0.00	0.158	9.40	4.00
ATOM	313	HA	VAL	345	-13.852	-2.708	-20.633	0.00	0.00	0.053	0.00	0.00
ATOM	314	C	VAL	345	-11.857	-2.638	-21.496	0.00	0.00	0.396	9.82	4.00
ATOM	315	O	VAL	345	-11.894	-3.537	-22.335	0.00	0.00	-0.396	8.17	-17.40
ATOM	316	CB	VAL	345	-13.636	-1.263	-22.215	0.00	0.00	-0.053	9.40	4.00
ATOM	317	HB	VAL	345	-14.156	-1.982	-22.848	0.00	0.00	0.053	0.00	0.00
ATOM	318	CG1	VAL	345	-14.616	-0.134	-21.884	0.00	0.00	-0.159	16.15	4.00
ATOM	319	HG11	VAL	345	-14.949	0.341	-22.807	0.00	0.00	0.053	0.00	0.00
ATOM	320	HG12	VAL	345	-15.477	-0.543	-21.355	0.00	0.00	0.053	0.00	0.00
ATOM	321	HG13	VAL	345	-14.121	0.605	-21.254	0.00	0.00	0.053	0.00	0.00
ATOM	322	CG2	VAL	345	-12.506	-0.921	-23.176	0.00	0.00	-0.159	16.15	4.00
ATOM	323	HG21	VAL	345	-12.911	-0.398	-24.042	0.00	0.00	0.053	0.00	0.00
ATOM	324	HG22	VAL	345	-11.781	-0.282	-22.672	0.00	0.00	0.053	0.00	0.00
ATOM	325	HG23	VAL	345	-12.016	-1.838	-23.503	0.00	0.00	0.053	0.00	0.00
ATOM	326	N	GLU	346	-10.691	-2.122	-21.067	0.00	0.00	-0.650	9.00	-17.40
ATOM	327	HN	GLU	346	-10.636	-1.267	-20.495	0.00	0.00	0.439	0.00	0.00
ATOM	328	CA	GLU	346	-9.542	-2.853	-21.468	0.00	0.00	0.158	9.40	4.00
ATOM	329	HA	GLU	346	-9.610	-2.878	-22.556	0.00	0.00	0.053	0.00	0.00
ATOM	330	C	GLU	346	-9.709	-4.171	-20.817	0.00	0.00	0.396	9.82	4.00
ATOM	331	O	GLU	346	-9.628	-5.209	-21.471	0.00	0.00	-0.396	8.17	-17.40
ATOM	332	CB	GLU	346	-8.193	-2.317	-20.949	0.00	0.00	-0.106	12.77	4.00
ATOM	333	HB1	GLU	346	-7.488	-3.148	-20.933	0.00	0.00	0.053	0.00	0.00
ATOM	334	HB2	GLU	346	-8.355	-1.921	-19.946	0.00	0.00	0.053	0.00	0.00
ATOM	335	CG	GLU	346	-7.548	-1.201	-21.770	0.00	0.00	-0.336	12.77	4.00
ATOM	336	HG1	GLU	346	-6.685	-0.822	-21.223	0.00	0.00	0.053	0.00	0.00
ATOM	337	HG2	GLU	346	-8.282	-0.408	-21.916	0.00	0.00	0.053	0.00	0.00
ATOM	338	CD	GLU	346	-7.115	-1.774	-23.111	0.00	0.00	0.297	9.82	4.00
ATOM	339	OE1	GLU	346	-7.943	-2.477	-23.747	0.00	0.00	-0.534	8.17	-18.95
ATOM	340	OE2	GLU	346	-5.950	-1.513	-23.517	0.00	0.00	-0.534	8.17	-18.95
ATOM	341	N	LEU	347	-9.973	-4.165	-19.496	0.00	0.00	-0.650	9.00	-17.40
ATOM	342	HN	LEU	347	-10.122	-3.299	-18.959	0.00	0.00	0.439	0.00	0.00
ATOM	343	CA	LEU	347	-10.028	-5.452	-18.910	0.00	0.00	0.158	9.40	4.00
ATOM	344	HA	LEU	347	-9.121	-6.001	-19.164	0.00	0.00	0.053	0.00	0.00
ATOM	345	C	LEU	347	-11.225	-6.183	-19.436	0.00	0.00	0.396	9.82	4.00
ATOM	346	O	LEU	347	-11.059	-7.053	-20.281	0.00	0.00	-0.396	8.17	-17.40
ATOM	347	CB	LEU	347	-9.967	-5.426	-17.377	0.00	0.00	-0.106	12.77	4.00
ATOM	348	HB1	LEU	347	-10.938	-5.206	-16.934	0.00	0.00	0.053	0.00	0.00
ATOM	349	HB2	LEU	347	-9.273	-4.670	-17.009	0.00	0.00	0.053	0.00	0.00
ATOM	350	CG	LEU	347	-9.507	-6.773	-16.797	0.00	0.00	-0.053	9.40	4.00
ATOM	351	HG	LEU	347	-8.652	-7.163	-17.349	0.00	0.00	0.053	0.00	0.00
ATOM	352	CD1	LEU	347	-9.094	-6.624	-15.327	0.00	0.00	-0.159	16.15	4.00
ATOM	353	HD11	LEU	347	-8.773	-7.591	-14.940	0.00	0.00	0.053	0.00	0.00
ATOM	354	HD12	LEU	347	-8.273	-5.911	-15.250	0.00	0.00	0.053	0.00	0.00
ATOM	355	HD13	LEU	347	-9.943	-6.264	-14.745	0.00	0.00	0.053	0.00	0.00
ATOM	356	CD2	LEU	347	-10.545	-7.881	-17.030	0.00	0.00	-0.159	16.15	4.00
ATOM	357	HD21	LEU	347	-10.181	-8.816	-16.605	0.00	0.00	0.053	0.00	0.00
ATOM	358	HD22	LEU	347	-11.484	-7.606	-16.551	0.00	0.00	0.053	0.00	0.00
ATOM	359	HD23	LEU	347	-10.708	-8.008	-18.100	0.00	0.00	0.053	0.00	0.00
ATOM	360	N	ILE	348	-12.469	-5.774	-19.107	0.00	0.00	-0.650	9.00	-17.40
ATOM	361	HN	ILE	348	-12.616	-4.940	-18.521	0.00	0.00	0.439	0.00	0.00
ATOM	362	CA	ILE	348	-13.586	-6.541	-19.601	0.00	0.00	0.158	9.40	4.00
ATOM	363	HA	ILE	348	-13.183	-7.481	-19.979	0.00	0.00	0.053	0.00	0.00
ATOM	364	C	ILE	348	-14.220	-5.737	-20.677	0.00	0.00	0.396	9.82	4.00
ATOM	365	O	ILE	348	-13.722	-4.673	-21.025	0.00	0.00	-0.396	8.17	-17.40
ATOM	366	CB	ILE	348	-14.687	-6.841	-18.614	0.00	0.00	-0.053	9.40	4.00
ATOM	367	HB	ILE	348	-14.243	-7.079	-17.647	0.00	0.00	0.053	0.00	0.00
ATOM	368	CG1	ILE	348	-15.476	-8.078	-19.082	0.00	0.00	-0.106	12.77	4.00
ATOM	369	HG11	ILE	348	-14.843	-8.923	-19.354	0.00	0.00	0.053	0.00	0.00
ATOM	370	HG12	ILE	348	-16.095	-7.895	-19.960	0.00	0.00	0.053	0.00	0.00
ATOM	371	CG2	ILE	348	-15.599	-5.601	-18.483	0.00	0.00	-0.159	16.15	4.00

ATOM	372	HG21	ILE	348	-16.397	-5.810	-17.771	0.00	0.00	0.053	0.00	0.00
ATOM	373	HG22	ILE	348	-15.012	-4.753	-18.131	0.00	0.00	0.053	0.00	0.00
ATOM	374	HG23	ILE	348	-16.032	-5.364	-19.455	0.00	0.00	0.053	0.00	0.00
ATOM	375	CD1	ILE	348	-16.435	-8.626	-18.029	0.00	0.00	-0.159	16.15	4.00
ATOM	376	HD11	ILE	348	-16.956	-9.496	-18.429	0.00	0.00	0.053	0.00	0.00
ATOM	377	HD12	ILE	348	-15.873	-8.916	-17.141	0.00	0.00	0.053	0.00	0.00
ATOM	378	HD13	ILE	348	-17.162	-7.858	-17.764	0.00	0.00	0.053	0.00	0.00
ATOM	379	N	TYR	349	-15.355	-6.227	-21.211	0.00	0.00	-0.650	9.00	-17.40
ATOM	380	HN	TYR	349	-15.747	-7.091	-20.809	0.00	0.00	0.439	0.00	0.00
ATOM	381	CA	TYR	349	-16.048	-5.618	-22.303	0.00	0.00	0.158	9.40	4.00
ATOM	382	HA	TYR	349	-15.476	-5.766	-23.219	0.00	0.00	0.053	0.00	0.00
ATOM	383	C	TYR	349	-16.201	-4.149	-22.034	0.00	0.00	0.396	9.82	4.00
ATOM	384	O	TYR	349	-16.089	-3.342	-22.956	0.00	0.00	-0.396	8.17	-17.40
ATOM	385	CB	TYR	349	-17.451	-6.220	-22.490	0.00	0.00	-0.106	12.77	4.00
ATOM	386	HB1	TYR	349	-18.078	-5.907	-21.655	0.00	0.00	0.053	0.00	0.00
ATOM	387	HB2	TYR	349	-17.364	-7.306	-22.511	0.00	0.00	0.053	0.00	0.00
ATOM	388	CG	TYR	349	-18.015	-5.722	-23.775	0.00	0.00	0.000	7.26	0.60
ATOM	389	CD1	TYR	349	-17.694	-6.354	-24.954	0.00	0.00	-0.127	10.80	0.60
ATOM	390	HD1	TYR	349	-17.025	-7.214	-24.939	0.00	0.00	0.127	0.00	0.00
ATOM	391	CD2	TYR	349	-18.864	-4.641	-23.807	0.00	0.00	-0.127	10.80	0.60
ATOM	392	HD2	TYR	349	-19.130	-4.134	-22.880	0.00	0.00	0.127	0.00	0.00
ATOM	393	CE1	TYR	349	-18.207	-5.913	-26.150	0.00	0.00	-0.127	10.80	0.60
ATOM	394	HE1	TYR	349	-17.944	-6.421	-27.078	0.00	0.00	0.127	0.00	0.00
ATOM	395	CE2	TYR	349	-19.380	-4.195	-25.002	0.00	0.00	-0.127	10.80	0.60
ATOM	396	HE2	TYR	349	-20.050	-3.336	-25.018	0.00	0.00	0.127	0.00	0.00
ATOM	397	CZ	TYR	349	-19.052	-4.831	-26.175	0.00	0.00	0.027	7.26	0.60
ATOM	398	OH	TYR	349	-19.580	-4.376	-27.402	0.00	0.00	-0.451	10.94	-17.40
ATOM	399	HH	TYR	349	-19.396	-3.368	-27.503	0.00	0.00	0.424	0.00	0.00
ATOM	400	N	ILE	350	-16.440	-3.747	-20.769	0.00	0.00	-0.650	9.00	-17.40
ATOM	401	HN	ILE	350	-16.492	-4.420	-19.991	0.00	0.00	0.439	0.00	0.00
ATOM	402	CA	ILE	350	-16.618	-2.339	-20.556	0.00	0.00	0.158	9.40	4.00
ATOM	403	HA	ILE	350	-16.237	-1.784	-21.414	0.00	0.00	0.053	0.00	0.00
ATOM	404	C	ILE	350	-15.871	-1.911	-19.321	0.00	0.00	0.396	9.82	4.00
ATOM	405	O	ILE	350	-15.575	-2.727	-18.450	0.00	0.00	-0.396	8.17	-17.40
ATOM	406	CB	ILE	350	-18.071	-1.983	-20.370	0.00	0.00	-0.053	9.40	4.00
ATOM	407	HB	ILE	350	-18.474	-2.531	-19.518	0.00	0.00	0.053	0.00	0.00
ATOM	408	CG1	ILE	350	-18.883	-2.445	-21.592	0.00	0.00	-0.106	12.77	4.00
ATOM	409	HG11	ILE	350	-18.674	-3.474	-21.886	0.00	0.00	0.053	0.00	0.00
ATOM	410	HG12	ILE	350	-18.699	-1.847	-22.485	0.00	0.00	0.053	0.00	0.00
ATOM	411	CG2	ILE	350	-18.201	-0.473	-20.115	0.00	0.00	-0.159	16.15	4.00
ATOM	412	HG21	ILE	350	-19.252	-0.216	-19.981	0.00	0.00	0.053	0.00	0.00
ATOM	413	HG22	ILE	350	-17.644	-0.206	-19.217	0.00	0.00	0.053	0.00	0.00
ATOM	414	HG23	ILE	350	-17.799	0.076	-20.967	0.00	0.00	0.053	0.00	0.00
ATOM	415	CD1	ILE	350	-20.394	-2.387	-21.373	0.00	0.00	-0.159	16.15	4.00
ATOM	416	HD11	ILE	350	-20.905	-2.726	-22.274	0.00	0.00	0.053	0.00	0.00
ATOM	417	HD12	ILE	350	-20.665	-3.032	-20.537	0.00	0.00	0.053	0.00	0.00
ATOM	418	HD13	ILE	350	-20.690	-1.362	-21.152	0.00	0.00	0.053	0.00	0.00
ATOM	419	N	ASP	351	-15.515	-0.603	-19.282	0.00	0.00	-0.650	9.00	-17.40
ATOM	420	HN	ASP	351	-15.672	-0.075	-20.152	0.00	0.00	0.439	0.00	0.00
ATOM	421	CA	ASP	351	-14.950	0.149	-18.199	0.00	0.00	0.158	9.40	4.00
ATOM	422	HA	ASP	351	-15.725	0.800	-17.793	0.00	0.00	0.053	0.00	0.00
ATOM	423	C	ASP	351	-13.779	1.019	-18.592	0.00	0.00	0.396	9.82	4.00
ATOM	424	O	ASP	351	-13.505	1.215	-19.774	0.00	0.00	-0.396	8.17	-17.40
ATOM	425	CB	ASP	351	-14.807	-0.619	-16.892	0.00	0.00	-0.336	12.77	4.00
ATOM	426	HB1	ASP	351	-14.150	-0.006	-16.276	0.00	0.00	0.053	0.00	0.00
ATOM	427	HB2	ASP	351	-14.371	-1.577	-17.175	0.00	0.00	0.053	0.00	0.00
ATOM	428	CG	ASP	351	-16.222	-0.732	-16.346	0.00	0.00	0.297	9.82	4.00
ATOM	429	OD1	ASP	351	-16.748	0.308	-15.863	0.00	0.00	-0.534	8.17	-18.95
ATOM	430	OD2	ASP	351	-16.807	-1.845	-16.412	0.00	0.00	-0.534	8.17	-18.95
ATOM	431	N	ILE	352	-13.068	1.584	-17.589	0.00	0.00	-0.650	9.00	-17.40
ATOM	432	HN	ILE	352	-13.182	1.214	-16.634	0.00	0.00	0.439	0.00	0.00
ATOM	433	CA	ILE	352	-12.155	2.685	-17.801	0.00	0.00	0.158	9.40	4.00
ATOM	434	HA	ILE	352	-12.709	3.454	-18.339	0.00	0.00	0.053	0.00	0.00
ATOM	435	C	ILE	352	-10.879	2.482	-18.588	0.00	0.00	0.396	9.82	4.00
ATOM	436	O	ILE	352	-10.619	3.275	-19.487	0.00	0.00	-0.396	8.17	-17.40
ATOM	437	CB	ILE	352	-11.803	3.419	-16.535	0.00	0.00	-0.053	9.40	4.00
ATOM	438	HB	ILE	352	-12.717	3.653	-15.989	0.00	0.00	0.053	0.00	0.00
ATOM	439	CG1	ILE	352	-11.175	4.779	-16.884	0.00	0.00	-0.106	12.77	4.00
ATOM	440	HG11	ILE	352	-10.324	4.699	-17.560	0.00	0.00	0.053	0.00	0.00
ATOM	441	HG12	ILE	352	-10.803	5.317	-16.012	0.00	0.00	0.053	0.00	0.00
ATOM	442	CG2	ILE	352	-10.898	2.532	-15.672	0.00	0.00	-0.159	16.15	4.00
ATOM	443	HG21	ILE	352	-10.640	3.060	-14.754	0.00	0.00	0.053	0.00	0.00
ATOM	444	HG22	ILE	352	-11.422	1.609	-15.425	0.00	0.00	0.053	0.00	0.00
ATOM	445	HG23	ILE	352	-9.987	2.296	-16.223	0.00	0.00	0.053	0.00	0.00
ATOM	446	CD1	ILE	352	-12.150	5.735	-17.568	0.00	0.00	-0.159	16.15	4.00
ATOM	447	HD11	ILE	352	-11.644	6.675	-17.787	0.00	0.00	0.053	0.00	0.00

ATOM	448	HD12	ILE	352	-12.505	5.289	-18.497	0.00	0.00	0.053	0.00	0.00
ATOM	449	HD13	ILE	352	-12.997	5.924	-16.909	0.00	0.00	0.053	0.00	0.00
ATOM	450	N	VAL	353	-10.041	1.459	-18.324	0.00	0.00	-0.650	9.00	-17.40
ATOM	451	HN	VAL	353	-10.310	0.715	-17.665	0.00	0.00	0.439	0.00	0.00
ATOM	452	CA	VAL	353	-8.755	1.431	-18.988	0.00	0.00	0.158	9.40	4.00
ATOM	453	HA	VAL	353	-8.189	2.335	-18.762	0.00	0.00	0.053	0.00	0.00
ATOM	454	C	VAL	353	-8.932	1.343	-20.466	0.00	0.00	0.396	9.82	4.00
ATOM	455	O	VAL	353	-8.302	2.088	-21.216	0.00	0.00	-0.396	8.17	-17.40
ATOM	456	CB	VAL	353	-7.857	0.307	-18.555	0.00	0.00	-0.053	9.40	4.00
ATOM	457	HB	VAL	353	-8.399	-0.630	-18.681	0.00	0.00	0.053	0.00	0.00
ATOM	458	CG1	VAL	353	-6.599	0.330	-19.438	0.00	0.00	-0.159	16.15	4.00
ATOM	459	HG11	VAL	353	-5.931	-0.479	-19.141	0.00	0.00	0.053	0.00	0.00
ATOM	460	HG12	VAL	353	-6.885	0.200	-20.482	0.00	0.00	0.053	0.00	0.00
ATOM	461	HG13	VAL	353	-6.088	1.285	-19.318	0.00	0.00	0.053	0.00	0.00
ATOM	462	CG2	VAL	353	-7.523	0.491	-17.065	0.00	0.00	-0.159	16.15	4.00
ATOM	463	HG21	VAL	353	-6.871	-0.318	-16.736	0.00	0.00	0.053	0.00	0.00
ATOM	464	HG22	VAL	353	-7.017	1.446	-16.921	0.00	0.00	0.053	0.00	0.00
ATOM	465	HG23	VAL	353	-8.443	0.476	-16.481	0.00	0.00	0.053	0.00	0.00
ATOM	466	N	GLY	354	-9.791	0.424	-20.934	0.00	0.00	-0.650	9.00	-17.40
ATOM	467	HN	GLY	354	-10.300	-0.188	-20.281	0.00	0.00	0.439	0.00	0.00
ATOM	468	CA	GLY	354	-9.996	0.299	-22.345	0.00	0.00	0.105	9.40	4.00
ATOM	469	HA1	GLY	354	-10.574	-0.600	-22.559	0.00	0.00	0.053	0.00	0.00
ATOM	470	HA2	GLY	354	-9.036	0.232	-22.856	0.00	0.00	0.053	0.00	0.00
ATOM	471	C	GLY	354	-10.739	1.489	-22.860	0.00	0.00	0.396	9.82	4.00
ATOM	472	O	GLY	354	-10.519	1.927	-23.987	0.00	0.00	-0.396	8.17	-17.40
ATOM	473	N	LEU	355	-11.675	2.029	-22.061	0.00	0.00	-0.650	9.00	-17.40
ATOM	474	HN	LEU	355	-11.838	1.644	-21.120	0.00	0.00	0.439	0.00	0.00
ATOM	475	CA	LEU	355	-12.446	3.145	-22.528	0.00	0.00	0.158	9.40	4.00
ATOM	476	HA	LEU	355	-12.932	2.839	-23.454	0.00	0.00	0.053	0.00	0.00
ATOM	477	C	LEU	355	-11.496	4.279	-22.755	0.00	0.00	0.396	9.82	4.00
ATOM	478	O	LEU	355	-11.586	4.988	-23.757	0.00	0.00	-0.396	8.17	-17.40
ATOM	479	CB	LEU	355	-13.517	3.573	-21.495	0.00	0.00	-0.106	12.77	4.00
ATOM	480	HB1	LEU	355	-12.993	3.968	-20.625	0.00	0.00	0.053	0.00	0.00
ATOM	481	HB2	LEU	355	-14.099	2.687	-21.240	0.00	0.00	0.053	0.00	0.00
ATOM	482	CG	LEU	355	-14.536	4.659	-21.926	0.00	0.00	-0.053	9.40	4.00
ATOM	483	HG	LEU	355	-15.099	4.322	-22.796	0.00	0.00	0.053	0.00	0.00
ATOM	484	CD1	LEU	355	-15.521	4.946	-20.780	0.00	0.00	-0.159	16.15	4.00
ATOM	485	HD11	LEU	355	-16.232	5.710	-21.094	0.00	0.00	0.053	0.00	0.00
ATOM	486	HD12	LEU	355	-16.059	4.033	-20.525	0.00	0.00	0.053	0.00	0.00
ATOM	487	HD13	LEU	355	-14.971	5.299	-19.907	0.00	0.00	0.053	0.00	0.00
ATOM	488	CD2	LEU	355	-13.883	5.954	-22.434	0.00	0.00	-0.159	16.15	4.00
ATOM	489	HD21	LEU	355	-14.658	6.666	-22.717	0.00	0.00	0.053	0.00	0.00
ATOM	490	HD22	LEU	355	-13.266	6.384	-21.645	0.00	0.00	0.053	0.00	0.00
ATOM	491	HD23	LEU	355	-13.261	5.732	-23.301	0.00	0.00	0.053	0.00	0.00
ATOM	492	N	ALA	356	-10.560	4.468	-21.809	0.00	0.00	-0.650	9.00	-17.40
ATOM	493	HN	ALA	356	-10.533	3.806	-21.021	0.00	0.00	0.439	0.00	0.00
ATOM	494	CA	ALA	356	-9.595	5.532	-21.824	0.00	0.00	0.158	9.40	4.00
ATOM	495	HA	ALA	356	-10.076	6.499	-21.973	0.00	0.00	0.053	0.00	0.00
ATOM	496	C	ALA	356	-8.599	5.345	-22.926	0.00	0.00	0.396	9.82	4.00
ATOM	497	O	ALA	356	-8.168	6.333	-23.519	0.00	0.00	-0.396	8.17	-17.40
ATOM	498	CB	ALA	356	-8.797	5.627	-20.511	0.00	0.00	-0.159	16.15	4.00
ATOM	499	HB1	ALA	356	-8.083	6.448	-20.578	0.00	0.00	0.053	0.00	0.00
ATOM	500	HB2	ALA	356	-9.481	5.808	-19.682	0.00	0.00	0.053	0.00	0.00
ATOM	501	HB3	ALA	356	-8.262	4.693	-20.342	0.00	0.00	0.053	0.00	0.00
ATOM	502	N	GLN	357	-8.210	4.078	-23.202	0.00	0.00	-0.650	9.00	-17.40
ATOM	503	HN	GLN	357	-8.669	3.319	-22.679	0.00	0.00	0.439	0.00	0.00
ATOM	504	CA	GLN	357	-7.205	3.702	-24.168	0.00	0.00	0.158	9.40	4.00
ATOM	505	HA	GLN	357	-6.204	3.819	-23.752	0.00	0.00	0.053	0.00	0.00
ATOM	506	C	GLN	357	-7.300	4.553	-25.392	0.00	0.00	0.396	9.82	4.00
ATOM	507	O	GLN	357	-8.265	4.470	-26.149	0.00	0.00	-0.396	8.17	-17.40
ATOM	508	CB	GLN	357	-7.377	2.248	-24.644	0.00	0.00	-0.106	12.77	4.00
ATOM	509	HB1	GLN	357	-8.386	2.135	-25.040	0.00	0.00	0.053	0.00	0.00
ATOM	510	HB2	GLN	357	-7.224	1.588	-23.790	0.00	0.00	0.053	0.00	0.00
ATOM	511	CG	GLN	357	-6.400	1.824	-25.738	0.00	0.00	-0.106	12.77	4.00
ATOM	512	HG1	GLN	357	-6.112	2.711	-26.302	0.00	0.00	0.053	0.00	0.00
ATOM	513	HG2	GLN	357	-6.902	1.104	-26.385	0.00	0.00	0.053	0.00	0.00
ATOM	514	CD	GLN	357	-5.188	1.194	-25.076	0.00	0.00	0.396	9.82	4.00
ATOM	515	OE1	GLN	357	-4.308	0.685	-25.766	0.00	0.00	-0.396	8.17	-17.40
ATOM	516	NE2	GLN	357	-5.142	1.209	-23.718	0.00	0.00	-0.879	13.25	-17.40
ATOM	517	HE21	GLN	357	-5.904	1.648	-23.182	0.00	0.00	0.439	0.00	0.00
ATOM	518	HE22	GLN	357	-4.345	0.781	-23.225	0.00	0.00	0.439	0.00	0.00
ATOM	519	N	PHE	358	-6.296	5.429	-25.599	0.00	0.00	-0.650	9.00	-17.40
ATOM	520	HN	PHE	358	-5.523	5.504	-24.922	0.00	0.00	0.439	0.00	0.00
ATOM	521	CA	PHE	358	-6.315	6.254	-26.768	0.00	0.00	0.158	9.40	4.00
ATOM	522	HA	PHE	358	-7.300	6.717	-26.825	0.00	0.00	0.053	0.00	0.00
ATOM	523	C	PHE	358	-6.058	5.368	-27.946	0.00	0.00	0.396	9.82	4.00

ATOM	524	O	PHE	358	-6.739	5.465	-28.966	0.00	0.00	-0.396	8.17	-17.40
ATOM	525	CB	PHE	358	-5.261	7.369	-26.758	0.00	0.00	-0.106	12.77	4.00
ATOM	526	HB1	PHE	358	-4.302	6.883	-26.937	0.00	0.00	0.053	0.00	0.00
ATOM	527	HB2	PHE	358	-5.317	7.832	-25.773	0.00	0.00	0.053	0.00	0.00
ATOM	528	CG	PHE	358	-5.637	8.307	-27.851	0.00	0.00	0.000	7.26	0.60
ATOM	529	CD1	PHE	358	-6.539	9.317	-27.607	0.00	0.00	-0.127	10.80	0.60
ATOM	530	HD1	PHE	358	-6.971	9.425	-26.612	0.00	0.00	0.127	0.00	0.00
ATOM	531	CD2	PHE	358	-5.106	8.179	-29.113	0.00	0.00	-0.127	10.80	0.60
ATOM	532	HD2	PHE	358	-4.395	7.380	-29.322	0.00	0.00	0.127	0.00	0.00
ATOM	533	CE1	PHE	358	-6.902	10.192	-28.603	0.00	0.00	-0.127	10.80	0.60
ATOM	534	HE1	PHE	358	-7.615	10.990	-28.396	0.00	0.00	0.127	0.00	0.00
ATOM	535	CE2	PHE	358	-5.465	9.051	-30.113	0.00	0.00	-0.127	10.80	0.60
ATOM	536	HE2	PHE	358	-5.035	8.943	-31.109	0.00	0.00	0.127	0.00	0.00
ATOM	537	CZ	PHE	358	-6.365	10.059	-29.860	0.00	0.00	-0.127	10.80	0.60
ATOM	538	HZ	PHE	358	-6.651	10.749	-30.653	0.00	0.00	0.127	0.00	0.00
ATOM	539	N	LYS	359	-5.053	4.470	-27.841	0.00	0.00	-0.650	9.00	-17.40
ATOM	540	HN	LYS	359	-4.455	4.435	-27.003	0.00	0.00	0.439	0.00	0.00
ATOM	541	CA	LYS	359	-4.848	3.570	-28.935	0.00	0.00	0.158	9.40	4.00
ATOM	542	HA	LYS	359	-5.794	3.349	-29.428	0.00	0.00	0.053	0.00	0.00
ATOM	543	C	LYS	359	-4.256	2.290	-28.452	0.00	0.00	0.396	9.82	4.00
ATOM	544	O	LYS	359	-3.419	2.254	-27.550	0.00	0.00	-0.396	8.17	-17.40
ATOM	545	CB	LYS	359	-3.966	4.089	-30.076	0.00	0.00	-0.106	12.77	4.00
ATOM	546	HB1	LYS	359	-2.926	4.156	-29.757	0.00	0.00	0.053	0.00	0.00
ATOM	547	HB2	LYS	359	-4.292	5.080	-30.393	0.00	0.00	0.053	0.00	0.00
ATOM	548	CG	LYS	359	-4.039	3.150	-31.284	0.00	0.00	-0.106	12.77	4.00
ATOM	549	HG1	LYS	359	-3.745	2.129	-31.041	0.00	0.00	0.053	0.00	0.00
ATOM	550	HG2	LYS	359	-3.390	3.465	-32.101	0.00	0.00	0.053	0.00	0.00
ATOM	551	CD	LYS	359	-5.449	3.056	-31.875	0.00	0.00	-0.106	12.77	4.00
ATOM	552	HD1	LYS	359	-5.750	4.050	-32.204	0.00	0.00	0.053	0.00	0.00
ATOM	553	HD2	LYS	359	-6.122	2.689	-31.100	0.00	0.00	0.053	0.00	0.00
ATOM	554	CE	LYS	359	-5.560	2.114	-33.074	0.00	0.00	0.099	12.77	4.00
ATOM	555	HE1	LYS	359	-6.599	2.049	-33.396	0.00	0.00	0.053	0.00	0.00
ATOM	556	HE2	LYS	359	-5.209	1.121	-32.795	0.00	0.00	0.053	0.00	0.00
ATOM	557	NZ	LYS	359	-4.736	2.626	-34.189	0.00	0.00	-0.045	13.25	-39.20
ATOM	558	HZ1	LYS	359	-4.813	1.989	-34.995	0.00	0.00	0.280	0.00	0.00
ATOM	559	HZ2	LYS	359	-5.068	3.563	-34.460	0.00	0.00	0.280	0.00	0.00
ATOM	560	HZ3	LYS	359	-3.752	2.684	-33.891	0.00	0.00	0.280	0.00	0.00
ATOM	561	N	LYS	360	-4.702	1.199	-29.098	0.00	0.00	-0.650	9.00	-17.40
ATOM	562	HN	LYS	360	-5.381	1.350	-29.857	0.00	0.00	0.439	0.00	0.00
ATOM	563	CA	LYS	360	-4.319	-0.152	-28.827	0.00	0.00	0.158	9.40	4.00
ATOM	564	HA	LYS	360	-4.521	-0.363	-27.777	0.00	0.00	0.053	0.00	0.00
ATOM	565	C	LYS	360	-2.859	-0.297	-29.120	0.00	0.00	0.396	9.82	4.00
ATOM	566	O	LYS	360	-2.127	-0.953	-28.381	0.00	0.00	-0.396	8.17	-17.40
ATOM	567	CB	LYS	360	-5.079	-1.117	-29.755	0.00	0.00	-0.106	12.77	4.00
ATOM	568	HB1	LYS	360	-4.827	-0.860	-30.784	0.00	0.00	0.053	0.00	0.00
ATOM	569	HB2	LYS	360	-6.145	-0.988	-29.570	0.00	0.00	0.053	0.00	0.00
ATOM	570	CG	LYS	360	-4.770	-2.603	-29.577	0.00	0.00	-0.106	12.77	4.00
ATOM	571	HG1	LYS	360	-4.865	-2.922	-28.539	0.00	0.00	0.053	0.00	0.00
ATOM	572	HG2	LYS	360	-3.756	-2.853	-29.888	0.00	0.00	0.053	0.00	0.00
ATOM	573	CD	LYS	360	-5.711	-3.492	-30.397	0.00	0.00	-0.106	12.77	4.00
ATOM	574	HD1	LYS	360	-5.759	-3.096	-31.411	0.00	0.00	0.053	0.00	0.00
ATOM	575	HD2	LYS	360	-6.696	-3.471	-29.930	0.00	0.00	0.053	0.00	0.00
ATOM	576	CE	LYS	360	-5.271	-4.953	-30.489	0.00	0.00	0.099	12.77	4.00
ATOM	577	HE1	LYS	360	-5.399	-5.441	-29.523	0.00	0.00	0.053	0.00	0.00
ATOM	578	HE2	LYS	360	-4.222	-5.007	-30.778	0.00	0.00	0.053	0.00	0.00
ATOM	579	NZ	LYS	360	-6.088	-5.663	-31.500	0.00	0.00	-0.045	13.25	-39.20
ATOM	580	HZ1	LYS	360	-5.786	-6.646	-31.557	0.00	0.00	0.280	0.00	0.00
ATOM	581	HZ2	LYS	360	-7.081	-5.624	-31.229	0.00	0.00	0.280	0.00	0.00
ATOM	582	HZ3	LYS	360	-5.966	-5.213	-32.418	0.00	0.00	0.280	0.00	0.00
ATOM	583	N	THR	361	-2.405	0.327	-30.220	0.00	0.00	-0.650	9.00	-17.40
ATOM	584	HN	THR	361	-3.053	0.916	-30.763	0.00	0.00	0.439	0.00	0.00
ATOM	585	CA	THR	361	-1.048	0.199	-30.661	0.00	0.00	0.158	9.40	4.00
ATOM	586	HA	THR	361	-0.790	-0.849	-30.817	0.00	0.00	0.053	0.00	0.00
ATOM	587	C	THR	361	-0.104	0.767	-29.644	0.00	0.00	0.396	9.82	4.00
ATOM	588	O	THR	361	0.890	0.132	-29.292	0.00	0.00	-0.396	8.17	-17.40
ATOM	589	CB	THR	361	-0.827	0.917	-31.964	0.00	0.00	0.060	9.40	4.00
ATOM	590	HB	THR	361	0.204	0.753	-32.278	0.00	0.00	0.053	0.00	0.00
ATOM	591	OG1	THR	361	-1.066	2.308	-31.805	0.00	0.00	-0.537	11.04	-17.40
ATOM	592	HG1	THR	361	-0.173	2.819	-31.858	0.00	0.00	0.424	0.00	0.00
ATOM	593	CG2	THR	361	-1.805	0.346	-33.007	0.00	0.00	-0.159	16.15	4.00
ATOM	594	HG21	THR	361	-1.659	0.855	-33.960	0.00	0.00	0.053	0.00	0.00
ATOM	595	HG22	THR	361	-1.620	-0.721	-33.134	0.00	0.00	0.053	0.00	0.00
ATOM	596	HG23	THR	361	-2.829	0.499	-32.667	0.00	0.00	0.053	0.00	0.00
ATOM	597	N	LEU	362	-0.389	1.980	-29.138	0.00	0.00	-0.650	9.00	-17.40
ATOM	598	HN	LEU	362	-1.261	2.456	-29.410	0.00	0.00	0.439	0.00	0.00
ATOM	599	CA	LEU	362	0.515	2.615	-28.221	0.00	0.00	0.158	9.40	4.00

ATOM	600	HA	LEU	362	1.527	2.638	-28.624	0.00	0.00	0.053	0.00	0.00
ATOM	601	C	LEU	362	0.556	1.881	-26.911	0.00	0.00	0.396	9.82	4.00
ATOM	602	O	LEU	362	1.633	1.683	-26.345	0.00	0.00	-0.396	8.17	-17.40
ATOM	603	CB	LEU	362	0.146	4.085	-27.946	0.00	0.00	-0.106	12.77	4.00
ATOM	604	HB1	LEU	362	0.866	4.492	-27.236	0.00	0.00	0.053	0.00	0.00
ATOM	605	HB2	LEU	362	-0.861	4.114	-27.530	0.00	0.00	0.053	0.00	0.00
ATOM	606	CG	LEU	362	0.162	4.984	-29.197	0.00	0.00	-0.053	9.40	4.00
ATOM	607	HG	LEU	362	1.118	4.928	-29.718	0.00	0.00	0.053	0.00	0.00
ATOM	608	CD1	LEU	362	-0.929	4.576	-30.198	0.00	0.00	-0.159	16.15	4.00
ATOM	609	HD11	LEU	362	-0.888	5.231	-31.068	0.00	0.00	0.053	0.00	0.00
ATOM	610	HD12	LEU	362	-0.767	3.545	-30.513	0.00	0.00	0.053	0.00	0.00
ATOM	611	HD13	LEU	362	-1.907	4.661	-29.725	0.00	0.00	0.053	0.00	0.00
ATOM	612	CD2	LEU	362	0.070	6.467	-28.812	0.00	0.00	-0.159	16.15	4.00
ATOM	613	HD21	LEU	362	0.083	7.079	-29.714	0.00	0.00	0.053	0.00	0.00
ATOM	614	HD22	LEU	362	-0.857	6.645	-28.267	0.00	0.00	0.053	0.00	0.00
ATOM	615	HD23	LEU	362	0.918	6.732	-28.181	0.00	0.00	0.053	0.00	0.00
ATOM	616	N	GLY	363	-0.607	1.442	-26.382	0.00	0.00	-0.650	9.00	-17.40
ATOM	617	HN	GLY	363	-1.503	1.564	-26.876	0.00	0.00	0.439	0.00	0.00
ATOM	618	CA	GLY	363	-0.539	0.797	-25.100	0.00	0.00	0.105	9.40	4.00
ATOM	619	HA1	GLY	363	-1.015	1.407	-24.332	0.00	0.00	0.053	0.00	0.00
ATOM	620	HA2	GLY	363	0.496	0.629	-24.803	0.00	0.00	0.053	0.00	0.00
ATOM	621	C	GLY	363	-1.232	-0.530	-25.132	0.00	0.00	0.396	9.82	4.00
ATOM	622	O	GLY	363	-2.401	-0.648	-24.770	0.00	0.00	-0.396	8.17	-17.40
ATOM	623	N	PRO	364	-0.520	-1.555	-25.510	0.00	0.00	-0.422	9.00	-17.40
ATOM	624	CA	PRO	364	-1.149	-2.844	-25.515	0.00	0.00	0.158	9.40	4.00
ATOM	625	HA	PRO	364	-2.138	-2.766	-25.966	0.00	0.00	0.053	0.00	0.00
ATOM	626	CD	PRO	364	0.461	-1.427	-26.575	0.00	0.00	0.105	12.77	4.00
ATOM	627	HD1	PRO	364	1.422	-1.326	-26.072	0.00	0.00	0.053	0.00	0.00
ATOM	628	HD2	PRO	364	0.170	-0.535	-27.130	0.00	0.00	0.053	0.00	0.00
ATOM	629	C	PRO	364	-1.281	-3.341	-24.114	0.00	0.00	0.396	9.82	4.00
ATOM	630	O	PRO	364	-0.393	-3.080	-23.302	0.00	0.00	-0.396	8.17	-17.40
ATOM	631	CB	PRO	364	-0.324	-3.727	-26.441	0.00	0.00	-0.106	12.77	4.00
ATOM	632	HB1	PRO	364	-0.959	-4.434	-26.975	0.00	0.00	0.053	0.00	0.00
ATOM	633	HB2	PRO	364	0.415	-4.299	-25.880	0.00	0.00	0.053	0.00	0.00
ATOM	634	CG	PRO	364	0.340	-2.720	-27.398	0.00	0.00	-0.106	12.77	4.00
ATOM	635	HG1	PRO	364	-0.350	-2.646	-28.239	0.00	0.00	0.053	0.00	0.00
ATOM	636	HG2	PRO	364	1.298	-3.174	-27.651	0.00	0.00	0.053	0.00	0.00
ATOM	637	N	SER	365	-2.370	-4.067	-23.804	0.00	0.00	-0.650	9.00	-17.40
ATOM	638	HN	SER	365	-3.067	-4.308	-24.523	0.00	0.00	0.439	0.00	0.00
ATOM	639	CA	SER	365	-2.536	-4.496	-22.449	0.00	0.00	0.158	9.40	4.00
ATOM	640	HA	SER	365	-1.844	-3.950	-21.808	0.00	0.00	0.053	0.00	0.00
ATOM	641	C	SER	365	-2.255	-5.961	-22.352	0.00	0.00	0.396	9.82	4.00
ATOM	642	O	SER	365	-2.814	-6.776	-23.089	0.00	0.00	-0.396	8.17	-17.40
ATOM	643	CB	SER	365	-3.953	-4.270	-21.895	0.00	0.00	0.007	12.77	4.00
ATOM	644	HB1	SER	365	-4.676	-4.821	-22.496	0.00	0.00	0.053	0.00	0.00
ATOM	645	HB2	SER	365	-4.197	-3.208	-21.927	0.00	0.00	0.053	0.00	0.00
ATOM	646	OG	SER	365	-4.022	-4.724	-20.550	0.00	0.00	-0.537	11.04	-17.40
ATOM	647	HG	SER	365	-4.349	-3.957	-19.945	0.00	0.00	0.424	0.00	0.00
ATOM	648	N	TRP	366	-1.345	-6.345	-21.437	0.00	0.00	-0.650	9.00	-17.40
ATOM	649	HN	TRP	366	-0.811	-5.664	-20.879	0.00	0.00	0.439	0.00	0.00
ATOM	650	CA	TRP	366	-1.166	-7.751	-21.288	0.00	0.00	0.158	9.40	4.00
ATOM	651	HA	TRP	366	-1.747	-8.300	-22.029	0.00	0.00	0.053	0.00	0.00
ATOM	652	C	TRP	366	-1.648	-8.013	-19.900	0.00	0.00	0.396	9.82	4.00
ATOM	653	O	TRP	366	-1.330	-7.281	-18.961	0.00	0.00	-0.396	8.17	-17.40
ATOM	654	CB	TRP	366	0.281	-8.257	-21.369	0.00	0.00	-0.106	12.77	4.00
ATOM	655	HB1	TRP	366	0.919	-7.621	-21.982	0.00	0.00	0.053	0.00	0.00
ATOM	656	HB2	TRP	366	0.358	-9.256	-21.798	0.00	0.00	0.053	0.00	0.00
ATOM	657	CG	TRP	366	0.948	-8.335	-20.028	0.00	0.00	0.000	7.26	0.60
ATOM	658	CD1	TRP	366	1.466	-7.357	-19.241	0.00	0.00	-0.177	10.80	0.60
ATOM	659	HD1	TRP	366	1.461	-6.293	-19.480	0.00	0.00	0.127	0.00	0.00
ATOM	660	CD2	TRP	366	1.154	-9.572	-19.337	0.00	0.00	0.000	6.80	0.60
ATOM	661	NE1	TRP	366	1.998	-7.907	-18.099	0.00	0.00	-0.292	9.00	-17.40
ATOM	662	HE1	TRP	366	2.459	-7.389	-17.338	0.00	0.00	0.393	0.00	0.00
ATOM	663	CE2	TRP	366	1.809	-9.270	-18.148	0.00	0.00	-0.050	6.80	0.60
ATOM	664	CE3	TRP	366	0.825	-10.856	-19.666	0.00	0.00	-0.127	10.80	0.60
ATOM	665	HE3	TRP	366	0.310	-11.092	-20.597	0.00	0.00	0.127	0.00	0.00
ATOM	666	CZ2	TRP	366	2.148	-10.253	-17.270	0.00	0.00	-0.127	10.80	0.60
ATOM	667	HZ2	TRP	366	2.661	-10.020	-16.337	0.00	0.00	0.127	0.00	0.00
ATOM	668	CZ3	TRP	366	1.174	-11.839	-18.767	0.00	0.00	-0.127	10.80	0.60
ATOM	669	HZ3	TRP	366	0.927	-12.876	-18.993	0.00	0.00	0.127	0.00	0.00
ATOM	670	CH2	TRP	366	1.824	-11.548	-17.594	0.00	0.00	-0.127	10.80	0.60
ATOM	671	HH2	TRP	366	2.087	-12.355	-16.910	0.00	0.00	0.127	0.00	0.00
ATOM	672	N	VAL	367	-2.473	-9.053	-19.722	0.00	0.00	-0.650	9.00	-17.40
ATOM	673	HN	VAL	367	-2.740	-9.677	-20.496	0.00	0.00	0.439	0.00	0.00
ATOM	674	CA	VAL	367	-2.958	-9.243	-18.397	0.00	0.00	0.158	9.40	4.00
ATOM	675	HA	VAL	367	-2.673	-8.365	-17.818	0.00	0.00	0.053	0.00	0.00

ATOM	676	C	VAL	367	-2.317	-10.487	-17.861	0.00	0.00	0.396	9.82	4.00
ATOM	677	O	VAL	367	-2.369	-11.557	-18.468	0.00	0.00	-0.396	8.17	-17.40
ATOM	678	CB	VAL	367	-4.462	-9.327	-18.328	0.00	0.00	-0.053	9.40	4.00
ATOM	679	HB	VAL	367	-4.918	-8.573	-18.970	0.00	0.00	0.053	0.00	0.00
ATOM	680	CG1	VAL	367	-4.947	-10.709	-18.787	0.00	0.00	-0.159	16.15	4.00
ATOM	681	HG11	VAL	367	-6.035	-10.750	-18.730	0.00	0.00	0.053	0.00	0.00
ATOM	682	HG12	VAL	367	-4.631	-10.883	-19.816	0.00	0.00	0.053	0.00	0.00
ATOM	683	HG13	VAL	367	-4.521	-11.477	-18.142	0.00	0.00	0.053	0.00	0.00
ATOM	684	CG2	VAL	367	-4.904	-8.914	-16.921	0.00	0.00	-0.159	16.15	4.00
ATOM	685	HG21	VAL	367	-5.990	-8.968	-16.850	0.00	0.00	0.053	0.00	0.00
ATOM	686	HG22	VAL	367	-4.459	-9.586	-16.188	0.00	0.00	0.053	0.00	0.00
ATOM	687	HG23	VAL	367	-4.578	-7.893	-16.722	0.00	0.00	0.053	0.00	0.00
ATOM	688	N	HIS	368	-1.642	-10.345	-16.705	0.00	0.00	-0.650	9.00	-17.40
ATOM	689	HN	HIS	368	-1.581	-9.409	-16.278	0.00	0.00	0.439	0.00	0.00
ATOM	690	CA	HIS	368	-1.006	-11.446	-16.046	0.00	0.00	0.158	9.40	4.00
ATOM	691	HA	HIS	368	-0.772	-12.161	-16.834	0.00	0.00	0.053	0.00	0.00
ATOM	692	C	HIS	368	-2.004	-11.956	-15.074	0.00	0.00	0.396	9.82	4.00
ATOM	693	O	HIS	368	-2.461	-11.217	-14.205	0.00	0.00	-0.396	8.17	-17.40
ATOM	694	CB	HIS	368	0.203	-11.031	-15.192	0.00	0.00	-0.106	12.77	4.00
ATOM	695	HB1	HIS	368	0.274	-9.954	-15.041	0.00	0.00	0.053	0.00	0.00
ATOM	696	HB2	HIS	368	1.158	-11.326	-15.626	0.00	0.00	0.053	0.00	0.00
ATOM	697	CG	HIS	368	0.189	-11.628	-13.813	0.00	0.00	0.241	7.26	0.60
ATOM	698	ND1	HIS	368	-0.014	-12.962	-13.539	0.00	0.00	-0.481	9.25	-17.40
ATOM	699	CD2	HIS	368	0.364	-11.024	-12.604	0.00	0.00	-0.177	10.80	0.60
ATOM	700	HD2	HIS	368	0.548	-9.959	-12.463	0.00	0.00	0.127	0.00	0.00
ATOM	701	CE1	HIS	368	0.049	-13.099	-12.190	0.00	0.00	0.064	10.80	0.60
ATOM	702	HE1	HIS	368	-0.074	-14.049	-11.670	0.00	0.00	0.127	0.00	0.00
ATOM	703	NE2	HIS	368	0.276	-11.950	-11.580	0.00	0.00	-0.292	9.25	-17.40
ATOM	704	HE2	HIS	368	0.367	-11.781	-10.568	0.00	0.00	0.393	0.00	0.00
ATOM	705	N	TYR	369	-2.379	-13.240	-15.183	0.00	0.00	-0.650	9.00	-17.40
ATOM	706	HN	TYR	369	-1.970	-13.866	-15.891	0.00	0.00	0.439	0.00	0.00
ATOM	707	CA	TYR	369	-3.376	-13.694	-14.265	0.00	0.00	0.158	9.40	4.00
ATOM	708	HA	TYR	369	-3.646	-12.873	-13.600	0.00	0.00	0.053	0.00	0.00
ATOM	709	C	TYR	369	-2.824	-14.831	-13.472	0.00	0.00	0.396	9.82	4.00
ATOM	710	O	TYR	369	-2.335	-15.816	-14.024	0.00	0.00	-0.396	8.17	-17.40
ATOM	711	CB	TYR	369	-4.662	-14.140	-14.988	0.00	0.00	-0.106	12.77	4.00
ATOM	712	HB1	TYR	369	-4.449	-14.978	-15.652	0.00	0.00	0.053	0.00	0.00
ATOM	713	HB2	TYR	369	-5.066	-13.318	-15.579	0.00	0.00	0.053	0.00	0.00
ATOM	714	CG	TYR	369	-5.689	-14.565	-13.996	0.00	0.00	0.000	7.26	0.60
ATOM	715	CD1	TYR	369	-6.254	-13.646	-13.142	0.00	0.00	-0.127	10.80	0.60
ATOM	716	HD1	TYR	369	-5.938	-12.604	-13.186	0.00	0.00	0.127	0.00	0.00
ATOM	717	CD2	TYR	369	-6.118	-15.871	-13.950	0.00	0.00	-0.127	10.80	0.60
ATOM	718	HD2	TYR	369	-5.694	-16.604	-14.637	0.00	0.00	0.127	0.00	0.00
ATOM	719	CE1	TYR	369	-7.213	-14.029	-12.234	0.00	0.00	-0.127	10.80	0.60
ATOM	720	HE1	TYR	369	-7.646	-13.295	-11.555	0.00	0.00	0.127	0.00	0.00
ATOM	721	CE2	TYR	369	-7.077	-16.259	-13.045	0.00	0.00	-0.127	10.80	0.60
ATOM	722	HE2	TYR	369	-7.404	-17.298	-13.010	0.00	0.00	0.127	0.00	0.00
ATOM	723	CZ	TYR	369	-7.624	-15.339	-12.184	0.00	0.00	0.027	7.26	0.60
ATOM	724	OH	TYR	369	-8.609	-15.742	-11.259	0.00	0.00	-0.451	10.94	-17.40
ATOM	725	HH	TYR	369	-9.127	-14.916	-10.926	0.00	0.00	0.424	0.00	0.00
ATOM	726	N	GLN	370	-2.875	-14.699	-12.131	0.00	0.00	-0.650	9.00	-17.40
ATOM	727	HN	GLN	370	-3.249	-13.830	-11.724	0.00	0.00	0.439	0.00	0.00
ATOM	728	CA	GLN	370	-2.420	-15.741	-11.259	0.00	0.00	0.158	9.40	4.00
ATOM	729	HA	GLN	370	-1.593	-16.212	-11.790	0.00	0.00	0.053	0.00	0.00
ATOM	730	C	GLN	370	-3.599	-16.636	-11.079	0.00	0.00	0.396	9.82	4.00
ATOM	731	O	GLN	370	-4.641	-16.421	-11.695	0.00	0.00	-0.396	8.17	-17.40
ATOM	732	CB	GLN	370	-2.016	-15.244	-9.856	0.00	0.00	-0.106	12.77	4.00
ATOM	733	HB1	GLN	370	-2.917	-14.924	-9.332	0.00	0.00	0.053	0.00	0.00
ATOM	734	HB2	GLN	370	-1.325	-14.409	-9.973	0.00	0.00	0.053	0.00	0.00
ATOM	735	CG	GLN	370	-1.325	-16.308	-8.995	0.00	0.00	-0.106	12.77	4.00
ATOM	736	HG1	GLN	370	-0.299	-16.428	-9.344	0.00	0.00	0.053	0.00	0.00
ATOM	737	HG2	GLN	370	-1.870	-17.247	-9.096	0.00	0.00	0.053	0.00	0.00
ATOM	738	CD	GLN	370	-1.337	-15.845	-7.545	0.00	0.00	0.396	9.82	4.00
ATOM	739	OE1	GLN	370	-1.929	-14.819	-7.212	0.00	0.00	-0.396	8.17	-17.40
ATOM	740	NE2	GLN	370	-0.670	-16.627	-6.654	0.00	0.00	-0.879	13.25	-17.40
ATOM	741	HE21	GLN	370	-0.188	-17.478	-6.976	0.00	0.00	0.439	0.00	0.00
ATOM	742	HE22	GLN	370	-0.647	-16.368	-5.657	0.00	0.00	0.439	0.00	0.00
ATOM	743	N	CYS	371	-3.472	-17.658	-10.208	0.00	0.00	-0.650	9.00	-17.40
ATOM	744	HN	CYS	371	-2.582	-17.767	-9.700	0.00	0.00	0.439	0.00	0.00
ATOM	745	CA	CYS	371	-4.525	-18.599	-9.960	0.00	0.00	0.158	9.40	4.00
ATOM	746	HA	CYS	371	-4.140	-19.450	-9.398	0.00	0.00	0.053	0.00	0.00
ATOM	747	C	CYS	371	-5.091	-19.089	-11.258	0.00	0.00	0.396	9.82	4.00
ATOM	748	O	CYS	371	-4.542	-18.870	-12.335	0.00	0.00	-0.396	8.17	-17.40
ATOM	749	CB	CYS	371	-5.667	-18.012	-9.115	0.00	0.00	-0.041	12.77	4.00
ATOM	750	HB1	CYS	371	-6.480	-18.726	-8.984	0.00	0.00	0.053	0.00	0.00
ATOM	751	HB2	CYS	371	-6.093	-17.121	-9.577	0.00	0.00	0.053	0.00	0.00

ATOM	752	SG	CYS	371	-5.099	-17.536	-7.456	0.00	0.00	-0.255	19.93	-6.40
ATOM	753	HG	CYS	371	-4.628	-16.282	-7.487	0.00	0.00	0.190	0.00	0.00
ATOM	754	N	MET	372	-6.186	-19.859	-11.188	0.00	0.00	-0.650	9.00	-17.40
ATOM	755	HN	MET	372	-6.624	-20.085	-10.284	0.00	0.00	0.439	0.00	0.00
ATOM	756	CA	MET	372	-6.723	-20.355	-12.418	0.00	0.00	0.158	9.40	4.00
ATOM	757	HA	MET	372	-6.234	-19.834	-13.241	0.00	0.00	0.053	0.00	0.00
ATOM	758	C	MET	372	-8.193	-20.091	-12.430	0.00	0.00	0.396	9.82	4.00
ATOM	759	O	MET	372	-8.972	-20.827	-11.827	0.00	0.00	-0.396	8.17	-17.40
ATOM	760	CB	MET	372	-6.523	-21.869	-12.596	0.00	0.00	-0.106	12.77	4.00
ATOM	761	HB1	MET	372	-7.001	-22.468	-11.821	0.00	0.00	0.053	0.00	0.00
ATOM	762	HB2	MET	372	-5.477	-22.177	-12.584	0.00	0.00	0.053	0.00	0.00
ATOM	763	CG	MET	372	-7.079	-22.411	-13.913	0.00	0.00	-0.041	12.77	4.00
ATOM	764	HG1	MET	372	-6.602	-21.874	-14.732	0.00	0.00	0.053	0.00	0.00
ATOM	765	HG2	MET	372	-8.157	-22.247	-13.922	0.00	0.00	0.053	0.00	0.00
ATOM	766	SD	MET	372	-6.790	-24.186	-14.177	0.00	0.00	-0.130	16.39	-6.40
ATOM	767	CE	MET	372	-7.914	-24.727	-12.857	0.00	0.00	-0.094	16.15	4.00
ATOM	768	HE1	MET	372	-7.920	-25.816	-12.808	0.00	0.00	0.053	0.00	0.00
ATOM	769	HE2	MET	372	-7.576	-24.322	-11.903	0.00	0.00	0.053	0.00	0.00
ATOM	770	HE3	MET	372	-8.922	-24.368	-13.067	0.00	0.00	0.053	0.00	0.00
ATOM	771	N	LEU	373	-8.604	-19.008	-13.116	0.00	0.00	-0.650	9.00	-17.40
ATOM	772	HN	LEU	373	-7.906	-18.394	-13.559	0.00	0.00	0.439	0.00	0.00
ATOM	773	CA	LEU	373	-9.998	-18.696	-13.240	0.00	0.00	0.158	9.40	4.00
ATOM	774	HA	LEU	373	-10.532	-19.636	-13.103	0.00	0.00	0.053	0.00	0.00
ATOM	775	C	LEU	373	-10.176	-18.128	-14.612	0.00	0.00	0.396	9.82	4.00
ATOM	776	O	LEU	373	-9.200	-17.914	-15.328	0.00	0.00	-0.396	8.17	-17.40
ATOM	777	CB	LEU	373	-10.504	-17.643	-12.238	0.00	0.00	-0.106	12.77	4.00
ATOM	778	HB1	LEU	373	-11.535	-17.396	-12.492	0.00	0.00	0.053	0.00	0.00
ATOM	779	HB2	LEU	373	-9.868	-16.762	-12.317	0.00	0.00	0.053	0.00	0.00
ATOM	780	CG	LEU	373	-10.482	-18.108	-10.767	0.00	0.00	-0.053	9.40	4.00
ATOM	781	HG	LEU	373	-11.000	-19.058	-10.634	0.00	0.00	0.053	0.00	0.00
ATOM	782	CD1	LEU	373	-9.048	-18.302	-10.250	0.00	0.00	-0.159	16.15	4.00
ATOM	783	HD11	LEU	373	-9.077	-18.630	-9.211	0.00	0.00	0.053	0.00	0.00
ATOM	784	HD12	LEU	373	-8.542	-19.055	-10.854	0.00	0.00	0.053	0.00	0.00
ATOM	785	HD13	LEU	373	-8.506	-17.359	-10.318	0.00	0.00	0.053	0.00	0.00
ATOM	786	CD2	LEU	373	-11.314	-17.172	-9.875	0.00	0.00	-0.159	16.15	4.00
ATOM	787	HD21	LEU	373	-11.279	-17.526	-8.845	0.00	0.00	0.053	0.00	0.00
ATOM	788	HD22	LEU	373	-10.906	-16.163	-9.926	0.00	0.00	0.053	0.00	0.00
ATOM	789	HD23	LEU	373	-12.348	-17.163	-10.221	0.00	0.00	0.053	0.00	0.00
ATOM	790	N	ARG	374	-11.438	-17.890	-15.032	0.00	0.00	-0.650	9.00	-17.40
ATOM	791	HN	ARG	374	-12.238	-18.103	-14.420	0.00	0.00	0.439	0.00	0.00
ATOM	792	CA	ARG	374	-11.653	-17.337	-16.339	0.00	0.00	0.158	9.40	4.00
ATOM	793	HA	ARG	374	-10.681	-17.105	-16.775	0.00	0.00	0.053	0.00	0.00
ATOM	794	C	ARG	374	-12.477	-16.095	-16.192	0.00	0.00	0.396	9.82	4.00
ATOM	795	O	ARG	374	-13.170	-15.925	-15.190	0.00	0.00	-0.396	8.17	-17.40
ATOM	796	CB	ARG	374	-12.414	-18.272	-17.295	0.00	0.00	-0.106	12.77	4.00
ATOM	797	HB1	ARG	374	-11.917	-19.228	-17.460	0.00	0.00	0.053	0.00	0.00
ATOM	798	HB2	ARG	374	-12.559	-17.855	-18.292	0.00	0.00	0.053	0.00	0.00
ATOM	799	CG	ARG	374	-13.819	-18.635	-16.810	0.00	0.00	-0.106	12.77	4.00
ATOM	800	HG1	ARG	374	-14.458	-17.769	-16.637	0.00	0.00	0.053	0.00	0.00
ATOM	801	HG2	ARG	374	-13.827	-19.186	-15.869	0.00	0.00	0.053	0.00	0.00
ATOM	802	CD	ARG	374	-14.598	-19.514	-17.792	0.00	0.00	0.374	12.77	4.00
ATOM	803	HD1	ARG	374	-14.546	-19.041	-18.773	0.00	0.00	0.053	0.00	0.00
ATOM	804	HD2	ARG	374	-15.627	-19.575	-17.438	0.00	0.00	0.053	0.00	0.00
ATOM	805	NE	ARG	374	-13.954	-20.857	-17.807	0.00	0.00	-0.819	9.00	-24.67
ATOM	806	HE	ARG	374	-13.053	-21.003	-17.329	0.00	0.00	0.407	0.00	0.00
ATOM	807	CZ	ARG	374	-14.559	-21.894	-18.455	0.00	0.00	0.796	6.95	4.00
ATOM	808	NH1	ARG	374	-15.748	-21.699	-19.096	0.00	0.00	-0.746	9.00	-24.67
ATOM	809	HH11	ARG	374	-16.204	-22.483	-19.585	0.00	0.00	0.407	0.00	0.00
ATOM	810	HH12	ARG	374	-16.189	-20.768	-19.091	0.00	0.00	0.407	0.00	0.00
ATOM	811	NH2	ARG	374	-13.976	-23.129	-18.462	0.00	0.00	-0.746	9.00	-24.67
ATOM	812	HH21	ARG	374	-14.433	-23.912	-18.951	0.00	0.00	0.407	0.00	0.00
ATOM	813	HH22	ARG	374	-13.079	-23.278	-17.978	0.00	0.00	0.407	0.00	0.00
ATOM	814	N	VAL	375	-12.403	-15.187	-17.194	0.00	0.00	-0.650	9.00	-17.40
ATOM	815	HN	VAL	375	-11.787	-15.376	-17.997	0.00	0.00	0.439	0.00	0.00
ATOM	816	CA	VAL	375	-13.162	-13.965	-17.167	0.00	0.00	0.158	9.40	4.00
ATOM	817	HA	VAL	375	-14.215	-14.195	-17.333	0.00	0.00	0.053	0.00	0.00
ATOM	818	C	VAL	375	-12.662	-13.050	-18.253	0.00	0.00	0.396	9.82	4.00
ATOM	819	O	VAL	375	-13.367	-12.786	-19.225	0.00	0.00	-0.396	8.17	-17.40
ATOM	820	CB	VAL	375	-13.105	-13.263	-15.831	0.00	0.00	-0.053	9.40	4.00
ATOM	821	HB	VAL	375	-13.643	-13.836	-15.076	0.00	0.00	0.053	0.00	0.00
ATOM	822	CG1	VAL	375	-11.645	-13.100	-15.370	0.00	0.00	-0.159	16.15	4.00
ATOM	823	HG11	VAL	375	-11.622	-12.592	-14.406	0.00	0.00	0.053	0.00	0.00
ATOM	824	HG12	VAL	375	-11.182	-14.082	-15.274	0.00	0.00	0.053	0.00	0.00
ATOM	825	HG13	VAL	375	-11.096	-12.510	-16.104	0.00	0.00	0.053	0.00	0.00
ATOM	826	CG2	VAL	375	-13.878	-11.941	-15.952	0.00	0.00	-0.159	16.15	4.00
ATOM	827	HG21	VAL	375	-13.851	-11.415	-14.998	0.00	0.00	0.053	0.00	0.00

ATOM	828	HG22	VAL	375	-13.419	-11.320	-16.722	0.00	0.00	0.053	0.00	0.00
ATOM	829	HG23	VAL	375	-14.913	-12.148	-16.223	0.00	0.00	0.053	0.00	0.00
ATOM	830	N	LEU	376	-11.418	-12.556	-18.118	0.00	0.00	-0.650	9.00	-17.40
ATOM	831	HN	LEU	376	-10.876	-12.842	-17.290	0.00	0.00	0.439	0.00	0.00
ATOM	832	CA	LEU	376	-10.794	-11.657	-19.049	0.00	0.00	0.158	9.40	4.00
ATOM	833	HA	LEU	376	-11.480	-10.817	-19.159	0.00	0.00	0.053	0.00	0.00
ATOM	834	C	LEU	376	-10.621	-12.434	-20.316	0.00	0.00	0.396	9.82	4.00
ATOM	835	O	LEU	376	-10.578	-11.885	-21.416	0.00	0.00	-0.396	8.17	-17.40
ATOM	836	CB	LEU	376	-9.439	-11.136	-18.520	0.00	0.00	-0.106	12.77	4.00
ATOM	837	HB1	LEU	376	-8.727	-11.960	-18.561	0.00	0.00	0.053	0.00	0.00
ATOM	838	HB2	LEU	376	-9.590	-10.798	-17.495	0.00	0.00	0.053	0.00	0.00
ATOM	839	CG	LEU	376	-8.806	-9.956	-19.294	0.00	0.00	-0.053	9.40	4.00
ATOM	840	HG	LEU	376	-9.524	-9.144	-19.410	0.00	0.00	0.053	0.00	0.00
ATOM	841	CD1	LEU	376	-7.581	-9.414	-18.544	0.00	0.00	-0.159	16.15	4.00
ATOM	842	HD11	LEU	376	-7.149	-8.584	-19.104	0.00	0.00	0.053	0.00	0.00
ATOM	843	HD12	LEU	376	-7.884	-9.067	-17.556	0.00	0.00	0.053	0.00	0.00
ATOM	844	HD13	LEU	376	-6.839	-10.206	-18.439	0.00	0.00	0.053	0.00	0.00
ATOM	845	CD2	LEU	376	-8.448	-10.313	-20.743	0.00	0.00	-0.159	16.15	4.00
ATOM	846	HD21	LEU	376	-8.008	-9.445	-21.234	0.00	0.00	0.053	0.00	0.00
ATOM	847	HD22	LEU	376	-7.732	-11.135	-20.749	0.00	0.00	0.053	0.00	0.00
ATOM	848	HD23	LEU	376	-9.349	-10.613	-21.277	0.00	0.00	0.053	0.00	0.00
ATOM	849	N	ASP	377	-10.588	-13.769	-20.171	0.00	0.00	-0.650	9.00	-17.40
ATOM	850	HN	ASP	377	-10.739	-14.152	-19.227	0.00	0.00	0.439	0.00	0.00
ATOM	851	CA	ASP	377	-10.358	-14.698	-21.236	0.00	0.00	0.158	9.40	4.00
ATOM	852	HA	ASP	377	-9.338	-14.566	-21.597	0.00	0.00	0.053	0.00	0.00
ATOM	853	C	ASP	377	-11.336	-14.419	-22.329	0.00	0.00	0.396	9.82	4.00
ATOM	854	O	ASP	377	-11.073	-14.753	-23.483	0.00	0.00	-0.396	8.17	-17.40
ATOM	855	CB	ASP	377	-10.556	-16.160	-20.794	0.00	0.00	-0.336	12.77	4.00
ATOM	856	HB1	ASP	377	-11.621	-16.344	-20.653	0.00	0.00	0.053	0.00	0.00
ATOM	857	HB2	ASP	377	-10.021	-16.321	-19.858	0.00	0.00	0.053	0.00	0.00
ATOM	858	CG	ASP	377	-10.005	-17.081	-21.876	0.00	0.00	0.297	9.82	4.00
ATOM	859	OD1	ASP	377	-9.405	-16.560	-22.854	0.00	0.00	-0.534	8.17	-18.95
ATOM	860	OD2	ASP	377	-10.174	-18.320	-21.735	0.00	0.00	-0.534	8.17	-18.95
ATOM	861	N	SER	378	-12.490	-13.808	-21.990	0.00	0.00	-0.650	9.00	-17.40
ATOM	862	HN	SER	378	-12.653	-13.542	-21.008	0.00	0.00	0.439	0.00	0.00
ATOM	863	CA	SER	378	-13.494	-13.523	-22.976	0.00	0.00	0.158	9.40	4.00
ATOM	864	HA	SER	378	-13.891	-14.475	-23.329	0.00	0.00	0.053	0.00	0.00
ATOM	865	C	SER	378	-12.838	-12.766	-24.086	0.00	0.00	0.396	9.82	4.00
ATOM	866	O	SER	378	-13.025	-13.098	-25.256	0.00	0.00	-0.396	8.17	-17.40
ATOM	867	CB	SER	378	-14.634	-12.647	-22.428	0.00	0.00	0.007	12.77	4.00
ATOM	868	HB1	SER	378	-14.238	-11.694	-22.078	0.00	0.00	0.053	0.00	0.00
ATOM	869	HB2	SER	378	-15.126	-13.151	-21.596	0.00	0.00	0.053	0.00	0.00
ATOM	870	OG	SER	378	-15.591	-12.400	-23.447	0.00	0.00	-0.537	11.04	-17.40
ATOM	871	HG	SER	378	-15.654	-11.387	-23.621	0.00	0.00	0.424	0.00	0.00
ATOM	872	N	PHE	379	-12.032	-11.739	-23.760	0.00	0.00	-0.650	9.00	-17.40
ATOM	873	HN	PHE	379	-11.924	-11.433	-22.782	0.00	0.00	0.439	0.00	0.00
ATOM	874	CA	PHE	379	-11.331	-11.088	-24.825	0.00	0.00	0.158	9.40	4.00
ATOM	875	HA	PHE	379	-11.072	-11.857	-25.553	0.00	0.00	0.053	0.00	0.00
ATOM	876	C	PHE	379	-10.117	-10.458	-24.228	0.00	0.00	0.396	9.82	4.00
ATOM	877	O	PHE	379	-10.180	-9.902	-23.133	0.00	0.00	-0.396	8.17	-17.40
ATOM	878	CB	PHE	379	-12.134	-9.973	-25.521	0.00	0.00	-0.106	12.77	4.00
ATOM	879	HB1	PHE	379	-13.111	-10.381	-25.779	0.00	0.00	0.053	0.00	0.00
ATOM	880	HB2	PHE	379	-11.582	-9.676	-26.413	0.00	0.00	0.053	0.00	0.00
ATOM	881	CG	PHE	379	-12.258	-8.842	-24.563	0.00	0.00	0.000	7.26	0.60
ATOM	882	CD1	PHE	379	-13.220	-8.841	-23.580	0.00	0.00	-0.127	10.80	0.60
ATOM	883	HD1	PHE	379	-13.910	-9.680	-23.495	0.00	0.00	0.127	0.00	0.00
ATOM	884	CD2	PHE	379	-11.393	-7.776	-24.656	0.00	0.00	-0.127	10.80	0.60
ATOM	885	HD2	PHE	379	-10.627	-7.771	-25.432	0.00	0.00	0.127	0.00	0.00
ATOM	886	CE1	PHE	379	-13.314	-7.785	-22.704	0.00	0.00	-0.127	10.80	0.60
ATOM	887	HE1	PHE	379	-14.079	-7.788	-21.928	0.00	0.00	0.127	0.00	0.00
ATOM	888	CE2	PHE	379	-11.481	-6.719	-23.785	0.00	0.00	-0.127	10.80	0.60
ATOM	889	HE2	PHE	379	-10.791	-5.880	-23.869	0.00	0.00	0.127	0.00	0.00
ATOM	890	CZ	PHE	379	-12.444	-6.726	-22.807	0.00	0.00	-0.127	10.80	0.60
ATOM	891	HZ	PHE	379	-12.519	-5.890	-22.111	0.00	0.00	0.127	0.00	0.00
ATOM	892	N	GLY	380	-8.962	-10.556	-24.920	0.00	0.00	-0.650	9.00	-17.40
ATOM	893	HN	GLY	380	-8.915	-11.094	-25.797	0.00	0.00	0.439	0.00	0.00
ATOM	894	CA	GLY	380	-7.802	-9.890	-24.400	0.00	0.00	0.105	9.40	4.00
ATOM	895	HA1	GLY	380	-7.968	-9.571	-23.371	0.00	0.00	0.053	0.00	0.00
ATOM	896	HA2	GLY	380	-7.563	-9.008	-24.994	0.00	0.00	0.053	0.00	0.00
ATOM	897	C	GLY	380	-6.609	-10.803	-24.419	0.00	0.00	0.396	9.82	4.00
ATOM	898	O	GLY	380	-6.712	-11.959	-24.827	0.00	0.00	-0.396	8.17	-17.40
ATOM	899	N	THR	381	-5.433	-10.282	-23.978	0.00	0.00	-0.650	9.00	-17.40
ATOM	900	HN	THR	381	-5.395	-9.298	-23.676	0.00	0.00	0.439	0.00	0.00
ATOM	901	CA	THR	381	-4.240	-11.088	-23.927	0.00	0.00	0.158	9.40	4.00
ATOM	902	HA	THR	381	-4.408	-11.947	-24.577	0.00	0.00	0.053	0.00	0.00
ATOM	903	C	THR	381	-4.050	-11.498	-22.501	0.00	0.00	0.396	9.82	4.00

ATOM	904	O	THR	381	-3.900	-10.645	-21.626	0.00	0.00	-0.396	8.17	-17.40
ATOM	905	CB	THR	381	-3.000	-10.356	-24.350	0.00	0.00	0.060	9.40	4.00
ATOM	906	HB	THR	381	-2.857	-9.503	-23.687	0.00	0.00	0.053	0.00	0.00
ATOM	907	OG1	THR	381	-3.140	-9.889	-25.685	0.00	0.00	-0.537	11.04	-17.40
ATOM	908	HG1	THR	381	-2.855	-8.901	-25.735	0.00	0.00	0.424	0.00	0.00
ATOM	909	CG2	THR	381	-1.805	-11.318	-24.249	0.00	0.00	-0.159	16.15	4.00
ATOM	910	HG21	THR	381	-0.895	-10.801	-24.553	0.00	0.00	0.053	0.00	0.00
ATOM	911	HG22	THR	381	-1.700	-11.661	-23.220	0.00	0.00	0.053	0.00	0.00
ATOM	912	HG23	THR	381	-1.971	-12.175	-24.902	0.00	0.00	0.053	0.00	0.00
ATOM	913	N	GLU	382	-4.053	-12.821	-22.219	0.00	0.00	-0.650	9.00	-17.40
ATOM	914	HN	GLU	382	-4.125	-13.529	-22.964	0.00	0.00	0.439	0.00	0.00
ATOM	915	CA	GLU	382	-3.951	-13.197	-20.834	0.00	0.00	0.158	9.40	4.00
ATOM	916	HA	GLU	382	-3.581	-12.365	-20.235	0.00	0.00	0.053	0.00	0.00
ATOM	917	C	GLU	382	-3.007	-14.352	-20.665	0.00	0.00	0.396	9.82	4.00
ATOM	918	O	GLU	382	-3.421	-15.503	-20.789	0.00	0.00	-0.396	8.17	-17.40
ATOM	919	CB	GLU	382	-5.278	-13.718	-20.255	0.00	0.00	-0.106	12.77	4.00
ATOM	920	HB1	GLU	382	-5.159	-13.834	-19.178	0.00	0.00	0.053	0.00	0.00
ATOM	921	HB2	GLU	382	-5.502	-14.677	-20.722	0.00	0.00	0.053	0.00	0.00
ATOM	922	CG	GLU	382	-6.473	-12.797	-20.492	0.00	0.00	-0.336	12.77	4.00
ATOM	923	HG1	GLU	382	-6.087	-11.779	-20.431	0.00	0.00	0.053	0.00	0.00
ATOM	924	HG2	GLU	382	-7.189	-13.022	-19.702	0.00	0.00	0.053	0.00	0.00
ATOM	925	CD	GLU	382	-7.003	-13.141	-21.879	0.00	0.00	0.297	9.82	4.00
ATOM	926	OE1	GLU	382	-6.405	-14.042	-22.526	0.00	0.00	-0.534	8.17	-18.95
ATOM	927	OE2	GLU	382	-8.010	-12.520	-22.310	0.00	0.00	-0.534	8.17	-18.95
ATOM	928	N	PRO	383	-1.752	-14.107	-20.406	0.00	0.00	-0.422	9.00	-17.40
ATOM	929	CA	PRO	383	-0.921	-15.252	-20.115	0.00	0.00	0.158	9.40	4.00
ATOM	930	HA	PRO	383	-1.232	-16.155	-20.640	0.00	0.00	0.053	0.00	0.00
ATOM	931	CD	PRO	383	-1.071	-13.197	-21.314	0.00	0.00	0.105	12.77	4.00
ATOM	932	HD1	PRO	383	-1.343	-12.199	-20.971	0.00	0.00	0.053	0.00	0.00
ATOM	933	HD2	PRO	383	-1.461	-13.438	-22.303	0.00	0.00	0.053	0.00	0.00
ATOM	934	C	PRO	383	-0.908	-15.623	-18.655	0.00	0.00	0.396	9.82	4.00
ATOM	935	O	PRO	383	-1.325	-14.810	-17.832	0.00	0.00	-0.396	8.17	-17.40
ATOM	936	CB	PRO	383	0.448	-14.994	-20.749	0.00	0.00	-0.106	12.77	4.00
ATOM	937	HB1	PRO	383	0.496	-15.678	-21.596	0.00	0.00	0.053	0.00	0.00
ATOM	938	HB2	PRO	383	1.167	-15.221	-19.962	0.00	0.00	0.053	0.00	0.00
ATOM	939	CG	PRO	383	0.421	-13.514	-21.152	0.00	0.00	-0.106	12.77	4.00
ATOM	940	HG1	PRO	383	0.989	-13.481	-22.082	0.00	0.00	0.053	0.00	0.00
ATOM	941	HG2	PRO	383	0.899	-13.002	-20.317	0.00	0.00	0.053	0.00	0.00
ATOM	942	N	GLU	384	-0.449	-16.856	-18.323	0.00	0.00	-0.650	9.00	-17.40
ATOM	943	HN	GLU	384	-0.120	-17.477	-19.076	0.00	0.00	0.439	0.00	0.00
ATOM	944	CA	GLU	384	-0.400	-17.338	-16.961	0.00	0.00	0.158	9.40	4.00
ATOM	945	HA	GLU	384	-0.368	-16.475	-16.296	0.00	0.00	0.053	0.00	0.00
ATOM	946	C	GLU	384	0.841	-18.179	-16.805	0.00	0.00	0.396	9.82	4.00
ATOM	947	O	GLU	384	1.652	-18.264	-17.725	0.00	0.00	-0.396	8.17	-17.40
ATOM	948	CB	GLU	384	-1.596	-18.226	-16.577	0.00	0.00	-0.106	12.77	4.00
ATOM	949	HB1	GLU	384	-1.501	-18.677	-15.589	0.00	0.00	0.053	0.00	0.00
ATOM	950	HB2	GLU	384	-1.752	-19.061	-17.260	0.00	0.00	0.053	0.00	0.00
ATOM	951	CG	GLU	384	-2.928	-17.474	-16.550	0.00	0.00	-0.336	12.77	4.00
ATOM	952	HG1	GLU	384	-3.107	-17.073	-17.548	0.00	0.00	0.053	0.00	0.00
ATOM	953	HG2	GLU	384	-2.846	-16.672	-15.816	0.00	0.00	0.053	0.00	0.00
ATOM	954	CD	GLU	384	-4.016	-18.462	-16.157	0.00	0.00	0.297	9.82	4.00
ATOM	955	OE1	GLU	384	-3.681	-19.661	-15.953	0.00	0.00	-0.534	8.17	-18.95
ATOM	956	OE2	GLU	384	-5.197	-18.034	-16.053	0.00	0.00	-0.534	8.17	-18.95
ATOM	957	N	PHE	385	1.040	-18.809	-15.618	0.00	0.00	-0.650	9.00	-17.40
ATOM	958	HN	PHE	385	0.341	-18.719	-14.867	0.00	0.00	0.439	0.00	0.00
ATOM	959	CA	PHE	385	2.223	-19.603	-15.402	0.00	0.00	0.158	9.40	4.00
ATOM	960	HA	PHE	385	2.582	-20.017	-16.344	0.00	0.00	0.053	0.00	0.00
ATOM	961	C	PHE	385	1.930	-20.738	-14.467	0.00	0.00	0.396	9.82	4.00
ATOM	962	O	PHE	385	0.823	-21.274	-14.437	0.00	0.00	-0.396	8.17	-17.40
ATOM	963	CB	PHE	385	3.384	-18.783	-14.803	0.00	0.00	-0.106	12.77	4.00
ATOM	964	HB1	PHE	385	3.617	-17.962	-15.481	0.00	0.00	0.053	0.00	0.00
ATOM	965	HB2	PHE	385	4.250	-19.436	-14.689	0.00	0.00	0.053	0.00	0.00
ATOM	966	CG	PHE	385	2.958	-18.252	-13.474	0.00	0.00	0.000	7.26	0.60
ATOM	967	CD1	PHE	385	2.027	-17.241	-13.397	0.00	0.00	-0.127	10.80	0.60
ATOM	968	HD1	PHE	385	1.598	-16.832	-14.312	0.00	0.00	0.127	0.00	0.00
ATOM	969	CD2	PHE	385	3.505	-18.737	-12.307	0.00	0.00	-0.127	10.80	0.60
ATOM	970	HD2	PHE	385	4.258	-19.524	-12.352	0.00	0.00	0.127	0.00	0.00
ATOM	971	CE1	PHE	385	1.632	-16.741	-12.178	0.00	0.00	-0.127	10.80	0.60
ATOM	972	HE1	PHE	385	0.888	-15.946	-12.132	0.00	0.00	0.127	0.00	0.00
ATOM	973	CE2	PHE	385	3.114	-18.241	-11.085	0.00	0.00	-0.127	10.80	0.60
ATOM	974	HE2	PHE	385	3.550	-18.640	-10.169	0.00	0.00	0.127	0.00	0.00
ATOM	975	CZ	PHE	385	2.173	-17.242	-11.019	0.00	0.00	-0.127	10.80	0.60
ATOM	976	HZ	PHE	385	1.858	-16.849	-10.052	0.00	0.00	0.127	0.00	0.00
ATOM	977	N	ASN	386	2.957	-21.137	-13.684	0.00	0.00	-0.650	9.00	-17.40
ATOM	978	HN	ASN	386	3.842	-20.613	-13.741	0.00	0.00	0.439	0.00	0.00
ATOM	979	CA	ASN	386	2.887	-22.250	-12.777	0.00	0.00	0.158	9.40	4.00

ATOM	980	HA	ASN	386	2.470	-23.114	-13.295	0.00	0.00	0.053	0.00	0.00
ATOM	981	C	ASN	386	2.013	-21.893	-11.618	0.00	0.00	0.396	9.82	4.00
ATOM	982	O	ASN	386	1.943	-20.738	-11.200	0.00	0.00	-0.396	8.17	-17.40
ATOM	983	CB	ASN	386	4.265	-22.651	-12.217	0.00	0.00	-0.106	12.77	4.00
ATOM	984	HB1	ASN	386	4.564	-21.933	-11.453	0.00	0.00	0.053	0.00	0.00
ATOM	985	HB2	ASN	386	4.994	-22.652	-13.027	0.00	0.00	0.053	0.00	0.00
ATOM	986	CG	ASN	386	4.171	-24.043	-11.607	0.00	0.00	0.396	9.82	4.00
ATOM	987	OD1	ASN	386	3.132	-24.698	-11.660	0.00	0.00	-0.396	8.17	-17.40
ATOM	988	ND2	ASN	386	5.298	-24.514	-11.008	0.00	0.00	-0.879	13.25	-17.40
ATOM	989	HD21	ASN	386	6.149	-23.935	-10.984	0.00	0.00	0.439	0.00	0.00
ATOM	990	HD22	ASN	386	5.300	-25.450	-10.578	0.00	0.00	0.439	0.00	0.00
ATOM	991	N	HIS	387	1.313	-22.906	-11.068	0.00	0.00	-0.650	9.00	-17.40
ATOM	992	HN	HIS	387	1.417	-23.856	-11.452	0.00	0.00	0.439	0.00	0.00
ATOM	993	CA	HIS	387	0.429	-22.691	-9.962	0.00	0.00	0.158	9.40	4.00
ATOM	994	HA	HIS	387	0.374	-21.615	-9.798	0.00	0.00	0.053	0.00	0.00
ATOM	995	C	HIS	387	1.015	-23.399	-8.785	0.00	0.00	0.396	9.82	4.00
ATOM	996	O	HIS	387	0.328	-23.638	-7.792	0.00	0.00	-0.396	8.17	-17.40
ATOM	997	CB	HIS	387	-0.955	-23.323	-10.190	0.00	0.00	-0.106	12.77	4.00
ATOM	998	HB1	HIS	387	-1.649	-23.147	-9.368	0.00	0.00	0.053	0.00	0.00
ATOM	999	HB2	HIS	387	-0.918	-24.405	-10.313	0.00	0.00	0.053	0.00	0.00
ATOM	1000	CG	HIS	387	-1.647	-22.805	-11.414	0.00	0.00	0.241	7.26	0.60
ATOM	1001	ND1	HIS	387	-1.455	-23.316	-12.678	0.00	0.00	-0.481	9.25	-17.40
ATOM	1002	CD2	HIS	387	-2.550	-21.796	-11.555	0.00	0.00	-0.177	10.80	0.60
ATOM	1003	HD2	HIS	387	-2.923	-21.178	-10.738	0.00	0.00	0.127	0.00	0.00
ATOM	1004	CE1	HIS	387	-2.245	-22.598	-13.516	0.00	0.00	0.064	10.80	0.60
ATOM	1005	HE1	HIS	387	-2.308	-22.772	-14.590	0.00	0.00	0.127	0.00	0.00
ATOM	1006	NE2	HIS	387	-2.928	-21.664	-12.879	0.00	0.00	-0.292	9.25	-17.40
ATOM	1007	HE2	HIS	387	-3.594	-20.988	-13.279	0.00	0.00	0.393	0.00	0.00
ATOM	1008	N	ALA	388	2.315	-23.737	-8.857	0.00	0.00	-0.650	9.00	-17.40
ATOM	1009	HN	ALA	388	2.872	-23.466	-9.680	0.00	0.00	0.439	0.00	0.00
ATOM	1010	CA	ALA	388	2.926	-24.473	-7.791	0.00	0.00	0.158	9.40	4.00
ATOM	1011	HA	ALA	388	2.309	-25.342	-7.564	0.00	0.00	0.053	0.00	0.00
ATOM	1012	C	ALA	388	3.029	-23.591	-6.593	0.00	0.00	0.396	9.82	4.00
ATOM	1013	O	ALA	388	3.122	-22.369	-6.701	0.00	0.00	-0.396	8.17	-17.40
ATOM	1014	CB	ALA	388	4.343	-24.975	-8.121	0.00	0.00	-0.159	16.15	4.00
ATOM	1015	HB1	ALA	388	4.743	-25.523	-7.268	0.00	0.00	0.053	0.00	0.00
ATOM	1016	HB2	ALA	388	4.303	-25.633	-8.989	0.00	0.00	0.053	0.00	0.00
ATOM	1017	HB3	ALA	388	4.988	-24.124	-8.340	0.00	0.00	0.053	0.00	0.00
ATOM	1018	N	ASN	389	2.990	-24.213	-5.400	0.00	0.00	-0.650	9.00	-17.40
ATOM	1019	HN	ASN	389	2.878	-25.236	-5.371	0.00	0.00	0.439	0.00	0.00
ATOM	1020	CA	ASN	389	3.100	-23.487	-4.171	0.00	0.00	0.158	9.40	4.00
ATOM	1021	HA	ASN	389	2.525	-22.570	-4.301	0.00	0.00	0.053	0.00	0.00
ATOM	1022	C	ASN	389	4.554	-23.220	-3.966	0.00	0.00	0.396	9.82	4.00
ATOM	1023	O	ASN	389	5.400	-23.911	-4.531	0.00	0.00	-0.396	8.17	-17.40
ATOM	1024	CB	ASN	389	2.599	-24.285	-2.956	0.00	0.00	-0.106	12.77	4.00
ATOM	1025	HB1	ASN	389	2.832	-23.716	-2.056	0.00	0.00	0.053	0.00	0.00
ATOM	1026	HB2	ASN	389	3.110	-25.248	-2.948	0.00	0.00	0.053	0.00	0.00
ATOM	1027	CG	ASN	389	1.096	-24.474	-3.100	0.00	0.00	0.396	9.82	4.00
ATOM	1028	OD1	ASN	389	0.359	-23.521	-3.347	0.00	0.00	-0.396	8.17	-17.40
ATOM	1029	ND2	ASN	389	0.626	-25.742	-2.951	0.00	0.00	-0.879	13.25	-17.40
ATOM	1030	HD21	ASN	389	1.278	-26.512	-2.744	0.00	0.00	0.439	0.00	0.00
ATOM	1031	HD22	ASN	389	-0.382	-25.932	-3.045	0.00	0.00	0.439	0.00	0.00
ATOM	1032	N	TYR	390	4.895	-22.191	-3.165	0.00	0.00	-0.650	9.00	-17.40
ATOM	1033	HN	TYR	390	4.179	-21.605	-2.713	0.00	0.00	0.439	0.00	0.00
ATOM	1034	CA	TYR	390	6.292	-21.944	-2.966	0.00	0.00	0.158	9.40	4.00
ATOM	1035	HA	TYR	390	6.856	-22.632	-3.596	0.00	0.00	0.053	0.00	0.00
ATOM	1036	C	TYR	390	6.609	-22.172	-1.528	0.00	0.00	0.396	9.82	4.00
ATOM	1037	O	TYR	390	5.781	-21.944	-0.644	0.00	0.00	-0.396	8.17	-17.40
ATOM	1038	CB	TYR	390	6.764	-20.527	-3.348	0.00	0.00	-0.106	12.77	4.00
ATOM	1039	HB1	TYR	390	6.420	-20.288	-4.354	0.00	0.00	0.053	0.00	0.00
ATOM	1040	HB2	TYR	390	7.853	-20.486	-3.317	0.00	0.00	0.053	0.00	0.00
ATOM	1041	CG	TYR	390	6.203	-19.540	-2.385	0.00	0.00	0.000	7.26	0.60
ATOM	1042	CD1	TYR	390	6.863	-19.254	-1.210	0.00	0.00	-0.127	10.80	0.60
ATOM	1043	HD1	TYR	390	7.803	-19.758	-0.985	0.00	0.00	0.127	0.00	0.00
ATOM	1044	CD2	TYR	390	5.022	-18.893	-2.660	0.00	0.00	-0.127	10.80	0.60
ATOM	1045	HD2	TYR	390	4.491	-19.105	-3.588	0.00	0.00	0.127	0.00	0.00
ATOM	1046	CE1	TYR	390	6.353	-18.343	-0.318	0.00	0.00	-0.127	10.80	0.60
ATOM	1047	HE1	TYR	390	6.884	-18.128	0.609	0.00	0.00	0.127	0.00	0.00
ATOM	1048	CE2	TYR	390	4.508	-17.981	-1.772	0.00	0.00	-0.127	10.80	0.60
ATOM	1049	HE2	TYR	390	3.570	-17.474	-1.997	0.00	0.00	0.127	0.00	0.00
ATOM	1050	CZ	TYR	390	5.171	-17.704	-0.600	0.00	0.00	0.027	7.26	0.60
ATOM	1051	OH	TYR	390	4.640	-16.767	0.311	0.00	0.00	-0.451	10.94	-17.40
ATOM	1052	HH	TYR	390	5.156	-15.879	0.230	0.00	0.00	0.424	0.00	0.00
ATOM	1053	N	ALA	391	7.841	-22.643	-1.267	0.00	0.00	-0.650	9.00	-17.40
ATOM	1054	HN	ALA	391	8.500	-22.806	-2.042	0.00	0.00	0.439	0.00	0.00
ATOM	1055	CA	ALA	391	8.245	-22.920	0.076	0.00	0.00	0.158	9.40	4.00

ATOM	1056	HA	ALA	391	7.483	-23.554	0.529	0.00	0.00	0.053	0.00	0.00
ATOM	1057	C	ALA	391	8.358	-21.620	0.795	0.00	0.00	0.396	9.82	4.00
ATOM	1058	O	ALA	391	8.960	-20.667	0.306	0.00	0.00	-0.396	8.17	-17.40
ATOM	1059	CB	ALA	391	9.602	-23.637	0.177	0.00	0.00	-0.159	16.15	4.00
ATOM	1060	HB1	ALA	391	9.843	-23.814	1.225	0.00	0.00	0.053	0.00	0.00
ATOM	1061	HB2	ALA	391	9.550	-24.590	-0.349	0.00	0.00	0.053	0.00	0.00
ATOM	1062	HB3	ALA	391	10.376	-23.016	-0.273	0.00	0.00	0.053	0.00	0.00
ATOM	1063	N	GLN	392	7.753	-21.565	1.992	0.00	0.00	-0.650	9.00	-17.40
ATOM	1064	HN	GLN	392	7.261	-22.401	2.339	0.00	0.00	0.439	0.00	0.00
ATOM	1065	CA	GLN	392	7.767	-20.387	2.803	0.00	0.00	0.158	9.40	4.00
ATOM	1066	HA	GLN	392	8.227	-19.586	2.224	0.00	0.00	0.053	0.00	0.00
ATOM	1067	C	GLN	392	8.562	-20.683	4.030	0.00	0.00	0.396	9.82	4.00
ATOM	1068	O	GLN	392	8.655	-21.831	4.463	0.00	0.00	-0.396	8.17	-17.40
ATOM	1069	CB	GLN	392	6.343	-19.936	3.186	0.00	0.00	-0.106	12.77	4.00
ATOM	1070	HB1	GLN	392	5.828	-19.620	2.279	0.00	0.00	0.053	0.00	0.00
ATOM	1071	HB2	GLN	392	6.423	-19.107	3.889	0.00	0.00	0.053	0.00	0.00
ATOM	1072	CG	GLN	392	5.495	-21.030	3.848	0.00	0.00	-0.106	12.77	4.00
ATOM	1073	HG1	GLN	392	5.734	-22.007	3.427	0.00	0.00	0.053	0.00	0.00
ATOM	1074	HG2	GLN	392	4.433	-20.839	3.691	0.00	0.00	0.053	0.00	0.00
ATOM	1075	CD	GLN	392	5.757	-21.076	5.344	0.00	0.00	0.396	9.82	4.00
ATOM	1076	OE1	GLN	392	5.387	-20.157	6.073	0.00	0.00	-0.396	8.17	-17.40
ATOM	1077	NE2	GLN	392	6.392	-22.180	5.822	0.00	0.00	-0.879	13.25	-17.40
ATOM	1078	HE21	GLN	392	6.685	-22.926	5.175	0.00	0.00	0.439	0.00	0.00
ATOM	1079	HE22	GLN	392	6.580	-22.270	6.831	0.00	0.00	0.439	0.00	0.00
ATOM	1080	N	SER	393	9.191	-19.641	4.606	0.00	0.00	-0.650	9.00	-17.40
ATOM	1081	HN	SER	393	9.106	-18.701	4.193	0.00	0.00	0.439	0.00	0.00
ATOM	1082	CA	SER	393	9.977	-19.828	5.788	0.00	0.00	0.158	9.40	4.00
ATOM	1083	HA	SER	393	10.663	-20.650	5.583	0.00	0.00	0.053	0.00	0.00
ATOM	1084	C	SER	393	9.026	-20.155	6.890	0.00	0.00	0.396	9.82	4.00
ATOM	1085	O	SER	393	7.821	-19.956	6.763	0.00	0.00	-0.396	8.17	-17.40
ATOM	1086	CB	SER	393	10.778	-18.583	6.204	0.00	0.00	0.007	12.77	4.00
ATOM	1087	HB1	SER	393	11.405	-18.248	5.378	0.00	0.00	0.053	0.00	0.00
ATOM	1088	HB2	SER	393	11.414	-18.815	7.058	0.00	0.00	0.053	0.00	0.00
ATOM	1089	OG	SER	393	9.893	-17.531	6.564	0.00	0.00	-0.537	11.04	-17.40
ATOM	1090	HG	SER	393	10.398	-16.633	6.539	0.00	0.00	0.424	0.00	0.00
ATOM	1091	N	LYS	394	9.550	-20.668	8.017	0.00	0.00	-0.650	9.00	-17.40
ATOM	1092	HN	LYS	394	10.571	-20.771	8.106	0.00	0.00	0.439	0.00	0.00
ATOM	1093	CA	LYS	394	8.698	-21.073	9.096	0.00	0.00	0.158	9.40	4.00
ATOM	1094	HA	LYS	394	8.015	-21.841	8.731	0.00	0.00	0.053	0.00	0.00
ATOM	1095	C	LYS	394	7.932	-19.882	9.572	0.00	0.00	0.396	9.82	4.00
ATOM	1096	O	LYS	394	6.758	-19.987	9.923	0.00	0.00	-0.396	8.17	-17.40
ATOM	1097	CB	LYS	394	9.478	-21.622	10.304	0.00	0.00	-0.106	12.77	4.00
ATOM	1098	HB1	LYS	394	8.772	-21.803	11.115	0.00	0.00	0.053	0.00	0.00
ATOM	1099	HB2	LYS	394	10.219	-20.880	10.600	0.00	0.00	0.053	0.00	0.00
ATOM	1100	CG	LYS	394	10.217	-22.934	10.028	0.00	0.00	-0.106	12.77	4.00
ATOM	1101	HG1	LYS	394	9.513	-23.639	9.586	0.00	0.00	0.053	0.00	0.00
ATOM	1102	HG2	LYS	394	10.600	-23.319	10.973	0.00	0.00	0.053	0.00	0.00
ATOM	1103	CD	LYS	394	11.399	-22.788	9.068	0.00	0.00	-0.106	12.77	4.00
ATOM	1104	HD1	LYS	394	12.165	-22.100	9.424	0.00	0.00	0.053	0.00	0.00
ATOM	1105	HD2	LYS	394	11.115	-22.415	8.084	0.00	0.00	0.053	0.00	0.00
ATOM	1106	CE	LYS	394	12.134	-24.103	8.802	0.00	0.00	0.099	12.77	4.00
ATOM	1107	HE1	LYS	394	11.452	-24.830	8.362	0.00	0.00	0.053	0.00	0.00
ATOM	1108	HE2	LYS	394	12.526	-24.508	9.735	0.00	0.00	0.053	0.00	0.00
ATOM	1109	NZ	LYS	394	13.260	-23.876	7.868	0.00	0.00	-0.045	13.25	-39.20
ATOM	1110	HZ1	LYS	394	13.748	-24.766	7.695	0.00	0.00	0.280	0.00	0.00
ATOM	1111	HZ2	LYS	394	12.899	-23.505	6.978	0.00	0.00	0.280	0.00	0.00
ATOM	1112	HZ3	LYS	394	13.918	-23.199	8.280	0.00	0.00	0.280	0.00	0.00
ATOM	1113	N	GLY	395	8.594	-18.713	9.603	0.00	0.00	-0.650	9.00	-17.40
ATOM	1114	HN	GLY	395	9.562	-18.684	9.254	0.00	0.00	0.439	0.00	0.00
ATOM	1115	CA	GLY	395	8.006	-17.505	10.103	0.00	0.00	0.105	9.40	4.00
ATOM	1116	HA1	GLY	395	8.729	-16.692	10.176	0.00	0.00	0.053	0.00	0.00
ATOM	1117	HA2	GLY	395	7.582	-17.632	11.099	0.00	0.00	0.053	0.00	0.00
ATOM	1118	C	GLY	395	6.894	-17.008	9.228	0.00	0.00	0.396	9.82	4.00
ATOM	1119	O	GLY	395	5.941	-16.412	9.727	0.00	0.00	-0.396	8.17	-17.40
ATOM	1120	N	HIS	396	6.979	-17.215	7.899	0.00	0.00	-0.650	9.00	-17.40
ATOM	1121	HN	HIS	396	7.720	-17.816	7.511	0.00	0.00	0.439	0.00	0.00
ATOM	1122	CA	HIS	396	6.021	-16.586	7.030	0.00	0.00	0.158	9.40	4.00
ATOM	1123	HA	HIS	396	5.541	-15.723	7.491	0.00	0.00	0.053	0.00	0.00
ATOM	1124	C	HIS	396	4.915	-17.512	6.626	0.00	0.00	0.396	9.82	4.00
ATOM	1125	O	HIS	396	4.625	-17.651	5.438	0.00	0.00	-0.396	8.17	-17.40
ATOM	1126	CB	HIS	396	6.691	-16.087	5.742	0.00	0.00	-0.106	12.77	4.00
ATOM	1127	HB1	HIS	396	5.966	-15.662	5.048	0.00	0.00	0.053	0.00	0.00
ATOM	1128	HB2	HIS	396	7.205	-16.891	5.216	0.00	0.00	0.053	0.00	0.00
ATOM	1129	CG	HIS	396	7.709	-15.023	6.021	0.00	0.00	0.241	7.26	0.60
ATOM	1130	ND1	HIS	396	8.698	-14.645	5.143	0.00	0.00	-0.481	9.25	-17.40
ATOM	1131	CD2	HIS	396	7.871	-14.242	7.124	0.00	0.00	-0.177	10.80	0.60

ATOM	1132	HD2	HIS	396	7.244	-14.287	8.015	0.00	0.00	0.127	0.00	0.00
ATOM	1133	CE1	HIS	396	9.406	-13.661	5.752	0.00	0.00	0.064	10.80	0.60
ATOM	1134	HE1	HIS	396	10.260	-13.157	5.299	0.00	0.00	0.127	0.00	0.00
ATOM	1135	NE2	HIS	396	8.942	-13.383	6.957	0.00	0.00	-0.292	9.25	-17.40
ATOM	1136	HE2	HIS	396	9.298	-12.683	7.623	0.00	0.00	0.393	0.00	0.00
ATOM	1137	N	LYS	397	4.225	-18.143	7.593	0.00	0.00	-0.650	9.00	-17.40
ATOM	1138	HN	LYS	397	4.457	-17.990	8.585	0.00	0.00	0.439	0.00	0.00
ATOM	1139	CA	LYS	397	3.161	-19.032	7.223	0.00	0.00	0.158	9.40	4.00
ATOM	1140	HA	LYS	397	3.551	-19.782	6.535	0.00	0.00	0.053	0.00	0.00
ATOM	1141	C	LYS	397	2.075	-18.240	6.558	0.00	0.00	0.396	9.82	4.00
ATOM	1142	O	LYS	397	1.586	-18.609	5.491	0.00	0.00	-0.396	8.17	-17.40
ATOM	1143	CB	LYS	397	2.529	-19.743	8.432	0.00	0.00	-0.106	12.77	4.00
ATOM	1144	HB1	LYS	397	1.649	-20.336	8.182	0.00	0.00	0.053	0.00	0.00
ATOM	1145	HB2	LYS	397	2.194	-19.063	9.215	0.00	0.00	0.053	0.00	0.00
ATOM	1146	CG	LYS	397	3.474	-20.719	9.136	0.00	0.00	-0.106	12.77	4.00
ATOM	1147	HG1	LYS	397	3.036	-21.199	10.011	0.00	0.00	0.053	0.00	0.00
ATOM	1148	HG2	LYS	397	4.391	-20.256	9.499	0.00	0.00	0.053	0.00	0.00
ATOM	1149	CD	LYS	397	3.941	-21.873	8.247	0.00	0.00	-0.106	12.77	4.00
ATOM	1150	HD1	LYS	397	4.486	-21.549	7.360	0.00	0.00	0.053	0.00	0.00
ATOM	1151	HD2	LYS	397	3.126	-22.490	7.868	0.00	0.00	0.053	0.00	0.00
ATOM	1152	CE	LYS	397	4.881	-22.850	8.954	0.00	0.00	0.099	12.77	4.00
ATOM	1153	HE1	LYS	397	4.381	-23.292	9.816	0.00	0.00	0.053	0.00	0.00
ATOM	1154	HE2	LYS	397	5.776	-22.328	9.294	0.00	0.00	0.053	0.00	0.00
ATOM	1155	NZ	LYS	397	5.281	-23.931	8.026	0.00	0.00	-0.045	13.25	-39.20
ATOM	1156	HZ1	LYS	397	5.914	-24.584	8.511	0.00	0.00	0.280	0.00	0.00
ATOM	1157	HZ2	LYS	397	4.443	-24.438	7.708	0.00	0.00	0.280	0.00	0.00
ATOM	1158	HZ3	LYS	397	5.765	-23.524	7.213	0.00	0.00	0.280	0.00	0.00
ATOM	1159	N	THR	398	1.682	-17.112	7.180	0.00	0.00	-0.650	9.00	-17.40
ATOM	1160	HN	THR	398	2.170	-16.833	8.043	0.00	0.00	0.439	0.00	0.00
ATOM	1161	CA	THR	398	0.614	-16.279	6.698	0.00	0.00	0.158	9.40	4.00
ATOM	1162	HA	THR	398	-0.293	-16.839	6.470	0.00	0.00	0.053	0.00	0.00
ATOM	1163	C	THR	398	0.968	-15.541	5.431	0.00	0.00	0.396	9.82	4.00
ATOM	1164	O	THR	398	0.064	-15.261	4.645	0.00	0.00	-0.396	8.17	-17.40
ATOM	1165	CB	THR	398	0.071	-15.319	7.730	0.00	0.00	0.060	9.40	4.00
ATOM	1166	HB	THR	398	-0.725	-14.737	7.265	0.00	0.00	0.053	0.00	0.00
ATOM	1167	OG1	THR	398	1.064	-14.416	8.190	0.00	0.00	-0.537	11.04	-17.40
ATOM	1168	HG1	THR	398	1.923	-14.537	7.634	0.00	0.00	0.424	0.00	0.00
ATOM	1169	CG2	THR	398	-0.471	-16.143	8.909	0.00	0.00	-0.159	16.15	4.00
ATOM	1170	HG21	THR	398	-0.870	-15.471	9.669	0.00	0.00	0.053	0.00	0.00
ATOM	1171	HG22	THR	398	-1.263	-16.804	8.557	0.00	0.00	0.053	0.00	0.00
ATOM	1172	HG23	THR	398	0.335	-16.739	9.338	0.00	0.00	0.053	0.00	0.00
ATOM	1173	N	PRO	399	2.204	-15.195	5.166	0.00	0.00	-0.422	9.00	-17.40
ATOM	1174	CA	PRO	399	2.481	-14.452	3.959	0.00	0.00	0.158	9.40	4.00
ATOM	1175	HA	PRO	399	1.729	-13.694	3.740	0.00	0.00	0.053	0.00	0.00
ATOM	1176	CD	PRO	399	3.104	-14.778	6.231	0.00	0.00	0.105	12.77	4.00
ATOM	1177	HD1	PRO	399	3.312	-15.686	6.797	0.00	0.00	0.053	0.00	0.00
ATOM	1178	HD2	PRO	399	2.546	-14.031	6.796	0.00	0.00	0.053	0.00	0.00
ATOM	1179	C	PRO	399	2.548	-15.314	2.741	0.00	0.00	0.396	9.82	4.00
ATOM	1180	O	PRO	399	3.141	-14.891	1.751	0.00	0.00	-0.396	8.17	-17.40
ATOM	1181	CB	PRO	399	3.762	-13.652	4.204	0.00	0.00	-0.106	12.77	4.00
ATOM	1182	HB1	PRO	399	3.435	-12.615	4.277	0.00	0.00	0.053	0.00	0.00
ATOM	1183	HB2	PRO	399	4.388	-13.853	3.335	0.00	0.00	0.053	0.00	0.00
ATOM	1184	CG	PRO	399	4.331	-14.211	5.514	0.00	0.00	-0.106	12.77	4.00
ATOM	1185	HG1	PRO	399	4.810	-13.425	6.098	0.00	0.00	0.053	0.00	0.00
ATOM	1186	HG2	PRO	399	5.074	-14.984	5.317	0.00	0.00	0.053	0.00	0.00
ATOM	1187	N	TRP	400	1.929	-16.504	2.778	0.00	0.00	-0.650	9.00	-17.40
ATOM	1188	HN	TRP	400	1.374	-16.740	3.613	0.00	0.00	0.439	0.00	0.00
ATOM	1189	CA	TRP	400	2.001	-17.463	1.715	0.00	0.00	0.158	9.40	4.00
ATOM	1190	HA	TRP	400	3.020	-17.838	1.623	0.00	0.00	0.053	0.00	0.00
ATOM	1191	C	TRP	400	1.596	-16.821	0.421	0.00	0.00	0.396	9.82	4.00
ATOM	1192	O	TRP	400	2.165	-17.158	-0.615	0.00	0.00	-0.396	8.17	-17.40
ATOM	1193	CB	TRP	400	1.064	-18.657	1.962	0.00	0.00	-0.106	12.77	4.00
ATOM	1194	HB1	TRP	400	0.043	-18.279	2.020	0.00	0.00	0.053	0.00	0.00
ATOM	1195	HB2	TRP	400	1.357	-19.128	2.900	0.00	0.00	0.053	0.00	0.00
ATOM	1196	CG	TRP	400	1.089	-19.725	0.896	0.00	0.00	0.000	7.26	0.60
ATOM	1197	CD1	TRP	400	0.340	-19.850	-0.238	0.00	0.00	-0.177	10.80	0.60
ATOM	1198	HD1	TRP	400	-0.419	-19.141	-0.569	0.00	0.00	0.127	0.00	0.00
ATOM	1199	CD2	TRP	400	1.958	-20.866	0.940	0.00	0.00	0.000	6.80	0.60
ATOM	1200	NE1	TRP	400	0.687	-21.004	-0.901	0.00	0.00	-0.292	9.00	-17.40
ATOM	1201	HE1	TRP	400	0.273	-21.339	-1.783	0.00	0.00	0.393	0.00	0.00
ATOM	1202	CE2	TRP	400	1.682	-21.637	-0.187	0.00	0.00	-0.050	6.80	0.60
ATOM	1203	CE3	TRP	400	2.905	-21.242	1.849	0.00	0.00	-0.127	10.80	0.60
ATOM	1204	HE3	TRP	400	3.116	-20.638	2.731	0.00	0.00	0.127	0.00	0.00
ATOM	1205	CZ2	TRP	400	2.353	-22.803	-0.421	0.00	0.00	-0.127	10.80	0.60
ATOM	1206	HZ2	TRP	400	2.137	-23.412	-1.299	0.00	0.00	0.127	0.00	0.00
ATOM	1207	CZ3	TRP	400	3.583	-22.416	1.606	0.00	0.00	-0.127	10.80	0.60

ATOM	1208	HZ3	TRP	400	4.349	-22.746	2.308	0.00	0.00	0.127	0.00	0.00
ATOM	1209	CH2	TRP	400	3.312	-23.182	0.492	0.00	0.00	-0.127	10.80	0.60
ATOM	1210	HH2	TRP	400	3.868	-24.106	0.331	0.00	0.00	0.127	0.00	0.00
ATOM	1211	N	GLY	401	0.602	-15.903	0.439	0.00	0.00	-0.650	9.00	-17.40
ATOM	1212	HN	GLY	401	0.162	-15.671	1.341	0.00	0.00	0.439	0.00	0.00
ATOM	1213	CA	GLY	401	0.131	-15.234	-0.751	0.00	0.00	0.105	9.40	4.00
ATOM	1214	HA1	GLY	401	-0.487	-14.382	-0.467	0.00	0.00	0.053	0.00	0.00
ATOM	1215	HA2	GLY	401	-0.459	-15.929	-1.348	0.00	0.00	0.053	0.00	0.00
ATOM	1216	C	GLY	401	1.306	-14.757	-1.553	0.00	0.00	0.396	9.82	4.00
ATOM	1217	O	GLY	401	1.948	-13.766	-1.211	0.00	0.00	-0.396	8.17	-17.40
ATOM	1218	N	LYS	402	1.601	-15.470	-2.663	0.00	0.00	-0.650	9.00	-17.40
ATOM	1219	HN	LYS	402	0.978	-16.244	-2.935	0.00	0.00	0.439	0.00	0.00
ATOM	1220	CA	LYS	402	2.750	-15.189	-3.476	0.00	0.00	0.158	9.40	4.00
ATOM	1221	HA	LYS	402	3.617	-14.972	-2.851	0.00	0.00	0.053	0.00	0.00
ATOM	1222	C	LYS	402	2.495	-14.010	-4.352	0.00	0.00	0.396	9.82	4.00
ATOM	1223	O	LYS	402	2.506	-14.109	-5.579	0.00	0.00	-0.396	8.17	-17.40
ATOM	1224	CB	LYS	402	3.170	-16.381	-4.352	0.00	0.00	-0.106	12.77	4.00
ATOM	1225	HB1	LYS	402	3.474	-17.197	-3.697	0.00	0.00	0.053	0.00	0.00
ATOM	1226	HB2	LYS	402	4.001	-16.066	-4.983	0.00	0.00	0.053	0.00	0.00
ATOM	1227	CG	LYS	402	2.065	-16.907	-5.267	0.00	0.00	-0.106	12.77	4.00
ATOM	1228	HG1	LYS	402	1.597	-16.125	-5.865	0.00	0.00	0.053	0.00	0.00
ATOM	1229	HG2	LYS	402	1.252	-17.387	-4.723	0.00	0.00	0.053	0.00	0.00
ATOM	1230	CD	LYS	402	2.562	-17.950	-6.269	0.00	0.00	-0.106	12.77	4.00
ATOM	1231	HD1	LYS	402	3.126	-18.764	-5.813	0.00	0.00	0.053	0.00	0.00
ATOM	1232	HD2	LYS	402	3.225	-17.545	-7.033	0.00	0.00	0.053	0.00	0.00
ATOM	1233	CE	LYS	402	1.442	-18.639	-7.049	0.00	0.00	0.099	12.77	4.00
ATOM	1234	HE1	LYS	402	0.893	-17.905	-7.639	0.00	0.00	0.053	0.00	0.00
ATOM	1235	HE2	LYS	402	0.753	-19.126	-6.359	0.00	0.00	0.053	0.00	0.00
ATOM	1236	NZ	LYS	402	2.012	-19.658	-7.958	0.00	0.00	-0.045	13.25	-39.20
ATOM	1237	HZ1	LYS	402	1.252	-20.117	-8.479	0.00	0.00	0.280	0.00	0.00
ATOM	1238	HZ2	LYS	402	2.657	-19.205	-8.621	0.00	0.00	0.280	0.00	0.00
ATOM	1239	HZ3	LYS	402	2.524	-20.362	-7.407	0.00	0.00	0.280	0.00	0.00
ATOM	1240	N	TRP	403	2.261	-12.848	-3.720	0.00	0.00	-0.650	9.00	-17.40
ATOM	1241	HN	TRP	403	2.201	-12.837	-2.692	0.00	0.00	0.439	0.00	0.00
ATOM	1242	CA	TRP	403	2.094	-11.629	-4.443	0.00	0.00	0.158	9.40	4.00
ATOM	1243	HA	TRP	403	1.332	-11.826	-5.197	0.00	0.00	0.053	0.00	0.00
ATOM	1244	C	TRP	403	3.420	-11.318	-5.039	0.00	0.00	0.396	9.82	4.00
ATOM	1245	O	TRP	403	3.505	-10.725	-6.101	0.00	0.00	-0.396	8.17	-17.40
ATOM	1246	CB	TRP	403	1.696	-10.438	-3.550	0.00	0.00	-0.106	12.77	4.00
ATOM	1247	HB1	TRP	403	0.746	-10.675	-3.070	0.00	0.00	0.053	0.00	0.00
ATOM	1248	HB2	TRP	403	1.599	-9.556	-4.183	0.00	0.00	0.053	0.00	0.00
ATOM	1249	CG	TRP	403	2.687	-10.108	-2.458	0.00	0.00	0.000	7.26	0.60
ATOM	1250	CD1	TRP	403	3.861	-9.417	-2.536	0.00	0.00	-0.177	10.80	0.60
ATOM	1251	HD1	TRP	403	4.276	-8.991	-3.449	0.00	0.00	0.127	0.00	0.00
ATOM	1252	CD2	TRP	403	2.524	-10.476	-1.079	0.00	0.00	0.000	6.80	0.60
ATOM	1253	NE1	TRP	403	4.443	-9.338	-1.293	0.00	0.00	-0.292	9.00	-17.40
ATOM	1254	HE1	TRP	403	5.337	-8.874	-1.076	0.00	0.00	0.393	0.00	0.00
ATOM	1255	CE2	TRP	403	3.629	-9.984	-0.386	0.00	0.00	-0.050	6.80	0.60
ATOM	1256	CE3	TRP	403	1.531	-11.164	-0.442	0.00	0.00	-0.127	10.80	0.60
ATOM	1257	HE3	TRP	403	0.666	-11.544	-0.985	0.00	0.00	0.127	0.00	0.00
ATOM	1258	CZ2	TRP	403	3.760	-10.175	0.960	0.00	0.00	-0.127	10.80	0.60
ATOM	1259	HZ2	TRP	403	4.622	-9.790	1.505	0.00	0.00	0.127	0.00	0.00
ATOM	1260	CZ3	TRP	403	1.667	-11.358	0.915	0.00	0.00	-0.127	10.80	0.60
ATOM	1261	HZ3	TRP	403	0.895	-11.905	1.456	0.00	0.00	0.127	0.00	0.00
ATOM	1262	CH2	TRP	403	2.761	-10.873	1.603	0.00	0.00	-0.127	10.80	0.60
ATOM	1263	HH2	TRP	403	2.836	-11.046	2.677	0.00	0.00	0.127	0.00	0.00
ATOM	1264	N	ASN	404	4.511	-11.679	-4.358	0.00	0.00	-0.650	9.00	-17.40
ATOM	1265	HN	ASN	404	4.411	-12.173	-3.460	0.00	0.00	0.439	0.00	0.00
ATOM	1266	CA	ASN	404	5.820	-11.386	-4.865	0.00	0.00	0.158	9.40	4.00
ATOM	1267	HA	ASN	404	5.893	-10.324	-5.099	0.00	0.00	0.053	0.00	0.00
ATOM	1268	C	ASN	404	6.069	-12.184	-6.107	0.00	0.00	0.396	9.82	4.00
ATOM	1269	O	ASN	404	6.571	-11.671	-7.108	0.00	0.00	-0.396	8.17	-17.40
ATOM	1270	CB	ASN	404	6.891	-11.794	-3.848	0.00	0.00	-0.106	12.77	4.00
ATOM	1271	HB1	ASN	404	6.933	-12.882	-3.789	0.00	0.00	0.053	0.00	0.00
ATOM	1272	HB2	ASN	404	6.634	-11.382	-2.872	0.00	0.00	0.053	0.00	0.00
ATOM	1273	CG	ASN	404	8.231	-11.254	-4.294	0.00	0.00	0.396	9.82	4.00
ATOM	1274	OD1	ASN	404	8.555	-11.183	-5.478	0.00	0.00	-0.396	8.17	-17.40
ATOM	1275	ND2	ASN	404	9.040	-10.854	-3.279	0.00	0.00	-0.879	13.25	-17.40
ATOM	1276	HD21	ASN	404	8.720	-10.935	-2.303	0.00	0.00	0.439	0.00	0.00
ATOM	1277	HD22	ASN	404	9.973	-10.470	-3.485	0.00	0.00	0.439	0.00	0.00
ATOM	1278	N	LEU	405	5.695	-13.473	-6.074	0.00	0.00	-0.650	9.00	-17.40
ATOM	1279	HN	LEU	405	5.173	-13.823	-5.258	0.00	0.00	0.439	0.00	0.00
ATOM	1280	CA	LEU	405	6.002	-14.375	-7.144	0.00	0.00	0.158	9.40	4.00
ATOM	1281	HA	LEU	405	7.082	-14.410	-7.289	0.00	0.00	0.053	0.00	0.00
ATOM	1282	C	LEU	405	5.345	-13.900	-8.396	0.00	0.00	0.396	9.82	4.00
ATOM	1283	O	LEU	405	5.964	-13.924	-9.458	0.00	0.00	-0.396	8.17	-17.40

ATOM	1284	CB	LEU	405	5.523	-15.816	-6.846	0.00	0.00	-0.106	12.77	4.00
ATOM	1285	HB1	LEU	405	4.433	-15.806	-6.856	0.00	0.00	0.053	0.00	0.00
ATOM	1286	HB2	LEU	405	5.910	-16.092	-5.865	0.00	0.00	0.053	0.00	0.00
ATOM	1287	CG	LEU	405	5.961	-16.940	-7.823	0.00	0.00	-0.053	9.40	4.00
ATOM	1288	HG	LEU	405	7.049	-17.007	-7.850	0.00	0.00	0.053	0.00	0.00
ATOM	1289	CD1	LEU	405	5.389	-18.289	-7.362	0.00	0.00	-0.159	16.15	4.00
ATOM	1290	HD11	LEU	405	5.701	-19.072	-8.053	0.00	0.00	0.053	0.00	0.00
ATOM	1291	HD12	LEU	405	5.759	-18.519	-6.363	0.00	0.00	0.053	0.00	0.00
ATOM	1292	HD13	LEU	405	4.301	-18.235	-7.343	0.00	0.00	0.053	0.00	0.00
ATOM	1293	CD2	LEU	405	5.606	-16.672	-9.298	0.00	0.00	-0.159	16.15	4.00
ATOM	1294	HD21	LEU	405	5.947	-17.506	-9.912	0.00	0.00	0.053	0.00	0.00
ATOM	1295	HD22	LEU	405	4.526	-16.566	-9.399	0.00	0.00	0.053	0.00	0.00
ATOM	1296	HD23	LEU	405	6.093	-15.755	-9.629	0.00	0.00	0.053	0.00	0.00
ATOM	1297	N	ASN	406	4.078	-13.452	-8.322	0.00	0.00	-0.650	9.00	-17.40
ATOM	1298	HN	ASN	406	3.598	-13.353	-7.416	0.00	0.00	0.439	0.00	0.00
ATOM	1299	CA	ASN	406	3.423	-13.118	-9.552	0.00	0.00	0.158	9.40	4.00
ATOM	1300	HA	ASN	406	3.425	-13.984	-10.214	0.00	0.00	0.053	0.00	0.00
ATOM	1301	C	ASN	406	4.148	-11.980	-10.217	0.00	0.00	0.396	9.82	4.00
ATOM	1302	O	ASN	406	4.476	-12.090	-11.396	0.00	0.00	-0.396	8.17	-17.40
ATOM	1303	CB	ASN	406	1.931	-12.774	-9.373	0.00	0.00	-0.106	12.77	4.00
ATOM	1304	HB1	ASN	406	1.516	-12.555	-10.357	0.00	0.00	0.053	0.00	0.00
ATOM	1305	HB2	ASN	406	1.863	-11.905	-8.719	0.00	0.00	0.053	0.00	0.00
ATOM	1306	CG	ASN	406	1.245	-13.976	-8.751	0.00	0.00	0.396	9.82	4.00
ATOM	1307	OD1	ASN	406	1.285	-15.088	-9.275	0.00	0.00	-0.396	8.17	-17.40
ATOM	1308	ND2	ASN	406	0.603	-13.739	-7.576	0.00	0.00	-0.879	13.25	-17.40
ATOM	1309	HD21	ASN	406	0.596	-12.790	-7.175	0.00	0.00	0.439	0.00	0.00
ATOM	1310	HD22	ASN	406	0.123	-14.508	-7.087	0.00	0.00	0.439	0.00	0.00
ATOM	1311	N	PRO	407	4.447	-10.898	-9.540	0.00	0.00	-0.422	9.00	-17.40
ATOM	1312	CA	PRO	407	5.217	-9.900	-10.205	0.00	0.00	0.158	9.40	4.00
ATOM	1313	HA	PRO	407	4.641	-9.543	-11.059	0.00	0.00	0.053	0.00	0.00
ATOM	1314	CD	PRO	407	3.398	-10.217	-8.808	0.00	0.00	0.105	12.77	4.00
ATOM	1315	HD1	PRO	407	3.302	-10.722	-7.847	0.00	0.00	0.053	0.00	0.00
ATOM	1316	HD2	PRO	407	2.489	-10.301	-9.404	0.00	0.00	0.053	0.00	0.00
ATOM	1317	C	PRO	407	6.533	-10.346	-10.720	0.00	0.00	0.396	9.82	4.00
ATOM	1318	O	PRO	407	6.929	-9.844	-11.768	0.00	0.00	-0.396	8.17	-17.40
ATOM	1319	CB	PRO	407	5.251	-8.708	-9.259	0.00	0.00	-0.106	12.77	4.00
ATOM	1320	HB1	PRO	407	5.440	-7.779	-9.797	0.00	0.00	0.053	0.00	0.00
ATOM	1321	HB2	PRO	407	6.035	-8.818	-8.509	0.00	0.00	0.053	0.00	0.00
ATOM	1322	CG	PRO	407	3.844	-8.751	-8.644	0.00	0.00	-0.106	12.77	4.00
ATOM	1323	HG1	PRO	407	3.266	-8.043	-9.238	0.00	0.00	0.053	0.00	0.00
ATOM	1324	HG2	PRO	407	3.991	-8.445	-7.608	0.00	0.00	0.053	0.00	0.00
ATOM	1325	N	GLN	408	7.225	-11.277	-10.044	0.00	0.00	-0.650	9.00	-17.40
ATOM	1326	HN	GLN	408	6.853	-11.700	-9.182	0.00	0.00	0.439	0.00	0.00
ATOM	1327	CA	GLN	408	8.500	-11.658	-10.570	0.00	0.00	0.158	9.40	4.00
ATOM	1328	HA	GLN	408	9.097	-10.747	-10.614	0.00	0.00	0.053	0.00	0.00
ATOM	1329	C	GLN	408	8.240	-12.234	-11.918	0.00	0.00	0.396	9.82	4.00
ATOM	1330	O	GLN	408	8.923	-11.912	-12.889	0.00	0.00	-0.396	8.17	-17.40
ATOM	1331	CB	GLN	408	9.211	-12.737	-9.723	0.00	0.00	-0.106	12.77	4.00
ATOM	1332	HB1	GLN	408	8.579	-13.625	-9.705	0.00	0.00	0.053	0.00	0.00
ATOM	1333	HB2	GLN	408	9.350	-12.341	-8.717	0.00	0.00	0.053	0.00	0.00
ATOM	1334	CG	GLN	408	10.595	-13.168	-10.243	0.00	0.00	-0.106	12.77	4.00
ATOM	1335	HG1	GLN	408	11.145	-13.686	-9.457	0.00	0.00	0.053	0.00	0.00
ATOM	1336	HG2	GLN	408	11.165	-12.293	-10.555	0.00	0.00	0.053	0.00	0.00
ATOM	1337	CD	GLN	408	10.436	-14.107	-11.436	0.00	0.00	0.396	9.82	4.00
ATOM	1338	OE1	GLN	408	9.567	-14.978	-11.442	0.00	0.00	-0.396	8.17	-17.40
ATOM	1339	NE2	GLN	408	11.271	-13.900	-12.490	0.00	0.00	-0.879	13.25	-17.40
ATOM	1340	HE21	GLN	408	11.985	-13.159	-12.443	0.00	0.00	0.439	0.00	0.00
ATOM	1341	HE22	GLN	408	11.189	-14.484	-13.334	0.00	0.00	0.439	0.00	0.00
ATOM	1342	N	GLN	409	7.220	-13.102	-12.012	0.00	0.00	-0.650	9.00	-17.40
ATOM	1343	HN	GLN	409	6.639	-13.319	-11.190	0.00	0.00	0.439	0.00	0.00
ATOM	1344	CA	GLN	409	6.956	-13.718	-13.271	0.00	0.00	0.158	9.40	4.00
ATOM	1345	HA	GLN	409	7.866	-14.163	-13.672	0.00	0.00	0.053	0.00	0.00
ATOM	1346	C	GLN	409	6.448	-12.704	-14.249	0.00	0.00	0.396	9.82	4.00
ATOM	1347	O	GLN	409	6.953	-12.617	-15.364	0.00	0.00	-0.396	8.17	-17.40
ATOM	1348	CB	GLN	409	5.940	-14.871	-13.172	0.00	0.00	-0.106	12.77	4.00
ATOM	1349	HB1	GLN	409	5.655	-15.267	-14.147	0.00	0.00	0.053	0.00	0.00
ATOM	1350	HB2	GLN	409	5.011	-14.574	-12.686	0.00	0.00	0.053	0.00	0.00
ATOM	1351	CG	GLN	409	6.473	-16.064	-12.371	0.00	0.00	-0.106	12.77	4.00
ATOM	1352	HG1	GLN	409	5.652	-16.762	-12.208	0.00	0.00	0.053	0.00	0.00
ATOM	1353	HG2	GLN	409	6.856	-15.695	-11.420	0.00	0.00	0.053	0.00	0.00
ATOM	1354	CD	GLN	409	7.585	-16.724	-13.177	0.00	0.00	0.396	9.82	4.00
ATOM	1355	OE1	GLN	409	7.730	-16.486	-14.376	0.00	0.00	-0.396	8.17	-17.40
ATOM	1356	NE2	GLN	409	8.392	-17.588	-12.505	0.00	0.00	-0.879	13.25	-17.40
ATOM	1357	HE21	GLN	409	8.239	-17.761	-11.501	0.00	0.00	0.439	0.00	0.00
ATOM	1358	HE22	GLN	409	9.156	-18.069	-13.000	0.00	0.00	0.439	0.00	0.00
ATOM	1359	N	PHE	410	5.466	-11.862	-13.881	0.00	0.00	-0.650	9.00	-17.40

ATOM	1360	HN	PHE	410	5.103	-11.811	-12.919	0.00	0.00	0.439	0.00	0.00
ATOM	1361	CA	PHE	410	4.970	-11.042	-14.948	0.00	0.00	0.158	9.40	4.00
ATOM	1362	HA	PHE	410	4.680	-11.622	-15.824	0.00	0.00	0.053	0.00	0.00
ATOM	1363	C	PHE	410	5.983	-10.041	-15.429	0.00	0.00	0.396	9.82	4.00
ATOM	1364	O	PHE	410	6.041	-9.761	-16.627	0.00	0.00	-0.396	8.17	-17.40
ATOM	1365	CB	PHE	410	3.601	-10.375	-14.731	0.00	0.00	-0.106	12.77	4.00
ATOM	1366	HB1	PHE	410	2.869	-11.161	-14.543	0.00	0.00	0.053	0.00	0.00
ATOM	1367	HB2	PHE	410	3.350	-9.818	-15.634	0.00	0.00	0.053	0.00	0.00
ATOM	1368	CG	PHE	410	3.529	-9.427	-13.596	0.00	0.00	0.000	7.26	0.60
ATOM	1369	CD1	PHE	410	4.191	-8.224	-13.641	0.00	0.00	-0.127	10.80	0.60
ATOM	1370	HD1	PHE	410	4.783	-7.964	-14.518	0.00	0.00	0.127	0.00	0.00
ATOM	1371	CD2	PHE	410	2.784	-9.749	-12.488	0.00	0.00	-0.127	10.80	0.60
ATOM	1372	HD2	PHE	410	2.259	-10.703	-12.445	0.00	0.00	0.127	0.00	0.00
ATOM	1373	CE1	PHE	410	4.111	-7.347	-12.586	0.00	0.00	-0.127	10.80	0.60
ATOM	1374	HE1	PHE	410	4.642	-6.396	-12.625	0.00	0.00	0.127	0.00	0.00
ATOM	1375	CE2	PHE	410	2.698	-8.874	-11.436	0.00	0.00	-0.127	10.80	0.60
ATOM	1376	HE2	PHE	410	2.102	-9.133	-10.561	0.00	0.00	0.127	0.00	0.00
ATOM	1377	CZ	PHE	410	3.361	-7.671	-11.482	0.00	0.00	-0.127	10.80	0.60
ATOM	1378	HZ	PHE	410	3.292	-6.976	-10.645	0.00	0.00	0.127	0.00	0.00
ATOM	1379	N	TYR	411	6.815	-9.469	-14.536	0.00	0.00	-0.650	9.00	-17.40
ATOM	1380	HN	TYR	411	6.744	-9.687	-13.532	0.00	0.00	0.439	0.00	0.00
ATOM	1381	CA	TYR	411	7.806	-8.545	-15.023	0.00	0.00	0.158	9.40	4.00
ATOM	1382	HA	TYR	411	7.305	-7.734	-15.551	0.00	0.00	0.053	0.00	0.00
ATOM	1383	C	TYR	411	8.732	-9.270	-15.956	0.00	0.00	0.396	9.82	4.00
ATOM	1384	O	TYR	411	9.152	-8.707	-16.962	0.00	0.00	-0.396	8.17	-17.40
ATOM	1385	CB	TYR	411	8.775	-7.956	-13.970	0.00	0.00	-0.106	12.77	4.00
ATOM	1386	HB1	TYR	411	9.622	-7.428	-14.407	0.00	0.00	0.053	0.00	0.00
ATOM	1387	HB2	TYR	411	9.215	-8.709	-13.316	0.00	0.00	0.053	0.00	0.00
ATOM	1388	CG	TYR	411	8.130	-6.971	-13.055	0.00	0.00	0.000	7.26	0.60
ATOM	1389	CD1	TYR	411	7.796	-5.706	-13.481	0.00	0.00	-0.127	10.80	0.60
ATOM	1390	HD1	TYR	411	7.993	-5.414	-14.513	0.00	0.00	0.127	0.00	0.00
ATOM	1391	CD2	TYR	411	7.901	-7.299	-11.743	0.00	0.00	-0.127	10.80	0.60
ATOM	1392	HD2	TYR	411	8.185	-8.288	-11.385	0.00	0.00	0.127	0.00	0.00
ATOM	1393	CE1	TYR	411	7.216	-4.806	-12.617	0.00	0.00	-0.127	10.80	0.60
ATOM	1394	HE1	TYR	411	6.946	-3.810	-12.969	0.00	0.00	0.127	0.00	0.00
ATOM	1395	CE2	TYR	411	7.323	-6.412	-10.871	0.00	0.00	-0.127	10.80	0.60
ATOM	1396	HE2	TYR	411	7.141	-6.700	-9.836	0.00	0.00	0.127	0.00	0.00
ATOM	1397	CZ	TYR	411	6.976	-5.160	-11.311	0.00	0.00	0.027	7.26	0.60
ATOM	1398	OH	TYR	411	6.384	-4.245	-10.418	0.00	0.00	-0.451	10.94	-17.40
ATOM	1399	HH	TYR	411	6.870	-3.339	-10.481	0.00	0.00	0.424	0.00	0.00
ATOM	1400	N	THR	412	9.098	-10.532	-15.655	0.00	0.00	-0.650	9.00	-17.40
ATOM	1401	HN	THR	412	8.699	-11.007	-14.833	0.00	0.00	0.439	0.00	0.00
ATOM	1402	CA	THR	412	10.051	-11.209	-16.492	0.00	0.00	0.158	9.40	4.00
ATOM	1403	HA	THR	412	10.956	-10.603	-16.517	0.00	0.00	0.053	0.00	0.00
ATOM	1404	C	THR	412	9.449	-11.336	-17.845	0.00	0.00	0.396	9.82	4.00
ATOM	1405	O	THR	412	10.143	-11.237	-18.855	0.00	0.00	-0.396	8.17	-17.40
ATOM	1406	CB	THR	412	10.447	-12.588	-16.018	0.00	0.00	0.060	9.40	4.00
ATOM	1407	HB	THR	412	10.645	-12.581	-14.946	0.00	0.00	0.053	0.00	0.00
ATOM	1408	OG1	THR	412	11.624	-13.011	-16.691	0.00	0.00	-0.537	11.04	-17.40
ATOM	1409	HG1	THR	412	11.620	-12.645	-17.654	0.00	0.00	0.424	0.00	0.00
ATOM	1410	CG2	THR	412	9.322	-13.597	-16.298	0.00	0.00	-0.159	16.15	4.00
ATOM	1411	HG21	THR	412	9.624	-14.585	-15.950	0.00	0.00	0.053	0.00	0.00
ATOM	1412	HG22	THR	412	8.418	-13.289	-15.773	0.00	0.00	0.053	0.00	0.00
ATOM	1413	HG23	THR	412	9.125	-13.634	-17.369	0.00	0.00	0.053	0.00	0.00
ATOM	1414	N	MET	413	8.126	-11.560	-17.894	0.00	0.00	-0.650	9.00	-17.40
ATOM	1415	HN	MET	413	7.584	-11.665	-17.025	0.00	0.00	0.439	0.00	0.00
ATOM	1416	CA	MET	413	7.479	-11.651	-19.163	0.00	0.00	0.158	9.40	4.00
ATOM	1417	HA	MET	413	7.932	-12.467	-19.726	0.00	0.00	0.053	0.00	0.00
ATOM	1418	C	MET	413	7.663	-10.358	-19.884	0.00	0.00	0.396	9.82	4.00
ATOM	1419	O	MET	413	7.962	-10.368	-21.070	0.00	0.00	-0.396	8.17	-17.40
ATOM	1420	CB	MET	413	5.975	-11.960	-19.052	0.00	0.00	-0.106	12.77	4.00
ATOM	1421	HB1	MET	413	5.399	-11.583	-19.897	0.00	0.00	0.053	0.00	0.00
ATOM	1422	HB2	MET	413	5.515	-11.526	-18.164	0.00	0.00	0.053	0.00	0.00
ATOM	1423	CG	MET	413	5.675	-13.461	-18.983	0.00	0.00	-0.041	12.77	4.00
ATOM	1424	HG1	MET	413	6.083	-13.926	-19.881	0.00	0.00	0.053	0.00	0.00
ATOM	1425	HG2	MET	413	4.593	-13.585	-18.936	0.00	0.00	0.053	0.00	0.00
ATOM	1426	SD	MET	413	6.374	-14.344	-17.561	0.00	0.00	-0.130	16.39	-6.40
ATOM	1427	CE	MET	413	5.950	-16.002	-18.163	0.00	0.00	-0.094	16.15	4.00
ATOM	1428	HE1	MET	413	6.286	-16.748	-17.442	0.00	0.00	0.053	0.00	0.00
ATOM	1429	HE2	MET	413	4.870	-16.079	-18.288	0.00	0.00	0.053	0.00	0.00
ATOM	1430	HE3	MET	413	6.439	-16.177	-19.121	0.00	0.00	0.053	0.00	0.00
ATOM	1431	N	PHE	414	7.511	-9.204	-19.211	0.00	0.00	-0.650	9.00	-17.40
ATOM	1432	HN	PHE	414	7.276	-9.214	-18.208	0.00	0.00	0.439	0.00	0.00
ATOM	1433	CA	PHE	414	7.680	-7.957	-19.903	0.00	0.00	0.158	9.40	4.00
ATOM	1434	HA	PHE	414	6.964	-7.926	-20.724	0.00	0.00	0.053	0.00	0.00
ATOM	1435	C	PHE	414	9.036	-7.733	-20.487	0.00	0.00	0.396	9.82	4.00

ATOM	1436	O	PHE	414	9.103	-7.591	-21.710	0.00	0.00	-0.396	8.17	-17.40
ATOM	1437	CB	PHE	414	7.256	-6.753	-19.068	0.00	0.00	-0.106	12.77	4.00
ATOM	1438	HB1	PHE	414	7.978	-5.938	-19.122	0.00	0.00	0.053	0.00	0.00
ATOM	1439	HB2	PHE	414	7.146	-7.000	-18.012	0.00	0.00	0.053	0.00	0.00
ATOM	1440	CG	PHE	414	5.994	-6.465	-19.738	0.00	0.00	0.000	7.26	0.60
ATOM	1441	CD1	PHE	414	5.166	-7.501	-20.084	0.00	0.00	-0.127	10.80	0.60
ATOM	1442	HD1	PHE	414	5.448	-8.526	-19.844	0.00	0.00	0.127	0.00	0.00
ATOM	1443	CD2	PHE	414	5.662	-5.172	-20.020	0.00	0.00	-0.127	10.80	0.60
ATOM	1444	HD2	PHE	414	6.325	-4.352	-19.744	0.00	0.00	0.127	0.00	0.00
ATOM	1445	CE1	PHE	414	3.987	-7.252	-20.729	0.00	0.00	-0.127	10.80	0.60
ATOM	1446	HE1	PHE	414	3.330	-8.074	-21.014	0.00	0.00	0.127	0.00	0.00
ATOM	1447	CE2	PHE	414	4.482	-4.932	-20.655	0.00	0.00	-0.127	10.80	0.60
ATOM	1448	HE2	PHE	414	4.199	-3.905	-20.884	0.00	0.00	0.127	0.00	0.00
ATOM	1449	CZ	PHE	414	3.640	-5.956	-21.013	0.00	0.00	-0.127	10.80	0.60
ATOM	1450	HZ	PHE	414	2.700	-5.740	-21.521	0.00	0.00	0.127	0.00	0.00
ATOM	1451	N	PRO	415	10.132	-7.649	-19.783	0.00	0.00	-0.422	9.00	-17.40
ATOM	1452	CA	PRO	415	11.291	-7.499	-20.602	0.00	0.00	0.158	9.40	4.00
ATOM	1453	HA	PRO	415	11.050	-6.791	-21.395	0.00	0.00	0.053	0.00	0.00
ATOM	1454	CD	PRO	415	10.231	-6.741	-18.645	0.00	0.00	0.105	12.77	4.00
ATOM	1455	HD1	PRO	415	9.688	-7.243	-17.844	0.00	0.00	0.053	0.00	0.00
ATOM	1456	HD2	PRO	415	9.760	-5.819	-18.987	0.00	0.00	0.053	0.00	0.00
ATOM	1457	C	PRO	415	11.796	-8.742	-21.265	0.00	0.00	0.396	9.82	4.00
ATOM	1458	O	PRO	415	12.422	-8.611	-22.315	0.00	0.00	-0.396	8.17	-17.40
ATOM	1459	CB	PRO	415	12.348	-6.745	-19.785	0.00	0.00	-0.106	12.77	4.00
ATOM	1460	HB1	PRO	415	12.474	-5.794	-20.303	0.00	0.00	0.053	0.00	0.00
ATOM	1461	HB2	PRO	415	13.231	-7.383	-19.818	0.00	0.00	0.053	0.00	0.00
ATOM	1462	CG	PRO	415	11.736	-6.609	-18.385	0.00	0.00	-0.106	12.77	4.00
ATOM	1463	HG1	PRO	415	11.987	-5.647	-17.939	0.00	0.00	0.053	0.00	0.00
ATOM	1464	HG2	PRO	415	12.102	-7.391	-17.720	0.00	0.00	0.053	0.00	0.00
ATOM	1465	N	HIS	416	11.588	-9.944	-20.690	0.00	0.00	-0.650	9.00	-17.40
ATOM	1466	HN	HIS	416	11.016	-10.042	-19.839	0.00	0.00	0.439	0.00	0.00
ATOM	1467	CA	HIS	416	12.201	-11.082	-21.319	0.00	0.00	0.158	9.40	4.00
ATOM	1468	HA	HIS	416	13.250	-10.842	-21.493	0.00	0.00	0.053	0.00	0.00
ATOM	1469	C	HIS	416	11.625	-11.502	-22.637	0.00	0.00	0.396	9.82	4.00
ATOM	1470	O	HIS	416	12.233	-11.299	-23.687	0.00	0.00	-0.396	8.17	-17.40
ATOM	1471	CB	HIS	416	12.174	-12.360	-20.461	0.00	0.00	-0.106	12.77	4.00
ATOM	1472	HB1	HIS	416	12.118	-13.276	-21.050	0.00	0.00	0.053	0.00	0.00
ATOM	1473	HB2	HIS	416	11.326	-12.405	-19.778	0.00	0.00	0.053	0.00	0.00
ATOM	1474	CG	HIS	416	13.384	-12.521	-19.597	0.00	0.00	0.241	7.26	0.60
ATOM	1475	ND1	HIS	416	13.614	-13.607	-18.782	0.00	0.00	-0.481	9.25	-17.40
ATOM	1476	CD2	HIS	416	14.471	-11.715	-19.454	0.00	0.00	-0.177	10.80	0.60
ATOM	1477	HD2	HIS	416	14.608	-10.762	-19.965	0.00	0.00	0.127	0.00	0.00
ATOM	1478	CE1	HIS	416	14.821	-13.407	-18.194	0.00	0.00	0.064	10.80	0.60
ATOM	1479	HE1	HIS	416	15.278	-14.104	-17.491	0.00	0.00	0.127	0.00	0.00
ATOM	1480	NE2	HIS	416	15.378	-12.271	-18.572	0.00	0.00	-0.292	9.25	-17.40
ATOM	1481	HE2	HIS	416	16.286	-11.885	-18.276	0.00	0.00	0.393	0.00	0.00
ATOM	1482	N	THR	417	10.415	-12.097	-22.606	0.00	0.00	-0.650	9.00	-17.40
ATOM	1483	HN	THR	417	9.839	-12.059	-21.753	0.00	0.00	0.439	0.00	0.00
ATOM	1484	CA	THR	417	9.934	-12.786	-23.777	0.00	0.00	0.158	9.40	4.00
ATOM	1485	HA	THR	417	10.797	-13.264	-24.240	0.00	0.00	0.053	0.00	0.00
ATOM	1486	C	THR	417	9.257	-12.013	-24.880	0.00	0.00	0.396	9.82	4.00
ATOM	1487	O	THR	417	9.592	-12.248	-26.039	0.00	0.00	-0.396	8.17	-17.40
ATOM	1488	CB	THR	417	9.008	-13.926	-23.465	0.00	0.00	0.060	9.40	4.00
ATOM	1489	HB	THR	417	8.847	-14.495	-24.381	0.00	0.00	0.053	0.00	0.00
ATOM	1490	OG1	THR	417	7.760	-13.444	-22.993	0.00	0.00	-0.537	11.04	-17.40
ATOM	1491	HG1	THR	417	7.787	-12.416	-22.937	0.00	0.00	0.424	0.00	0.00
ATOM	1492	CG2	THR	417	9.670	-14.803	-22.389	0.00	0.00	-0.159	16.15	4.00
ATOM	1493	HG21	THR	417	9.014	-15.639	-22.146	0.00	0.00	0.053	0.00	0.00
ATOM	1494	HG22	THR	417	10.620	-15.184	-22.764	0.00	0.00	0.053	0.00	0.00
ATOM	1495	HG23	THR	417	9.846	-14.208	-21.493	0.00	0.00	0.053	0.00	0.00
ATOM	1496	N	PRO	418	8.353	-11.106	-24.576	0.00	0.00	-0.422	9.00	-17.40
ATOM	1497	CA	PRO	418	7.407	-10.624	-25.561	0.00	0.00	0.158	9.40	4.00
ATOM	1498	HA	PRO	418	6.707	-11.430	-25.783	0.00	0.00	0.053	0.00	0.00
ATOM	1499	CD	PRO	418	8.745	-10.008	-23.715	0.00	0.00	0.105	12.77	4.00
ATOM	1500	HD1	PRO	418	9.778	-9.773	-23.973	0.00	0.00	0.053	0.00	0.00
ATOM	1501	HD2	PRO	418	8.643	-10.372	-22.693	0.00	0.00	0.053	0.00	0.00
ATOM	1502	C	PRO	418	8.012	-10.189	-26.854	0.00	0.00	0.396	9.82	4.00
ATOM	1503	O	PRO	418	7.589	-10.650	-27.910	0.00	0.00	-0.396	8.17	-17.40
ATOM	1504	CB	PRO	418	6.673	-9.479	-24.882	0.00	0.00	-0.106	12.77	4.00
ATOM	1505	HB1	PRO	418	5.842	-9.843	-24.278	0.00	0.00	0.053	0.00	0.00
ATOM	1506	HB2	PRO	418	6.266	-8.780	-25.613	0.00	0.00	0.053	0.00	0.00
ATOM	1507	CG	PRO	418	7.779	-8.849	-24.029	0.00	0.00	-0.106	12.77	4.00
ATOM	1508	HG1	PRO	418	7.266	-8.457	-23.151	0.00	0.00	0.053	0.00	0.00
ATOM	1509	HG2	PRO	418	8.215	-8.076	-24.662	0.00	0.00	0.053	0.00	0.00
ATOM	1510	N	ASP	419	9.001	-9.299	-26.774	0.00	0.00	-0.650	9.00	-17.40
ATOM	1511	HN	ASP	419	9.255	-8.968	-25.832	0.00	0.00	0.439	0.00	0.00

ATOM	1512	CA	ASP	419	9.742	-8.761	-27.869	0.00	0.00	0.158	9.40	4.00
ATOM	1513	HA	ASP	419	10.333	-9.520	-28.381	0.00	0.00	0.053	0.00	0.00
ATOM	1514	C	ASP	419	10.551	-7.785	-27.119	0.00	0.00	0.396	9.82	4.00
ATOM	1515	O	ASP	419	10.328	-6.578	-27.205	0.00	0.00	-0.396	8.17	-17.40
ATOM	1516	CB	ASP	419	8.880	-7.978	-28.880	0.00	0.00	-0.336	12.77	4.00
ATOM	1517	HB1	ASP	419	8.448	-7.111	-28.380	0.00	0.00	0.053	0.00	0.00
ATOM	1518	HB2	ASP	419	8.087	-8.629	-29.249	0.00	0.00	0.053	0.00	0.00
ATOM	1519	CG	ASP	419	9.763	-7.525	-30.038	0.00	0.00	0.297	9.82	4.00
ATOM	1520	OD1	ASP	419	10.919	-7.110	-29.763	0.00	0.00	-0.534	8.17	-18.95
ATOM	1521	OD2	ASP	419	9.290	-7.576	-31.205	0.00	0.00	-0.534	8.17	-18.95
ATOM	1522	N	ASN	420	11.514	-8.322	-26.348	0.00	0.00	-0.650	9.00	-17.40
ATOM	1523	HN	ASN	420	11.746	-9.319	-26.459	0.00	0.00	0.439	0.00	0.00
ATOM	1524	CA	ASN	420	12.221	-7.550	-25.382	0.00	0.00	0.158	9.40	4.00
ATOM	1525	HA	ASN	420	12.768	-8.266	-24.769	0.00	0.00	0.053	0.00	0.00
ATOM	1526	C	ASN	420	11.185	-6.809	-24.615	0.00	0.00	0.396	9.82	4.00
ATOM	1527	O	ASN	420	10.066	-7.289	-24.473	0.00	0.00	-0.396	8.17	-17.40
ATOM	1528	CB	ASN	420	13.354	-6.633	-25.912	0.00	0.00	-0.106	12.77	4.00
ATOM	1529	HB1	ASN	420	14.117	-7.185	-26.461	0.00	0.00	0.053	0.00	0.00
ATOM	1530	HB2	ASN	420	13.876	-6.107	-25.112	0.00	0.00	0.053	0.00	0.00
ATOM	1531	CG	ASN	420	12.842	-5.561	-26.860	0.00	0.00	0.396	9.82	4.00
ATOM	1532	OD1	ASN	420	12.028	-4.719	-26.486	0.00	0.00	-0.396	8.17	-17.40
ATOM	1533	ND2	ASN	420	13.345	-5.582	-28.124	0.00	0.00	-0.879	13.25	-17.40
ATOM	1534	HD21	ASN	420	14.026	-6.306	-28.395	0.00	0.00	0.439	0.00	0.00
ATOM	1535	HD22	ASN	420	13.045	-4.874	-28.809	0.00	0.00	0.439	0.00	0.00
ATOM	1536	N	SER	421	11.496	-5.628	-24.086	0.00	0.00	-0.650	9.00	-17.40
ATOM	1537	HN	SER	421	12.397	-5.177	-24.300	0.00	0.00	0.439	0.00	0.00
ATOM	1538	CA	SER	421	10.557	-5.001	-23.217	0.00	0.00	0.158	9.40	4.00
ATOM	1539	HA	SER	421	9.695	-5.653	-23.074	0.00	0.00	0.053	0.00	0.00
ATOM	1540	C	SER	421	10.107	-3.724	-23.807	0.00	0.00	0.396	9.82	4.00
ATOM	1541	O	SER	421	9.481	-3.694	-24.858	0.00	0.00	-0.396	8.17	-17.40
ATOM	1542	CB	SER	421	11.227	-4.717	-21.871	0.00	0.00	0.007	12.77	4.00
ATOM	1543	HB1	SER	421	11.303	-5.656	-21.323	0.00	0.00	0.053	0.00	0.00
ATOM	1544	HB2	SER	421	10.609	-4.003	-21.327	0.00	0.00	0.053	0.00	0.00
ATOM	1545	OG	SER	421	12.516	-4.177	-22.122	0.00	0.00	-0.537	11.04	-17.40
ATOM	1546	HG	SER	421	13.197	-4.599	-21.475	0.00	0.00	0.424	0.00	0.00
ATOM	1547	N	PHE	422	10.398	-2.647	-23.070	0.00	0.00	-0.650	9.00	-17.40
ATOM	1548	HN	PHE	422	10.940	-2.826	-22.212	0.00	0.00	0.439	0.00	0.00
ATOM	1549	CA	PHE	422	10.058	-1.285	-23.314	0.00	0.00	0.158	9.40	4.00
ATOM	1550	HA	PHE	422	10.678	-0.855	-24.101	0.00	0.00	0.053	0.00	0.00
ATOM	1551	C	PHE	422	10.313	-0.672	-22.000	0.00	0.00	0.396	9.82	4.00
ATOM	1552	O	PHE	422	11.432	-0.504	-21.522	0.00	0.00	-0.396	8.17	-17.40
ATOM	1553	CB	PHE	422	8.536	-0.990	-23.401	0.00	0.00	-0.106	12.77	4.00
ATOM	1554	HB1	PHE	422	8.381	0.022	-23.026	0.00	0.00	0.053	0.00	0.00
ATOM	1555	HB2	PHE	422	8.028	-1.730	-22.782	0.00	0.00	0.053	0.00	0.00
ATOM	1556	CG	PHE	422	7.872	-1.042	-24.739	0.00	0.00	0.000	7.26	0.60
ATOM	1557	CD1	PHE	422	7.840	0.096	-25.511	0.00	0.00	-0.127	10.80	0.60
ATOM	1558	HD1	PHE	422	8.314	1.005	-25.140	0.00	0.00	0.127	0.00	0.00
ATOM	1559	CD2	PHE	422	7.235	-2.168	-25.207	0.00	0.00	-0.127	10.80	0.60
ATOM	1560	HD2	PHE	422	7.220	-3.072	-24.599	0.00	0.00	0.127	0.00	0.00
ATOM	1561	CE1	PHE	422	7.224	0.113	-26.738	0.00	0.00	-0.127	10.80	0.60
ATOM	1562	HE1	PHE	422	7.220	1.023	-27.337	0.00	0.00	0.127	0.00	0.00
ATOM	1563	CE2	PHE	422	6.617	-2.163	-26.436	0.00	0.00	-0.127	10.80	0.60
ATOM	1564	HE2	PHE	422	6.129	-3.066	-26.802	0.00	0.00	0.127	0.00	0.00
ATOM	1565	CZ	PHE	422	6.613	-1.023	-27.205	0.00	0.00	-0.127	10.80	0.60
ATOM	1566	HZ	PHE	422	6.127	-1.022	-28.181	0.00	0.00	0.127	0.00	0.00
ATOM	1567	N	LEU	423	9.167	-0.353	-21.405	0.00	0.00	-0.650	9.00	-17.40
ATOM	1568	HN	LEU	423	8.317	-0.556	-21.950	0.00	0.00	0.439	0.00	0.00
ATOM	1569	CA	LEU	423	8.946	0.224	-20.133	0.00	0.00	0.158	9.40	4.00
ATOM	1570	HA	LEU	423	9.722	-0.038	-19.413	0.00	0.00	0.053	0.00	0.00
ATOM	1571	C	LEU	423	7.632	-0.412	-19.872	0.00	0.00	0.396	9.82	4.00
ATOM	1572	O	LEU	423	7.130	-1.114	-20.748	0.00	0.00	-0.396	8.17	-17.40
ATOM	1573	CB	LEU	423	8.670	1.738	-20.217	0.00	0.00	-0.106	12.77	4.00
ATOM	1574	HB1	LEU	423	8.696	2.144	-19.206	0.00	0.00	0.053	0.00	0.00
ATOM	1575	HB2	LEU	423	7.687	1.879	-20.665	0.00	0.00	0.053	0.00	0.00
ATOM	1576	CG	LEU	423	9.685	2.543	-21.065	0.00	0.00	-0.053	9.40	4.00
ATOM	1577	HG	LEU	423	10.714	2.329	-20.775	0.00	0.00	0.053	0.00	0.00
ATOM	1578	CD1	LEU	423	9.561	2.218	-22.565	0.00	0.00	-0.159	16.15	4.00
ATOM	1579	HD11	LEU	423	10.290	2.803	-23.126	0.00	0.00	0.053	0.00	0.00
ATOM	1580	HD12	LEU	423	9.749	1.156	-22.724	0.00	0.00	0.053	0.00	0.00
ATOM	1581	HD13	LEU	423	8.556	2.464	-22.909	0.00	0.00	0.053	0.00	0.00
ATOM	1582	CD2	LEU	423	9.561	4.052	-20.808	0.00	0.00	-0.159	16.15	4.00
ATOM	1583	HD21	LEU	423	10.288	4.586	-21.420	0.00	0.00	0.053	0.00	0.00
ATOM	1584	HD22	LEU	423	8.556	4.384	-21.067	0.00	0.00	0.053	0.00	0.00
ATOM	1585	HD23	LEU	423	9.751	4.259	-19.755	0.00	0.00	0.053	0.00	0.00
ATOM	1586	N	GLY	424	7.032	-0.231	-18.693	0.00	0.00	-0.650	9.00	-17.40
ATOM	1587	HN	GLY	424	7.464	0.310	-17.930	0.00	0.00	0.439	0.00	0.00

ATOM	1588	CA	GLY	424	5.747	-0.843	-18.568	0.00	0.00	0.105	9.40	4.00
ATOM	1589	HA1	GLY	424	5.910	-1.905	-18.385	0.00	0.00	0.053	0.00	0.00
ATOM	1590	HA2	GLY	424	5.215	-0.675	-19.505	0.00	0.00	0.053	0.00	0.00
ATOM	1591	C	GLY	424	5.058	-0.193	-17.426	0.00	0.00	0.396	9.82	4.00
ATOM	1592	O	GLY	424	5.705	0.205	-16.456	0.00	0.00	-0.396	8.17	-17.40
ATOM	1593	N	PHE	425	3.722	-0.031	-17.508	0.00	0.00	-0.650	9.00	-17.40
ATOM	1594	HN	PHE	425	3.167	-0.263	-18.344	0.00	0.00	0.439	0.00	0.00
ATOM	1595	CA	PHE	425	3.163	0.498	-16.305	0.00	0.00	0.158	9.40	4.00
ATOM	1596	HA	PHE	425	4.013	0.766	-15.677	0.00	0.00	0.053	0.00	0.00
ATOM	1597	C	PHE	425	2.337	-0.599	-15.727	0.00	0.00	0.396	9.82	4.00
ATOM	1598	O	PHE	425	1.537	-1.237	-16.413	0.00	0.00	-0.396	8.17	-17.40
ATOM	1599	CB	PHE	425	2.388	1.843	-16.398	0.00	0.00	-0.106	12.77	4.00
ATOM	1600	HB1	PHE	425	2.850	2.433	-17.190	0.00	0.00	0.053	0.00	0.00
ATOM	1601	HB2	PHE	425	2.475	2.338	-15.431	0.00	0.00	0.053	0.00	0.00
ATOM	1602	CG	PHE	425	0.928	1.783	-16.713	0.00	0.00	0.000	7.26	0.60
ATOM	1603	CD1	PHE	425	0.048	1.561	-15.678	0.00	0.00	-0.127	10.80	0.60
ATOM	1604	HD1	PHE	425	0.435	1.415	-14.670	0.00	0.00	0.127	0.00	0.00
ATOM	1605	CD2	PHE	425	0.423	2.001	-17.977	0.00	0.00	-0.127	10.80	0.60
ATOM	1606	HD2	PHE	425	1.102	2.207	-18.805	0.00	0.00	0.127	0.00	0.00
ATOM	1607	CE1	PHE	425	-1.308	1.520	-15.891	0.00	0.00	-0.127	10.80	0.60
ATOM	1608	HE1	PHE	425	-1.988	1.332	-15.060	0.00	0.00	0.127	0.00	0.00
ATOM	1609	CE2	PHE	425	-0.937	1.960	-18.199	0.00	0.00	-0.127	10.80	0.60
ATOM	1610	HE2	PHE	425	-1.328	2.121	-19.204	0.00	0.00	0.127	0.00	0.00
ATOM	1611	CZ	PHE	425	-1.802	1.717	-17.157	0.00	0.00	-0.127	10.80	0.60
ATOM	1612	HZ	PHE	425	-2.877	1.681	-17.336	0.00	0.00	0.127	0.00	0.00
ATOM	1613	N	VAL	426	2.552	-0.875	-14.428	0.00	0.00	-0.650	9.00	-17.40
ATOM	1614	HN	VAL	426	3.190	-0.297	-13.862	0.00	0.00	0.439	0.00	0.00
ATOM	1615	CA	VAL	426	1.871	-1.992	-13.856	0.00	0.00	0.158	9.40	4.00
ATOM	1616	HA	VAL	426	1.595	-2.690	-14.647	0.00	0.00	0.053	0.00	0.00
ATOM	1617	C	VAL	426	0.645	-1.517	-13.158	0.00	0.00	0.396	9.82	4.00
ATOM	1618	O	VAL	426	0.687	-0.584	-12.354	0.00	0.00	-0.396	8.17	-17.40
ATOM	1619	CB	VAL	426	2.697	-2.798	-12.894	0.00	0.00	-0.053	9.40	4.00
ATOM	1620	HB	VAL	426	3.662	-3.030	-13.345	0.00	0.00	0.053	0.00	0.00
ATOM	1621	CG1	VAL	426	2.920	-1.992	-11.603	0.00	0.00	-0.159	16.15	4.00
ATOM	1622	HG11	VAL	426	3.519	-2.579	-10.907	0.00	0.00	0.053	0.00	0.00
ATOM	1623	HG12	VAL	426	3.442	-1.064	-11.839	0.00	0.00	0.053	0.00	0.00
ATOM	1624	HG13	VAL	426	1.957	-1.761	-11.147	0.00	0.00	0.053	0.00	0.00
ATOM	1625	CG2	VAL	426	1.986	-4.141	-12.685	0.00	0.00	-0.159	16.15	4.00
ATOM	1626	HG21	VAL	426	2.561	-4.753	-11.990	0.00	0.00	0.053	0.00	0.00
ATOM	1627	HG22	VAL	426	0.991	-3.966	-12.277	0.00	0.00	0.053	0.00	0.00
ATOM	1628	HG23	VAL	426	1.901	-4.660	-13.640	0.00	0.00	0.053	0.00	0.00
ATOM	1629	N	VAL	427	-0.503	-2.148	-13.476	0.00	0.00	-0.650	9.00	-17.40
ATOM	1630	HN	VAL	427	-0.519	-2.918	-14.160	0.00	0.00	0.439	0.00	0.00
ATOM	1631	CA	VAL	427	-1.696	-1.708	-12.827	0.00	0.00	0.158	9.40	4.00
ATOM	1632	HA	VAL	427	-1.407	-1.053	-12.005	0.00	0.00	0.053	0.00	0.00
ATOM	1633	C	VAL	427	-2.417	-2.919	-12.322	0.00	0.00	0.396	9.82	4.00
ATOM	1634	O	VAL	427	-2.628	-3.898	-13.039	0.00	0.00	-0.396	8.17	-17.40
ATOM	1635	CB	VAL	427	-2.584	-0.904	-13.743	0.00	0.00	-0.053	9.40	4.00
ATOM	1636	HB	VAL	427	-2.050	-0.589	-14.639	0.00	0.00	0.053	0.00	0.00
ATOM	1637	CG1	VAL	427	-3.806	-1.718	-14.197	0.00	0.00	-0.159	16.15	4.00
ATOM	1638	HG11	VAL	427	-4.425	-1.109	-14.856	0.00	0.00	0.053	0.00	0.00
ATOM	1639	HG12	VAL	427	-3.473	-2.607	-14.732	0.00	0.00	0.053	0.00	0.00
ATOM	1640	HG13	VAL	427	-4.389	-2.016	-13.325	0.00	0.00	0.053	0.00	0.00
ATOM	1641	CG2	VAL	427	-2.854	0.451	-13.079	0.00	0.00	-0.159	16.15	4.00
ATOM	1642	HG21	VAL	427	-3.495	1.051	-13.724	0.00	0.00	0.053	0.00	0.00
ATOM	1643	HG22	VAL	427	-3.349	0.294	-12.120	0.00	0.00	0.053	0.00	0.00
ATOM	1644	HG23	VAL	427	-1.910	0.972	-12.919	0.00	0.00	0.053	0.00	0.00
ATOM	1645	N	GLU	428	-2.809	-2.885	-11.036	0.00	0.00	-0.650	9.00	-17.40
ATOM	1646	HN	GLU	428	-2.637	-2.048	-10.461	0.00	0.00	0.439	0.00	0.00
ATOM	1647	CA	GLU	428	-3.466	-4.023	-10.477	0.00	0.00	0.158	9.40	4.00
ATOM	1648	HA	GLU	428	-2.985	-4.927	-10.850	0.00	0.00	0.053	0.00	0.00
ATOM	1649	C	GLU	428	-4.909	-4.002	-10.887	0.00	0.00	0.396	9.82	4.00
ATOM	1650	O	GLU	428	-5.448	-2.995	-11.343	0.00	0.00	-0.396	8.17	-17.40
ATOM	1651	CB	GLU	428	-3.332	-4.129	-8.945	0.00	0.00	-0.106	12.77	4.00
ATOM	1652	HB1	GLU	428	-2.714	-4.978	-8.654	0.00	0.00	0.053	0.00	0.00
ATOM	1653	HB2	GLU	428	-4.302	-4.256	-8.465	0.00	0.00	0.053	0.00	0.00
ATOM	1654	CG	GLU	428	-2.689	-2.871	-8.346	0.00	0.00	-0.336	12.77	4.00
ATOM	1655	HG1	GLU	428	-3.469	-2.164	-8.063	0.00	0.00	0.053	0.00	0.00
ATOM	1656	HG2	GLU	428	-2.033	-2.412	-9.085	0.00	0.00	0.053	0.00	0.00
ATOM	1657	CD	GLU	428	-1.877	-3.254	-7.112	0.00	0.00	0.297	9.82	4.00
ATOM	1658	OE1	GLU	428	-1.264	-4.353	-7.111	0.00	0.00	-0.534	8.17	-18.95
ATOM	1659	OE2	GLU	428	-1.869	-2.441	-6.147	0.00	0.00	-0.534	8.17	-18.95
ATOM	1660	N	GLN	429	-5.566	-5.166	-10.716	0.00	0.00	-0.650	9.00	-17.40
ATOM	1661	HN	GLN	429	-5.044	-5.937	-10.275	0.00	0.00	0.439	0.00	0.00
ATOM	1662	CA	GLN	429	-6.928	-5.431	-11.093	0.00	0.00	0.158	9.40	4.00
ATOM	1663	HA	GLN	429	-7.046	-5.312	-12.170	0.00	0.00	0.053	0.00	0.00

ATOM	1664	C	GLN	429	-7.845	-4.479	-10.395	0.00	0.00	0.396	9.82	4.00
ATOM	1665	O	GLN	429	-8.883	-4.085	-10.928	0.00	0.00	-0.396	8.17	-17.40
ATOM	1666	CB	GLN	429	-7.356	-6.825	-10.618	0.00	0.00	-0.106	12.77	4.00
ATOM	1667	HB1	GLN	429	-7.081	-6.930	-9.568	0.00	0.00	0.053	0.00	0.00
ATOM	1668	HB2	GLN	429	-6.839	-7.569	-11.225	0.00	0.00	0.053	0.00	0.00
ATOM	1669	CG	GLN	429	-8.855	-7.087	-10.736	0.00	0.00	-0.106	12.77	4.00
ATOM	1670	HG1	GLN	429	-9.054	-7.299	-11.786	0.00	0.00	0.053	0.00	0.00
ATOM	1671	HG2	GLN	429	-9.359	-6.181	-10.398	0.00	0.00	0.053	0.00	0.00
ATOM	1672	CD	GLN	429	-9.162	-8.280	-9.843	0.00	0.00	0.396	9.82	4.00
ATOM	1673	OE1	GLN	429	-8.401	-9.244	-9.778	0.00	0.00	-0.396	8.17	-17.40
ATOM	1674	NE2	GLN	429	-10.313	-8.209	-9.124	0.00	0.00	-0.879	13.25	-17.40
ATOM	1675	HE21	GLN	429	-10.922	-7.383	-9.208	0.00	0.00	0.439	0.00	0.00
ATOM	1676	HE22	GLN	429	-10.576	-8.981	-8.495	0.00	0.00	0.439	0.00	0.00
ATOM	1677	N	HIS	430	-7.476	-4.131	-9.156	0.00	0.00	-0.650	9.00	-17.40
ATOM	1678	HN	HIS	430	-6.554	-4.465	-8.842	0.00	0.00	0.439	0.00	0.00
ATOM	1679	CA	HIS	430	-8.221	-3.346	-8.219	0.00	0.00	0.158	9.40	4.00
ATOM	1680	HA	HIS	430	-9.234	-3.725	-8.081	0.00	0.00	0.053	0.00	0.00
ATOM	1681	C	HIS	430	-8.350	-1.912	-8.660	0.00	0.00	0.396	9.82	4.00
ATOM	1682	O	HIS	430	-9.312	-1.238	-8.302	0.00	0.00	-0.396	8.17	-17.40
ATOM	1683	CB	HIS	430	-7.503	-3.356	-6.867	0.00	0.00	-0.106	12.77	4.00
ATOM	1684	HB1	HIS	430	-8.216	-3.198	-6.058	0.00	0.00	0.053	0.00	0.00
ATOM	1685	HB2	HIS	430	-6.754	-2.565	-6.830	0.00	0.00	0.053	0.00	0.00
ATOM	1686	CG	HIS	430	-6.816	-4.677	-6.649	0.00	0.00	0.241	7.26	0.60
ATOM	1687	ND1	HIS	430	-7.466	-5.879	-6.472	0.00	0.00	-0.481	9.25	-17.40
ATOM	1688	CD2	HIS	430	-5.486	-4.968	-6.613	0.00	0.00	-0.177	10.80	0.60
ATOM	1689	HD2	HIS	430	-4.688	-4.234	-6.723	0.00	0.00	0.127	0.00	0.00
ATOM	1690	CE1	HIS	430	-6.505	-6.828	-6.338	0.00	0.00	0.064	10.80	0.60
ATOM	1691	HE1	HIS	430	-6.714	-7.886	-6.183	0.00	0.00	0.127	0.00	0.00
ATOM	1692	NE2	HIS	430	-5.287	-6.323	-6.417	0.00	0.00	-0.292	9.25	-17.40
ATOM	1693	HE2	HIS	430	-4.390	-6.825	-6.348	0.00	0.00	0.393	0.00	0.00
ATOM	1694	N	LEU	431	-7.384	-1.383	-9.429	0.00	0.00	-0.650	9.00	-17.40
ATOM	1695	HN	LEU	431	-6.649	-1.981	-9.833	0.00	0.00	0.439	0.00	0.00
ATOM	1696	CA	LEU	431	-7.394	0.035	-9.678	0.00	0.00	0.158	9.40	4.00
ATOM	1697	HA	LEU	431	-7.813	0.606	-8.849	0.00	0.00	0.053	0.00	0.00
ATOM	1698	C	LEU	431	-8.201	0.406	-10.885	0.00	0.00	0.396	9.82	4.00
ATOM	1699	O	LEU	431	-8.345	-0.364	-11.835	0.00	0.00	-0.396	8.17	-17.40
ATOM	1700	CB	LEU	431	-5.978	0.591	-9.892	0.00	0.00	-0.106	12.77	4.00
ATOM	1701	HB1	LEU	431	-5.986	1.677	-9.990	0.00	0.00	0.053	0.00	0.00
ATOM	1702	HB2	LEU	431	-5.522	0.186	-10.795	0.00	0.00	0.053	0.00	0.00
ATOM	1703	CG	LEU	431	-5.051	0.243	-8.713	0.00	0.00	-0.053	9.40	4.00
ATOM	1704	HG	LEU	431	-4.842	-0.825	-8.652	0.00	0.00	0.053	0.00	0.00
ATOM	1705	CD1	LEU	431	-3.693	0.947	-8.813	0.00	0.00	-0.159	16.15	4.00
ATOM	1706	HD11	LEU	431	-3.075	0.669	-7.959	0.00	0.00	0.053	0.00	0.00
ATOM	1707	HD12	LEU	431	-3.194	0.646	-9.734	0.00	0.00	0.053	0.00	0.00
ATOM	1708	HD13	LEU	431	-3.842	2.027	-8.817	0.00	0.00	0.053	0.00	0.00
ATOM	1709	CD2	LEU	431	-5.745	0.497	-7.370	0.00	0.00	-0.159	16.15	4.00
ATOM	1710	HD21	LEU	431	-5.066	0.242	-6.556	0.00	0.00	0.053	0.00	0.00
ATOM	1711	HD22	LEU	431	-6.021	1.549	-7.296	0.00	0.00	0.053	0.00	0.00
ATOM	1712	HD23	LEU	431	-6.641	-0.119	-7.301	0.00	0.00	0.053	0.00	0.00
ATOM	1713	N	ASN	432	-8.776	1.630	-10.845	0.00	0.00	-0.650	9.00	-17.40
ATOM	1714	HN	ASN	432	-8.706	2.182	-9.978	0.00	0.00	0.439	0.00	0.00
ATOM	1715	CA	ASN	432	-9.479	2.187	-11.964	0.00	0.00	0.158	9.40	4.00
ATOM	1716	HA	ASN	432	-9.819	1.315	-12.523	0.00	0.00	0.053	0.00	0.00
ATOM	1717	C	ASN	432	-8.451	3.003	-12.666	0.00	0.00	0.396	9.82	4.00
ATOM	1718	O	ASN	432	-7.267	2.865	-12.382	0.00	0.00	-0.396	8.17	-17.40
ATOM	1719	CB	ASN	432	-10.613	3.156	-11.593	0.00	0.00	-0.106	12.77	4.00
ATOM	1720	HB1	ASN	432	-10.952	3.662	-12.497	0.00	0.00	0.053	0.00	0.00
ATOM	1721	HB2	ASN	432	-10.232	3.883	-10.876	0.00	0.00	0.053	0.00	0.00
ATOM	1722	CG	ASN	432	-11.752	2.363	-10.979	0.00	0.00	0.396	9.82	4.00
ATOM	1723	OD1	ASN	432	-11.654	1.151	-10.791	0.00	0.00	-0.396	8.17	-17.40
ATOM	1724	ND2	ASN	432	-12.871	3.069	-10.669	0.00	0.00	-0.879	13.25	-17.40
ATOM	1725	HD21	ASN	432	-12.905	4.083	-10.845	0.00	0.00	0.439	0.00	0.00
ATOM	1726	HD22	ASN	432	-13.685	2.590	-10.258	0.00	0.00	0.439	0.00	0.00
ATOM	1727	N	SER	433	-8.850	3.869	-13.615	0.00	0.00	-0.650	9.00	-17.40
ATOM	1728	HN	SER	433	-9.844	3.957	-13.872	0.00	0.00	0.439	0.00	0.00
ATOM	1729	CA	SER	433	-7.844	4.665	-14.257	0.00	0.00	0.158	9.40	4.00
ATOM	1730	HA	SER	433	-6.992	4.740	-13.582	0.00	0.00	0.053	0.00	0.00
ATOM	1731	C	SER	433	-8.427	6.014	-14.531	0.00	0.00	0.396	9.82	4.00
ATOM	1732	O	SER	433	-9.642	6.196	-14.494	0.00	0.00	-0.396	8.17	-17.40
ATOM	1733	CB	SER	433	-7.380	4.094	-15.607	0.00	0.00	0.007	12.77	4.00
ATOM	1734	HB1	SER	433	-7.029	3.070	-15.479	0.00	0.00	0.053	0.00	0.00
ATOM	1735	HB2	SER	433	-6.566	4.698	-16.008	0.00	0.00	0.053	0.00	0.00
ATOM	1736	OG	SER	433	-8.457	4.099	-16.534	0.00	0.00	-0.537	11.04	-17.40
ATOM	1737	HG	SER	433	-8.714	5.071	-16.757	0.00	0.00	0.424	0.00	0.00
ATOM	1738	N	SER	434	-7.549	7.001	-14.805	0.00	0.00	-0.650	9.00	-17.40
ATOM	1739	HN	SER	434	-6.541	6.787	-14.800	0.00	0.00	0.439	0.00	0.00

ATOM	1740	CA	SER	434	-7.974	8.341	-15.104	0.00	0.00	0.158	9.40	4.00
ATOM	1741	HA	SER	434	-9.061	8.314	-15.179	0.00	0.00	0.053	0.00	0.00
ATOM	1742	C	SER	434	-7.328	8.716	-16.400	0.00	0.00	0.396	9.82	4.00
ATOM	1743	O	SER	434	-7.362	7.952	-17.362	0.00	0.00	-0.396	8.17	-17.40
ATOM	1744	CB	SER	434	-7.545	9.377	-14.051	0.00	0.00	0.007	12.77	4.00
ATOM	1745	HB1	SER	434	-7.783	10.382	-14.400	0.00	0.00	0.053	0.00	0.00
ATOM	1746	HB2	SER	434	-6.471	9.307	-13.876	0.00	0.00	0.053	0.00	0.00
ATOM	1747	OG	SER	434	-8.229	9.138	-12.829	0.00	0.00	-0.537	11.04	-17.40
ATOM	1748	HG	SER	434	-8.558	10.033	-12.438	0.00	0.00	0.424	0.00	0.00
ATOM	1749	N	ASP	435	-6.709	9.918	-16.451	0.00	0.00	-0.650	9.00	-17.40
ATOM	1750	HN	ASP	435	-6.730	10.496	-15.598	0.00	0.00	0.439	0.00	0.00
ATOM	1751	CA	ASP	435	-6.022	10.459	-17.598	0.00	0.00	0.158	9.40	4.00
ATOM	1752	HA	ASP	435	-6.636	10.218	-18.466	0.00	0.00	0.053	0.00	0.00
ATOM	1753	C	ASP	435	-4.684	9.789	-17.643	0.00	0.00	0.396	9.82	4.00
ATOM	1754	O	ASP	435	-3.700	10.361	-18.108	0.00	0.00	-0.396	8.17	-17.40
ATOM	1755	CB	ASP	435	-5.705	11.946	-17.387	0.00	0.00	-0.336	12.77	4.00
ATOM	1756	HB1	ASP	435	-5.225	12.302	-18.299	0.00	0.00	0.053	0.00	0.00
ATOM	1757	HB2	ASP	435	-5.039	12.011	-16.527	0.00	0.00	0.053	0.00	0.00
ATOM	1758	CG	ASP	435	-7.023	12.648	-17.133	0.00	0.00	0.297	9.82	4.00
ATOM	1759	OD1	ASP	435	-7.651	13.088	-18.130	0.00	0.00	-0.534	8.17	-18.95
ATOM	1760	OD2	ASP	435	-7.419	12.749	-15.940	0.00	0.00	-0.534	8.17	-18.95
ATOM	1761	N	ILE	436	-4.644	8.537	-17.167	0.00	0.00	-0.650	9.00	-17.40
ATOM	1762	HN	ILE	436	-5.545	8.085	-16.956	0.00	0.00	0.439	0.00	0.00
ATOM	1763	CA	ILE	436	-3.462	7.776	-16.927	0.00	0.00	0.158	9.40	4.00
ATOM	1764	HA	ILE	436	-2.796	8.366	-16.297	0.00	0.00	0.053	0.00	0.00
ATOM	1765	C	ILE	436	-2.713	7.411	-18.161	0.00	0.00	0.396	9.82	4.00
ATOM	1766	O	ILE	436	-1.485	7.427	-18.144	0.00	0.00	-0.396	8.17	-17.40
ATOM	1767	CB	ILE	436	-3.750	6.501	-16.174	0.00	0.00	-0.053	9.40	4.00
ATOM	1768	HB	ILE	436	-2.798	5.984	-16.051	0.00	0.00	0.053	0.00	0.00
ATOM	1769	CG1	ILE	436	-4.635	5.518	-16.971	0.00	0.00	-0.106	12.77	4.00
ATOM	1770	HG11	ILE	436	-5.373	6.098	-17.525	0.00	0.00	0.053	0.00	0.00
ATOM	1771	HG12	ILE	436	-5.123	4.849	-16.262	0.00	0.00	0.053	0.00	0.00
ATOM	1772	CG2	ILE	436	-4.361	6.908	-14.824	0.00	0.00	-0.159	16.15	4.00
ATOM	1773	HG21	ILE	436	-4.587	6.014	-14.242	0.00	0.00	0.053	0.00	0.00
ATOM	1774	HG22	ILE	436	-3.652	7.528	-14.276	0.00	0.00	0.053	0.00	0.00
ATOM	1775	HG23	ILE	436	-5.279	7.471	-14.995	0.00	0.00	0.053	0.00	0.00
ATOM	1776	CD1	ILE	436	-3.885	4.647	-17.981	0.00	0.00	-0.159	16.15	4.00
ATOM	1777	HD11	ILE	436	-4.591	3.991	-18.490	0.00	0.00	0.053	0.00	0.00
ATOM	1778	HD12	ILE	436	-3.389	5.284	-18.713	0.00	0.00	0.053	0.00	0.00
ATOM	1779	HD13	ILE	436	-3.141	4.045	-17.460	0.00	0.00	0.053	0.00	0.00
ATOM	1780	N	HIS	437	-3.407	7.102	-19.267	0.00	0.00	-0.650	9.00	-17.40
ATOM	1781	HN	HIS	437	-4.411	7.315	-19.349	0.00	0.00	0.439	0.00	0.00
ATOM	1782	CA	HIS	437	-2.690	6.464	-20.328	0.00	0.00	0.158	9.40	4.00
ATOM	1783	HA	HIS	437	-2.295	5.520	-19.952	0.00	0.00	0.053	0.00	0.00
ATOM	1784	C	HIS	437	-1.545	7.245	-20.865	0.00	0.00	0.396	9.82	4.00
ATOM	1785	O	HIS	437	-1.487	8.471	-20.791	0.00	0.00	-0.396	8.17	-17.40
ATOM	1786	CB	HIS	437	-3.562	5.966	-21.496	0.00	0.00	-0.106	12.77	4.00
ATOM	1787	HB1	HIS	437	-2.967	5.687	-22.365	0.00	0.00	0.053	0.00	0.00
ATOM	1788	HB2	HIS	437	-4.270	6.723	-21.834	0.00	0.00	0.053	0.00	0.00
ATOM	1789	CG	HIS	437	-4.372	4.757	-21.125	0.00	0.00	0.241	7.26	0.60
ATOM	1790	ND1	HIS	437	-3.821	3.506	-20.957	0.00	0.00	-0.481	9.25	-17.40
ATOM	1791	CD2	HIS	437	-5.701	4.614	-20.871	0.00	0.00	-0.177	10.80	0.60
ATOM	1792	HD2	HIS	437	-6.433	5.420	-20.920	0.00	0.00	0.127	0.00	0.00
ATOM	1793	CE1	HIS	437	-4.834	2.676	-20.606	0.00	0.00	0.064	10.80	0.60
ATOM	1794	HE1	HIS	437	-4.705	1.613	-20.401	0.00	0.00	0.127	0.00	0.00
ATOM	1795	NE2	HIS	437	-5.995	3.302	-20.541	0.00	0.00	-0.292	9.25	-17.40
ATOM	1796	HE2	HIS	437	-6.913	2.903	-20.299	0.00	0.00	0.393	0.00	0.00
ATOM	1797	N	HIS	438	-0.531	6.475	-21.307	0.00	0.00	-0.650	9.00	-17.40
ATOM	1798	HN	HIS	438	-0.577	5.462	-21.128	0.00	0.00	0.439	0.00	0.00
ATOM	1799	CA	HIS	438	0.603	6.982	-22.009	0.00	0.00	0.158	9.40	4.00
ATOM	1800	HA	HIS	438	0.962	7.906	-21.555	0.00	0.00	0.053	0.00	0.00
ATOM	1801	C	HIS	438	0.090	7.211	-23.388	0.00	0.00	0.396	9.82	4.00
ATOM	1802	O	HIS	438	0.412	8.198	-24.041	0.00	0.00	-0.396	8.17	-17.40
ATOM	1803	CB	HIS	438	1.749	5.962	-22.085	0.00	0.00	-0.106	12.77	4.00
ATOM	1804	HB1	HIS	438	1.380	5.078	-22.605	0.00	0.00	0.053	0.00	0.00
ATOM	1805	HB2	HIS	438	2.050	5.716	-21.067	0.00	0.00	0.053	0.00	0.00
ATOM	1806	CG	HIS	438	2.975	6.426	-22.811	0.00	0.00	0.241	7.26	0.60
ATOM	1807	ND1	HIS	438	4.151	6.805	-22.199	0.00	0.00	-0.481	9.25	-17.40
ATOM	1808	CD2	HIS	438	3.201	6.538	-24.147	0.00	0.00	-0.177	10.80	0.60
ATOM	1809	HD2	HIS	438	2.467	6.314	-24.921	0.00	0.00	0.127	0.00	0.00
ATOM	1810	CE1	HIS	438	5.021	7.125	-23.190	0.00	0.00	0.064	10.80	0.60
ATOM	1811	HE1	HIS	438	6.041	7.467	-23.016	0.00	0.00	0.127	0.00	0.00
ATOM	1812	NE2	HIS	438	4.490	6.975	-24.389	0.00	0.00	-0.292	9.25	-17.40
ATOM	1813	HE2	HIS	438	4.936	7.146	-25.301	0.00	0.00	0.393	0.00	0.00
ATOM	1814	N	ILE	439	-0.757	6.283	-23.870	0.00	0.00	-0.650	9.00	-17.40
ATOM	1815	HN	ILE	439	-0.980	5.434	-23.330	0.00	0.00	0.439	0.00	0.00

ATOM	1816	CA	ILE	439	-1.336	6.513	-25.152	0.00	0.00	0.158	9.40	4.00
ATOM	1817	HA	ILE	439	-0.567	6.655	-25.912	0.00	0.00	0.053	0.00	0.00
ATOM	1818	C	ILE	439	-2.138	7.745	-24.933	0.00	0.00	0.396	9.82	4.00
ATOM	1819	O	ILE	439	-2.254	8.603	-25.807	0.00	0.00	-0.396	8.17	-17.40
ATOM	1820	CB	ILE	439	-2.289	5.445	-25.604	0.00	0.00	-0.053	9.40	4.00
ATOM	1821	HB	ILE	439	-3.101	5.446	-24.877	0.00	0.00	0.053	0.00	0.00
ATOM	1822	CG1	ILE	439	-1.629	4.054	-25.598	0.00	0.00	-0.106	12.77	4.00
ATOM	1823	HG11	ILE	439	-0.703	4.113	-26.170	0.00	0.00	0.053	0.00	0.00
ATOM	1824	HG12	ILE	439	-2.320	3.346	-26.056	0.00	0.00	0.053	0.00	0.00
ATOM	1825	CG2	ILE	439	-2.745	5.862	-27.011	0.00	0.00	-0.159	16.15	4.00
ATOM	1826	HG21	ILE	439	-3.445	5.123	-27.401	0.00	0.00	0.053	0.00	0.00
ATOM	1827	HG22	ILE	439	-3.235	6.834	-26.961	0.00	0.00	0.053	0.00	0.00
ATOM	1828	HG23	ILE	439	-1.879	5.925	-27.670	0.00	0.00	0.053	0.00	0.00
ATOM	1829	CD1	ILE	439	-1.280	3.524	-24.208	0.00	0.00	-0.159	16.15	4.00
ATOM	1830	HD11	ILE	439	-0.820	2.540	-24.299	0.00	0.00	0.053	0.00	0.00
ATOM	1831	HD12	ILE	439	-0.583	4.207	-23.723	0.00	0.00	0.053	0.00	0.00
ATOM	1832	HD13	ILE	439	-2.188	3.446	-23.610	0.00	0.00	0.053	0.00	0.00
ATOM	1833	N	ASN	440	-2.698	7.844	-23.713	0.00	0.00	-0.650	9.00	-17.40
ATOM	1834	HN	ASN	440	-2.585	7.066	-23.047	0.00	0.00	0.439	0.00	0.00
ATOM	1835	CA	ASN	440	-3.443	8.992	-23.314	0.00	0.00	0.158	9.40	4.00
ATOM	1836	HA	ASN	440	-3.988	9.317	-24.200	0.00	0.00	0.053	0.00	0.00
ATOM	1837	C	ASN	440	-2.435	9.994	-22.854	0.00	0.00	0.396	9.82	4.00
ATOM	1838	O	ASN	440	-1.247	9.894	-23.155	0.00	0.00	-0.396	8.17	-17.40
ATOM	1839	CB	ASN	440	-4.419	8.716	-22.155	0.00	0.00	-0.106	12.77	4.00
ATOM	1840	HB1	ASN	440	-3.886	8.706	-21.204	0.00	0.00	0.053	0.00	0.00
ATOM	1841	HB2	ASN	440	-4.905	7.750	-22.290	0.00	0.00	0.053	0.00	0.00
ATOM	1842	CG	ASN	440	-5.496	9.799	-22.097	0.00	0.00	0.396	9.82	4.00
ATOM	1843	OD1	ASN	440	-6.254	9.866	-21.129	0.00	0.00	-0.396	8.17	-17.40
ATOM	1844	ND2	ASN	440	-5.579	10.657	-23.149	0.00	0.00	-0.879	13.25	-17.40
ATOM	1845	HD21	ASN	440	-4.925	10.567	-23.940	0.00	0.00	0.439	0.00	0.00
ATOM	1846	HD22	ASN	440	-6.296	11.397	-23.155	0.00	0.00	0.439	0.00	0.00
ATOM	1847	N	GLU	441	-2.904	11.004	-22.114	0.00	0.00	-0.650	9.00	-17.40
ATOM	1848	HN	GLU	441	-3.888	10.976	-21.811	0.00	0.00	0.439	0.00	0.00
ATOM	1849	CA	GLU	441	-2.099	12.125	-21.723	0.00	0.00	0.158	9.40	4.00
ATOM	1850	HA	GLU	441	-1.602	12.499	-22.618	0.00	0.00	0.053	0.00	0.00
ATOM	1851	C	GLU	441	-1.014	11.887	-20.700	0.00	0.00	0.396	9.82	4.00
ATOM	1852	O	GLU	441	0.153	12.158	-20.978	0.00	0.00	-0.396	8.17	-17.40
ATOM	1853	CB	GLU	441	-3.001	13.248	-21.188	0.00	0.00	-0.106	12.77	4.00
ATOM	1854	HB1	GLU	441	-3.744	13.561	-21.921	0.00	0.00	0.053	0.00	0.00
ATOM	1855	HB2	GLU	441	-2.432	14.138	-20.919	0.00	0.00	0.053	0.00	0.00
ATOM	1856	CG	GLU	441	-3.770	12.821	-19.936	0.00	0.00	-0.336	12.77	4.00
ATOM	1857	HG1	GLU	441	-3.218	13.176	-19.066	0.00	0.00	0.053	0.00	0.00
ATOM	1858	HG2	GLU	441	-3.837	11.733	-19.938	0.00	0.00	0.053	0.00	0.00
ATOM	1859	CD	GLU	441	-5.151	13.451	-19.998	0.00	0.00	0.297	9.82	4.00
ATOM	1860	OE1	GLU	441	-5.889	13.099	-20.956	0.00	0.00	-0.534	8.17	-18.95
ATOM	1861	OE2	GLU	441	-5.495	14.269	-19.103	0.00	0.00	-0.534	8.17	-18.95
ATOM	1862	N	ILE	442	-1.343	11.353	-19.503	0.00	0.00	-0.650	9.00	-17.40
ATOM	1863	HN	ILE	442	-2.258	10.902	-19.363	0.00	0.00	0.439	0.00	0.00
ATOM	1864	CA	ILE	442	-0.384	11.427	-18.422	0.00	0.00	0.158	9.40	4.00
ATOM	1865	HA	ILE	442	-0.084	12.470	-18.316	0.00	0.00	0.053	0.00	0.00
ATOM	1866	C	ILE	442	0.870	10.631	-18.583	0.00	0.00	0.396	9.82	4.00
ATOM	1867	O	ILE	442	1.965	11.191	-18.522	0.00	0.00	-0.396	8.17	-17.40
ATOM	1868	CB	ILE	442	-0.942	11.031	-17.085	0.00	0.00	-0.053	9.40	4.00
ATOM	1869	HB	ILE	442	-1.416	10.057	-17.206	0.00	0.00	0.053	0.00	0.00
ATOM	1870	CG1	ILE	442	-2.054	11.992	-16.638	0.00	0.00	-0.106	12.77	4.00
ATOM	1871	HG11	ILE	442	-2.821	12.146	-17.397	0.00	0.00	0.053	0.00	0.00
ATOM	1872	HG12	ILE	442	-1.688	12.988	-16.390	0.00	0.00	0.053	0.00	0.00
ATOM	1873	CG2	ILE	442	0.235	10.966	-16.097	0.00	0.00	-0.159	16.15	4.00
ATOM	1874	HG21	ILE	442	-0.133	10.680	-15.111	0.00	0.00	0.053	0.00	0.00
ATOM	1875	HG22	ILE	442	0.959	10.228	-16.442	0.00	0.00	0.053	0.00	0.00
ATOM	1876	HG23	ILE	442	0.714	11.943	-16.036	0.00	0.00	0.053	0.00	0.00
ATOM	1877	CD1	ILE	442	-2.803	11.513	-15.394	0.00	0.00	-0.159	16.15	4.00
ATOM	1878	HD11	ILE	442	-3.574	12.237	-15.132	0.00	0.00	0.053	0.00	0.00
ATOM	1879	HD12	ILE	442	-3.266	10.547	-15.597	0.00	0.00	0.053	0.00	0.00
ATOM	1880	HD13	ILE	442	-2.103	11.412	-14.564	0.00	0.00	0.053	0.00	0.00
ATOM	1881	N	LYS	443	0.767	9.311	-18.809	0.00	0.00	-0.650	9.00	-17.40
ATOM	1882	HN	LYS	443	-0.138	8.869	-19.026	0.00	0.00	0.439	0.00	0.00
ATOM	1883	CA	LYS	443	1.978	8.548	-18.734	0.00	0.00	0.158	9.40	4.00
ATOM	1884	HA	LYS	443	2.491	8.698	-17.784	0.00	0.00	0.053	0.00	0.00
ATOM	1885	C	LYS	443	2.933	8.923	-19.813	0.00	0.00	0.396	9.82	4.00
ATOM	1886	O	LYS	443	4.137	8.994	-19.578	0.00	0.00	-0.396	8.17	-17.40
ATOM	1887	CB	LYS	443	1.780	7.027	-18.740	0.00	0.00	-0.106	12.77	4.00
ATOM	1888	HB1	LYS	443	1.427	6.682	-19.712	0.00	0.00	0.053	0.00	0.00
ATOM	1889	HB2	LYS	443	1.047	6.725	-17.992	0.00	0.00	0.053	0.00	0.00
ATOM	1890	CG	LYS	443	3.090	6.302	-18.433	0.00	0.00	-0.106	12.77	4.00
ATOM	1891	HG1	LYS	443	3.760	6.886	-17.803	0.00	0.00	0.053	0.00	0.00

ATOM	1892	HG2	LYS	443	3.661	6.060	-19.330	0.00	0.00	0.053	0.00	0.00
ATOM	1893	CD	LYS	443	2.879	4.979	-17.703	0.00	0.00	-0.106	12.77	4.00
ATOM	1894	HD1	LYS	443	3.828	4.493	-17.478	0.00	0.00	0.053	0.00	0.00
ATOM	1895	HD2	LYS	443	2.289	4.284	-18.301	0.00	0.00	0.053	0.00	0.00
ATOM	1896	CE	LYS	443	2.142	5.184	-16.376	0.00	0.00	0.099	12.77	4.00
ATOM	1897	HE1	LYS	443	2.337	4.344	-15.709	0.00	0.00	0.053	0.00	0.00
ATOM	1898	HE2	LYS	443	1.069	5.254	-16.554	0.00	0.00	0.053	0.00	0.00
ATOM	1899	NZ	LYS	443	2.607	6.434	-15.727	0.00	0.00	-0.045	13.25	-39.20
ATOM	1900	HZ1	LYS	443	2.107	6.565	-14.836	0.00	0.00	0.280	0.00	0.00
ATOM	1901	HZ2	LYS	443	3.619	6.372	-15.547	0.00	0.00	0.280	0.00	0.00
ATOM	1902	HZ3	LYS	443	2.418	7.234	-16.347	0.00	0.00	0.280	0.00	0.00
ATOM	1903	N	ARG	444	2.437	9.161	-21.035	0.00	0.00	-0.650	9.00	-17.40
ATOM	1904	HN	ARG	444	1.428	9.078	-21.222	0.00	0.00	0.439	0.00	0.00
ATOM	1905	CA	ARG	444	3.349	9.533	-22.072	0.00	0.00	0.158	9.40	4.00
ATOM	1906	HA	ARG	444	4.146	8.790	-22.093	0.00	0.00	0.053	0.00	0.00
ATOM	1907	C	ARG	444	3.882	10.889	-21.742	0.00	0.00	0.396	9.82	4.00
ATOM	1908	O	ARG	444	4.992	11.246	-22.140	0.00	0.00	-0.396	8.17	-17.40
ATOM	1909	CB	ARG	444	2.720	9.503	-23.463	0.00	0.00	-0.106	12.77	4.00
ATOM	1910	HB1	ARG	444	2.006	10.325	-23.522	0.00	0.00	0.053	0.00	0.00
ATOM	1911	HB2	ARG	444	2.223	8.540	-23.581	0.00	0.00	0.053	0.00	0.00
ATOM	1912	CG	ARG	444	3.671	9.658	-24.651	0.00	0.00	-0.106	12.77	4.00
ATOM	1913	HG1	ARG	444	4.241	8.740	-24.795	0.00	0.00	0.053	0.00	0.00
ATOM	1914	HG2	ARG	444	4.364	10.479	-24.469	0.00	0.00	0.053	0.00	0.00
ATOM	1915	CD	ARG	444	2.874	9.953	-25.925	0.00	0.00	0.374	12.77	4.00
ATOM	1916	HD1	ARG	444	2.078	10.656	-25.680	0.00	0.00	0.053	0.00	0.00
ATOM	1917	HD2	ARG	444	2.455	9.017	-26.295	0.00	0.00	0.053	0.00	0.00
ATOM	1918	NE	ARG	444	3.795	10.543	-26.931	0.00	0.00	-0.819	9.00	-24.67
ATOM	1919	HE	ARG	444	4.292	11.424	-26.739	0.00	0.00	0.407	0.00	0.00
ATOM	1920	CZ	ARG	444	3.965	9.890	-28.111	0.00	0.00	0.796	6.95	4.00
ATOM	1921	NH1	ARG	444	3.315	8.704	-28.296	0.00	0.00	-0.746	9.00	-24.67
ATOM	1922	HH11	ARG	444	3.426	8.188	-29.181	0.00	0.00	0.407	0.00	0.00
ATOM	1923	HH12	ARG	444	2.713	8.325	-27.551	0.00	0.00	0.407	0.00	0.00
ATOM	1924	NH2	ARG	444	4.786	10.403	-29.075	0.00	0.00	-0.746	9.00	-24.67
ATOM	1925	HH21	ARG	444	4.909	9.902	-29.966	0.00	0.00	0.407	0.00	0.00
ATOM	1926	HH22	ARG	444	5.281	11.291	-28.910	0.00	0.00	0.407	0.00	0.00
ATOM	1927	N	GLN	445	3.085	11.690	-21.006	0.00	0.00	-0.650	9.00	-17.40
ATOM	1928	HN	GLN	445	2.149	11.367	-20.722	0.00	0.00	0.439	0.00	0.00
ATOM	1929	CA	GLN	445	3.542	12.989	-20.620	0.00	0.00	0.158	9.40	4.00
ATOM	1930	HA	GLN	445	3.674	13.576	-21.529	0.00	0.00	0.053	0.00	0.00
ATOM	1931	C	GLN	445	4.835	12.816	-19.895	0.00	0.00	0.396	9.82	4.00
ATOM	1932	O	GLN	445	5.880	13.141	-20.453	0.00	0.00	-0.396	8.17	-17.40
ATOM	1933	CB	GLN	445	2.557	13.669	-19.651	0.00	0.00	-0.106	12.77	4.00
ATOM	1934	HB1	GLN	445	2.453	13.037	-18.769	0.00	0.00	0.053	0.00	0.00
ATOM	1935	HB2	GLN	445	1.599	13.780	-20.159	0.00	0.00	0.053	0.00	0.00
ATOM	1936	CG	GLN	445	2.996	15.053	-19.180	0.00	0.00	-0.106	12.77	4.00
ATOM	1937	HG1	GLN	445	3.101	15.675	-20.069	0.00	0.00	0.053	0.00	0.00
ATOM	1938	HG2	GLN	445	3.946	14.927	-18.660	0.00	0.00	0.053	0.00	0.00
ATOM	1939	CD	GLN	445	1.910	15.573	-18.253	0.00	0.00	0.396	9.82	4.00
ATOM	1940	OE1	GLN	445	1.714	15.071	-17.145	0.00	0.00	-0.396	8.17	-17.40
ATOM	1941	NE2	GLN	445	1.165	16.604	-18.729	0.00	0.00	-0.879	13.25	-17.40
ATOM	1942	HE21	GLN	445	1.362	16.995	-19.661	0.00	0.00	0.439	0.00	0.00
ATOM	1943	HE22	GLN	445	0.403	16.995	-18.158	0.00	0.00	0.439	0.00	0.00
ATOM	1944	N	ASN	446	4.778	12.157	-18.714	0.00	0.00	-0.650	9.00	-17.40
ATOM	1945	HN	ASN	446	3.875	11.724	-18.472	0.00	0.00	0.439	0.00	0.00
ATOM	1946	CA	ASN	446	5.848	11.996	-17.758	0.00	0.00	0.158	9.40	4.00
ATOM	1947	HA	ASN	446	6.285	12.957	-17.488	0.00	0.00	0.053	0.00	0.00
ATOM	1948	C	ASN	446	6.943	11.140	-18.308	0.00	0.00	0.396	9.82	4.00
ATOM	1949	O	ASN	446	8.065	11.181	-17.803	0.00	0.00	-0.396	8.17	-17.40
ATOM	1950	CB	ASN	446	5.430	11.333	-16.430	0.00	0.00	-0.106	12.77	4.00
ATOM	1951	HB1	ASN	446	4.466	11.732	-16.114	0.00	0.00	0.053	0.00	0.00
ATOM	1952	HB2	ASN	446	6.180	11.545	-15.668	0.00	0.00	0.053	0.00	0.00
ATOM	1953	CG	ASN	446	5.318	9.825	-16.630	0.00	0.00	0.396	9.82	4.00
ATOM	1954	OD1	ASN	446	4.295	9.281	-17.043	0.00	0.00	-0.396	8.17	-17.40
ATOM	1955	ND2	ASN	446	6.433	9.110	-16.319	0.00	0.00	-0.879	13.25	-17.40
ATOM	1956	HD21	ASN	446	7.275	9.593	-15.975	0.00	0.00	0.439	0.00	0.00
ATOM	1957	HD22	ASN	446	6.435	8.086	-16.427	0.00	0.00	0.439	0.00	0.00
ATOM	1958	N	GLN	447	6.639	10.336	-19.343	0.00	0.00	-0.650	9.00	-17.40
ATOM	1959	HN	GLN	447	5.690	10.386	-19.739	0.00	0.00	0.439	0.00	0.00
ATOM	1960	CA	GLN	447	7.571	9.414	-19.921	0.00	0.00	0.158	9.40	4.00
ATOM	1961	HA	GLN	447	7.753	8.620	-19.196	0.00	0.00	0.053	0.00	0.00
ATOM	1962	C	GLN	447	8.827	10.157	-20.222	0.00	0.00	0.396	9.82	4.00
ATOM	1963	O	GLN	447	9.915	9.620	-20.067	0.00	0.00	-0.396	8.17	-17.40
ATOM	1964	CB	GLN	447	7.050	8.836	-21.252	0.00	0.00	-0.106	12.77	4.00
ATOM	1965	HB1	GLN	447	6.787	9.669	-21.904	0.00	0.00	0.053	0.00	0.00
ATOM	1966	HB2	GLN	447	6.175	8.223	-21.037	0.00	0.00	0.053	0.00	0.00
ATOM	1967	CG	GLN	447	8.052	7.957	-22.009	0.00	0.00	-0.106	12.77	4.00

ATOM	1968	HG1	GLN	447	7.537	7.109	-22.460	0.00	0.00	0.053	0.00	0.00
ATOM	1969	HG2	GLN	447	8.813	7.585	-21.323	0.00	0.00	0.053	0.00	0.00
ATOM	1970	CD	GLN	447	8.731	8.771	-23.113	0.00	0.00	0.396	9.82	4.00
ATOM	1971	OE1	GLN	447	9.219	9.883	-22.915	0.00	0.00	-0.396	8.17	-17.40
ATOM	1972	NE2	GLN	447	8.761	8.189	-24.341	0.00	0.00	-0.879	13.25	-17.40
ATOM	1973	HE21	GLN	447	8.345	7.257	-24.479	0.00	0.00	0.439	0.00	0.00
ATOM	1974	HE22	GLN	447	9.200	8.680	-25.133	0.00	0.00	0.439	0.00	0.00
ATOM	1975	N	SER	448	8.743	11.419	-20.664	0.00	0.00	-0.650	9.00	-17.40
ATOM	1976	HN	SER	448	7.832	11.887	-20.776	0.00	0.00	0.439	0.00	0.00
ATOM	1977	CA	SER	448	9.967	12.093	-20.975	0.00	0.00	0.158	9.40	4.00
ATOM	1978	HA	SER	448	10.522	11.537	-21.731	0.00	0.00	0.053	0.00	0.00
ATOM	1979	C	SER	448	10.820	12.215	-19.744	0.00	0.00	0.396	9.82	4.00
ATOM	1980	O	SER	448	12.033	12.030	-19.814	0.00	0.00	-0.396	8.17	-17.40
ATOM	1981	CB	SER	448	9.747	13.501	-21.554	0.00	0.00	0.007	12.77	4.00
ATOM	1982	HB1	SER	448	10.705	14.010	-21.660	0.00	0.00	0.053	0.00	0.00
ATOM	1983	HB2	SER	448	9.107	14.078	-20.887	0.00	0.00	0.053	0.00	0.00
ATOM	1984	OG	SER	448	9.127	13.405	-22.828	0.00	0.00	-0.537	11.04	-17.40
ATOM	1985	HG	SER	448	8.911	14.350	-23.177	0.00	0.00	0.424	0.00	0.00
ATOM	1986	N	LEU	449	10.231	12.546	-18.578	0.00	0.00	-0.650	9.00	-17.40
ATOM	1987	HN	LEU	449	9.212	12.686	-18.521	0.00	0.00	0.439	0.00	0.00
ATOM	1988	CA	LEU	449	11.062	12.698	-17.416	0.00	0.00	0.158	9.40	4.00
ATOM	1989	HA	LEU	449	11.854	13.426	-17.594	0.00	0.00	0.053	0.00	0.00
ATOM	1990	C	LEU	449	11.708	11.397	-17.042	0.00	0.00	0.396	9.82	4.00
ATOM	1991	O	LEU	449	12.931	11.322	-16.932	0.00	0.00	-0.396	8.17	-17.40
ATOM	1992	CB	LEU	449	10.291	13.206	-16.182	0.00	0.00	-0.106	12.77	4.00
ATOM	1993	HB1	LEU	449	9.479	12.510	-15.974	0.00	0.00	0.053	0.00	0.00
ATOM	1994	HB2	LEU	449	9.897	14.197	-16.407	0.00	0.00	0.053	0.00	0.00
ATOM	1995	CG	LEU	449	11.151	13.320	-14.907	0.00	0.00	-0.053	9.40	4.00
ATOM	1996	HG	LEU	449	11.542	12.351	-14.596	0.00	0.00	0.053	0.00	0.00
ATOM	1997	CD1	LEU	449	12.357	14.249	-15.115	0.00	0.00	-0.159	16.15	4.00
ATOM	1998	HD11	LEU	449	12.938	14.303	-14.194	0.00	0.00	0.053	0.00	0.00
ATOM	1999	HD12	LEU	449	12.983	13.858	-15.917	0.00	0.00	0.053	0.00	0.00
ATOM	2000	HD13	LEU	449	12.007	15.246	-15.382	0.00	0.00	0.053	0.00	0.00
ATOM	2001	CD2	LEU	449	10.297	13.742	-13.701	0.00	0.00	-0.159	16.15	4.00
ATOM	2002	HD21	LEU	449	10.929	13.815	-12.816	0.00	0.00	0.053	0.00	0.00
ATOM	2003	HD22	LEU	449	9.839	14.711	-13.901	0.00	0.00	0.053	0.00	0.00
ATOM	2004	HD23	LEU	449	9.517	13.000	-13.530	0.00	0.00	0.053	0.00	0.00
ATOM	2005	N	VAL	450	10.905	10.331	-16.843	0.00	0.00	-0.650	9.00	-17.40
ATOM	2006	HN	VAL	450	9.891	10.418	-17.000	0.00	0.00	0.439	0.00	0.00
ATOM	2007	CA	VAL	450	11.457	9.073	-16.413	0.00	0.00	0.158	9.40	4.00
ATOM	2008	HA	VAL	450	12.108	9.204	-15.548	0.00	0.00	0.053	0.00	0.00
ATOM	2009	C	VAL	450	12.266	8.438	-17.501	0.00	0.00	0.396	9.82	4.00
ATOM	2010	O	VAL	450	13.414	8.058	-17.291	0.00	0.00	-0.396	8.17	-17.40
ATOM	2011	CB	VAL	450	10.405	8.095	-15.966	0.00	0.00	-0.053	9.40	4.00
ATOM	2012	HB	VAL	450	9.874	8.499	-15.104	0.00	0.00	0.053	0.00	0.00
ATOM	2013	CG1	VAL	450	9.408	7.851	-17.113	0.00	0.00	-0.159	16.15	4.00
ATOM	2014	HG11	VAL	450	8.646	7.142	-16.788	0.00	0.00	0.053	0.00	0.00
ATOM	2015	HG12	VAL	450	8.933	8.793	-17.389	0.00	0.00	0.053	0.00	0.00
ATOM	2016	HG13	VAL	450	9.937	7.445	-17.975	0.00	0.00	0.053	0.00	0.00
ATOM	2017	CG2	VAL	450	11.112	6.820	-15.476	0.00	0.00	-0.159	16.15	4.00
ATOM	2018	HG21	VAL	450	10.368	6.095	-15.146	0.00	0.00	0.053	0.00	0.00
ATOM	2019	HG22	VAL	450	11.698	6.393	-16.290	0.00	0.00	0.053	0.00	0.00
ATOM	2020	HG23	VAL	450	11.772	7.067	-14.644	0.00	0.00	0.053	0.00	0.00
ATOM	2021	N	TYR	451	11.687	8.325	-18.708	0.00	0.00	-0.650	9.00	-17.40
ATOM	2022	HN	TYR	451	10.724	8.672	-18.823	0.00	0.00	0.439	0.00	0.00
ATOM	2023	CA	TYR	451	12.342	7.746	-19.843	0.00	0.00	0.158	9.40	4.00
ATOM	2024	HA	TYR	451	12.706	6.768	-19.529	0.00	0.00	0.053	0.00	0.00
ATOM	2025	C	TYR	451	13.447	8.661	-20.208	0.00	0.00	0.396	9.82	4.00
ATOM	2026	O	TYR	451	13.336	9.877	-20.076	0.00	0.00	-0.396	8.17	-17.40
ATOM	2027	CB	TYR	451	11.425	7.570	-21.069	0.00	0.00	-0.106	12.77	4.00
ATOM	2028	HB1	TYR	451	10.895	8.506	-21.244	0.00	0.00	0.053	0.00	0.00
ATOM	2029	HB2	TYR	451	10.717	6.767	-20.862	0.00	0.00	0.053	0.00	0.00
ATOM	2030	CG	TYR	451	12.268	7.225	-22.247	0.00	0.00	0.000	7.26	0.60
ATOM	2031	CD1	TYR	451	12.802	5.966	-22.390	0.00	0.00	-0.127	10.80	0.60
ATOM	2032	HD1	TYR	451	12.612	5.208	-21.630	0.00	0.00	0.127	0.00	0.00
ATOM	2033	CD2	TYR	451	12.507	8.167	-23.220	0.00	0.00	-0.127	10.80	0.60
ATOM	2034	HD2	TYR	451	12.080	9.165	-23.121	0.00	0.00	0.127	0.00	0.00
ATOM	2035	CE1	TYR	451	13.574	5.656	-23.484	0.00	0.00	-0.127	10.80	0.60
ATOM	2036	HE1	TYR	451	13.996	4.656	-23.587	0.00	0.00	0.127	0.00	0.00
ATOM	2037	CE2	TYR	451	13.278	7.863	-24.316	0.00	0.00	-0.127	10.80	0.60
ATOM	2038	HE2	TYR	451	13.464	8.619	-25.079	0.00	0.00	0.127	0.00	0.00
ATOM	2039	CZ	TYR	451	13.814	6.605	-24.449	0.00	0.00	0.027	7.26	0.60
ATOM	2040	OH	TYR	451	14.607	6.287	-25.573	0.00	0.00	-0.451	10.94	-17.40
ATOM	2041	HH	TYR	451	14.581	7.068	-26.244	0.00	0.00	0.424	0.00	0.00
ATOM	2042	N	GLY	452	14.578	8.092	-20.656	0.00	0.00	-0.650	9.00	-17.40
ATOM	2043	HN	GLY	452	14.628	7.075	-20.809	0.00	0.00	0.439	0.00	0.00

ATOM	2044	CA	GLY	452	15.710	8.924	-20.916	0.00	0.00	0.105	9.40	4.00
ATOM	2045	HA1	GLY	452	15.282	9.860	-21.274	0.00	0.00	0.053	0.00	0.00
ATOM	2046	HA2	GLY	452	16.279	8.380	-21.669	0.00	0.00	0.053	0.00	0.00
ATOM	2047	C	GLY	452	16.399	9.036	-19.598	0.00	0.00	0.396	9.82	4.00
ATOM	2048	O	GLY	452	17.513	9.552	-19.508	0.00	0.00	-0.396	8.17	-17.40
ATOM	2049	N	LYS	453	15.711	8.517	-18.557	0.00	0.00	-0.650	9.00	-17.40
ATOM	2050	HN	LYS	453	14.787	8.117	-18.776	0.00	0.00	0.439	0.00	0.00
ATOM	2051	CA	LYS	453	16.117	8.458	-17.185	0.00	0.00	0.158	9.40	4.00
ATOM	2052	HA	LYS	453	15.237	8.422	-16.542	0.00	0.00	0.053	0.00	0.00
ATOM	2053	C	LYS	453	16.921	9.663	-16.847	0.00	0.00	0.396	9.82	4.00
ATOM	2054	O	LYS	453	17.949	9.569	-16.178	0.00	0.00	-0.396	8.17	-17.40
ATOM	2055	CB	LYS	453	16.931	7.191	-16.868	0.00	0.00	-0.106	12.77	4.00
ATOM	2056	HB1	LYS	453	17.248	7.150	-15.826	0.00	0.00	0.053	0.00	0.00
ATOM	2057	HB2	LYS	453	17.838	7.119	-17.468	0.00	0.00	0.053	0.00	0.00
ATOM	2058	CG	LYS	453	16.138	5.906	-17.129	0.00	0.00	-0.106	12.77	4.00
ATOM	2059	HG1	LYS	453	15.704	5.969	-18.127	0.00	0.00	0.053	0.00	0.00
ATOM	2060	HG2	LYS	453	15.356	5.828	-16.374	0.00	0.00	0.053	0.00	0.00
ATOM	2061	CD	LYS	453	16.972	4.624	-17.067	0.00	0.00	-0.106	12.77	4.00
ATOM	2062	HD1	LYS	453	18.038	4.794	-17.221	0.00	0.00	0.053	0.00	0.00
ATOM	2063	HD2	LYS	453	16.687	3.886	-17.817	0.00	0.00	0.053	0.00	0.00
ATOM	2064	CE	LYS	453	16.868	3.897	-15.725	0.00	0.00	0.099	12.77	4.00
ATOM	2065	HE1	LYS	453	17.389	2.941	-15.778	0.00	0.00	0.053	0.00	0.00
ATOM	2066	HE2	LYS	453	15.821	3.717	-15.480	0.00	0.00	0.053	0.00	0.00
ATOM	2067	NZ	LYS	453	17.478	4.719	-14.657	0.00	0.00	-0.045	13.25	-39.20
ATOM	2068	HZ1	LYS	453	17.404	4.223	-13.757	0.00	0.00	0.280	0.00	0.00
ATOM	2069	HZ2	LYS	453	18.470	4.886	-14.876	0.00	0.00	0.280	0.00	0.00
ATOM	2070	HZ3	LYS	453	16.985	5.621	-14.593	0.00	0.00	0.280	0.00	0.00
ATOM	2071	N	VAL	454	16.470	10.840	-17.321	0.00	0.00	-0.650	9.00	-17.40
ATOM	2072	HN	VAL	454	15.607	10.877	-17.882	0.00	0.00	0.439	0.00	0.00
ATOM	2073	CA	VAL	454	17.197	12.038	-17.041	0.00	0.00	0.158	9.40	4.00
ATOM	2074	HA	VAL	454	18.236	11.902	-17.342	0.00	0.00	0.053	0.00	0.00
ATOM	2075	C	VAL	454	17.125	12.321	-15.573	0.00	0.00	0.396	9.82	4.00
ATOM	2076	O	VAL	454	18.135	12.629	-14.944	0.00	0.00	-0.396	8.17	-17.40
ATOM	2077	CB	VAL	454	16.668	13.227	-17.784	0.00	0.00	-0.053	9.40	4.00
ATOM	2078	HB	VAL	454	15.607	13.335	-17.558	0.00	0.00	0.053	0.00	0.00
ATOM	2079	CG1	VAL	454	17.440	14.475	-17.327	0.00	0.00	-0.159	16.15	4.00
ATOM	2080	HG11	VAL	454	17.066	15.349	-17.859	0.00	0.00	0.053	0.00	0.00
ATOM	2081	HG12	VAL	454	17.302	14.616	-16.255	0.00	0.00	0.053	0.00	0.00
ATOM	2082	HG13	VAL	454	18.501	14.346	-17.542	0.00	0.00	0.053	0.00	0.00
ATOM	2083	CG2	VAL	454	16.798	12.939	-19.290	0.00	0.00	-0.159	16.15	4.00
ATOM	2084	HG21	VAL	454	16.420	13.790	-19.857	0.00	0.00	0.053	0.00	0.00
ATOM	2085	HG22	VAL	454	17.846	12.774	-19.540	0.00	0.00	0.053	0.00	0.00
ATOM	2086	HG23	VAL	454	16.221	12.049	-19.542	0.00	0.00	0.053	0.00	0.00
ATOM	2087	N	ASP	455	15.920	12.194	-14.984	0.00	0.00	-0.650	9.00	-17.40
ATOM	2088	HN	ASP	455	15.114	11.880	-15.544	0.00	0.00	0.439	0.00	0.00
ATOM	2089	CA	ASP	455	15.738	12.488	-13.591	0.00	0.00	0.158	9.40	4.00
ATOM	2090	HA	ASP	455	16.437	13.285	-13.338	0.00	0.00	0.053	0.00	0.00
ATOM	2091	C	ASP	455	16.033	11.232	-12.834	0.00	0.00	0.396	9.82	4.00
ATOM	2092	O	ASP	455	16.031	10.136	-13.394	0.00	0.00	-0.396	8.17	-17.40
ATOM	2093	CB	ASP	455	14.284	12.914	-13.266	0.00	0.00	-0.336	12.77	4.00
ATOM	2094	HB1	ASP	455	13.654	12.025	-13.282	0.00	0.00	0.053	0.00	0.00
ATOM	2095	HB2	ASP	455	13.958	13.628	-14.023	0.00	0.00	0.053	0.00	0.00
ATOM	2096	CG	ASP	455	14.118	13.579	-11.894	0.00	0.00	0.297	9.82	4.00
ATOM	2097	OD1	ASP	455	15.079	13.623	-11.082	0.00	0.00	-0.534	8.17	-18.95
ATOM	2098	OD2	ASP	455	12.983	14.070	-11.647	0.00	0.00	-0.534	8.17	-18.95
ATOM	2099	N	SER	456	16.330	11.387	-11.531	0.00	0.00	-0.650	9.00	-17.40
ATOM	2100	HN	SER	456	16.383	12.349	-11.168	0.00	0.00	0.439	0.00	0.00
ATOM	2101	CA	SER	456	16.578	10.321	-10.611	0.00	0.00	0.158	9.40	4.00
ATOM	2102	HA	SER	456	17.341	9.694	-11.072	0.00	0.00	0.053	0.00	0.00
ATOM	2103	C	SER	456	15.278	9.609	-10.440	0.00	0.00	0.396	9.82	4.00
ATOM	2104	O	SER	456	15.243	8.472	-9.973	0.00	0.00	-0.396	8.17	-17.40
ATOM	2105	CB	SER	456	17.065	10.803	-9.234	0.00	0.00	0.007	12.77	4.00
ATOM	2106	HB1	SER	456	16.314	11.449	-8.779	0.00	0.00	0.053	0.00	0.00
ATOM	2107	HB2	SER	456	17.995	11.361	-9.343	0.00	0.00	0.053	0.00	0.00
ATOM	2108	OG	SER	456	17.292	9.689	-8.383	0.00	0.00	-0.537	11.04	-17.40
ATOM	2109	HG	SER	456	16.585	9.679	-7.634	0.00	0.00	0.424	0.00	0.00
ATOM	2110	N	PHE	457	14.179	10.313	-10.782	0.00	0.00	-0.650	9.00	-17.40
ATOM	2111	HN	PHE	457	14.331	11.282	-11.095	0.00	0.00	0.439	0.00	0.00
ATOM	2112	CA	PHE	457	12.815	9.850	-10.755	0.00	0.00	0.158	9.40	4.00
ATOM	2113	HA	PHE	457	12.492	9.901	-9.715	0.00	0.00	0.053	0.00	0.00
ATOM	2114	C	PHE	457	12.833	8.444	-11.278	0.00	0.00	0.396	9.82	4.00
ATOM	2115	O	PHE	457	12.847	8.223	-12.487	0.00	0.00	-0.396	8.17	-17.40
ATOM	2116	CB	PHE	457	11.979	10.743	-11.704	0.00	0.00	-0.106	12.77	4.00
ATOM	2117	HB1	PHE	457	12.281	10.517	-12.727	0.00	0.00	0.053	0.00	0.00
ATOM	2118	HB2	PHE	457	12.189	11.783	-11.454	0.00	0.00	0.053	0.00	0.00
ATOM	2119	CG	PHE	457	10.496	10.570	-11.639	0.00	0.00	0.000	7.26	0.60

ATOM	2120	CD1	PHE	457	9.770	11.252	-10.694	0.00	0.00	-0.127	10.80	0.60
ATOM	2121	HD1	PHE	457	10.289	11.904	-9.992	0.00	0.00	0.127	0.00	0.00
ATOM	2122	CD2	PHE	457	9.820	9.767	-12.530	0.00	0.00	-0.127	10.80	0.60
ATOM	2123	HD2	PHE	457	10.374	9.224	-13.296	0.00	0.00	0.127	0.00	0.00
ATOM	2124	CE1	PHE	457	8.403	11.131	-10.614	0.00	0.00	-0.127	10.80	0.60
ATOM	2125	HE1	PHE	457	7.850	11.676	-9.849	0.00	0.00	0.127	0.00	0.00
ATOM	2126	CE2	PHE	457	8.451	9.644	-12.461	0.00	0.00	-0.127	10.80	0.60
ATOM	2127	HE2	PHE	457	7.929	9.004	-13.173	0.00	0.00	0.127	0.00	0.00
ATOM	2128	CZ	PHE	457	7.737	10.322	-11.501	0.00	0.00	-0.127	10.80	0.60
ATOM	2129	HZ	PHE	457	6.653	10.218	-11.445	0.00	0.00	0.127	0.00	0.00
ATOM	2130	N	TRP	458	12.878	7.445	-10.367	0.00	0.00	-0.650	9.00	-17.40
ATOM	2131	HN	TRP	458	12.835	7.654	-9.359	0.00	0.00	0.439	0.00	0.00
ATOM	2132	CA	TRP	458	12.987	6.089	-10.826	0.00	0.00	0.158	9.40	4.00
ATOM	2133	HA	TRP	458	13.736	6.015	-11.615	0.00	0.00	0.053	0.00	0.00
ATOM	2134	C	TRP	458	11.680	5.618	-11.366	0.00	0.00	0.396	9.82	4.00
ATOM	2135	O	TRP	458	11.644	4.800	-12.282	0.00	0.00	-0.396	8.17	-17.40
ATOM	2136	CB	TRP	458	13.507	5.054	-9.800	0.00	0.00	-0.106	12.77	4.00
ATOM	2137	HB1	TRP	458	14.382	5.484	-9.313	0.00	0.00	0.053	0.00	0.00
ATOM	2138	HB2	TRP	458	13.764	4.148	-10.348	0.00	0.00	0.053	0.00	0.00
ATOM	2139	CG	TRP	458	12.561	4.641	-8.702	0.00	0.00	0.000	7.26	0.60
ATOM	2140	CD1	TRP	458	11.461	5.272	-8.214	0.00	0.00	-0.177	10.80	0.60
ATOM	2141	HD1	TRP	458	11.095	6.241	-8.553	0.00	0.00	0.127	0.00	0.00
ATOM	2142	CD2	TRP	458	12.671	3.400	-7.987	0.00	0.00	0.000	6.80	0.60
ATOM	2143	NE1	TRP	458	10.878	4.510	-7.230	0.00	0.00	-0.292	9.00	-17.40
ATOM	2144	HE1	TRP	458	10.036	4.762	-6.693	0.00	0.00	0.393	0.00	0.00
ATOM	2145	CE2	TRP	458	11.611	3.351	-7.083	0.00	0.00	-0.050	6.80	0.60
ATOM	2146	CE3	TRP	458	13.575	2.380	-8.080	0.00	0.00	-0.127	10.80	0.60
ATOM	2147	HE3	TRP	458	14.400	2.417	-8.791	0.00	0.00	0.127	0.00	0.00
ATOM	2148	CZ2	TRP	458	11.438	2.278	-6.256	0.00	0.00	-0.127	10.80	0.60
ATOM	2149	HZ2	TRP	458	10.607	2.234	-5.552	0.00	0.00	0.127	0.00	0.00
ATOM	2150	CZ3	TRP	458	13.402	1.302	-7.239	0.00	0.00	-0.127	10.80	0.60
ATOM	2151	HZ3	TRP	458	14.107	0.472	-7.282	0.00	0.00	0.127	0.00	0.00
ATOM	2152	CH2	TRP	458	12.354	1.253	-6.345	0.00	0.00	-0.127	10.80	0.60
ATOM	2153	HH2	TRP	458	12.248	0.385	-5.695	0.00	0.00	0.127	0.00	0.00
ATOM	2154	N	LYS	459	10.555	6.088	-10.799	0.00	0.00	-0.650	9.00	-17.40
ATOM	2155	HN	LYS	459	10.585	6.764	-10.023	0.00	0.00	0.439	0.00	0.00
ATOM	2156	CA	LYS	459	9.317	5.606	-11.323	0.00	0.00	0.158	9.40	4.00
ATOM	2157	HA	LYS	459	9.488	5.246	-12.338	0.00	0.00	0.053	0.00	0.00
ATOM	2158	C	LYS	459	8.342	6.722	-11.327	0.00	0.00	0.396	9.82	4.00
ATOM	2159	O	LYS	459	8.469	7.678	-10.564	0.00	0.00	-0.396	8.17	-17.40
ATOM	2160	CB	LYS	459	8.711	4.431	-10.524	0.00	0.00	-0.106	12.77	4.00
ATOM	2161	HB1	LYS	459	9.440	3.620	-10.516	0.00	0.00	0.053	0.00	0.00
ATOM	2162	HB2	LYS	459	7.792	4.125	-11.023	0.00	0.00	0.053	0.00	0.00
ATOM	2163	CG	LYS	459	8.352	4.728	-9.062	0.00	0.00	-0.106	12.77	4.00
ATOM	2164	HG1	LYS	459	9.205	5.221	-8.596	0.00	0.00	0.053	0.00	0.00
ATOM	2165	HG2	LYS	459	8.135	3.782	-8.566	0.00	0.00	0.053	0.00	0.00
ATOM	2166	CD	LYS	459	7.135	5.637	-8.873	0.00	0.00	-0.106	12.77	4.00
ATOM	2167	HD1	LYS	459	6.272	5.343	-9.470	0.00	0.00	0.053	0.00	0.00
ATOM	2168	HD2	LYS	459	7.320	6.677	-9.140	0.00	0.00	0.053	0.00	0.00
ATOM	2169	CE	LYS	459	6.621	5.684	-7.432	0.00	0.00	0.099	12.77	4.00
ATOM	2170	HE1	LYS	459	6.306	4.691	-7.111	0.00	0.00	0.053	0.00	0.00
ATOM	2171	HE2	LYS	459	5.770	6.361	-7.357	0.00	0.00	0.053	0.00	0.00
ATOM	2172	NZ	LYS	459	7.687	6.160	-6.523	0.00	0.00	-0.045	13.25	-39.20
ATOM	2173	HZ1	LYS	459	7.329	6.187	-5.558	0.00	0.00	0.280	0.00	0.00
ATOM	2174	HZ2	LYS	459	8.492	5.520	-6.572	0.00	0.00	0.280	0.00	0.00
ATOM	2175	HZ3	LYS	459	7.983	7.105	-6.806	0.00	0.00	0.280	0.00	0.00
ATOM	2176	N	ASN	460	7.345	6.625	-12.225	0.00	0.00	-0.650	9.00	-17.40
ATOM	2177	HN	ASN	460	7.323	5.832	-12.882	0.00	0.00	0.439	0.00	0.00
ATOM	2178	CA	ASN	460	6.319	7.614	-12.273	0.00	0.00	0.158	9.40	4.00
ATOM	2179	HA	ASN	460	6.724	8.462	-11.721	0.00	0.00	0.053	0.00	0.00
ATOM	2180	C	ASN	460	5.148	6.978	-11.616	0.00	0.00	0.396	9.82	4.00
ATOM	2181	O	ASN	460	4.683	5.917	-12.025	0.00	0.00	-0.396	8.17	-17.40
ATOM	2182	CB	ASN	460	5.907	8.027	-13.694	0.00	0.00	-0.106	12.77	4.00
ATOM	2183	HB1	ASN	460	5.312	7.210	-14.102	0.00	0.00	0.053	0.00	0.00
ATOM	2184	HB2	ASN	460	6.827	8.181	-14.258	0.00	0.00	0.053	0.00	0.00
ATOM	2185	CG	ASN	460	5.098	9.309	-13.565	0.00	0.00	0.396	9.82	4.00
ATOM	2186	OD1	ASN	460	5.629	10.409	-13.713	0.00	0.00	-0.396	8.17	-17.40
ATOM	2187	ND2	ASN	460	3.777	9.169	-13.276	0.00	0.00	-0.879	13.25	-17.40
ATOM	2188	HD21	ASN	460	3.372	8.229	-13.160	0.00	0.00	0.439	0.00	0.00
ATOM	2189	HD22	ASN	460	3.181	10.003	-13.173	0.00	0.00	0.439	0.00	0.00
ATOM	2190	N	LYS	461	4.651	7.644	-10.563	0.00	0.00	-0.650	9.00	-17.40
ATOM	2191	HN	LYS	461	5.034	8.576	-10.350	0.00	0.00	0.439	0.00	0.00
ATOM	2192	CA	LYS	461	3.621	7.130	-9.725	0.00	0.00	0.158	9.40	4.00
ATOM	2193	HA	LYS	461	3.531	6.052	-9.859	0.00	0.00	0.053	0.00	0.00
ATOM	2194	C	LYS	461	2.323	7.763	-10.063	0.00	0.00	0.396	9.82	4.00
ATOM	2195	O	LYS	461	2.232	8.972	-10.263	0.00	0.00	-0.396	8.17	-17.40

ATOM	2196	CB	LYS	461	3.862	7.501	-8.263	0.00	0.00	-0.106	12.77	4.00
ATOM	2197	HB1	LYS	461	4.124	8.554	-8.162	0.00	0.00	0.053	0.00	0.00
ATOM	2198	HB2	LYS	461	4.676	6.914	-7.837	0.00	0.00	0.053	0.00	0.00
ATOM	2199	CG	LYS	461	2.626	7.252	-7.424	0.00	0.00	-0.106	12.77	4.00
ATOM	2200	HG1	LYS	461	1.770	7.785	-7.838	0.00	0.00	0.053	0.00	0.00
ATOM	2201	HG2	LYS	461	2.783	7.595	-6.401	0.00	0.00	0.053	0.00	0.00
ATOM	2202	CD	LYS	461	2.299	5.775	-7.388	0.00	0.00	-0.106	12.77	4.00
ATOM	2203	HD1	LYS	461	3.205	5.236	-7.110	0.00	0.00	0.053	0.00	0.00
ATOM	2204	HD2	LYS	461	1.960	5.481	-8.381	0.00	0.00	0.053	0.00	0.00
ATOM	2205	CE	LYS	461	1.210	5.368	-6.400	0.00	0.00	0.099	12.77	4.00
ATOM	2206	HE1	LYS	461	0.953	6.175	-5.713	0.00	0.00	0.053	0.00	0.00
ATOM	2207	HE2	LYS	461	1.507	4.519	-5.784	0.00	0.00	0.053	0.00	0.00
ATOM	2208	NZ	LYS	461	-0.036	4.980	-7.074	0.00	0.00	-0.045	13.25	-39.20
ATOM	2209	HZ1	LYS	461	-0.739	4.714	-6.370	0.00	0.00	0.280	0.00	0.00
ATOM	2210	HZ2	LYS	461	-0.388	5.773	-7.628	0.00	0.00	0.280	0.00	0.00
ATOM	2211	HZ3	LYS	461	0.145	4.180	-7.697	0.00	0.00	0.280	0.00	0.00
ATOM	2212	N	LYS	462	1.287	6.912	-10.136	0.00	0.00	-0.650	9.00	-17.40
ATOM	2213	HN	LYS	462	1.489	5.910	-10.008	0.00	0.00	0.439	0.00	0.00
ATOM	2214	CA	LYS	462	-0.070	7.281	-10.376	0.00	0.00	0.158	9.40	4.00
ATOM	2215	HA	LYS	462	-0.145	7.895	-11.274	0.00	0.00	0.053	0.00	0.00
ATOM	2216	C	LYS	462	-0.610	8.061	-9.224	0.00	0.00	0.396	9.82	4.00
ATOM	2217	O	LYS	462	-1.193	9.127	-9.411	0.00	0.00	-0.396	8.17	-17.40
ATOM	2218	CB	LYS	462	-0.927	6.009	-10.553	0.00	0.00	-0.106	12.77	4.00
ATOM	2219	HB1	LYS	462	-0.576	5.273	-9.830	0.00	0.00	0.053	0.00	0.00
ATOM	2220	HB2	LYS	462	-0.787	5.658	-11.575	0.00	0.00	0.053	0.00	0.00
ATOM	2221	CG	LYS	462	-2.438	6.147	-10.340	0.00	0.00	-0.106	12.77	4.00
ATOM	2222	HG1	LYS	462	-2.919	5.263	-10.758	0.00	0.00	0.053	0.00	0.00
ATOM	2223	HG2	LYS	462	-2.770	7.049	-10.854	0.00	0.00	0.053	0.00	0.00
ATOM	2224	CD	LYS	462	-2.892	6.264	-8.875	0.00	0.00	-0.106	12.77	4.00
ATOM	2225	HD1	LYS	462	-3.806	6.857	-8.847	0.00	0.00	0.053	0.00	0.00
ATOM	2226	HD2	LYS	462	-2.099	6.753	-8.309	0.00	0.00	0.053	0.00	0.00
ATOM	2227	CE	LYS	462	-3.187	4.926	-8.197	0.00	0.00	0.099	12.77	4.00
ATOM	2228	HE1	LYS	462	-2.302	4.291	-8.230	0.00	0.00	0.053	0.00	0.00
ATOM	2229	HE2	LYS	462	-4.006	4.423	-8.711	0.00	0.00	0.053	0.00	0.00
ATOM	2230	NZ	LYS	462	-3.569	5.151	-6.783	0.00	0.00	-0.045	13.25	-39.20
ATOM	2231	HZ1	LYS	462	-3.766	4.246	-6.332	0.00	0.00	0.280	0.00	0.00
ATOM	2232	HZ2	LYS	462	-2.796	5.619	-6.288	0.00	0.00	0.280	0.00	0.00
ATOM	2233	HZ3	LYS	462	-4.410	5.744	-6.744	0.00	0.00	0.280	0.00	0.00
ATOM	2234	N	ILE	463	-0.412	7.573	-7.983	0.00	0.00	-0.650	9.00	-17.40
ATOM	2235	HN	ILE	463	0.209	6.772	-7.799	0.00	0.00	0.439	0.00	0.00
ATOM	2236	CA	ILE	463	-1.124	8.244	-6.938	0.00	0.00	0.158	9.40	4.00
ATOM	2237	HA	ILE	463	-1.930	8.857	-7.342	0.00	0.00	0.053	0.00	0.00
ATOM	2238	C	ILE	463	-0.225	9.133	-6.164	0.00	0.00	0.396	9.82	4.00
ATOM	2239	O	ILE	463	0.955	8.856	-5.962	0.00	0.00	-0.396	8.17	-17.40
ATOM	2240	CB	ILE	463	-1.833	7.363	-5.940	0.00	0.00	-0.053	9.40	4.00
ATOM	2241	HB	ILE	463	-2.279	6.521	-6.469	0.00	0.00	0.053	0.00	0.00
ATOM	2242	CG1	ILE	463	-2.934	8.153	-5.220	0.00	0.00	-0.106	12.77	4.00
ATOM	2243	HG11	ILE	463	-3.591	8.702	-5.895	0.00	0.00	0.053	0.00	0.00
ATOM	2244	HG12	ILE	463	-2.552	8.902	-4.526	0.00	0.00	0.053	0.00	0.00
ATOM	2245	CG2	ILE	463	-0.817	6.862	-4.916	0.00	0.00	-0.159	16.15	4.00
ATOM	2246	HG21	ILE	463	-1.318	6.223	-4.189	0.00	0.00	0.053	0.00	0.00
ATOM	2247	HG22	ILE	463	-0.039	6.292	-5.424	0.00	0.00	0.053	0.00	0.00
ATOM	2248	HG23	ILE	463	-0.367	7.712	-4.403	0.00	0.00	0.053	0.00	0.00
ATOM	2249	CD1	ILE	463	-3.869	7.279	-4.383	0.00	0.00	-0.159	16.15	4.00
ATOM	2250	HD11	ILE	463	-4.621	7.906	-3.904	0.00	0.00	0.053	0.00	0.00
ATOM	2251	HD12	ILE	463	-4.361	6.551	-5.028	0.00	0.00	0.053	0.00	0.00
ATOM	2252	HD13	ILE	463	-3.292	6.756	-3.620	0.00	0.00	0.053	0.00	0.00
ATOM	2253	N	TYR	464	-0.799	10.259	-5.710	0.00	0.00	-0.650	9.00	-17.40
ATOM	2254	HN	TYR	464	-1.780	10.460	-5.950	0.00	0.00	0.439	0.00	0.00
ATOM	2255	CA	TYR	464	-0.071	11.182	-4.900	0.00	0.00	0.158	9.40	4.00
ATOM	2256	HA	TYR	464	0.905	11.398	-5.335	0.00	0.00	0.053	0.00	0.00
ATOM	2257	C	TYR	464	0.053	10.483	-3.597	0.00	0.00	0.396	9.82	4.00
ATOM	2258	O	TYR	464	-0.493	9.389	-3.455	0.00	0.00	-0.396	8.17	-17.40
ATOM	2259	CB	TYR	464	-0.826	12.514	-4.672	0.00	0.00	-0.106	12.77	4.00
ATOM	2260	HB1	TYR	464	-1.726	12.347	-4.080	0.00	0.00	0.053	0.00	0.00
ATOM	2261	HB2	TYR	464	-1.118	12.956	-5.625	0.00	0.00	0.053	0.00	0.00
ATOM	2262	CG	TYR	464	0.043	13.493	-3.944	0.00	0.00	0.000	7.26	0.60
ATOM	2263	CD1	TYR	464	1.055	14.149	-4.604	0.00	0.00	-0.127	10.80	0.60
ATOM	2264	HD1	TYR	464	1.214	13.944	-5.663	0.00	0.00	0.127	0.00	0.00
ATOM	2265	CD2	TYR	464	-0.148	13.778	-2.612	0.00	0.00	-0.127	10.80	0.60
ATOM	2266	HD2	TYR	464	-0.949	13.285	-2.061	0.00	0.00	0.127	0.00	0.00
ATOM	2267	CE1	TYR	464	1.871	15.052	-3.974	0.00	0.00	-0.127	10.80	0.60
ATOM	2268	HE1	TYR	464	2.667	15.552	-4.526	0.00	0.00	0.127	0.00	0.00
ATOM	2269	CE2	TYR	464	0.667	14.683	-1.971	0.00	0.00	-0.127	10.80	0.60
ATOM	2270	HE2	TYR	464	0.507	14.896	-0.914	0.00	0.00	0.127	0.00	0.00
ATOM	2271	CZ	TYR	464	1.678	15.321	-2.645	0.00	0.00	0.027	7.26	0.60

ATOM	2272	OH	TYR	464	2.511	16.247	-1.983	0.00	0.00	-0.451	10.94	-17.40
ATOM	2273	HH	TYR	464	3.351	16.422	-2.552	0.00	0.00	0.424	0.00	0.00
ATOM	2274	N	LEU	465	0.769	11.113	-2.638	0.00	0.00	-0.650	9.00	-17.40
ATOM	2275	HN	LEU	465	1.183	12.018	-2.903	0.00	0.00	0.439	0.00	0.00
ATOM	2276	CA	LEU	465	1.022	10.671	-1.294	0.00	0.00	0.158	9.40	4.00
ATOM	2277	HA	LEU	465	1.886	10.009	-1.346	0.00	0.00	0.053	0.00	0.00
ATOM	2278	C	LEU	465	-0.210	9.962	-0.846	0.00	0.00	0.396	9.82	4.00
ATOM	2279	O	LEU	465	-1.310	10.349	-1.242	0.00	0.00	-0.396	8.17	-17.40
ATOM	2280	CB	LEU	465	1.337	11.880	-0.379	0.00	0.00	-0.106	12.77	4.00
ATOM	2281	HB1	LEU	465	0.422	12.467	-0.298	0.00	0.00	0.053	0.00	0.00
ATOM	2282	HB2	LEU	465	2.138	12.443	-0.858	0.00	0.00	0.053	0.00	0.00
ATOM	2283	CG	LEU	465	1.807	11.626	1.074	0.00	0.00	-0.053	9.40	4.00
ATOM	2284	HG	LEU	465	2.729	11.045	1.068	0.00	0.00	0.053	0.00	0.00
ATOM	2285	CD1	LEU	465	2.062	12.967	1.782	0.00	0.00	-0.159	16.15	4.00
ATOM	2286	HD11	LEU	465	2.392	12.782	2.804	0.00	0.00	0.053	0.00	0.00
ATOM	2287	HD12	LEU	465	2.833	13.521	1.246	0.00	0.00	0.053	0.00	0.00
ATOM	2288	HD13	LEU	465	1.142	13.551	1.798	0.00	0.00	0.053	0.00	0.00
ATOM	2289	CD2	LEU	465	0.838	10.762	1.893	0.00	0.00	-0.159	16.15	4.00
ATOM	2290	HD21	LEU	465	1.233	10.627	2.900	0.00	0.00	0.053	0.00	0.00
ATOM	2291	HD22	LEU	465	-0.132	11.255	1.947	0.00	0.00	0.053	0.00	0.00
ATOM	2292	HD23	LEU	465	0.724	9.789	1.414	0.00	0.00	0.053	0.00	0.00
ATOM	2293	N	ASP	466	-0.036	8.907	-0.027	0.00	0.00	-0.650	9.00	-17.40
ATOM	2294	HN	ASP	466	0.913	8.726	0.330	0.00	0.00	0.439	0.00	0.00
ATOM	2295	CA	ASP	466	-1.086	8.021	0.379	0.00	0.00	0.158	9.40	4.00
ATOM	2296	HA	ASP	466	-1.352	7.427	-0.496	0.00	0.00	0.053	0.00	0.00
ATOM	2297	C	ASP	466	-2.211	8.873	0.837	0.00	0.00	0.396	9.82	4.00
ATOM	2298	O	ASP	466	-3.375	8.565	0.588	0.00	0.00	-0.396	8.17	-17.40
ATOM	2299	CB	ASP	466	-0.695	7.139	1.576	0.00	0.00	-0.336	12.77	4.00
ATOM	2300	HB1	ASP	466	-1.570	6.573	1.896	0.00	0.00	0.053	0.00	0.00
ATOM	2301	HB2	ASP	466	-0.346	7.780	2.386	0.00	0.00	0.053	0.00	0.00
ATOM	2302	CG	ASP	466	0.413	6.191	1.145	0.00	0.00	0.297	9.82	4.00
ATOM	2303	OD1	ASP	466	0.720	6.150	-0.076	0.00	0.00	-0.534	8.17	-18.95
ATOM	2304	OD2	ASP	466	0.970	5.499	2.038	0.00	0.00	-0.534	8.17	-18.95
ATOM	2305	N	ILE	467	-1.891	9.990	1.510	0.00	0.00	-0.650	9.00	-17.40
ATOM	2306	HN	ILE	467	-0.919	10.205	1.775	0.00	0.00	0.439	0.00	0.00
ATOM	2307	CA	ILE	467	-2.969	10.862	1.838	0.00	0.00	0.158	9.40	4.00
ATOM	2308	HA	ILE	467	-3.828	10.223	2.045	0.00	0.00	0.053	0.00	0.00
ATOM	2309	C	ILE	467	-3.183	11.740	0.636	0.00	0.00	0.396	9.82	4.00
ATOM	2310	O	ILE	467	-2.868	12.929	0.612	0.00	0.00	-0.396	8.17	-17.40
ATOM	2311	CB	ILE	467	-2.746	11.636	3.120	0.00	0.00	-0.053	9.40	4.00
ATOM	2312	HB	ILE	467	-2.568	10.945	3.944	0.00	0.00	0.053	0.00	0.00
ATOM	2313	CG1	ILE	467	-4.044	12.308	3.607	0.00	0.00	-0.106	12.77	4.00
ATOM	2314	HG11	ILE	467	-3.831	12.811	4.550	0.00	0.00	0.053	0.00	0.00
ATOM	2315	HG12	ILE	467	-4.796	11.531	3.743	0.00	0.00	0.053	0.00	0.00
ATOM	2316	CG2	ILE	467	-1.529	12.558	2.968	0.00	0.00	-0.159	16.15	4.00
ATOM	2317	HG21	ILE	467	-1.374	13.112	3.894	0.00	0.00	0.053	0.00	0.00
ATOM	2318	HG22	ILE	467	-0.644	11.960	2.751	0.00	0.00	0.053	0.00	0.00
ATOM	2319	HG23	ILE	467	-1.703	13.258	2.151	0.00	0.00	0.053	0.00	0.00
ATOM	2320	CD1	ILE	467	-4.634	13.351	2.659	0.00	0.00	-0.159	16.15	4.00
ATOM	2321	HD11	ILE	467	-5.544	13.764	3.093	0.00	0.00	0.053	0.00	0.00
ATOM	2322	HD12	ILE	467	-3.911	14.152	2.503	0.00	0.00	0.053	0.00	0.00
ATOM	2323	HD13	ILE	467	-4.868	12.883	1.703	0.00	0.00	0.053	0.00	0.00
ATOM	2324	N	ILE	468	-3.710	11.108	-0.430	0.00	0.00	-0.650	9.00	-17.40
ATOM	2325	HN	ILE	468	-3.869	10.094	-0.339	0.00	0.00	0.439	0.00	0.00
ATOM	2326	CA	ILE	468	-4.071	11.711	-1.678	0.00	0.00	0.158	9.40	4.00
ATOM	2327	HA	ILE	468	-3.185	12.269	-1.981	0.00	0.00	0.053	0.00	0.00
ATOM	2328	C	ILE	468	-5.240	12.570	-1.356	0.00	0.00	0.396	9.82	4.00
ATOM	2329	O	ILE	468	-5.531	13.541	-2.053	0.00	0.00	-0.396	8.17	-17.40
ATOM	2330	CB	ILE	468	-4.474	10.667	-2.688	0.00	0.00	-0.053	9.40	4.00
ATOM	2331	HB	ILE	468	-3.694	9.906	-2.697	0.00	0.00	0.053	0.00	0.00
ATOM	2332	CG1	ILE	468	-4.470	11.199	-4.135	0.00	0.00	-0.106	12.77	4.00
ATOM	2333	HG11	ILE	468	-4.625	10.354	-4.806	0.00	0.00	0.053	0.00	0.00
ATOM	2334	HG12	ILE	468	-3.504	11.669	-4.319	0.00	0.00	0.053	0.00	0.00
ATOM	2335	CG2	ILE	468	-5.824	10.086	-2.233	0.00	0.00	-0.159	16.15	4.00
ATOM	2336	HG21	ILE	468	-6.150	9.324	-2.941	0.00	0.00	0.053	0.00	0.00
ATOM	2337	HG22	ILE	468	-5.713	9.639	-1.245	0.00	0.00	0.053	0.00	0.00
ATOM	2338	HG23	ILE	468	-6.567	10.882	-2.190	0.00	0.00	0.053	0.00	0.00
ATOM	2339	CD1	ILE	468	-5.545	12.234	-4.454	0.00	0.00	-0.159	16.15	4.00
ATOM	2340	HD11	ILE	468	-5.455	12.543	-5.495	0.00	0.00	0.053	0.00	0.00
ATOM	2341	HD12	ILE	468	-6.530	11.798	-4.288	0.00	0.00	0.053	0.00	0.00
ATOM	2342	HD13	ILE	468	-5.419	13.101	-3.806	0.00	0.00	0.053	0.00	0.00
ATOM	2343	N	HIS	469	-5.930	12.185	-0.264	0.00	0.00	-0.650	9.00	-17.40
ATOM	2344	HN	HIS	469	-5.569	11.367	0.247	0.00	0.00	0.439	0.00	0.00
ATOM	2345	CA	HIS	469	-7.115	12.799	0.258	0.00	0.00	0.158	9.40	4.00
ATOM	2346	HA	HIS	469	-7.982	12.446	-0.300	0.00	0.00	0.053	0.00	0.00
ATOM	2347	C	HIS	469	-7.006	14.281	0.124	0.00	0.00	0.396	9.82	4.00

ATOM	2348	O	HIS	469	-5.915	14.850	0.085	0.00	0.00	-0.396	8.17	-17.40
ATOM	2349	CB	HIS	469	-7.318	12.524	1.758	0.00	0.00	-0.106	12.77	4.00
ATOM	2350	HB1	HIS	469	-8.287	12.927	2.052	0.00	0.00	0.053	0.00	0.00
ATOM	2351	HB2	HIS	469	-6.515	13.015	2.308	0.00	0.00	0.053	0.00	0.00
ATOM	2352	CG	HIS	469	-7.299	11.070	2.126	0.00	0.00	0.241	7.26	0.60
ATOM	2353	ND1	HIS	469	-6.237	10.232	1.865	0.00	0.00	-0.481	9.25	-17.40
ATOM	2354	CD2	HIS	469	-8.215	10.313	2.789	0.00	0.00	-0.177	10.80	0.60
ATOM	2355	HD2	HIS	469	-9.181	10.674	3.142	0.00	0.00	0.127	0.00	0.00
ATOM	2356	CE1	HIS	469	-6.559	9.019	2.381	0.00	0.00	0.064	10.80	0.60
ATOM	2357	HE1	HIS	469	-5.910	8.145	2.329	0.00	0.00	0.127	0.00	0.00
ATOM	2358	NE2	HIS	469	-7.749	9.020	2.953	0.00	0.00	-0.292	9.25	-17.40
ATOM	2359	HE2	HIS	469	-8.225	8.234	3.418	0.00	0.00	0.393	0.00	0.00
ATOM	2360	N	THR	470	-8.172	14.940	0.029	0.00	0.00	-0.650	9.00	-17.40
ATOM	2361	HN	THR	470	-9.051	14.404	0.051	0.00	0.00	0.439	0.00	0.00
ATOM	2362	CA	THR	470	-8.230	16.363	-0.102	0.00	0.00	0.158	9.40	4.00
ATOM	2363	HA	THR	470	-7.632	16.648	-0.968	0.00	0.00	0.053	0.00	0.00
ATOM	2364	C	THR	470	-7.678	16.965	1.143	0.00	0.00	0.396	9.82	4.00
ATOM	2365	O	THR	470	-7.049	18.021	1.109	0.00	0.00	-0.396	8.17	-17.40
ATOM	2366	CB	THR	470	-9.629	16.885	-0.241	0.00	0.00	0.060	9.40	4.00
ATOM	2367	HB	THR	470	-10.096	16.411	-1.104	0.00	0.00	0.053	0.00	0.00
ATOM	2368	OG1	THR	470	-9.598	18.291	-0.439	0.00	0.00	-0.537	11.04	-17.40
ATOM	2369	HG1	THR	470	-8.629	18.629	-0.350	0.00	0.00	0.424	0.00	0.00
ATOM	2370	CG2	THR	470	-10.413	16.547	1.038	0.00	0.00	-0.159	16.15	4.00
ATOM	2371	HG21	THR	470	-11.433	16.922	0.949	0.00	0.00	0.053	0.00	0.00
ATOM	2372	HG22	THR	470	-10.434	15.466	1.177	0.00	0.00	0.053	0.00	0.00
ATOM	2373	HG23	THR	470	-9.928	17.013	1.896	0.00	0.00	0.053	0.00	0.00
ATOM	2374	N	TYR	471	-7.884	16.277	2.279	0.00	0.00	-0.650	9.00	-17.40
ATOM	2375	HN	TYR	471	-8.318	15.345	2.222	0.00	0.00	0.439	0.00	0.00
ATOM	2376	CA	TYR	471	-7.523	16.791	3.565	0.00	0.00	0.158	9.40	4.00
ATOM	2377	HA	TYR	471	-8.144	17.652	3.813	0.00	0.00	0.053	0.00	0.00
ATOM	2378	C	TYR	471	-6.090	17.215	3.565	0.00	0.00	0.396	9.82	4.00
ATOM	2379	O	TYR	471	-5.765	18.276	4.095	0.00	0.00	-0.396	8.17	-17.40
ATOM	2380	CB	TYR	471	-7.678	15.742	4.681	0.00	0.00	-0.106	12.77	4.00
ATOM	2381	HB1	TYR	471	-7.354	16.196	5.618	0.00	0.00	0.053	0.00	0.00
ATOM	2382	HB2	TYR	471	-7.053	14.886	4.428	0.00	0.00	0.053	0.00	0.00
ATOM	2383	CG	TYR	471	-9.114	15.350	4.749	0.00	0.00	0.000	7.26	0.60
ATOM	2384	CD1	TYR	471	-10.019	16.104	5.460	0.00	0.00	-0.127	10.80	0.60
ATOM	2385	HD1	TYR	471	-9.684	17.001	5.980	0.00	0.00	0.127	0.00	0.00
ATOM	2386	CD2	TYR	471	-9.555	14.221	4.098	0.00	0.00	-0.127	10.80	0.60
ATOM	2387	HD2	TYR	471	-8.848	13.616	3.531	0.00	0.00	0.127	0.00	0.00
ATOM	2388	CE1	TYR	471	-11.343	15.736	5.520	0.00	0.00	-0.127	10.80	0.60
ATOM	2389	HE1	TYR	471	-12.051	16.341	6.087	0.00	0.00	0.127	0.00	0.00
ATOM	2390	CE2	TYR	471	-10.877	13.847	4.154	0.00	0.00	-0.127	10.80	0.60
ATOM	2391	HE2	TYR	471	-11.213	12.950	3.634	0.00	0.00	0.127	0.00	0.00
ATOM	2392	CZ	TYR	471	-11.774	14.606	4.866	0.00	0.00	0.027	7.26	0.60
ATOM	2393	OH	TYR	471	-13.131	14.226	4.926	0.00	0.00	-0.451	10.94	-17.40
ATOM	2394	HH	TYR	471	-13.723	15.068	4.946	0.00	0.00	0.424	0.00	0.00
ATOM	2395	N	MET	472	-5.184	16.417	2.966	0.00	0.00	-0.650	9.00	-17.40
ATOM	2396	HN	MET	472	-5.474	15.566	2.464	0.00	0.00	0.439	0.00	0.00
ATOM	2397	CA	MET	472	-3.803	16.792	3.051	0.00	0.00	0.158	9.40	4.00
ATOM	2398	HA	MET	472	-3.517	16.956	4.090	0.00	0.00	0.053	0.00	0.00
ATOM	2399	C	MET	472	-3.558	18.052	2.287	0.00	0.00	0.396	9.82	4.00
ATOM	2400	O	MET	472	-4.471	18.816	1.981	0.00	0.00	-0.396	8.17	-17.40
ATOM	2401	CB	MET	472	-2.793	15.787	2.483	0.00	0.00	-0.106	12.77	4.00
ATOM	2402	HB1	MET	472	-2.950	14.781	2.873	0.00	0.00	0.053	0.00	0.00
ATOM	2403	HB2	MET	472	-1.765	16.058	2.722	0.00	0.00	0.053	0.00	0.00
ATOM	2404	CG	MET	472	-2.876	15.684	0.963	0.00	0.00	-0.041	12.77	4.00
ATOM	2405	HG1	MET	472	-3.497	16.501	0.596	0.00	0.00	0.053	0.00	0.00
ATOM	2406	HG2	MET	472	-3.320	14.722	0.707	0.00	0.00	0.053	0.00	0.00
ATOM	2407	SD	MET	472	-1.266	15.792	0.130	0.00	0.00	-0.130	16.39	-6.40
ATOM	2408	CE	MET	472	-0.503	14.302	0.832	0.00	0.00	-0.094	16.15	4.00
ATOM	2409	HE1	MET	472	0.507	14.190	0.437	0.00	0.00	0.053	0.00	0.00
ATOM	2410	HE2	MET	472	-0.461	14.392	1.917	0.00	0.00	0.053	0.00	0.00
ATOM	2411	HE3	MET	472	-1.097	13.428	0.563	0.00	0.00	0.053	0.00	0.00
ATOM	2412	N	GLU	473	-2.273	18.264	1.942	0.00	0.00	-0.650	9.00	-17.40
ATOM	2413	HN	GLU	473	-1.584	17.536	2.177	0.00	0.00	0.439	0.00	0.00
ATOM	2414	CA	GLU	473	-1.806	19.438	1.269	0.00	0.00	0.158	9.40	4.00
ATOM	2415	HA	GLU	473	-1.975	20.299	1.915	0.00	0.00	0.053	0.00	0.00
ATOM	2416	C	GLU	473	-2.564	19.589	-0.002	0.00	0.00	0.396	9.82	4.00
ATOM	2417	O	GLU	473	-3.012	20.686	-0.329	0.00	0.00	-0.396	8.17	-17.40
ATOM	2418	CB	GLU	473	-0.315	19.344	0.902	0.00	0.00	-0.106	12.77	4.00
ATOM	2419	HB1	GLU	473	-0.076	18.512	0.240	0.00	0.00	0.053	0.00	0.00
ATOM	2420	HB2	GLU	473	0.343	19.214	1.761	0.00	0.00	0.053	0.00	0.00
ATOM	2421	CG	GLU	473	0.223	20.581	0.183	0.00	0.00	-0.336	12.77	4.00
ATOM	2422	HG1	GLU	473	0.089	21.436	0.846	0.00	0.00	0.053	0.00	0.00
ATOM	2423	HG2	GLU	473	-0.347	20.705	-0.737	0.00	0.00	0.053	0.00	0.00

ATOM	2424	CD	GLU	473	1.696	20.342	-0.113	0.00	0.00	0.297	9.82	4.00
ATOM	2425	OE1	GLU	473	2.014	19.291	-0.731	0.00	0.00	-0.534	8.17	-18.95
ATOM	2426	OE2	GLU	473	2.524	21.206	0.282	0.00	0.00	-0.534	8.17	-18.95
ATOM	2427	N	VAL	474	-2.730	18.482	-0.752	0.00	0.00	-0.650	9.00	-17.40
ATOM	2428	HN	VAL	474	-2.331	17.583	-0.445	0.00	0.00	0.439	0.00	0.00
ATOM	2429	CA	VAL	474	-3.465	18.563	-1.979	0.00	0.00	0.158	9.40	4.00
ATOM	2430	HA	VAL	474	-2.910	19.246	-2.622	0.00	0.00	0.053	0.00	0.00
ATOM	2431	C	VAL	474	-4.812	19.084	-1.623	0.00	0.00	0.396	9.82	4.00
ATOM	2432	O	VAL	474	-5.289	18.874	-0.510	0.00	0.00	-0.396	8.17	-17.40
ATOM	2433	CB	VAL	474	-3.631	17.240	-2.661	0.00	0.00	-0.053	9.40	4.00
ATOM	2434	HB	VAL	474	-4.289	17.376	-3.519	0.00	0.00	0.053	0.00	0.00
ATOM	2435	CG1	VAL	474	-2.245	16.752	-3.115	0.00	0.00	-0.159	16.15	4.00
ATOM	2436	HG11	VAL	474	-2.344	15.788	-3.615	0.00	0.00	0.053	0.00	0.00
ATOM	2437	HG12	VAL	474	-1.813	17.476	-3.806	0.00	0.00	0.053	0.00	0.00
ATOM	2438	HG13	VAL	474	-1.595	16.645	-2.247	0.00	0.00	0.053	0.00	0.00
ATOM	2439	CG2	VAL	474	-4.329	16.278	-1.684	0.00	0.00	-0.159	16.15	4.00
ATOM	2440	HG21	VAL	474	-4.460	15.307	-2.161	0.00	0.00	0.053	0.00	0.00
ATOM	2441	HG22	VAL	474	-3.719	16.163	-0.788	0.00	0.00	0.053	0.00	0.00
ATOM	2442	HG23	VAL	474	-5.303	16.682	-1.409	0.00	0.00	0.053	0.00	0.00
ATOM	2443	N	HIS	475	-5.456	19.814	-2.548	0.00	0.00	-0.650	9.00	-17.40
ATOM	2444	HN	HIS	475	-5.045	19.974	-3.479	0.00	0.00	0.439	0.00	0.00
ATOM	2445	CA	HIS	475	-6.729	20.361	-2.200	0.00	0.00	0.158	9.40	4.00
ATOM	2446	HA	HIS	475	-6.996	20.059	-1.187	0.00	0.00	0.053	0.00	0.00
ATOM	2447	C	HIS	475	-7.769	19.864	-3.150	0.00	0.00	0.396	9.82	4.00
ATOM	2448	O	HIS	475	-7.496	19.607	-4.322	0.00	0.00	-0.396	8.17	-17.40
ATOM	2449	CB	HIS	475	-6.761	21.898	-2.188	0.00	0.00	-0.106	12.77	4.00
ATOM	2450	HB1	HIS	475	-7.764	22.313	-2.287	0.00	0.00	0.053	0.00	0.00
ATOM	2451	HB2	HIS	475	-6.184	22.351	-2.994	0.00	0.00	0.053	0.00	0.00
ATOM	2452	CG	HIS	475	-6.211	22.499	-0.926	0.00	0.00	0.241	7.26	0.60
ATOM	2453	ND1	HIS	475	-6.913	22.551	0.258	0.00	0.00	-0.481	9.25	-17.40
ATOM	2454	CD2	HIS	475	-5.013	23.092	-0.672	0.00	0.00	-0.177	10.80	0.60
ATOM	2455	HD2	HIS	475	-4.214	23.215	-1.403	0.00	0.00	0.127	0.00	0.00
ATOM	2456	CE1	HIS	475	-6.112	23.169	1.163	0.00	0.00	0.064	10.80	0.60
ATOM	2457	HE1	HIS	475	-6.396	23.356	2.199	0.00	0.00	0.127	0.00	0.00
ATOM	2458	NE2	HIS	475	-4.949	23.518	0.643	0.00	0.00	-0.292	9.25	-17.40
ATOM	2459	HE2	HIS	475	-4.169	24.000	1.112	0.00	0.00	0.393	0.00	0.00
ATOM	2460	N	ALA	476	-9.006	19.713	-2.627	0.00	0.00	-0.650	9.00	-17.40
ATOM	2461	HN	ALA	476	-9.151	19.959	-1.637	0.00	0.00	0.439	0.00	0.00
ATOM	2462	CA	ALA	476	-10.127	19.228	-3.380	0.00	0.00	0.158	9.40	4.00
ATOM	2463	HA	ALA	476	-9.804	18.336	-3.917	0.00	0.00	0.053	0.00	0.00
ATOM	2464	C	ALA	476	-10.538	20.305	-4.322	0.00	0.00	0.396	9.82	4.00
ATOM	2465	O	ALA	476	-9.715	20.835	-5.063	0.00	0.00	-0.396	8.17	-17.40
ATOM	2466	CB	ALA	476	-11.353	18.894	-2.513	0.00	0.00	-0.159	16.15	4.00
ATOM	2467	HB1	ALA	476	-12.161	18.533	-3.149	0.00	0.00	0.053	0.00	0.00
ATOM	2468	HB2	ALA	476	-11.088	18.122	-1.790	0.00	0.00	0.053	0.00	0.00
ATOM	2469	HB3	ALA	476	-11.679	19.789	-1.984	0.00	0.00	0.053	0.00	0.00
ATOM	2470	N	THR	477	-11.844	20.636	-4.341	0.00	0.00	-0.650	9.00	-17.40
ATOM	2471	HN	THR	477	-12.516	20.151	-3.729	0.00	0.00	0.439	0.00	0.00
ATOM	2472	CA	THR	477	-12.281	21.673	-5.226	0.00	0.00	0.158	9.40	4.00
ATOM	2473	HA	THR	477	-11.442	21.965	-5.858	0.00	0.00	0.053	0.00	0.00
ATOM	2474	C	THR	477	-12.744	22.833	-4.406	0.00	0.00	0.396	9.82	4.00
ATOM	2475	O	THR	477	-13.531	22.686	-3.471	0.00	0.00	-0.396	8.17	-17.40
ATOM	2476	CB	THR	477	-13.410	21.268	-6.134	0.00	0.00	0.060	9.40	4.00
ATOM	2477	HB	THR	477	-13.132	20.368	-6.683	0.00	0.00	0.053	0.00	0.00
ATOM	2478	OG1	THR	477	-13.666	22.294	-7.082	0.00	0.00	-0.537	11.04	-17.40
ATOM	2479	HG1	THR	477	-13.027	23.084	-6.915	0.00	0.00	0.424	0.00	0.00
ATOM	2480	CG2	THR	477	-14.669	20.986	-5.297	0.00	0.00	-0.159	16.15	4.00
ATOM	2481	HG21	THR	477	-15.486	20.693	-5.956	0.00	0.00	0.053	0.00	0.00
ATOM	2482	HG22	THR	477	-14.464	20.180	-4.592	0.00	0.00	0.053	0.00	0.00
ATOM	2483	HG23	THR	477	-14.950	21.885	-4.749	0.00	0.00	0.053	0.00	0.00
ATOM	2484	N	VAL	478	-12.216	24.026	-4.729	0.00	0.00	-0.650	9.00	-17.40
ATOM	2485	HN	VAL	478	-11.500	24.071	-5.468	0.00	0.00	0.439	0.00	0.00
ATOM	2486	CA	VAL	478	-12.617	25.236	-4.079	0.00	0.00	0.158	9.40	4.00
ATOM	2487	HA	VAL	478	-13.696	25.287	-4.224	0.00	0.00	0.053	0.00	0.00
ATOM	2488	C	VAL	478	-11.867	26.314	-4.783	0.00	0.00	0.396	9.82	4.00
ATOM	2489	O	VAL	478	-11.321	26.092	-5.862	0.00	0.00	-0.396	8.17	-17.40
ATOM	2490	CB	VAL	478	-12.260	25.315	-2.619	0.00	0.00	-0.053	9.40	4.00
ATOM	2491	HB	VAL	478	-12.525	24.374	-2.137	0.00	0.00	0.053	0.00	0.00
ATOM	2492	CG1	VAL	478	-10.750	25.564	-2.486	0.00	0.00	-0.159	16.15	4.00
ATOM	2493	HG11	VAL	478	-10.482	25.623	-1.431	0.00	0.00	0.053	0.00	0.00
ATOM	2494	HG12	VAL	478	-10.204	24.745	-2.954	0.00	0.00	0.053	0.00	0.00
ATOM	2495	HG13	VAL	478	-10.491	26.501	-2.979	0.00	0.00	0.053	0.00	0.00
ATOM	2496	CG2	VAL	478	-13.127	26.397	-1.956	0.00	0.00	-0.159	16.15	4.00
ATOM	2497	HG21	VAL	478	-12.878	26.464	-0.897	0.00	0.00	0.053	0.00	0.00
ATOM	2498	HG22	VAL	478	-12.939	27.358	-2.435	0.00	0.00	0.053	0.00	0.00
ATOM	2499	HG23	VAL	478	-14.180	26.137	-2.065	0.00	0.00	0.053	0.00	0.00

ATOM	2500	N	TYR	479	-11.830	27.523	-4.201	0.00	0.00	-0.650	9.00	-17.40
ATOM	2501	HN	TYR	479	-12.328	27.699	-3.317	0.00	0.00	0.439	0.00	0.00
ATOM	2502	CA	TYR	479	-11.083	28.557	-4.838	0.00	0.00	0.158	9.40	4.00
ATOM	2503	HA	TYR	479	-11.281	28.458	-5.905	0.00	0.00	0.053	0.00	0.00
ATOM	2504	C	TYR	479	-9.648	28.305	-4.491	0.00	0.00	0.396	9.82	4.00
ATOM	2505	O	TYR	479	-9.160	28.773	-3.463	0.00	0.00	-0.396	8.17	-17.40
ATOM	2506	CB	TYR	479	-11.470	29.956	-4.324	0.00	0.00	-0.106	12.77	4.00
ATOM	2507	HB1	TYR	479	-11.218	30.027	-3.266	0.00	0.00	0.053	0.00	0.00
ATOM	2508	HB2	TYR	479	-12.542	30.100	-4.462	0.00	0.00	0.053	0.00	0.00
ATOM	2509	CG	TYR	479	-10.715	30.981	-5.096	0.00	0.00	0.000	7.26	0.60
ATOM	2510	CD1	TYR	479	-11.145	31.356	-6.347	0.00	0.00	-0.127	10.80	0.60
ATOM	2511	HD1	TYR	479	-12.038	30.896	-6.770	0.00	0.00	0.127	0.00	0.00
ATOM	2512	CD2	TYR	479	-9.590	31.575	-4.571	0.00	0.00	-0.127	10.80	0.60
ATOM	2513	HD2	TYR	479	-9.242	31.291	-3.578	0.00	0.00	0.127	0.00	0.00
ATOM	2514	CE1	TYR	479	-10.462	32.304	-7.070	0.00	0.00	-0.127	10.80	0.60
ATOM	2515	HE1	TYR	479	-10.812	32.591	-8.061	0.00	0.00	0.127	0.00	0.00
ATOM	2516	CE2	TYR	479	-8.902	32.524	-5.290	0.00	0.00	-0.127	10.80	0.60
ATOM	2517	HE2	TYR	479	-8.011	32.987	-4.867	0.00	0.00	0.127	0.00	0.00
ATOM	2518	CZ	TYR	479	-9.337	32.889	-6.541	0.00	0.00	0.027	7.26	0.60
ATOM	2519	OH	TYR	479	-8.634	33.863	-7.281	0.00	0.00	-0.451	10.94	-17.40
ATOM	2520	HH	TYR	479	-7.792	34.149	-6.761	0.00	0.00	0.424	0.00	0.00
ATOM	2521	N	GLY	480	-8.934	27.541	-5.346	0.00	0.00	-0.650	9.00	-17.40
ATOM	2522	HN	GLY	480	-9.388	27.146	-6.182	0.00	0.00	0.439	0.00	0.00
ATOM	2523	CA	GLY	480	-7.546	27.278	-5.094	0.00	0.00	0.105	9.40	4.00
ATOM	2524	HA1	GLY	480	-7.253	27.724	-4.144	0.00	0.00	0.053	0.00	0.00
ATOM	2525	HA2	GLY	480	-6.939	27.705	-5.893	0.00	0.00	0.053	0.00	0.00
ATOM	2526	C	GLY	480	-7.313	25.796	-5.036	0.00	0.00	0.396	9.82	4.00
ATOM	2527	O	GLY	480	-6.307	25.305	-5.546	0.00	0.00	-0.396	8.17	-17.40
ATOM	2528	N	SER	481	-8.235	25.042	-4.409	0.00	0.00	-0.650	9.00	-17.40
ATOM	2529	HN	SER	481	-9.070	25.498	-4.015	0.00	0.00	0.439	0.00	0.00
ATOM	2530	CA	SER	481	-8.088	23.622	-4.273	0.00	0.00	0.158	9.40	4.00
ATOM	2531	HA	SER	481	-7.129	23.411	-3.801	0.00	0.00	0.053	0.00	0.00
ATOM	2532	C	SER	481	-8.140	23.000	-5.628	0.00	0.00	0.396	9.82	4.00
ATOM	2533	O	SER	481	-7.439	22.028	-5.896	0.00	0.00	-0.396	8.17	-17.40
ATOM	2534	CB	SER	481	-9.207	22.981	-3.429	0.00	0.00	0.007	12.77	4.00
ATOM	2535	HB1	SER	481	-9.148	21.893	-3.471	0.00	0.00	0.053	0.00	0.00
ATOM	2536	HB2	SER	481	-10.188	23.282	-3.796	0.00	0.00	0.053	0.00	0.00
ATOM	2537	OG	SER	481	-9.102	23.378	-2.068	0.00	0.00	-0.537	11.04	-17.40
ATOM	2538	HG	SER	481	-8.805	24.363	-2.019	0.00	0.00	0.424	0.00	0.00
ATOM	2539	N	SER	482	-8.971	23.550	-6.529	0.00	0.00	-0.650	9.00	-17.40
ATOM	2540	HN	SER	482	-9.479	24.415	-6.297	0.00	0.00	0.439	0.00	0.00
ATOM	2541	CA	SER	482	-9.153	22.937	-7.812	0.00	0.00	0.158	9.40	4.00
ATOM	2542	HA	SER	482	-9.577	21.943	-7.668	0.00	0.00	0.053	0.00	0.00
ATOM	2543	C	SER	482	-7.828	22.838	-8.488	0.00	0.00	0.396	9.82	4.00
ATOM	2544	O	SER	482	-7.469	21.793	-9.026	0.00	0.00	-0.396	8.17	-17.40
ATOM	2545	CB	SER	482	-10.065	23.751	-8.744	0.00	0.00	0.007	12.77	4.00
ATOM	2546	HB1	SER	482	-10.998	23.995	-8.236	0.00	0.00	0.053	0.00	0.00
ATOM	2547	HB2	SER	482	-10.293	23.176	-9.641	0.00	0.00	0.053	0.00	0.00
ATOM	2548	OG	SER	482	-9.421	24.959	-9.125	0.00	0.00	-0.537	11.04	-17.40
ATOM	2549	HG	SER	482	-8.440	24.939	-8.812	0.00	0.00	0.424	0.00	0.00
ATOM	2550	N	THR	483	-7.047	23.928	-8.449	0.00	0.00	-0.650	9.00	-17.40
ATOM	2551	HN	THR	483	-7.358	24.770	-7.945	0.00	0.00	0.439	0.00	0.00
ATOM	2552	CA	THR	483	-5.781	23.914	-9.111	0.00	0.00	0.158	9.40	4.00
ATOM	2553	HA	THR	483	-5.971	23.731	-10.169	0.00	0.00	0.053	0.00	0.00
ATOM	2554	C	THR	483	-4.974	22.816	-8.500	0.00	0.00	0.396	9.82	4.00
ATOM	2555	O	THR	483	-4.267	22.085	-9.192	0.00	0.00	-0.396	8.17	-17.40
ATOM	2556	CB	THR	483	-5.031	25.199	-8.925	0.00	0.00	0.060	9.40	4.00
ATOM	2557	HB	THR	483	-4.857	25.354	-7.860	0.00	0.00	0.053	0.00	0.00
ATOM	2558	OG1	THR	483	-5.795	26.283	-9.434	0.00	0.00	-0.537	11.04	-17.40
ATOM	2559	HG1	THR	483	-5.239	27.149	-9.385	0.00	0.00	0.424	0.00	0.00
ATOM	2560	CG2	THR	483	-3.691	25.104	-9.670	0.00	0.00	-0.159	16.15	4.00
ATOM	2561	HG21	THR	483	-3.137	26.034	-9.542	0.00	0.00	0.053	0.00	0.00
ATOM	2562	HG22	THR	483	-3.109	24.276	-9.267	0.00	0.00	0.053	0.00	0.00
ATOM	2563	HG23	THR	483	-3.876	24.935	-10.731	0.00	0.00	0.053	0.00	0.00
ATOM	2564	N	LYS	484	-5.079	22.671	-7.171	0.00	0.00	-0.650	9.00	-17.40
ATOM	2565	HN	LYS	484	-5.719	23.285	-6.647	0.00	0.00	0.439	0.00	0.00
ATOM	2566	CA	LYS	484	-4.323	21.685	-6.464	0.00	0.00	0.158	9.40	4.00
ATOM	2567	HA	LYS	484	-3.265	21.851	-6.667	0.00	0.00	0.053	0.00	0.00
ATOM	2568	C	LYS	484	-4.742	20.335	-6.945	0.00	0.00	0.396	9.82	4.00
ATOM	2569	O	LYS	484	-3.915	19.494	-7.288	0.00	0.00	-0.396	8.17	-17.40
ATOM	2570	CB	LYS	484	-4.621	21.725	-4.957	0.00	0.00	-0.106	12.77	4.00
ATOM	2571	HB1	LYS	484	-3.988	21.052	-4.378	0.00	0.00	0.053	0.00	0.00
ATOM	2572	HB2	LYS	484	-5.646	21.443	-4.716	0.00	0.00	0.053	0.00	0.00
ATOM	2573	CG	LYS	484	-4.420	23.110	-4.343	0.00	0.00	-0.106	12.77	4.00
ATOM	2574	HG1	LYS	484	-4.637	23.149	-3.276	0.00	0.00	0.053	0.00	0.00
ATOM	2575	HG2	LYS	484	-5.050	23.880	-4.789	0.00	0.00	0.053	0.00	0.00

ATOM	2576	CD	LYS	484	-2.992	23.636	-4.478	0.00	0.00	-0.106	12.77	4.00
ATOM	2577	HD1	LYS	484	-2.924	24.722	-4.416	0.00	0.00	0.053	0.00	0.00
ATOM	2578	HD2	LYS	484	-2.522	23.371	-5.425	0.00	0.00	0.053	0.00	0.00
ATOM	2579	CE	LYS	484	-2.048	23.110	-3.397	0.00	0.00	0.099	12.77	4.00
ATOM	2580	HE1	LYS	484	-1.019	23.367	-3.649	0.00	0.00	0.053	0.00	0.00
ATOM	2581	HE2	LYS	484	-2.139	22.026	-3.324	0.00	0.00	0.053	0.00	0.00
ATOM	2582	NZ	LYS	484	-2.395	23.716	-2.092	0.00	0.00	-0.045	13.25	-39.20
ATOM	2583	HZ1	LYS	484	-1.757	23.359	-1.367	0.00	0.00	0.280	0.00	0.00
ATOM	2584	HZ2	LYS	484	-2.305	24.740	-2.154	0.00	0.00	0.280	0.00	0.00
ATOM	2585	HZ3	LYS	484	-3.365	23.471	-1.846	0.00	0.00	0.280	0.00	0.00
ATOM	2586	N	ASN	485	-6.063	20.108	-7.015	0.00	0.00	-0.650	9.00	-17.40
ATOM	2587	HN	ASN	485	-6.720	20.869	-6.790	0.00	0.00	0.439	0.00	0.00
ATOM	2588	CA	ASN	485	-6.573	18.829	-7.396	0.00	0.00	0.158	9.40	4.00
ATOM	2589	HA	ASN	485	-6.178	18.096	-6.693	0.00	0.00	0.053	0.00	0.00
ATOM	2590	C	ASN	485	-6.107	18.556	-8.784	0.00	0.00	0.396	9.82	4.00
ATOM	2591	O	ASN	485	-5.709	17.438	-9.109	0.00	0.00	-0.396	8.17	-17.40
ATOM	2592	CB	ASN	485	-8.112	18.787	-7.379	0.00	0.00	-0.106	12.77	4.00
ATOM	2593	HB1	ASN	485	-8.486	19.345	-8.237	0.00	0.00	0.053	0.00	0.00
ATOM	2594	HB2	ASN	485	-8.463	19.240	-6.452	0.00	0.00	0.053	0.00	0.00
ATOM	2595	CG	ASN	485	-8.561	17.335	-7.459	0.00	0.00	0.396	9.82	4.00
ATOM	2596	OD1	ASN	485	-8.471	16.697	-8.507	0.00	0.00	-0.396	8.17	-17.40
ATOM	2597	ND2	ASN	485	-9.057	16.795	-6.315	0.00	0.00	-0.879	13.25	-17.40
ATOM	2598	HD21	ASN	485	-9.115	17.365	-5.459	0.00	0.00	0.439	0.00	0.00
ATOM	2599	HD22	ASN	485	-9.375	15.816	-6.304	0.00	0.00	0.439	0.00	0.00
ATOM	2600	N	ILE	486	-6.116	19.597	-9.635	0.00	0.00	-0.650	9.00	-17.40
ATOM	2601	HN	ILE	486	-6.399	20.528	-9.296	0.00	0.00	0.439	0.00	0.00
ATOM	2602	CA	ILE	486	-5.738	19.429	-11.005	0.00	0.00	0.158	9.40	4.00
ATOM	2603	HA	ILE	486	-6.405	18.695	-11.457	0.00	0.00	0.053	0.00	0.00
ATOM	2604	C	ILE	486	-4.326	18.951	-11.046	0.00	0.00	0.396	9.82	4.00
ATOM	2605	O	ILE	486	-3.371	19.702	-10.857	0.00	0.00	-0.396	8.17	-17.40
ATOM	2606	CB	ILE	486	-5.804	20.702	-11.792	0.00	0.00	-0.053	9.40	4.00
ATOM	2607	HB	ILE	486	-5.204	21.452	-11.277	0.00	0.00	0.053	0.00	0.00
ATOM	2608	CG1	ILE	486	-7.240	21.251	-11.791	0.00	0.00	-0.106	12.77	4.00
ATOM	2609	HG11	ILE	486	-7.699	21.265	-10.802	0.00	0.00	0.053	0.00	0.00
ATOM	2610	HG12	ILE	486	-7.925	20.677	-12.415	0.00	0.00	0.053	0.00	0.00
ATOM	2611	CG2	ILE	486	-5.243	20.427	-13.196	0.00	0.00	-0.159	16.15	4.00
ATOM	2612	HG21	ILE	486	-5.281	21.341	-13.788	0.00	0.00	0.053	0.00	0.00
ATOM	2613	HG22	ILE	486	-4.210	20.090	-13.115	0.00	0.00	0.053	0.00	0.00
ATOM	2614	HG23	ILE	486	-5.840	19.655	-13.682	0.00	0.00	0.053	0.00	0.00
ATOM	2615	CD1	ILE	486	-7.343	22.687	-12.300	0.00	0.00	-0.159	16.15	4.00
ATOM	2616	HD11	ILE	486	-8.384	23.009	-12.272	0.00	0.00	0.053	0.00	0.00
ATOM	2617	HD12	ILE	486	-6.743	23.341	-11.667	0.00	0.00	0.053	0.00	0.00
ATOM	2618	HD13	ILE	486	-6.975	22.737	-13.325	0.00	0.00	0.053	0.00	0.00
ATOM	2619	N	PRO	487	-4.207	17.684	-11.301	0.00	0.00	-0.422	9.00	-17.40
ATOM	2620	CA	PRO	487	-2.931	17.040	-11.373	0.00	0.00	0.158	9.40	4.00
ATOM	2621	HA	PRO	487	-2.466	17.109	-10.389	0.00	0.00	0.053	0.00	0.00
ATOM	2622	CD	PRO	487	-5.205	16.985	-12.087	0.00	0.00	0.105	12.77	4.00
ATOM	2623	HD1	PRO	487	-5.569	17.718	-12.807	0.00	0.00	0.053	0.00	0.00
ATOM	2624	HD2	PRO	487	-5.964	16.669	-11.372	0.00	0.00	0.053	0.00	0.00
ATOM	2625	C	PRO	487	-2.123	17.747	-12.394	0.00	0.00	0.396	9.82	4.00
ATOM	2626	O	PRO	487	-0.898	17.746	-12.276	0.00	0.00	-0.396	8.17	-17.40
ATOM	2627	CB	PRO	487	-3.214	15.623	-11.853	0.00	0.00	-0.106	12.77	4.00
ATOM	2628	HB1	PRO	487	-3.406	14.954	-11.015	0.00	0.00	0.053	0.00	0.00
ATOM	2629	HB2	PRO	487	-2.369	15.220	-12.412	0.00	0.00	0.053	0.00	0.00
ATOM	2630	CG	PRO	487	-4.457	15.810	-12.740	0.00	0.00	-0.106	12.77	4.00
ATOM	2631	HG1	PRO	487	-5.065	14.905	-12.753	0.00	0.00	0.053	0.00	0.00
ATOM	2632	HG2	PRO	487	-4.171	16.038	-13.767	0.00	0.00	0.053	0.00	0.00
ATOM	2633	N	SER	488	-2.776	18.321	-13.418	0.00	0.00	-0.650	9.00	-17.40
ATOM	2634	HN	SER	488	-3.803	18.279	-13.479	0.00	0.00	0.439	0.00	0.00
ATOM	2635	CA	SER	488	-2.012	18.989	-14.418	0.00	0.00	0.158	9.40	4.00
ATOM	2636	HA	SER	488	-1.360	18.220	-14.833	0.00	0.00	0.053	0.00	0.00
ATOM	2637	C	SER	488	-1.285	20.055	-13.693	0.00	0.00	0.396	9.82	4.00
ATOM	2638	O	SER	488	-0.065	20.165	-13.814	0.00	0.00	-0.396	8.17	-17.40
ATOM	2639	CB	SER	488	-2.876	19.662	-15.496	0.00	0.00	0.007	12.77	4.00
ATOM	2640	HB1	SER	488	-3.532	20.405	-15.042	0.00	0.00	0.053	0.00	0.00
ATOM	2641	HB2	SER	488	-3.488	18.918	-16.006	0.00	0.00	0.053	0.00	0.00
ATOM	2642	OG	SER	488	-2.050	20.307	-16.453	0.00	0.00	-0.537	11.04	-17.40
ATOM	2643	HG	SER	488	-1.409	20.954	-15.973	0.00	0.00	0.424	0.00	0.00
ATOM	2644	N	TYR	489	-2.025	20.795	-12.837	0.00	0.00	-0.650	9.00	-17.40
ATOM	2645	HN	TYR	489	-3.028	20.587	-12.731	0.00	0.00	0.439	0.00	0.00
ATOM	2646	CA	TYR	489	-1.448	21.860	-12.074	0.00	0.00	0.158	9.40	4.00
ATOM	2647	HA	TYR	489	-2.291	22.377	-11.615	0.00	0.00	0.053	0.00	0.00
ATOM	2648	C	TYR	489	-0.710	22.699	-13.060	0.00	0.00	0.396	9.82	4.00
ATOM	2649	O	TYR	489	-1.052	22.716	-14.244	0.00	0.00	-0.396	8.17	-17.40
ATOM	2650	CB	TYR	489	-0.420	21.293	-11.086	0.00	0.00	-0.106	12.77	4.00
ATOM	2651	HB1	TYR	489	0.549	21.199	-11.575	0.00	0.00	0.053	0.00	0.00

ATOM	2652	HB2	TYR	489	-0.743	20.311	-10.741	0.00	0.00	0.053	0.00	0.00
ATOM	2653	CG	TYR	489	-0.291	22.199	-9.922	0.00	0.00	0.000	7.26	0.60
ATOM	2654	CD1	TYR	489	-1.257	22.125	-8.949	0.00	0.00	-0.127	10.80	0.60
ATOM	2655	HD1	TYR	489	-2.082	21.422	-9.062	0.00	0.00	0.127	0.00	0.00
ATOM	2656	CD2	TYR	489	0.757	23.078	-9.774	0.00	0.00	-0.127	10.80	0.60
ATOM	2657	HD2	TYR	489	1.533	23.137	-10.537	0.00	0.00	0.127	0.00	0.00
ATOM	2658	CE1	TYR	489	-1.196	22.924	-7.838	0.00	0.00	-0.127	10.80	0.60
ATOM	2659	HE1	TYR	489	-1.970	22.859	-7.073	0.00	0.00	0.127	0.00	0.00
ATOM	2660	CE2	TYR	489	0.822	23.883	-8.660	0.00	0.00	-0.127	10.80	0.60
ATOM	2661	HE2	TYR	489	1.649	24.583	-8.542	0.00	0.00	0.127	0.00	0.00
ATOM	2662	CZ	TYR	489	-0.156	23.806	-7.694	0.00	0.00	0.027	7.26	0.60
ATOM	2663	OH	TYR	489	-0.097	24.626	-6.548	0.00	0.00	-0.451	10.94	-17.40
ATOM	2664	HH	TYR	489	0.482	25.454	-6.747	0.00	0.00	0.424	0.00	0.00
ATOM	2665	N	VAL	490	0.268	23.499	-12.604	0.00	0.00	-0.650	9.00	-17.40
ATOM	2666	HN	VAL	490	0.442	23.668	-11.603	0.00	0.00	0.439	0.00	0.00
ATOM	2667	CA	VAL	490	1.041	24.090	-13.645	0.00	0.00	0.158	9.40	4.00
ATOM	2668	HA	VAL	490	0.411	24.640	-14.344	0.00	0.00	0.053	0.00	0.00
ATOM	2669	C	VAL	490	1.680	22.891	-14.277	0.00	0.00	0.396	9.82	4.00
ATOM	2670	O	VAL	490	2.373	22.113	-13.624	0.00	0.00	-0.396	8.17	-17.40
ATOM	2671	CB	VAL	490	2.057	25.081	-13.165	0.00	0.00	-0.053	9.40	4.00
ATOM	2672	HB	VAL	490	2.698	24.600	-12.426	0.00	0.00	0.053	0.00	0.00
ATOM	2673	CG1	VAL	490	2.898	25.553	-14.364	0.00	0.00	-0.159	16.15	4.00
ATOM	2674	HG11	VAL	490	3.641	26.275	-14.025	0.00	0.00	0.053	0.00	0.00
ATOM	2675	HG12	VAL	490	3.402	24.698	-14.814	0.00	0.00	0.053	0.00	0.00
ATOM	2676	HG13	VAL	490	2.248	26.021	-15.103	0.00	0.00	0.053	0.00	0.00
ATOM	2677	CG2	VAL	490	1.289	26.226	-12.478	0.00	0.00	-0.159	16.15	4.00
ATOM	2678	HG21	VAL	490	1.996	26.971	-12.113	0.00	0.00	0.053	0.00	0.00
ATOM	2679	HG22	VAL	490	0.610	26.690	-13.194	0.00	0.00	0.053	0.00	0.00
ATOM	2680	HG23	VAL	490	0.716	25.829	-11.640	0.00	0.00	0.053	0.00	0.00
ATOM	2681	N	LYS	491	1.408	22.708	-15.580	0.00	0.00	-0.650	9.00	-17.40
ATOM	2682	HN	LYS	491	0.944	23.478	-16.083	0.00	0.00	0.439	0.00	0.00
ATOM	2683	CA	LYS	491	1.715	21.520	-16.324	0.00	0.00	0.158	9.40	4.00
ATOM	2684	HA	LYS	491	1.081	20.712	-15.959	0.00	0.00	0.053	0.00	0.00
ATOM	2685	C	LYS	491	3.139	21.075	-16.200	0.00	0.00	0.396	9.82	4.00
ATOM	2686	O	LYS	491	3.988	21.759	-15.631	0.00	0.00	-0.396	8.17	-17.40
ATOM	2687	CB	LYS	491	1.342	21.656	-17.807	0.00	0.00	-0.106	12.77	4.00
ATOM	2688	HB1	LYS	491	1.766	20.859	-18.418	0.00	0.00	0.053	0.00	0.00
ATOM	2689	HB2	LYS	491	1.692	22.593	-18.241	0.00	0.00	0.053	0.00	0.00
ATOM	2690	CG	LYS	491	-0.170	21.615	-18.036	0.00	0.00	-0.106	12.77	4.00
ATOM	2691	HG1	LYS	491	-0.561	20.718	-17.555	0.00	0.00	0.053	0.00	0.00
ATOM	2692	HG2	LYS	491	-0.349	21.588	-19.111	0.00	0.00	0.053	0.00	0.00
ATOM	2693	CD	LYS	491	-0.945	22.805	-17.476	0.00	0.00	-0.106	12.77	4.00
ATOM	2694	HD1	LYS	491	-0.593	23.754	-17.880	0.00	0.00	0.053	0.00	0.00
ATOM	2695	HD2	LYS	491	-0.861	22.879	-16.392	0.00	0.00	0.053	0.00	0.00
ATOM	2696	CE	LYS	491	-2.440	22.724	-17.793	0.00	0.00	0.099	12.77	4.00
ATOM	2697	HE1	LYS	491	-2.946	23.618	-17.428	0.00	0.00	0.053	0.00	0.00
ATOM	2698	HE2	LYS	491	-2.875	21.848	-17.311	0.00	0.00	0.053	0.00	0.00
ATOM	2699	NZ	LYS	491	-2.640	22.619	-19.256	0.00	0.00	-0.045	13.25	-39.20
ATOM	2700	HZ1	LYS	491	-3.648	22.565	-19.462	0.00	0.00	0.280	0.00	0.00
ATOM	2701	HZ2	LYS	491	-2.239	23.448	-19.718	0.00	0.00	0.280	0.00	0.00
ATOM	2702	HZ3	LYS	491	-2.172	21.771	-19.607	0.00	0.00	0.280	0.00	0.00
ATOM	2703	N	ASN	492	3.399	19.865	-16.755	0.00	0.00	-0.650	9.00	-17.40
ATOM	2704	HN	ASN	492	2.617	19.385	-17.223	0.00	0.00	0.439	0.00	0.00
ATOM	2705	CA	ASN	492	4.671	19.192	-16.748	0.00	0.00	0.158	9.40	4.00
ATOM	2706	HA	ASN	492	5.361	19.867	-16.242	0.00	0.00	0.053	0.00	0.00
ATOM	2707	C	ASN	492	5.026	18.969	-18.196	0.00	0.00	0.396	9.82	4.00
ATOM	2708	O	ASN	492	4.132	18.867	-19.033	0.00	0.00	-0.396	8.17	-17.40
ATOM	2709	CB	ASN	492	4.535	17.774	-16.204	0.00	0.00	-0.106	12.77	4.00
ATOM	2710	HB1	ASN	492	5.500	17.524	-15.764	0.00	0.00	0.053	0.00	0.00
ATOM	2711	HB2	ASN	492	4.289	17.143	-17.058	0.00	0.00	0.053	0.00	0.00
ATOM	2712	CG	ASN	492	3.422	17.821	-15.177	0.00	0.00	0.396	9.82	4.00
ATOM	2713	OD1	ASN	492	3.509	18.436	-14.120	0.00	0.00	-0.396	8.17	-17.40
ATOM	2714	ND2	ASN	492	2.296	17.149	-15.534	0.00	0.00	-0.879	13.25	-17.40
ATOM	2715	HD21	ASN	492	2.260	16.643	-16.431	0.00	0.00	0.439	0.00	0.00
ATOM	2716	HD22	ASN	492	1.478	17.145	-14.908	0.00	0.00	0.439	0.00	0.00
ATOM	2717	N	HIS	493	6.333	18.905	-18.550	0.00	0.00	-0.650	9.00	-17.40
ATOM	2718	HN	HIS	493	7.074	19.059	-17.851	0.00	0.00	0.439	0.00	0.00
ATOM	2719	CA	HIS	493	6.666	18.617	-19.922	0.00	0.00	0.158	9.40	4.00
ATOM	2720	HA	HIS	493	6.337	17.600	-20.137	0.00	0.00	0.053	0.00	0.00
ATOM	2721	C	HIS	493	8.157	18.747	-20.068	0.00	0.00	0.396	9.82	4.00
ATOM	2722	O	HIS	493	8.846	19.118	-19.120	0.00	0.00	-0.396	8.17	-17.40
ATOM	2723	CB	HIS	493	5.983	19.562	-20.948	0.00	0.00	-0.106	12.77	4.00
ATOM	2724	HB1	HIS	493	5.214	20.127	-20.422	0.00	0.00	0.053	0.00	0.00
ATOM	2725	HB2	HIS	493	5.546	18.944	-21.732	0.00	0.00	0.053	0.00	0.00
ATOM	2726	CG	HIS	493	6.882	20.563	-21.624	0.00	0.00	0.241	7.26	0.60
ATOM	2727	ND1	HIS	493	7.414	20.337	-22.876	0.00	0.00	-0.481	9.25	-17.40

ATOM	2728	CD2	HIS	493	7.369	21.771	-21.230	0.00	0.00	-0.177	10.80	0.60
ATOM	2729	HD2	HIS	493	7.143	22.250	-20.278	0.00	0.00	0.127	0.00	0.00
ATOM	2730	CE1	HIS	493	8.187	21.410	-23.175	0.00	0.00	0.064	10.80	0.60
ATOM	2731	HE1	HIS	493	8.740	21.520	-24.108	0.00	0.00	0.127	0.00	0.00
ATOM	2732	NE2	HIS	493	8.192	22.307	-22.206	0.00	0.00	-0.292	9.25	-17.40
ATOM	2733	HE2	HIS	493	8.696	23.205	-22.182	0.00	0.00	0.393	0.00	0.00
ATOM	2734	N	GLY	494	8.696	18.406	-21.262	0.00	0.00	-0.650	9.00	-17.40
ATOM	2735	HN	GLY	494	8.079	18.030	-21.996	0.00	0.00	0.439	0.00	0.00
ATOM	2736	CA	GLY	494	10.095	18.549	-21.543	0.00	0.00	0.105	9.40	4.00
ATOM	2737	HA1	GLY	494	10.539	17.563	-21.407	0.00	0.00	0.053	0.00	0.00
ATOM	2738	HA2	GLY	494	10.479	19.279	-20.830	0.00	0.00	0.053	0.00	0.00
ATOM	2739	C	GLY	494	10.195	19.028	-22.958	0.00	0.00	0.396	9.82	4.00
ATOM	2740	O	GLY	494	9.335	18.724	-23.783	0.00	0.00	-0.396	8.17	-17.40
ATOM	2741	N	ILE	495	11.248	19.808	-23.277	0.00	0.00	-0.650	9.00	-17.40
ATOM	2742	HN	ILE	495	11.943	20.049	-22.557	0.00	0.00	0.439	0.00	0.00
ATOM	2743	CA	ILE	495	11.405	20.304	-24.616	0.00	0.00	0.158	9.40	4.00
ATOM	2744	HA	ILE	495	10.661	19.814	-25.245	0.00	0.00	0.053	0.00	0.00
ATOM	2745	C	ILE	495	12.792	19.973	-25.070	0.00	0.00	0.396	9.82	4.00
ATOM	2746	O	ILE	495	13.749	20.122	-24.315	0.00	0.00	-0.396	8.17	-17.40
ATOM	2747	CB	ILE	495	11.221	21.802	-24.691	0.00	0.00	-0.053	9.40	4.00
ATOM	2748	HB	ILE	495	10.253	22.046	-24.253	0.00	0.00	0.053	0.00	0.00
ATOM	2749	CG1	ILE	495	11.078	22.314	-26.137	0.00	0.00	-0.106	12.77	4.00
ATOM	2750	HG11	ILE	495	10.818	23.372	-26.101	0.00	0.00	0.053	0.00	0.00
ATOM	2751	HG12	ILE	495	10.290	21.741	-26.626	0.00	0.00	0.053	0.00	0.00
ATOM	2752	CG2	ILE	495	12.363	22.463	-23.899	0.00	0.00	-0.159	16.15	4.00
ATOM	2753	HG21	ILE	495	12.253	23.547	-23.938	0.00	0.00	0.053	0.00	0.00
ATOM	2754	HG22	ILE	495	12.326	22.131	-22.861	0.00	0.00	0.053	0.00	0.00
ATOM	2755	HG23	ILE	495	13.320	22.180	-24.336	0.00	0.00	0.053	0.00	0.00
ATOM	2756	CD1	ILE	495	12.342	22.177	-26.980	0.00	0.00	-0.159	16.15	4.00
ATOM	2757	HD11	ILE	495	12.154	22.561	-27.983	0.00	0.00	0.053	0.00	0.00
ATOM	2758	HD12	ILE	495	13.150	22.746	-26.519	0.00	0.00	0.053	0.00	0.00
ATOM	2759	HD13	ILE	495	12.627	21.127	-27.041	0.00	0.00	0.053	0.00	0.00
ATOM	2760	N	LEU	496	12.950	19.498	-26.321	0.00	0.00	-0.650	9.00	-17.40
ATOM	2761	HN	LEU	496	12.139	19.349	-26.938	0.00	0.00	0.439	0.00	0.00
ATOM	2762	CA	LEU	496	14.281	19.206	-26.767	0.00	0.00	0.158	9.40	4.00
ATOM	2763	HA	LEU	496	14.811	18.743	-25.934	0.00	0.00	0.053	0.00	0.00
ATOM	2764	C	LEU	496	14.914	20.499	-27.165	0.00	0.00	0.396	9.82	4.00
ATOM	2765	O	LEU	496	14.878	20.879	-28.334	0.00	0.00	-0.396	8.17	-17.40
ATOM	2766	CB	LEU	496	14.356	18.299	-28.011	0.00	0.00	-0.106	12.77	4.00
ATOM	2767	HB1	LEU	496	15.385	18.307	-28.371	0.00	0.00	0.053	0.00	0.00
ATOM	2768	HB2	LEU	496	13.677	18.702	-28.762	0.00	0.00	0.053	0.00	0.00
ATOM	2769	CG	LEU	496	13.963	16.824	-27.787	0.00	0.00	-0.053	9.40	4.00
ATOM	2770	HG	LEU	496	13.911	16.280	-28.730	0.00	0.00	0.053	0.00	0.00
ATOM	2771	CD1	LEU	496	14.984	16.104	-26.892	0.00	0.00	-0.159	16.15	4.00
ATOM	2772	HD11	LEU	496	14.679	15.067	-26.753	0.00	0.00	0.053	0.00	0.00
ATOM	2773	HD12	LEU	496	15.966	16.133	-27.364	0.00	0.00	0.053	0.00	0.00
ATOM	2774	HD13	LEU	496	15.032	16.601	-25.923	0.00	0.00	0.053	0.00	0.00
ATOM	2775	CD2	LEU	496	12.517	16.687	-27.287	0.00	0.00	-0.159	16.15	4.00
ATOM	2776	HD21	LEU	496	12.280	15.633	-27.142	0.00	0.00	0.053	0.00	0.00
ATOM	2777	HD22	LEU	496	12.407	17.217	-26.341	0.00	0.00	0.053	0.00	0.00
ATOM	2778	HD23	LEU	496	11.836	17.114	-28.023	0.00	0.00	0.053	0.00	0.00
ATOM	2779	N	SER	497	15.507	21.230	-26.199	0.00	0.00	-0.650	9.00	-17.40
ATOM	2780	HN	SER	497	15.494	20.925	-25.215	0.00	0.00	0.439	0.00	0.00
ATOM	2781	CA	SER	497	16.155	22.446	-26.592	0.00	0.00	0.158	9.40	4.00
ATOM	2782	HA	SER	497	16.934	22.208	-27.316	0.00	0.00	0.053	0.00	0.00
ATOM	2783	C	SER	497	16.753	23.083	-25.380	0.00	0.00	0.396	9.82	4.00
ATOM	2784	O	SER	497	16.077	23.275	-24.370	0.00	0.00	-0.396	8.17	-17.40
ATOM	2785	CB	SER	497	15.200	23.475	-27.219	0.00	0.00	0.007	12.77	4.00
ATOM	2786	HB1	SER	497	14.422	23.743	-26.504	0.00	0.00	0.053	0.00	0.00
ATOM	2787	HB2	SER	497	14.734	23.054	-28.110	0.00	0.00	0.053	0.00	0.00
ATOM	2788	OG	SER	497	15.919	24.644	-27.581	0.00	0.00	-0.537	11.04	-17.40
ATOM	2789	HG	SER	497	16.893	24.563	-27.255	0.00	0.00	0.424	0.00	0.00
ATOM	2790	N	GLY	498	18.050	23.438	-25.472	0.00	0.00	-0.650	9.00	-17.40
ATOM	2791	HN	GLY	498	18.567	23.250	-26.343	0.00	0.00	0.439	0.00	0.00
ATOM	2792	CA	GLY	498	18.719	24.073	-24.376	0.00	0.00	0.105	9.40	4.00
ATOM	2793	HA1	GLY	498	18.252	25.047	-24.232	0.00	0.00	0.053	0.00	0.00
ATOM	2794	HA2	GLY	498	19.770	24.169	-24.649	0.00	0.00	0.053	0.00	0.00
ATOM	2795	C	GLY	498	18.542	23.200	-23.183	0.00	0.00	0.396	9.82	4.00
ATOM	2796	O	GLY	498	18.502	21.976	-23.292	0.00	0.00	-0.396	8.17	-17.40
ATOM	2797	N	ARG	499	18.435	23.825	-21.996	0.00	0.00	-0.650	9.00	-17.40
ATOM	2798	HN	ARG	499	18.505	24.851	-21.939	0.00	0.00	0.439	0.00	0.00
ATOM	2799	CA	ARG	499	18.224	23.049	-20.817	0.00	0.00	0.158	9.40	4.00
ATOM	2800	HA	ARG	499	18.703	22.086	-20.995	0.00	0.00	0.053	0.00	0.00
ATOM	2801	C	ARG	499	16.750	22.929	-20.655	0.00	0.00	0.396	9.82	4.00
ATOM	2802	O	ARG	499	15.986	23.629	-21.317	0.00	0.00	-0.396	8.17	-17.40
ATOM	2803	CB	ARG	499	18.860	23.660	-19.565	0.00	0.00	-0.106	12.77	4.00

ATOM	2804	HB1	ARG	499	18.546	23.123	-18.670	0.00	0.00	0.053	0.00	0.00
ATOM	2805	HB2	ARG	499	18.569	24.704	-19.453	0.00	0.00	0.053	0.00	0.00
ATOM	2806	CG	ARG	499	20.386	23.598	-19.646	0.00	0.00	-0.106	12.77	4.00
ATOM	2807	HG1	ARG	499	20.702	24.106	-20.557	0.00	0.00	0.053	0.00	0.00
ATOM	2808	HG2	ARG	499	20.686	22.550	-19.668	0.00	0.00	0.053	0.00	0.00
ATOM	2809	CD	ARG	499	21.098	24.261	-18.472	0.00	0.00	0.374	12.77	4.00
ATOM	2810	HD1	ARG	499	20.882	25.328	-18.532	0.00	0.00	0.053	0.00	0.00
ATOM	2811	HD2	ARG	499	22.162	24.054	-18.589	0.00	0.00	0.053	0.00	0.00
ATOM	2812	NE	ARG	499	20.547	23.652	-17.233	0.00	0.00	-0.819	9.00	-24.67
ATOM	2813	HE	ARG	499	19.595	23.259	-17.229	0.00	0.00	0.407	0.00	0.00
ATOM	2814	CZ	ARG	499	21.307	23.616	-16.102	0.00	0.00	0.796	6.95	4.00
ATOM	2815	NH1	ARG	499	22.583	24.100	-16.120	0.00	0.00	-0.746	9.00	-24.67
ATOM	2816	HH11	ARG	499	23.156	24.072	-15.265	0.00	0.00	0.407	0.00	0.00
ATOM	2817	HH12	ARG	499	22.973	24.493	-16.989	0.00	0.00	0.407	0.00	0.00
ATOM	2818	NH2	ARG	499	20.790	23.087	-14.954	0.00	0.00	-0.746	9.00	-24.67
ATOM	2819	HH21	ARG	499	21.361	23.058	-14.097	0.00	0.00	0.407	0.00	0.00
ATOM	2820	HH22	ARG	499	19.829	22.717	-14.945	0.00	0.00	0.407	0.00	0.00
ATOM	2821	N	ASP	500	16.301	22.034	-19.761	0.00	0.00	-0.650	9.00	-17.40
ATOM	2822	HN	ASP	500	16.942	21.556	-19.112	0.00	0.00	0.439	0.00	0.00
ATOM	2823	CA	ASP	500	14.898	21.774	-19.749	0.00	0.00	0.158	9.40	4.00
ATOM	2824	HA	ASP	500	14.399	22.203	-20.618	0.00	0.00	0.053	0.00	0.00
ATOM	2825	C	ASP	500	14.243	22.342	-18.548	0.00	0.00	0.396	9.82	4.00
ATOM	2826	O	ASP	500	14.844	22.532	-17.496	0.00	0.00	-0.396	8.17	-17.40
ATOM	2827	CB	ASP	500	14.566	20.276	-19.673	0.00	0.00	-0.336	12.77	4.00
ATOM	2828	HB1	ASP	500	13.486	20.176	-19.564	0.00	0.00	0.053	0.00	0.00
ATOM	2829	HB2	ASP	500	15.085	19.860	-18.809	0.00	0.00	0.053	0.00	0.00
ATOM	2830	CG	ASP	500	15.043	19.627	-20.954	0.00	0.00	0.297	9.82	4.00
ATOM	2831	OD1	ASP	500	14.814	20.241	-22.027	0.00	0.00	-0.534	8.17	-18.95
ATOM	2832	OD2	ASP	500	15.634	18.516	-20.887	0.00	0.00	-0.534	8.17	-18.95
ATOM	2833	N	LEU	501	12.960	22.672	-18.730	0.00	0.00	-0.650	9.00	-17.40
ATOM	2834	HN	LEU	501	12.592	22.750	-19.689	0.00	0.00	0.439	0.00	0.00
ATOM	2835	CA	LEU	501	12.092	22.917	-17.633	0.00	0.00	0.158	9.40	4.00
ATOM	2836	HA	LEU	501	12.630	23.072	-16.698	0.00	0.00	0.053	0.00	0.00
ATOM	2837	C	LEU	501	11.346	21.626	-17.708	0.00	0.00	0.396	9.82	4.00
ATOM	2838	O	LEU	501	10.991	21.207	-18.808	0.00	0.00	-0.396	8.17	-17.40
ATOM	2839	CB	LEU	501	11.121	24.092	-17.876	0.00	0.00	-0.106	12.77	4.00
ATOM	2840	HB1	LEU	501	10.396	24.231	-17.074	0.00	0.00	0.053	0.00	0.00
ATOM	2841	HB2	LEU	501	10.525	23.984	-18.782	0.00	0.00	0.053	0.00	0.00
ATOM	2842	CG	LEU	501	11.830	25.460	-18.021	0.00	0.00	-0.053	9.40	4.00
ATOM	2843	HG	LEU	501	12.447	25.683	-17.151	0.00	0.00	0.053	0.00	0.00
ATOM	2844	CD1	LEU	501	12.746	25.490	-19.256	0.00	0.00	-0.159	16.15	4.00
ATOM	2845	HD11	LEU	501	13.228	26.465	-19.328	0.00	0.00	0.053	0.00	0.00
ATOM	2846	HD12	LEU	501	13.507	24.715	-19.164	0.00	0.00	0.053	0.00	0.00
ATOM	2847	HD13	LEU	501	12.153	25.312	-20.153	0.00	0.00	0.053	0.00	0.00
ATOM	2848	CD2	LEU	501	10.830	26.630	-18.004	0.00	0.00	-0.159	16.15	4.00
ATOM	2849	HD21	LEU	501	11.370	27.571	-18.108	0.00	0.00	0.053	0.00	0.00
ATOM	2850	HD22	LEU	501	10.128	26.521	-18.831	0.00	0.00	0.053	0.00	0.00
ATOM	2851	HD23	LEU	501	10.283	26.628	-17.061	0.00	0.00	0.053	0.00	0.00
ATOM	2852	N	GLN	502	11.078	20.914	-16.599	0.00	0.00	-0.650	9.00	-17.40
ATOM	2853	HN	GLN	502	11.257	21.252	-15.643	0.00	0.00	0.439	0.00	0.00
ATOM	2854	CA	GLN	502	10.512	19.626	-16.901	0.00	0.00	0.158	9.40	4.00
ATOM	2855	HA	GLN	502	10.071	19.567	-17.896	0.00	0.00	0.053	0.00	0.00
ATOM	2856	C	GLN	502	9.417	19.220	-15.964	0.00	0.00	0.396	9.82	4.00
ATOM	2857	O	GLN	502	8.727	20.060	-15.400	0.00	0.00	-0.396	8.17	-17.40
ATOM	2858	CB	GLN	502	11.573	18.516	-17.007	0.00	0.00	-0.106	12.77	4.00
ATOM	2859	HB1	GLN	502	12.268	18.791	-17.801	0.00	0.00	0.053	0.00	0.00
ATOM	2860	HB2	GLN	502	11.060	17.583	-17.242	0.00	0.00	0.053	0.00	0.00
ATOM	2861	CG	GLN	502	12.403	18.268	-15.749	0.00	0.00	-0.106	12.77	4.00
ATOM	2862	HG1	GLN	502	11.705	17.897	-14.998	0.00	0.00	0.053	0.00	0.00
ATOM	2863	HG2	GLN	502	12.837	19.232	-15.482	0.00	0.00	0.053	0.00	0.00
ATOM	2864	CD	GLN	502	13.453	17.236	-16.138	0.00	0.00	0.396	9.82	4.00
ATOM	2865	OE1	GLN	502	13.602	16.914	-17.316	0.00	0.00	-0.396	8.17	-17.40
ATOM	2866	NE2	GLN	502	14.198	16.703	-15.133	0.00	0.00	-0.879	13.25	-17.40
ATOM	2867	HE21	GLN	502	14.039	17.002	-14.160	0.00	0.00	0.439	0.00	0.00
ATOM	2868	HE22	GLN	502	14.921	16.000	-15.345	0.00	0.00	0.439	0.00	0.00
ATOM	2869	N	PHE	503	9.219	17.895	-15.798	0.00	0.00	-0.650	9.00	-17.40
ATOM	2870	HN	PHE	503	9.899	17.244	-16.216	0.00	0.00	0.439	0.00	0.00
ATOM	2871	CA	PHE	503	8.108	17.344	-15.068	0.00	0.00	0.158	9.40	4.00
ATOM	2872	HA	PHE	503	7.223	17.392	-15.703	0.00	0.00	0.053	0.00	0.00
ATOM	2873	C	PHE	503	7.794	18.060	-13.800	0.00	0.00	0.396	9.82	4.00
ATOM	2874	O	PHE	503	8.639	18.232	-12.923	0.00	0.00	-0.396	8.17	-17.40
ATOM	2875	CB	PHE	503	8.176	15.820	-14.913	0.00	0.00	-0.106	12.77	4.00
ATOM	2876	HB1	PHE	503	7.549	15.446	-14.103	0.00	0.00	0.053	0.00	0.00
ATOM	2877	HB2	PHE	503	9.182	15.459	-14.700	0.00	0.00	0.053	0.00	0.00
ATOM	2878	CG	PHE	503	7.683	15.515	-16.268	0.00	0.00	0.000	7.26	0.60
ATOM	2879	CD1	PHE	503	6.327	15.447	-16.464	0.00	0.00	-0.127	10.80	0.60

ATOM	2880	HD1	PHE	503	5.649	15.586	-15.622	0.00	0.00	0.127	0.00	0.00
ATOM	2881	CD2	PHE	503	8.553	15.371	-17.320	0.00	0.00	-0.127	10.80	0.60
ATOM	2882	HD2	PHE	503	9.628	15.449	-17.160	0.00	0.00	0.127	0.00	0.00
ATOM	2883	CE1	PHE	503	5.822	15.206	-17.710	0.00	0.00	-0.127	10.80	0.60
ATOM	2884	HE1	PHE	503	4.747	15.138	-17.874	0.00	0.00	0.127	0.00	0.00
ATOM	2885	CE2	PHE	503	8.057	15.128	-18.572	0.00	0.00	-0.127	10.80	0.60
ATOM	2886	HE2	PHE	503	8.731	14.997	-19.418	0.00	0.00	0.127	0.00	0.00
ATOM	2887	CZ	PHE	503	6.701	15.052	-18.745	0.00	0.00	-0.127	10.80	0.60
ATOM	2888	HZ	PHE	503	6.308	14.862	-19.744	0.00	0.00	0.127	0.00	0.00
ATOM	2889	N	LEU	504	6.523	18.529	-13.733	0.00	0.00	-0.650	9.00	-17.40
ATOM	2890	HN	LEU	504	5.882	18.298	-14.505	0.00	0.00	0.439	0.00	0.00
ATOM	2891	CA	LEU	504	6.018	19.325	-12.655	0.00	0.00	0.158	9.40	4.00
ATOM	2892	HA	LEU	504	6.901	19.729	-12.159	0.00	0.00	0.053	0.00	0.00
ATOM	2893	C	LEU	504	5.240	18.380	-11.800	0.00	0.00	0.396	9.82	4.00
ATOM	2894	O	LEU	504	4.881	17.289	-12.234	0.00	0.00	-0.396	8.17	-17.40
ATOM	2895	CB	LEU	504	5.083	20.450	-13.180	0.00	0.00	-0.106	12.77	4.00
ATOM	2896	HB1	LEU	504	4.104	19.995	-13.333	0.00	0.00	0.053	0.00	0.00
ATOM	2897	HB2	LEU	504	5.520	20.809	-14.112	0.00	0.00	0.053	0.00	0.00
ATOM	2898	CG	LEU	504	4.813	21.724	-12.339	0.00	0.00	-0.053	9.40	4.00
ATOM	2899	HG	LEU	504	4.061	22.323	-12.854	0.00	0.00	0.053	0.00	0.00
ATOM	2900	CD1	LEU	504	4.297	21.439	-10.927	0.00	0.00	-0.159	16.15	4.00
ATOM	2901	HD11	LEU	504	4.133	22.380	-10.403	0.00	0.00	0.053	0.00	0.00
ATOM	2902	HD12	LEU	504	3.358	20.888	-10.987	0.00	0.00	0.053	0.00	0.00
ATOM	2903	HD13	LEU	504	5.032	20.845	-10.384	0.00	0.00	0.053	0.00	0.00
ATOM	2904	CD2	LEU	504	5.981	22.719	-12.404	0.00	0.00	-0.159	16.15	4.00
ATOM	2905	HD21	LEU	504	5.746	23.595	-11.800	0.00	0.00	0.053	0.00	0.00
ATOM	2906	HD22	LEU	504	6.884	22.245	-12.020	0.00	0.00	0.053	0.00	0.00
ATOM	2907	HD23	LEU	504	6.142	23.024	-13.438	0.00	0.00	0.053	0.00	0.00
ATOM	2908	N	LEU	505	5.060	18.764	-10.527	0.00	0.00	-0.650	9.00	-17.40
ATOM	2909	HN	LEU	505	5.520	19.643	-10.249	0.00	0.00	0.439	0.00	0.00
ATOM	2910	CA	LEU	505	4.307	18.100	-9.511	0.00	0.00	0.158	9.40	4.00
ATOM	2911	HA	LEU	505	3.437	18.722	-9.298	0.00	0.00	0.053	0.00	0.00
ATOM	2912	C	LEU	505	5.195	17.969	-8.323	0.00	0.00	0.396	9.82	4.00
ATOM	2913	O	LEU	505	6.232	18.626	-8.248	0.00	0.00	-0.396	8.17	-17.40
ATOM	2914	CB	LEU	505	3.578	16.788	-9.872	0.00	0.00	-0.106	12.77	4.00
ATOM	2915	HB1	LEU	505	3.403	16.162	-8.997	0.00	0.00	0.053	0.00	0.00
ATOM	2916	HB2	LEU	505	4.146	16.185	-10.580	0.00	0.00	0.053	0.00	0.00
ATOM	2917	CG	LEU	505	2.192	17.049	-10.519	0.00	0.00	-0.053	9.40	4.00
ATOM	2918	HG	LEU	505	1.589	16.144	-10.447	0.00	0.00	0.053	0.00	0.00
ATOM	2919	CD1	LEU	505	1.500	18.196	-9.776	0.00	0.00	-0.159	16.15	4.00
ATOM	2920	HD11	LEU	505	0.525	18.385	-10.225	0.00	0.00	0.053	0.00	0.00
ATOM	2921	HD12	LEU	505	1.370	17.925	-8.728	0.00	0.00	0.053	0.00	0.00
ATOM	2922	HD13	LEU	505	2.112	19.096	-9.845	0.00	0.00	0.053	0.00	0.00
ATOM	2923	CD2	LEU	505	2.173	17.224	-12.045	0.00	0.00	-0.159	16.15	4.00
ATOM	2924	HD21	LEU	505	1.150	17.400	-12.378	0.00	0.00	0.053	0.00	0.00
ATOM	2925	HD22	LEU	505	2.796	18.074	-12.322	0.00	0.00	0.053	0.00	0.00
ATOM	2926	HD23	LEU	505	2.559	16.322	-12.520	0.00	0.00	0.053	0.00	0.00
ATOM	2927	N	ARG	506	4.823	17.117	-7.358	0.00	0.00	-0.650	9.00	-17.40
ATOM	2928	HN	ARG	506	4.004	16.503	-7.476	0.00	0.00	0.439	0.00	0.00
ATOM	2929	CA	ARG	506	5.600	17.089	-6.160	0.00	0.00	0.158	9.40	4.00
ATOM	2930	HA	ARG	506	6.242	17.969	-6.196	0.00	0.00	0.053	0.00	0.00
ATOM	2931	C	ARG	506	6.370	15.817	-6.198	0.00	0.00	0.396	9.82	4.00
ATOM	2932	O	ARG	506	5.911	14.817	-6.747	0.00	0.00	-0.396	8.17	-17.40
ATOM	2933	CB	ARG	506	4.692	17.125	-4.917	0.00	0.00	-0.106	12.77	4.00
ATOM	2934	HB1	ARG	506	4.482	16.096	-4.623	0.00	0.00	0.053	0.00	0.00
ATOM	2935	HB2	ARG	506	3.774	17.648	-5.186	0.00	0.00	0.053	0.00	0.00
ATOM	2936	CG	ARG	506	5.275	17.834	-3.696	0.00	0.00	-0.106	12.77	4.00
ATOM	2937	HG1	ARG	506	5.954	18.628	-4.005	0.00	0.00	0.053	0.00	0.00
ATOM	2938	HG2	ARG	506	5.827	17.130	-3.074	0.00	0.00	0.053	0.00	0.00
ATOM	2939	CD	ARG	506	4.157	18.453	-2.852	0.00	0.00	0.374	12.77	4.00
ATOM	2940	HD1	ARG	506	4.656	19.064	-2.099	0.00	0.00	0.053	0.00	0.00
ATOM	2941	HD2	ARG	506	3.610	17.614	-2.421	0.00	0.00	0.053	0.00	0.00
ATOM	2942	NE	ARG	506	3.330	19.260	-3.799	0.00	0.00	-0.819	9.00	-24.67
ATOM	2943	HE	ARG	506	2.608	18.793	-4.365	0.00	0.00	0.407	0.00	0.00
ATOM	2944	CZ	ARG	506	3.516	20.606	-3.926	0.00	0.00	0.796	6.95	4.00
ATOM	2945	NH1	ARG	506	4.338	21.271	-3.064	0.00	0.00	-0.746	9.00	-24.67
ATOM	2946	HH11	ARG	506	4.475	22.287	-3.164	0.00	0.00	0.407	0.00	0.00
ATOM	2947	HH12	ARG	506	4.821	20.757	-2.313	0.00	0.00	0.407	0.00	0.00
ATOM	2948	NH2	ARG	506	2.879	21.292	-4.921	0.00	0.00	-0.746	9.00	-24.67
ATOM	2949	HH21	ARG	506	3.019	22.308	-5.017	0.00	0.00	0.407	0.00	0.00
ATOM	2950	HH22	ARG	506	2.259	20.793	-5.575	0.00	0.00	0.407	0.00	0.00
ATOM	2951	N	GLU	507	7.593	15.825	-5.649	0.00	0.00	-0.650	9.00	-17.40
ATOM	2952	HN	GLU	507	7.966	16.663	-5.180	0.00	0.00	0.439	0.00	0.00
ATOM	2953	CA	GLU	507	8.355	14.623	-5.742	0.00	0.00	0.158	9.40	4.00
ATOM	2954	HA	GLU	507	7.812	13.946	-6.401	0.00	0.00	0.053	0.00	0.00
ATOM	2955	C	GLU	507	8.476	14.064	-4.357	0.00	0.00	0.396	9.82	4.00

ATOM	2956	O	GLU	507	8.864	14.772	-3.429	0.00	0.00	-0.396	8.17	-17.40
ATOM	2957	CB	GLU	507	9.705	14.898	-6.417	0.00	0.00	-0.106	12.77	4.00
ATOM	2958	HB1	GLU	507	10.271	13.967	-6.444	0.00	0.00	0.053	0.00	0.00
ATOM	2959	HB2	GLU	507	10.234	15.651	-5.832	0.00	0.00	0.053	0.00	0.00
ATOM	2960	CG	GLU	507	9.438	15.410	-7.842	0.00	0.00	-0.336	12.77	4.00
ATOM	2961	HG1	GLU	507	8.765	16.268	-7.835	0.00	0.00	0.053	0.00	0.00
ATOM	2962	HG2	GLU	507	8.981	14.638	-8.461	0.00	0.00	0.053	0.00	0.00
ATOM	2963	CD	GLU	507	10.725	15.842	-8.523	0.00	0.00	0.297	9.82	4.00
ATOM	2964	OE1	GLU	507	11.744	16.043	-7.809	0.00	0.00	-0.534	8.17	-18.95
ATOM	2965	OE2	GLU	507	10.708	15.964	-9.777	0.00	0.00	-0.534	8.17	-18.95
ATOM	2966	N	THR	508	8.111	12.772	-4.177	0.00	0.00	-0.650	9.00	-17.40
ATOM	2967	HN	THR	508	7.836	12.194	-4.984	0.00	0.00	0.439	0.00	0.00
ATOM	2968	CA	THR	508	8.109	12.212	-2.853	0.00	0.00	0.158	9.40	4.00
ATOM	2969	HA	THR	508	8.456	12.935	-2.115	0.00	0.00	0.053	0.00	0.00
ATOM	2970	C	THR	508	8.998	11.023	-2.766	0.00	0.00	0.396	9.82	4.00
ATOM	2971	O	THR	508	9.220	10.289	-3.729	0.00	0.00	-0.396	8.17	-17.40
ATOM	2972	CB	THR	508	6.776	11.733	-2.357	0.00	0.00	0.060	9.40	4.00
ATOM	2973	HB	THR	508	6.051	12.533	-2.507	0.00	0.00	0.053	0.00	0.00
ATOM	2974	OG1	THR	508	6.865	11.385	-0.982	0.00	0.00	-0.537	11.04	-17.40
ATOM	2975	HG1	THR	508	6.649	12.210	-0.404	0.00	0.00	0.424	0.00	0.00
ATOM	2976	CG2	THR	508	6.388	10.489	-3.162	0.00	0.00	-0.159	16.15	4.00
ATOM	2977	HG21	THR	508	5.421	10.121	-2.820	0.00	0.00	0.053	0.00	0.00
ATOM	2978	HG22	THR	508	6.325	10.745	-4.220	0.00	0.00	0.053	0.00	0.00
ATOM	2979	HG23	THR	508	7.142	9.714	-3.020	0.00	0.00	0.053	0.00	0.00
ATOM	2980	N	LYS	509	9.520	10.837	-1.545	0.00	0.00	-0.650	9.00	-17.40
ATOM	2981	HN	LYS	509	9.235	11.506	-0.815	0.00	0.00	0.439	0.00	0.00
ATOM	2982	CA	LYS	509	10.429	9.810	-1.150	0.00	0.00	0.158	9.40	4.00
ATOM	2983	HA	LYS	509	11.242	9.721	-1.870	0.00	0.00	0.053	0.00	0.00
ATOM	2984	C	LYS	509	9.723	8.483	-1.065	0.00	0.00	0.396	9.82	4.00
ATOM	2985	O	LYS	509	10.332	7.443	-1.306	0.00	0.00	-0.396	8.17	-17.40
ATOM	2986	CB	LYS	509	11.028	10.126	0.230	0.00	0.00	-0.106	12.77	4.00
ATOM	2987	HB1	LYS	509	11.697	9.337	0.573	0.00	0.00	0.053	0.00	0.00
ATOM	2988	HB2	LYS	509	10.256	10.242	0.991	0.00	0.00	0.053	0.00	0.00
ATOM	2989	CG	LYS	509	11.840	11.425	0.216	0.00	0.00	-0.106	12.77	4.00
ATOM	2990	HG1	LYS	509	11.293	12.162	-0.372	0.00	0.00	0.053	0.00	0.00
ATOM	2991	HG2	LYS	509	12.810	11.215	-0.235	0.00	0.00	0.053	0.00	0.00
ATOM	2992	CD	LYS	509	12.095	12.034	1.596	0.00	0.00	-0.106	12.77	4.00
ATOM	2993	HD1	LYS	509	12.619	11.356	2.270	0.00	0.00	0.053	0.00	0.00
ATOM	2994	HD2	LYS	509	11.178	12.315	2.113	0.00	0.00	0.053	0.00	0.00
ATOM	2995	CE	LYS	509	12.947	13.305	1.540	0.00	0.00	0.099	12.77	4.00
ATOM	2996	HE1	LYS	509	12.614	13.946	0.724	0.00	0.00	0.053	0.00	0.00
ATOM	2997	HE2	LYS	509	13.994	13.050	1.379	0.00	0.00	0.053	0.00	0.00
ATOM	2998	NZ	LYS	509	12.831	14.055	2.810	0.00	0.00	-0.045	13.25	-39.20
ATOM	2999	HZ1	LYS	509	13.408	14.907	2.760	0.00	0.00	0.280	0.00	0.00
ATOM	3000	HZ2	LYS	509	11.847	14.316	2.967	0.00	0.00	0.280	0.00	0.00
ATOM	3001	HZ3	LYS	509	13.157	13.465	3.589	0.00	0.00	0.280	0.00	0.00
ATOM	3002	N	LEU	510	8.419	8.477	-0.715	0.00	0.00	-0.650	9.00	-17.40
ATOM	3003	HN	LEU	510	7.911	9.368	-0.624	0.00	0.00	0.439	0.00	0.00
ATOM	3004	CA	LEU	510	7.732	7.235	-0.467	0.00	0.00	0.158	9.40	4.00
ATOM	3005	HA	LEU	510	8.409	6.507	-0.020	0.00	0.00	0.053	0.00	0.00
ATOM	3006	C	LEU	510	7.197	6.660	-1.756	0.00	0.00	0.396	9.82	4.00
ATOM	3007	O	LEU	510	6.411	7.297	-2.454	0.00	0.00	-0.396	8.17	-17.40
ATOM	3008	CB	LEU	510	6.552	7.418	0.512	0.00	0.00	-0.106	12.77	4.00
ATOM	3009	HB1	LEU	510	5.753	7.935	-0.019	0.00	0.00	0.053	0.00	0.00
ATOM	3010	HB2	LEU	510	6.906	8.009	1.357	0.00	0.00	0.053	0.00	0.00
ATOM	3011	CG	LEU	510	5.945	6.120	1.090	0.00	0.00	-0.053	9.40	4.00
ATOM	3012	HG	LEU	510	5.157	6.315	1.818	0.00	0.00	0.053	0.00	0.00
ATOM	3013	CD1	LEU	510	5.318	5.230	0.006	0.00	0.00	-0.159	16.15	4.00
ATOM	3014	HD11	LEU	510	4.906	4.332	0.466	0.00	0.00	0.053	0.00	0.00
ATOM	3015	HD12	LEU	510	4.521	5.777	-0.498	0.00	0.00	0.053	0.00	0.00
ATOM	3016	HD13	LEU	510	6.081	4.949	-0.720	0.00	0.00	0.053	0.00	0.00
ATOM	3017	CD2	LEU	510	6.961	5.380	1.976	0.00	0.00	-0.159	16.15	4.00
ATOM	3018	HD21	LEU	510	6.507	4.471	2.369	0.00	0.00	0.053	0.00	0.00
ATOM	3019	HD22	LEU	510	7.839	5.120	1.384	0.00	0.00	0.053	0.00	0.00
ATOM	3020	HD23	LEU	510	7.259	6.024	2.804	0.00	0.00	0.053	0.00	0.00
ATOM	3021	N	PHE	511	7.606	5.409	-2.075	0.00	0.00	-0.650	9.00	-17.40
ATOM	3022	HN	PHE	511	8.247	4.942	-1.418	0.00	0.00	0.439	0.00	0.00
ATOM	3023	CA	PHE	511	7.222	4.671	-3.257	0.00	0.00	0.158	9.40	4.00
ATOM	3024	HA	PHE	511	7.271	5.337	-4.118	0.00	0.00	0.053	0.00	0.00
ATOM	3025	C	PHE	511	5.831	4.166	-3.077	0.00	0.00	0.396	9.82	4.00
ATOM	3026	O	PHE	511	5.579	3.223	-2.329	0.00	0.00	-0.396	8.17	-17.40
ATOM	3027	CB	PHE	511	8.145	3.462	-3.509	0.00	0.00	-0.106	12.77	4.00
ATOM	3028	HB1	PHE	511	8.284	2.889	-2.592	0.00	0.00	0.053	0.00	0.00
ATOM	3029	HB2	PHE	511	9.123	3.793	-3.858	0.00	0.00	0.053	0.00	0.00
ATOM	3030	CG	PHE	511	7.557	2.560	-4.543	0.00	0.00	0.000	7.26	0.60
ATOM	3031	CD1	PHE	511	7.651	2.846	-5.886	0.00	0.00	-0.127	10.80	0.60

ATOM	3032	HD1	PHE	511	8.159	3.754	-6.211	0.00	0.00	0.127	0.00	0.00
ATOM	3033	CD2	PHE	511	6.924	1.399	-4.157	0.00	0.00	-0.127	10.80	0.60
ATOM	3034	HD2	PHE	511	6.853	1.153	-3.097	0.00	0.00	0.127	0.00	0.00
ATOM	3035	CE1	PHE	511	7.109	1.996	-6.822	0.00	0.00	-0.127	10.80	0.60
ATOM	3036	HE1	PHE	511	7.185	2.237	-7.882	0.00	0.00	0.127	0.00	0.00
ATOM	3037	CE2	PHE	511	6.381	0.546	-5.088	0.00	0.00	-0.127	10.80	0.60
ATOM	3038	HE2	PHE	511	5.879	-0.366	-4.765	0.00	0.00	0.127	0.00	0.00
ATOM	3039	CZ	PHE	511	6.472	0.844	-6.426	0.00	0.00	-0.127	10.80	0.60
ATOM	3040	HZ	PHE	511	6.042	0.172	-7.168	0.00	0.00	0.127	0.00	0.00
ATOM	3041	N	VAL	512	4.875	4.831	-3.743	0.00	0.00	-0.650	9.00	-17.40
ATOM	3042	HN	VAL	512	5.139	5.606	-4.368	0.00	0.00	0.439	0.00	0.00
ATOM	3043	CA	VAL	512	3.496	4.483	-3.601	0.00	0.00	0.158	9.40	4.00
ATOM	3044	HA	VAL	512	3.327	4.209	-2.560	0.00	0.00	0.053	0.00	0.00
ATOM	3045	C	VAL	512	3.006	3.329	-4.445	0.00	0.00	0.396	9.82	4.00
ATOM	3046	O	VAL	512	2.026	2.691	-4.067	0.00	0.00	-0.396	8.17	-17.40
ATOM	3047	CB	VAL	512	2.607	5.684	-3.513	0.00	0.00	-0.053	9.40	4.00
ATOM	3048	HB	VAL	512	2.694	6.123	-2.519	0.00	0.00	0.053	0.00	0.00
ATOM	3049	CG1	VAL	512	3.035	6.706	-4.568	0.00	0.00	-0.159	16.15	4.00
ATOM	3050	HG11	VAL	512	2.390	7.583	-4.508	0.00	0.00	0.053	0.00	0.00
ATOM	3051	HG12	VAL	512	4.068	7.003	-4.389	0.00	0.00	0.053	0.00	0.00
ATOM	3052	HG13	VAL	512	2.952	6.262	-5.560	0.00	0.00	0.053	0.00	0.00
ATOM	3053	CG2	VAL	512	1.145	5.221	-3.468	0.00	0.00	-0.159	16.15	4.00
ATOM	3054	HG21	VAL	512	0.490	6.090	-3.404	0.00	0.00	0.053	0.00	0.00
ATOM	3055	HG22	VAL	512	0.914	4.658	-4.372	0.00	0.00	0.053	0.00	0.00
ATOM	3056	HG23	VAL	512	0.991	4.586	-2.596	0.00	0.00	0.053	0.00	0.00
ATOM	3057	N	GLY	513	3.626	3.008	-5.602	0.00	0.00	-0.650	9.00	-17.40
ATOM	3058	HN	GLY	513	4.414	3.575	-5.946	0.00	0.00	0.439	0.00	0.00
ATOM	3059	CA	GLY	513	3.169	1.859	-6.352	0.00	0.00	0.105	9.40	4.00
ATOM	3060	HA1	GLY	513	3.005	1.025	-5.670	0.00	0.00	0.053	0.00	0.00
ATOM	3061	HA2	GLY	513	3.924	1.585	-7.089	0.00	0.00	0.053	0.00	0.00
ATOM	3062	C	GLY	513	1.889	2.198	-7.047	0.00	0.00	0.396	9.82	4.00
ATOM	3063	O	GLY	513	1.857	3.143	-7.824	0.00	0.00	-0.396	8.17	-17.40
ATOM	3064	N	LEU	514	0.834	1.373	-6.852	0.00	0.00	-0.650	9.00	-17.40
ATOM	3065	HN	LEU	514	1.001	0.516	-6.305	0.00	0.00	0.439	0.00	0.00
ATOM	3066	CA	LEU	514	-0.507	1.591	-7.345	0.00	0.00	0.158	9.40	4.00
ATOM	3067	HA	LEU	514	-1.087	0.672	-7.429	0.00	0.00	0.053	0.00	0.00
ATOM	3068	C	LEU	514	-0.539	2.213	-8.708	0.00	0.00	0.396	9.82	4.00
ATOM	3069	O	LEU	514	-1.078	3.304	-8.886	0.00	0.00	-0.396	8.17	-17.40
ATOM	3070	CB	LEU	514	-1.371	2.452	-6.408	0.00	0.00	-0.106	12.77	4.00
ATOM	3071	HB1	LEU	514	-2.333	2.726	-6.840	0.00	0.00	0.053	0.00	0.00
ATOM	3072	HB2	LEU	514	-0.899	3.395	-6.131	0.00	0.00	0.053	0.00	0.00
ATOM	3073	CG	LEU	514	-1.704	1.756	-5.077	0.00	0.00	-0.053	9.40	4.00
ATOM	3074	HG	LEU	514	-2.184	0.790	-5.233	0.00	0.00	0.053	0.00	0.00
ATOM	3075	CD1	LEU	514	-0.446	1.500	-4.235	0.00	0.00	-0.159	16.15	4.00
ATOM	3076	HD11	LEU	514	-0.726	1.007	-3.304	0.00	0.00	0.053	0.00	0.00
ATOM	3077	HD12	LEU	514	0.241	0.862	-4.791	0.00	0.00	0.053	0.00	0.00
ATOM	3078	HD13	LEU	514	0.041	2.449	-4.011	0.00	0.00	0.053	0.00	0.00
ATOM	3079	CD2	LEU	514	-2.785	2.526	-4.307	0.00	0.00	-0.159	16.15	4.00
ATOM	3080	HD21	LEU	514	-3.001	2.012	-3.370	0.00	0.00	0.053	0.00	0.00
ATOM	3081	HD22	LEU	514	-2.431	3.535	-4.094	0.00	0.00	0.053	0.00	0.00
ATOM	3082	HD23	LEU	514	-3.692	2.579	-4.909	0.00	0.00	0.053	0.00	0.00
ATOM	3083	N	GLY	515	0.032	1.547	-9.723	0.00	0.00	-0.650	9.00	-17.40
ATOM	3084	HN	GLY	515	0.487	0.636	-9.571	0.00	0.00	0.439	0.00	0.00
ATOM	3085	CA	GLY	515	-0.012	2.144	-11.024	0.00	0.00	0.105	9.40	4.00
ATOM	3086	HA1	GLY	515	-0.894	2.784	-11.064	0.00	0.00	0.053	0.00	0.00
ATOM	3087	HA2	GLY	515	-0.076	1.338	-11.755	0.00	0.00	0.053	0.00	0.00
ATOM	3088	C	GLY	515	1.235	2.933	-11.199	0.00	0.00	0.396	9.82	4.00
ATOM	3089	O	GLY	515	1.255	4.143	-10.970	0.00	0.00	-0.396	8.17	-17.40
ATOM	3090	N	PHE	516	2.322	2.257	-11.611	0.00	0.00	-0.650	9.00	-17.40
ATOM	3091	HN	PHE	516	2.274	1.246	-11.802	0.00	0.00	0.439	0.00	0.00
ATOM	3092	CA	PHE	516	3.547	2.978	-11.777	0.00	0.00	0.158	9.40	4.00
ATOM	3093	HA	PHE	516	3.323	4.003	-12.074	0.00	0.00	0.053	0.00	0.00
ATOM	3094	C	PHE	516	4.370	2.314	-12.836	0.00	0.00	0.396	9.82	4.00
ATOM	3095	O	PHE	516	4.431	1.087	-12.931	0.00	0.00	-0.396	8.17	-17.40
ATOM	3096	CB	PHE	516	4.367	3.041	-10.479	0.00	0.00	-0.106	12.77	4.00
ATOM	3097	HB1	PHE	516	3.774	3.636	-9.785	0.00	0.00	0.053	0.00	0.00
ATOM	3098	HB2	PHE	516	5.310	3.517	-10.749	0.00	0.00	0.053	0.00	0.00
ATOM	3099	CG	PHE	516	4.533	1.629	-10.040	0.00	0.00	0.000	7.26	0.60
ATOM	3100	CD1	PHE	516	3.549	1.016	-9.297	0.00	0.00	-0.127	10.80	0.60
ATOM	3101	HD1	PHE	516	2.650	1.571	-9.029	0.00	0.00	0.127	0.00	0.00
ATOM	3102	CD2	PHE	516	5.659	0.918	-10.376	0.00	0.00	-0.127	10.80	0.60
ATOM	3103	HD2	PHE	516	6.442	1.392	-10.968	0.00	0.00	0.127	0.00	0.00
ATOM	3104	CE1	PHE	516	3.689	-0.289	-8.890	0.00	0.00	-0.127	10.80	0.60
ATOM	3105	HE1	PHE	516	2.904	-0.765	-8.302	0.00	0.00	0.127	0.00	0.00
ATOM	3106	CE2	PHE	516	5.804	-0.387	-9.971	0.00	0.00	-0.127	10.80	0.60
ATOM	3107	HE2	PHE	516	6.702	-0.943	-10.241	0.00	0.00	0.127	0.00	0.00

ATOM	3108	CZ	PHE	516	4.820	-0.993	-9.226	0.00	0.00	-0.127	10.80	0.60
ATOM	3109	HZ	PHE	516	4.937	-2.028	-8.903	0.00	0.00	0.127	0.00	0.00
ATOM	3110	N	PRO	517	4.961	3.119	-13.682	0.00	0.00	-0.422	9.00	-17.40
ATOM	3111	CA	PRO	517	5.839	2.555	-14.670	0.00	0.00	0.158	9.40	4.00
ATOM	3112	HA	PRO	517	5.553	1.546	-14.968	0.00	0.00	0.053	0.00	0.00
ATOM	3113	CD	PRO	517	4.205	4.231	-14.235	0.00	0.00	0.105	12.77	4.00
ATOM	3114	HD1	PRO	517	4.170	4.971	-13.435	0.00	0.00	0.053	0.00	0.00
ATOM	3115	HD2	PRO	517	3.231	3.810	-14.485	0.00	0.00	0.053	0.00	0.00
ATOM	3116	C	PRO	517	7.254	2.453	-14.203	0.00	0.00	0.396	9.82	4.00
ATOM	3117	O	PRO	517	7.660	3.250	-13.355	0.00	0.00	-0.396	8.17	-17.40
ATOM	3118	CB	PRO	517	5.692	3.398	-15.938	0.00	0.00	-0.106	12.77	4.00
ATOM	3119	HB1	PRO	517	5.075	2.787	-16.597	0.00	0.00	0.053	0.00	0.00
ATOM	3120	HB2	PRO	517	6.715	3.538	-16.288	0.00	0.00	0.053	0.00	0.00
ATOM	3121	CG	PRO	517	5.012	4.686	-15.460	0.00	0.00	-0.106	12.77	4.00
ATOM	3122	HG1	PRO	517	4.369	5.100	-16.237	0.00	0.00	0.053	0.00	0.00
ATOM	3123	HG2	PRO	517	5.750	5.444	-15.198	0.00	0.00	0.053	0.00	0.00
ATOM	3124	N	TYR	518	8.024	1.485	-14.751	0.00	0.00	-0.650	9.00	-17.40
ATOM	3125	HN	TYR	518	7.604	0.792	-15.387	0.00	0.00	0.439	0.00	0.00
ATOM	3126	CA	TYR	518	9.424	1.423	-14.448	0.00	0.00	0.158	9.40	4.00
ATOM	3127	HA	TYR	518	9.593	2.238	-13.744	0.00	0.00	0.053	0.00	0.00
ATOM	3128	C	TYR	518	10.110	1.613	-15.766	0.00	0.00	0.396	9.82	4.00
ATOM	3129	O	TYR	518	9.489	1.447	-16.815	0.00	0.00	-0.396	8.17	-17.40
ATOM	3130	CB	TYR	518	9.920	0.162	-13.707	0.00	0.00	-0.106	12.77	4.00
ATOM	3131	HB1	TYR	518	9.265	-0.145	-12.892	0.00	0.00	0.053	0.00	0.00
ATOM	3132	HB2	TYR	518	10.904	0.286	-13.255	0.00	0.00	0.053	0.00	0.00
ATOM	3133	CG	TYR	518	10.038	-1.028	-14.587	0.00	0.00	0.000	7.26	0.60
ATOM	3134	CD1	TYR	518	8.938	-1.761	-14.960	0.00	0.00	-0.127	10.80	0.60
ATOM	3135	HD1	TYR	518	7.947	-1.464	-14.617	0.00	0.00	0.127	0.00	0.00
ATOM	3136	CD2	TYR	518	11.283	-1.429	-15.014	0.00	0.00	-0.127	10.80	0.60
ATOM	3137	HD2	TYR	518	12.163	-0.862	-14.711	0.00	0.00	0.127	0.00	0.00
ATOM	3138	CE1	TYR	518	9.081	-2.867	-15.763	0.00	0.00	-0.127	10.80	0.60
ATOM	3139	HE1	TYR	518	8.203	-3.440	-16.060	0.00	0.00	0.127	0.00	0.00
ATOM	3140	CE2	TYR	518	11.432	-2.532	-15.816	0.00	0.00	-0.127	10.80	0.60
ATOM	3141	HE2	TYR	518	12.424	-2.834	-16.153	0.00	0.00	0.127	0.00	0.00
ATOM	3142	CZ	TYR	518	10.327	-3.253	-16.192	0.00	0.00	0.027	7.26	0.60
ATOM	3143	OH	TYR	518	10.474	-4.390	-17.015	0.00	0.00	-0.451	10.94	-17.40
ATOM	3144	HH	TYR	518	9.728	-4.400	-17.725	0.00	0.00	0.424	0.00	0.00
ATOM	3145	N	GLU	519	11.414	1.944	-15.752	0.00	0.00	-0.650	9.00	-17.40
ATOM	3146	HN	GLU	519	11.988	1.786	-14.912	0.00	0.00	0.439	0.00	0.00
ATOM	3147	CA	GLU	519	11.987	2.522	-16.935	0.00	0.00	0.158	9.40	4.00
ATOM	3148	HA	GLU	519	11.200	2.600	-17.686	0.00	0.00	0.053	0.00	0.00
ATOM	3149	C	GLU	519	13.109	1.755	-17.551	0.00	0.00	0.396	9.82	4.00
ATOM	3150	O	GLU	519	13.365	0.589	-17.245	0.00	0.00	-0.396	8.17	-17.40
ATOM	3151	CB	GLU	519	12.560	3.907	-16.601	0.00	0.00	-0.106	12.77	4.00
ATOM	3152	HB1	GLU	519	11.774	4.585	-16.267	0.00	0.00	0.053	0.00	0.00
ATOM	3153	HB2	GLU	519	13.038	4.353	-17.473	0.00	0.00	0.053	0.00	0.00
ATOM	3154	CG	GLU	519	13.607	3.814	-15.486	0.00	0.00	-0.336	12.77	4.00
ATOM	3155	HG1	GLU	519	14.547	3.458	-15.908	0.00	0.00	0.053	0.00	0.00
ATOM	3156	HG2	GLU	519	13.256	3.118	-14.725	0.00	0.00	0.053	0.00	0.00
ATOM	3157	CD	GLU	519	13.805	5.191	-14.874	0.00	0.00	0.297	9.82	4.00
ATOM	3158	OE1	GLU	519	13.847	6.185	-15.644	0.00	0.00	-0.534	8.17	-18.95
ATOM	3159	OE2	GLU	519	13.911	5.267	-13.621	0.00	0.00	-0.534	8.17	-18.95
ATOM	3160	N	GLY	520	13.758	2.468	-18.506	0.00	0.00	-0.650	9.00	-17.40
ATOM	3161	HN	GLY	520	13.389	3.411	-18.693	0.00	0.00	0.439	0.00	0.00
ATOM	3162	CA	GLY	520	14.894	2.072	-19.288	0.00	0.00	0.105	9.40	4.00
ATOM	3163	HA1	GLY	520	15.654	1.694	-18.604	0.00	0.00	0.053	0.00	0.00
ATOM	3164	HA2	GLY	520	15.251	2.951	-19.825	0.00	0.00	0.053	0.00	0.00
ATOM	3165	C	GLY	520	14.449	1.014	-20.230	0.00	0.00	0.396	9.82	4.00
ATOM	3166	O	GLY	520	13.300	0.962	-20.658	0.00	0.00	-0.396	8.17	-17.40
ATOM	3167	N	PRO	521	15.390	0.170	-20.559	0.00	0.00	-0.422	9.00	-17.40
ATOM	3168	CA	PRO	521	15.083	-1.006	-21.334	0.00	0.00	0.158	9.40	4.00
ATOM	3169	HA	PRO	521	14.319	-0.669	-22.034	0.00	0.00	0.053	0.00	0.00
ATOM	3170	CD	PRO	521	16.717	0.685	-20.862	0.00	0.00	0.105	12.77	4.00
ATOM	3171	HD1	PRO	521	17.307	0.520	-19.961	0.00	0.00	0.053	0.00	0.00
ATOM	3172	HD2	PRO	521	16.575	1.741	-21.093	0.00	0.00	0.053	0.00	0.00
ATOM	3173	C	PRO	521	14.597	-1.993	-20.320	0.00	0.00	0.396	9.82	4.00
ATOM	3174	O	PRO	521	14.352	-3.148	-20.652	0.00	0.00	-0.396	8.17	-17.40
ATOM	3175	CB	PRO	521	16.391	-1.431	-21.996	0.00	0.00	-0.106	12.77	4.00
ATOM	3176	HB1	PRO	521	16.208	-1.842	-22.989	0.00	0.00	0.053	0.00	0.00
ATOM	3177	HB2	PRO	521	16.897	-2.193	-21.403	0.00	0.00	0.053	0.00	0.00
ATOM	3178	CG	PRO	521	17.211	-0.133	-22.064	0.00	0.00	-0.106	12.77	4.00
ATOM	3179	HG1	PRO	521	16.953	0.294	-23.033	0.00	0.00	0.053	0.00	0.00
ATOM	3180	HG2	PRO	521	18.245	-0.468	-21.983	0.00	0.00	0.053	0.00	0.00
ATOM	3181	N	ALA	522	14.493	-1.517	-19.069	0.00	0.00	-0.650	9.00	-17.40
ATOM	3182	HN	ALA	522	14.727	-0.519	-18.968	0.00	0.00	0.439	0.00	0.00
ATOM	3183	CA	ALA	522	14.113	-2.164	-17.860	0.00	0.00	0.158	9.40	4.00

ATOM	3184	HA	ALA	522	13.342	-1.541	-17.407	0.00	0.00	0.053	0.00	0.00
ATOM	3185	C	ALA	522	15.352	-2.245	-17.015	0.00	0.00	0.396	9.82	4.00
ATOM	3186	O	ALA	522	15.721	-3.359	-16.646	0.00	0.00	-0.396	8.17	-17.40
ATOM	3187	CB	ALA	522	13.588	-3.596	-18.059	0.00	0.00	-0.159	16.15	4.00
ATOM	3188	HB1	ALA	522	13.319	-4.022	-17.093	0.00	0.00	0.053	0.00	0.00
ATOM	3189	HB2	ALA	522	12.709	-3.575	-18.704	0.00	0.00	0.053	0.00	0.00
ATOM	3190	HB3	ALA	522	14.363	-4.207	-18.522	0.00	0.00	0.053	0.00	0.00
ATOM	3191	N	PRO	523	16.066	-1.182	-16.680	0.00	0.00	-0.422	9.00	-17.40
ATOM	3192	CA	PRO	523	17.192	-1.369	-15.818	0.00	0.00	0.158	9.40	4.00
ATOM	3193	HA	PRO	523	17.738	-2.247	-16.163	0.00	0.00	0.053	0.00	0.00
ATOM	3194	CD	PRO	523	16.160	0.085	-17.393	0.00	0.00	0.105	12.77	4.00
ATOM	3195	HD1	PRO	523	15.146	0.486	-17.397	0.00	0.00	0.053	0.00	0.00
ATOM	3196	HD2	PRO	523	16.527	-0.173	-18.386	0.00	0.00	0.053	0.00	0.00
ATOM	3197	C	PRO	523	16.685	-1.569	-14.441	0.00	0.00	0.396	9.82	4.00
ATOM	3198	O	PRO	523	17.374	-2.184	-13.629	0.00	0.00	-0.396	8.17	-17.40
ATOM	3199	CB	PRO	523	18.069	-0.124	-15.952	0.00	0.00	-0.106	12.77	4.00
ATOM	3200	HB1	PRO	523	18.889	-0.435	-16.599	0.00	0.00	0.053	0.00	0.00
ATOM	3201	HB2	PRO	523	18.375	0.106	-14.931	0.00	0.00	0.053	0.00	0.00
ATOM	3202	CG	PRO	523	17.147	0.931	-16.579	0.00	0.00	-0.106	12.77	4.00
ATOM	3203	HG1	PRO	523	17.709	1.620	-17.209	0.00	0.00	0.053	0.00	0.00
ATOM	3204	HG2	PRO	523	16.643	1.519	-15.812	0.00	0.00	0.053	0.00	0.00
ATOM	3205	N	LEU	524	15.483	-1.043	-14.147	0.00	0.00	-0.650	9.00	-17.40
ATOM	3206	HN	LEU	524	14.912	-0.561	-14.855	0.00	0.00	0.439	0.00	0.00
ATOM	3207	CA	LEU	524	15.045	-1.191	-12.800	0.00	0.00	0.158	9.40	4.00
ATOM	3208	HA	LEU	524	15.829	-0.758	-12.179	0.00	0.00	0.053	0.00	0.00
ATOM	3209	C	LEU	524	14.880	-2.652	-12.580	0.00	0.00	0.396	9.82	4.00
ATOM	3210	O	LEU	524	15.391	-3.211	-11.611	0.00	0.00	-0.396	8.17	-17.40
ATOM	3211	CB	LEU	524	13.706	-0.491	-12.500	0.00	0.00	-0.106	12.77	4.00
ATOM	3212	HB1	LEU	524	12.881	-0.865	-13.106	0.00	0.00	0.053	0.00	0.00
ATOM	3213	HB2	LEU	524	13.734	0.584	-12.677	0.00	0.00	0.053	0.00	0.00
ATOM	3214	CG	LEU	524	13.249	-0.655	-11.036	0.00	0.00	-0.053	9.40	4.00
ATOM	3215	HG	LEU	524	13.144	-1.708	-10.774	0.00	0.00	0.053	0.00	0.00
ATOM	3216	CD1	LEU	524	14.263	-0.028	-10.067	0.00	0.00	-0.159	16.15	4.00
ATOM	3217	HD11	LEU	524	13.915	-0.158	-9.042	0.00	0.00	0.053	0.00	0.00
ATOM	3218	HD12	LEU	524	15.230	-0.516	-10.187	0.00	0.00	0.053	0.00	0.00
ATOM	3219	HD13	LEU	524	14.364	1.036	-10.284	0.00	0.00	0.053	0.00	0.00
ATOM	3220	CD2	LEU	524	11.828	-0.108	-10.827	0.00	0.00	-0.159	16.15	4.00
ATOM	3221	HD21	LEU	524	11.537	-0.239	-9.785	0.00	0.00	0.053	0.00	0.00
ATOM	3222	HD22	LEU	524	11.805	0.952	-11.079	0.00	0.00	0.053	0.00	0.00
ATOM	3223	HD23	LEU	524	11.132	-0.648	-11.469	0.00	0.00	0.053	0.00	0.00
ATOM	3224	N	GLU	525	14.216	-3.321	-13.540	0.00	0.00	-0.650	9.00	-17.40
ATOM	3225	HN	GLU	525	13.904	-2.822	-14.385	0.00	0.00	0.439	0.00	0.00
ATOM	3226	CA	GLU	525	13.938	-4.719	-13.400	0.00	0.00	0.158	9.40	4.00
ATOM	3227	HA	GLU	525	13.360	-4.871	-12.488	0.00	0.00	0.053	0.00	0.00
ATOM	3228	C	GLU	525	15.233	-5.460	-13.320	0.00	0.00	0.396	9.82	4.00
ATOM	3229	O	GLU	525	15.414	-6.324	-12.463	0.00	0.00	-0.396	8.17	-17.40
ATOM	3230	CB	GLU	525	13.136	-5.282	-14.591	0.00	0.00	-0.106	12.77	4.00
ATOM	3231	HB1	GLU	525	13.784	-5.285	-15.468	0.00	0.00	0.053	0.00	0.00
ATOM	3232	HB2	GLU	525	12.271	-4.639	-14.754	0.00	0.00	0.053	0.00	0.00
ATOM	3233	CG	GLU	525	12.620	-6.712	-14.391	0.00	0.00	-0.336	12.77	4.00
ATOM	3234	HG1	GLU	525	11.680	-6.833	-14.929	0.00	0.00	0.053	0.00	0.00
ATOM	3235	HG2	GLU	525	12.461	-6.891	-13.328	0.00	0.00	0.053	0.00	0.00
ATOM	3236	CD	GLU	525	13.650	-7.698	-14.929	0.00	0.00	0.297	9.82	4.00
ATOM	3237	OE1	GLU	525	14.046	-7.552	-16.116	0.00	0.00	-0.534	8.17	-18.95
ATOM	3238	OE2	GLU	525	14.050	-8.612	-14.160	0.00	0.00	-0.534	8.17	-18.95
ATOM	3239	N	ALA	526	16.182	-5.111	-14.204	0.00	0.00	-0.650	9.00	-17.40
ATOM	3240	HN	ALA	526	16.014	-4.326	-14.849	0.00	0.00	0.439	0.00	0.00
ATOM	3241	CA	ALA	526	17.425	-5.820	-14.259	0.00	0.00	0.158	9.40	4.00
ATOM	3242	HA	ALA	526	17.254	-6.886	-14.410	0.00	0.00	0.053	0.00	0.00
ATOM	3243	C	ALA	526	18.190	-5.644	-12.986	0.00	0.00	0.396	9.82	4.00
ATOM	3244	O	ALA	526	18.708	-6.613	-12.434	0.00	0.00	-0.396	8.17	-17.40
ATOM	3245	CB	ALA	526	18.333	-5.339	-15.404	0.00	0.00	-0.159	16.15	4.00
ATOM	3246	HB1	ALA	526	19.261	-5.911	-15.398	0.00	0.00	0.053	0.00	0.00
ATOM	3247	HB2	ALA	526	17.824	-5.484	-16.357	0.00	0.00	0.053	0.00	0.00
ATOM	3248	HB3	ALA	526	18.558	-4.281	-15.270	0.00	0.00	0.053	0.00	0.00
ATOM	3249	N	ILE	527	18.257	-4.407	-12.461	0.00	0.00	-0.650	9.00	-17.40
ATOM	3250	HN	ILE	527	17.703	-3.635	-12.857	0.00	0.00	0.439	0.00	0.00
ATOM	3251	CA	ILE	527	19.119	-4.191	-11.337	0.00	0.00	0.158	9.40	4.00
ATOM	3252	HA	ILE	527	20.079	-4.689	-11.473	0.00	0.00	0.053	0.00	0.00
ATOM	3253	C	ILE	527	18.513	-4.716	-10.082	0.00	0.00	0.396	9.82	4.00
ATOM	3254	O	ILE	527	17.296	-4.739	-9.906	0.00	0.00	-0.396	8.17	-17.40
ATOM	3255	CB	ILE	527	19.467	-2.752	-11.092	0.00	0.00	-0.053	9.40	4.00
ATOM	3256	HB	ILE	527	20.095	-2.707	-10.202	0.00	0.00	0.053	0.00	0.00
ATOM	3257	CG1	ILE	527	18.213	-1.937	-10.739	0.00	0.00	-0.106	12.77	4.00
ATOM	3258	HG11	ILE	527	17.578	-2.425	-9.999	0.00	0.00	0.053	0.00	0.00
ATOM	3259	HG12	ILE	527	17.568	-1.748	-11.597	0.00	0.00	0.053	0.00	0.00

ATOM	3260	CG2	ILE	527	20.221	-2.233	-12.327	0.00	0.00	-0.159	16.15	4.00
ATOM	3261	HG21	ILE	527	20.488	-1.187	-12.177	0.00	0.00	0.053	0.00	0.00
ATOM	3262	HG22	ILE	527	21.127	-2.821	-12.474	0.00	0.00	0.053	0.00	0.00
ATOM	3263	HG23	ILE	527	19.584	-2.323	-13.207	0.00	0.00	0.053	0.00	0.00
ATOM	3264	CD1	ILE	527	18.534	-0.561	-10.158	0.00	0.00	-0.159	16.15	4.00
ATOM	3265	HD11	ILE	527	17.606	-0.037	-9.930	0.00	0.00	0.053	0.00	0.00
ATOM	3266	HD12	ILE	527	19.118	-0.679	-9.245	0.00	0.00	0.053	0.00	0.00
ATOM	3267	HD13	ILE	527	19.108	0.016	-10.884	0.00	0.00	0.053	0.00	0.00
ATOM	3268	N	ALA	528	19.396	-5.184	-9.180	0.00	0.00	-0.650	9.00	-17.40
ATOM	3269	HN	ALA	528	20.394	-5.201	-9.433	0.00	0.00	0.439	0.00	0.00
ATOM	3270	CA	ALA	528	19.012	-5.658	-7.887	0.00	0.00	0.158	9.40	4.00
ATOM	3271	HA	ALA	528	18.120	-5.090	-7.623	0.00	0.00	0.053	0.00	0.00
ATOM	3272	C	ALA	528	20.176	-5.371	-6.997	0.00	0.00	0.396	9.82	4.00
ATOM	3273	O	ALA	528	21.257	-5.929	-7.180	0.00	0.00	-0.396	8.17	-17.40
ATOM	3274	CB	ALA	528	18.768	-7.175	-7.834	0.00	0.00	-0.159	16.15	4.00
ATOM	3275	HB1	ALA	528	18.480	-7.462	-6.823	0.00	0.00	0.053	0.00	0.00
ATOM	3276	HB2	ALA	528	17.969	-7.440	-8.527	0.00	0.00	0.053	0.00	0.00
ATOM	3277	HB3	ALA	528	19.681	-7.700	-8.115	0.00	0.00	0.053	0.00	0.00
ATOM	3278	N	ASN	529	19.996	-4.469	-6.013	0.00	0.00	-0.650	9.00	-17.40
ATOM	3279	HN	ASN	529	19.086	-4.002	-5.892	0.00	0.00	0.439	0.00	0.00
ATOM	3280	CA	ASN	529	21.089	-4.169	-5.138	0.00	0.00	0.158	9.40	4.00
ATOM	3281	HA	ASN	529	21.866	-4.911	-5.321	0.00	0.00	0.053	0.00	0.00
ATOM	3282	C	ASN	529	20.576	-4.249	-3.740	0.00	0.00	0.396	9.82	4.00
ATOM	3283	O	ASN	529	19.423	-3.921	-3.469	0.00	0.00	-0.396	8.17	-17.40
ATOM	3284	CB	ASN	529	21.674	-2.759	-5.344	0.00	0.00	-0.106	12.77	4.00
ATOM	3285	HB1	ASN	529	20.933	-2.024	-5.030	0.00	0.00	0.053	0.00	0.00
ATOM	3286	HB2	ASN	529	21.910	-2.629	-6.400	0.00	0.00	0.053	0.00	0.00
ATOM	3287	CG	ASN	529	22.938	-2.626	-4.501	0.00	0.00	0.396	9.82	4.00
ATOM	3288	OD1	ASN	529	22.887	-2.582	-3.273	0.00	0.00	-0.396	8.17	-17.40
ATOM	3289	ND2	ASN	529	24.112	-2.560	-5.184	0.00	0.00	-0.879	13.25	-17.40
ATOM	3290	HD21	ASN	529	24.112	-2.600	-6.213	0.00	0.00	0.439	0.00	0.00
ATOM	3291	HD22	ASN	529	25.001	-2.470	-4.672	0.00	0.00	0.439	0.00	0.00
ATOM	3292	N	GLY	530	21.433	-4.714	-2.812	0.00	0.00	-0.650	9.00	-17.40
ATOM	3293	HN	GLY	530	22.382	-5.006	-3.088	0.00	0.00	0.439	0.00	0.00
ATOM	3294	CA	GLY	530	21.027	-4.803	-1.444	0.00	0.00	0.105	9.40	4.00
ATOM	3295	HA1	GLY	530	20.191	-4.118	-1.299	0.00	0.00	0.053	0.00	0.00
ATOM	3296	HA2	GLY	530	21.878	-4.519	-0.825	0.00	0.00	0.053	0.00	0.00
ATOM	3297	C	GLY	530	20.618	-6.212	-1.181	0.00	0.00	0.396	9.82	4.00
ATOM	3298	O	GLY	530	21.190	-7.155	-1.727	0.00	0.00	-0.396	8.17	-17.40
ATOM	3299	N	CYS	531	19.602	-6.380	-0.316	0.00	0.00	-0.650	9.00	-17.40
ATOM	3300	HN	CYS	531	19.159	-5.553	0.109	0.00	0.00	0.439	0.00	0.00
ATOM	3301	CA	CYS	531	19.125	-7.684	0.025	0.00	0.00	0.158	9.40	4.00
ATOM	3302	HA	CYS	531	19.987	-8.351	0.042	0.00	0.00	0.053	0.00	0.00
ATOM	3303	C	CYS	531	18.144	-8.086	-1.021	0.00	0.00	0.396	9.82	4.00
ATOM	3304	O	CYS	531	18.365	-7.878	-2.213	0.00	0.00	-0.396	8.17	-17.40
ATOM	3305	CB	CYS	531	18.404	-7.733	1.382	0.00	0.00	-0.041	12.77	4.00
ATOM	3306	HB1	CYS	531	17.978	-8.714	1.591	0.00	0.00	0.053	0.00	0.00
ATOM	3307	HB2	CYS	531	17.581	-7.021	1.441	0.00	0.00	0.053	0.00	0.00
ATOM	3308	SG	CYS	531	19.514	-7.350	2.771	0.00	0.00	-0.255	19.93	-6.40
ATOM	3309	HG	CYS	531	20.053	-6.136	2.591	0.00	0.00	0.190	0.00	0.00
ATOM	3310	N	ALA	532	17.025	-8.696	-0.590	0.00	0.00	-0.650	9.00	-17.40
ATOM	3311	HN	ALA	532	16.885	-8.855	0.418	0.00	0.00	0.439	0.00	0.00
ATOM	3312	CA	ALA	532	16.029	-9.125	-1.523	0.00	0.00	0.158	9.40	4.00
ATOM	3313	HA	ALA	532	16.493	-9.854	-2.187	0.00	0.00	0.053	0.00	0.00
ATOM	3314	C	ALA	532	15.570	-7.922	-2.275	0.00	0.00	0.396	9.82	4.00
ATOM	3315	O	ALA	532	14.952	-7.031	-1.697	0.00	0.00	-0.396	8.17	-17.40
ATOM	3316	CB	ALA	532	14.798	-9.756	-0.848	0.00	0.00	-0.159	16.15	4.00
ATOM	3317	HB1	ALA	532	14.081	-10.060	-1.610	0.00	0.00	0.053	0.00	0.00
ATOM	3318	HB2	ALA	532	15.106	-10.628	-0.272	0.00	0.00	0.053	0.00	0.00
ATOM	3319	HB3	ALA	532	14.334	-9.027	-0.183	0.00	0.00	0.053	0.00	0.00
ATOM	3320	N	PHE	533	15.865	-7.881	-3.591	0.00	0.00	-0.650	9.00	-17.40
ATOM	3321	HN	PHE	533	16.350	-8.684	-4.017	0.00	0.00	0.439	0.00	0.00
ATOM	3322	CA	PHE	533	15.528	-6.762	-4.415	0.00	0.00	0.158	9.40	4.00
ATOM	3323	HA	PHE	533	14.682	-6.206	-4.011	0.00	0.00	0.053	0.00	0.00
ATOM	3324	C	PHE	533	15.156	-7.190	-5.802	0.00	0.00	0.396	9.82	4.00
ATOM	3325	O	PHE	533	15.049	-8.379	-6.093	0.00	0.00	-0.396	8.17	-17.40
ATOM	3326	CB	PHE	533	16.585	-5.658	-4.423	0.00	0.00	-0.106	12.77	4.00
ATOM	3327	HB1	PHE	533	16.373	-4.902	-5.179	0.00	0.00	0.053	0.00	0.00
ATOM	3328	HB2	PHE	533	17.579	-6.053	-4.634	0.00	0.00	0.053	0.00	0.00
ATOM	3329	CG	PHE	533	16.452	-5.140	-3.035	0.00	0.00	0.000	7.26	0.60
ATOM	3330	CD1	PHE	533	15.291	-4.498	-2.661	0.00	0.00	-0.127	10.80	0.60
ATOM	3331	HD1	PHE	533	14.486	-4.375	-3.386	0.00	0.00	0.127	0.00	0.00
ATOM	3332	CD2	PHE	533	17.460	-5.289	-2.113	0.00	0.00	-0.127	10.80	0.60
ATOM	3333	HD2	PHE	533	18.384	-5.793	-2.397	0.00	0.00	0.127	0.00	0.00
ATOM	3334	CE1	PHE	533	15.136	-4.012	-1.387	0.00	0.00	-0.127	10.80	0.60
ATOM	3335	HE1	PHE	533	14.214	-3.505	-1.104	0.00	0.00	0.127	0.00	0.00

ATOM	3336	CE2	PHE	533	17.310	-4.805	-0.833	0.00	0.00	-0.127	10.80	0.60
ATOM	3337	HE2	PHE	533	18.114	-4.928	-0.107	0.00	0.00	0.127	0.00	0.00
ATOM	3338	CZ	PHE	533	16.147	-4.167	-0.470	0.00	0.00	-0.127	10.80	0.60
ATOM	3339	HZ	PHE	533	16.028	-3.785	0.544	0.00	0.00	0.127	0.00	0.00
ATOM	3340	N	LEU	534	15.030	-6.210	-6.720	0.00	0.00	-0.650	9.00	-17.40
ATOM	3341	HN	LEU	534	15.502	-5.305	-6.580	0.00	0.00	0.439	0.00	0.00
ATOM	3342	CA	LEU	534	14.237	-6.435	-7.888	0.00	0.00	0.158	9.40	4.00
ATOM	3343	HA	LEU	534	13.200	-6.550	-7.572	0.00	0.00	0.053	0.00	0.00
ATOM	3344	C	LEU	534	14.588	-7.645	-8.691	0.00	0.00	0.396	9.82	4.00
ATOM	3345	O	LEU	534	13.808	-8.593	-8.683	0.00	0.00	-0.396	8.17	-17.40
ATOM	3346	CB	LEU	534	14.157	-5.189	-8.803	0.00	0.00	-0.106	12.77	4.00
ATOM	3347	HB1	LEU	534	15.066	-5.154	-9.404	0.00	0.00	0.053	0.00	0.00
ATOM	3348	HB2	LEU	534	14.078	-4.308	-8.166	0.00	0.00	0.053	0.00	0.00
ATOM	3349	CG	LEU	534	12.955	-5.157	-9.784	0.00	0.00	-0.053	9.40	4.00
ATOM	3350	HG	LEU	534	12.010	-5.236	-9.247	0.00	0.00	0.053	0.00	0.00
ATOM	3351	CD1	LEU	534	12.934	-3.848	-10.586	0.00	0.00	-0.159	16.15	4.00
ATOM	3352	HD11	LEU	534	12.082	-3.851	-11.266	0.00	0.00	0.053	0.00	0.00
ATOM	3353	HD12	LEU	534	12.849	-3.004	-9.902	0.00	0.00	0.053	0.00	0.00
ATOM	3354	HD13	LEU	534	13.856	-3.758	-11.160	0.00	0.00	0.053	0.00	0.00
ATOM	3355	CD2	LEU	534	12.883	-6.380	-10.710	0.00	0.00	-0.159	16.15	4.00
ATOM	3356	HD21	LEU	534	12.018	-6.288	-11.367	0.00	0.00	0.053	0.00	0.00
ATOM	3357	HD22	LEU	534	13.791	-6.436	-11.311	0.00	0.00	0.053	0.00	0.00
ATOM	3358	HD23	LEU	534	12.789	-7.285	-10.110	0.00	0.00	0.053	0.00	0.00
ATOM	3359	N	ASN	535	15.742	-7.721	-9.375	0.00	0.00	-0.650	9.00	-17.40
ATOM	3360	HN	ASN	535	16.522	-7.056	-9.276	0.00	0.00	0.439	0.00	0.00
ATOM	3361	CA	ASN	535	15.745	-8.850	-10.262	0.00	0.00	0.158	9.40	4.00
ATOM	3362	HA	ASN	535	14.811	-8.848	-10.824	0.00	0.00	0.053	0.00	0.00
ATOM	3363	C	ASN	535	15.858	-10.190	-9.557	0.00	0.00	0.396	9.82	4.00
ATOM	3364	O	ASN	535	14.842	-10.879	-9.513	0.00	0.00	-0.396	8.17	-17.40
ATOM	3365	CB	ASN	535	16.754	-8.685	-11.423	0.00	0.00	-0.106	12.77	4.00
ATOM	3366	HB1	ASN	535	17.767	-8.799	-11.038	0.00	0.00	0.053	0.00	0.00
ATOM	3367	HB2	ASN	535	16.638	-7.694	-11.863	0.00	0.00	0.053	0.00	0.00
ATOM	3368	CG	ASN	535	16.484	-9.750	-12.480	0.00	0.00	0.396	9.82	4.00
ATOM	3369	OD1	ASN	535	15.799	-10.744	-12.240	0.00	0.00	-0.396	8.17	-17.40
ATOM	3370	ND2	ASN	535	17.052	-9.540	-13.697	0.00	0.00	-0.879	13.25	-17.40
ATOM	3371	HD21	ASN	535	17.619	-8.696	-13.862	0.00	0.00	0.439	0.00	0.00
ATOM	3372	HD22	ASN	535	16.915	-10.225	-14.454	0.00	0.00	0.439	0.00	0.00
ATOM	3373	N	PRO	536	16.947	-10.662	-8.978	0.00	0.00	-0.422	9.00	-17.40
ATOM	3374	CA	PRO	536	16.790	-11.968	-8.375	0.00	0.00	0.158	9.40	4.00
ATOM	3375	HA	PRO	536	15.997	-12.493	-8.908	0.00	0.00	0.053	0.00	0.00
ATOM	3376	CD	PRO	536	18.244	-10.566	-9.640	0.00	0.00	0.105	12.77	4.00
ATOM	3377	HD1	PRO	536	18.866	-9.936	-9.004	0.00	0.00	0.053	0.00	0.00
ATOM	3378	HD2	PRO	536	18.057	-10.117	-10.615	0.00	0.00	0.053	0.00	0.00
ATOM	3379	C	PRO	536	16.423	-11.965	-6.925	0.00	0.00	0.396	9.82	4.00
ATOM	3380	O	PRO	536	15.913	-12.968	-6.429	0.00	0.00	-0.396	8.17	-17.40
ATOM	3381	CB	PRO	536	18.109	-12.713	-8.571	0.00	0.00	-0.106	12.77	4.00
ATOM	3382	HB1	PRO	536	17.810	-13.739	-8.786	0.00	0.00	0.053	0.00	0.00
ATOM	3383	HB2	PRO	536	18.631	-12.592	-7.622	0.00	0.00	0.053	0.00	0.00
ATOM	3384	CG	PRO	536	18.778	-11.997	-9.748	0.00	0.00	-0.106	12.77	4.00
ATOM	3385	HG1	PRO	536	18.504	-12.461	-10.695	0.00	0.00	0.053	0.00	0.00
ATOM	3386	HG2	PRO	536	19.864	-12.031	-9.661	0.00	0.00	0.053	0.00	0.00
ATOM	3387	N	LYS	537	16.702	-10.846	-6.242	0.00	0.00	-0.650	9.00	-17.40
ATOM	3388	HN	LYS	537	16.889	-9.980	-6.767	0.00	0.00	0.439	0.00	0.00
ATOM	3389	CA	LYS	537	16.750	-10.806	-4.813	0.00	0.00	0.158	9.40	4.00
ATOM	3390	HA	LYS	537	17.305	-11.689	-4.496	0.00	0.00	0.053	0.00	0.00
ATOM	3391	C	LYS	537	15.480	-10.815	-3.984	0.00	0.00	0.396	9.82	4.00
ATOM	3392	O	LYS	537	15.499	-11.419	-2.914	0.00	0.00	-0.396	8.17	-17.40
ATOM	3393	CB	LYS	537	17.789	-9.773	-4.347	0.00	0.00	-0.106	12.77	4.00
ATOM	3394	HB1	LYS	537	18.781	-10.207	-4.224	0.00	0.00	0.053	0.00	0.00
ATOM	3395	HB2	LYS	537	17.529	-9.325	-3.388	0.00	0.00	0.053	0.00	0.00
ATOM	3396	CG	LYS	537	17.946	-8.613	-5.337	0.00	0.00	-0.106	12.77	4.00
ATOM	3397	HG1	LYS	537	17.018	-8.074	-5.528	0.00	0.00	0.053	0.00	0.00
ATOM	3398	HG2	LYS	537	18.300	-8.923	-6.320	0.00	0.00	0.053	0.00	0.00
ATOM	3399	CD	LYS	537	18.937	-7.547	-4.877	0.00	0.00	-0.106	12.77	4.00
ATOM	3400	HD1	LYS	537	18.728	-7.189	-3.869	0.00	0.00	0.053	0.00	0.00
ATOM	3401	HD2	LYS	537	18.932	-6.667	-5.520	0.00	0.00	0.053	0.00	0.00
ATOM	3402	CE	LYS	537	20.379	-8.056	-4.859	0.00	0.00	0.099	12.77	4.00
ATOM	3403	HE1	LYS	537	20.676	-8.386	-5.854	0.00	0.00	0.053	0.00	0.00
ATOM	3404	HE2	LYS	537	20.475	-8.895	-4.170	0.00	0.00	0.053	0.00	0.00
ATOM	3405	NZ	LYS	537	21.296	-6.982	-4.425	0.00	0.00	-0.045	13.25	-39.20
ATOM	3406	HZ1	LYS	537	22.263	-7.338	-4.417	0.00	0.00	0.280	0.00	0.00
ATOM	3407	HZ2	LYS	537	21.228	-6.188	-5.077	0.00	0.00	0.280	0.00	0.00
ATOM	3408	HZ3	LYS	537	21.037	-6.671	-3.478	0.00	0.00	0.280	0.00	0.00
ATOM	3409	N	PHE	538	14.337	-10.213	-4.383	0.00	0.00	-0.650	9.00	-17.40
ATOM	3410	HN	PHE	538	14.207	-9.847	-5.337	0.00	0.00	0.439	0.00	0.00
ATOM	3411	CA	PHE	538	13.311	-10.123	-3.368	0.00	0.00	0.158	9.40	4.00

ATOM	3412	HA	PHE	538	13.790	-10.199	-2.392	0.00	0.00	0.053	0.00	0.00
ATOM	3413	C	PHE	538	12.260	-11.195	-3.440	0.00	0.00	0.396	9.82	4.00
ATOM	3414	O	PHE	538	11.439	-11.233	-4.355	0.00	0.00	-0.396	8.17	-17.40
ATOM	3415	CB	PHE	538	12.599	-8.750	-3.335	0.00	0.00	-0.106	12.77	4.00
ATOM	3416	HB1	PHE	538	13.311	-7.927	-3.266	0.00	0.00	0.053	0.00	0.00
ATOM	3417	HB2	PHE	538	11.926	-8.664	-2.482	0.00	0.00	0.053	0.00	0.00
ATOM	3418	CG	PHE	538	11.779	-8.520	-4.567	0.00	0.00	0.000	7.26	0.60
ATOM	3419	CD1	PHE	538	12.352	-8.128	-5.752	0.00	0.00	-0.127	10.80	0.60
ATOM	3420	HD1	PHE	538	13.431	-7.978	-5.800	0.00	0.00	0.127	0.00	0.00
ATOM	3421	CD2	PHE	538	10.416	-8.694	-4.540	0.00	0.00	-0.127	10.80	0.60
ATOM	3422	HD2	PHE	538	9.937	-9.000	-3.610	0.00	0.00	0.127	0.00	0.00
ATOM	3423	CE1	PHE	538	11.592	-7.921	-6.880	0.00	0.00	-0.127	10.80	0.60
ATOM	3424	HE1	PHE	538	12.071	-7.612	-7.809	0.00	0.00	0.127	0.00	0.00
ATOM	3425	CE2	PHE	538	9.643	-8.491	-5.659	0.00	0.00	-0.127	10.80	0.60
ATOM	3426	HE2	PHE	538	8.564	-8.638	-5.611	0.00	0.00	0.127	0.00	0.00
ATOM	3427	CZ	PHE	538	10.231	-8.103	-6.837	0.00	0.00	-0.127	10.80	0.60
ATOM	3428	HZ	PHE	538	9.625	-7.941	-7.728	0.00	0.00	0.127	0.00	0.00
ATOM	3429	N	ASN	539	12.306	-12.141	-2.475	0.00	0.00	-0.650	9.00	-17.40
ATOM	3430	HN	ASN	539	13.124	-12.169	-1.849	0.00	0.00	0.439	0.00	0.00
ATOM	3431	CA	ASN	539	11.259	-13.111	-2.286	0.00	0.00	0.158	9.40	4.00
ATOM	3432	HA	ASN	539	10.762	-13.358	-3.224	0.00	0.00	0.053	0.00	0.00
ATOM	3433	C	ASN	539	10.187	-12.606	-1.334	0.00	0.00	0.396	9.82	4.00
ATOM	3434	O	ASN	539	9.033	-13.001	-1.492	0.00	0.00	-0.396	8.17	-17.40
ATOM	3435	CB	ASN	539	11.744	-14.538	-1.911	0.00	0.00	-0.106	12.77	4.00
ATOM	3436	HB1	ASN	539	12.365	-14.996	-2.681	0.00	0.00	0.053	0.00	0.00
ATOM	3437	HB2	ASN	539	10.926	-15.238	-1.741	0.00	0.00	0.053	0.00	0.00
ATOM	3438	CG	ASN	539	12.579	-14.572	-0.641	0.00	0.00	0.396	9.82	4.00
ATOM	3439	OD1	ASN	539	13.565	-13.850	-0.511	0.00	0.00	-0.396	8.17	-17.40
ATOM	3440	ND2	ASN	539	12.175	-15.438	0.326	0.00	0.00	-0.879	13.25	-17.40
ATOM	3441	HD21	ASN	539	11.342	-16.025	0.176	0.00	0.00	0.439	0.00	0.00
ATOM	3442	HD22	ASN	539	12.702	-15.507	1.208	0.00	0.00	0.439	0.00	0.00
ATOM	3443	N	PRO	540	10.477	-11.768	-0.351	0.00	0.00	-0.422	9.00	-17.40
ATOM	3444	CA	PRO	540	9.438	-11.278	0.539	0.00	0.00	0.158	9.40	4.00
ATOM	3445	HA	PRO	540	8.633	-12.008	0.624	0.00	0.00	0.053	0.00	0.00
ATOM	3446	CD	PRO	540	11.761	-11.845	0.336	0.00	0.00	0.105	12.77	4.00
ATOM	3447	HD1	PRO	540	12.499	-11.415	-0.341	0.00	0.00	0.053	0.00	0.00
ATOM	3448	HD2	PRO	540	11.944	-12.902	0.530	0.00	0.00	0.053	0.00	0.00
ATOM	3449	C	PRO	540	8.857	-9.983	0.013	0.00	0.00	0.396	9.82	4.00
ATOM	3450	O	PRO	540	9.441	-9.505	-0.957	0.00	0.00	-0.396	8.17	-17.40
ATOM	3451	CB	PRO	540	10.119	-11.161	1.914	0.00	0.00	-0.106	12.77	4.00
ATOM	3452	HB1	PRO	540	9.861	-12.077	2.445	0.00	0.00	0.053	0.00	0.00
ATOM	3453	HB2	PRO	540	9.697	-10.267	2.373	0.00	0.00	0.053	0.00	0.00
ATOM	3454	CG	PRO	540	11.612	-11.037	1.620	0.00	0.00	-0.106	12.77	4.00
ATOM	3455	HG1	PRO	540	12.211	-11.445	2.434	0.00	0.00	0.053	0.00	0.00
ATOM	3456	HG2	PRO	540	11.904	-9.995	1.486	0.00	0.00	0.053	0.00	0.00
ATOM	3457	N	PRO	541	7.809	-9.385	0.595	0.00	0.00	-0.422	9.00	-17.40
ATOM	3458	CA	PRO	541	7.139	-8.226	0.036	0.00	0.00	0.158	9.40	4.00
ATOM	3459	HA	PRO	541	6.414	-8.584	-0.695	0.00	0.00	0.053	0.00	0.00
ATOM	3460	CD	PRO	541	7.567	-9.460	2.032	0.00	0.00	0.105	12.77	4.00
ATOM	3461	HD1	PRO	541	8.536	-9.654	2.493	0.00	0.00	0.053	0.00	0.00
ATOM	3462	HD2	PRO	541	6.862	-10.279	2.178	0.00	0.00	0.053	0.00	0.00
ATOM	3463	C	PRO	541	7.993	-7.223	-0.664	0.00	0.00	0.396	9.82	4.00
ATOM	3464	O	PRO	541	8.879	-6.615	-0.062	0.00	0.00	-0.396	8.17	-17.40
ATOM	3465	CB	PRO	541	6.303	-7.605	1.156	0.00	0.00	-0.106	12.77	4.00
ATOM	3466	HB1	PRO	541	5.266	-7.937	1.098	0.00	0.00	0.053	0.00	0.00
ATOM	3467	HB2	PRO	541	6.312	-6.517	1.091	0.00	0.00	0.053	0.00	0.00
ATOM	3468	CG	PRO	541	6.983	-8.100	2.438	0.00	0.00	-0.106	12.77	4.00
ATOM	3469	HG1	PRO	541	6.262	-8.197	3.250	0.00	0.00	0.053	0.00	0.00
ATOM	3470	HG2	PRO	541	7.760	-7.407	2.760	0.00	0.00	0.053	0.00	0.00
ATOM	3471	N	LYS	542	7.687	-7.049	-1.961	0.00	0.00	-0.650	9.00	-17.40
ATOM	3472	HN	LYS	542	6.865	-7.555	-2.319	0.00	0.00	0.439	0.00	0.00
ATOM	3473	CA	LYS	542	8.396	-6.228	-2.888	0.00	0.00	0.158	9.40	4.00
ATOM	3474	HA	LYS	542	9.459	-6.466	-2.910	0.00	0.00	0.053	0.00	0.00
ATOM	3475	C	LYS	542	8.280	-4.777	-2.548	0.00	0.00	0.396	9.82	4.00
ATOM	3476	O	LYS	542	9.266	-4.049	-2.623	0.00	0.00	-0.396	8.17	-17.40
ATOM	3477	CB	LYS	542	7.869	-6.388	-4.323	0.00	0.00	-0.106	12.77	4.00
ATOM	3478	HB1	LYS	542	6.817	-6.122	-4.427	0.00	0.00	0.053	0.00	0.00
ATOM	3479	HB2	LYS	542	7.949	-7.408	-4.699	0.00	0.00	0.053	0.00	0.00
ATOM	3480	CG	LYS	542	8.611	-5.520	-5.337	0.00	0.00	-0.106	12.77	4.00
ATOM	3481	HG1	LYS	542	9.682	-5.649	-5.181	0.00	0.00	0.053	0.00	0.00
ATOM	3482	HG2	LYS	542	8.323	-4.481	-5.175	0.00	0.00	0.053	0.00	0.00
ATOM	3483	CD	LYS	542	8.308	-5.866	-6.795	0.00	0.00	-0.106	12.77	4.00
ATOM	3484	HD1	LYS	542	8.213	-6.937	-6.973	0.00	0.00	0.053	0.00	0.00
ATOM	3485	HD2	LYS	542	9.077	-5.525	-7.488	0.00	0.00	0.053	0.00	0.00
ATOM	3486	CE	LYS	542	7.004	-5.253	-7.303	0.00	0.00	0.099	12.77	4.00
ATOM	3487	HE1	LYS	542	6.162	-5.644	-6.732	0.00	0.00	0.053	0.00	0.00

DEMANDE OU BREVET VOLUMINEUX

LA PRÉSENTE PARTIE DE CETTE DEMANDE OU CE BREVET COMPREND PLUS D'UN TOME.

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JUMBO APPLICATIONS/PATENTS

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NOTE POUR LE TOME / VOLUME NOTE:

WE CLAIM

1. A model or secondary, tertiary, and/or quanternary structure for a ligand binding domain of a glycosyltransferase.

2. A model as claimed in claim 1 wherein the ligand binding domain is a binding domain for a disphosphate group of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a nitrogeneous heterocyclic base of a sugar nucleotide donor, a sugar of a nucleotide of a sugar nucleotide donor, a selected sugar of a sugar nucleotide donor that is transferred to an acceptor, or an acceptor.

3. A model as claimed in claim 1 wherein the ligand binding domain is defined by (a) one or more amino acid residues of a GnT1 shown in Table 10; (b) one or more amino acid residues of a GnTV shown in Table 11; (c) one or more amino acid residues of a core 2L/T1 shown in Table 12; and (d) one or more amino acid residues of a core 2b/2M/T2 shown in Table 13.

4. A model as claimed in claim 1 defined by the structural coordinates of one or more of the atomic contacts or atomic interactions as shown in Table 10, Table 11, Table 12, or Table 13.

5. A model as claimed in claim 4 wherein each of the atomic interactions is defined in Table 10, 11, 12, or 13 by an atomic contact (more preferably a specific atom where indicated) on a sugar nucleotide donor or part thereof and an atomic contact (more preferably a specific atom where indicated) on the glycosyltransferase.

6. A model as claimed in claim 1 for a transition state of a glycosyltransferase.

7. A model as claimed in claim 1 wherein the glycosyltransferases is selected from the group consisting of GnT1, GnTV, Core 2L/T1, and Core 2b/M/T2, and the ligand binding domain is defined by selected atomic interactions or contacts in the ligand binding domain, as follows:

   (a) one or more of atomic interactions or atomic contacts for GnT1 shown in Table 10;

   (b) one or more of atomic interactions or atomic contacts for GnTV shown in Table 11;

   (c) one or more of atomic interactions or atomic contacts for Core 2L/T1 shown in Table 12; or

   (d) one or more of atomic interactions or atomic contacts for Core 2b/T shown in Table 13.

8. A model as claimed in claim 1 wherein the glycosyltransferase is selected from the group consisting of GnT1, GnTV, Core 2L/T1, Core 2b/M/T2, Core 2c, and Core 3 comprising the following atomic structural coordinates:

   Table 1 – Structural coordinates for GnT1.

   Table 2 – Structural coordinates for GnTV.

   Table 3, 4, or 5 – Structural coordinates for core 2L or T1

   Table 6 – Structural coordinates for core 2b/core M/core 2 T2.

   Table 7 – Structural coordinates for core 2C (human)

   Table 8 – Structural coordinates for core 3.

9. A model as claimed in claim 2 wherein the ligand binding domain associates with a diphosphate of a sugar nucleotide donor and comprises (a) atomic interaction 7 listed in Table 10 (GnT1 Table); (b) at least two of atomic interactions 9, 10, 11, 12, and 13 listed in Table 12 (Core 2L Table); (c) at least two of atomic interactions 11, 12, 13, 14, and 15 listed in Table 13 (Core2b/M); or (d) atomic interaction 8 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the diphosphate of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase.

10. A model as claimed in claim 2 wherein the ligand binding domain associates with a heterocyclic amine base, preferably uracil, of a sugar nucleotide donor and comprises at least two of the following atomic interactions (a) 1, 2, 3, and 4 listed in Table 10 (GnT1 Table); (b) 1, 2, 3, 4, 5 listed in Table 12 (Core 2L Table); (c) 1, 2, 3, and 4 listed in Table 13 (Core2b/M); or (d) 1, 2, 3, and 4, listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the heterocyclic amine base of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase.

11. A model as claimed in claim 2 wherein the ligand binding domain associates with a sugar, preferably ribose, of the nucleotide of a sugar nucleotide donor and comprises atomic interactions 5 and 6 listed in Table 10 (GnT1 Table); at least two of atomic interactions 6, 7, and 8 listed in Table 12 (Core 2L Table), or atomic interaction 5 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the sugar of the nucleotide of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase.

12. A model as claimed in claim 2 wherein the ligand binding domain associates with the sugar, preferably GlcNAc, of a sugar nucleotide donor and comprises at least two of atomic interactions 8, 9, 10, 11, or 12 listed in Table 10 (GnT1 Table); at least two of atomic interactions 14, 15, 16, 17, and 18 listed in Table 12 (Core 2L Table), atomic interactions 16 and/or 17 listed in Table 13 (Core2b/M), or at least two of atomic interactions 9, 10, 11, 12 and 13 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the sugar of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase.

13. A model as claimed in claim 2 wherein the ligand binding domain associates with UDP and is characterized by (a) a hydrogen bond between an Asp side chain of the glycosyltransferase with position 3 of the uracil ring of UDP; (b) a stacking interaction between either a disulfide or an aromatic group (Phe or Tyr) of the glycosyltransferase and the uracil ring of the UDP; (c) a stacking interaction between either an Ile or a Thr of the glycosyltransferase and the ribose ring of the UDP; and (d) metal mediated charge interactions between a well-conserved Asp/Glu of the glycosyltransferase and a pyrophosphate oxygen of the UDP.

14. A model as claimed in claim 2 wherein the ligand binding domain associates with a nucleotide, preferably UDP, of a sugar nucleotide donor comprising at least two of (a) atomic interactions 1, 2, 3, 4, 5, 6, andr 7 listed in Table 10 (GnT1 Table); (b) atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, and 13 listed in Table 12 (Core 2L Table); (c) atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, and 15 listed in Table 13 (Core2b/M); or (d) atomic interactions 1, 2, 3, 4, 5, 6, 7, and 8 listed in Table 11 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the nucleotide of the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase.

15. A model as claimed in claim 2 wherein the ligand binding domain associates with a sugar nucleotide donor, preferably UDP-GlcNAc comprising at least two of (a) atomic interactions 1, 2,3, 4, 5, 6, 7, 8, 9, 10, 11, and 12 listed in Table 10 (GnT1 Table); (b) atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, and 18 listed in Table 12 (Core 2L Table); (c) atomic interactions 1, 2, 3, 4, 5, 6, 9, 10, 11, 12, 13, 14, 15, 16, and 17 listed in Table 13 (Core2b/M), or (d) atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10,

11, 12, and 13 listed in Table 13 (GNTV Table), each atomic interaction defined therein by a residue (more preferably a specific atom where indicated) on the sugar nucleotide donor and an amino acid, (more preferably a specific atom where indicated), on the glycosyltransferase.

16. A model as claimed in claim 2 wherein the ligand binding domain is a loop structure that associates with a pyrophosphate of a sugar nucleotide donor comprising the structural coordinates for the loop structure of GnT1 listed in Table 21; Core 2L listed in Table 22; or GnTV listed in Table 24.

17. A model as claimed in claim 6 wherein the ligand binding domain is a GlcNAc transition state ligand binding domain of a glycosyltransferase comprising a hydrophobic pocket that is 1.9 to 3.5 Å, preferably 2.2 to 3.0Å, from the pyrophosphate binding cavity for the glycosyltransferase.

18. A model as claimed in claim 17 wherein the ligand binding domain is further characterized as follows: amino acid residues in the domain that associate with C2 and C4 positions of the sugar comprise the structural coordinates of Leu-331, and Leu 269 in Table 1, or the structural coordinates of Leu –116 and Val-81 of Table 3, 4, or 5.

19. A model as claimed in claim 18 wherein the ligand binding domain comprises atomic interactions 14 to 18 in Table 12, atomic interactions 9 to 12 of Table 10, or the particular structural coordinates for the atoms of the atomic contacts of the atomic interactions as set out in Tables 1, 3, 4, or 5.

20. A model according to any preceding claims in association with a ligand or substrate.

21. A computer readable medium having stored thereon a model according to any preceding claim.

22. A computerized representation of a model according to any of the preceding claims.

23. A method of screening for a ligand capable of binding a ligand binding domain of a glycosyltransferase comprising the use of a model according to any preceding claim.

24. A ligand identified by a method according to claim 23.

25. A ligand according to claim 24 that is capable of associating with one or more atomic contacts of a glycosyltransferase as shown in Table 10, 11, 12, or 13.

26. A method of identifying a modulator of a glycosyltransferase or a ligand binding domain thereof comprising the step of using the structural coordinates of a glycosyltransferase or a ligand binding domain thereof as shown in Table 1, 2, 3, 4, 5, 6, 7, or 8, or a model according to any preceding claim to computationally evaluate a test compound for its ability to associate with the glycosyltransferase or binding domain or binding site thereof.

27. A method for identifying a potential modulator of a glycosyltransferase by determining binding interactions between a test compound and atomic contacts of a model of a ligand binding domain of a glycosyltransferase as claimed in any preceding claim comprising:

(a) generating the atomic contacts on a computer screen;

(b) generating test compounds with their spatial structure on the computer screen; and

(c) determining whether the compounds associate or interact with the atomic contacts defining the glycosyltransferase;

(d) identifying test compounds that are potential modulators by their ability to enter into a selected number of atomic contacts.

28. A method for identifying a potential modulator of a glycosyltransferase function by docking a computer representation of a test compound with a computer representation of a model of a glycosyltransferase or a ligand binding domain as claimed in any preceding claim.

29. A method for the design of ligands for glycosyltransferase based on a secondary, tertiary, or quanternary structure or model of a sugar nucleotide donor or part thereof comprising using the structural coordinates shown in Table 14, 15, or 16.

30. A method as claimed in claim 29 comprising (a) generating a computer representation of a sugar nucleotide donor, or part thereof, defined by the structural coordinates shown in Table 14, 15, or 16; (b) searching for molecules in a data base that are similar to the defined sugar nucleotide donor, or part thereof, using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

31. A method as claimed in claim 30 comprising one or more of the following additional steps:

(a) testing whether the ligand is a modulator of the activity of a glycosyltransferase in cellular assays and animal model assays;

(b) modifying the ligand;

(c) optionally rerunning steps (a) or (b); and

(d) preparing a pharmaceutical composition comprising the modulator.

32. A method for designing potential modulators that are inhibitors of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L GnT, comprising the step of using one or more (preferably all) of the structural coordinates of uracil, uridine, ribose, pyrophosphate, or UDP of Tables 14, 15 or 16, as follows:

Table 14 for GnT1 Ground State

Table 15 for GntV

Table 16 for core 2L

to generate a compound for associating with a ligand binding domain of a glycosyltransferase that associates with uracil, uridine, ribose, pyrophosphate, or UDP.

33. A method for generating a compound for associating with the active site of a glycosyltransferase comprising the following steps: (a) generating a computer representation of uracil, uridine, or UDP defined by structural coordinates of Tables 14, 15 or 16; (b) searching for molecules in a data base that are structurally or chemically similar to the defined uracil, uridine, or UDP using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound-building computer program.

34. A method for designing potential modulators that are inhibitors of a glycosyltransferase preferably GnT I, GnT V. and/or Core 2L GnT, comprising the step of using one or more (preferably all) of the structural coordinates of UDP-GlcNAc of Tables 17, 18, or 19 as follows:

Table 17 for GnT1 transition state

Table 18 for GnTV

Table 19 for core 2 L transition state

to generate a compound for associating with a ligand binding domain of a glycosyltransferase that associates with UDP-GlcNAc.

35. A method for designing potential modulators that are inhibitors of a glycosyltransferase preferably GnT I, GnT V, and/or Core 2L GnT, comprising : (a) generating a computer representation of UDP-GlcNAc defined by the one or more (preferably all) of the structural coordinates of Table 17, 18, or 19 appropriate for a specific glycosyltransferase; (b) searching for molecules in a data base that are structurally or chemically similar to the defined UDP-GlcNAc using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

36. A method for designing potential modulators that are inhibitors of GnT I comprising the step of using one or more (preferably all) of the structural coordinates of Table 20 for an oligosaccharide acceptor, to generate a compound for associating with a ligand binding domain of a glycosyltransferase that associates with the acceptor.

37. A method as claimed in claim 36 comprising: (a) generating a computer representation of an oligosaccharide acceptor defined by the one or more (preferably all) of the structural coordinates of Table 20 appropriate for a specific glycosyltransferase; (b) searching for molecules in a data base that are structurally or chemically similar to the defined oligosaccharide acceptor using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

38. A modulator identified by a method of claim 27, 28, 31, 32, 34, 35, 36, or 37.

39. A modulator of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L GnT, comprising the structure of uracil, uridine, ribose, pyrophosphate, or UDP with one or more (preferably all) of the structural coordinates of uracil, uridine, ribose, pyrophosphate, or UDP of Tables 14, 15 or 16 as follows:

Table 14 for Gnt1 Ground State

Table 15 for GnTV

Table 16 for core 2L

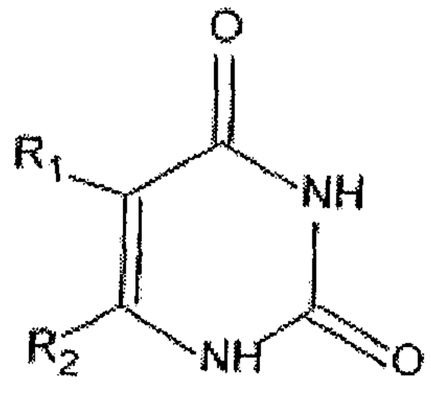
40. A modulator of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L GnT, comprising the structure of UDP-GlcNAc and having one or more (preferably all) of the structural coordinates of UDP-GlcNAc of Tables 17, 18, or 19 as follows:

Table 17 for GnT1 transition state

Table 18 for GnTV,

Table 19 for core 2L

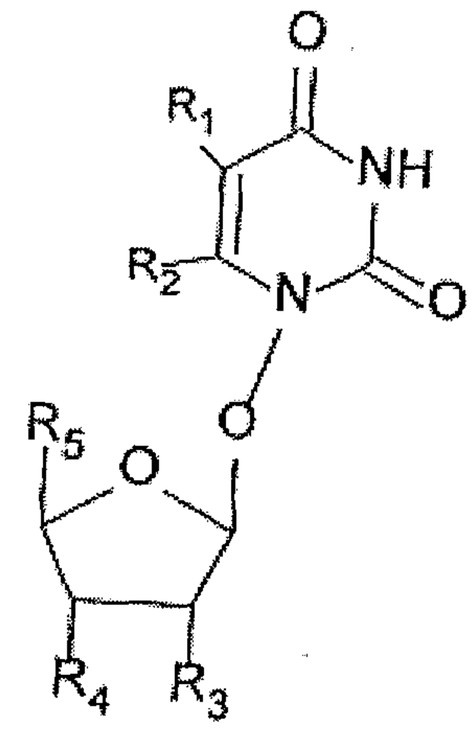
41. A modulator of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L, of the Formula I having the structural coordinates of uracil of Table 14, 15 or 16



wherein R_1 and R_2 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, pyrophophate, gallic acid, phosphonates, thioamide, and $-OR_{10}$ where R_{10} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring;

and salts and optically active and racemic forms of a compound of the formula I.

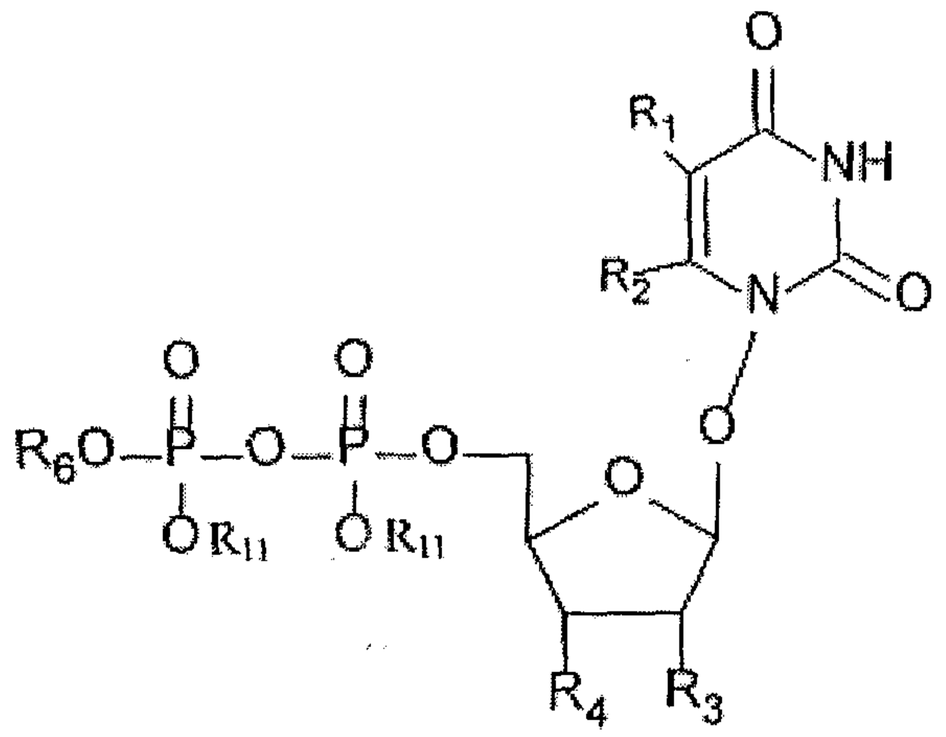
42. A modulator of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L, of the formula II having the structural coordinates of uridine of Table 14, 15, or 16



wherein R_1, R_2, R_3, R_4, and R_5 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, pyrophosphate, gallic acid, phosphonates, thioamide, and $-OR_{10}$ where R_{10} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring,

and salts and optically active and racemic forms of a compound of the formula II.

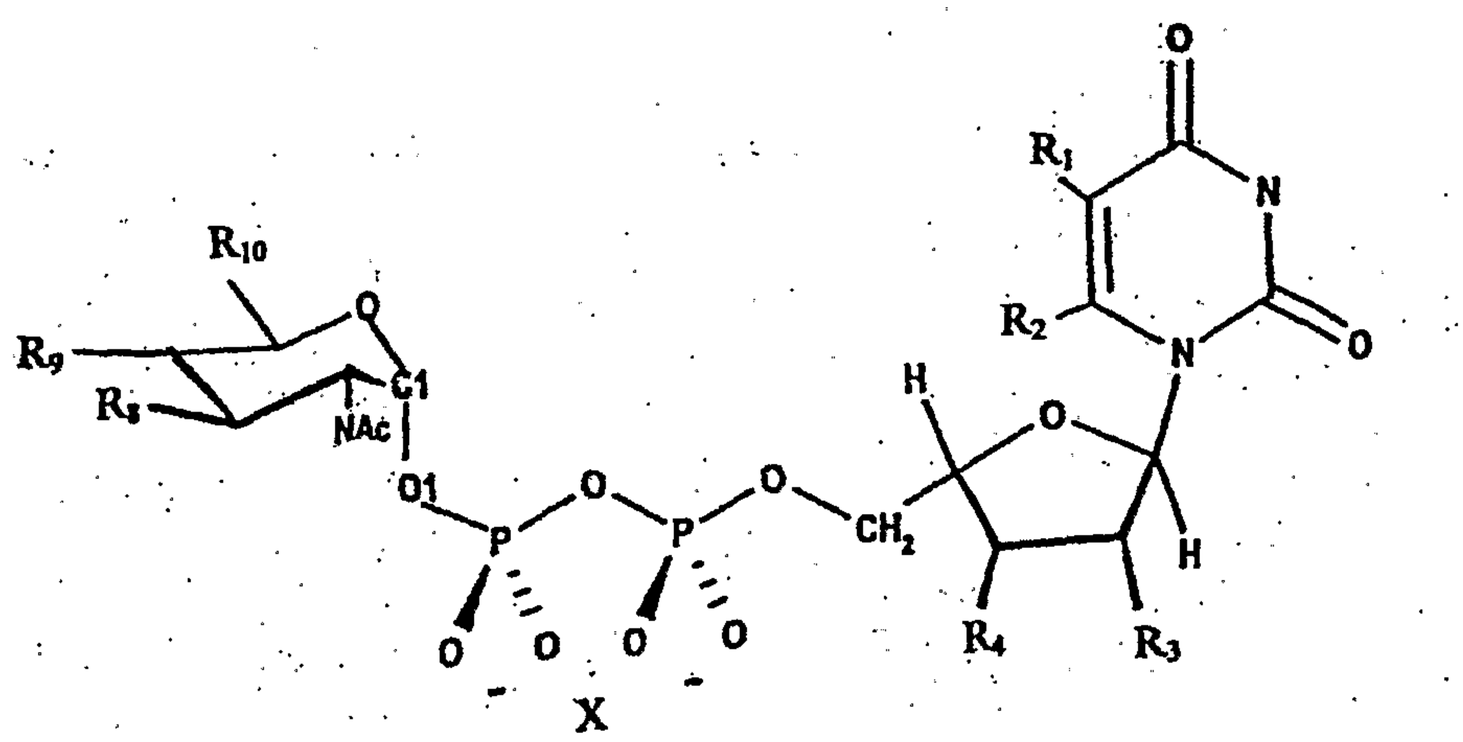
43. A modulator of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L of the formula III having the structural coordinates of UDP of Tables 14, 15, or 16



wherein R_1, R_2, R_3, R_4, R_5, and R_6 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, gallic acid, phosphonates, thioamide, and $-OR_{10}$ where R_{10} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring, R_6 may be a monosaccharide or disaccharide, preferably a monosaccharide, including GlcNAc, glucose, and mannose,

and salts and optically active and racemic forms of a compound of the formula III.

44. A modulator of a glycosyltransferase, preferably GnT I, GnT V, and/or Core 2L of the formula IV having the structural coordinates of UDP-GlcNAc of Table 17, 18, or 19



wherein R_1, R_2, R_3, R_4, and R_5 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate,

gallic acid, phosphonates, thioamide, and $-OR_{10}$ where R_{10} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring,

and salts and optically active and racemic forms of a compound of the formula IV.

45. A modulator of a glycosyltransferase comprising the structure of an acceptor of a glycosyltransferase, preferably as shown in Figure 19A or 33, and the structural coordinates as shown in Table 20.

46. A modulator of a transition state of a glycosyltransferase comprising the structural coordinates of GlcNAc in the transition state of a reaction catalyzed by a glycosyltransferase, preferably Core 2 GnT-L and GnT-I, wherein the GlcNAc has a half chair or distorted chair conformation, a partial double bond between C1 and 05, and a hybridization Sp^2 at C1.

47. A modulator as claimed in claim 46 wherein the GlcNAc is directly or indirectly linked to a pyrophosphate group and the distance between the pyrophosphate group and the GlcNAc is about 1.9 to 3.5 Å, preferably 2.2 to 3.0Å.

48. A peptide of the following formula which interferes with the association of the loop structure of a Core 2 transferase and a pyrophosphate group of a sugar nucleotide donor for the Core 2 transferase:

$$X\text{-}X^1\text{-}X^2\text{-}X^3\text{-}X^4$$

wherein X represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids, X^1 and X^2 independently represent an amino acid with a charged polar group, preferably Glu, Asp, Asn, or Gln, X^3 represents a basic amino acid, preferably Arg, His, or Lys, and X^4 represents 0 to 70, preferably 0 to 50 amino acids, more preferably 2 to 20 amino acids.

49. A pharmaceutical composition comprising a ligand or modulator according to any preceding claim, and optionally a pharmaceutically acceptable carrier, diluent, excipient, or adjuvant or any combination thereof.

50. A method of treating and/or preventing disease comprising the step of administering a ligand or modulator according to any preceding claim or pharmaceutical composition comprising a modulator to a mammalian patient.

51. A method of treating a disease associated with a glycosyltransferase with inappropriate activity in a cellular organism, comprising:

(a) administering a modulator as claimed in any of the preceding claims in an acceptable pharmaceutical preparation; and

(b) activating or inhibiting a glycosyltransferase to treat the disease.

52. Use of a modulator as claimed in any of the preceding claims in the preparation of a medicament to treat a disease associated with a glycosyltransferase with inappropriate activity in a cellular organism.

53. Use of the structural coordinates of a glycosyltransferase as shown in Table 1, 2, 3, 4, 5, 6, 7, or 8 in the manufacture of a medicament.

54. A computer for producing a model or three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a glycosyltransferase or ligand binding domain thereof defined by structural coordinates of glycosyltransferase amino acids or a ligand binding domain thereof, or comprises structural coordinates of atoms of a ligand or substrate, or a three-dimensional representation of a homologue of said molecule or molecular complex, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates of glycosyltransferase amino acids according to Table 1, 3, 4, 5, 6, 7, or 8 or a ligand binding domain thereof, or a ligand according to any one of Table 14 through 23;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

55. A method of conducting a drug discovery business comprising:

(a) providing one or more systems or methods for identifying modulators based on a model according to any preceding claim;

(b) conducting therapeutic profiling of modulators identified in step (a), or further analogs thereof, for efficacy and toxicity in animals; and

(c) formulating a pharmaceutical composition including one or more agents identified in step (b) as having an acceptable therapeutic profile.

56. A method as claimed in claim 55 including establishing a distribution system for distributing the pharmaceutical composition for sale, and optionally establishing a sales group for marketing the pharmaceutical composition.

57. A method of conducting a target discovery business comprising:

(a) providing one or more system or method for identifying modulators based on a model as claimed in any preceding claim;

(b) optionally conducting therapeutic profiling of modulators identified in (a) for efficacy and toxicity in animals; and

(c) licensing to a third party the rights for further drug development and/or sales for agents identified in step (a), or analogs thereof.

FIGURE 1 (a)

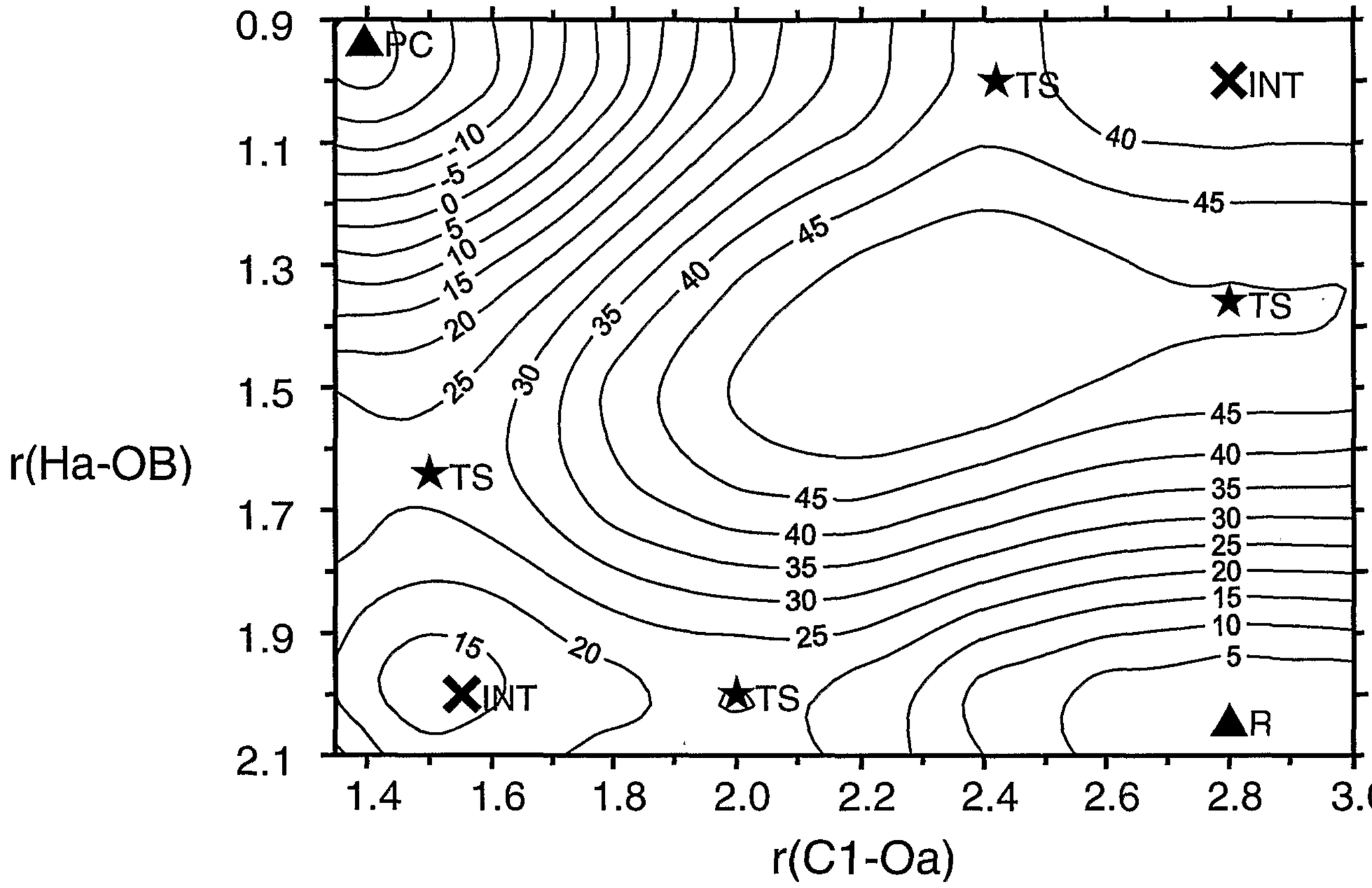

PC
TS
INT
TS
TS
INT
TS
R
-10
-5
0
5
10
15
20
25
30
35
40
45
0.9
1.1
1.3
1.5
1.7
1.9
2.1
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
r(Ha-OB)
r(C1-Oa)

FIGURE 1 (b)

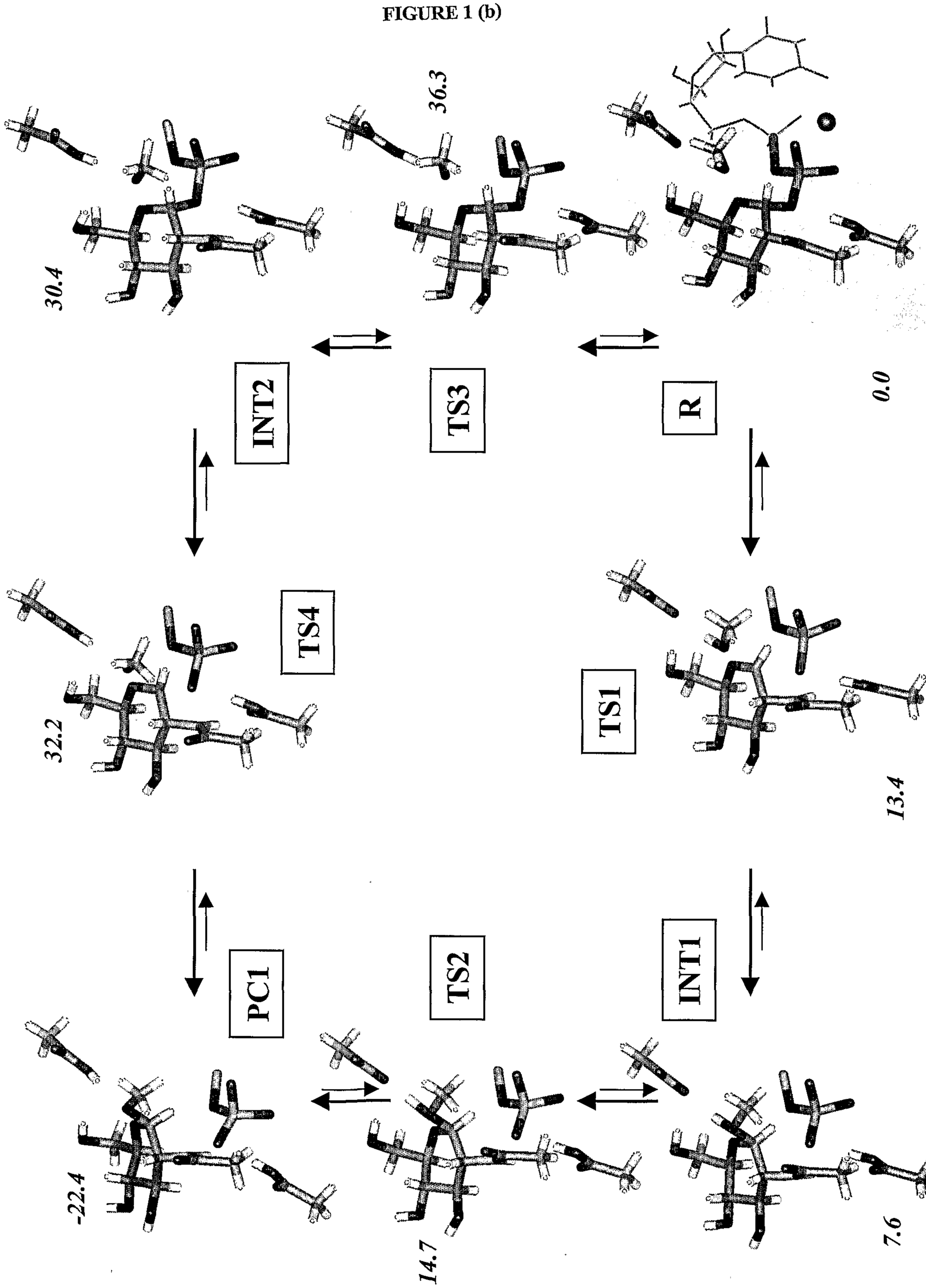


FIGURE 2 (a)

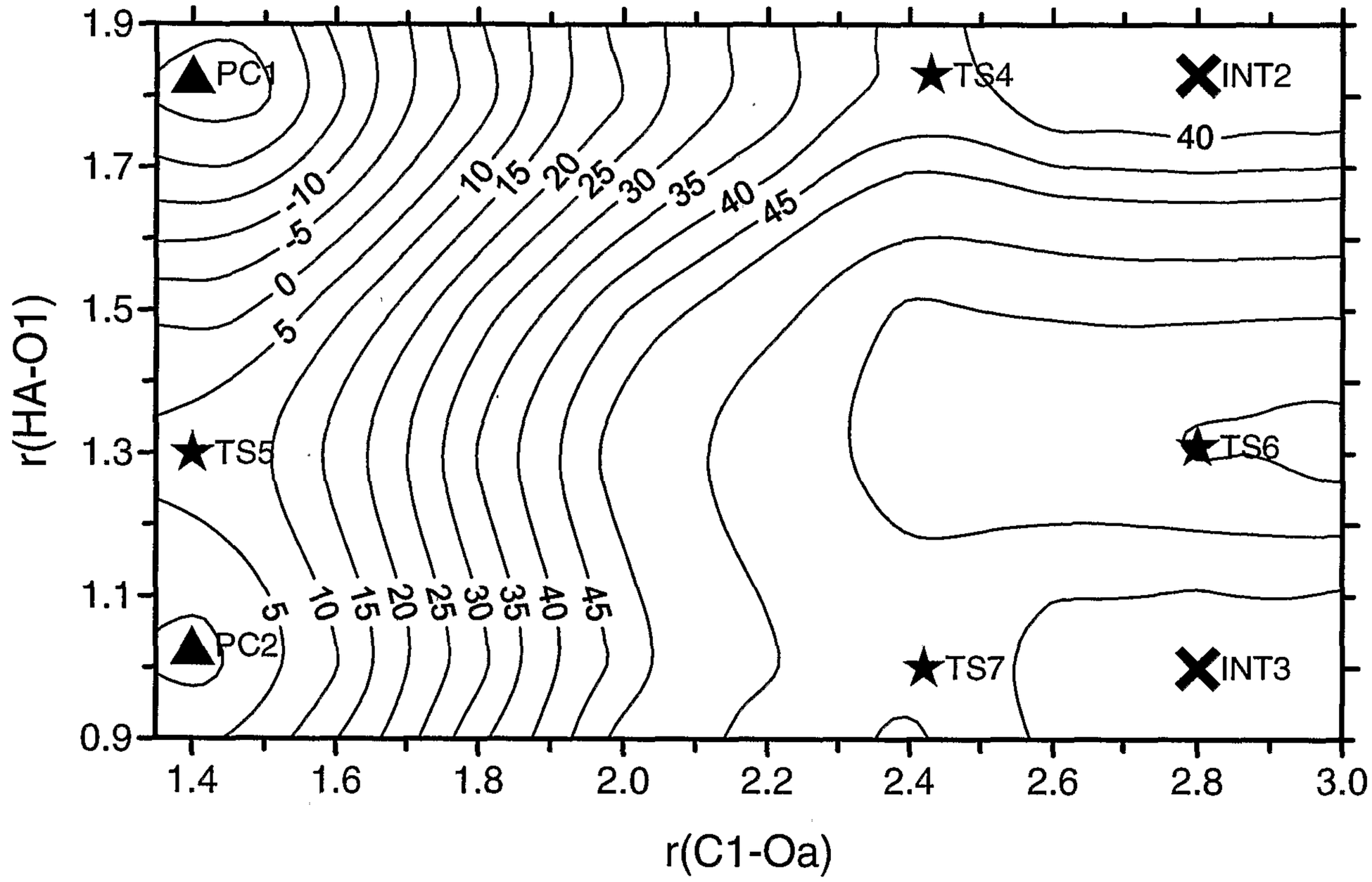

PC1
TS4
INT2
TS5
TS6
PC2
TS7
INT3
-10
-5
0
5
10
15
20
25
30
35
40
45
1.9
1.7
1.5
1.3
1.1
0.9
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
r(HA-O1)
r(C1-Oa)

FIGURE 2 (b)

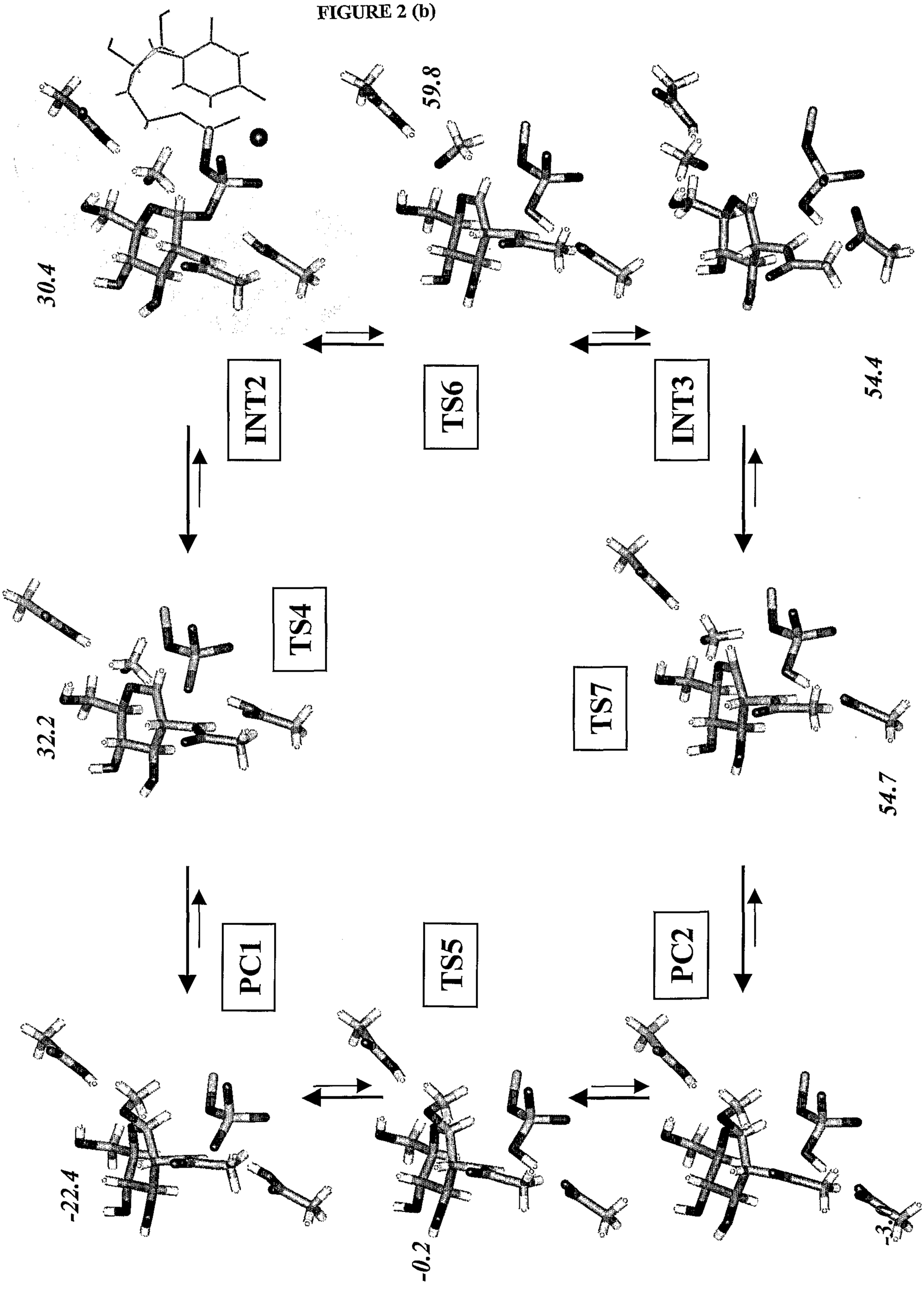


FIGURE 3 (a)

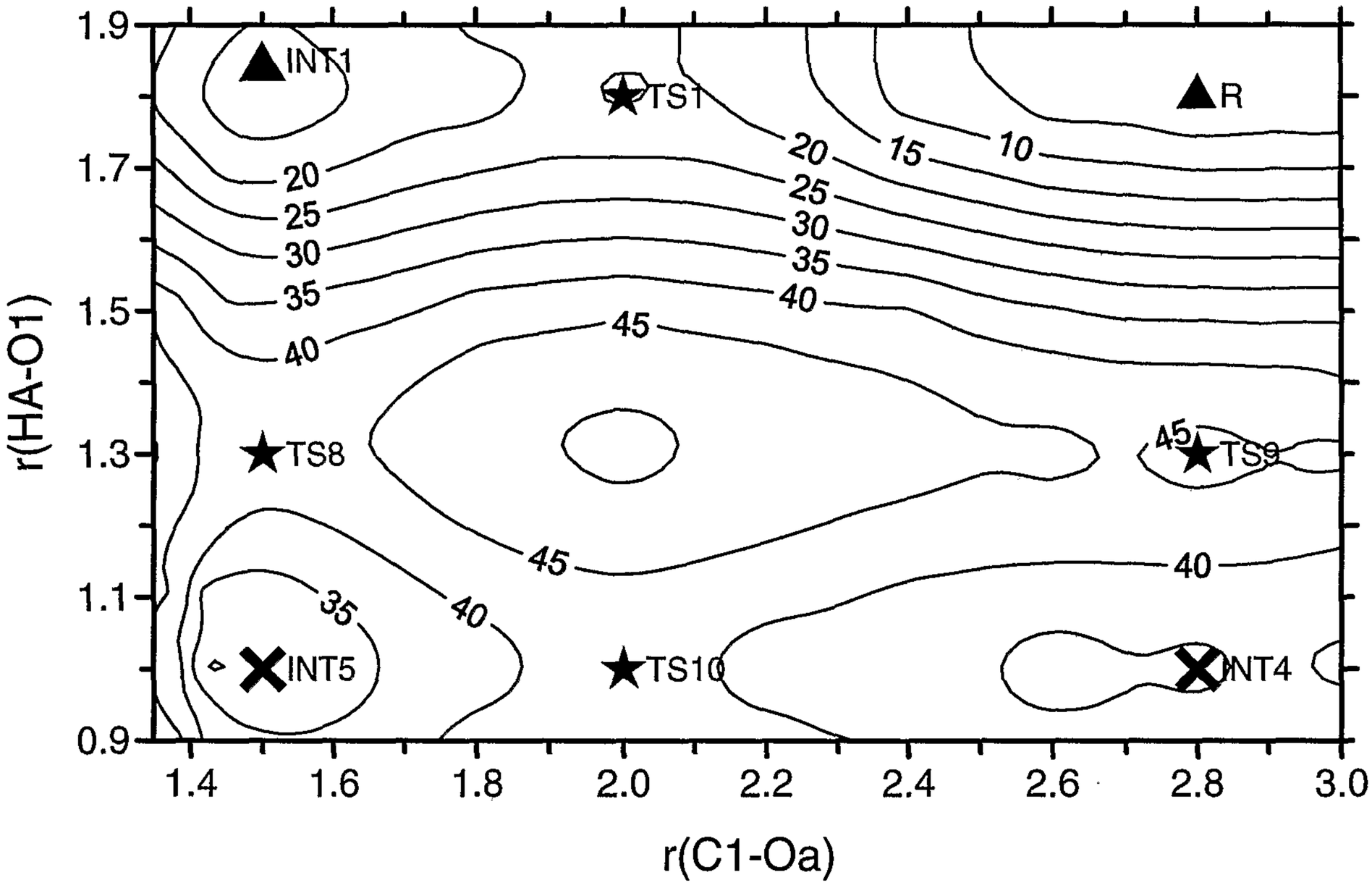

INT1
TS1
R
TS8
TS9
INT5
TS10
INT4
20
25
30
35
40
45
15
10
r(HA-O1)
r(C1-Oa)
1.9
1.7
1.5
1.3
1.1
0.9
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0

FIGURE 3 (b)

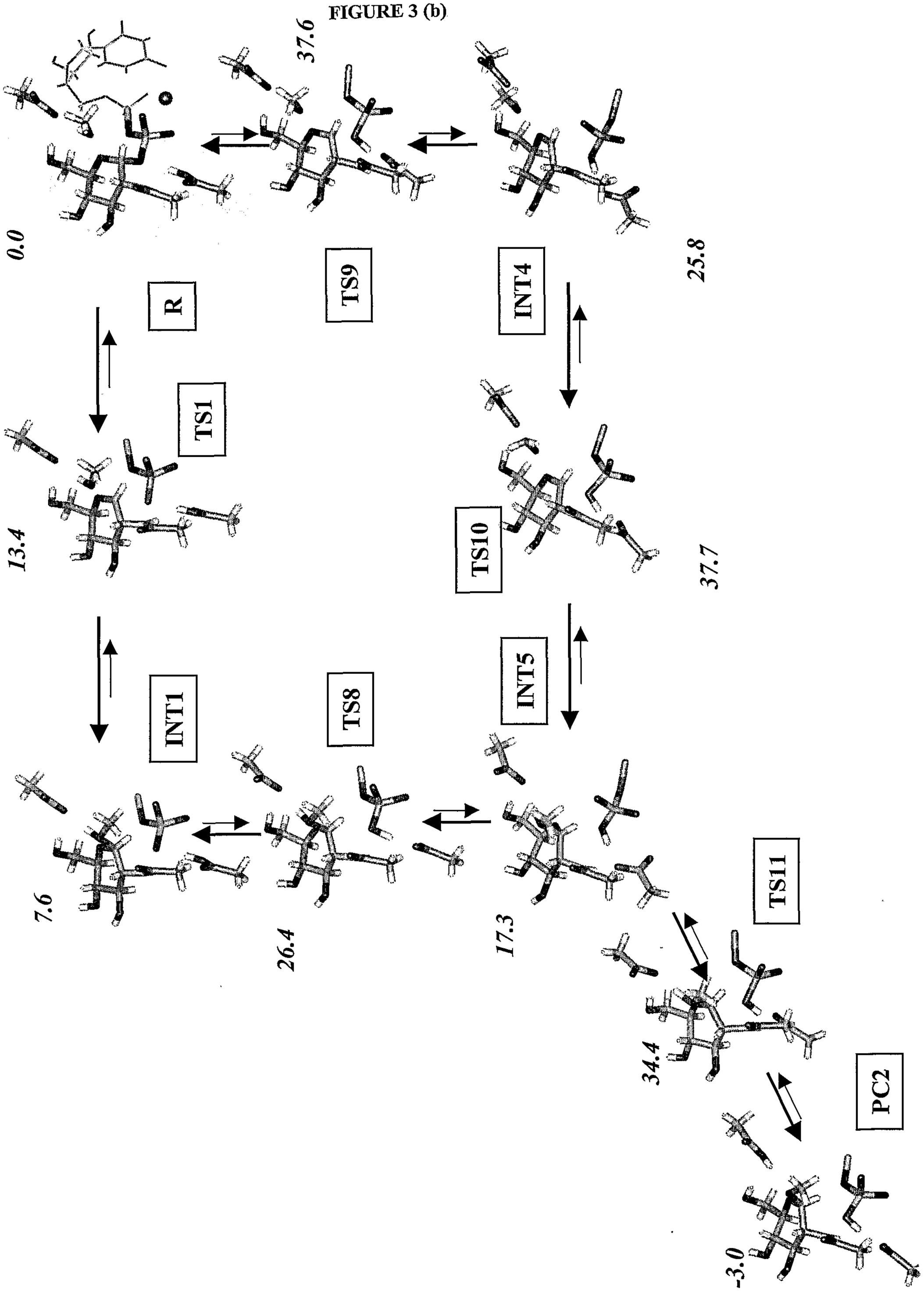
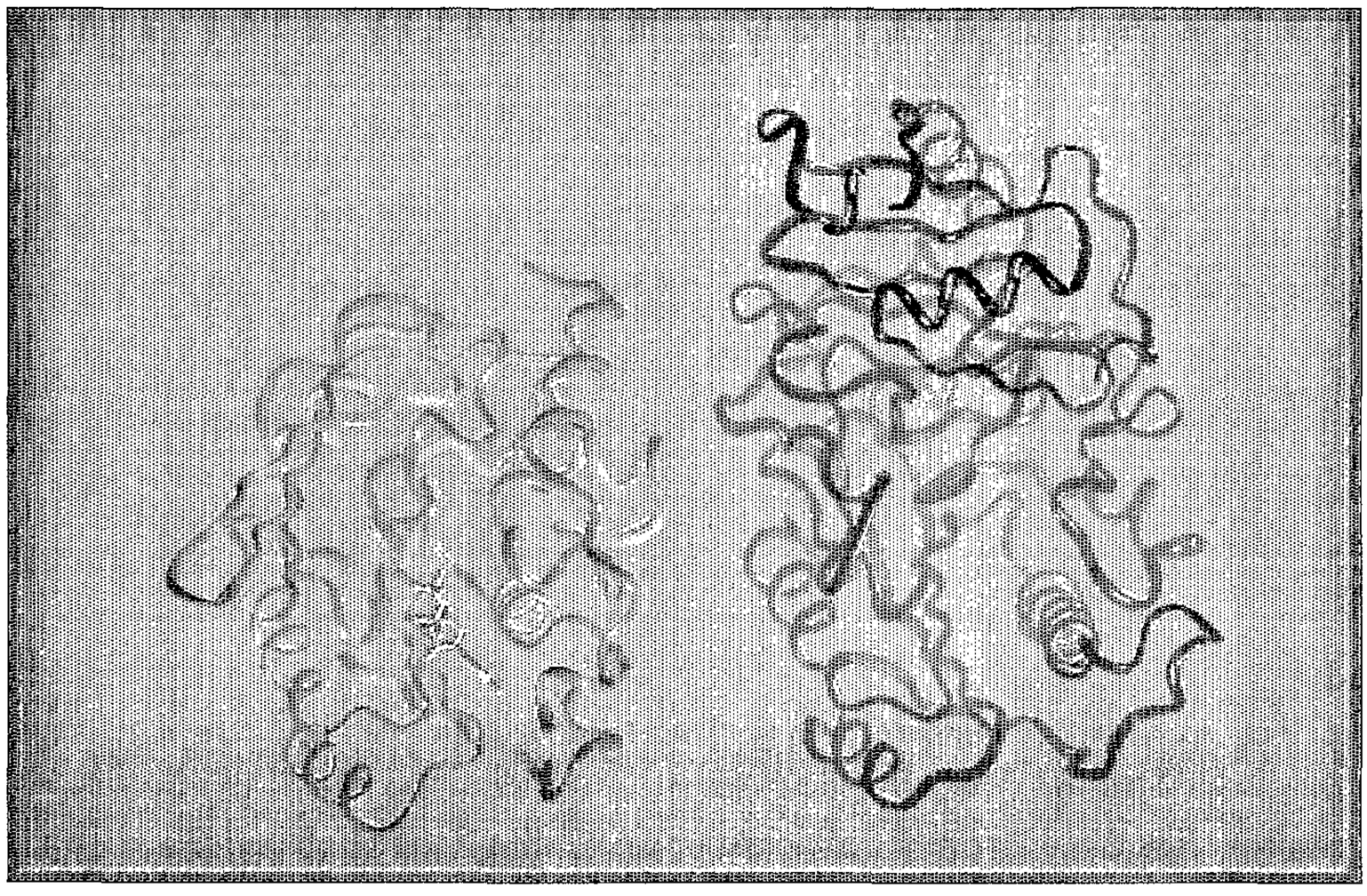

0.0
37.6
25.8
13.4
R
TS1
TS9
INT4
TS10
37.7
INT1
TS8
INT5
7.6
26.4
17.3
TS11
34.4
PC2
-3.0

FIGURE 4

(a)



(b)

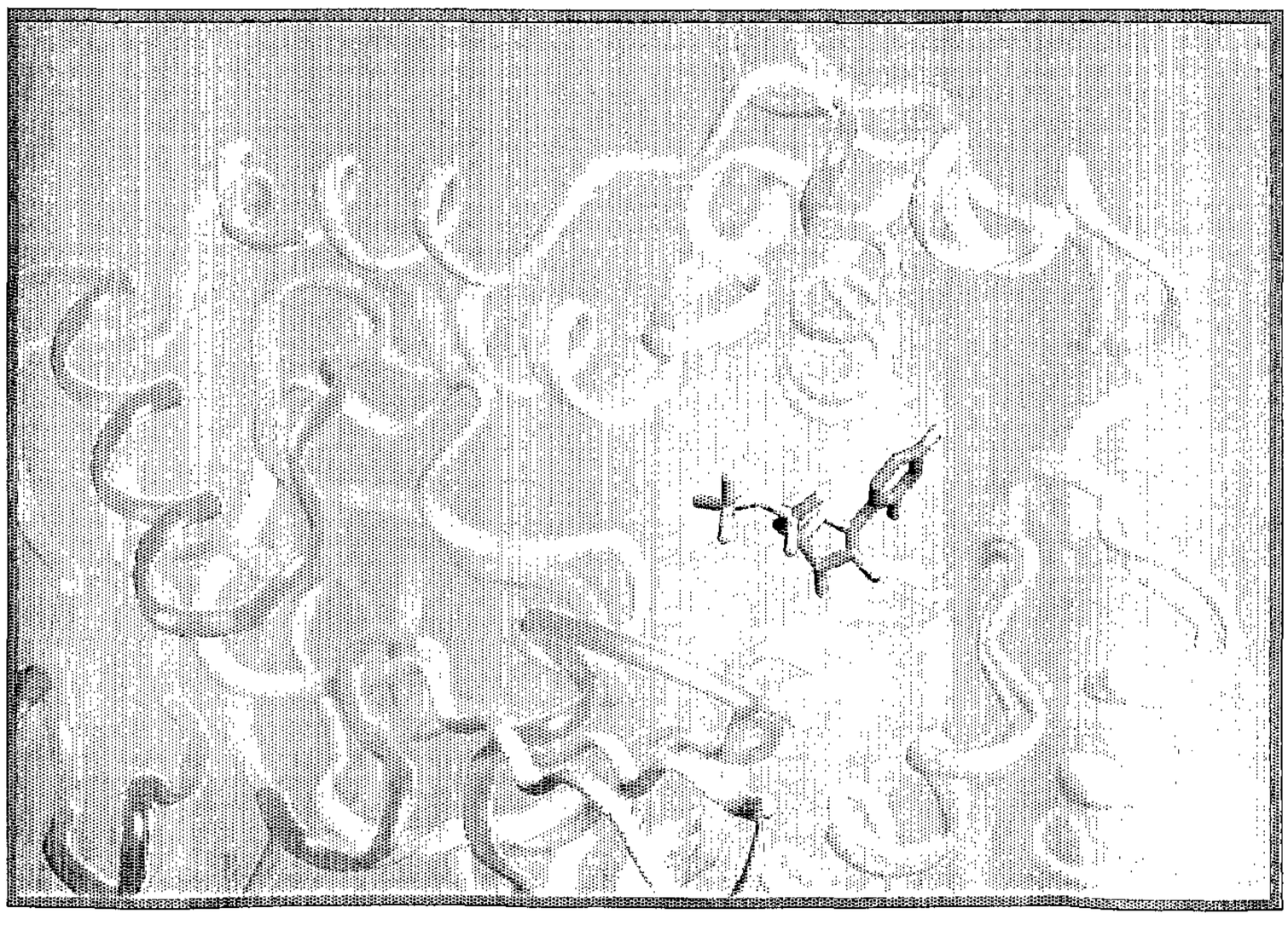


FIGURE 5

GNT1_D (105) LAVI-PILVIACDR------STVRRC-LDKL-LHY--RPSAELF--PIIVSQDC (145)
CORE2 (1) lagenpssdincktkvlqgdvneiqkvkleiltvkfkkrprwt-pddyinmtsdc (53)
GNT1_D (146) GHEETAQVIASYGSAVTHIRQPDLSNIAVQPDHRKFQGYYKIARH----YRWAL (195)
CORE2 (54) s----------sfikrrkyivep-lskeeaef----playsivvhhkiemldrll (93)
GNT1_D (196) GQI--FHNFNYPAAVVV--EDD-LEVAPDFFEYFQATYP---LLKADPSLWC-V (240)
CORE2 (94) raiympqnf-ycvhvdtksedsyllaavmgiascfsnvfvasrlesvvyaswsrv (146)
GNT1_D (241) SAWNDNG--KE--QMVDSSKPEL-LYRTDFF----PGLGW---LLLAELWAELE (282)
CORE2 (147) qa--dlncmkdlyamsanwkylinlcgmdfpiktnleivrklkllmge--nnle (196)
GNT1_D (283) PKW-P--KAFWDDWMRRPEQRKGRACVRPEISRTMTFG|HLKFIKLNQQFVPFT (344)
CORE2 (197) termpshke--erwkkryevvngk------ltntgt-------vkm----lpp-(gap)
GNT1_D (345) QLDLSYL-QQEAYDRDFL-ARVYGAPQLQVEKV-----RTNDRKELGE-VRVQY (390)
CORE2 (gap) -le-tplfsgsay---fvvsreyvgyvlqnekiqklmewaqdtyspdeylwa--(gap)
GNT1_D (391) TGRDSFKAFAKALGV----MDDLKSGV-P--RAGYRGIVT----FLF-RGRRVH (432)
CORE2 (278) tiqripevpgslpashkydlsdmqavarfvkwqyfegdvskgapyppcdgvhvr (331)
GNT1_D (gap) -LAPPQTWDGYDPSWT|?|?|?|?|? (452)
CORE2 (332) svcifga--g-dlnwm-l-r-k-h-hlfankfdvdvdlfaiqcldehlrhkale (377)

FIGURE 6

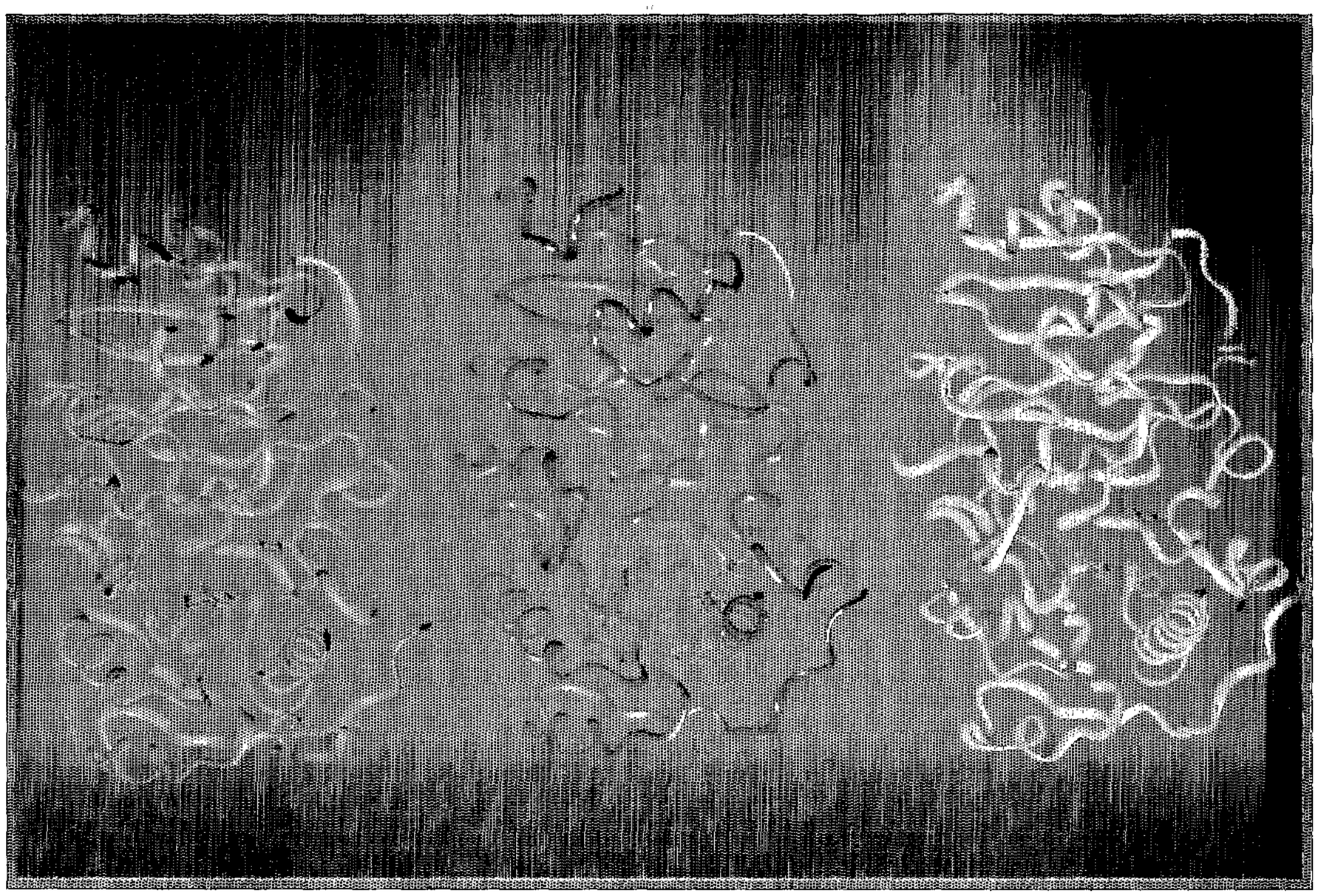


FIGURE 7.

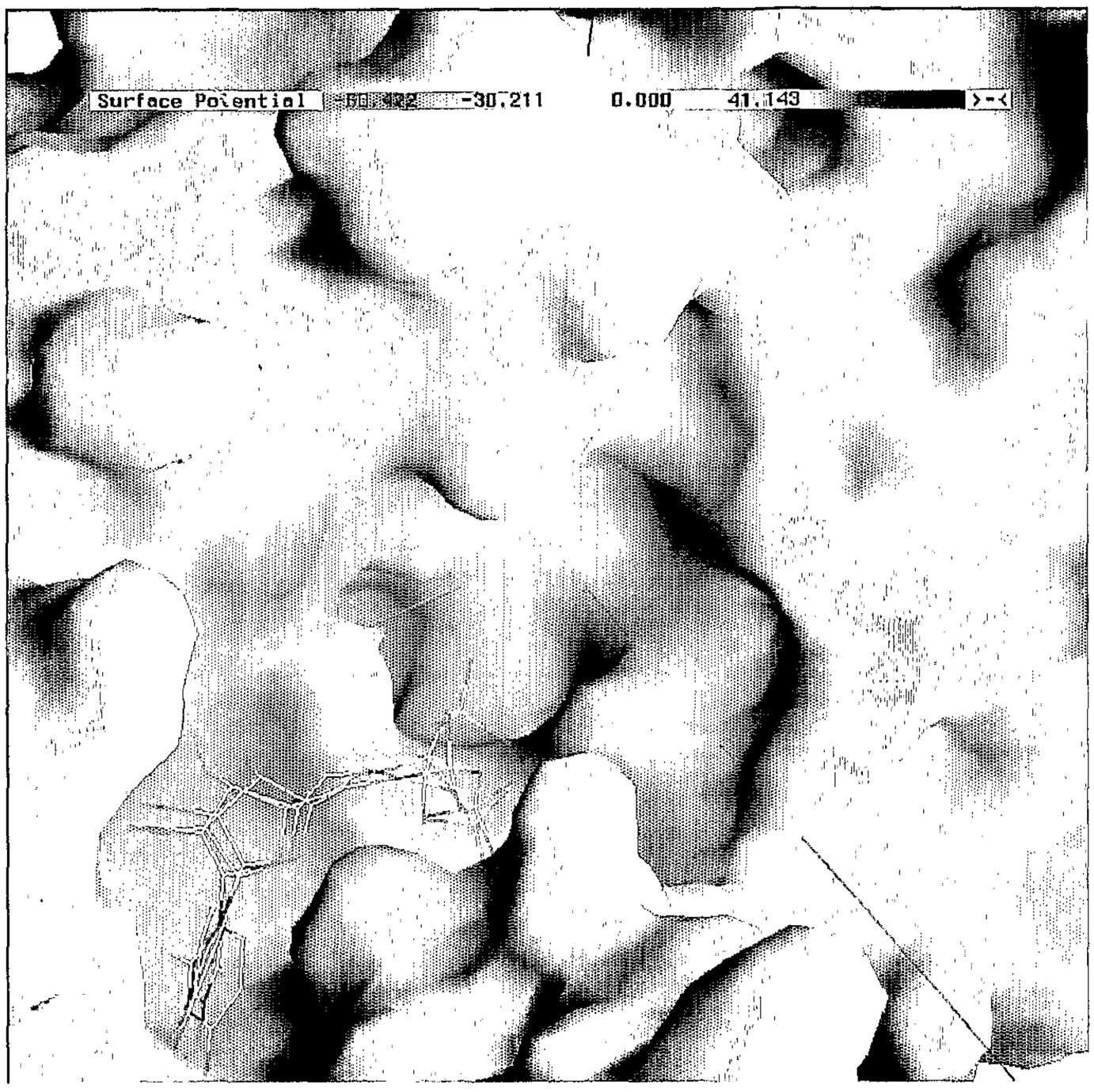


FIGURE 8

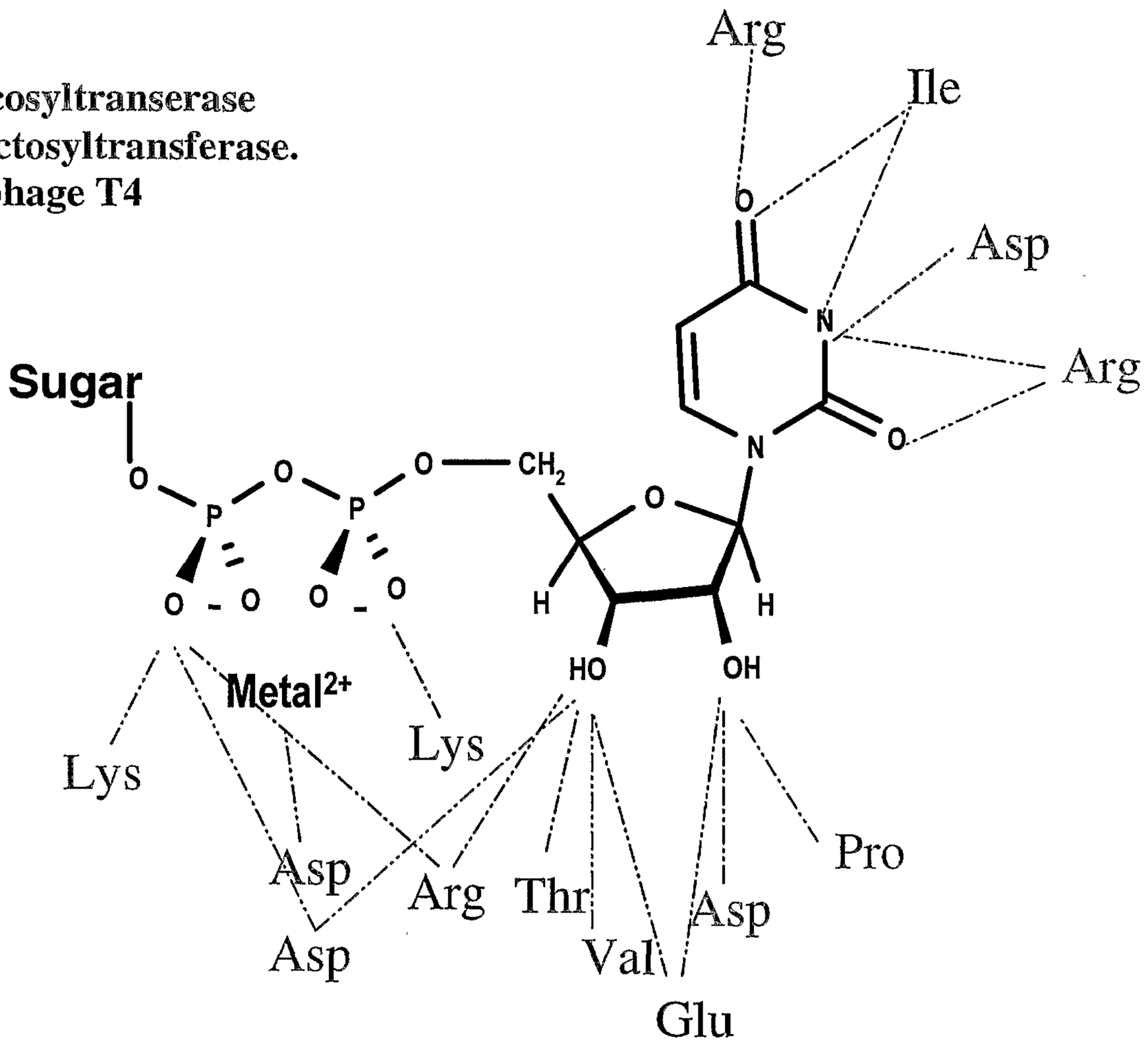

SpsA glycosyltranserase
β1,4-galactosyltransferase.
Bacteriophage T4
Sugar
Metal2+
Lys
Lys
Asp
Asp
Arg
Thr
Val
Glu
Asp
Pro
Arg
Asp
Arg
Ile
N
N
O
O
O
O
O
O
O
O
P
P
CH2
H
H
HO
OH

FIGURE 9/

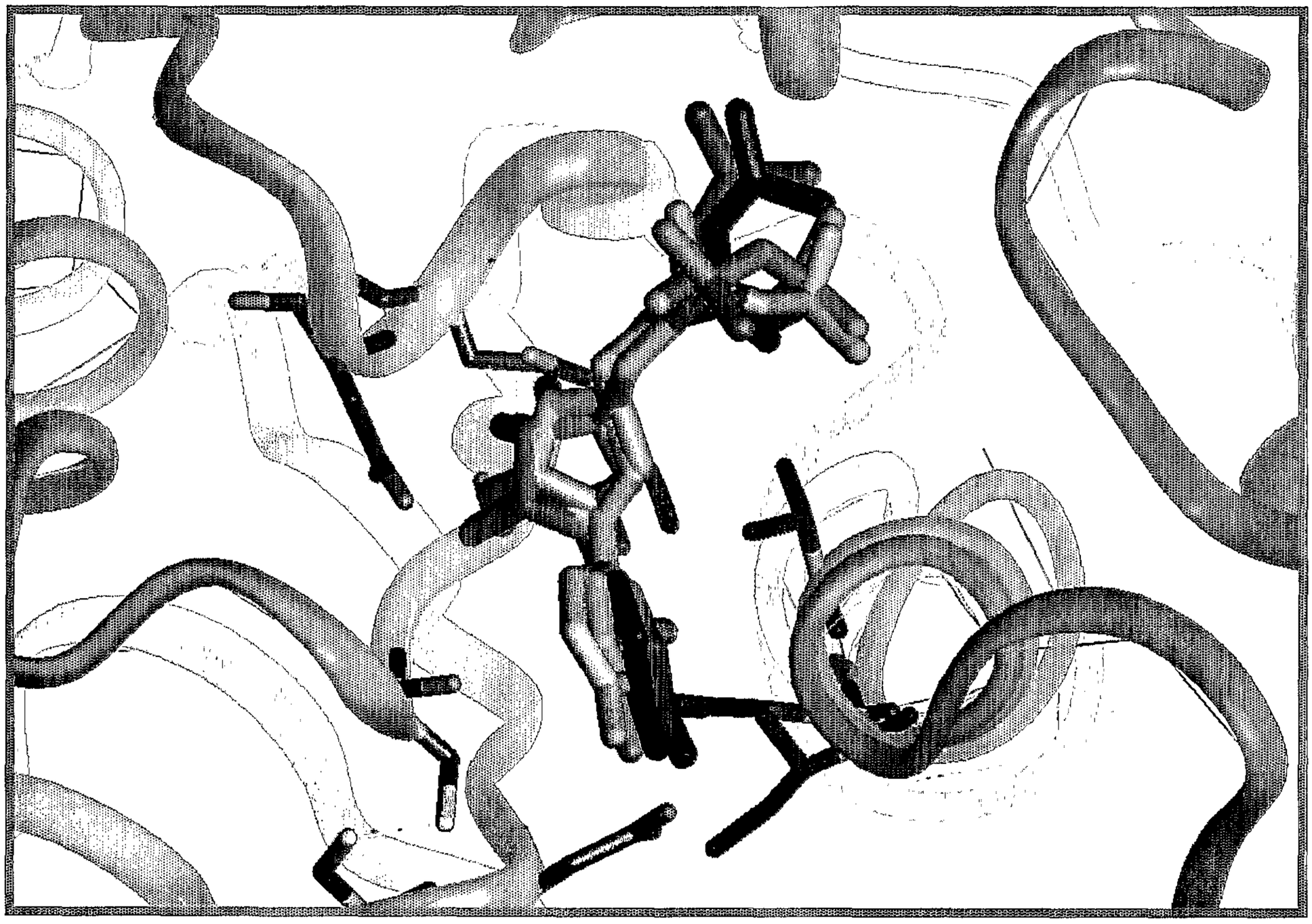
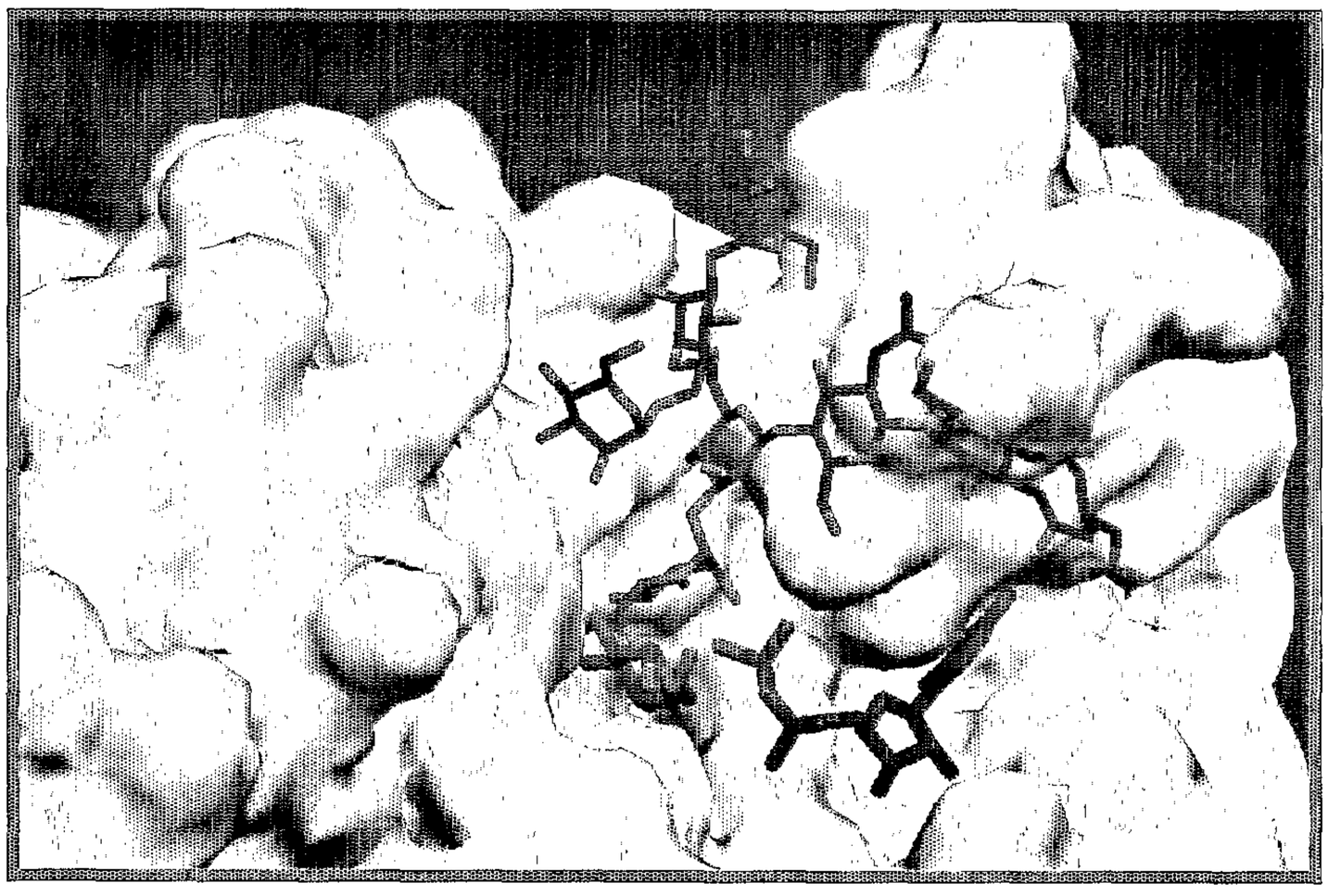


FIGURE 10

(a)



(b)

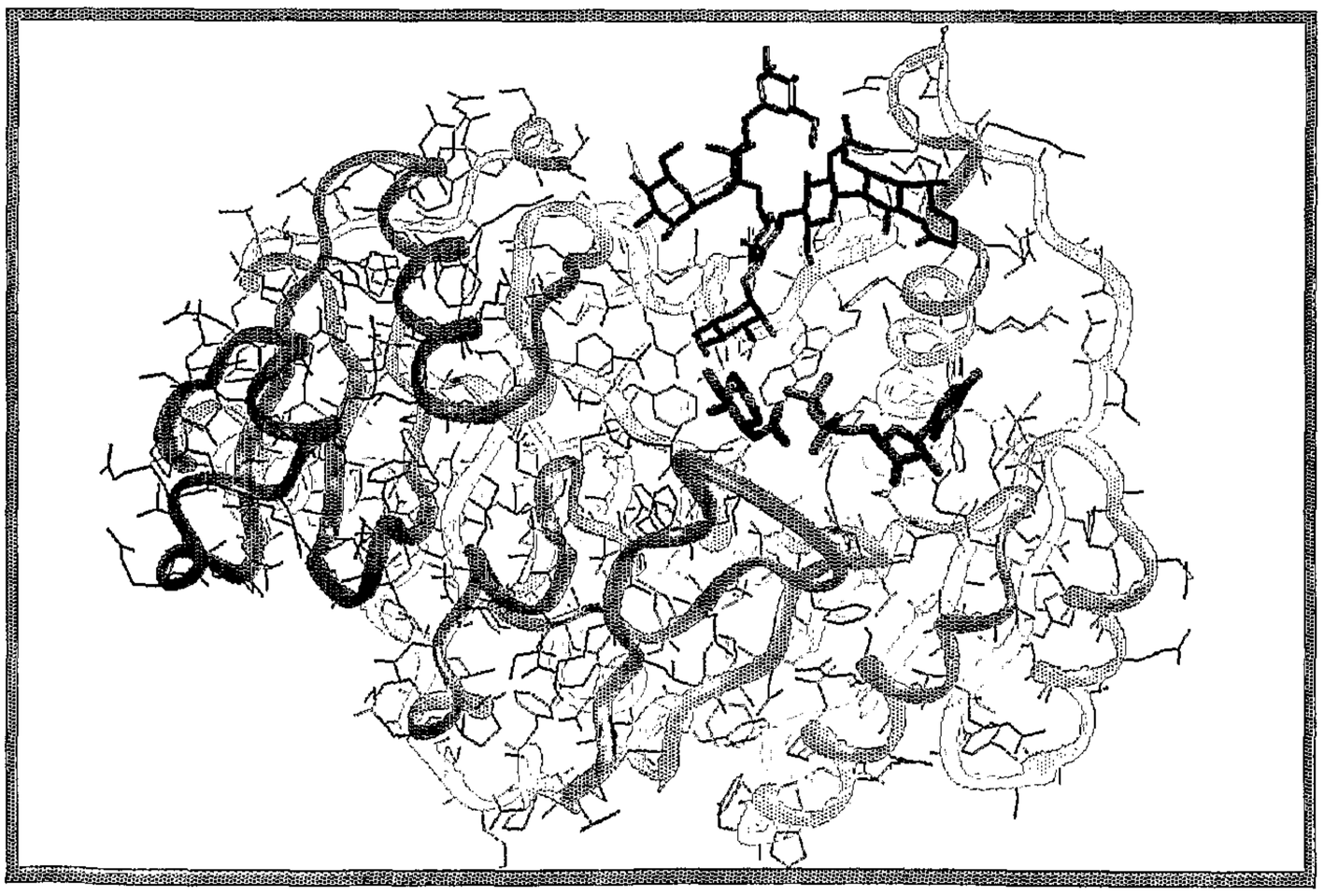


FIGURE 11

FIGURE 12

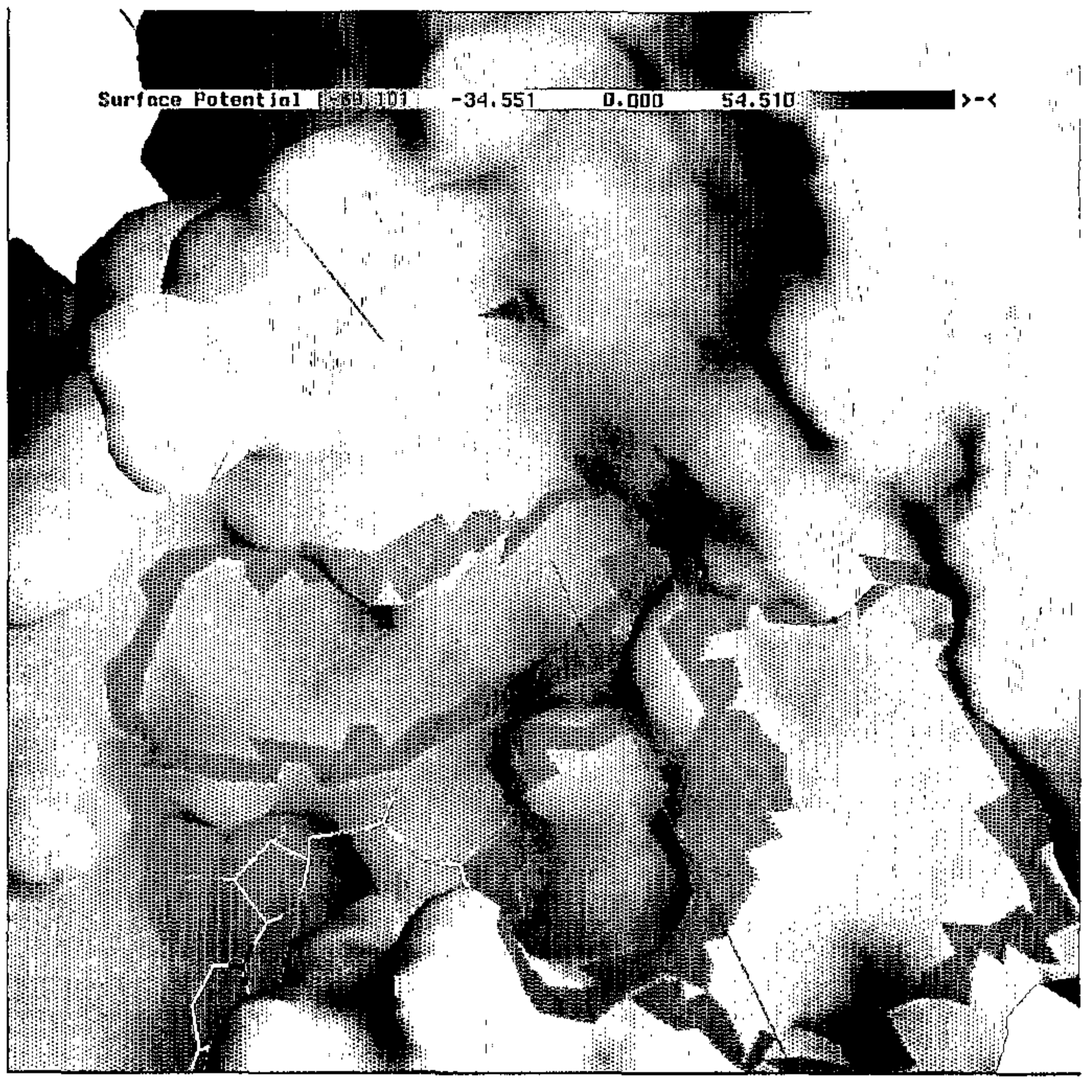


FIGURE 13

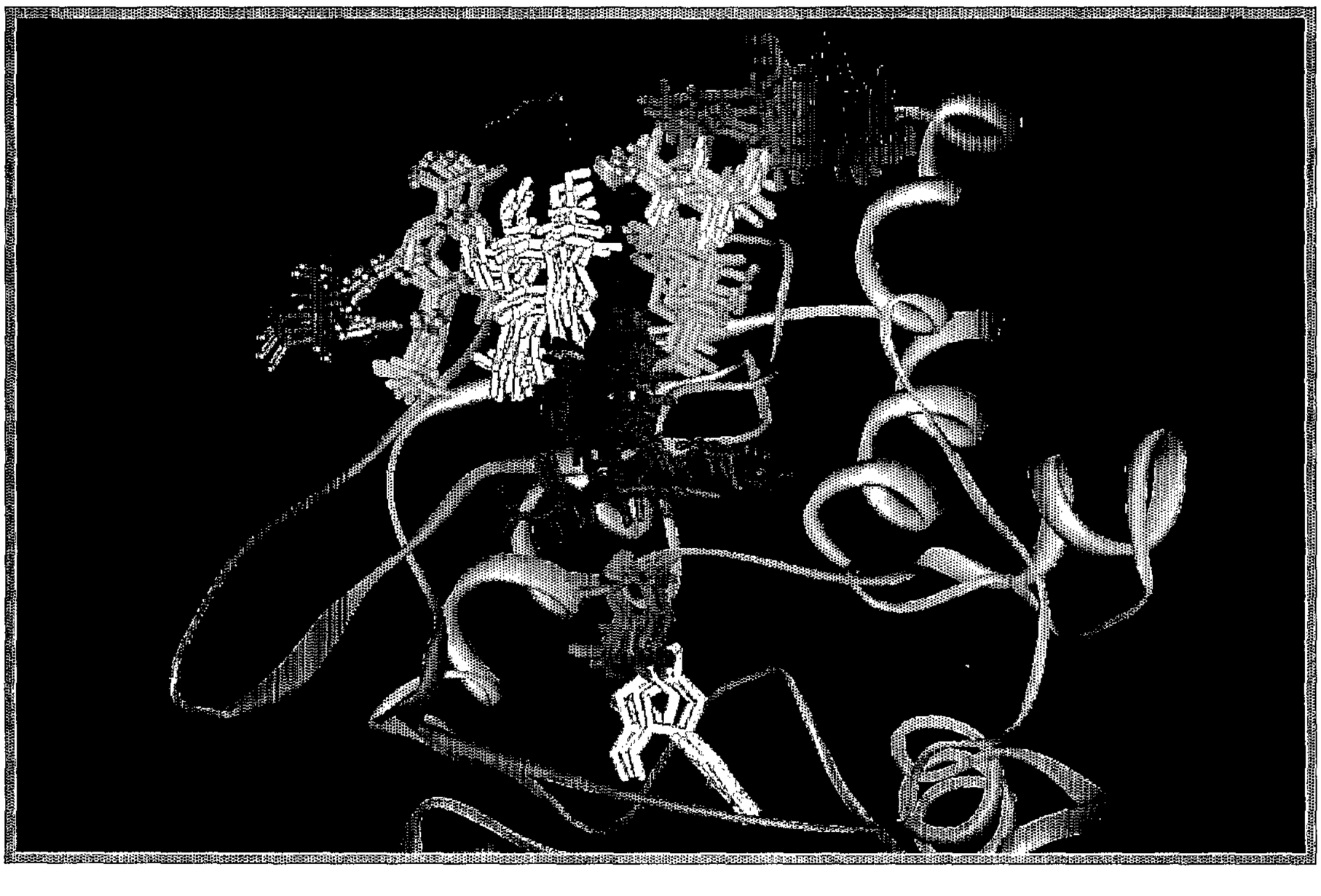


FIGURE 14/

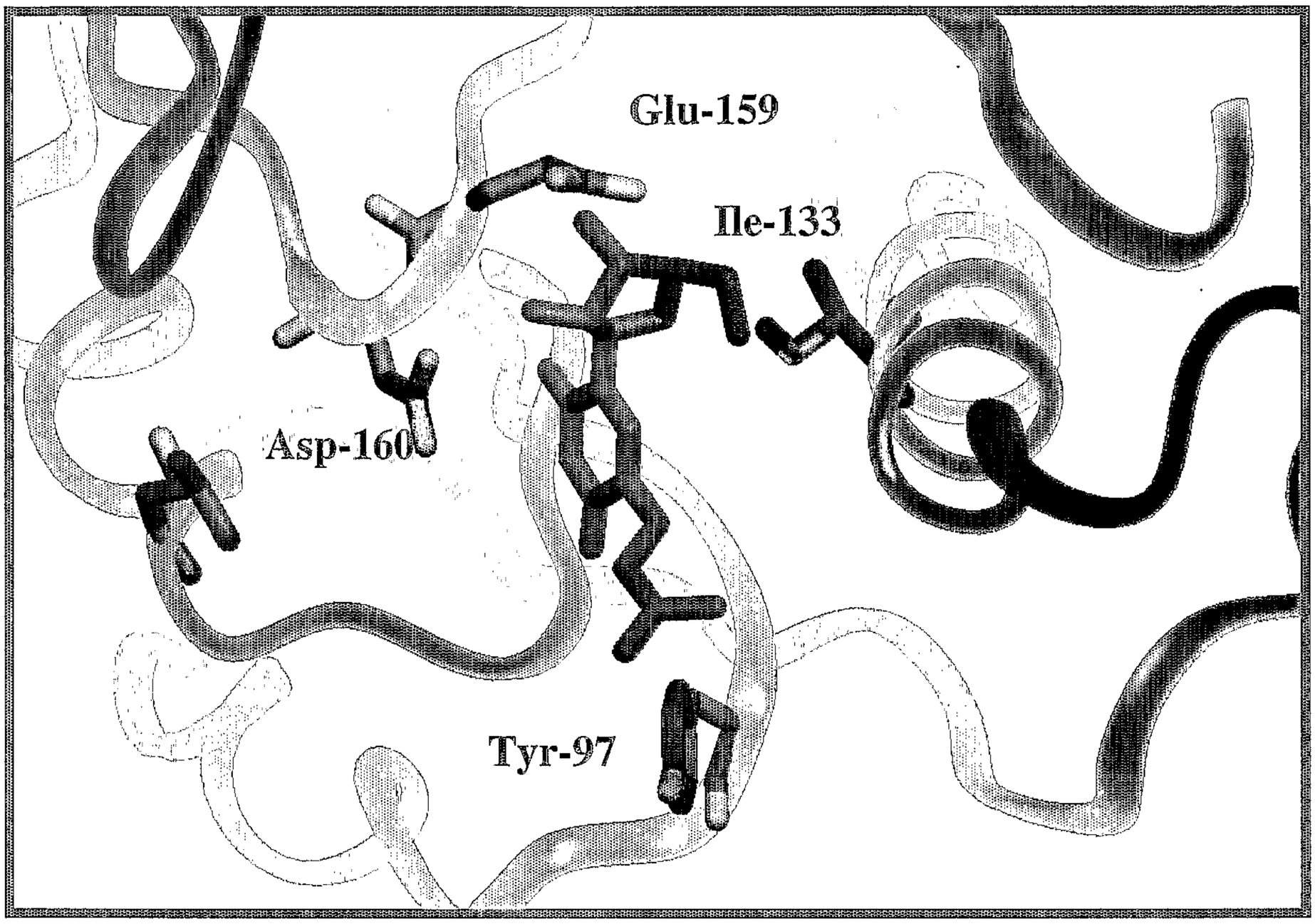


FIGURE 15

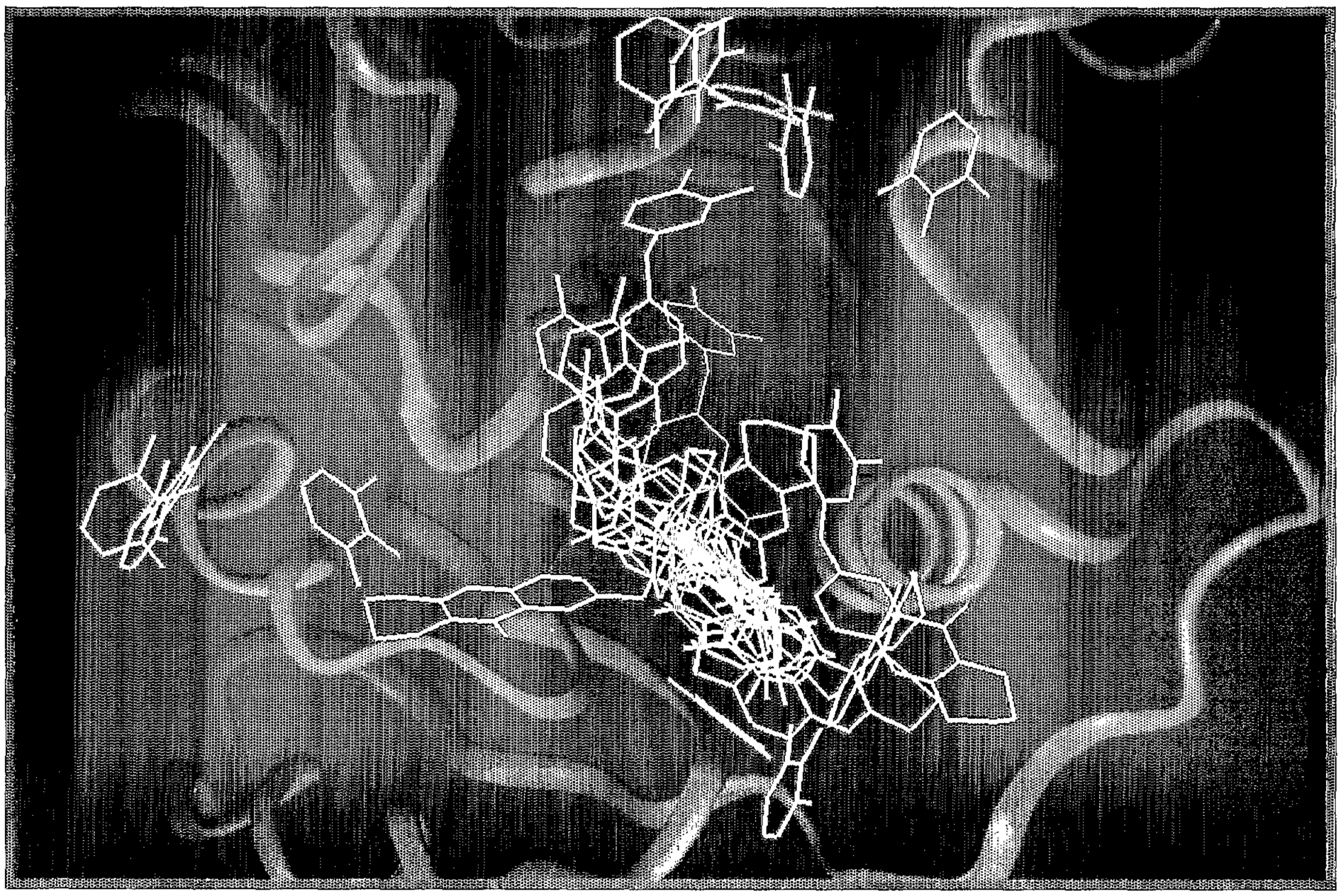
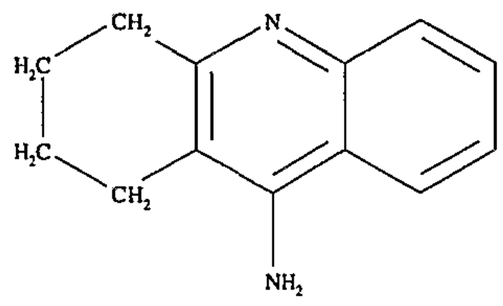


FIGURE 16

(a)



(b)

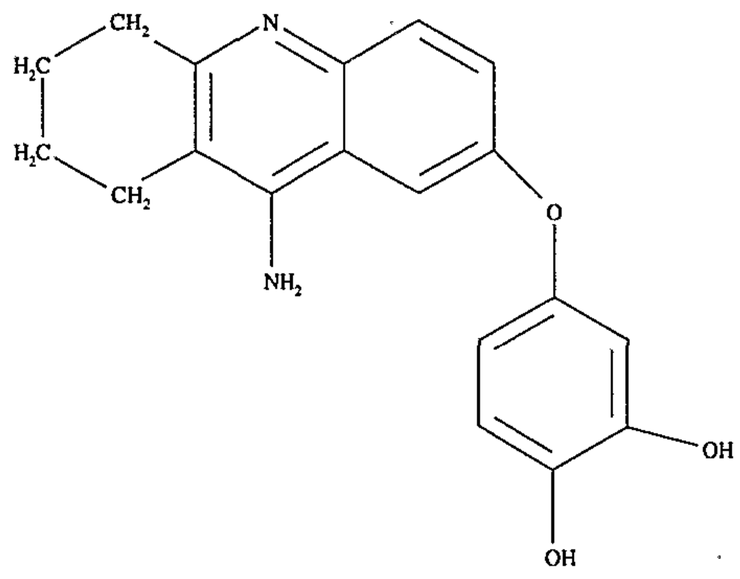


FIGURE 17

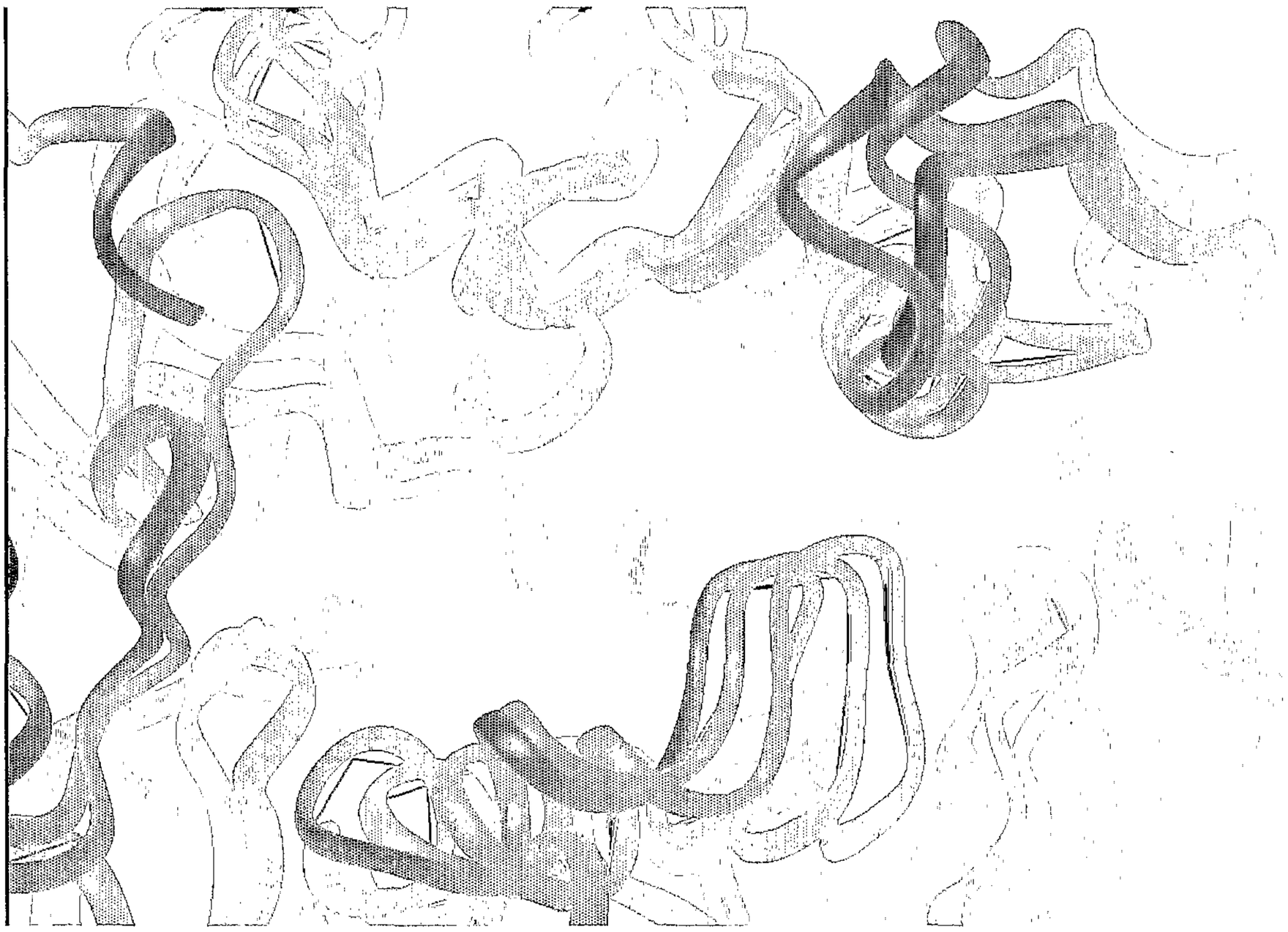


FIGURE 18 (a)

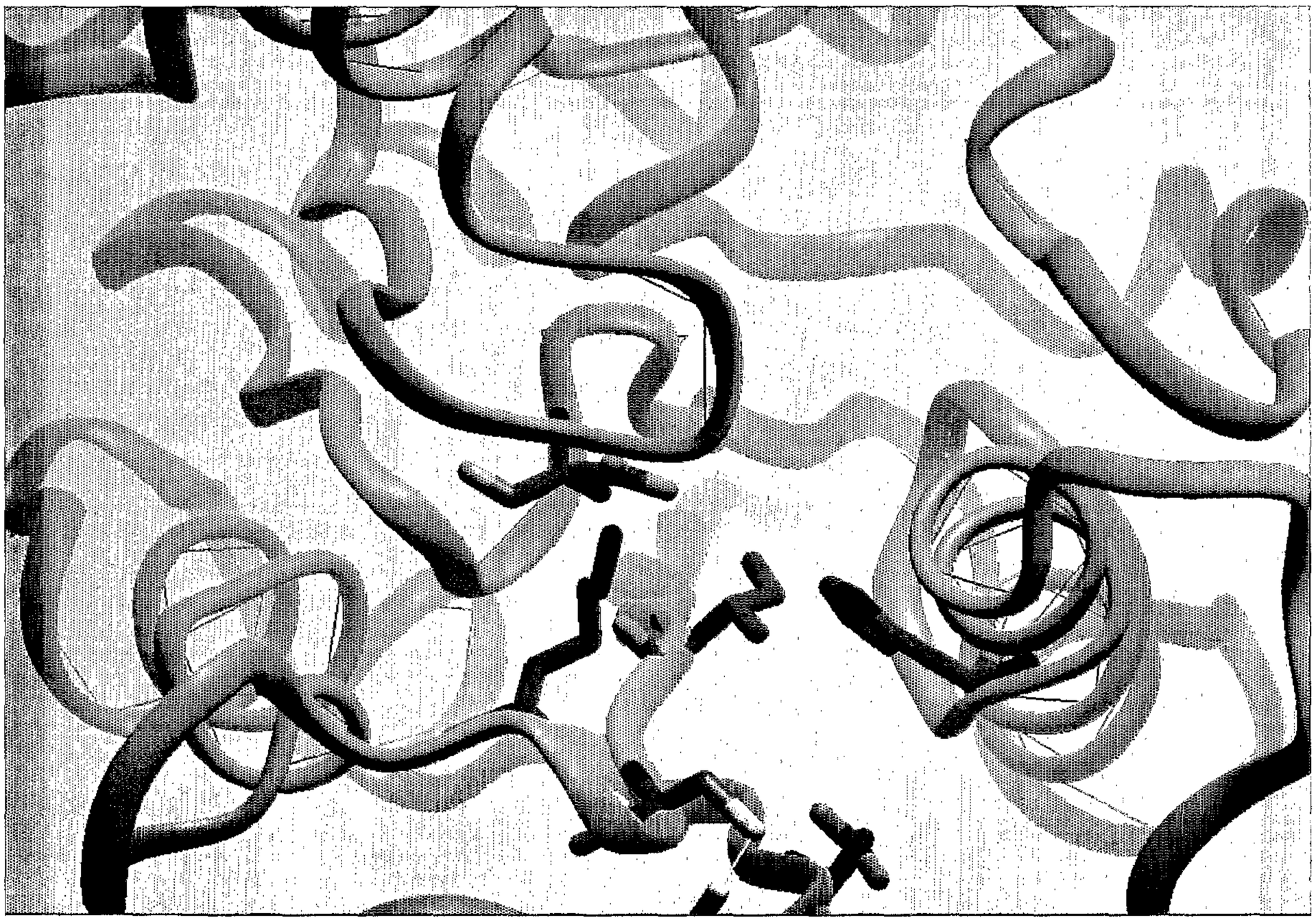


FIGURE 18 (b)

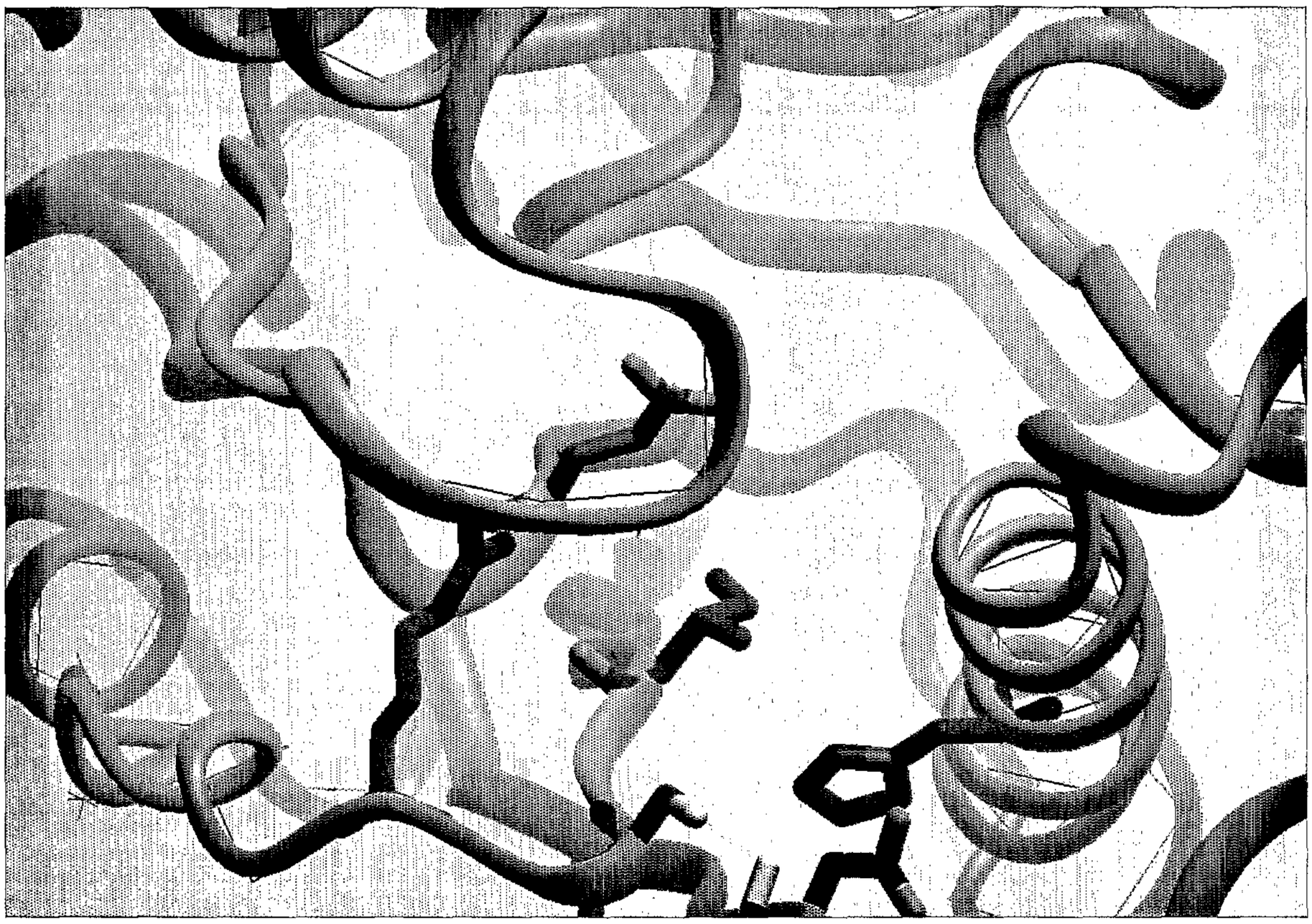


FIGURE 18 (c)

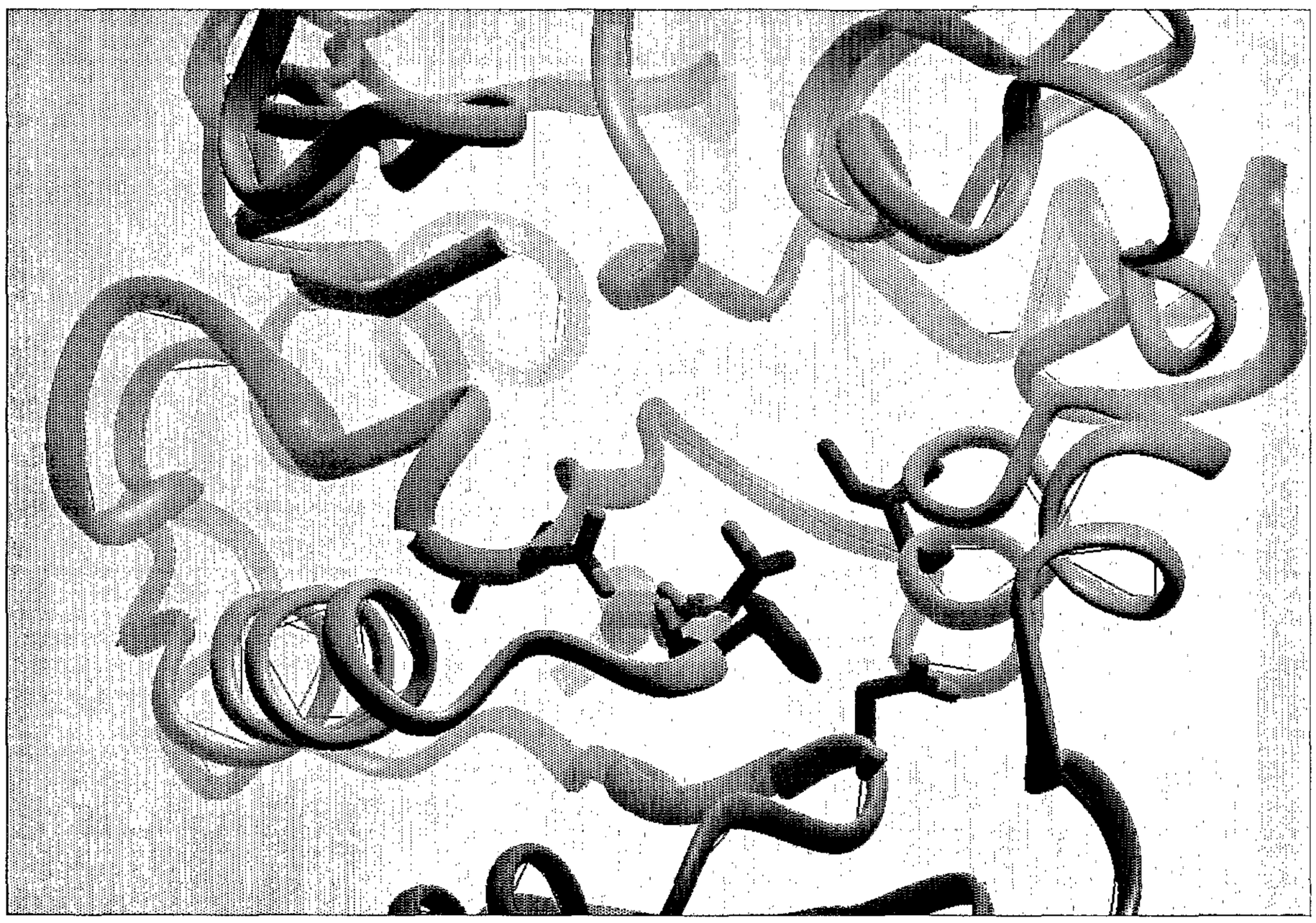


FIGURE 18 (d)

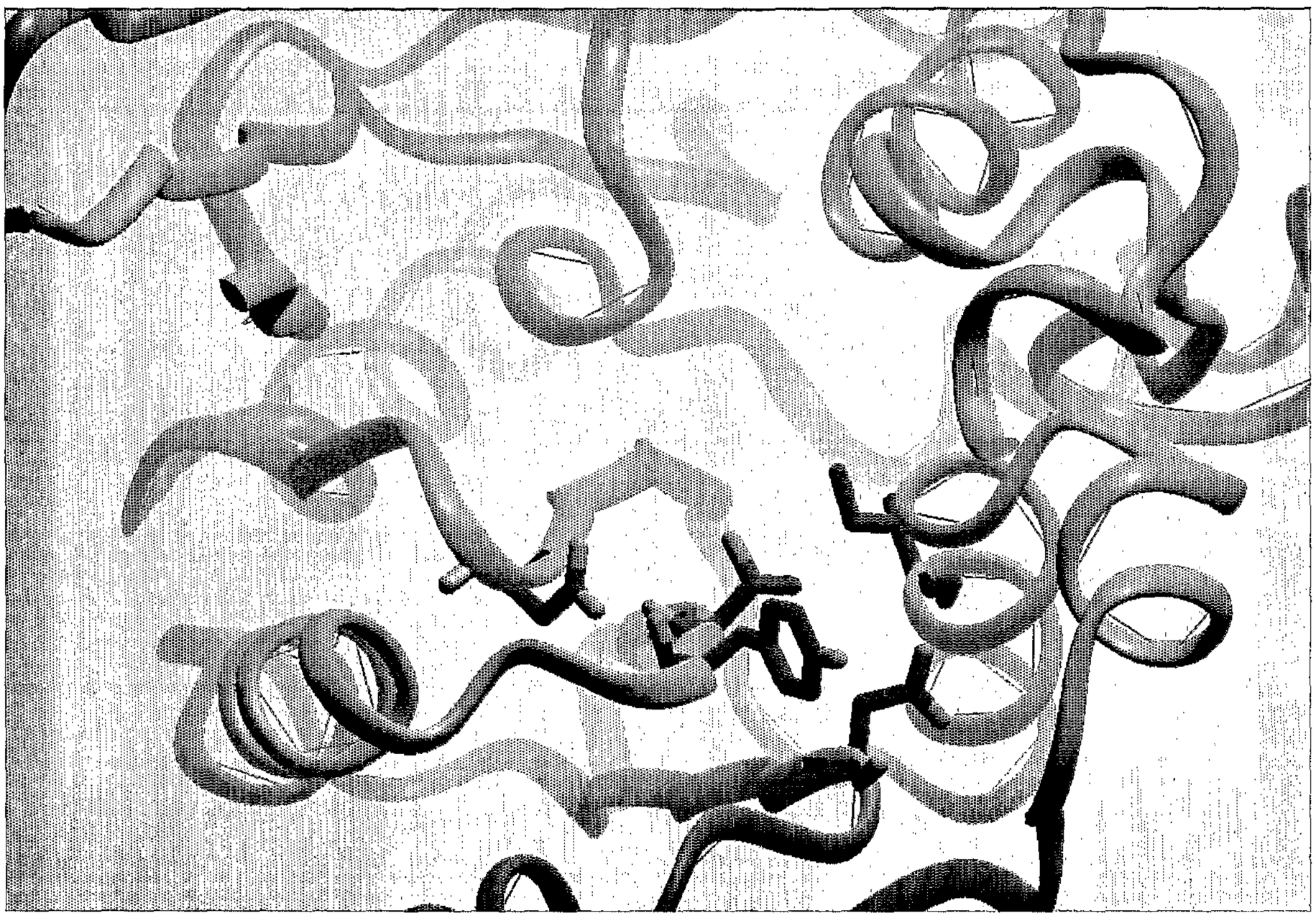


FIGURE 18 (e)

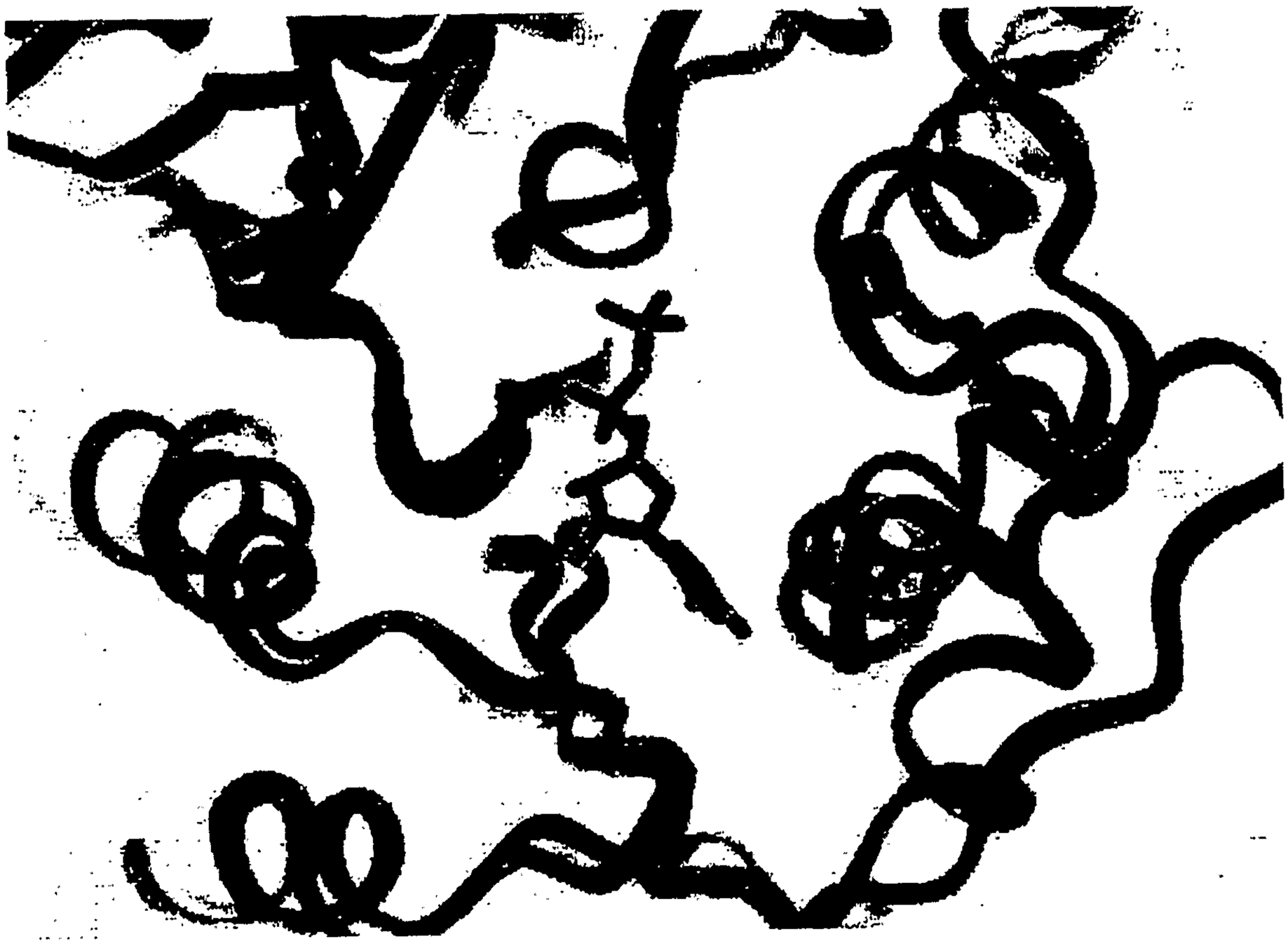
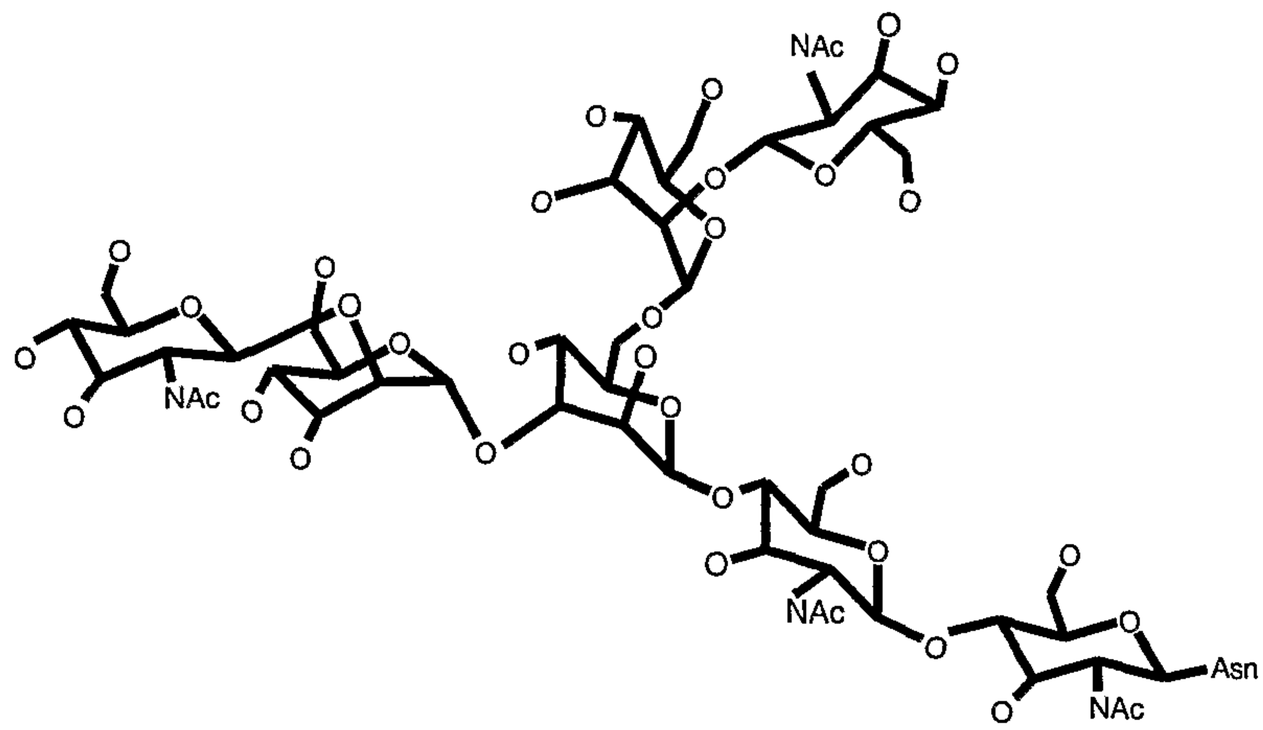


FIGURE 19

(a)



(b)

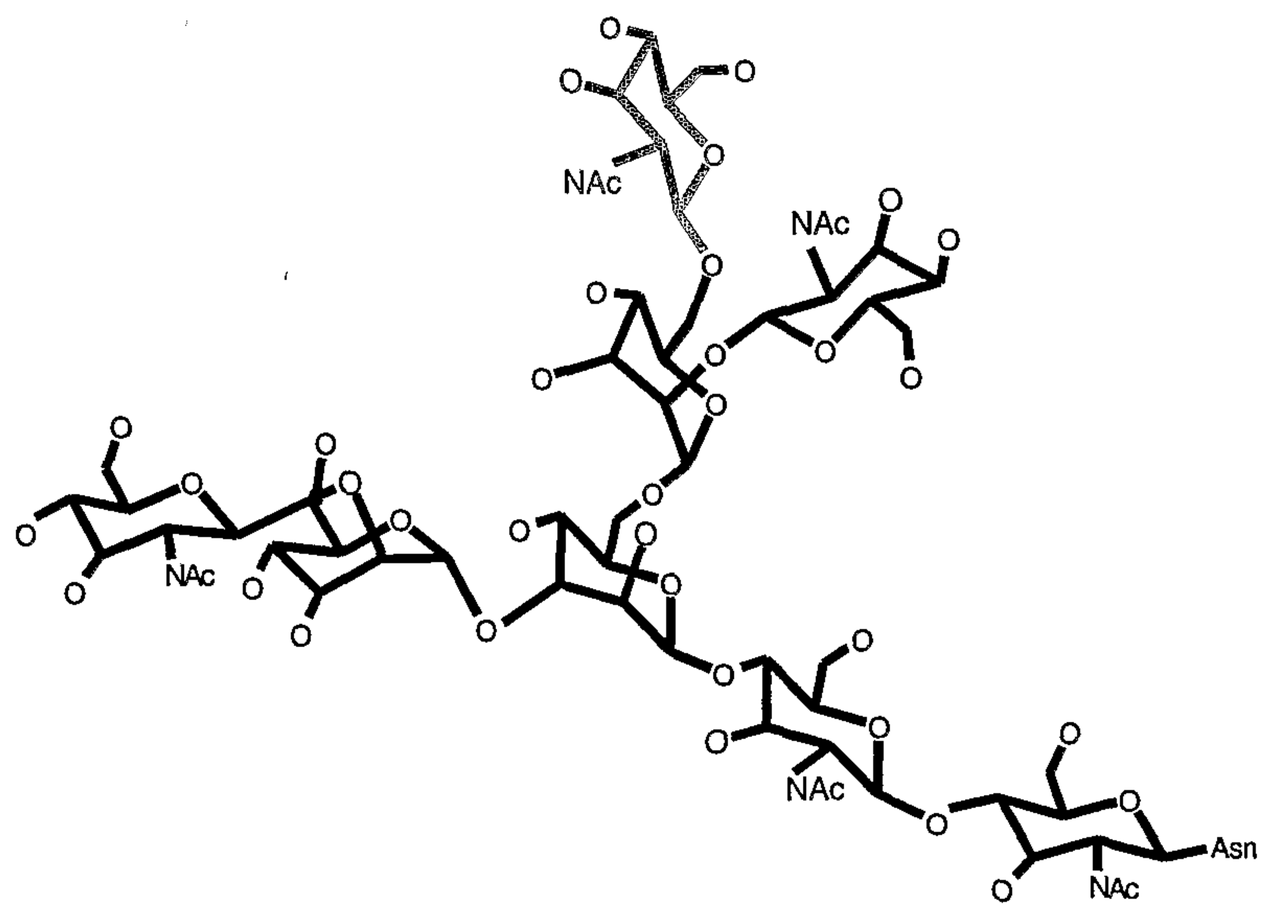


FIGURE 20

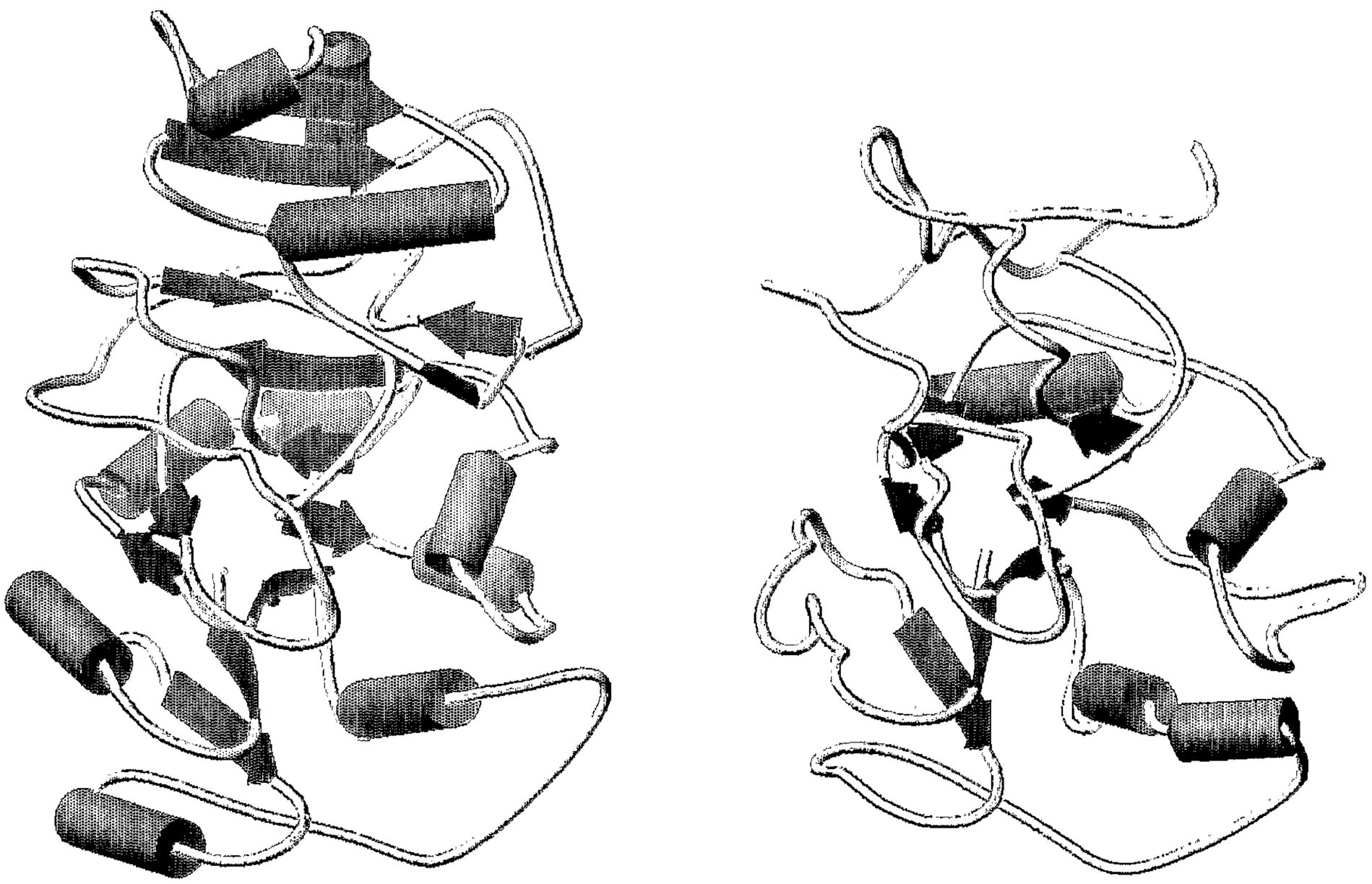


FIGURE 21

FIGURE 22/

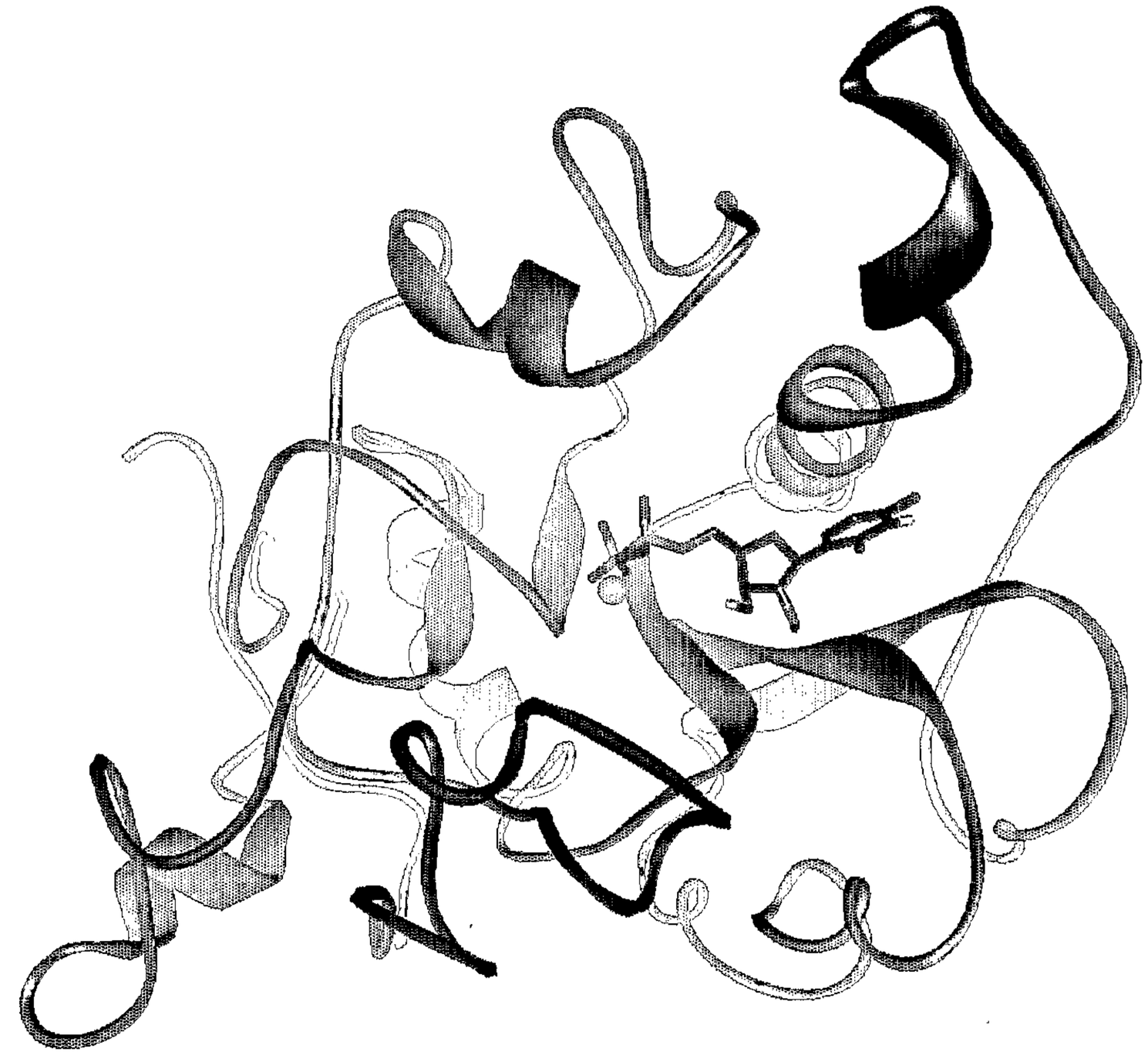


FIGURE 23/

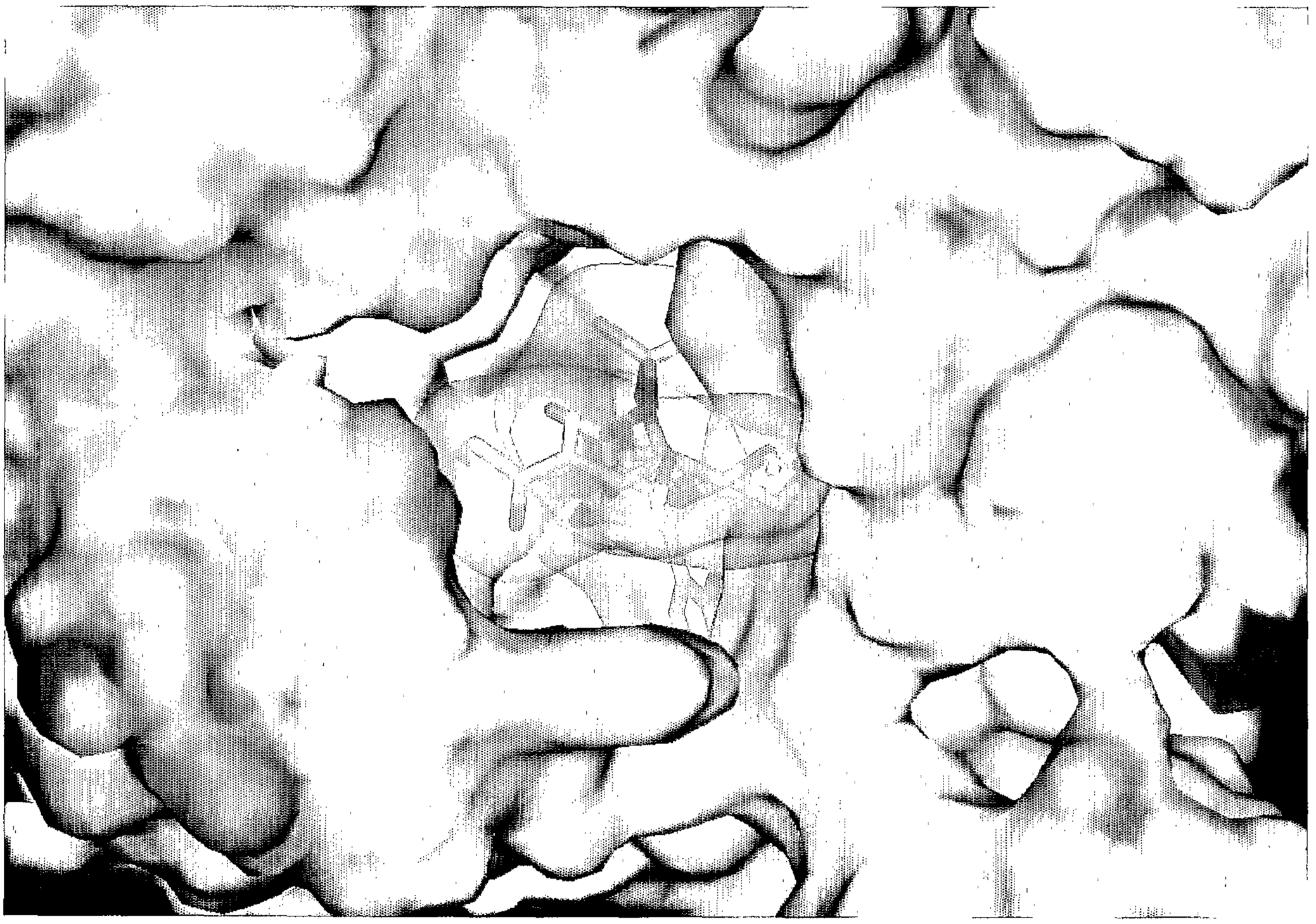


FIGURE 24

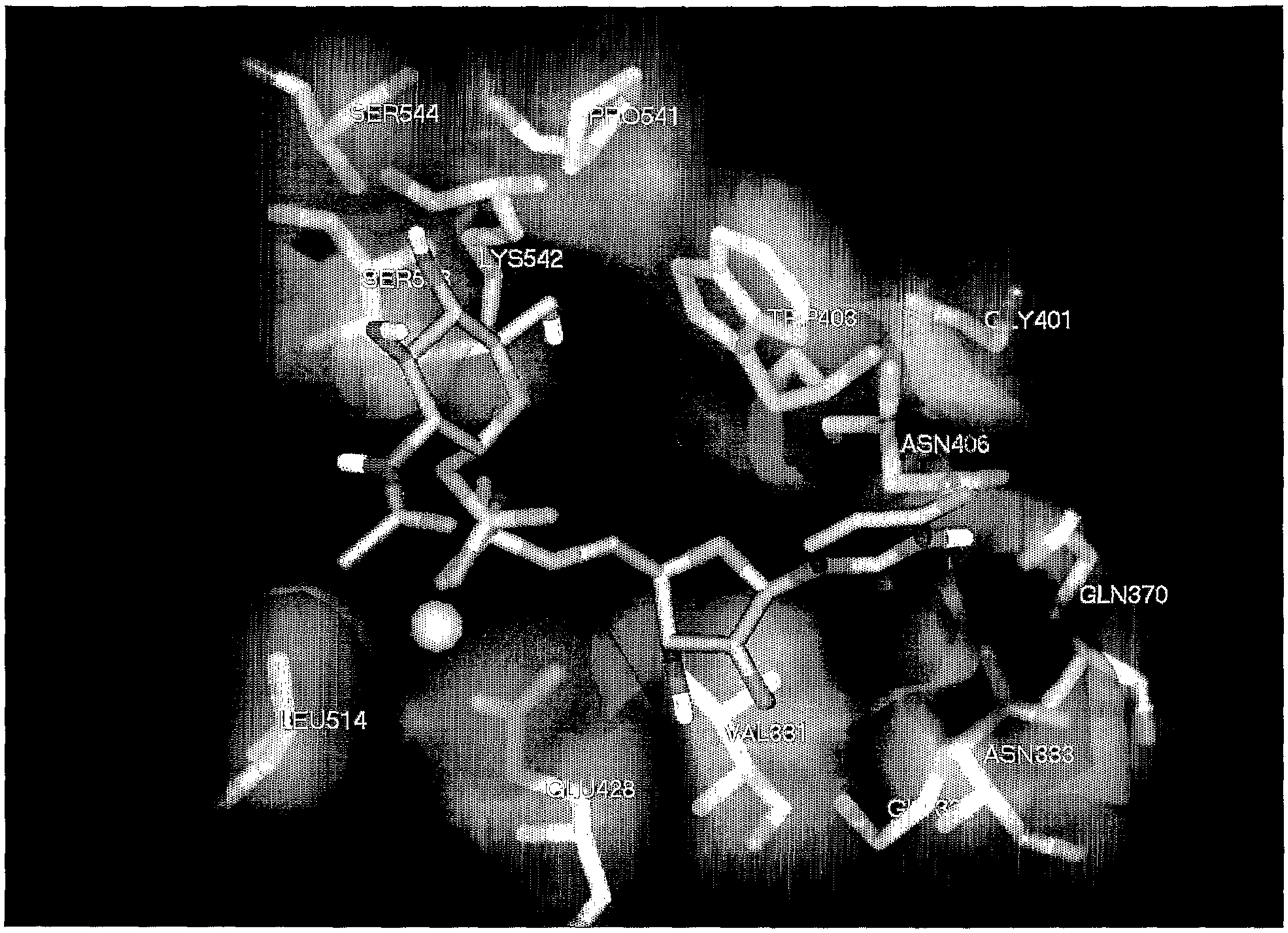

SER544
PRO541
LYS542
SER5
TR 2408
GLY401
ASN406
GLN370
LEU514
VAL831
ASN383
GLU428

FIGURE 25 (a)

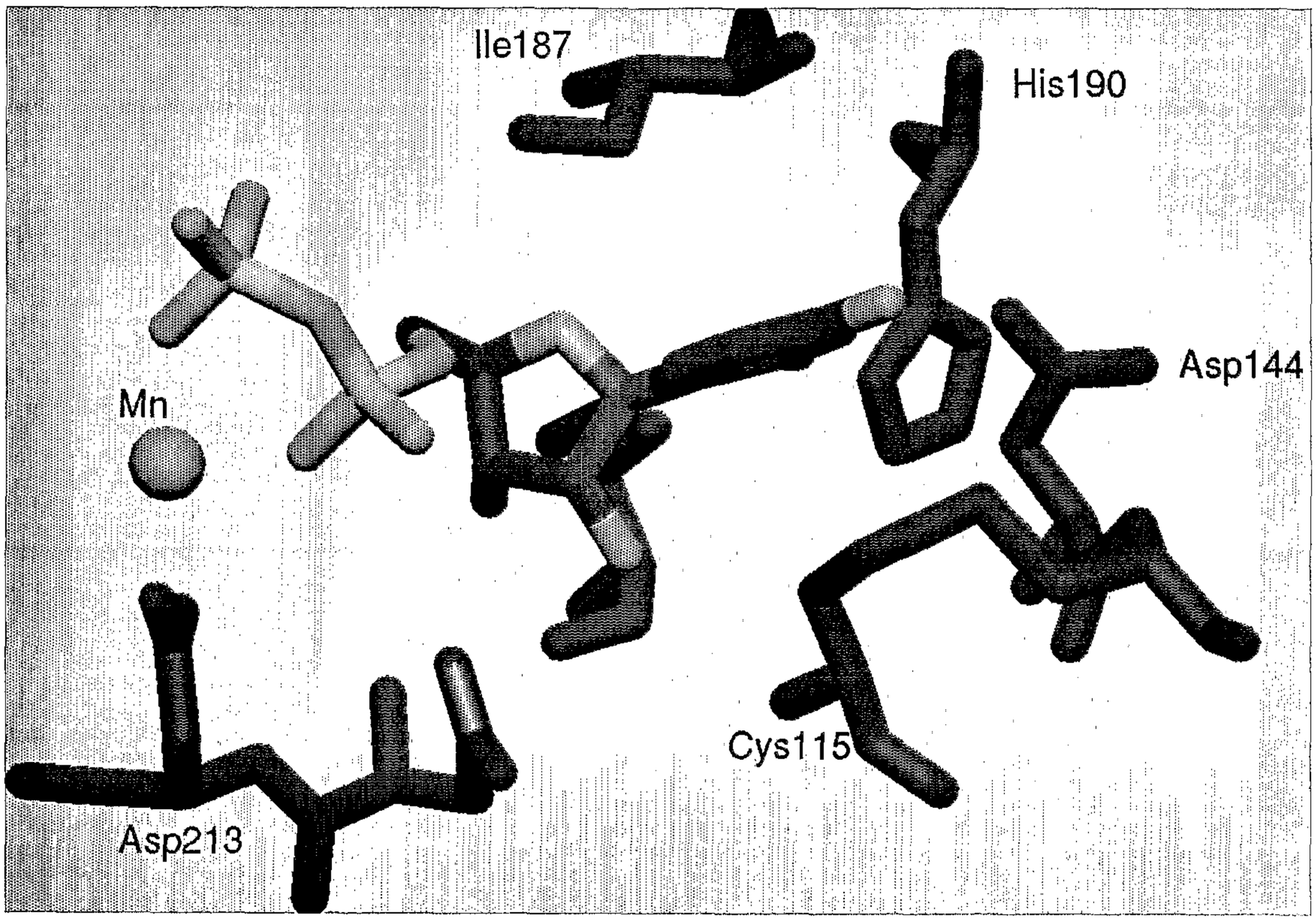


FIGURE 25 (b)

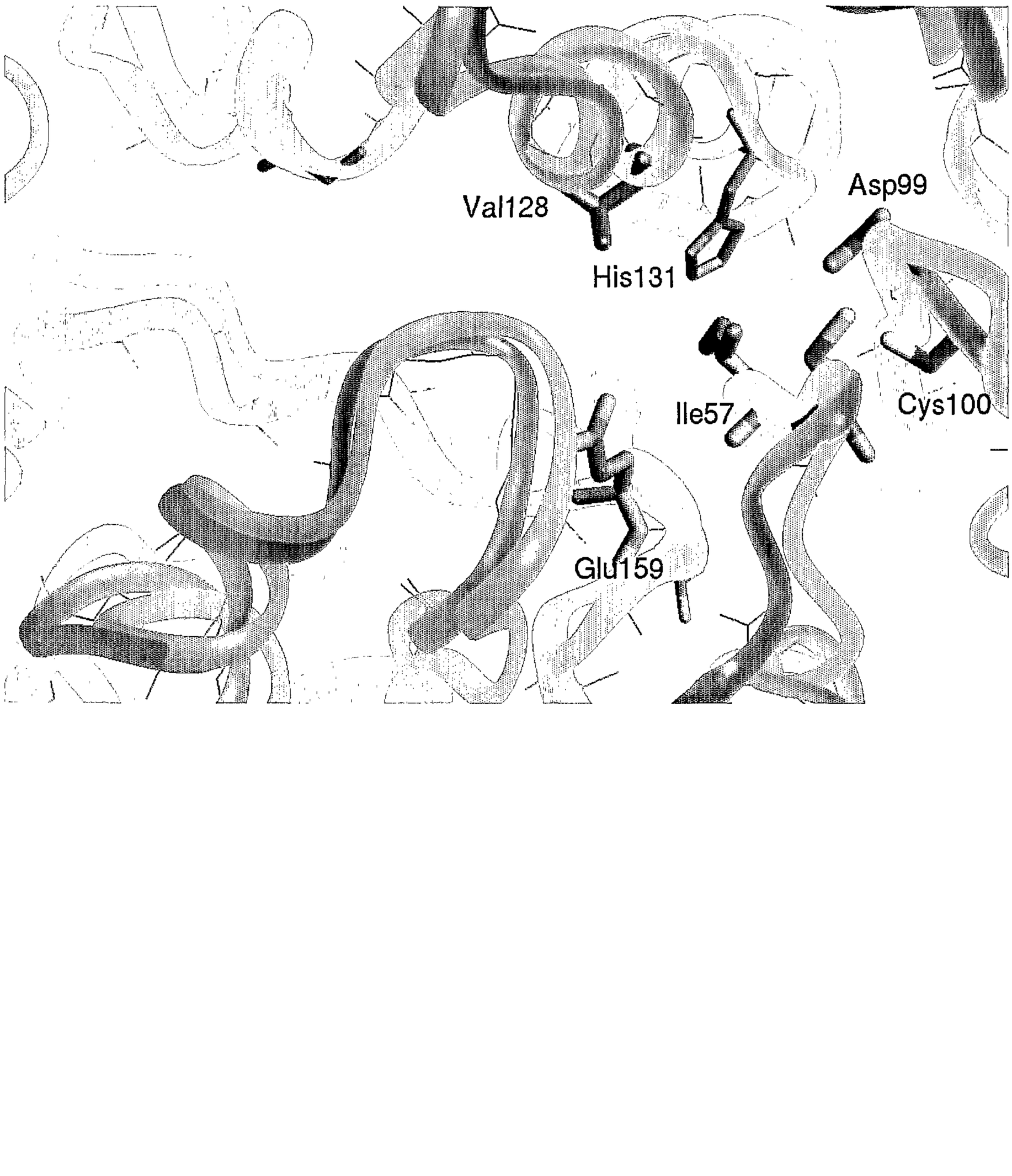


FIGURE 26

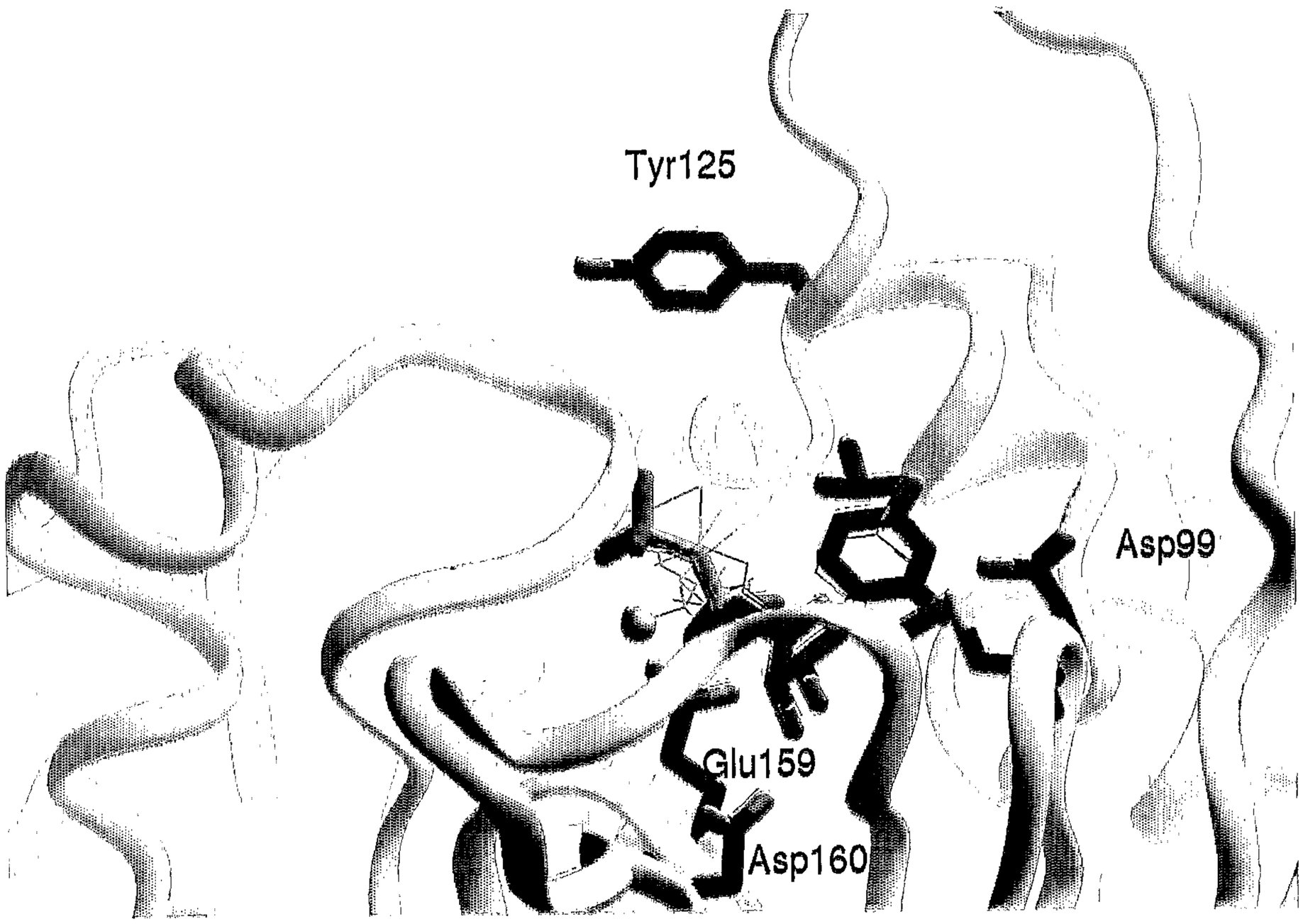


FIGURE 27.

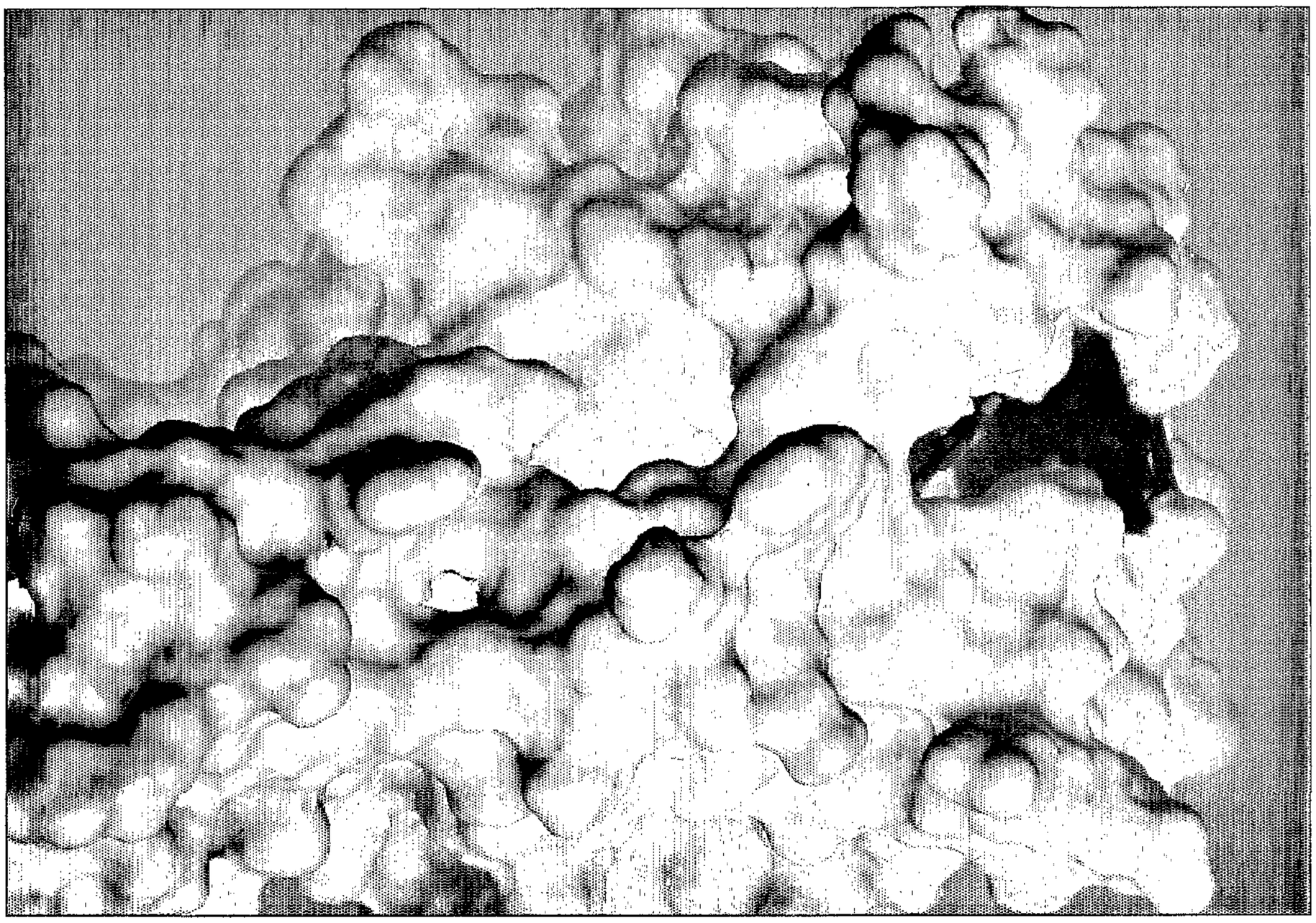


FIGURE 28.

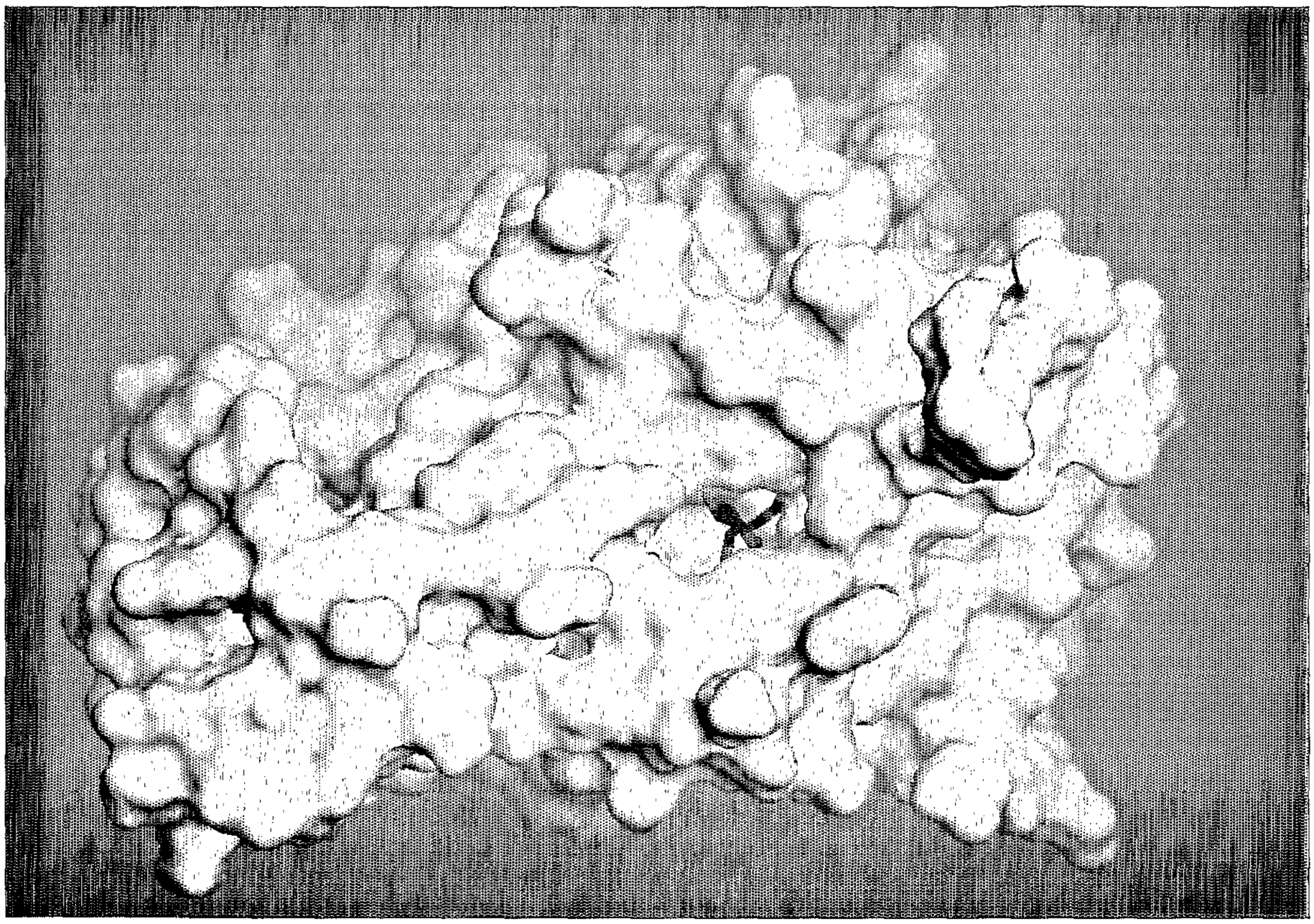


FIGURE 29

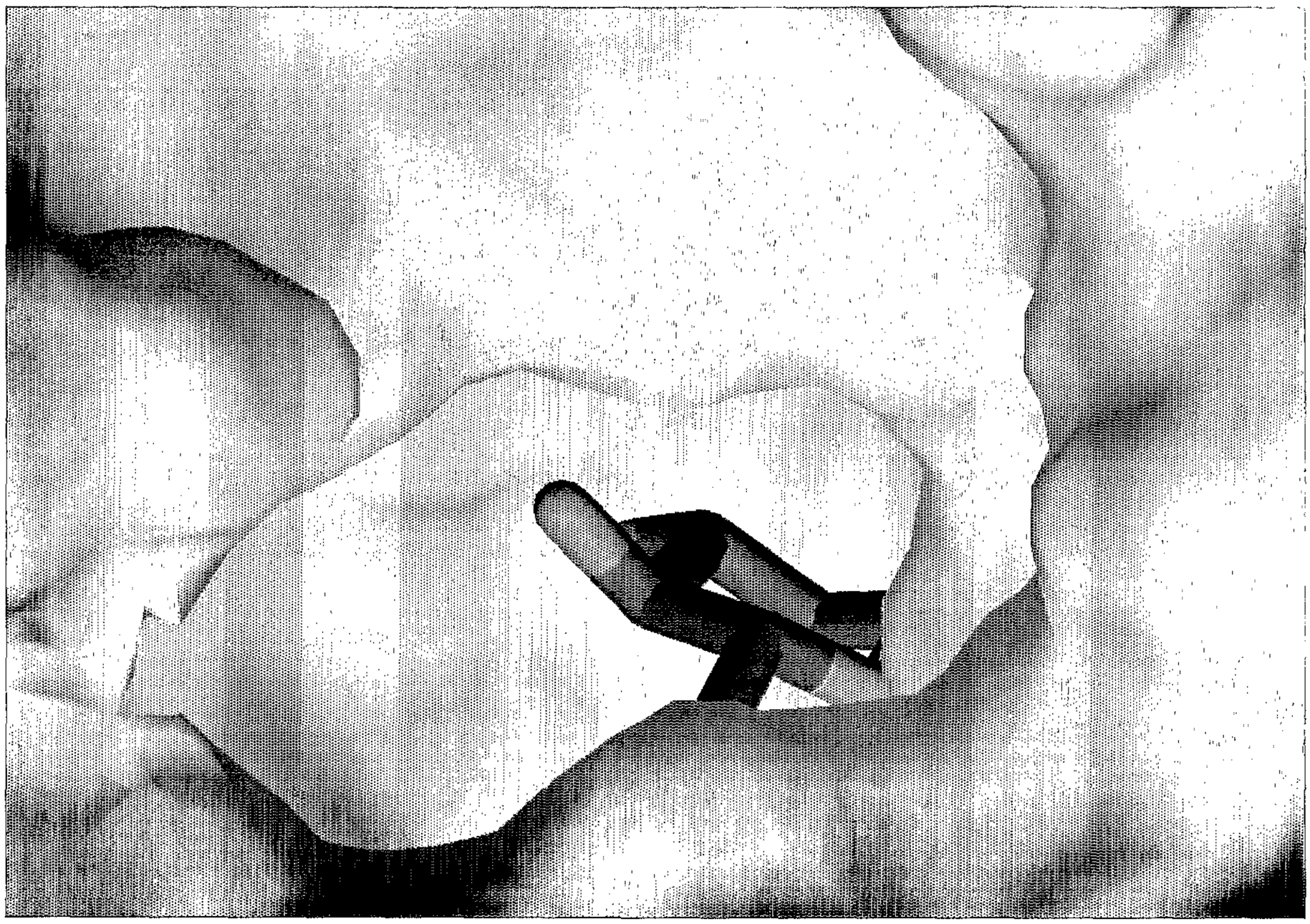


FIGURE 30

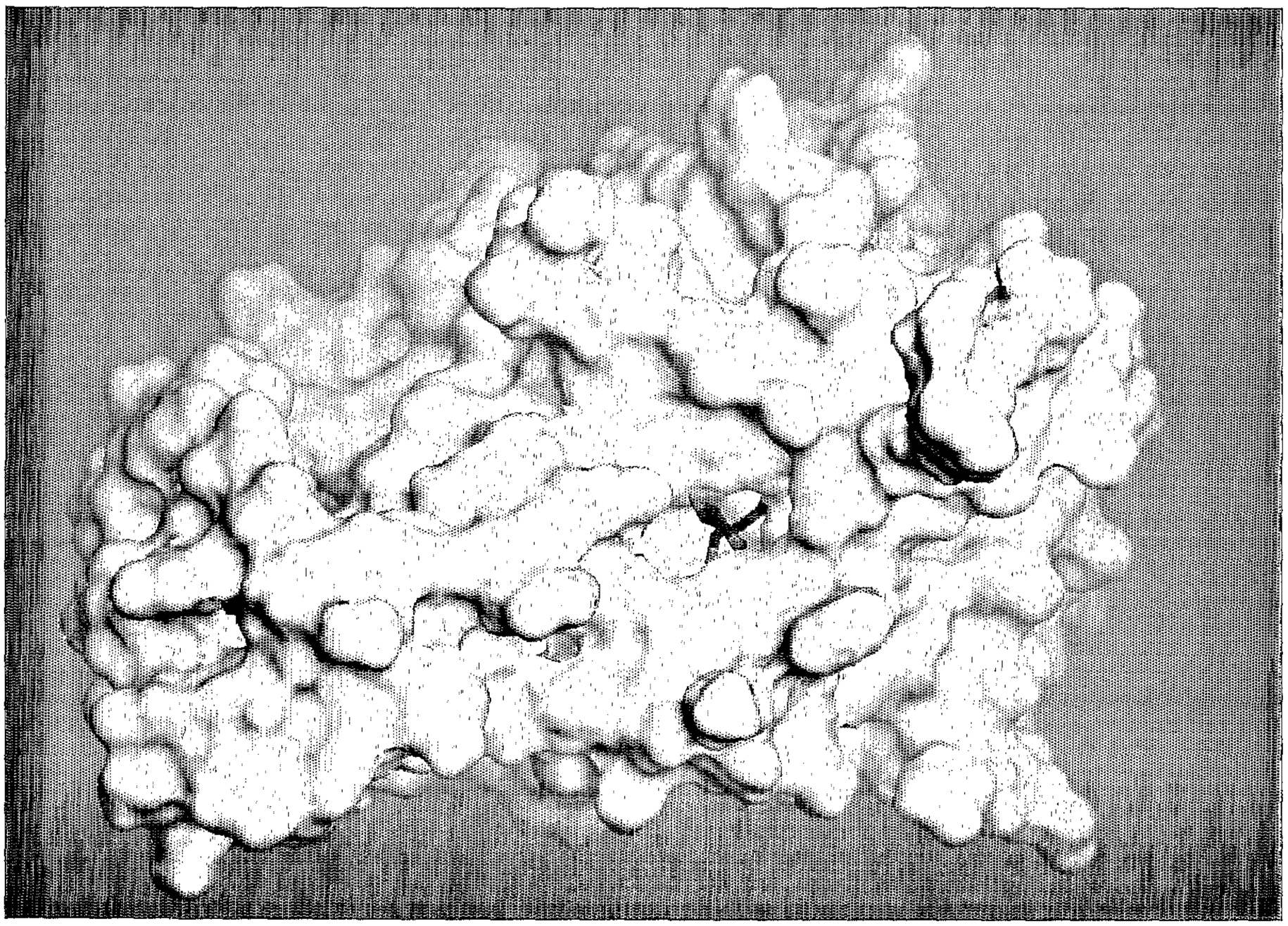


FIGURE 31

FIGURE 32

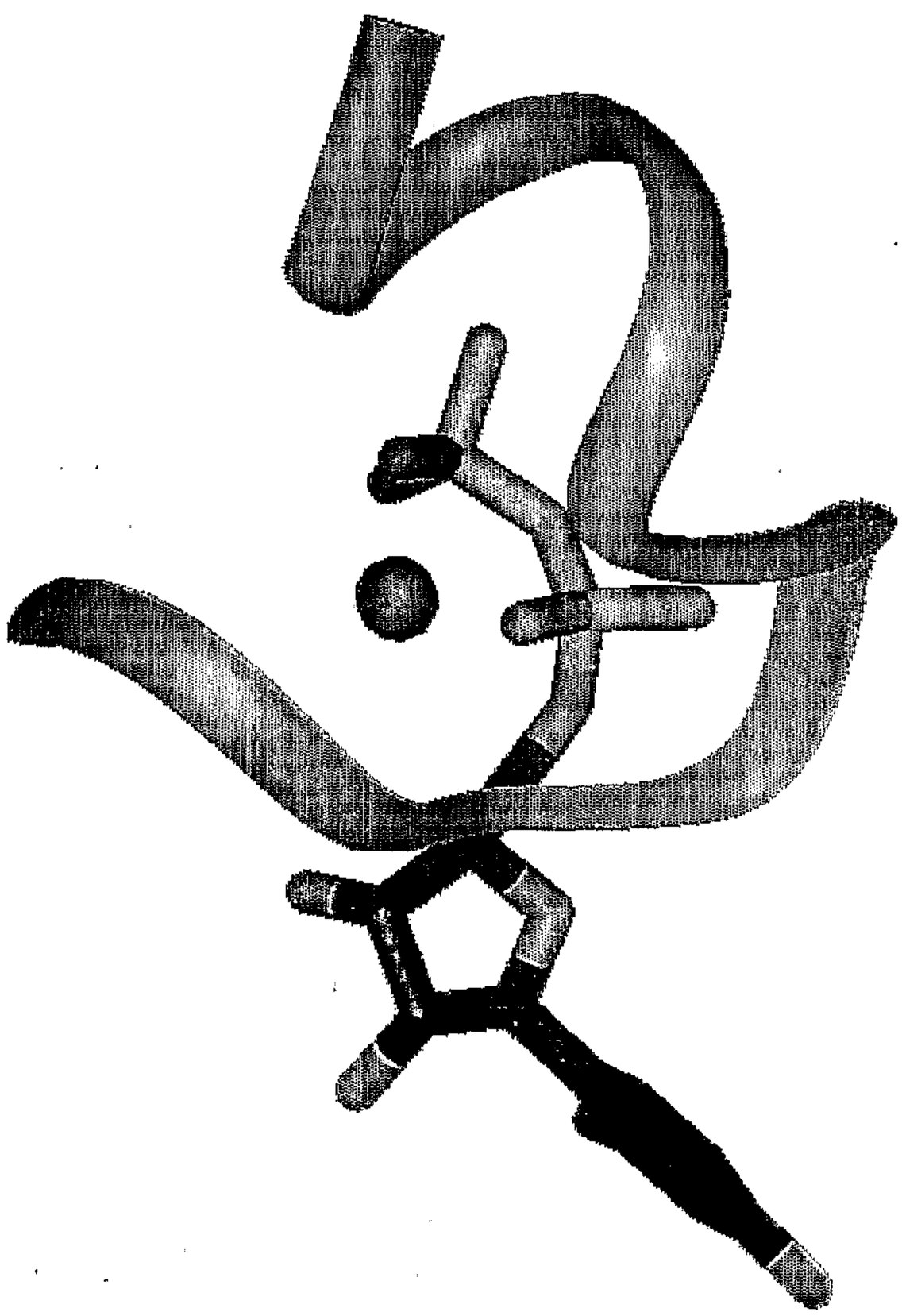


FIGURE 33

GnTI acceptor

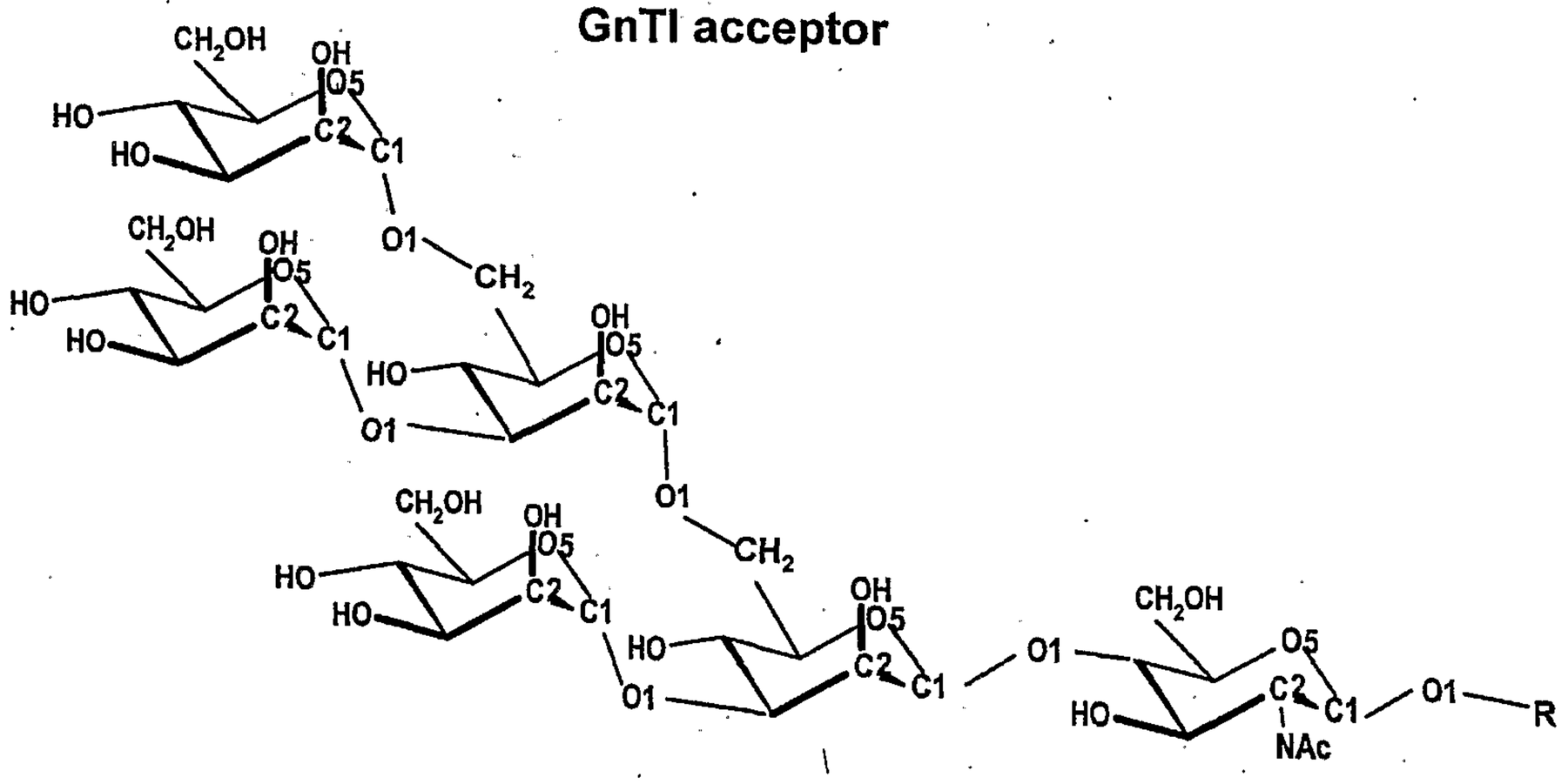


FIGURE 34

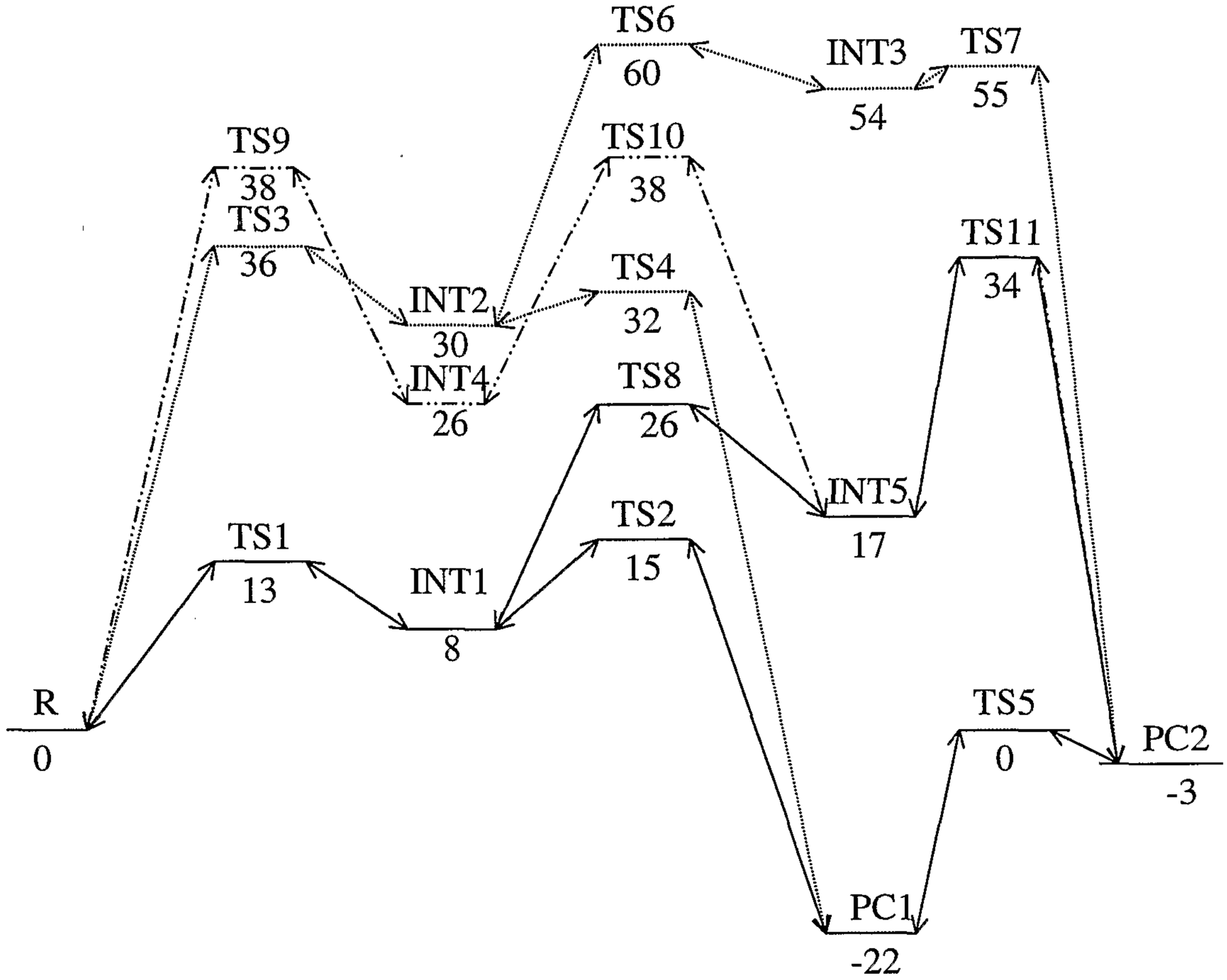

TS6
60
INT3
54
TS7
55
TS9
38
TS10
38
TS3
36
TS11
34
TS4
32
INT2
30
INT4
26
TS8
26
INT5
17
TS1
13
INT1
8
TS2
15
R
0
TS5
0
PC2
-3
PC1
-22

FIGURE 35

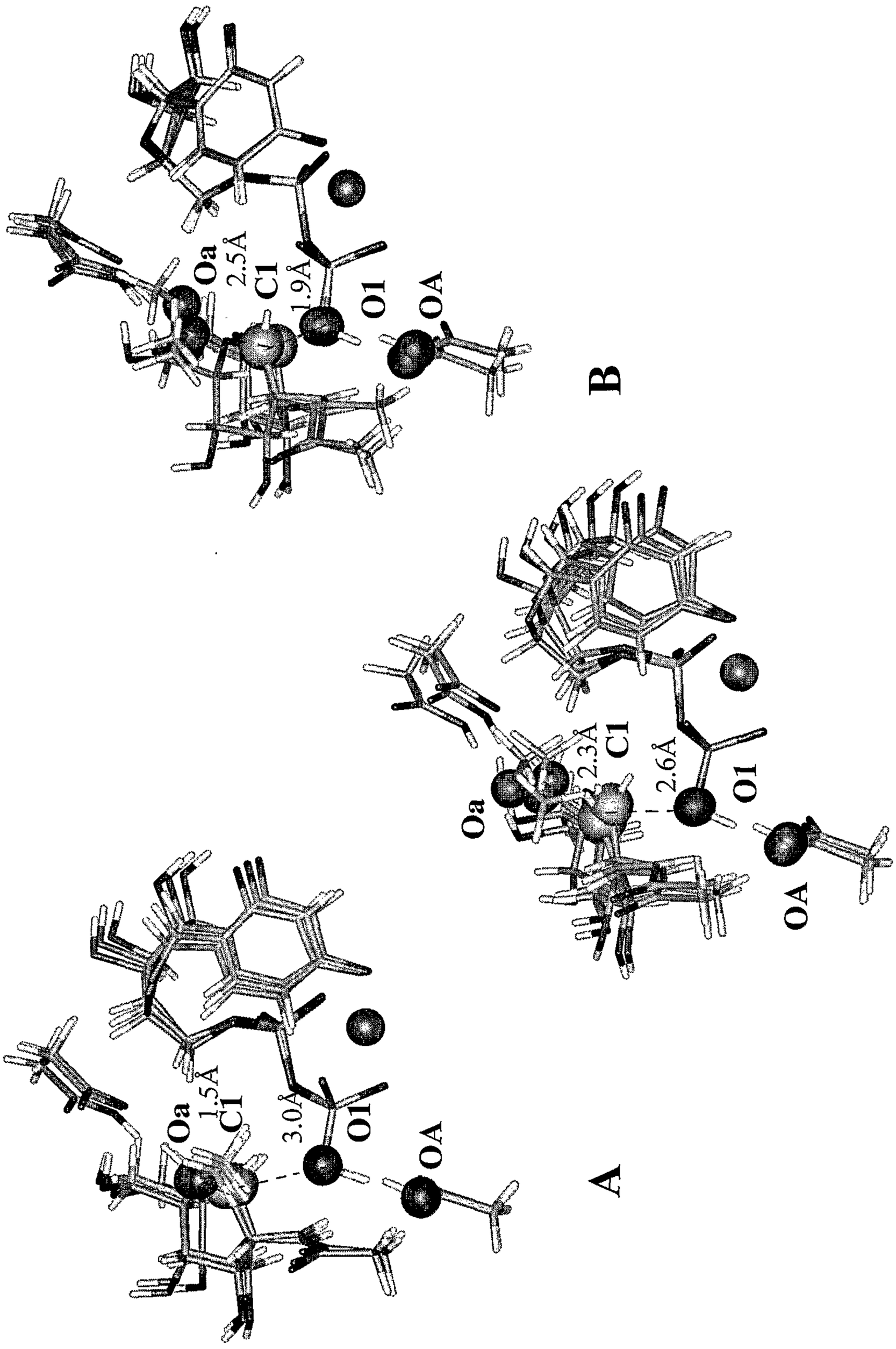
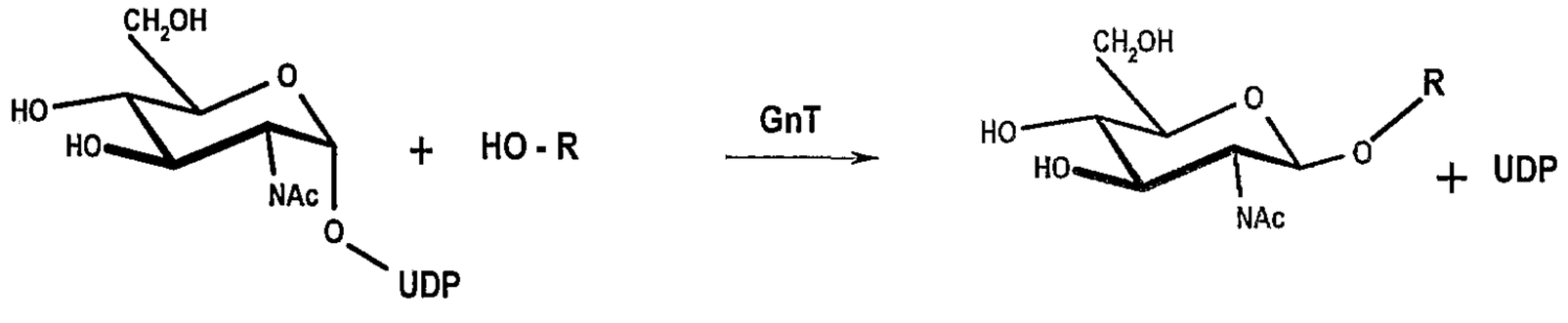
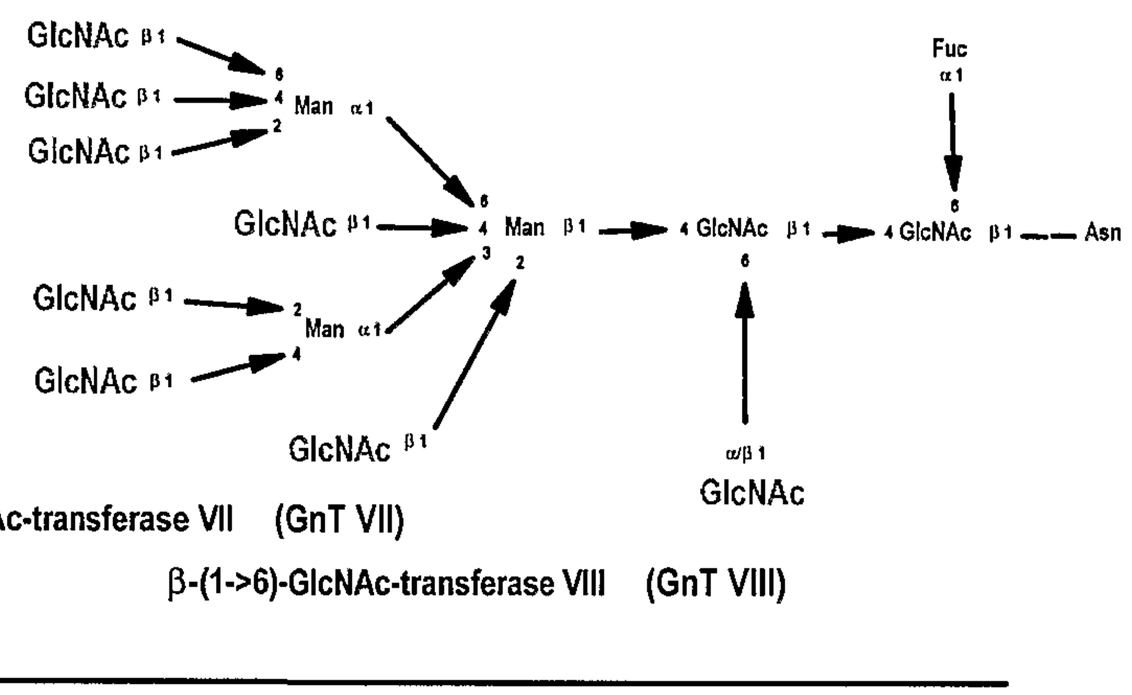
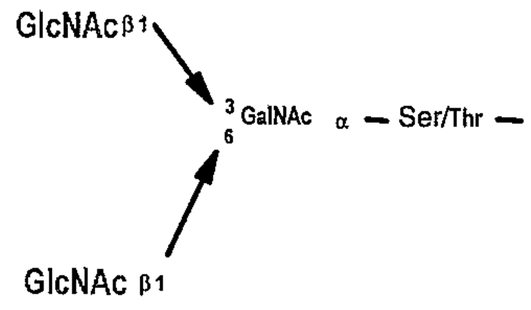
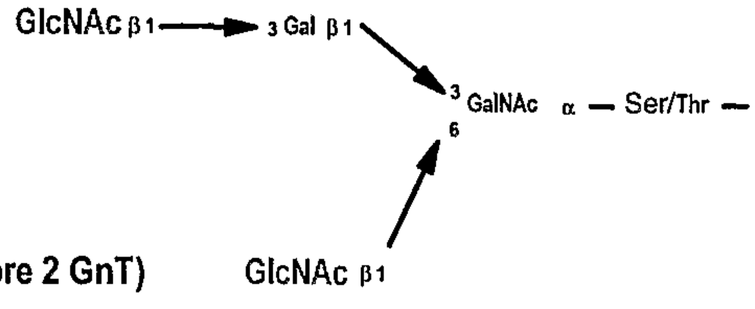
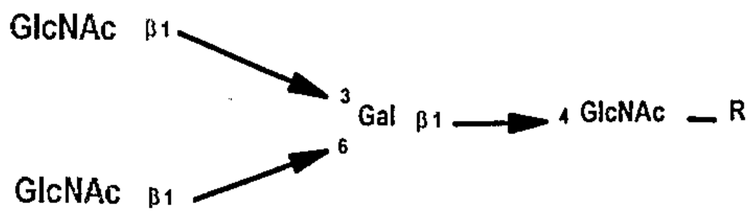


FIGURE 36

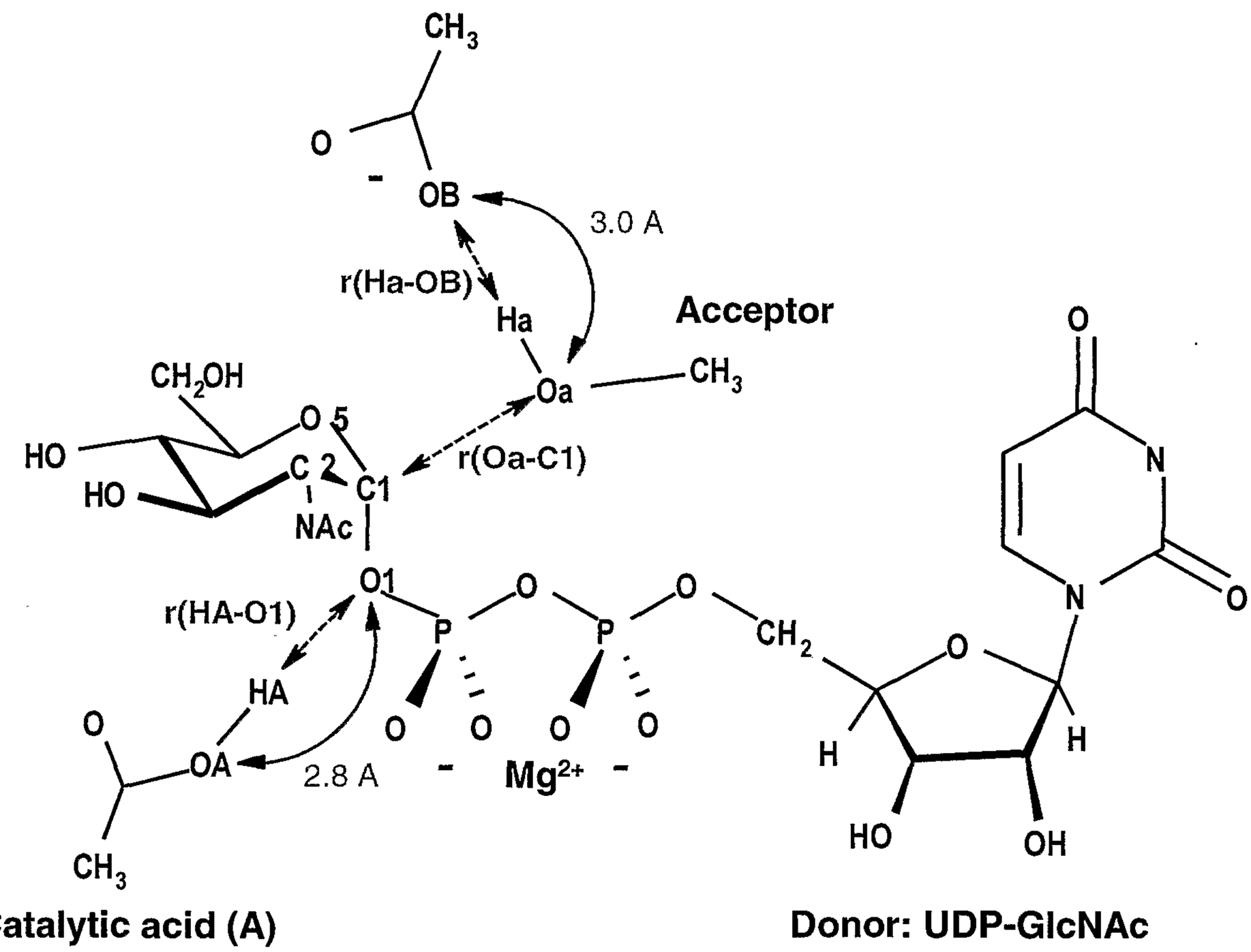


(UDP - uridine diphosphate; R - oligosaccharide part of glycoprotein)

N-acetylglucosaminyltransferase		Oligosaccharide (R)
β-(1-->6)-GlcNAc-transferase V	(GnT V)	
β-(1->4)-GlcNAc-transferase VI	(GnT VI)	
β-(1->2)-GlcNAc-transferase II	(GnT II)	
β-(1->4)-GlcNAc-transferase III	(GnT III)	
β-(1->2)-GlcNAc-transferase I	(GnT I)	
β-(1->4)-GlcNAc-transferase IV	(GnT IV)	
β-(1->2)-GlcNAc-transferase VII	(GnT VII)	
β-(1->6)-GlcNAc-transferase VIII	(GnT VIII)	
O-glycan core 3 β-(1->3)-GlcNAc-transferase	(Core 3 GnT)	
O-glycan core 4 β-(1->6)-GlcNAc-transferase	(Core 4 GnT)	
Core 2 elongation β-(1->3)-GlcNAc-transferase		
Core 1 elongation β-(1->3)-GlcNAc-transferase		
O-glycan core 2 β-(1->6)-GlcNAc-transferase	(Core 2 GnT)	
Blood group i β-(1->3)-GlcNAc-transferase		
Blood group I β-(1->6)-GlcNAc-transferase		

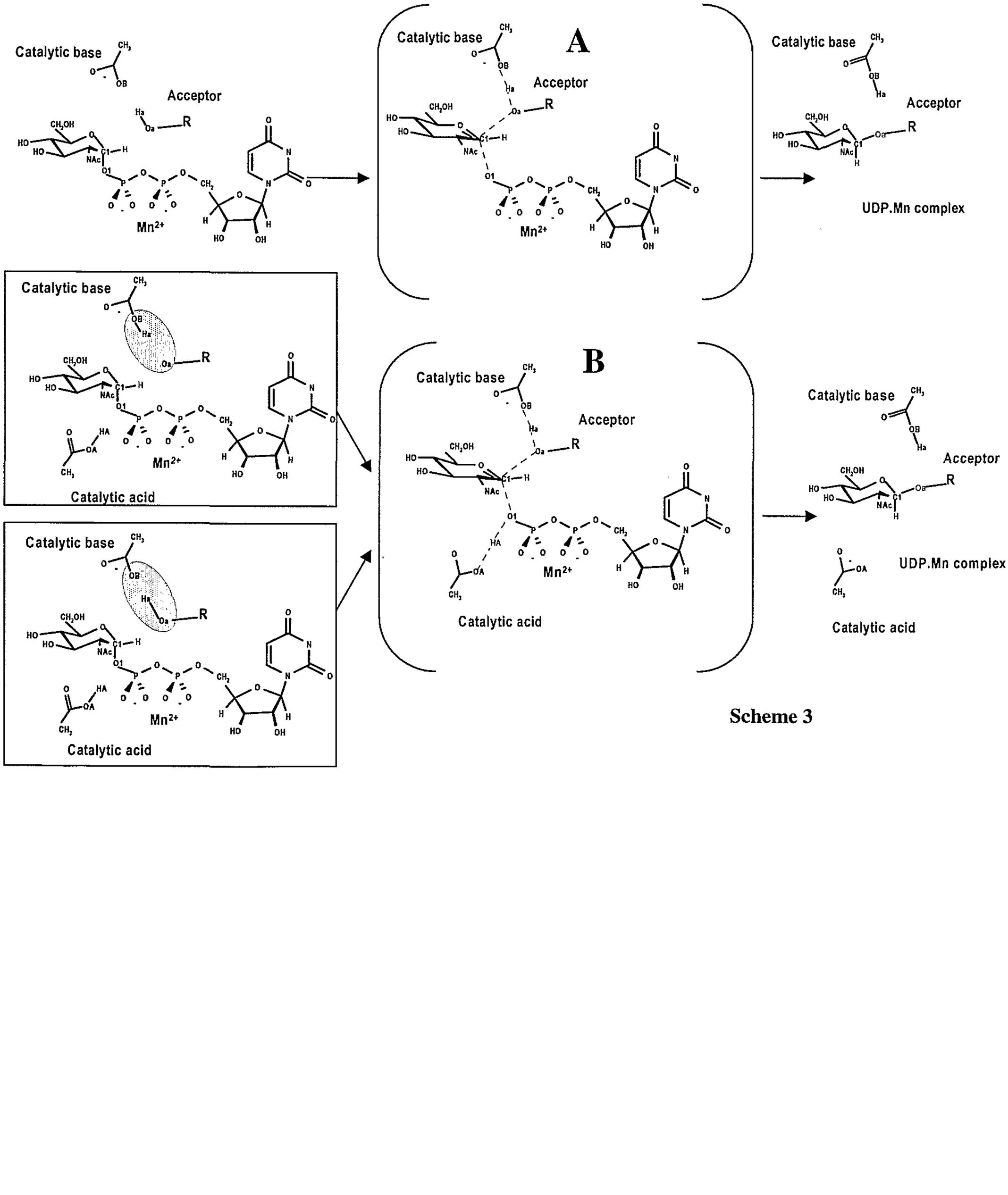
Scheme 1

FIGURE 37



Scheme 2

FIGURE 38



Scheme 3