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(54) Title: COMPOUNDS THAT MODULATE HSP90 ACTIVITY AND METHODS FOR IDENTIFYING SAME

(57) Abstract: The present invention relates to compositions and methods related to inhibitors of Hsp90, including substituted triazole compounds and compositions comprising substituted triazole compounds. The invention further relates to methods of inhibiting the activity of Hsp90 in a subject in need thereof and methods for preventing or treating hyperproliferative disorders, such as cancer, in a subject in need thereof comprising administering to the subject a substituted triazole compound of the invention, or a composition comprising such a compound. The invention further provides methods for designing and identifying inhibitors of Hsp90.



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COMPOUNDS THAT MODULATE HSP90 ACTIVITY AND METHODS FOR
IDENTIFYING SAME

RELATED APPLICATION

This application claims the benefit of U.S. Provisional Application No. 60/808,362,
5 filed on May 25, 2006. The entire teachings of the above application is incorporated herein
by reference.

BACKGROUND OF THE INVENTION

Although tremendous advances have been made in elucidating the genomic
abnormalities that cause malignant cancer cells, currently available chemotherapy remains
10 unsatisfactory, and the prognosis for the majority of patients diagnosed with cancer remains
dismal. Most chemotherapeutic agents act on a specific molecular target thought to be
involved in the development of the malignant phenotype. However, a complex network of
signaling pathways regulate cell proliferation, and the majority of malignant cancers are
facilitated by multiple genetic abnormalities in these pathway. Therefore, it is unlikely that
15 a therapeutic agent that acts on one molecular target will be fully effective in curing a
patient who has cancer.

Heat shock proteins (HSPs) are a class of chaperone proteins that are up-regulated
in response to elevated temperature and other environmental stresses, such as ultraviolet
light, nutrient deprivation, and oxygen deprivation. HSPs act as chaperones to other cellular
20 proteins (called client proteins) and facilitate their proper folding and repair, and aid in the
refolding of misfolded client proteins. There are several known families of HSPs, each
having its own set of client proteins. The Hsp90 family is one of the most abundant HSP
families, accounting for about 1-2% of proteins in a cell that is not under stress and
increasing to about 4-6% in a cell under stress. Inhibition of Hsp90 results in degradation of
25 its client proteins via the ubiquitin proteasome pathway. Unlike other chaperone proteins,
the client proteins of Hsp90 are mostly protein kinases or transcription factors involved in
signal transduction, and a number of its client proteins have been shown to be involved in
the progression of cancer.

Examples of Hsp90 client proteins that have been implicated in the progression of
30 cancer are described below.

Her-2 is a transmembrane tyrosine kinase cell surface growth factor receptor that is
expressed in normal epithelial cells. Her2 has an extracellular domain that interacts with
extracellular growth factors and an internal tyrosine kinase portion that transmits the
external growth signal to the nucleus of the cell. Her2 is overexpressed in a significant
35 proportion of malignancies, such as breast cancer, ovarian cancer, prostate cancer, and
gastric cancers, and is typically associated with a poor prognosis.

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c-Kit is a membrane receptor protein tyrosine kinase which binds Stem Cell Factor (SCF) to its extraellular domain. c-Kit is involved in the development of melanocytes, mast, germ and hematopoietic cells, and there is evidence that it plays a role in several types of cancer including leukemias, mast cell tumors, small cell lung cancer, testicular cancer, 5 cancers of the gastointesinal tract and cancers of the central nervous system.

c-Met is a receptor tyrosine kinase that is encoded by the Met protooncogene and transduces the biological effects of hepatocyte growth factor (HGF), which is also referred to as scatter factor (SF). Jiang *et al.*, *Crit. Rev. Oncol. Hemtol.* 29: 209-248 (1999), the entire teachings of which are incorporated herein by reference. c-Met and HGF are 10 expressed in numerous tissues, although their expression is normally confined predominantly to cells of epithelial and mesenchymal origin, respectively. c-Met and HGF are required for normal mammalian development and have been shown to be important in cell migration, cell proliferation and survival, morphogenic differentiation, and organization of 3-dimensional tubular structures (e.g., renal tubular cells, gland formation, etc.). The c- 15 Met receptor has been shown to be expressed in a number of human cancers. c-Met and its ligand, HGF, have also been shown to be co-expressed at elevated levels in a variety of human cancers (particularly sarcomas). However, because the receptor and ligand are usually expressed by different cell types, c-Met signaling is most commonly regulated by tumor-stroma (tumor-host) interactions. Furthermore, c-Met gene amplification, mutation, 20 and rearrangement have been observed in a subset of human cancers. Families with germline mutations that activate c-Met kinase are prone to multiple kidney tumors as well as tumors in other tissues. Numerous studies have correlated the expression of c-Met and/or HGF/SF with the state of disease progression of different types of cancer (including lung, colon, breast, prostate, liver, pancreas, brain, kidney, ovaries, stomach, skin, and bone 25 cancers). Furthermore, the overexpression of c-Met or HGF have been shown to correlate with poor prognosis and disease outcome in a number of major human cancers including lung, liver, gastric, and breast.

Akt kinase is a serine/threonine kinase which is a downstream effector molecule of phosphoinositide 3-kinase and is involved in protecting the cell from apoptosis. Akt kinase 30 is thought to be involved in the progression of cancer because it stimulates cell proliferation and suppresses apoptosis.

Cdk4/cyclin D complexes are involved in phosphorylation of retinoblastoma protein which is an essential step in progression of a cell through the G1 phase of the cell cycle. Disruption of Hsp90 activity has been shown to decrease the half life of newly synthesized 35 Cdk4.

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Raf-1 is a MAP 3-kinase (MAP3K) which when activated can phosphorylate and activate the serine/threonine specific protein kinases ERK1 and ERK2. Activated ERKs play an important role in the control of gene expression involved in the cell division cycle, apoptosis, cell differentiation and cell migration.

5 The transforming protein of Rous sarcoma virus, v-src, is a prototype of an oncogene family that induces cellular transformation (i.e., tumorigenesis) by non-regulated kinase activity. Hsp90 has been shown to complex with v-src and inhibit its degradation.

10 The BCR-ABL fusion protein associated with chronic myelogenous leukemia and in a subset of patients with acute lymphoblastic leukemia. The fusion protein is a consequence of exchange of genetic material from the long arms of chromosomes 9 and 22 and results in unregulated tyrosine kinase activity. BCR-ABL exists as a complex with Hsp90 and is rapidly degraded when the action of Hsp90 is inhibited.

15 Hsp90 is required to maintain steroid hormone receptors in a conformation capable of binding hormone with high affinity. Inhibition of the action of Hsp90 therefore is expected to be useful in treating hormone-associated malignancies such as breast cancer.

20 p53 is a tumor suppressor protein that causes cell cycle arrest and apoptosis. Mutation of the p53 gene is found in about half of all human cancers making it one of the most common genetic alterations found in cancerous cells. In addition, p53 mutation is associated with a poor prognosis. Wild-type p53 has been shown to interact with Hsp90, but mutated p53 forms a more stable association than wild-type p53 as a result of its misfolded conformations. A stronger interaction with Hsp90 protects the mutated protein from normal proteolytic degradation and prolongs its half-life. In a cell that is heterozygous for mutated and wild-type p53, inhibition of the stabilizing effect of Hsp90 causes mutant p53 to be degraded and restores the normal transcriptional activity of wild-type p53.

25 Hif-1 α is a hypoxia-inducible transcription factor that is up-regulated under low oxygen conditions. Under normal oxygen conditions Hif-1 α associates with Von Hippel-Lindau (VHL) tumor suppressor protein and is degraded. Low oxygen conditions inhibits this association and allows Hif-1 α to accumulate and complex with Hif-1 β to form an active transcription complex that associates with hypoxia-response elements to activate the transcription of vascular endothelial growth factor (VEGF). Increased Hif-1 α is associated with increased metastasis and a poor prognosis.

30 Hsp90 has been shown by mutational analysis to be necessary for the survival of normal eukaryotic cells. However, Hsp90 is over expressed in many tumor types indicating that it may play a significant role in the survival of cancer cells and that cancer cells may be more sensitive to inhibition of Hsp90 than normal cells. For example, cancer cells typically

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have a large number of mutated and overexpressed oncoproteins that are dependent on Hsp90 for folding. In addition, because the environment of a tumor is typically hostile due to hypoxia, nutrient deprivation, acidosis, etc., tumor cells may be especially dependent on Hsp90 for survival. Moreover, inhibition of Hsp90 causes simultaneous inhibition of a number of oncoproteins, as well as hormone receptors and transcription factors making it an attractive target for an anti-cancer agent. In fact, benzoquinone ansamycins, a family of natural products that inhibit Hsp90, has shown evidence of therapeutic activity in clinical trials.

Although promising, benzoquinone ansamycins, and their derivatives, suffer from a number of limitations. For example, they have low oral bioavailability, and their limited solubility makes them difficult to formulate. In addition, they are metabolized by polymorphic cytochrome P450 CYP3A4 and are a substrate for P-glycoprotein export pump involved in the development of multidrug resistance.

Therefore, a need exists for new therapeutics, and methods of identifying new therapeutics, that improve the prognosis of cancer patients and that reduces or overcomes the limitations of currently used anti-cancer agents. In particular, a need exists for improved inhibitors of Hsp90, as well as methods for identifying such inhibitors.

SUMMARY OF THE INVENTION

The present invention provides novel compounds and methods of identifying novel compounds which inhibit the activity of Hsp90 and are useful in the treatment of proliferative disorders, such as cancer. The present invention also provides new uses for previously disclosed compounds.

The present invention relates to compositions of matter comprising a compound that binds to the N-terminal ADP/ATP binding site of Hsp90, wherein the compound interacts with the amino acid residue Lys58 of Hsp90, and wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of Hsp90, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below.

The present invention also relates to compositions of matter comprising an inhibitor and Hsp90, wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 3.

The present invention also relates to compositions of matter, comprising a compound that binds to the N-terminal ADP/ATP binding site of Hsp90, wherein the

compound interacts with the amino acid residue Gly97 of Hsp90, and wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of Hsp90, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below.

5 The present invention also relates to compositions of matter comprising an inhibitor and Hsp90, wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 4.

10 The present invention also relates to compositions of matter comprising an inhibitor and Hsp90, wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 5.

15 Another aspect of the present invention is methods of inhibiting Hsp90 activity comprising exposing a compound to Hsp90, wherein the compound interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 in the absence of the compound, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below.

20 The present invention also provides methods of identifying inhibitors for Hsp90 comprising obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90; determining a three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90 by computing atomic coordinates from X-ray diffraction data of the co-crystal; and designing a compound capable of binding to the N-terminal ADP/ATP binding site of Hsp90 based on a three-dimensional shape complementarity or estimated interaction energy of the N-terminal ADP/ATP binding site of Hsp90.

30 The present invention also provides methods of identifying inhibitors for Hsp90, comprising obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90; determining a three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90 by computing atomic coordinates from X-ray diffraction data of the co-crystal; and designing a compound capable of binding to the N-terminal ADP/ATP binding site of Hsp90 based on a three-dimensional shape complementarity or estimated interaction energy of the N-terminal ADP/ATP binding site of Hsp90.

35 The present invention also provides methods of identifying inhibitors for Hsp90, comprising obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90; determining a three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90 by computing atomic coordinates from X-ray diffraction data of the co-crystal; and designing a compound capable of binding to the N-terminal ADP/ATP binding site of Hsp90 based on a three-dimensional shape complementarity or estimated interaction energy of the N-terminal ADP/ATP binding site of Hsp90.

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Hsp90; using the X-ray diffraction data to generate an electron density map consistent with the three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90; and developing compounds for an inhibitor of Hsp90 based on the electron density map.

Another aspect of the present invention provides methods of inhibiting Hsp90 activity, comprising exposing a compound to Hsp90, wherein the compound interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 in the absence of the compound, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below.

The present invention also provides methods of identifying an inhibitor for Hsp90, comprising obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90; determining a three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90 by computing atomic coordinates from X-ray diffraction data of the co-crystal; and designing a compound capable of binding to the N-terminal ADP/ATP binding site of Hsp90 based on a three-dimensional shape complementarity or estimated interaction energy of the N-terminal ADP/ATP binding site of Hsp90.

The present invention also provides methods of identifying an inhibitor for Hsp90, comprising obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90; using the X-ray diffraction data to generate an electron density map consistent with the three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90; and developing compounds for an inhibitor of Hsp90 based on the electron density map.

Compounds of the present invention inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of the present invention are particularly useful in treating cancer when given in combination with other anti-cancer agent.

The compounds of the present invention, or tautomers, pharmaceutically acceptable salts, solvates, clathrates, hydrates, polymorphs or prodrugs thereof, inhibit the activity of

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Hsp90 and, thereby facilitates the degradation of Hsp90 client proteins. Hsp90 is necessary for the survival of normal eukaryotic cells. However, Hsp90 is over expressed in many tumor types indicating that it may play a significant role in the survival of cancer cells and that cancer cells may be more sensitive to inhibition of Hsp90 than normal cells.

5 Although chemotherapeutic agents initially cause tumor regression, most agents that are currently used to treat cancer target only one pathway to tumor progression. Therefore, in many instances, after treatment with one or more chemotherapeutic agents, a tumor develops multidrug resistance and no longer responds positively to treatment. One of the advantages of inhibiting Hsp90 activity is that several of its client proteins, which are
10 mostly protein kinases or transcription factors involved in signal transduction, have been shown to be involved in the progression of cancer. Thus, inhibition of Hsp90 provides a method of short circuiting several pathways for tumor progression simultaneously. Therefore, treatment of tumors with an Hsp90 inhibitor of the invention either alone, or in combination with other chemotherapeutic agents, is more likely to result in regression or
15 elimination of the tumor, and less likely to result in the development of more aggressive multidrug resistant tumors than other currently available therapies.

BRIEF DESCRIPTION OF THE DRAWINGS

The foregoing and other objects, features and advantages of the invention will be apparent from the following more particular description of preferred embodiments of the
20 invention, as illustrated in the accompanying drawings in which like reference characters refer to the same parts throughout the different views. The drawings are not necessarily to scale, emphasis instead being placed upon illustrating the principles of the invention.

Figure 1 is a graph showing the ATPase activity of Hsp90 when untreated, when treated with 40 mM of Geldanamycin, a known Hsp90 inhibitor as a positive control, and
25 when treated with 40 μ M or 4 μ M of Compound 108 of the invention;

Figure 2 is gel showing the amount of Her2, an Hsp90 client protein, in cells that are untreated, in cells that have been treated with 0.5 μ M, 2 μ M, or 5 μ M of 17AAG, a known Hsp90 inhibitor, and in cells that have been treated with 0.5 μ M, 2 μ M, or 5 μ M of Compound 108 or Compound 49;

30 Figure 3 is a graph showing an FACSCalibur flow cytometer analysis of the c-kit positive population of HEL92.1.7 cells treated with Hsp90 inhibitors of the invention or 17AAG (as a positive control). The results indicate that the Hsp90 inhibitors of the invention induce c-kit degradation at a lower concentration than 17AAG, an Hsp90 inhibitor that is currently in phase II clinical trials.

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Figure 4 is a graph showing an FACSCalibur flow cytometer analysis of the c-kit positive population of Kasumi-1 cells treated with Hsp90 inhibitors of the invention or 17AAG (as a positive control). The results indicate that the Hsp90 inhibitors of the invention induce c-kit degradation at a lower concentration than 17AAG, an Hsp90 inhibitor that is currently in phase II clinical trials.

Figure 5 is a Western blot analysis of the c-kit from Kasumi-1 cells treated with Hsp90 inhibitors of the invention or 17AAG (as a positive control).

Figure 6 is a Western blot analysis of the c-met from NCI-H1193 cells treated with Hsp90 inhibitors of the invention or 17AAG (as a positive control).

Figure 7 displays the results of a *nude* mouse xenograft study to determine the effect of Compound 49 on the *in vivo* growth rate of the human tumor cell line MDA-MB-435S. Tumor bearing animals (8 mice/group) were intraperitoneal (IP) injected 5 times per week for 3 weeks (hatched bar) and the average tumor volumes for each group (+/- SEM) were determined every 3-5 days. Treatment with a dose of 300 mg/kg body weight of Compound 49 decreased the growth rate of MDA-MB-435S cells in *nude* mice to a greater extent than did a dose of 100 mg/kg body weight of the Hsp90 inhibitor 17-allylamino-17-demethoxygeldanamycin (17-AAG);

Figure 8 demonstrates that treatment with Compound 49 did not cause toxicity in a *nude* mouse xenograft model using the human tumor cell line MDA-MB-435S (tumor growth data from the same study is presented in Figure 3). Tumor bearing animals (8 mice/group) were intraperitoneal (IP) injected 5 times per week for 3 weeks (hatched bar) and the average percent changes in body weights for each group relative to the start of dosing were determined every 1-3 days (error bars not shown for clarity; mean coefficient of variation = 18%). Treatment with a dose of 300 mg/kg body weight of Compound 49 was not toxic, as indicated by its lack of an effect on the body weights in animals treated with Compound 49 versus vehicle treated animals;

Figure 9 displays the results of a *nude* mouse xenograft study to determine the effect of Compound 188 on the *in vivo* growth rate of RERF-LC-AI^{IVP} human lung tumor cells. Tumor bearing animals (8 mice/group) were i.p. injected 5 times per week for a total of 15 doses (hatched bar) and the average tumor volumes for each group (error bars represent SEM) were determined every 3-4 days. Treatment with a dose of 200 mg/kg body weight of Compound 188 inhibited tumor growth, as did a dose of 75 mg/kg body weight of 17-AAG (both compounds were dosed at approximately their maximum tolerated doses in *nude* mice); and

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Figure 10 demonstrates that treatment with Compound 188 does not cause overt toxicity in a *nude* mouse xenograft model using RERF-LC-AI^{IVP} human lung tumor cells (data derived from the same study presented in Figure 5). Tumor bearing animals (8 mice/group) were i.p. injected 5 times per week for a total of 15 doses (hatched bar) and the cumulative average percent changes in body weights for each group relative to the start of dosing were determined every 2-3 days. Treatment with a dose of 200 mg/kg body weight of Compound 188 was not overtly toxic, as indicated by the minimal effects on the animal body weights in the test article-treated versus vehicle-treated groups; and

Figure 11 illustrates binding interactions between Hsp90 and Hsp90 inhibitors according to some embodiments of the invention.

DETAILED DESCRIPTION OF THE INVENTION

Methods for identifying new therapeutic agents which are able to inhibit HSPs would have broad application. For example, an X-ray crystal structure of Hsp90 complexed with an inhibitor would provide information relating to the interaction between Hsp90 and an inhibitor, which may be useful in the study of Hsp90 interaction and function, the structure-function relationship of Hsp90 and other molecules, and the rational design of agents useful in modulating Hsp90 activity or activation. A description of preferred embodiments of the invention follows.

The present invention provides design and identification of compounds, compounds, and uses of said compounds. The present invention encompasses the use of the compounds of the invention to inhibit Hsp90 activity and for the treatment of a proliferative disorder, such as cancer. In particular, the present invention encompasses the use of compounds of the invention to slow or stop the growth of cancerous cells or to reduce or eliminate cancerous cells in a mammal.

In certain embodiments, the compounds of the invention can be used in combination with other chemotherapeutic agents and may help to prevent or reduce the development of multidrug resistant cancerous cells in a mammal. In this embodiment, the compounds of the invention may allow a reduced efficacious amount of a second chemotherapeutic agent given to a mammal, because compounds of the invention should inhibit the development of multidrug resistant cancerous cells.

A. Terminology

Unless otherwise specified, the below terms used herein are defined as follows:

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The term "binding site," as used herein, refers to a region of a molecule or molecular complex (e.g., a protein/inhibitor complex) that, as a result of its shape, distribution of electrostatic charge, and/or distribution of nonpolar regions, favorably associates with a ligand. A binding site may include features such as cavities, surfaces, or interfaces between domains. Ligands that may associate with a binding site include, but are not limited to, inhibitors, cofactors, substrates, receptors, agonists, and antagonists. In some cases, the binding site may be capable of structural binding, wherein the ligand is in sufficient proximity to the molecule or molecular complex to exclude solvent (e.g., water) from the space between the ligand and the molecule or molecular complex. For example, amino acid residues of a protein may form a binding site, wherein a change in interaction between a ligand and the amino acid residues may not cause any change in a biochemical assay, a cell-based assay, or an *in vivo* assay used to define a functional binding site but may contribute to the formation of a three dimensional structure. In some cases, the binding site may be capable of functional binding site, wherein amino acid residues may be identified as binding site residues based upon loss or gain of function, for example, loss of binding to ligand upon mutation of the residue. In some embodiments, the amino acid residues of a functional binding site are a subset of the amino acid residues of the structural binding site.

The term "Hsp90 binding site" includes all or a portion of a molecule or molecular complex whose shape, distribution of electrostatic charge, and/or distribution of nonpolar regions is sufficiently similar to at least a portion of a binding site on Hsp90 as to be expected to bind, for example, an inhibitor of Hsp90. In some embodiments, a binding site for an inhibitor of Hsp90 comprises, consists essentially of, or consists of at least one amino acid residue of Hsp90 corresponding to Lys58, Gly97, or mixtures thereof.

The term "crystal" is given its ordinary meaning in the art and refers to one form of a solid state of matter in which atoms are arranged in a pattern that repeats periodically in three-dimensions, typically forming a lattice.

The term "co-crystal" is given its ordinary meaning in the art and refers a crystal containing a ligand bonded to a molecule (e.g., protein), wherein the crystal is solid at room temperature.

The term "complementary or complement" as used herein, refers the fit or relationship between two molecules (e.g., between a protein and a ligand) that permits interaction, including for example, space, charge, three-dimensional configuration, and the like.

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The term "ligand", as used herein, refers to an agent and/or compound that associates with a binding site on a molecule, for example, an HSP binding site, and may be an inhibitor of HSP activity.

5 The term "X-ray diffraction pattern" is given its ordinary meaning in the art and refers to the pattern obtained from X-ray scattering of the periodic assembly of molecules or atoms in a crystal. Based on the X-ray diffraction pattern obtained, a set of X-ray structure coordinates defining a three-dimensional configuration of points in space may be obtained.

10 The term "crystal structure" generally refers to the three-dimensional or lattice spacing arrangement of repeating atomic or molecular units in a crystalline material. The crystal structure of a crystalline material can be determined by X-ray crystallographic methods, as described in, for example, "Principles of Protein X-Ray Crystallography," by Jan Drenth; Springer Advanced Texts in Chemistry, Springer Verlag; 2nd ed., February 1999, ISBN: 0387985875, and "Introduction to Macromolecular Crystallography," by Alexander McPherson, Wiley-Liss, Oct. 18, 2002, ISBN: 0471251224.

15 As used herein, the term "alkyl" means a saturated straight chain or branched non-cyclic hydrocarbon having from 1 to 10 carbon atoms. Representative saturated straight chain alkyls include methyl, ethyl, n-propyl, n-butyl, n-pentyl, n-hexyl, n-heptyl, n-octyl, n-nonyl and n-decyl; while saturated branched alkyls include isopropyl, *sec*-butyl, isobutyl, *tert*-butyl, isopentyl, 2-methylbutyl, 3-methylbutyl, 2-methylpentyl, 3-methylpentyl, 4-methylpentyl, 2-methylhexyl, 3-methylhexyl, 4-methylhexyl, 5-methylhexyl, 2,3-dimethylbutyl, 2,3-dimethylpentyl, 2,4-dimethylpentyl, 2,3-dimethylhexyl, 2,4-dimethylhexyl, 2,5-dimethylhexyl, 2,2-dimethylpentyl, 2,2-dimethylhexyl, 3,3-dimethylpentyl, 3,3-dimethylhexyl, 4,4-dimethylhexyl, 2-ethylpentyl, 3-ethylpentyl, 2-ethylhexyl, 3-ethylhexyl, 4-ethylhexyl, 2-methyl-2-ethylpentyl, 2-methyl-3-ethylpentyl, 2-methyl-4-ethylpentyl, 2-methyl-2-ethylhexyl, 2-methyl-3-ethylhexyl, 2-methyl-4-ethylhexyl, 2,2-diethylpentyl, 3,3-diethylhexyl, 2,2-diethylhexyl, 3,3-diethylhexyl and the like. The term "(C₁-C₆)alkyl" means a saturated straight chain or branched non-cyclic hydrocarbon having from 1 to 6 carbon atoms. Representative (C₁-C₆)alkyl groups are those shown above having from 1 to 6 carbon atoms. Alkyl groups included in compounds of this invention may be optionally substituted with one or more substituents.

35 As used herein, the term "alkenyl" means a saturated straight chain or branched non-cyclic hydrocarbon having from 2 to 10 carbon atoms and having at least one carbon-carbon double bond. Representative straight chain and branched (C₂-C₁₀)alkenyls include vinyl, allyl, 1-butenyl, 2-butenyl, isobutylenyl, 1-pentenyl, 2-pentenyl, 3-methyl-1-butenyl, 2-methyl-2-butenyl, 2,3-dimethyl-2-butenyl, 1-hexenyl, 2-hexenyl, 3-hexenyl, 1-heptenyl,

2-heptenyl, 3-heptenyl, 1-octenyl, 2-octenyl, 3-octenyl, 1-nonenyl, 2-nonenyl, 3-nonenyl, 1-decenyl, 2-decenyl, 3-decenyl and the like. Alkenyl groups may be optionally substituted with one or more substituents.

As used herein, the term "alkynyl" means a saturated straight chain or branched non-cyclic hydrocarbon having from 2 to 10 carbon atoms and having at least one carbon-carbon triple bond. Representative straight chain and branched alkynyls include acetylenyl, propynyl, 1-butylnyl, 2-butylnyl, 1-pentylnyl, 2-pentylnyl, 3-methyl-1-butylnyl, 4-pentylnyl, 1-hexynyl, 2-hexynyl, 5-hexynyl, 1-heptynyl, 2-heptynyl, 6-heptynyl, 1-octynyl, 2-octynyl, 7-octynyl, 1-nonylnyl, 2-nonylnyl, 8-nonylnyl, 1-decynyl, 2-decynyl, 9-decynyl, and the like. Alkynyl groups may be optionally substituted with one or more substituents.

As used herein, the term "cycloalkyl" means a saturated, mono- or polycyclic alkyl radical having from 3 to 20 carbon atoms. Representative cycloalkyls include cyclopropyl, 1-methylcyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, cycloheptyl, cyclooctyl, cyclononyl, -cyclodecyl, octahydro-pentalenyl, and the like. Cycloalkyl groups may be optionally substituted with one or more substituents.

As used herein, the term "cycloalkenyl" means a mono- or poly- cyclic non-aromatic alkyl radical having at least one carbon-carbon double bond in the cyclic system and from 3 to 20 carbon atoms. Representative cycloalkenyls include cyclopentenyl, cyclopentadienyl, cyclohexenyl, cyclohexadienyl, cycloheptenyl, cycloheptadienyl, cycloheptatrienyl, cyclooctenyl, cyclooctadienyl, cyclooctatrienyl, cyclooctatetraenyl, cyclononenyl, cyclononadienyl, cyclodecenyl, cyclodecadienyl, 1,2,3,4,5,8-hexahydronaphthalenyl and the like. Cycloalkenyl groups may be optionally substituted with one or more substituents.

As used herein, the term "haloalkyl" means an alkyl group in which one or more (including all) the hydrogen radicals are replaced by a halo group, wherein each halo group is independently selected from -F, -Cl, -Br, and -I. The term "halomethyl" means a methyl in which one to three hydrogen radical(s) have been replaced by a halo group. Representative haloalkyl groups include trifluoromethyl, bromomethyl, 1,2-dichloroethyl, 4-iodobutyl, 2-fluoropentyl, and the like.

As used herein, an "alkoxy" is an alkyl group which is attached to another moiety via an oxygen linker.

As used herein, an "haloalkoxy" is a haloalkyl group which is attached to another moiety via an oxygen linker.

As used herein, the term an "aromatic ring" or "aryl" means a hydrocarbon monocyclic or polycyclic radical in which at least one ring is aromatic. Examples of

suitable aryl groups include, but are not limited to, phenyl, tolyl, anthracenyl, fluorenyl, indenyl, azulenyl, and naphthyl, as well as benzo-fused carbocyclic moieties such as 5,6,7,8-tetrahydronaphthyl. Aryl groups may be optionally substituted with one or more substituents. In one embodiment, the aryl group is a monocyclic ring, wherein the ring
5 comprises 6 carbon atoms, referred to herein as “(C₆)aryl.”

As used herein, the term “aralkyl” means an aryl group that is attached to another group by a (C₁-C₆)alkylene group. Representative aralkyl groups include benzyl, 2-phenylethyl, naphth-3-yl-methyl and the like. Aralkyl groups may be optionally substituted with one or more substituents.

10 As used herein, the term “alkylene” refers to an alkyl group that has two points of attachment. The term “(C₁-C₆)alkylene” refers to an alkylene group that has from one to six carbon atoms. Straight chain (C₁-C₆)alkylene groups are preferred. Non-limiting examples of alkylene groups include methylene (-CH₂-), ethylene (-CH₂CH₂-), n-propylene (-CH₂CH₂CH₂-), isopropylene (-CH₂CH(CH₃)-), and the like. Alkylene groups may be
15 optionally substituted with one or more substituents.

As used herein, the term “heterocyclyl” means a monocyclic (typically having 3- to 10-members) or a polycyclic (typically having 7- to 20-members) heterocyclic ring system which is either a saturated ring or a unsaturated non-aromatic ring. A 3- to 10-membered heterocycle can contain up to 5 heteroatoms; and a 7- to 20-membered heterocycle can
20 contain up to 7 heteroatoms. Typically, a heterocycle has at least one carbon atom ring member. Each heteroatom is independently selected from nitrogen, which can be oxidized (e.g., N(O)) or quaternized; oxygen; and sulfur, including sulfoxide and sulfone. The heterocycle may be attached via any heteroatom or carbon atom. Representative heterocycles include morpholinyl, thiomorpholinyl, pyrrolidinonyl, pyrrolidinyl, piperidinyl,
25 piperazinyl, hydantoinyl, valerolactamyl, oxiranyl, oxetanyl, tetrahydrofuranyl, tetrahydropyranyl, tetrahydropyrindinyl, tetrahydropyrimidinyl, tetrahydrothiophenyl, tetrahydrothiopyranyl, and the like. A heteroatom may be substituted with a protecting group known to those of ordinary skill in the art, for example, the hydrogen on a nitrogen may be substituted with a tert-butoxycarbonyl group. Furthermore, the heterocyclyl may be
30 optionally substituted with one or more substituents. Only stable isomers of such substituted heterocyclic groups are contemplated in this definition.

As used herein, the term “heteroaromatic”, “heteroaryl” or like terms means a monocyclic or polycyclic heteroaromatic ring comprising carbon atom ring members and one or more heteroatom ring members. Each heteroatom is independently selected from
35 nitrogen, which can be oxidized (e.g., N(O)) or quaternized; oxygen; and sulfur, including

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sulfoxide and sulfone. Representative heteroaryl groups include pyridyl, 1-oxo-pyridyl, furanyl, benzo[1,3]dioxolyl, benzo[1,4]dioxinyl, thienyl, pyrrolyl, oxazolyl, imidazolyl, thiazolyl, a isoxazolyl, quinolinyl, pyrazolyl, isothiazolyl, pyridazinyl, pyrimidinyl, pyrazinyl, a triazinyl, triazolyl, thiadiazolyl, isoquinolinyl, indazolyl, benzoxazolyl, benzofuryl, indoliziny, imidazopyridyl, tetrazolyl, benzimidazolyl, benzothiazolyl, benzothiadiazo, benzoxadiazolyl, indolyl, tetrahydroindolyl, azaindolyl, imidazopyridyl, quinazolinyl, purinyl, pyrrolo[2,3]pyrimidinyl, pyrazolo[3,4]pyrimidinyl, imidazo[1,2-a]pyridyl, and benzothienyl. In one embodiment, the heteroaromatic ring is selected from 5-8 membered monocyclic heteroaryl rings. The point of attachment of a heteroaromatic or heteroaryl ring to another group may be at either a carbon atom or a heteroatom of the heteroaromatic or heteroaryl rings. Heteroaryl groups may be optionally substituted with one or more substituents.

As used herein, the term “(C₅)heteroaryl” means an aromatic heterocyclic ring of 5 members, wherein at least one carbon atom of the ring is replaced with a heteroatom such as, for example, oxygen, sulfur or nitrogen. Representative (C₅)heteroaryls include furanyl, thienyl, pyrrolyl, oxazolyl, imidazolyl, thiazolyl, isoxazolyl, pyrazolyl, isothiazolyl, pyrazinyl, triazolyl, thiadiazolyl, and the like.

As used herein, the term “(C₆)heteroaryl” means an aromatic heterocyclic ring of 6 members, wherein at least one carbon atom of the ring is replaced with a heteroatom such as, for example, oxygen, nitrogen or sulfur. Representative (C₆)heteroaryls include pyridyl, pyridazinyl, pyrazinyl, triazinyl, tetrazinyl and the like.

As used herein, the term “heteroaralkyl” means a heteroaryl group that is attached to another group by a (C₁-C₆)alkylene. Representative heteroaralkyls include 2-(pyridin-4-yl)-propyl, 2-(thien-3-yl)-ethyl, imidazol-4-yl-methyl and the like. Heteroaralkyl groups may be optionally substituted with one or more substituents.

As used herein, the term “halogen” or “halo” means -F, -Cl, -Br or -I.

Suitable substituents for an alkyl, alkylene, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocyclyl, aryl, aralkyl, heteroaryl, and heteroaralkyl groups include any substituent which will form a stable compound of the invention. Examples of substituents for an alkyl, alkylene, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocyclyl, aryl, aralkyl, heteroaryl, and heteroarylalkyl include an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, a haloalkyl, -C(O)NR₂₈R₂₉, -C(S)NR₂₈R₂₉,

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-C(NR₃₂)NR₂₈R₂₉, -NR₃₀C(O)R₃₁, -NR₃₀C(S)R₃₁, -NR₃₀C(NR₃₂)R₃₁, halo, -OR₃₀, cyano, nitro, haloalkoxy, -C(O)R₃₀, -C(S)R₃₀, -C(NR₃₂)R₃₀, -NR₂₈R₂₉, -C(O)OR₃₀, -C(S)OR₃₀, -C(NR₃₂)OR₃₀, -OC(O)R₃₀, -OC(S)R₃₀, -OC(NR₃₂)R₃₀, -NR₃₀C(O)NR₂₈R₂₉, -NR₃₀C(S)NR₂₈R₂₉, -NR₃₀C(NR₃₂)NR₂₈R₂₉, -OC(O)NR₂₈R₂₉, -OC(S)NR₂₈R₂₉,
 5 -OC(NR₃₂)NR₂₈R₂₉, -NR₃₀C(O)OR₃₁, -NR₃₀C(S)OR₃₁, -NR₃₀C(NR₃₂)OR₃₁, -S(O)_hR₃₀, -OS(O)_pR₃₀, -NR₃₀S(O)_pR₃₀, -S(O)_pNR₂₈R₂₉, -OS(O)_pNR₂₈R₂₉, or -NR₃₀S(O)_pNR₂₈R₂₉, wherein R₂₈ and R₂₉, for each occurrence are, independently, H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted
 10 heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₂₈ and R₂₉ taken together with the nitrogen to which they are attached is optionally substituted heterocyclyl or optionally substituted heteroaryl;

R₃₀ and R₃₁ for each occurrence are, independently, H, an optionally substituted
 15 alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; and

R₃₂, for each occurrence is, independently, H, an optionally substituted alkyl, an
 20 optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, -C(O)R₃₀, -C(O)NR₂₈R₂₉, -S(O)_pR₃₀, or -S(O)_pNR₂₈R₂₉;

25 p, for each occurrence, is independently, 1 or 2; and
 h is 0, 1 or 2.

In addition, alkyl, cycloalkyl, alkylene, a heterocyclyl, and any saturated portion of a alkenyl, cycloalkenyl, alkynyl, aralkyl, and heteroaralkyl groups, may also be substituted with =O, =S, =N-R₃₂.

30 When a heterocyclyl, heteroaryl, or heteroaralkyl group contains a nitrogen atom, it may be substituted or unsubstituted. When a nitrogen atom in the aromatic ring of a heteroaryl group has a substituent the nitrogen may be a quaternary nitrogen.

As used herein, the terms "subject", "patient" and "mammal" are used interchangeably. The terms "subject" and "patient" refer to an animal (*e.g.*, a bird such as a
 35 chicken, quail or turkey, or a mammal), preferably a mammal including a non-primate (*e.g.*,

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a cow, pig, horse, sheep, rabbit, guinea pig, rat, cat, dog, and mouse) and a primate (*e.g.*, a monkey, chimpanzee and a human), and more preferably a human. In one embodiment, the subject is a non-human animal such as a farm animal (*e.g.*, a horse, cow, pig or sheep), or a pet (*e.g.*, a dog, cat, guinea pig or rabbit). In a preferred embodiment, the subject is a
5 human.

As used herein, the term "lower" refers to a group having up to four atoms. For example, a "lower alkyl" refers to an alkyl radical having from 1 to 4 carbon atoms, "lower alkoxy" refers to " $-\text{O}-(\text{C}_1-\text{C}_4)\text{alkyl}$ " and a "lower alkenyl" or "lower alkynyl" refers to an alkenyl or alkynyl radical having from 2 to 4 carbon atoms, respectively.

10 Unless indicated otherwise, the compounds of the invention containing reactive functional groups (such as (without limitation) carboxy, hydroxy, thiol, and amino moieties) also include protected derivatives thereof. "Protected derivatives" are those compounds in which a reactive site or sites are blocked with one or more protecting groups. Examples of suitable protecting groups for hydroxyl groups include benzyl, methoxymethyl, allyl,
15 trimethylsilyl, tert-butyldimethylsilyl, acetate, and the like. Examples of suitable amine protecting groups include benzyloxycarbonyl, tert-butoxycarbonyl, tert-butyl, benzyl and fluorenylmethyloxy-carbonyl (Fmoc). Examples of suitable thiol protecting groups include benzyl, tert-butyl, acetyl, methoxymethyl and the like. Other suitable protecting groups are well known to those of ordinary skill in the art and include those found in T. W. Greene,
20 Protecting Groups in Organic Synthesis, John Wiley & Sons, Inc. 1981.

As used herein, the term "compound(s) of this invention" and similar terms refers to a compound or a pharmaceutically acceptable salt, solvate, clathrate, hydrate, polymorph, prodrugs and protected derivatives thereof, that binds to the N-terminal ADP/ATP binding site of Hsp90, wherein the compound interacts with the amino acid residue Lys58 of Hsp90,
25 and wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of Hsp90; and a compound that binds to the N-terminal ADP/ATP binding site of Hsp90, wherein the compound interacts with the amino acid residue Gly97 of Hsp90, and wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of Hsp90.

30 The compounds of the invention may contain one or more chiral centers and/or double bonds and, therefore, exist as stereoisomers, such as double-bond isomers (*i.e.*, geometric isomers), enantiomers, or diastereomers. According to this invention, the chemical structures depicted herein, including the compounds of this invention, encompass all of the corresponding compounds' enantiomers, diastereomers and geometric isomers,
35 that is, both the stereochemically pure form (*e.g.*, geometrically pure, enantiomerically pure,

or diastereomerically pure) and isomeric mixtures (e.g., enantiomeric, diastereomeric and geometric isomeric mixtures). In some cases, one enantiomer, diastereomer or geometric isomer will possess superior activity or an improved toxicity or kinetic profile compared to other isomers. In those cases, such enantiomers, diastereomers and geometric isomers of
5 compounds of this invention are preferred.

As used herein, the term "polymorph" means solid crystalline forms of a compound of the present invention or complex thereof. Different polymorphs of the same compound can exhibit different physical, chemical and/or spectroscopic properties. Different physical properties include, but are not limited to stability (e.g., to heat or light), compressibility and
10 density (important in formulation and product manufacturing), and dissolution rates (which can affect bioavailability). Differences in stability can result from changes in chemical reactivity (e.g., differential oxidation, such that a dosage form discolors more rapidly when comprised of one polymorph than when comprised of another polymorph) or mechanical characteristics (e.g., tablets crumble on storage as a kinetically favored polymorph converts
15 to thermodynamically more stable polymorph) or both (e.g., tablets of one polymorph are more susceptible to breakdown at high humidity). Different physical properties of polymorphs can affect their processing. For example, one polymorph might be more likely to form solvates or might be more difficult to filter or wash free of impurities than another due to, for example, the shape or size distribution of particles of it.

20 As used herein, the term "hydrate" means a compound of the present invention or a salt thereof, that further includes a stoichiometric or non-stoichiometric amount of water bound by non-covalent intermolecular forces.

As used herein, the term "clathrate" means a compound of the present invention or a salt thereof in the form of a crystal lattice that contains spaces (e.g., channels) that have a
25 guest molecule (e.g., a solvent or water) trapped within.

As used herein and unless otherwise indicated, the term "prodrug" means a derivative of a compound that can hydrolyze, oxidize, or otherwise react under biological conditions (*in vitro* or *in vivo*) to provide a compound of this invention. Prodrugs may become active upon such reaction under biological conditions, or they may have activity in
30 their unreacted forms. Examples of prodrugs contemplated in this invention include, but are not limited to, analogs or derivatives of compounds of compounds of the present invention, that comprise biohydrolyzable moieties such as biohydrolyzable amides, biohydrolyzable esters, biohydrolyzable carbamates, biohydrolyzable carbonates, biohydrolyzable ureides, and biohydrolyzable phosphate analogues as well as -NO, -NO₂, -ONO, or -ONO₂ moieties.
35 Prodrugs can typically be prepared using well-known methods, such as those described by 1

BURGER'S MEDICINAL CHEMISTRY AND DRUG DISCOVERY (1995) 172-178, 949-982 (Manfred E. Wolff ed., 5th ed).

As used herein and unless otherwise indicated, the terms "biohydrolyzable amide", "biohydrolyzable ester", "biohydrolyzable carbamate", "biohydrolyzable carbonate",
5 "biohydrolyzable ureide" and "biohydrolyzable phosphate analogue" mean an amide, ester, carbamate, carbonate, ureide, or phosphate analogue, respectively, that either: 1) does not destroy the biological activity of the compound and confers upon that compound advantageous properties *in vivo*, such as improved water solubility, improved circulating half-life in the blood (e.g., because of reduced metabolism of the prodrug), improved
10 uptake, improved duration of action, or improved onset of action; or 2) is itself biologically inactive but is converted *in vivo* to a biologically active compound. Examples of biohydrolyzable amides include, but are not limited to, lower alkyl amides, α -amino acid amides, alkoxyacyl amides, and alkylaminoalkylcarbonyl amides. Examples of biohydrolyzable esters include, but are not limited to, lower alkyl esters, alkoxyacyloxy
15 esters, alkyl acylamino alkyl esters, and choline esters. Examples of biohydrolyzable carbamates include, but are not limited to, lower alkylamines, substituted ethylenediamines, aminoacids, hydroxyalkylamines, heterocyclic and heteroaromatic amines, and polyether amines.

As used herein, "Hsp90" includes each member of the family of heat shock proteins
20 having a mass of about 90-kiloDaltons. For example, in humans the highly conserved Hsp90 family includes cytosolic Hsp90 α and Hsp90 β isoforms, as well as GRP94, which is found in the endoplasmic reticulum, and HSP75/TRAP1, which is found in the mitochondrial matrix.

The term "c-kit" or "c-kit kinase" refers to a membrane receptor protein tyrosine
25 kinase which is preferably activated upon binding Stem Cell Factor (SCF) to its extracellular domain (Yarden et al., 1987; Qiu et al., 1988). The full length amino acid sequence of a c-kit kinase preferably is as set forth in Yarden, *et al.*, 1987, *EMBO J.*, 11:3341-3351; and Qiu, *et al.*, 1988, *EMBO J.*, 7:1003-1011, which are incorporated by reference herein in their entirety, including any drawings. Mutant versions of c-kit kinase
30 are encompassed by the term "c-kit kinase" and include those that fall into two classes: (1) having a single amino acid substitution at codon 816 of the human c-kit kinase, or its equivalent position in other species (Ma *et al.*, 1999, *J. Invest Dermatol.*, 112:165-170), and (2) those which have mutations involving the putative juxtamembrane α -helix of the protein (Ma, *et al.*, 1999, *J. Biol. Chem.*, 274:13399-13402). Both of these publications are
35 incorporated by reference herein in their entirety, including any drawings.

As used herein, a "proliferative disorder" or a "hyperproliferative disorder," and other equivalent terms, means a disease or medical condition involving pathological growth of cells. Proliferative disorders include cancer, smooth muscle cell proliferation, systemic sclerosis, cirrhosis of the liver, adult respiratory distress syndrome, idiopathic
5 cardiomyopathy, lupus erythematosus, retinopathy, e.g., diabetic retinopathy or other retinopathies, cardiac hyperplasia, reproductive system associated disorders such as benign prostatic hyperplasia and ovarian cysts, pulmonary fibrosis, endometriosis, fibromatosis, hamartomas, lymphangiomatosis, sarcoidosis, desmoid tumors,

Smooth muscle cell proliferation includes hyperproliferation of cells in the
10 vasculature, for example, intimal smooth muscle cell hyperplasia, restenosis and vascular occlusion, particularly stenosis following biologically- or mechanically-mediated vascular injury, e.g., vascular injury associated with angioplasty. Moreover, intimal smooth muscle cell hyperplasia can include hyperplasia in smooth muscle other than the vasculature, e.g., bile duct blockage, bronchial airways of the lung in patients with asthma, in the kidneys of
15 patients with renal interstitial fibrosis, and the like.

Non-cancerous proliferative disorders also include hyperproliferation of cells in the skin such as psoriasis and its varied clinical forms, Reiter's syndrome, pityriasis rubra
pilaris, and hyperproliferative variants of disorders of keratinization (e.g., actinic keratosis, senile keratosis), scleroderma, and the like.

20 In a preferred embodiment, the proliferative disorder is cancer. Cancers that can be treated or prevented by the methods of the present invention include, but are not limited to human sarcomas and carcinomas, e.g., fibrosarcoma, myxosarcoma, liposarcoma, chondrosarcoma, osteogenic sarcoma, chordoma, angiosarcoma, endotheliosarcoma, lymphangiosarcoma, lymphangioendotheliosarcoma, synovioma, mesothelioma, Ewing's
25 tumor, leiomyosarcoma, rhabdomyosarcoma, colon carcinoma, pancreatic cancer, breast cancer, ovarian cancer, prostate cancer, squamous cell carcinoma, basal cell carcinoma, adenocarcinoma, sweat gland carcinoma, sebaceous gland carcinoma, papillary carcinoma, papillary adenocarcinomas, cystadenocarcinoma, medullary carcinoma, bronchogenic carcinoma, renal cell carcinoma, hepatoma, bile duct carcinoma, choriocarcinoma,
30 seminoma, embryonal carcinoma, Wilms' tumor, cervical cancer, testicular tumor, lung carcinoma, small cell lung carcinoma, bladder carcinoma, epithelial carcinoma, glioma, astrocytoma, medulloblastoma, craniopharyngioma, ependymoma, pinealoma, hemangioblastoma, acoustic neuroma, oligodendroglioma, meningioma, melanoma, neuroblastoma, retinoblastoma; leukemias, e.g., acute lymphocytic leukemia and acute
35 myelocytic leukemia (myeloblastic, promyelocytic, myelomonocytic, monocytic and

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erythroleukemia); chronic leukemia (chronic myelocytic (granulocytic) leukemia and chronic lymphocytic leukemia); and polycythemia vera, lymphoma (Hodgkin's disease and non-Hodgkin's disease), multiple myeloma, Waldenstrom's macroglobulinemia, and heavy chain disease.

5 Other examples of leukemias include acute and/or chronic leukemias, e.g., lymphocytic leukemia (e.g., as exemplified by the p388 (murine) cell line), large granular lymphocytic leukemia, and lymphoblastic leukemia; T-cell leukemias, e.g., T-cell leukemia (e.g., as exemplified by the CEM, Jurkat, and HSB-2 (acute), YAC-1 (murine) cell lines), T-lymphocytic leukemia, and T-lymphoblastic leukemia; B cell leukemia (e.g., as exemplified
10 by the SB (acute) cell line), and B-lymphocytic leukemia; mixed cell leukemias, e.g., B and T cell leukemia and B and T lymphocytic leukemia; myeloid leukemias, e.g., granulocytic leukemia, myelocytic leukemia (e.g., as exemplified by the HL-60 (promyelocyte) cell line), and myelogenous leukemia (e.g., as exemplified by the K562 (chronic) cell line); neutrophilic leukemia; eosinophilic leukemia; monocytic leukemia (e.g., as exemplified by the THP-
15 1 (acute) cell line); myelomonocytic leukemia; Naegeli-type myeloid leukemia; and nonlymphocytic leukemia. Other examples of leukemias are described in Chapter 60 of *The Chemotherapy Sourcebook*, Michael C. Perry Ed., Williams & Williams (1992) and Section 36 of *Holland Frie Cancer Medicine* 5th Ed., Bast et al. Eds., B.C. Decker Inc. (2000). The entire teachings of the preceding references are incorporated herein by reference.

20 In one embodiment, the disclosed method is believed to be particularly effective in treating subject with non-solid tumors such as multiple myeloma. In another embodiment, the disclosed method is believed to be particularly effective against T-leukemia (e.g., as exemplified by Jurkat and CEM cell lines); B-leukemia (e.g., as exemplified by the SB cell line); promyelocytes (e.g., as exemplified by the HL-60 cell line); uterine sarcoma (e.g., as
25 exemplified by the MES-SA cell line); monocytic leukemia (e.g., as exemplified by the THP-1 (acute) cell line); and lymphoma (e.g., as exemplified by the U937 cell line).

 Some of the disclosed methods can be particularly effective at treating subjects whose cancer has become "multi-drug resistant". A cancer which initially responded to an anti-cancer drug becomes resistant to the anti-cancer drug when the anti-cancer drug is no
30 longer effective in treating the subject with the cancer. For example, many tumors will initially respond to treatment with an anti-cancer drug by decreasing in size or even going into remission, only to develop resistance to the drug. Drug resistant tumors are characterized by a resumption of their growth and/or reappearance after having seemingly gone into remission, despite the administration of increased dosages of the anti-cancer drug.
35 Cancers that have developed resistance to two or more anti-cancer drugs are said to be

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“multi-drug resistant”. For example, it is common for cancers to become resistant to three or more anti-cancer agents, often five or more anti-cancer agents and at times ten or more anti-cancer agents.

As used herein, the term “c-kit associated cancer” refers to a cancer which has
5 aberrant expression and/or activation of c-kit. c-Kit associated cancers include leukemias, mast cell tumors, small cell lung cancer, testicular cancer, some cancers of the gastrointestinal tract and some central nervous system. In addition, c-kit has been implicated in playing a role in carcinogenesis of the female genital tract (Inoue, *et al.*, 1994, *Cancer Res.*, 54(11):3049-3053), sarcomas of neuroectodermal origin (Ricotti, *et al.*, 1998, *Blood*,
10 91:2397-2405), and Schwann cell neoplasia associated with neurofibromatosis (Ryan, *et al.*, 1994, *J. Neuro. Res.*, 37:415-432).

As used herein, the term “pharmaceutically acceptable salt,” is a salt formed from, for example, an acid and a basic group of one of the compounds of the present invention. Illustrative salts include, but are not limited, to sulfate, citrate, acetate, oxalate, chloride,
15 bromide, iodide, nitrate, bisulfate, phosphate, acid phosphate, isonicotinate, lactate, salicylate, acid citrate, tartrate, oleate, tannate, pantothenate, bitartrate, ascorbate, succinate, maleate, besylate, gentisinate, fumarate, gluconate, glucaronate, saccharate, formate, benzoate, glutamate, methanesulfonate, ethanesulfonate, benzenesulfonate, *p*-toluenesulfonate, and pamoate (*i.e.*, 1,1'-methylene-bis-(2-hydroxy-3-naphthoate)) salts.
20 The term “pharmaceutically acceptable salt” also refers to a salt prepared from a compound of the present invention, having an acidic functional group, such as a carboxylic acid functional group, and a pharmaceutically acceptable inorganic or organic base. Suitable bases include, but are not limited to, hydroxides of alkali metals such as sodium, potassium, and lithium; hydroxides of alkaline earth metal such as calcium and magnesium; hydroxides
25 of other metals, such as aluminum and zinc; ammonia, and organic amines, such as unsubstituted or hydroxy-substituted mono-, di-, or trialkylamines; dicyclohexylamine; tributyl amine; pyridine; N-methyl,N-ethylamine; diethylamine; triethylamine; mono-, bis-, or tris-(2-hydroxy-lower alkyl amines), such as mono-, bis-, or tris-(2-hydroxyethyl)amine, 2-hydroxy-tert-butylamine, or tris-(hydroxymethyl)methylamine, N, N,-di-lower alkyl-N-(hydroxy lower alkyl)-amines, such as N,N-dimethyl-N-(2-hydroxyethyl)amine, or tri-(2-hydroxyethyl)amine; N-methyl-D-glucamine; and amino acids such as arginine, lysine, and the like. The term “pharmaceutically acceptable salt” also refers to a salt prepared from a
30 compound of the present invention, having a basic functional group, such as an amine functional group, and a pharmaceutically acceptable inorganic or organic acid.. Suitable acids include, but are not limited to, hydrogen sulfate, citric acid, acetic acid, oxalic acid,
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hydrochloric acid (HCl), hydrogen bromide (HBr), hydrogen iodide (HI), nitric acid, hydrogen bisulfide, phosphoric acid, lactic acid, salicylic acid, tartaric acid, bitartratic acid, ascorbic acid, succinic acid, maleic acid, besylic acid, fumaric acid, gluconic acid, glucaronic acid, formic acid, benzoic acid, glutamic acid, methanesulfonic acid, ethanesulfonic acid, benzenesulfonic acid, and *p*-toluenesulfonic acid.

As used herein, the term "pharmaceutically acceptable solvate," is a solvate formed from the association of one or more pharmaceutically acceptable solvent molecules to one of the compounds of the present invention. The term solvate includes hydrates (*e.g.*, hemihydrate, monohydrate, dihydrate, trihydrate, tetrahydrate, and the like).

A pharmaceutically acceptable carrier may contain inert ingredients which do not unduly inhibit the biological activity of the compounds. The pharmaceutically acceptable carriers should be biocompatible, *i.e.*, non-toxic, non-inflammatory, non-immunogenic and devoid of other undesired reactions upon the administration to a subject. Standard pharmaceutical formulation techniques can be employed, such as those described in Remington's Pharmaceutical Sciences, *ibid*. Suitable pharmaceutical carriers for parenteral administration include, for example, sterile water, physiological saline, bacteriostatic saline (saline containing about 0.9% mg/ml benzyl alcohol), phosphate-buffered saline, Hank's solution, Ringer's-lactate and the like. Methods for encapsulating compositions (such as in a coating of hard gelatin or cyclodextran) are known in the art (Baker, *et al.*, "Controlled Release of Biological Active Agents", John Wiley and Sons, 1986).

As used herein, the term "effective amount" refers to an amount of a compound of this invention which is sufficient to reduce or ameliorate the severity, duration, progression, or onset of a proliferative disorder, prevent the advancement of a proliferative disorder, cause the regression of a proliferative, prevent the recurrence, development, onset or progression of a symptom associated with a proliferative disorder, or enhance or improve the prophylactic or therapeutic effect(s) of another therapy. The precise amount of compound administered to a subject will depend on the mode of administration, the type and severity of the disease or condition and on the characteristics of the subject, such as general health, age, sex, body weight and tolerance to drugs. It will also depend on the degree, severity and type of cell proliferation, and the mode of administration. The skilled artisan will be able to determine appropriate dosages depending on these and other factors. When co-administered with other agents, *e.g.*, when co-administered with an anti-cancer agent, an "effective amount" of the second agent will depend on the type of drug used. Suitable dosages are known for approved agents and can be adjusted by the skilled artisan according to the condition of the subject, the type of condition(s) being treated and the amount of a

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compound of the invention being used. In cases where no amount is expressly noted, an effective amount should be assumed.

Non-limiting examples of an effective amount of a compound of the invention are provided herein below. In a specific embodiment, the invention provides a method of preventing, treating, managing, or ameliorating a proliferative disorder or one or more symptoms thereof, said methods comprising administering to a subject in need thereof a dose of at least 150 $\mu\text{g/kg}$, preferably at least 250 $\mu\text{g/kg}$, at least 500 $\mu\text{g/kg}$, at least 1 mg/kg, at least 5 mg/kg, at least 10 mg/kg, at least 25 mg/kg, at least 50 mg/kg, at least 75 mg/kg, at least 100 mg/kg, at least 125 mg/kg, at least 150 mg/kg, or at least 200 mg/kg or more of one or more compounds of the invention once every day, preferably, once every 2 days, once every 3 days, once every 4 days, once every 5 days, once every 6 days, once every 7 days, once every 8 days, once every 10 days, once every two weeks, once every three weeks, or once a month.

The dosages of a chemotherapeutic agents other than compounds of the invention, which have been or are currently being used to prevent, treat, manage, or ameliorate a proliferative disorder, or one or more symptoms thereof, can be used in the combination therapies of the invention. Preferably, dosages lower than those which have been or are currently being used to prevent, treat, manage, or ameliorate a proliferative disorder, or one or more symptoms thereof, are used in the combination therapies of the invention. The recommended dosages of agents currently used for the prevention, treatment, management, or amelioration of a proliferative disorder, or one or more symptoms thereof, can obtained from any reference in the art including, but not limited to, Hardman *et al.*, eds., 1996, Goodman & Gilman's The Pharmacological Basis Of Basis Of Therapeutics 9th Ed, McGraw-Hill, New York; Physician's Desk Reference (PDR) 57th Ed., 2003, Medical Economics Co., Inc., Montvale, NJ, which are incorporated herein by reference in its entirety.

As used herein, the terms "treat", "treatment" and "treating" refer to the reduction or amelioration of the progression, severity and/or duration of a proliferative disorder, or the amelioration of one or more symptoms (preferably, one or more discernible symptoms) of a proliferative disorder resulting from the administration of one or more therapies (e.g., one or more therapeutic agents such as a compound of the invention). In specific embodiments, the terms "treat", "treatment" and "treating" refer to the amelioration of at least one measurable physical parameter of a proliferative disorder, such as growth of a tumor, not necessarily discernible by the patient. In other embodiments the terms "treat", "treatment" and "treating" refer to the inhibition of the progression of a proliferative disorder, either

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physically by, *e.g.*, stabilization of a discernible symptom, physiologically by, *e.g.*, stabilization of a physical parameter, or both. In other embodiments the terms “treat”, “treatment” and “treating” refer to the reduction or stabilization of tumor size or cancerous cell count.

5 As used herein, the terms “prevent”, “prevention” and “preventing” refer to the reduction in the risk of acquiring or developing a given proliferative disorder, or the reduction or inhibition of the recurrence or a proliferative disorder. In one embodiment, a compound of the invention is administered as a preventative measure to a patient, preferably a human, having a genetic predisposition to any of the disorders described herein.

10 As used herein, the terms “therapeutic agent” and “therapeutic agents” refer to any agent(s) which can be used in the treatment, management, or amelioration of a proliferative disorder or one or more symptoms thereof. In certain embodiments, the term “therapeutic agent” refers to a compound of the invention. In certain other embodiments, the term “therapeutic agent” refers does not refer to a compound of the invention. Preferably, a
15 therapeutic agent is an agent which is known to be useful for, or has been or is currently being used for the treatment, management, prevention, or amelioration a proliferative disorder or one or more symptoms thereof.

 As used herein, the term “synergistic” refers to a combination of a compound of the invention and another therapy (*e.g.*, a prophylactic or therapeutic agent), which is more
20 effective than the additive effects of the therapies. A synergistic effect of a combination of therapies (*e.g.*, a combination of prophylactic or therapeutic agents) permits the use of lower dosages of one or more of the therapies and/or less frequent administration of said therapies to a subject with a proliferative disorder. The ability to utilize lower dosages of a therapy (*e.g.*, a prophylactic or therapeutic agent) and/or to administer said therapy less frequently
25 reduces the toxicity associated with the administration of said therapy to a subject without reducing the efficacy of said therapy in the prevention, management or treatment of a proliferative disorder. In addition, a synergistic effect can result in improved efficacy of agents in the prevention, management or treatment of a proliferative disorder. Finally, a synergistic effect of a combination of therapies (*e.g.*, a combination of prophylactic or
30 therapeutic agents) may avoid or reduce adverse or unwanted side effects associated with the use of either therapy alone.

 As used herein, the phrase “side effects” encompasses unwanted and adverse effects of a therapy (*e.g.*, a prophylactic or therapeutic agent). Side effects are always unwanted, but unwanted effects are not necessarily adverse. An adverse effect from a therapy (*e.g.*,
35 prophylactic or therapeutic agent) might be harmful or uncomfortable or risky. Side effects

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include, but are not limited to fever, chills, lethargy, gastrointestinal toxicities (including gastric and intestinal ulcerations and erosions), nausea, vomiting, neurotoxicities, nephrotoxicities, renal toxicities (including such conditions as papillary necrosis and chronic interstitial nephritis), hepatic toxicities (including elevated serum liver enzyme levels),
5 myelotoxicities (including leukopenia, myelosuppression, thrombocytopenia and anemia), dry mouth, metallic taste, prolongation of gestation, weakness, somnolence, pain (including muscle pain, bone pain and headache), hair loss, asthenia, dizziness, extra-pyramidal symptoms, akathisia, cardiovascular disturbances and sexual dysfunction.

As used herein, the term "in combination" refers to the use of more than one
10 therapies (e.g., one or more prophylactic and/or therapeutic agents). The use of the term "in combination" does not restrict the order in which therapies (e.g., prophylactic and/or therapeutic agents) are administered to a subject with a proliferative disorder. A first therapy (e.g., a prophylactic or therapeutic agent such as a compound of the invention) can be administered prior to (e.g., 5 minutes, 15 minutes, 30 minutes, 45 minutes, 1 hour, 2
15 hours, 4 hours, 6 hours, 12 hours, 24 hours, 48 hours, 72 hours, 96 hours, 1 week, 2 weeks, 3 weeks, 4 weeks, 5 weeks, 6 weeks, 8 weeks, or 12 weeks before), concomitantly with, or subsequent to (e.g., 5 minutes, 15 minutes, 30 minutes, 45 minutes, 1 hour, 2 hours, 4 hours, 6 hours, 12 hours, 24 hours, 48 hours, 72 hours, 96 hours, 1 week, 2 weeks, 3 weeks, 4 weeks, 5 weeks, 6 weeks, 8 weeks, or 12 weeks after) the administration of a second therapy
20 (e.g., a prophylactic or therapeutic agent such as an anti-cancer agent) to a subject with a proliferative disorder, such as cancer.

As used herein, the terms "therapies" and "therapy" can refer to any protocol(s), method(s), and/or agent(s) that can be used in the prevention, treatment, management, or amelioration of a proliferative disorder or one or more symptoms thereof.

25 As used herein, a "protocol" includes dosing schedules and dosing regimens. The protocols herein are methods of use and include prophylactic and therapeutic protocols.

As used herein, the terms "manage," "managing," and "management" refer to the beneficial effects that a subject derives from a therapy (e.g., a prophylactic or therapeutic agent), which does not result in a cure of the disease. In certain embodiments, a subject is
30 administered one or more therapies (e.g., one or more prophylactic or therapeutic agents) to "manage" a disease so as to prevent the progression or worsening of the disease.

As used herein, a composition that "substantially" comprises a compound means that the composition contains more than about 80% by weight, more preferably more than about 90% by weight, even more preferably more than about 95% by weight, and most
35 preferably more than about 97% by weight of the compound.

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As used herein, a reaction that is "substantially complete" means that the reaction contains more than about 80% by weight of the desired product, more preferably more than about 90% by weight of the desired product, even more preferably more than about 95% by weight of the desired product, and most preferably more than about 97% by weight of the desired product.

As used herein, a racemic mixture means about 50% of one enantiomer and about 50% of is corresponding enantiomer relative to a chiral center in the molecule. The invention encompasses all enantiomerically-pure, enantiomerically-enriched, diastereomerically pure, diastereomerically enriched, and racemic mixtures of the compounds of the invention.

Enantiomeric and diastereomeric mixtures can be resolved into their component enantiomers or diastereomers by well known methods, such as chiral-phase gas chromatography, chiral-phase high performance liquid chromatography, crystallizing the compound as a chiral salt complex, or crystallizing the compound in a chiral solvent. Enantiomers and diastereomers can also be obtained from diastereomerically- or enantiomerically-pure intermediates, reagents, and catalysts by well known asymmetric synthetic methods.

The compounds of the invention are defined herein by their chemical structures and/or chemical names. Where a compound is referred to by both a chemical structure and a chemical name, and the chemical structure and chemical name conflict, the chemical structure is determinative of the compound's identity.

When administered to a patient, *e.g.*, to a non-human animal for veterinary use or for improvement of livestock, or to a human for clinical use, the compounds of the invention are administered in isolated form or as the isolated form in a pharmaceutical composition. As used herein, "isolated" means that the compounds of the invention are separated from other components of either (a) a natural source, such as a plant or cell, preferably bacterial culture, or (b) a synthetic organic chemical reaction mixture. Preferably, the compounds of the invention are purified via conventional techniques. As used herein, "purified" means that when isolated, the isolate contains at least 95%, preferably at least 98%, of a compound of the invention by weight of the isolate either as a mixture of stereoisomers or as a diastereomeric or enantiomeric pure isolate.

As used herein, a composition that is "substantially free" of a compound means that the composition contains less than about 20% by weight, more preferably less than about 10% by weight, even more preferably less than about 5% by weight, and most preferably less than about 3% by weight of the compound.

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Only those choices and combinations of substituents that result in a stable structure are contemplated. Such choices and combinations will be apparent to those of ordinary skill in the art and may be determined without undue experimentation.

5 The invention can be understood more fully by reference to the detailed description and illustrative examples below, which are intended to exemplify non-limiting embodiments of the invention.

B. Hsp90 Binding Site and Identification of Inhibitors of Hsp90

10 Identification of the key interactions between ligands with the binding site of a protein not only helps to understand the basis of many biological mechanisms of action but may also have significant utility in the field of drug discovery. Many therapeutic agents (e.g. inhibitors) can exert their biological effects through interaction with the binding sites of proteins. An understanding of such interactions may help lead to the design of agents having more favorable associations with their target, and thus improved biological effects.

15 The present invention describes the use of X-ray diffraction data obtained from crystal (e.g., co-crystal) structures of Hsp90 complexed with various Hsp90 inhibitors to aid in the design, identification, and/or improvement of agents that can inhibit the activity of Hsp90. The three-dimensional configuration of points derived from the structural coordinates of the crystal structures may provide information relating to the preferred size, shape, electrostatic charge distribution, substitution pattern, and/or conformation of
20 compounds that may effectively inhibit Hsp90 activity. The three-dimensional configuration of points in space may be visualized as, for example, a holographic image, a stereodiagram, a model, a computer-displayed image, or other methods known to those of skill in the art.

25 In one embodiment, the present invention provides methods of identifying inhibitors for Hsp90 comprising obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, and determining a three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90 by computing the atomic coordinates from X-ray diffraction data of the co-crystal. For example, in one embodiment, X-ray diffraction data of a co-crystal of Hsp90 and a bound
30 inhibitor reveals that the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90, relative to the three-dimensional orientation of the same amino acid residue Lys58 in a crystal of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site. In one embodiment, using the obtained X-ray diffraction data, compound capable of binding to the N-terminal ADP/ATP binding
35 site of Hsp90 may be designed based on a three-dimensional shape complementarity or

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estimated interaction energy of the N-terminal ADP/ATP binding site of Hsp90. In another embodiment, the X-ray diffraction data may be used to generate an electron density map consistent with the three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90, and compounds for inhibitor of Hsp90 may be developed based on the electron density map.

As described herein, candidate inhibitors of Hsp90 may be designed and/or identified using various methods, including determining the optimal sites for interaction between an inhibitor and Hsp90 via observation of the X-ray crystal structures. Potential sites for modification of the inhibitor compound may be identified to achieve more efficient binding interactions, for example, enhanced hydrogen bonding, van der Waals interactions, hydrophobic interactions, and/or electrostatic interactions, and the like, between Hsp90 and an inhibitor, as described more fully below. Also, the shape complementarity of an inhibitor to the conformation of the Hsp90 binding site may be evaluated. In some embodiments, the inhibitor may be designed to be able, sterically and energetically, to assume a conformation that allows it to associate with the Hsp90 binding site. Other conformational considerations include the overall three-dimensional structure and orientation of the inhibitor in relation to the binding site of Hsp90, and the spacing between various functional groups of a ligand that directly interact with the binding site.

A compound that is identified or designed as a result of any of these methods can be obtained (e.g., synthesized) and its biological activity confirmed by performing functional assays, for example, binding to Hsp90 binding site and/or modulation (e.g., inhibition) of Hsp90 activity. Optionally, the potential binding of a ligand to a Hsp90 binding site may be analyzed using computer modeling techniques prior to the actual synthesis and testing of the ligand. If these computational experiments suggest insufficient interaction and association between it and the Hsp90 binding site, testing of the ligand may be obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to or interfere with the Hsp90 binding site. Binding assays to determine if a compound actually modulates with Hsp90 activity can also be performed and are well known in the art. Those of ordinary skill in the art, with the benefit of this disclosure, would be able to screen, identify, select, and/or design ligands (e.g., inhibitors) capable of associating with Hsp90 or related proteins.

In some embodiments, compounds for the inhibition of Hsp90 activity may be identified by the determination of key binding interactions between Hsp90 inhibitors and the N-terminal ADP/ATP binding site of Hsp90, e.g., via examination of X-ray crystal structures of co-crystals of Hsp90 and an inhibitor bound to Hsp90. For example, the three-

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dimensional structure of the Hsp90 binding site and/or other structural features produced using the structural coordinates of a co-crystal of Hsp90 and an inhibitor compound bound to the binding site of Hsp90, such as those provided in Tables 3-5, may aid in the identification of candidate Hsp90 inhibitors. In some cases, the present invention describes the identification of at least one amino acid residue of Hsp90 that substantially contributes to the binding of an Hsp90 inhibitor. For example, an Hsp90 inhibitor may interact with (e.g., form a hydrogen bond with) at least one of Hsp90 residue corresponding to Lys58, Gly97, Thr184, Asp93, Asn51, Ser52, Phe 138, Leu107, or Val150, as described more fully below.

10 In some embodiments, the present invention provides compositions of matter comprising a compound that binds to the N-terminal ADP/ATP binding site of Hsp90, wherein the compound interacts with the amino acid residue Lys58 and wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of Hsp90. In some cases, the compound can interact with the amino acid residue Lys58 of Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 in the absence of the compound. For example, the compound may form a hydrogen bond with the amine group of the side chain of Lys58, pulling the side chain closer to the inhibitor. In some embodiments, the compound further interacts with other amino acid residues of Hsp90. For example, the compound may further interact with at least one of Gly97, Thr184, Asp93, Asn51, Ser52, Phe138, Leu107, Val150, or any combination thereof. In some cases, the amino acid residue or residues, when interacting with the compound, can have a three-dimensional orientation substantially corresponding to the atomic coordinates corresponding to the residue or residues represented in, for example, Table 3.

25 In some cases, the present invention provides methods of inhibiting Hsp90 activity, comprising exposing a compound to Hsp90, wherein the compound interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 in the absence of the compound. For example, the may compound interact with Hsp90 to arrange the amino acid residue Lys58 of Hsp90 into a three-dimensional orientation substantially corresponding to the atomic coordinates represented in Table 3.

In other embodiments, the present invention provides compositions of matter comprising a compound that binds to the N-terminal ADP/ATP binding site of Hsp90, wherein the compound interacts with the amino acid residue Gly97 and wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of

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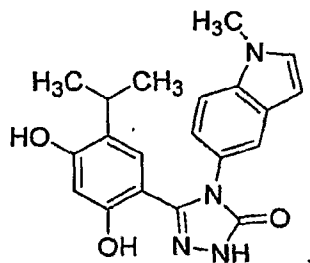
Hsp90. In some cases, the compound can interact with the amino acid residue Gly97 of Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 in the absence of the compound. For example, the compound may form a hydrogen bond with the carbonyl group of Gly97, pulling the residue closer to the inhibitor. In some embodiments, the compound further interacts with other amino acid residues of Hsp90. For example, the compound may further interact with at least one of Thr184, Asp93, Asn51, Ser52, Phe138, Leu107, Val150, or any combination thereof. In some cases, the amino acid residue or residues, when interacting with the compound, can have a three-dimensional orientation substantially corresponding to the atomic coordinates corresponding to the residue or residues represented in, for example, Table 4 or Table 5.

In some cases, the present invention provides methods of inhibiting Hsp90 activity, comprising exposing a compound to Hsp90, wherein the compound interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 in the absence of the compound. For example, the may compound interact with Hsp90 to arrange the amino acid residue Gly97 of Hsp90 into a three-dimensional orientation substantially corresponding to the atomic coordinates represented in Table 4 or Table 5.

In one embodiment, the present invention provides a composition of matter comprising an inhibitor and Hsp90, wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 3. In one embodiment, the present invention provides a composition of matter comprising an inhibitor and Hsp90, wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 4. In one embodiment, the present invention provides a composition of matter comprising an inhibitor and Hsp90, wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 5.

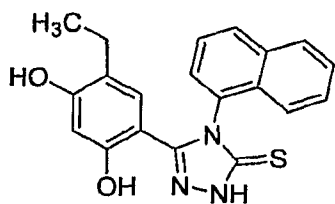
In some embodiments, the compound bound to Hsp90 has a three-dimensional orientation substantially corresponding to atomic coordinates corresponding to LIG represented in Table 3. In a particular embodiment, the compound has the structure,

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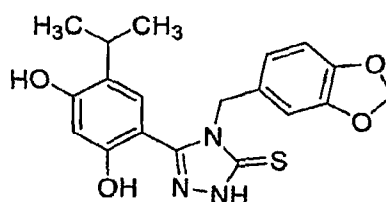
wherein the compound interacts with the binding site of Hsp90, as described more fully below.

In some embodiments, the compound bound to Hsp90 has a three-dimensional
 5 orientation substantially corresponding to atomic coordinates corresponding to LIG
 represented in Table 4 or Table 5. In one particular embodiment, the compound has the
 structure,



wherein the compound interacts with the binding site of Hsp90, as described more fully
 10 below.

In one particular embodiment, the compound has the structure,



wherein the compound interacts with the binding site of Hsp90, as described more fully
 15 below.

The present invention also provides compounds (e.g., inhibitors) that may exhibit or
 may be expected to exhibit substantially similar binding interaction(s) as the inhibitors
 described herein. In some cases, at least a portion of the compounds may be similar in size,
 shape, and/or electrostatic charge distribution to the inhibitors described herein. In some
 20 cases, at least a portion of the compounds may not have similar size, shape, and/or
 electrostatic charge distribution to the inhibitors described herein, but may exhibit similar
 binding interaction(s) to certain amino acid residues of Hsp90. For example, the present
 invention encompasses compounds that bind to Hsp90 via interaction (e.g., formation of a

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hydrogen-bond) with Lys58, Gly97, or combinations thereof. In some embodiments, the compound may interact with (e.g., form a hydrogen bond with) at least one Hsp90 residue corresponding to Lys58, Gly97, Thr184, Asp93, Asn51, Ser52, Phe 138, Leu107, or Val150, or combinations thereof.

5 In some embodiments, Hsp90 inhibitors may possess a structure corresponding in size and shape to a 3,4-diaryl triazoles. As used herein, the term "3,4-diaryl triazoles" includes triazoles substituted with aryl and heteroaryls. Sterically, the shape and size of a 3,4-diaryl triazole may complement the size and shape of the Hsp90 binding site. Identification of key binding interactions between inhibitors and amino acid residues within
10 the binding site may help in determining, for example, appropriate substitution of the 3,4-diaryl triazole core to effect certain interactions between amino acid residues and functional groups of the inhibitor. Substitution of the inhibitor with an electron-donating (e.g., carbonyl, heteroatom, etc.) or electron-accepting group (e.g., protons of hydroxyls, amines, thiols, etc.) may enable the formation of a hydrogen-bond with an adjacent amino acid
15 residue when the inhibitor is bound in the binding site. For example, substitution of the inhibitor with a carbonyl group may allow the carbonyl group to act as an electron-donor, forming hydrogen-bonds with amino acid side chains of amino acid residues comprising protons capable of accepting electrons (e.g., serine, cysteine, lysine, etc.).

 It should be understood that the present invention includes compounds which are
20 structurally equivalent to 3,4-diaryl triazoles, e.g., structures at least a portion of which are of similar size and shape which form similar hydrogen-bonds with the amino acid residues of Hsp90 as described herein, but differ slightly in chemical structure from 3,4-diaryl triazoles. For example, compounds wherein a nitrogen in the triazole ring is substituted with, for example, a carbon, may exhibit or may be expected to exhibit substantially similar
25 binding as the inhibitors described herein. Also, the aryl and/or heteroaryl substituents of the triazole ring may be replaced by aralkyl and/or heteroaralkyl substituents. In other embodiments, the triazole ring may be replaced by imidazole, pyrazole, or the like. In other embodiments, the resorcinol moiety may be replaced with indole, wherein the nitrogen of the indole can have similar interaction (e.g., hydrogen bonding) with the binding site of
30 Hsp90 as the resorcinol moiety.

 It should be understood that the compositions and methods of the present invention may also be suitable for use with proteins which are structurally equivalent to Hsp90. As used herein, a protein that is "structurally equivalent" or "structurally homologous" to Hsp90 may contain one or more amino acid substitutions, deletions, additions, or
35 rearrangements with respect to the amino acid sequence of Hsp90, but may exhibit or may

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be reasonably expected to exhibit similar properties to Hsp90. For example, a protein that is structurally equivalent to Hsp90 may exhibit at least a portion of the three-dimensional orientation of at least a portion of an Hsp90 protein or Hsp90:inhibitor complex, or may contain one or more structural features that are similar to structural features of at least a portion of an Hsp90 protein or an Hsp90:inhibitor complex. Other features that can be structurally equivalent Hsp90 or an Hsp90:inhibitor complex include, for example, regions of amino acid identity, conserved active site or binding site motifs (e.g. binding site for Hsp90 inhibitor), and similarly arranged secondary structural elements.

“Structurally equivalent” proteins may be proteins that have been chemically or enzymatically derivatized at one or more constituent amino acid, including side chain modifications, backbone modifications, and N- and C-terminal modifications including acetylation, hydroxylation, hylation, amidation, and the attachment of carbohydrate or lipid moieties, cofactors, and the like. In some cases, a protein that is structurally equivalent to Hsp90, when crystallized, may comprise structural coordinates that substantially correspond to the structural coordinates described in Table 3-5 of the invention. Structural coordinates that are substantially similar to those described in Table 3-5 of the invention differ within an acceptable margin of error, but may exhibit or may be reasonably expected to exhibit at least a portion of the three-dimensional structures described in Tables 3-5. The margin of error can be calculated using methods known to those of skill in the art. For example, the relative position of atoms in a three-dimensional structure may acceptably vary by less than 5.0, or, more preferably, less than 2.5, less than 1.5, less than 1.0, less than 0.9, less than 0.8, less than 0.7, less than 0.6, less than 0.5, less than 0.4, less than 0.3, less than 0.2, or less than 0.1 Angstroms.

It will be appreciated that amino acid residues in a structurally equivalent protein identified as corresponding to Hsp90 may have different amino acid numbering.

Various computational analyses can be used to determine whether a molecule or portions of the molecule defining structure features are structurally equivalent, defined in terms of its three-dimensional structure or orientation, to all or part of Hsp90, an Hsp90:inhibitor complex or its binding sites. For example, the structural coordinates as set forth in Tables 3-5 could be manipulated by crystallographic permutations of the structural coordinates, fractionalization of the structural coordinates, integer additions or subtractions to sets of the structural coordinates, inversion of the structure coordinates, or any combination of the above. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be structurally equivalent. It should be noted that slight variations in individual structural

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coordinates of the Hsp90:inhibitor complex would not be expected to significantly alter the nature of chemical entities such as ligands that could interact with (e.g., via hydrogen bonding, van der Waals forces, electrostatic interactions, covalent bonding, non-covalent bonding, and the like) a binding site or other structural features of Hsp90.

5 Methods for obtaining crystal structures of proteins and/or protein:ligand complexes (e.g., Hsp90:inhibitor complex) are known in the art. For example, vapor diffusion is a commonly used method for protein crystallization including the “hanging drop” and “sitting drop” methods. Both methods may involve equilibrating, in a closed system (e.g., an airtight container or high-vacuum grease between glass surfaces), a droplet containing
10 purified protein, buffer, and precipitant with a larger reservoir containing similar buffers and precipitants in higher concentrations. In the hanging drop method, the droplet may be positioned on a surface directly above the surface of the reservoir, such that the droplet is suspended over the reservoir. In the sitting drop method, the droplet may be positioned on a surface adjacent to the reservoir within the closed system. As water transfers from the
15 droplet to the reservoir, the precipitant concentration within the droplet increases to a level optimal for crystallization, which is maintained at equilibrium until the crystallization is complete. It should be understood that other crystallization methods known in the art are also suitable for use in the present invention.

 The droplet may further comprise a ligand (e.g., inhibitor), wherein the ligand and
20 protein are crystallized together to form a co-crystal. Within the co-crystal, the ligand may bind to the protein via non-covalent bonds, such as hydrogen-bonds or pi-bonds. Alternatively, the protein may be crystallized first, followed by diffusion of a ligand into the crystallized protein to form a co-crystal.

 X-ray diffraction of such co-crystals may provide three-dimensional structural
25 coordinates for the protein:ligand complexes. The term “structural coordinates” or “atomic coordinates” refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a protein:ligand (e.g., Hsp90:inhibitor) complex in crystal form. The diffraction data may then be used to calculate an electron density map of the repeating unit
30 of the crystal to establish the positions of the individual atoms of the protein:ligand complex.

C. Illustrative Hsp90 Binders

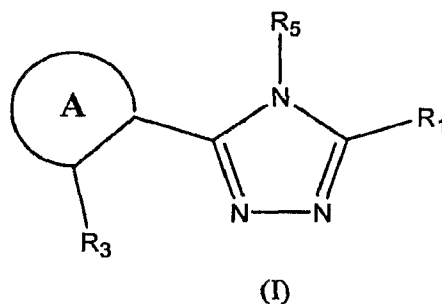
 In certain embodiments, the present invention is a compound that binds to the N-terminal
35 ADP/ATP binding site of Hsp90, wherein the compound interacts with the amino acid

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residue Lys58 of Hsp90, and wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of Hsp90, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below.

- 5 In another embodiment, the present invention is a compound that binds to the N-terminal ADP/ATP binding site of Hsp90, wherein the compound interacts with the amino acid residue Gly97 of Hsp90, and wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of Hsp90, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) -
- 10 (XXXIX) as defined below.

Structural formula (I):



and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof.

- 15 In formula (I):
ring A is an aryl or a heteroaryl, wherein the aryl or the heteroaryl are optionally further substituted with one or more substituents in addition to R₃;

- R₁ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;
- 20
- 25

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- R_3 is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

- R_5 is an optionally substituted heteroaryl or an optionally substituted 6 to 14 membered aryl, or an optionally substituted heteroaralkyl or an optionally substituted 8 to 14 membered aralkyl, or an optionally substituted cycloalkyl, and optionally substituted cycloalkenyl, or an optionally substituted alkyl;

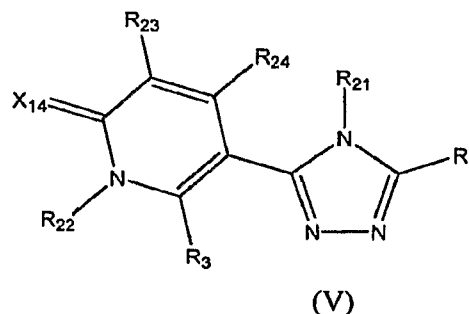
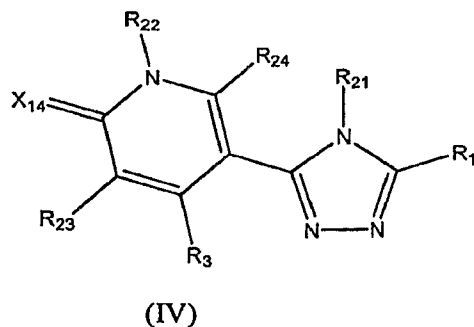
- R_7 and R_8 , for each occurrence, are, independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

- R_{10} and R_{11} , for each occurrence, are independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{10} and R_{11} , taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

- R_{26} is a lower alkyl;
- p , for each occurrence, is, independently, 1 or 2; and
- m , for each occurrence, is independently, 1, 2, 3, or 4.

Structural formula (IV) and structural formula (V):

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and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof.

In formulas (IV) and (V), R_1 and R_3 are defined as for formula (I); and

5 X_{14} is O, S, or NR_7 ;

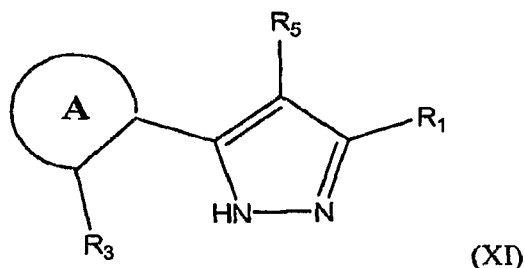
R_{21} is an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

R_{22} , for each occurrence, is independently -H or is selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, a haloalkyl, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-S(O)_pR_7$, $-S(O)_pOR_7$, or $-S(O)_pNR_{10}R_{11}$; and

R_{23} and R_{24} , for each occurrence, are independently -H or are selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, or $-S(O)_pNR_{10}R_{11}$.

Structural formula (XI):

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or a tautomer, pharmaceutically acceptable salt, solvate, clathrate, or a prodrug thereof. In formula (XI):

ring A is an aryl or a heteroaryl, wherein the aryl or the heteroaryl are optionally further substituted with one or more substituents in addition to R₃;

R₁ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, or -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, -SP(O)(OR₇)₂;

R₃ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)OH, -C(O)NHR₈, -C(O)SH, -S(O)OH, -S(O)₂OH, -S(O)NHR₈, -S(O)₂NHR₈, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

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R₅ is an optionally substituted heteroaryl or an optionally substituted 6 to 14-membered aryl, or an optionally substituted cycloalkyl, and optionally substituted cycloalkenyl, or an optionally substituted alkyl;

5 R₇ and R₈, for each occurrence, are, independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

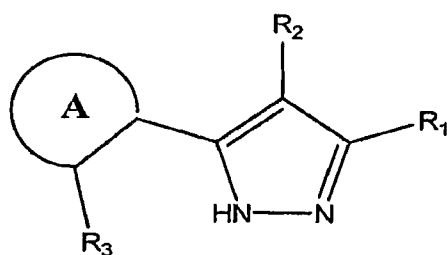
10 R₁₀ and R₁₁, for each occurrence, are independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken together with the nitrogen to which they are attached, form an optionally substituted
15 heterocyclyl or an optionally substituted heteroaryl;

R₂₆ is a lower alkyl;

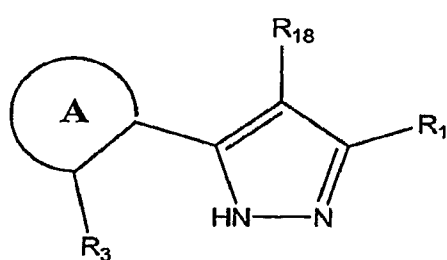
p, for each occurrence, is, independently, 0, 1 or 2; and

m, for each occurrence, is independently, 1, 2, 3, or 4.

20 Examples of a compound of formula (XI) include compounds of formulas (XII) and (XIII):



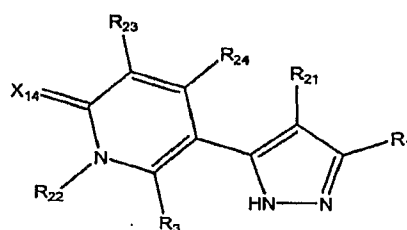
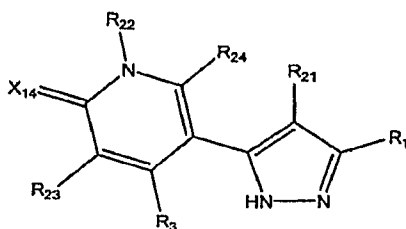
(XII)



(XIII)

Variables R₂ and R₁₈ are defined below with respect to formulas (II) and (III).

Structural formulas (XXXV) and (XXXVI):



25

(XXXV)

(XXXVI)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate, or a prodrug thereof. In formulas (XXXV) and (XXXVI):

X_{14} is O, S, or NR_7 ;

- 5 R_1 is -OH, -SH, $-NR_7H$, $-OR_{26}$, $-SR_{26}$, $-NHR_{26}$, $-O(CH_2)_mOH$, $-O(CH_2)_mSH$, $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$, $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$, $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$, $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$, $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$, $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$, $-OCH_2C(O)NR_{10}R_{11}$, $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_7S(O)_pR_7$, $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$, $-OS(O)_pOR_7$, $-SS(O)_pOR_7$, $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$, $-OC(S)OR_7$, $-SC(S)OR_7$, $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$, $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, or $-NR_7C(NR_8)NR_{10}R_{11}$, $-OP(O)(OR_7)_2$, $-SP(O)(OR_7)_2$;
- 10 R_3 is -OH, -SH, $-NR_7H$, $-OR_{26}$, $-SR_{26}$, $-NHR_{26}$, $-O(CH_2)_mOH$, $-O(CH_2)_mSH$, $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$, $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$, $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$, $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$, $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$, $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$, $-OCH_2C(O)NR_{10}R_{11}$, $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_7S(O)_pR_7$, $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$, $-OS(O)_pOR_7$, $-SS(O)_pOR_7$, $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$, $-OC(S)OR_7$, $-SC(S)OR_7$, $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$, $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, $-NR_7C(NR_8)NR_{10}R_{11}$, $-C(O)OH$, $-C(O)NHR_8$, $-C(O)SH$, $-S(O)OH$, $-S(O)_2OH$, $-S(O)NHR_8$, $-S(O)_2NHR_8$, $-OP(O)(OR_7)_2$, or $-SP(O)(OR_7)_2$;
- 20 R_7 and R_8 , for each occurrence, are, independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;
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- 30

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R₁₀ and R₁₁, for each occurrence, are independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R₂₁ is an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

R₂₂, for each occurrence, is independently a substituent selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, a haloalkyl, -C(O)R₇, -C(O)OR₇, -OC(O)R₇, -C(O)NR₁₀R₁₁, -NR₈C(O)R₇, -S(O)_pR₇, -S(O)_pOR₇, or -S(O)_pNR₁₀R₁₁; and

R₂₃ and R₂₄, for each occurrence, are independently a substituent selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, -NR₁₀R₁₁, -OR₇, -C(O)R₇, -C(O)OR₇, -OC(O)R₇, -C(O)NR₁₀R₁₁, -NR₈C(O)R₇, -SR₇, -S(O)_pR₇, -OS(O)_pR₇, -S(O)_pOR₇, -NR₈S(O)_pR₇, or -S(O)_pNR₁₀R₁₁;

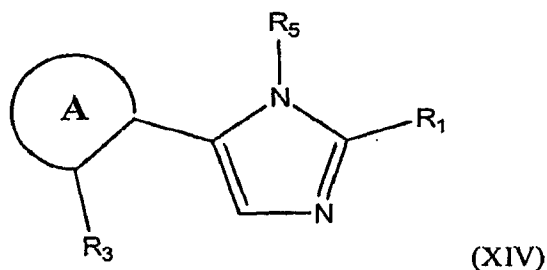
R₂₆ is a lower alkyl;

p, for each occurrence, is, independently, 0, 1 or 2; and

m, for each occurrence, is independently, 1, 2, 3, or 4.

Structural formula (XIV):

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or a tautomer, pharmaceutically acceptable salt, solvate, clathrate, or a prodrug thereof. In formula (XIV):

- ring A is an aryl or a heteroaryl, wherein the aryl or the heteroaryl are optionally
 5 further substituted with one or more substituents in addition to R₃;

- R₁ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, or -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, -SP(O)(OR₇)₂;

- R₃ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)OH, -C(O)NHR₈, -C(O)SH, -S(O)OH, -S(O)₂OH, -S(O)NHR₈, -S(O)₂NHR₈, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

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R₅ is an optionally substituted heteroaryl or an optionally substituted 6 to 14-membered aryl, or an optionally substituted cycloalkyl, and optionally substituted cycloalkenyl, or an optionally substituted alkyl;

R₇ and R₈, for each occurrence, are, independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

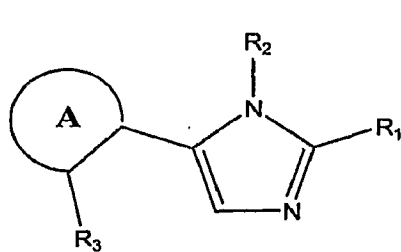
R₁₀ and R₁₁, for each occurrence, are independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R₂₆ is a lower alkyl;

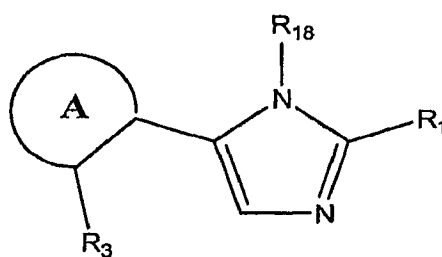
p, for each occurrence, is, independently, 0, 1 or 2; and

m, for each occurrence, is independently, 1, 2, 3, or 4.

Examples of a compound of formula (XIV) are compounds of formulas (XV) and (XVI):



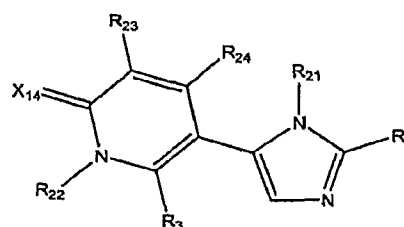
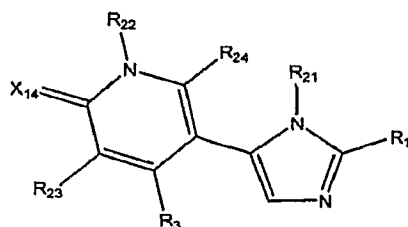
(XV)



(XVI).

In formulas (XV) and (XVI), variables R₂ and R₅ are as defined below with respect to formulas (II) and (III).

Structural formulas (XXXVII) and (XXXVIII):



(XXXVII)

(XXXVIII)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate, or a prodrug thereof. In structural formulas (XXXVII) and (XXXVIII):

X_{14} is O, S, or NR_7 ;

- 5 R_1 is -OH, -SH, $-NR_7H$, $-OR_{26}$, $-SR_{26}$, $-NHR_{26}$, $-O(CH_2)_mOH$, $-O(CH_2)_mSH$, $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$, $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$, $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$, $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$, $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$, $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$, $-OCH_2C(O)NR_{10}R_{11}$, $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_7S(O)_pR_7$, $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$, $-OS(O)_pOR_7$, $-SS(O)_pOR_7$, $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$, $-OC(S)OR_7$, $-SC(S)OR_7$, $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$, $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, or $-NR_7C(NR_8)NR_{10}R_{11}$, $-OP(O)(OR_7)_2$, $-SP(O)(OR_7)_2$;

- 10 R_3 is -OH, -SH, $-NR_7H$, $-OR_{26}$, $-SR_{26}$, $-NHR_{26}$, $-O(CH_2)_mOH$, $-O(CH_2)_mSH$, $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$, $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$, $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$, $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$, $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$, $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$, $-OCH_2C(O)NR_{10}R_{11}$, $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_7S(O)_pR_7$, $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$, $-OS(O)_pOR_7$, $-SS(O)_pOR_7$, $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$, $-OC(S)OR_7$, $-SC(S)OR_7$, $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$, $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, $-NR_7C(NR_8)NR_{10}R_{11}$, $-C(O)OH$, $-C(O)NHR_8$, $-C(O)SH$, $-S(O)OH$, $-S(O)_2OH$, $-S(O)NHR_8$, $-S(O)_2NHR_8$, $-OP(O)(OR_7)_2$, or $-SP(O)(OR_7)_2$;

- 20 R_7 and R_8 , for each occurrence, are, independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

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R_{10} and R_{11} , for each occurrence, are independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{10} and R_{11} , taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R_{21} is an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

R_{22} , for each occurrence, is independently -H or is selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, a haloalkyl, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-S(O)_pR_7$, $-S(O)_pOR_7$, or $-S(O)_pNR_{10}R_{11}$; and

R_{23} and R_{24} , for each occurrence, are independently -H, or are selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, or $-S(O)_pNR_{10}R_{11}$;

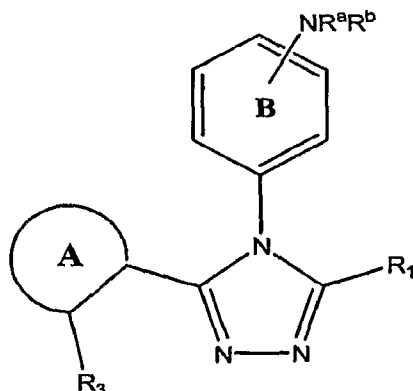
R_{26} is a lower alkyl;

p , for each occurrence, is, independently, 0, 1 or 2; and

m , for each occurrence, is independently, 1, 2, 3, or 4.

Structural formula (XVII):

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(XVII)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof.

- In formula (XVII), ring A is an aryl or a heteroaryl, wherein the aryl or the
 5 heteroaryl are optionally further substituted with one or more substituents in addition to R_3 ;

- R_1 is -OH, -SH, - NR_7H , - OR_{26} , - SR_{26} , - NHR_{26} , - $\text{O}(\text{CH}_2)_m\text{OH}$, - $\text{O}(\text{CH}_2)_m\text{SH}$,
 - $\text{O}(\text{CH}_2)_m\text{NR}_7\text{H}$, - $\text{S}(\text{CH}_2)_m\text{OH}$, - $\text{S}(\text{CH}_2)_m\text{SH}$, - $\text{S}(\text{CH}_2)_m\text{NR}_7\text{H}$, - $\text{OC}(\text{O})\text{NR}_{10}\text{R}_{11}$,
 - $\text{SC}(\text{O})\text{NR}_{10}\text{R}_{11}$, - $\text{NR}_7\text{C}(\text{O})\text{NR}_{10}\text{R}_{11}$, - $\text{OC}(\text{O})\text{R}_7$, - $\text{SC}(\text{O})\text{R}_7$, - $\text{NR}_7\text{C}(\text{O})\text{R}_7$, - $\text{OC}(\text{O})\text{OR}_7$,
 - $\text{SC}(\text{O})\text{OR}_7$, - $\text{NR}_7\text{C}(\text{O})\text{OR}_7$, - $\text{OCH}_2\text{C}(\text{O})\text{R}_7$, - $\text{SCH}_2\text{C}(\text{O})\text{R}_7$, - $\text{NR}_7\text{CH}_2\text{C}(\text{O})\text{R}_7$,
 10 - $\text{OCH}_2\text{C}(\text{O})\text{OR}_7$, - $\text{SCH}_2\text{C}(\text{O})\text{OR}_7$, - $\text{NR}_7\text{CH}_2\text{C}(\text{O})\text{OR}_7$, - $\text{OCH}_2\text{C}(\text{O})\text{NR}_{10}\text{R}_{11}$,
 - $\text{SCH}_2\text{C}(\text{O})\text{NR}_{10}\text{R}_{11}$, - $\text{NR}_7\text{CH}_2\text{C}(\text{O})\text{NR}_{10}\text{R}_{11}$, - $\text{OS}(\text{O})_p\text{R}_7$, - $\text{SS}(\text{O})_p\text{R}_7$, - $\text{S}(\text{O})_p\text{OR}_7$,
 - $\text{NR}_7\text{S}(\text{O})_p\text{R}_7$, - $\text{OS}(\text{O})_p\text{NR}_{10}\text{R}_{11}$, - $\text{SS}(\text{O})_p\text{NR}_{10}\text{R}_{11}$, - $\text{NR}_7\text{S}(\text{O})_p\text{NR}_{10}\text{R}_{11}$, - $\text{OS}(\text{O})_p\text{OR}_7$,
 - $\text{SS}(\text{O})_p\text{OR}_7$, - $\text{NR}_7\text{S}(\text{O})_p\text{OR}_7$, - $\text{OC}(\text{S})\text{R}_7$, - $\text{SC}(\text{S})\text{R}_7$, - $\text{NR}_7\text{C}(\text{S})\text{R}_7$, - $\text{OC}(\text{S})\text{OR}_7$,
 - $\text{SC}(\text{S})\text{OR}_7$, - $\text{NR}_7\text{C}(\text{S})\text{OR}_7$, - $\text{OC}(\text{S})\text{NR}_{10}\text{R}_{11}$, - $\text{SC}(\text{S})\text{NR}_{10}\text{R}_{11}$, - $\text{NR}_7\text{C}(\text{S})\text{NR}_{10}\text{R}_{11}$,
 15 - $\text{OC}(\text{NR}_8)\text{R}_7$, - $\text{SC}(\text{NR}_8)\text{R}_7$, - $\text{NR}_7\text{C}(\text{NR}_8)\text{R}_7$, - $\text{OC}(\text{NR}_8)\text{OR}_7$, - $\text{SC}(\text{NR}_8)\text{OR}_7$,
 - $\text{NR}_7\text{C}(\text{NR}_8)\text{OR}_7$, - $\text{OC}(\text{NR}_8)\text{NR}_{10}\text{R}_{11}$, - $\text{SC}(\text{NR}_8)\text{NR}_{10}\text{R}_{11}$, or - $\text{NR}_7\text{C}(\text{NR}_8)\text{NR}_{10}\text{R}_{11}$,
 - $\text{OP}(\text{O})(\text{OR}_7)_2$ or - $\text{SP}(\text{O})(\text{OR}_7)_2$;

- R_3 is -OH, -SH, - NR_7H , - NHR_{26} , - $\text{O}(\text{CH}_2)_m\text{OH}$, - $\text{O}(\text{CH}_2)_m\text{SH}$, - $\text{O}(\text{CH}_2)_m\text{NR}_7\text{H}$,
 - $\text{S}(\text{CH}_2)_m\text{OH}$, - $\text{S}(\text{CH}_2)_m\text{SH}$, - $\text{S}(\text{CH}_2)_m\text{NR}_7\text{H}$, - $\text{OC}(\text{O})\text{NR}_{10}\text{R}_{11}$, - $\text{SC}(\text{O})\text{NR}_{10}\text{R}_{11}$,
 20 - $\text{NR}_7\text{C}(\text{O})\text{NR}_{10}\text{R}_{11}$, - $\text{OC}(\text{O})\text{R}_7$, - $\text{SC}(\text{O})\text{R}_7$, - $\text{NR}_7\text{C}(\text{O})\text{R}_7$, - $\text{OC}(\text{O})\text{OR}_7$, - $\text{SC}(\text{O})\text{OR}_7$,
 - $\text{NR}_7\text{C}(\text{O})\text{OR}_7$, - $\text{OCH}_2\text{C}(\text{O})\text{R}_7$, - $\text{SCH}_2\text{C}(\text{O})\text{R}_7$, - $\text{NR}_7\text{CH}_2\text{C}(\text{O})\text{R}_7$, - $\text{OCH}_2\text{C}(\text{O})\text{OR}_7$,
 - $\text{SCH}_2\text{C}(\text{O})\text{OR}_7$, - $\text{NR}_7\text{CH}_2\text{C}(\text{O})\text{OR}_7$, - $\text{OCH}_2\text{C}(\text{O})\text{NR}_{10}\text{R}_{11}$, - $\text{SCH}_2\text{C}(\text{O})\text{NR}_{10}\text{R}_{11}$,
 - $\text{NR}_7\text{CH}_2\text{C}(\text{O})\text{NR}_{10}\text{R}_{11}$, - $\text{OS}(\text{O})_p\text{R}_7$, - $\text{SS}(\text{O})_p\text{R}_7$, - $\text{S}(\text{O})_p\text{OR}_7$, - $\text{NR}_7\text{S}(\text{O})_p\text{R}_7$,
 - $\text{OS}(\text{O})_p\text{NR}_{10}\text{R}_{11}$, - $\text{SS}(\text{O})_p\text{NR}_{10}\text{R}_{11}$, - $\text{NR}_7\text{S}(\text{O})_p\text{NR}_{10}\text{R}_{11}$, - $\text{OS}(\text{O})_p\text{OR}_7$, - $\text{SS}(\text{O})_p\text{OR}_7$,
 25 - $\text{NR}_7\text{S}(\text{O})_p\text{OR}_7$, - $\text{OC}(\text{S})\text{R}_7$, - $\text{SC}(\text{S})\text{R}_7$, - $\text{NR}_7\text{C}(\text{S})\text{R}_7$, - $\text{OC}(\text{S})\text{OR}_7$, - $\text{SC}(\text{S})\text{OR}_7$,
 - $\text{NR}_7\text{C}(\text{S})\text{OR}_7$, - $\text{OC}(\text{S})\text{NR}_{10}\text{R}_{11}$, - $\text{SC}(\text{S})\text{NR}_{10}\text{R}_{11}$, - $\text{NR}_7\text{C}(\text{S})\text{NR}_{10}\text{R}_{11}$, - $\text{OC}(\text{NR}_8)\text{R}_7$,
 - $\text{SC}(\text{NR}_8)\text{R}_7$, - $\text{NR}_7\text{C}(\text{NR}_8)\text{R}_7$, - $\text{OC}(\text{NR}_8)\text{OR}_7$, - $\text{SC}(\text{NR}_8)\text{OR}_7$, - $\text{NR}_7\text{C}(\text{NR}_8)\text{OR}_7$,

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-OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)OH, -C(O)NHR₈,
 -C(O)SH, -S(O)OH, -S(O)₂OH, -S(O)NHR₈, -S(O)₂NHR₈, -OP(O)(OR₇)₂, or
 -SP(O)(OR₇)₂. In another embodiment, -OR₂₆ and -SR₂₆, are additional values for R₃;

ring B is further optionally substituted with one or more substituents in addition to
 5 -NR^aR^b;

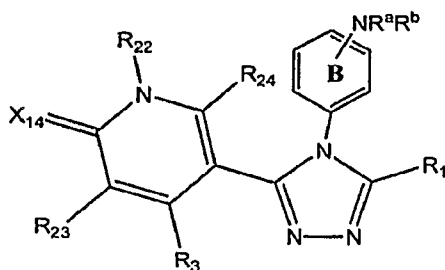
R^a and R^b, for each occurrence, is independently -H, an optionally substituted alkyl,
 an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted
 cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an
 optionally substituted aryl or heteroaryl, an optionally substituted aralkyl; or R^a and R^b,
 10 taken together with the nitrogen to which they are attached, form an optionally substituted
 heteroaryl or heterocyclyl;

R₇ and R₈, for each occurrence, is independently, -H, an optionally substituted alkyl,
 an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted
 cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an
 15 optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted
 aralkyl, or an optionally substituted heteraralkyl;

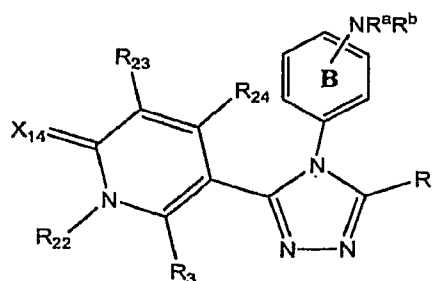
R₁₀ and R₁₁, for each occurrence, is independently -H, an optionally substituted
 alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally
 substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted
 20 heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an
 optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken
 together with the nitrogen to which they are attached, form an optionally substituted
 heterocyclyl or an optionally substituted heteroaryl;

R₂₆ is a C1-C6 alkyl;
 25 p, for each occurrence, is independently, 0, 1 or 2; and
 m, for each occurrence, is independently, 1, 2, 3 or 4.

Structural formulas (XVIII) and (XIX):



(XVIII)



(XIX)

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or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof.

In formulas (XVIII) and (XIX), ring B is further optionally substituted with one or more substituents in addition to $-NR^aR^b$;

R_1 is -OH, -SH, $-NR_7H$, $-OR_{26}$, $-SR_{26}$, $-NHR_{26}$, $-O(CH_2)_mOH$, $-O(CH_2)_mSH$,
 5 $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$, $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$,
 $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$, $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$,
 $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$, $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$,
 $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$, $-OCH_2C(O)NR_{10}R_{11}$,
 $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$, $-NR_7S(O)_pR_7$,
 10 $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$, $-OS(O)_pOR_7$, $-SS(O)_pOR_7$,
 $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$, $-OC(S)OR_7$, $-SC(S)OR_7$,
 $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$,
 $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$, $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$,
 $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, or $-NR_7C(NR_8)NR_{10}R_{11}$, $-S(O)_pOR_7$, $-OP(O)(OR_7)_2$
 15 or $-SP(O)(OR_7)_2$.

R_3 is -OH, -SH, $-NR_7H$, $-OR_{26}$, $-SR_{26}$, $-NHR_{26}$, $-O(CH_2)_mOH$, $-O(CH_2)_mSH$,
 $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$, $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$,
 $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$, $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$,
 $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$, $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$,
 20 $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$, $-OCH_2C(O)NR_{10}R_{11}$,
 $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$, $-NR_7S(O)_pR_7$,
 $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$, $-OS(O)_pOR_7$, $-SS(O)_pOR_7$,
 $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$, $-OC(S)OR_7$, $-SC(S)OR_7$,
 $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$,
 25 $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$, $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$,
 $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, $-NR_7C(NR_8)NR_{10}R_{11}$, $-C(O)OH$, $-C(O)NHR_8$,
 $-C(O)SH$, $-S(O)OH$, $-S(O)_2OH$, $-S(O)NHR_8$, $-S(O)_2NHR_8$, $-S(O)_pOR_7$, $-OP(O)(OR_7)_2$, or
 $-SP(O)(OR_7)_2$;

R_7 and R_8 , for each occurrence, is independently, -H, an optionally substituted alkyl,
 30 an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted
 cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an
 optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted
 aralkyl, or an optionally substituted heteraralkyl;

R_{10} and R_{11} , for each occurrence, is independently -H, an optionally substituted
 35 alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally

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substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{10} and R_{11} , taken together with the nitrogen to which they are attached, form an optionally substituted
 5 heterocyclyl or an optionally substituted heteroaryl;

R_{22} , for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted
 10 aralkyl, or an optionally substituted heteraralkyl, a haloalkyl, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-S(O)_pR_7$, $-S(O)_pOR_7$, or $-S(O)_pNR_{10}R_{11}$;

R_{23} and R_{24} , for each occurrence, is independently -H, an optionally substituted alky, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted
 15 heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, or $-S(O)_pNR_{10}R_{11}$;

20 R_{26} is a C1-C6 alkyl;

R^a and R^b , for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl or heteroaryl, an optionally substituted aralkyl; or R^a and R^b ,
 25 taken together with the nitrogen to which they are attached, form an optionally substituted heteroaryl or heterocyclyl;

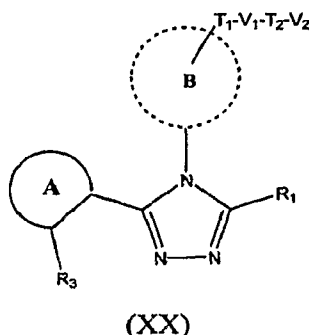
X_{14} is O, S, or NR_7 . Preferably, X_{14} is O;

p , for each occurrence, is independently, 0, 1 or 2; and

m , for each occurrence, is independently, 1, 2, 3, or 4.

30 Structural formula (XX):

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or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof. In formula (XX):

5 ring A is an aryl or a heteroaryl, wherein the aryl or the heteroaryl are optionally further substituted with one or more substituents in addition to R₃;

ring B is an aryl or a heteroaryl, wherein the aryl or the heteroaryl are optionally further substituted with one or more substituents in addition to -T₁-V₁-T₂-V₂;

R₁ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH,
 10 -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁,
 -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇,
 -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇,
 -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁,
 -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇,
 15 -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇,
 -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇,
 -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁,
 -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇,
 -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁,
 20 -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

R₃ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH,
 -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁,
 -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇,
 -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇,
 25 -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁,
 -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇,
 -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇,
 -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇,
 -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁,

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-OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇,
 -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)OH,
 -C(O)NHR₈, -C(O)SH, -S(O)OH, -S(O)₂OH, -S(O)NHR₈, -S(O)₂NHR₈, -OP(O)(OR₇)₂ or
 -SP(O)(OR₇)₂;

5 R₇ and R₈, for each occurrence, is independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteroaralkyl;

10 R₁₀ and R₁₁, for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteroaralkyl; or R₁₀ and R₁₁,
 15 taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R₂₆ is a C1-C6 alkyl;

T₁ is absent or a C1-C4 alkylene;

20 T₂ is absent or a C1-C4 alkylene, V₁ is absent and V₂ is -NR^aR^b, -NR^aS(O)₂R^{**}, -S(O)NR^aR^b, -S(O)₂NR^aR^b or -C(O)NR^aR^b; or T₂ is absent or a C1-C4 alkylene, V₁ is -O-, -S-, -N(R^{*})- or -C(O)N(R^{*})- and V₂ is -S(O)NR^aR^b, -S(O)₂NR^aR^b or -C(O)NR^aR^b; or T₂ is a C2-C4 alkylene, V₁ is -O-, -S-, -N(R^{*})-, -C(O)O-, C(O)N(R^{*})- and V₂ is -NR^aR^b, or -NR^aS(O)₂R^{**};

Each R^{*} is independently -H or C1-C3 alkyl;

25 Each R^{**} is independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteroaralkyl;

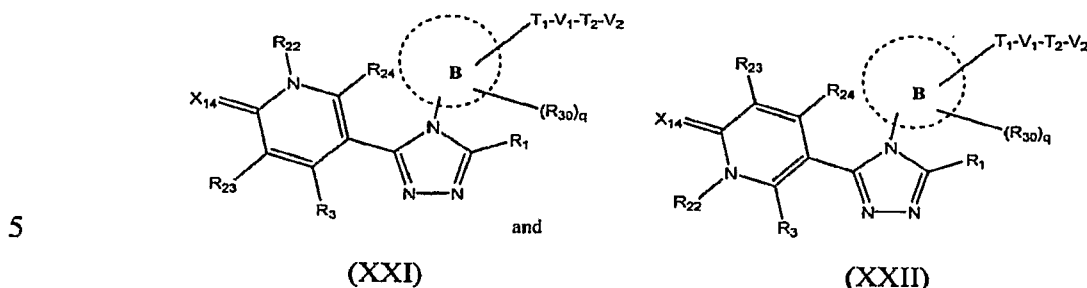
30 R^a and R^b, for each occurrence, are independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl or heteroaryl, or an optionally substituted aralkyl; or R^a and R^b, taken together with the nitrogen to which they are attached, form an
 35 optionally substituted heteroaryl or heterocyclyl;

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p, for each occurrence, is independently, 0, 1 or 2;

m, for each occurrence, is independently, 1, 2, 3 or 4;

Structural formulas (XXI) and (XXII):



or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof. In structural formulas (XXI) and (XXII):

ring B is an aryl or a heteroaryl, wherein the aryl or the heteroaryl are optionally further substituted with one or more substituents in addition to -T₁-V₁-T₂-V₂.

X₁₄ is O, S or NR₇.

R₁ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -S(O)_pOR₇, -OP(O)(OR₇)₂ or -SP(O)(OR₇)₂.

R₃ is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇,

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-NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇,
 -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇,
 -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)OH, -C(O)NHR₈,
 -C(O)SH, -S(O)OH, -S(O)₂OH, -S(O)NHR₈, -S(O)₂NHR₈, -S(O)_pOR₇, -OP(O)(OR₇)₂ or
 5 -SP(O)(OR₇)₂.

R₇ and R₈, for each occurrence, is independently, -H, an optionally substituted alkyl,
 an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted
 cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an
 optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted
 10 aralkyl or an optionally substituted heteroaralkyl.

R₁₀ and R₁₁, for each occurrence, is independently -H, an optionally substituted
 alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally
 substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted
 heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an
 15 optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken
 together with the nitrogen to which they are attached, form an optionally substituted
 heterocyclyl or an optionally substituted heteroaryl.

R₂₂, for each occurrence, is independently -H, an optionally substituted alkyl, an
 optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted
 20 cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an
 optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted
 aralkyl, or an optionally substituted heteraralkyl, a haloalkyl, -C(O)R₇, -C(O)OR₇,
 -OC(O)R₇, -C(O)NR₁₀R₁₁, -NR₈C(O)R₇, -S(O)_pR₇, -S(O)_pOR₇ or -S(O)_pNR₁₀R₁₁.

R₂₃ and R₂₄, for each occurrence, is independently -H, an optionally substituted
 25 alky, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally
 substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted
 heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an
 optionally substituted aralkyl, or an optionally substituted heteraralkyl, halo, cyano, nitro,
 guanadino, a haloalkyl, a heteroalkyl, -NR₁₀R₁₁, -OR₇, -C(O)R₇, -C(O)OR₇, -OC(O)R₇,
 30 -C(O)NR₁₀R₁₁, -NR₈C(O)R₇, -SR₇, -S(O)_pR₇, -OS(O)_pR₇, -S(O)_pOR₇, -NR₈S(O)_pR₇ or
 -S(O)_pNR₁₀R₁₁.

R₂₆ is a C1-C6 alkyl.

R^a and R^b, for each occurrence, is independently -H, an optionally substituted alkyl,
 an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted
 35 cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an

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optionally substituted aryl or heteroaryl, an optionally substituted aralkyl; or R^a and R^b , taken together with the nitrogen to which they are attached, form an optionally substituted heteroaryl or heterocyclyl.

T_1 is absent or a C1-C4 alkylene.

- 5 T_2 is absent or a C1-C4 alkylene, V_1 is absent and V_2 is $-NR^aR^b$, $-NR^aS(O)_2R^{**}$, $-S(O)NR^aR^b$, $-S(O)_2NR^aR^b$ or $-C(O)NR^aR^b$; or T_2 is absent or a C1-C4 alkylene, V_1 is $-O-$, $-S-$, $-N(R^*)-$ or $-C(O)N(R^*)-$ and V_2 is $-S(O)NR^aR^b$, $-S(O)_2NR^aR^b$ or $-C(O)NR^aR^b$; or T_2 is a C2-C4 alkylene, V_1 is $-O-$, $-S-$, $-N(R^*)-$, $-C(O)O-$, $C(O)N(R^*)-$ and V_2 is $-NR^aR^b$, or $-NR^aS(O)_2R^{**}$.

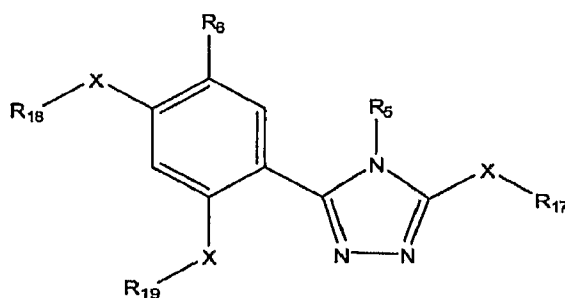
- 10 Each R^* is independently $-H$ or C1-C3 alkyl.

- Each R^{**} is independently, $-H$, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an
- 15 optionally substituted heteroaralkyl.

p , for each occurrence, is independently, 0, 1 or 2.

m , for each occurrence, is independently, 1, 2, 3 or 4.

Structural formula (XXIII):



20

(XXIII),

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof.

In formula (XXIII):

X is $-O-$ or $-S-$;

R_5 is an optionally substituted heteroaryl or an optionally substituted aryl;

- 25 R_6 is $-H$, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, cyano, halo, nitro, an optionally substituted cycloalkyl, haloalkyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteroaralkyl, $-OR_7$, $-SR_7$, $-NR_{10}R_{11}$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$,

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- SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇,
 -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇,
 -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇,
 -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇,
 5 -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇,
 -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁,
 -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇,
 -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)R₇,
 -C(O)OR₇, -C(O)NR₁₀R₁₁, -C(O)SR₇, -C(S)R₇, -C(S)OR₇, -C(S)NR₁₀R₁₁, -C(S)SR₇,
 10 -C(NR₈)OR₇, -C(NR₈)R₇, -C(NR₈)NR₁₀R₁₁, -C(NR₈)SR₇, -S(O)_pOR₇, -S(O)_pNR₁₀R₁₁, or
 -S(O)_pR₇;

R₇ and R₈, for each occurrence, is independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

- 15 R₁₀ and R₁₁, for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

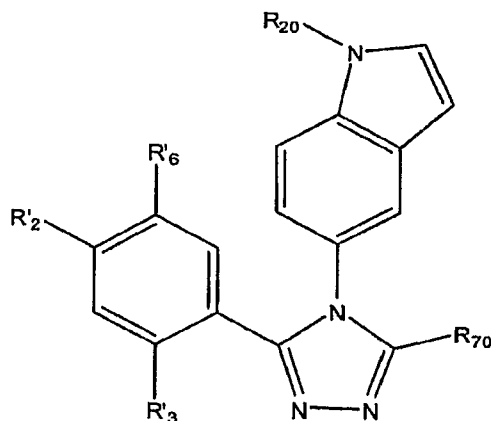
R₁₇, R₁₈, and R₁₉ are each, independently, -H, -C(O)R₂₂, or (alk)O(alk);

- 25 R₂₂, for each occurrence is independently optionally substituted alkyl, optionally substituted aryl, -O(alk), amino, alkyl amino, or dialkyl amino;
 alk is a lower alkyl;

p, for each occurrence, is independently 1 or 2.

Structural formula (XXXIX):

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(XXXIX)

In formula (XXXIX):

- R'_6 is -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, cyano, halo, nitro, an optionally substituted cycloalkyl, haloalkyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteroaralkyl, -OR₇, -SR₇, -NR₁₀R₁₁, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)R₇, -C(O)OR₇, -C(O)NR₁₀R₁₁, -C(O)SR₇, -C(S)R₇, -C(S)OR₇, -C(S)NR₁₀R₁₁, -C(S)SR₇, -C(NR₈)OR₇, -C(NR₈)R₇, -C(NR₈)NR₁₀R₁₁, -C(NR₈)SR₇, -S(O)_pOR₇, -S(O)_pNR₁₀R₁₁, or -S(O)_pR₇;
- R₇ and R₈, for each occurrence, is independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;
- R₁₀ and R₁₁, for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally

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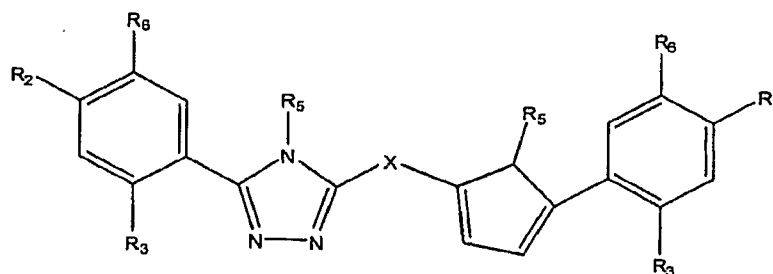
substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{10} and R_{11} , taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R_{70} , R'_{23} , and R'_{33} are, independently, -OH, -SH, or -NHR₇; R_{20} is C(O)R_y; and R_y is an optionally substituted alkyl;

p, for each occurrence, is independently 1 or 2;

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof.

Structural formula (XXIV):



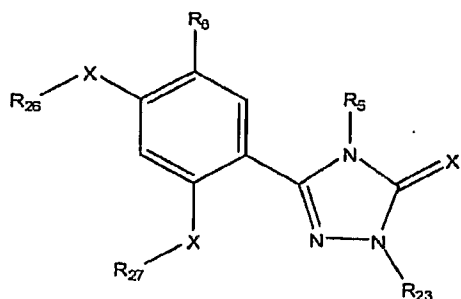
(XXIV)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof

In formula (XXIV):

X is -O-O- or -S-S-; R_2 and R_3 are, independently, -OH, -SH, or -NHR₇, and R_5 and R_6 are defined as for formula (XXIII).

Structural formula (XXV):



(XXV),

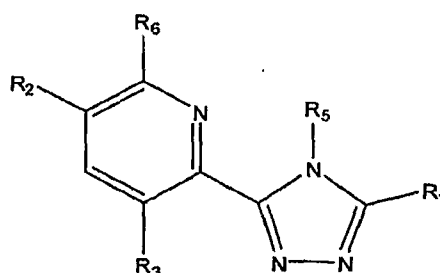
or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof.

In formula (XXV): X is -O- or -S-; X_1 is O or S; R_{26} and R_{27} are each, independently, -H, -C(O)R₂₂, or (alk)O(alk); R_{22} , for each occurrence is independently optionally substituted alkyl, optionally substituted aryl, -O(alk), amino, alkyl amino, or

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dialkyl amino; R_{23} is $-C(O)R_{22}$ or $-alk-O-C(O)R_{22}$; alk is a lower alkyl; and R_5 and R_6 are defined as for formula (XXIII).

Structural formula (XXVI):



(XXVI)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof.

In structural formula (XXVI):

- R_1 , R_2 , and R_3 are each, independently, $-OH$, $-SH$, $-NHR_7$, $-OR_{26}$, $-SR_{26}$,
 10 $-O(CH_2)_mOH$, $-O(CH_2)_mSH$, $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$,
 $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$,
 $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$, $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$,
 $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$, $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$,
 $-OCH_2C(O)NR_{10}R_{11}$, $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$,
 15 $-S(O)_pOR_7$, $-NR_7S(O)_pR_7$, $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$,
 $-OS(O)_pOR_7$, $-SS(O)_pOR_7$, $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$,
 $-OC(S)OR_7$, $-SC(S)OR_7$, $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$,
 $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$,
 $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$,
 20 $-NR_7C(NR_8)NR_{10}R_{11}$, $-OP(O)(OR_7)_2$, or $-SP(O)(OR_7)_2$;

R_5 is an optionally substituted alkyl; an optionally substituted heteroaryl or an optionally substituted aryl;

- R_6 is an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, cyano, halo, nitro, an optionally substituted cycloalkyl, haloalkyl, an
 25 optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteroaralkyl, $-OR_7$,
 $-SR_7$, $-NR_{10}R_{11}$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$,
 $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$, $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$,
 $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$, $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$,
 30 $-OCH_2C(O)NR_{10}R_{11}$, $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$,

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- NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇,
 -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇,
 -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁,
 -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇,
 5 -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)R₇,
 -C(O)OR₇, -C(O)NR₁₀R₁₁, -C(O)SR₇, -C(S)R₇, -C(S)OR₇, -C(S)NR₁₀R₁₁, -C(S)SR₇,
 -C(NR₈)OR₇, -C(NR₈)R₇, -C(NR₈)NR₁₀R₁₁, -C(NR₈)SR₇, -S(O)_pOR₇, -S(O)_pNR₁₀R₁₁, or
 -S(O)_pR₇;

- R₇ and R₈, for each occurrence, is independently, -H, an optionally substituted alkyl,
 10 an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted
 cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an
 optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted
 aralkyl, or an optionally substituted heteraralkyl;

- R₁₀ and R₁₁, for each occurrence, is independently -H, an optionally substituted
 15 alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally
 substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted
 heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an
 optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken
 together with the nitrogen to which they are attached, form an optionally substituted
 20 heterocyclyl or an optionally substituted heteroaryl;

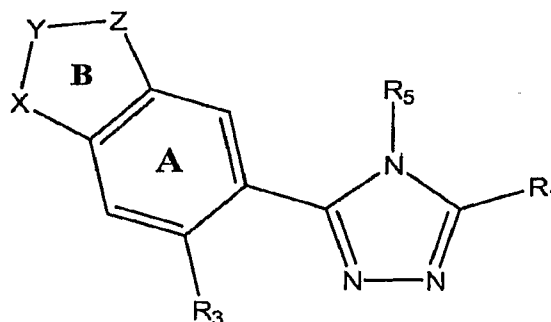
R₂₆ is a lower alkyl;

p, for each occurrence, is independently, 1 or 2; and

m, for each occurrence, is independently, 1, 2, 3 or 4.

Structural formula (XXVII):

25



(XXVII)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate, or a prodrug thereof.

In structural formula (XXVII):

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ring A is optionally further substituted with one or two independently selected substituents in addition to R₃;

ring B is aromatic or non-aromatic;

X is -O-, -NR₇-, or -S-;

5 Y is -(CR₃₈R₃₉)_l-, -C(O)-, -C(S)-, -C(NR₈)-, -CR₇=, -O-, -NR₇-, -N=, or -S-;

Z is -(CR₃₈R₃₉)_l-, =CR₇-, -O-, -S-, -NR₇-, =N-, or -CR₄₀=CR₄₁-;

R₁ and R₃ are each, independently, -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆,

-O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH,

-S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇,

10 -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇,

-SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇,

-OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇,

-S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁,

-OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇,

15 -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁,

-NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇,

-SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁,

-NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

R₅ is an optionally substituted aryl or an optionally substituted heteroaryl;

20 R₇ and R₈, for each occurrence, are, independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

25 R₁₀ and R₁₁, for each occurrence, are independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken
30 together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R₂₆, for each occurrence is, independently, a C1-C6 alkyl;

35 R₃₈ and R₃₉, for each occurrence, are independently H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted

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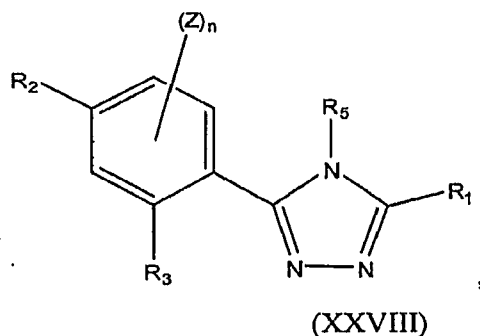
- heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteroaralkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, alkoxy, haloalkoxy, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-C(S)R_7$, $-C(O)SR_7$, $-C(S)SR_7$, $-C(S)OR_7$, $-C(S)NR_{10}R_{11}$, $-C(NR_8)OR_7$,
 5 $-C(NR_8)R_7$, $-C(NR_8)NR_{10}R_{11}$, $-C(NR_8)SR_7$, $-OC(O)R_7$, $-OC(O)OR_7$, $-OC(S)OR_7$, $-OC(NR_8)OR_7$, $-SC(O)R_7$, $-SC(O)OR_7$, $-SC(NR_8)OR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-SC(S)OR_7$, $-OC(O)NR_{10}R_{11}$, $-OC(S)NR_{10}R_{11}$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-NR_7C(S)R_7$, $-NR_7C(S)OR_7$, $-NR_7C(NR_8)R_7$, $-NR_7C(O)OR_7$, $-NR_7C(NR_8)OR_7$, $-NR_7C(O)NR_{10}R_{11}$,
 10 $-NR_7C(S)NR_{10}R_{11}$, $-NR_7C(NR_8)NR_{10}R_{11}$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-OS(O)_pOR_7$, $-OS(O)_pNR_{10}R_{11}$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, $-NR_7S(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pOR_7$, $-S(O)_pNR_{10}R_{11}$, $-SS(O)_pR_7$, $-SS(O)_pOR_7$, $-SS(O)_pNR_{10}R_{11}$, $-OP(O)(OR_7)_2$, or $-SP(O)(OR_7)_2$; or R_{38} and R_{39} together with the carbon or carbon atoms to which they are attached form a three to eight membered cycloalkyl or a three to eight membered cycloalkenyl;
- 15 R_{40} and R_{41} , for each occurrence, are, independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{40} and R_{41} ,
 20 together with the carbon atoms to which they are attached form a three to eight membered cycloalkenyl;

p , for each occurrence, is, independently, 1 or 2; and

m , for each occurrence, is independently, 1, 2, 3, or 4; and

t is 1 or 2.

- 25 Structural formula:



or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or prodrug thereof.

In formula (XXVIII):

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R_1 is, $-NHR_7$, $-NHC(O)NR_{10}R_{11}$, $-NHC(O)R_7$, $-NHC(O)OR_7$, $-NHCH_2C(O)R_7$, $-NHCH_2C(O)OR_7$, $-NHCH_2C(O)NR_{10}R_{11}$, $-NHS(O)_pR_7$, $-NHS(O)_pNR_{10}R_{11}$, $-NHS(O)_pOR_7$, $-NHC(S)R_7$, $-NHC(S)OR_7$, $-NHC(S)NR_{10}R_{11}$, $-NHC(NR_8)R_7$, $-NHC(NR_8)OR_7$, or $-NHC(NR_8)NR_{10}R_{11}$;

- 5 R_2 is $-OH$, $-SH$, $-NR_7H$, $-OR_{26}$, $-SR_{26}$, $-O(CH_2)_mOH$, $-O(CH_2)_mSH$, $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$, $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$, $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$, $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$, $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$, $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$, $-OCH_2C(O)NR_{10}R_{11}$, $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_7S(O)_pR_7$, $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$, $-OS(O)_pOR_7$, $-SS(O)_pOR_7$, $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$, $-OC(S)OR_7$, $-SC(S)OR_7$, $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$, $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, $-NR_7C(NR_8)NR_{10}R_{11}$, $-OP(O)(OR_7)_2$, or $-SP(O)(OR_7)_2$;

R_3 is $-OH$, $-SH$, or $-NHR_7$;

R_5 is an optionally substituted heteroaryl or an optionally substituted aryl;

- 20 R_7 and R_8 , for each occurrence, is independently, $-H$, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

- 25 R_{10} and R_{11} , for each occurrence, is independently $-H$, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{10} and R_{11} , taken together with the nitrogen to which they are attached, form an optionally substituted
- 30 heterocyclyl or an optionally substituted heteroaryl;

R_{26} is a lower alkyl;

Z is a substituent;

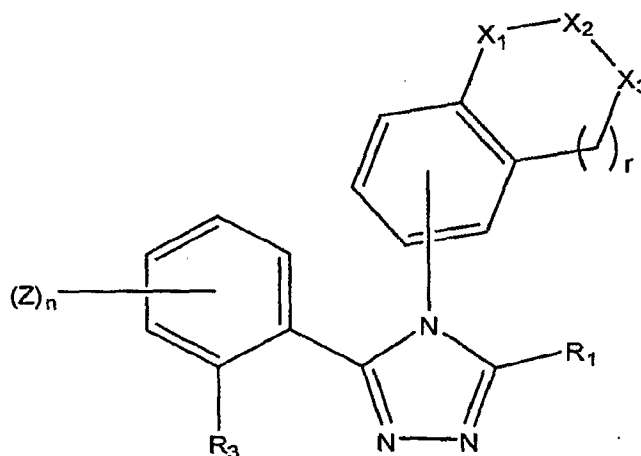
p , for each occurrence, is independently, 1 or 2;

m , for each occurrence, is independently, 1, 2, 3 or 4; and

- 35 n is 0, 1, 2, or 3.

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Structural formula (XXIX):



(XXIX)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof. In

5 formula (XXIX):

- R_1 and R_3 are, independently, -OH, -SH, -NHR₇, -OR₂₆, -SR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

R_7 and R_8 , for each occurrence, is independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

R_{10} and R_{11} , for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an

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optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R₂₆ is a lower alkyl;

5 X₁, X₂, and X₃ are each independently C(R₂₇)₂, NR₇₇, C(O), S(O)₂, O or S;

R₂₇, for each occurrence, is independently a substituent selected from the group consisting of -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, halo, cyano, nitro, guanadino, a hydroxyalkyl, alkoxyalkyl, haloalkyl, a heteroalkyl, -NR₁₀R₁₁, -OR₇, -C(O)R₇, -C(O)OR₇, -OC(O)R₇, -C(O)NR₁₀R₁₁, -NR₈C(O)R₇, -SR₇, -S(O)_pR₇, -OS(O)_pR₇, -S(O)_pOR₇, -NR₈S(O)_pR₇, or -S(O)_pNR₁₀R₁₁, -S(O)_pOR₇, -OP(O)(OR₇)₂, -SP(O)(OR₇)₂, -S(O)_pOR₇, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

15 or two R₂₇ groups taken together with the carbon atom to which they are attached form an optionally substituted cycloalkyl or optionally substituted heterocyclyl ring;

R₇₇, for each occurrence, is independently a substituent selected from the group consisting of -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, halo, guanadino, a hydroxyalkyl, alkoxyalkyl, haloalkyl, a heteroalkyl, -OR₇, -C(O)R₇, -C(O)OR₇, -OC(O)R₇, -C(O)NR₁₀R₁₁, -SR₇, -S(O)_pR₇, -OS(O)_pR₇, -S(O)_pOR₇, -S(O)_pNR₁₀R₁₁, -S(O)_pOR₇, -OP(O)(OR₇)₂, -SP(O)(OR₇)₂, -S(O)_pOR₇, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

Z is a substituent;

p, for each occurrence, is independently, 1 or 2;

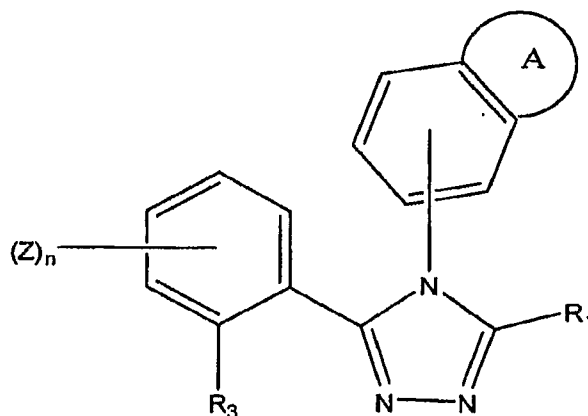
m, for each occurrence, is independently, 1, 2, 3 or 4;

n is 0, 1, 2, or 3;

30 r is 0 or 1.

Structural formula (XXX):

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(XXX)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof. In formula (XXX), ring A is an optionally substituted heteroaromatic ring, selected from the group consisting of furanyl, oxazolyl, thiazolyl, indazolyl, thiophenyl, triazolyl, or pyridyl;

R₁ and R₃ are, independently, -OH, -SH, -NHR₇, -OR₂₆, -SR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

R₇ and R₈, for each occurrence, is independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

R₁₀ and R₁₁, for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken

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together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R_{26} is a lower alkyl;

Z is a substituent;

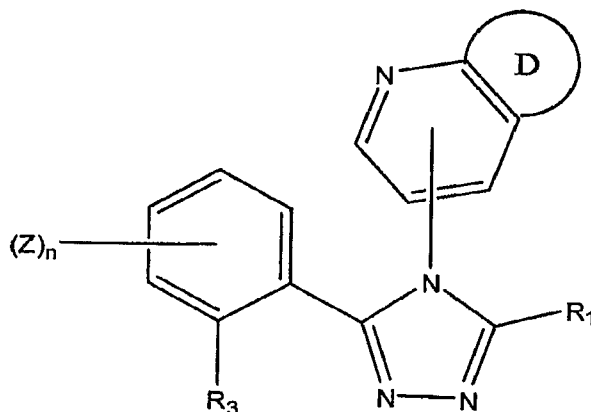
5

p, for each occurrence, is independently, 1 or 2;

m, for each occurrence, is independently, 1, 2, 3 or 4;

n is 0, 1, 2, or 3.

Structural formula (XXXI):



10

(XXXI)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof. In formula (XXXI);

ring D is an optionally substituted aryl or an optionally substituted heteroaryl;

- R_1 and R_3 are, independently, -OH, -SH, -NHR₇, -OR₂₆, -SR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

25

R_7 and R_8 , for each occurrence, is independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted

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cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

- 5 R_{10} and R_{11} , for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{10} and R_{11} , taken together with the nitrogen to which they are attached, form an optionally substituted
- 10 heterocyclyl or an optionally substituted heteroaryl;

R_{26} is a lower alkyl;

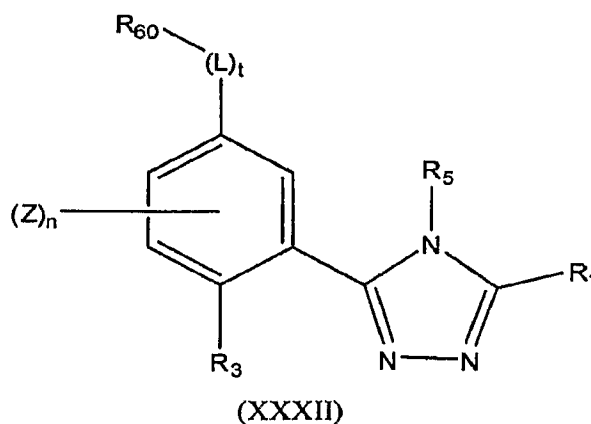
Z is a substituent;

p, for each occurrence, is independently, 1 or 2;

m, for each occurrence, is independently, 1, 2, 3 or 4; and

- 15 n is 0, 1, 2, or 3.

Structural formula (XXXII):



- or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof. In
- 20 formula (XXXII):

- R_1 and R_3 are, independently, -OH, -SH, -NHR₇, -OR₂₆, -SR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁,
- 25

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- OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇,
 -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁,
 -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇,
 -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁,
 5 -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

R₅ and R₆₀ are each, independently, an optionally substituted heteroaryl or an optionally substituted aryl;

- R₇ and R₈, for each occurrence, is independently, -H, an optionally substituted alkyl,
 an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted
 10 cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an
 optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted
 aralkyl, or an optionally substituted heteraralkyl;

- R₁₀ and R₁₁, for each occurrence, is independently -H, an optionally substituted
 alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally
 15 substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted
 heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an
 optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R₁₀ and R₁₁, taken
 together with the nitrogen to which they are attached, form an optionally substituted
 heterocyclyl or an optionally substituted heteroaryl;

- 20 R₂₆ is a lower alkyl;

L is an optionally substituted 1 to 6 atom linker, wherein each linker atom is
 independently selected from the group consisting of C, O, S or N;

Z is a substituent;

p, for each occurrence, is independently, 1 or 2;

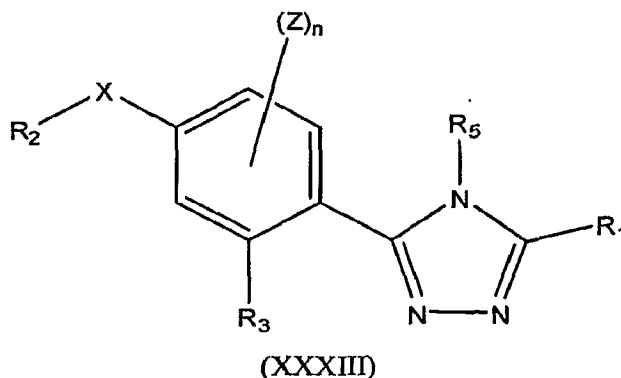
- 25 m, for each occurrence, is independently, 1, 2, 3 or 4;

n is 0, 1, 2, or 3; and

t is 0 or 1.

Structural formula (XXXIII):

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or a tautomer, pharmaceutically acceptable salt, solvate, clathrate or a prodrug thereof. In formula (XXXIII):

- 5 R_1 and R_3 are, independently, -OH, -SH, -NHR₇, -OR₂₆, -SR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

R_2 is -OH, -SH, -NHR₇;

R_5 is an optionally substituted heteroaryl or an optionally substituted aryl;

- 20 R_7 and R_8 , for each occurrence, is independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

- 25 R_{10} and R_{11} , for each occurrence, is independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{10} and R_{11} , taken

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together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R_{26} is a lower alkyl;

5 X is an optionally substituted 1 to 6 atom linker, wherein each linker atom is independently selected from the group consisting of C, O, P, N, or S;

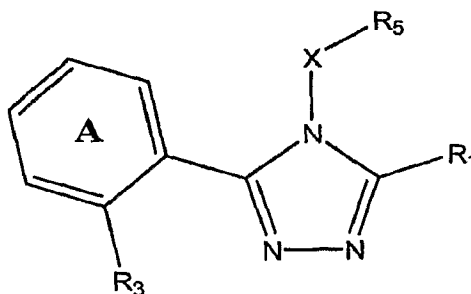
Z is a substituent;

p, for each occurrence, is independently, 1 or 2;

m, for each occurrence, is independently, 1, 2, 3 or 4;

n is 0, 1, or 2.

10 Structural formula (XXXIV):



(XXXIV)

or a tautomer, pharmaceutically acceptable salt, solvate, clathrate, or a prodrug thereof. In formula (XXXIV):

15 ring A is optionally further substituted with one to four independently selected substituents in addition to R_3 ;

X is a C1-C4 alkyl, NR_7 , C(O), C(S), C(NR_8), or S(O)_p;

20 R_1 is -OH, -SH, - NR_7H , - OR_{26} , - $O(CH_2)_mOH$, - $O(CH_2)_mSH$, - $O(CH_2)_mNR_7H$, - $S(CH_2)_mOH$, - $S(CH_2)_mSH$, - $S(CH_2)_mNR_7H$, - $OC(O)NR_{10}R_{11}$, - $SC(O)NR_{10}R_{11}$, - $NR_7C(O)NR_{10}R_{11}$, - $OC(O)R_7$, - $SC(O)R_7$, - $NR_7C(O)R_7$, - $OC(O)OR_7$, - $SC(O)OR_7$, - $NR_7C(O)OR_7$, - $OCH_2C(O)R_7$, - $NR_7CH_2C(O)R_7$, - $OCH_2C(O)OR_7$, - $NR_7CH_2C(O)OR_7$, - $OCH_2C(O)NR_{10}R_{11}$, - $NR_7CH_2C(O)NR_{10}R_{11}$, - $OS(O)_pR_7$, - $SS(O)_pR_7$, - $S(O)_pOR_7$, - $NR_7S(O)_pR_7$, - $OS(O)_pNR_{10}R_{11}$, - $SS(O)_pNR_{10}R_{11}$, - $NR_7S(O)_pNR_{10}R_{11}$, - $OS(O)_pOR_7$, - $SS(O)_pOR_7$, - $NR_7S(O)_pOR_7$, - $OC(S)R_7$, - $SC(S)R_7$, - $NR_7C(S)R_7$, - $OC(S)OR_7$, - $SC(S)OR_7$, - $NR_7C(S)OR_7$, - $OC(S)NR_{10}R_{11}$, - $SC(S)NR_{10}R_{11}$, - $NR_7C(S)NR_{10}R_{11}$, - $OC(NR_8)R_7$, - $SC(NR_8)R_7$, - $NR_7C(NR_8)R_7$, - $OC(NR_8)OR_7$, - $SC(NR_8)OR_7$, - $NR_7C(NR_8)OR_7$, - $OC(NR_8)NR_{10}R_{11}$, - $SC(NR_8)NR_{10}R_{11}$, - $NR_7C(NR_8)NR_{10}R_{11}$, - $OP(O)(OR_7)_2$, or - $SP(O)(OR_7)_2$;

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- R_3 is -OH, -SH, -NR₇H, -OR₂₆, -SR₂₆, -NHR₂₆, -O(CH₂)_mOH, -O(CH₂)_mSH, -O(CH₂)_mNR₇H, -S(CH₂)_mOH, -S(CH₂)_mSH, -S(CH₂)_mNR₇H, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -S(O)_pOR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

R_5 is an optionally substituted aryl or an optionally substituted heteroaryl;

- R_7 and R_8 , for each occurrence, are, independently, -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

- R_{10} and R_{11} , for each occurrence, are independently -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl; or R_{10} and R_{11} , taken together with the nitrogen to which they are attached, form an optionally substituted heterocyclyl or an optionally substituted heteroaryl;

R_{26} , for each occurrence is, independently, a C1-C6 alkyl;

p , for each occurrence, is, independently, 1 or 2; and

m , for each occurrence, is independently, 1, 2, 3, or 4.

- The compounds of formulas (I) through (XXXIX) are disclosed in the following publication, the entire teachings of which are incorporated herein by reference: US2006/0167070; WO2007/021966; US2007/0287998; co-pending U.S. Patent Application No. 11/506,185; co-pending U.S. Patent Application filed on even date herewith under the attorney's docket 3211.1045-005, claiming the benefit of the filing date of the U.S. provisional applications 60/808,253, 60/808,284, 60/808,255, and 60/808,339; co-pending U.S. Patent Application filed on even date herewith under the attorney's docket 3211.1057-

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003, claiming the benefit of the filing date of the U.S. provisional applications 60/808,425, 60/808,248, and 60/808,256; and co-pending U.S. Patent Application filed on even date herewith under the attorney's docket 3211.1059-001, claiming the benefit of the filing date of the U.S. provisional application 60/808,251. Any compound disclosed in the U.S.

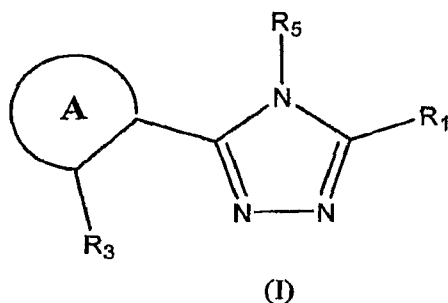
5 publications, PCT publications and the co-pending U.S. and International applications recited above and incorporated herein by reference are not the compounds of the present invention.

In another embodiment, the present invention is a composition of matter comprising an inhibitor and Hsp90, wherein, when the inhibitor is bound to Hsp90, the composition has
10 a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 3.

Examples of the inhibitors of the present invention are provided by the structural formulas below.

Compounds of formula (I) as set forth below:

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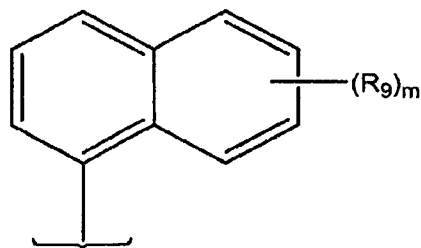
and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof, wherein ring A, R₁, R₃ and R₅ are defined as above.

20 Compounds of formula (I) inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of formula (I) are particularly useful in treating cancer when given in combination with other anti-cancer agent.

In one embodiment, in the compounds of formula (I), R₅ is an optionally substituted
25 naphthyl.

In another embodiment, in the compounds of formula (I), R₅ is represented by the following formula:

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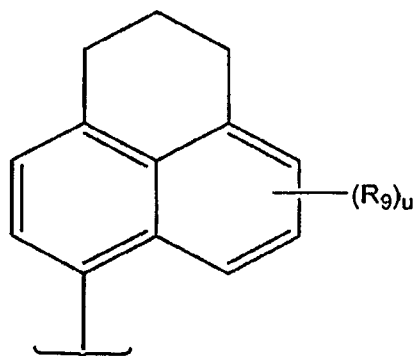
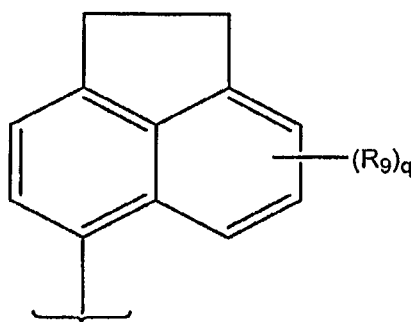
wherein:

- R_9 , for each occurrence, is independently a substituent selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, hydroxyalkyl, alkoxyalkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, or $-S(O)_pNR_{10}R_{11}$, $-S(O)_pOR_7$, $-OP(O)(OR_7)_2$, or $-SP(O)(OR_7)_2$;

or two R_9 groups taken together with the carbon atoms to which they are attached form a fused ring; and

- m is zero or an integer from 1 to 7, wherein R_7 , R_8 , R_{10} , R_{11} , and p are defined as above.

Compounds represented by formula (I), wherein R_5 is represented by one of the following formulas:

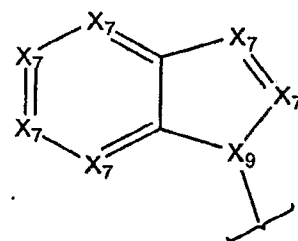
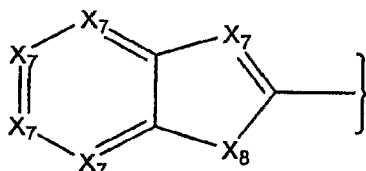
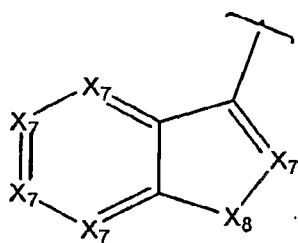
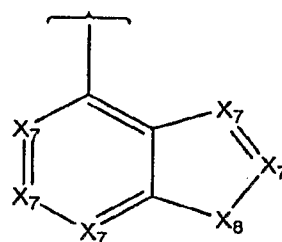
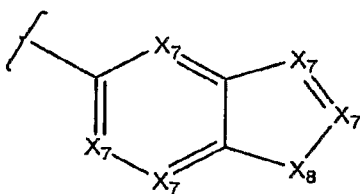
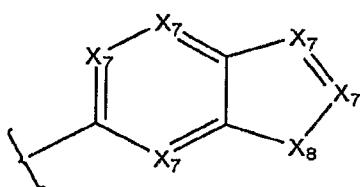
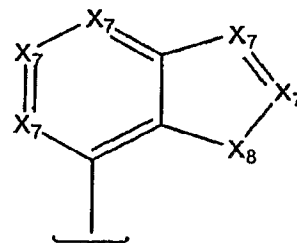
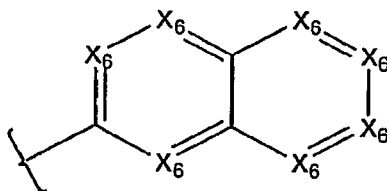
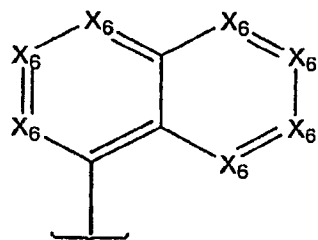


wherein R_9 is defined as above;

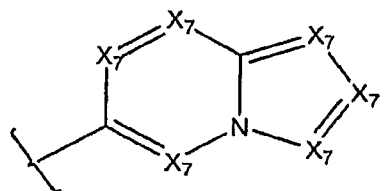
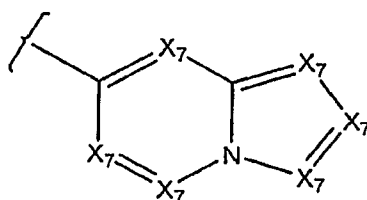
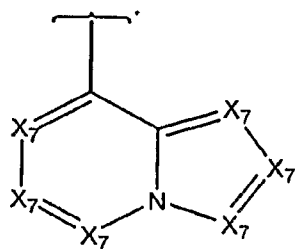
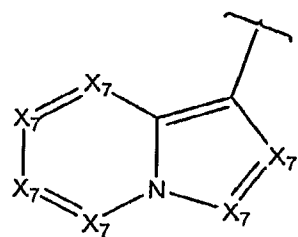
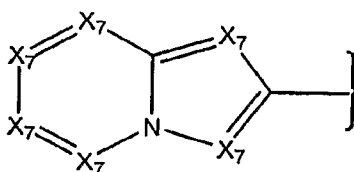
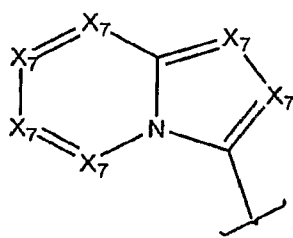
- q is zero or an integer from 1 to 7; and
 u is zero or an integer from 1 to 8.

Compounds represented by formula (I), wherein R_5 is selected from the group consisting of:

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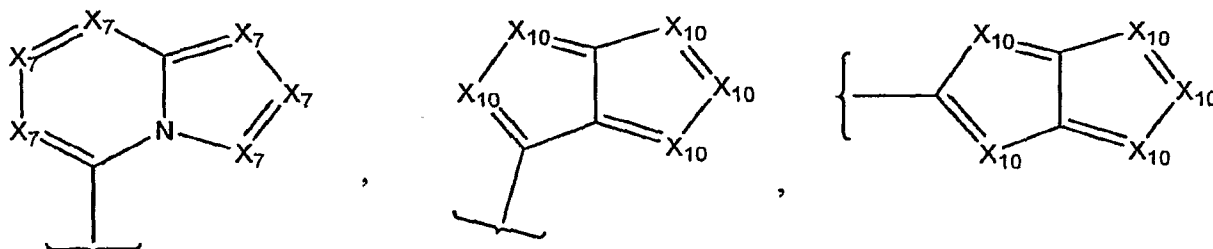


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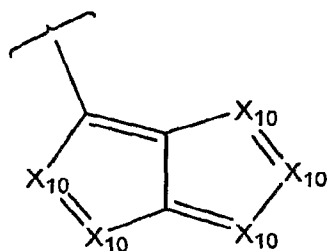


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and



wherein:

- 5 X_6 , for each occurrence, is independently CH, CR₉, N, N(O), N⁺(R₁₇);
 X_7 , for each occurrence, is independently CH, CR₉, N, N(O), N⁺(R₁₇);
 X_8 , for each occurrence, is independently CH₂, CHR₉, CR₉R₉, O, S, S(O)_p, NR₇, or NR₁₇;
 X_9 , for each occurrence, is independently N or CH;
10 X_{10} , for each occurrence, is independently CH, CR₉, N, N(O), N⁺(R₁₇);
R₁₇, for each occurrence, is independently -H, an alkyl, an aralkyl, -C(O)R₇, -C(O)OR₇, or -C(O)NR₁₀R₁₁; wherein R₇, R₉, R₁₀, R₁₁ and p are defined as above.

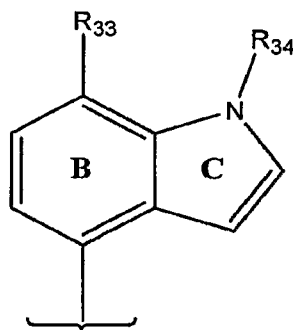
Compounds represented by formula (I), wherein R₅ is an optionally substituted indolyl, an optionally substituted benzoimidazolyl, an optionally substituted indazolyl, an optionally substituted 3*H*-indazolyl, an optionally substituted indoliziny, an optionally substituted quinoliny, an optionally substituted isoquinoliny, an optionally substituted benzoxazolyl, an optionally substituted benzo[1,3]dioxolyl, an optionally substituted benzofuryl, an optionally substituted benzothiazolyl, an optionally substituted benzo[d]isoxazolyl, an optionally substituted benzo[d]isothiazolyl, an optionally substituted thiazolo[4,5-*c*]pyridiny, an optionally substituted thiazolo[5,4-*c*]pyridiny, an optionally substituted thiazolo[4,5-*b*]pyridiny, an optionally substituted thiazolo[5,4-*b*]pyridiny, an optionally substituted oxazolo[4,5-*c*]pyridiny, an optionally substituted oxazolo[5,4-*c*]pyridiny, an optionally substituted oxazolo[4,5-*b*]pyridiny, an optionally substituted oxazolo[5,4-*b*]pyridiny, an optionally substituted imidazopyridiny, an optionally substituted benzothiadiazolyl, benzoxadiazolyl, an optionally substituted benzotriazolyl, an

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optionally substituted tetrahydroindolyl, an optionally substituted azaindolyl, an optionally substituted quinazoliny, an optionally substituted puriny, an optionally substituted imidazo[4,5-a]pyridiny, an optionally substituted imidazo[1,2-a]pyridiny, an optionally substituted 3*H*-imidazo[4,5-b]pyridiny, an optionally substituted 1*H*-imidazo[4,5-b]pyridiny, an optionally substituted 1*H*-imidazo[4,5-c]pyridiny, an optionally substituted 3*H*-imidazo[4,5-c]pyridiny, an optionally substituted pyridopyrdaziny, and optionally substituted pyridopyrimidiny, an optionally substituted pyrrolo[2,3]pyrimidyl, an optionally substituted pyrazolo[3,4]pyrimidyl an optionally substituted cyclopentaimidazolyl, an optionally substituted cyclopentatriazolyl, an optionally substituted pyrrolopyrazolyl, an optionally substituted pyrroloimidazolyl, an optionally substituted pyrrolotriazolyl, an optionally substituted benzo(b)thienyl, or an optionally substituted heteroaralkyl or aralkyl derivatives thereof.

Compounds represented by formula (I), wherein R_5 is an optionally substituted indolyl. Preferably, R_5 is an indolyl represented by the following structural formula:



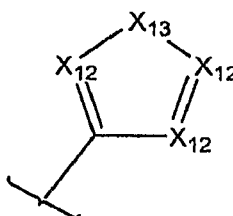
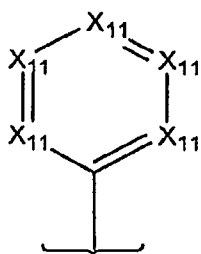
wherein:

R_{33} is a halo, lower alkyl, a lower alkoxy, a lower haloalkyl, a lower haloalkoxy, and lower alkyl sulfanyl;

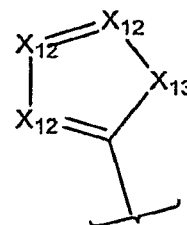
R_{34} is H, a lower alkyl, or a lower alkylcarbonyl; and

Ring B and Ring C are optionally substituted with one or more substituents.

Compounds represented by formula (I), wherein R_5 is selected from the group consisting of:



and



wherein:

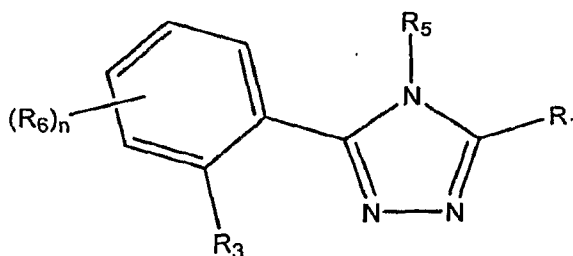
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X_{11} , for each occurrence, is independently CH, CR_9 , N, N(O), or $N^+(R_{17})$;

X_{12} , for each occurrence, is independently CH, CR_9 , N, N(O), $N^+(R_{17})$;

X_{13} , for each occurrence, is independently O, S, S(O)_p, NR_7 , or NR_{17} ; wherein R_7 , R_9 and R_{17} are defined as above.

- 5 Compounds represented by formula (I), or any of the embodiments of formula (I) in which particular groups are disclosed, the compound is represented by the following structural formula:

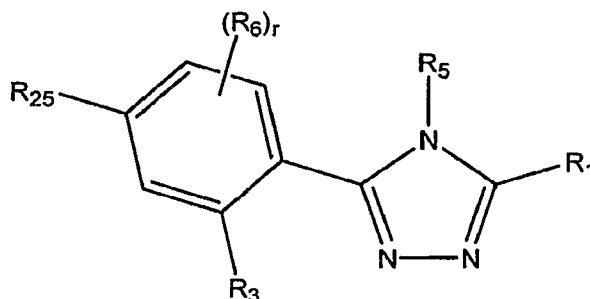


- 10 wherein R_1 , R_3 , and R_5 are defined as above; and

- R_6 , for each occurrence, is independently an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted
- 15 aralkyl, an optionally substituted heteroaralkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, alkoxy, haloalkoxy, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-C(S)R_7$, $-C(O)SR_7$, $-C(S)SR_7$, $-C(S)OR_7$, $-C(S)NR_{10}R_{11}$, $-C(NR_8)OR_7$, $-C(NR_8)R_7$, $-C(NR_8)NR_{10}R_{11}$, $-C(NR_8)SR_7$, $-OC(O)R_7$, $-OC(O)OR_7$, $-OC(S)OR_7$, $-OC(NR_8)OR_7$, $-SC(O)R_7$, $-SC(O)OR_7$, $-SC(NR_8)OR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-SC(S)OR_7$, $-OC(O)NR_{10}R_{11}$, $-OC(S)NR_{10}R_{11}$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-NR_7C(S)R_7$, $-NR_7C(S)OR_7$, $-NR_7C(NR_8)R_7$, $-NR_7C(O)OR_7$, $-NR_7C(NR_8)OR_7$, $-NR_7C(O)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-NR_7C(NR_8)NR_{10}R_{11}$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-OS(O)_pOR_7$, $-OS(O)_pNR_{10}R_{11}$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, $-NR_7S(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pOR_7$, $-S(O)_pNR_{10}R_{11}$, $-SS(O)_pR_7$, $-SS(O)_pOR_7$, $-SS(O)_pNR_{10}R_{11}$, $-OP(O)(OR_7)_2$, or $-SP(O)(OR_7)_2$; and
- 25 n is zero of an integer from 1 to 4, wherein R_7 , R_8 , R_{10} , R_{11} , and p are defined as above.

- 30 Compounds represented by formula (I), or any of the embodiments of formula (I) in which particular groups are disclosed, the compound is represented by the following structural formula:

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wherein R₁, R₃, R₅, and R₆ are defined as above; and

R₂₅ is an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteroaralkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, alkoxy, haloalkoxy, -NR₁₀R₁₁, -OR₇, -C(O)R₇, -C(O)OR₇, -C(S)R₇, -C(OS)R₇, -C(S)SR₇, -C(S)OR₇, -C(S)NR₁₀R₁₁, -C(NR₈)OR₇, -C(NR₈)R₇, -C(NR₈)NR₁₀R₁₁, -C(NR₈)SR₇, -OC(O)R₇, -OC(O)OR₇, -OC(S)OR₇, -OC(NR₈)OR₇, -SC(O)R₇, -SC(O)OR₇, -SC(NR₈)OR₇, -OC(S)R₇, -SC(S)R₇, -SC(S)OR₇, -OC(O)NR₁₀R₁₁, -OC(S)NR₁₀R₁₁, -OC(NR₈)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -C(O)NR₁₀R₁₁, -NR₈C(O)R₇, -NR₇C(S)R₇, -NR₇C(S)OR₇, -NR₇C(NR₈)R₇, -NR₇C(O)OR₇, -NR₇C(NR₈)OR₇, -NR₇C(O)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -SR₇, -S(O)_pR₇, -OS(O)_pR₇, -OS(O)_pOR₇, -OS(O)_pNR₁₀R₁₁, -S(O)_pOR₇, -NR₈S(O)_pR₇, -NR₇S(O)_pNR₁₀R₁₁, -NR₇S(O)_pOR₇, -S(O)_pNR₁₀R₁₁, -SS(O)_pR₇, -SS(O)_pOR₇, -SS(O)_pNR₁₀R₁₁, -OP(O)(OR₇)₂, or -SP(O)(OR₇)₂;

k is 1, 2, 3, or 4; and

r is zero or an integer from 1 to 3, wherein R₇, R₈, R₁₀, R₁₁, and p are defined as above.

Compound represented by the above formula, wherein R₁, R₃ and R₂₅ are each independently -OH, -SH, -NHR₇, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -OS(O)_pR₇, -S(O)_pOR₇, -SS(O)_pR₇, -OS(O)_pOR₇, -SS(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -OP(O)(OR₇)₂ or -SP(O)(OR₇)₂.

Compound represented by the above formula, wherein R₁ and R₃ are each, independently, -OH, -SH, or -NHR₇. In this case, R₆ can be an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, cyano, halo, nitro,

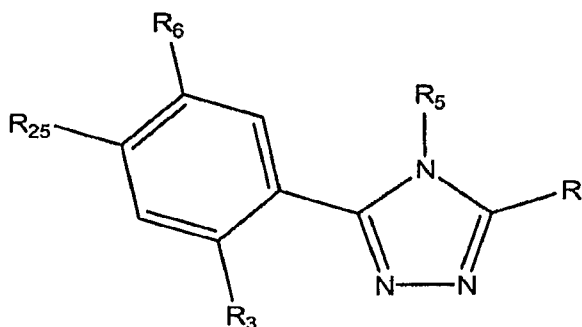
-79-

- an optionally substituted cycloalkyl, haloalkyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteroaralkyl, -OR₇, -SR₇, -NR₁₀R₁₁, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇,
 5 -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇,
 10 -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)R₇, -C(O)OR₇, -C(O)NR₁₀R₁₁, -C(O)SR₇, -C(S)R₇, -C(S)OR₇, -C(S)NR₁₀R₁₁, -C(S)SR₇, -C(NR₈)OR₇, -C(NR₈)R₇, -C(NR₈)NR₁₀R₁₁, -C(NR₈)SR₇, -S(O)_pOR₇, -S(O)_pNR₁₀R₁₁, or -S(O)_pR₇.

- 15 The above compound, wherein R₁ is -SH or -OH; R₃ and R₂₅ are -OH; R₆ is a lower alkyl, C3-C6 cycloalkyl, lower alkoxy, a lower alkyl sulfanyl, or -NR₁₀R₁₁; and R₉, for each occurrence, is independently selected from the group consisting of -OH, -SH, halo, a lower haloalkyl, cyano, a lower alkyl, a lower alkoxy, and a lower alkyl sulfanyl.

- 20 Compounds represented by formula (I), or any of the embodiments of formula (I) in which particular groups are disclosed, R₁ and R₃ are each, independently, -OH, -SH, or -NHR₇.

Compounds represented by formula (I), or any of the embodiments of formula (I) in which particular groups are disclosed, the compound is represented by the following structural formula:



25

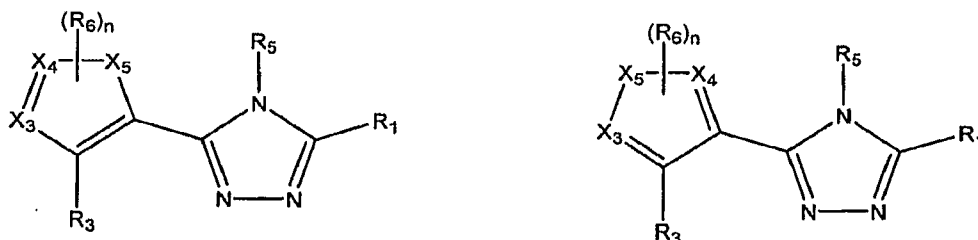
wherein R₁, R₃, R₅, and R₂₅ are defined as above; and

R₆ is an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, cyano, halo, nitro, an optionally substituted cycloalkyl, haloalkyl, an

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- optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteroaralkyl, -OR₇, -SR₇, -NR₁₀R₁₁, -OC(O)NR₁₀R₁₁, -SC(O)NR₁₀R₁₁, -NR₇C(O)NR₁₀R₁₁, -OC(O)R₇, -SC(O)R₇, -NR₇C(O)R₇, -OC(O)OR₇, -SC(O)OR₇, -NR₇C(O)OR₇, -OCH₂C(O)R₇, -SCH₂C(O)R₇, -NR₇CH₂C(O)R₇, -OCH₂C(O)OR₇, -SCH₂C(O)OR₇, -NR₇CH₂C(O)OR₇, -OCH₂C(O)NR₁₀R₁₁, -SCH₂C(O)NR₁₀R₁₁, -NR₇CH₂C(O)NR₁₀R₁₁, -OS(O)_pR₇, -SS(O)_pR₇, -NR₇S(O)_pR₇, -OS(O)_pNR₁₀R₁₁, -SS(O)_pNR₁₀R₁₁, -NR₇S(O)_pNR₁₀R₁₁, -OS(O)_pOR₇, -SS(O)_pOR₇, -NR₇S(O)_pOR₇, -OC(S)R₇, -SC(S)R₇, -NR₇C(S)R₇, -OC(S)OR₇, -SC(S)OR₇, -NR₇C(S)OR₇, -OC(S)NR₁₀R₁₁, -SC(S)NR₁₀R₁₁, -NR₇C(S)NR₁₀R₁₁, -OC(NR₈)R₇, -SC(NR₈)R₇, -NR₇C(NR₈)R₇, -OC(NR₈)OR₇, -SC(NR₈)OR₇, -NR₇C(NR₈)OR₇, -OC(NR₈)NR₁₀R₁₁, -SC(NR₈)NR₁₀R₁₁, -NR₇C(NR₈)NR₁₀R₁₁, -C(O)R₇, -C(O)OR₇, -C(O)NR₁₀R₁₁, -C(O)SR₇, -C(S)R₇, -C(S)OR₇, -C(S)NR₁₀R₁₁, -C(S)SR₇, -C(NR₈)OR₇, -C(NR₈)R₇, -C(NR₈)NR₁₀R₁₁, -C(NR₈)SR₇, -S(O)_pOR₇, -S(O)_pNR₁₀R₁₁, or -S(O)_pR₇, wherein R₇, R₈, R₁₀, R₁₁, and p are defined as above. In a preferred embodiment, R₁ is -SH or -OH; R₃ and R₂₅ are -OH; R₁₂ is a lower alkyl, lower alkoxy, a lower alkyl sulfanyl, or -NR₁₀R₁₁; and R₉, for each occurrence, is independently selected from the group consisting of -OH, -SH, halo, a lower haloalkyl, cyano, a lower alkyl, a lower alkoxy, and a lower alkyl sulfanyl.

- Compounds represented by formula (I), or any of the embodiments of formula (I) in which particular groups are disclosed, the compound is represented by one of the following structural formulas:



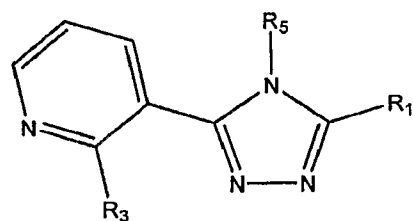
wherein R₁, R₃, R₅, R₆ and n are as defined above; and

X₃ and X₄ are each, independently, N, N(O), N⁺(R₁₇), CH or CR₆; and

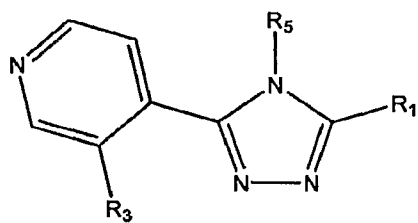
- X₅ is O, S, NR₁₇, CH=CH, CH=CR₆, CR₆=CH, CR₆=CR₆, CH=N, CR₆=N, CH=N(O), CR₆=N(O), N=CH, N=CR₆, N(O)=CH, N(O)=CR₆, N⁺(R₁₇)=CH, N⁺(R₁₇)=CR₆, CH=N⁺(R₁₇), CR₆=N⁺(R₁₇), or N=N; wherein R₁₇ is defined as above.

- Compounds represented by formula (I), or any of the embodiments of formula (I) in which particular groups are disclosed, the compound is selected from the group consisting of:

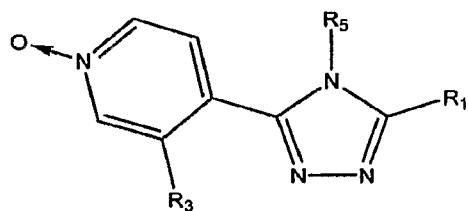
-81-



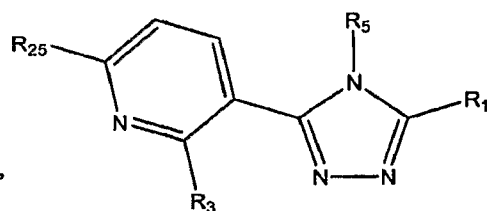
,



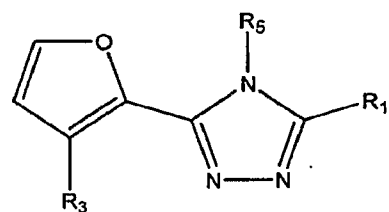
;



,

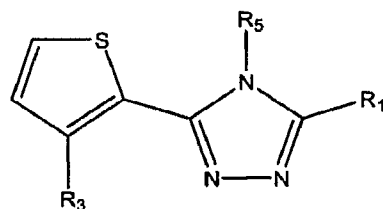


;

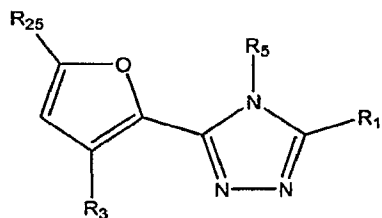


5

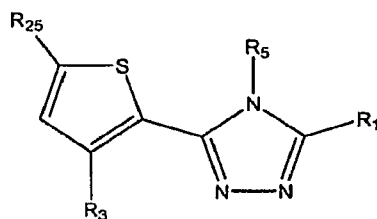
,



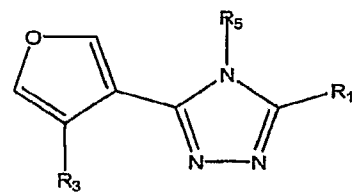
;



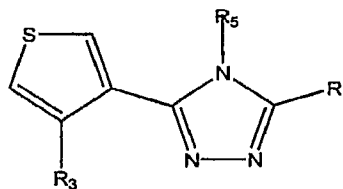
,



;



and



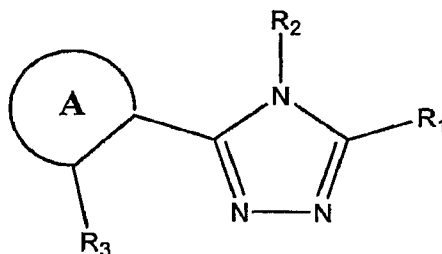
;

10

wherein R_1 , R_3 , R_5 , and R_{25} are defined as above.

Compounds of formula (II) as set forth below:

-82-



(II)

and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof, wherein ring A, R₁ and R₃ are defined as above; and

5 R₂ is a substituted phenyl, wherein the phenyl group is substituted with:

- i) one substituent selected from nitro, cyano, a haloalkoxy, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, hydroxylalkyl, alkoxyalkyl, guanadino, -NR₁₀R₁₁, -O-R₂₀, -C(O)R₇, -C(O)OR₂₀, -OC(O)R₇, -C(O)NR₁₀R₁₁, -NR₈C(O)R₇, -SR₇, -S(O)_pR₇, -OS(O)_pR₇, -S(O)_pOR₇, -NR₈S(O)_pR₇, or -S(O)_pNR₁₀R₁₁,
10 or
- ii) two to five substituents selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, hydroxyalkyl, alkoxyalkyl, -F, -Br, -I, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, -NR₁₀R₁₁, -OR₇, -C(O)R₇, -C(O)OR₇, -OC(O)R₇, -C(O)NR₁₀R₁₁, -NR₈C(O)R₇, -SR₇, -S(O)_pR₇, -OS(O)_pR₇, -S(O)_pOR₇, -NR₈S(O)_pR₇, or -S(O)_pNR₁₀R₁₁;
15 20

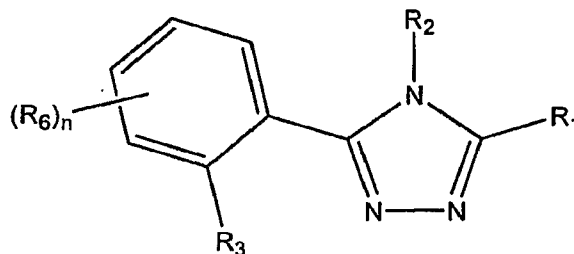
25 R₂₀, for each occurrence, is independently an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

30 p, for each occurrence, is, independently, 1 or 2.

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Compounds of formula (II) inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of formula (II) are particularly useful in treating cancer when given in combination with other anti-cancer agent.

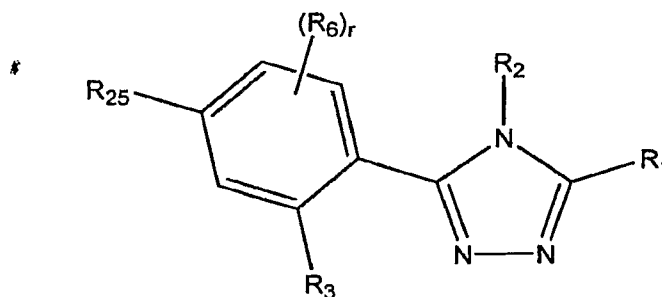
- 5 Compounds represented by formula (II), or any of the embodiments of formula (II) in which particular groups are disclosed, the compound is represented by the following structural formula:



10

wherein R_1 , R_2 , R_3 , R_6 , and n are defined as above.

Compound is represented by the following structural formula:

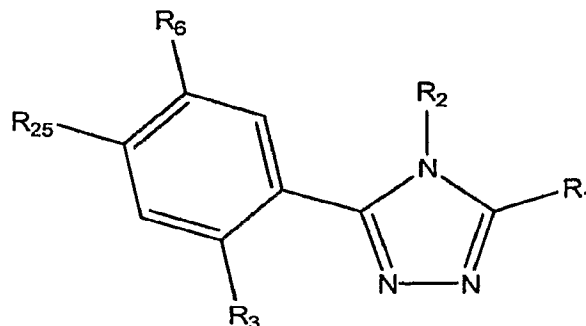


wherein R_1 , R_2 , R_3 , R_6 , R_{25} and r are defined as above.

- 15 Compounds represented by formula (II), or any of the embodiments of formula (II) in which particular groups are disclosed, R_1 and R_3 are each, independently, -OH, -SH, or -NHR₇.

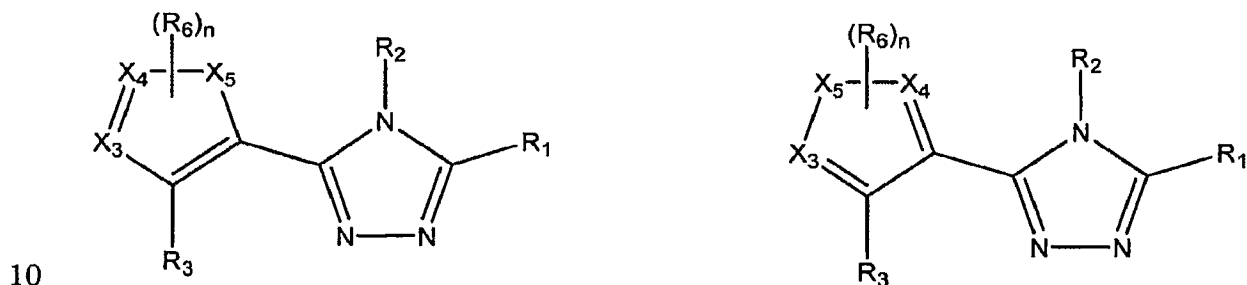
- 20 Compounds represented by formula (II), or any of the embodiments of formula (II) in which particular groups are disclosed, the compound is represented by the following structural formula:

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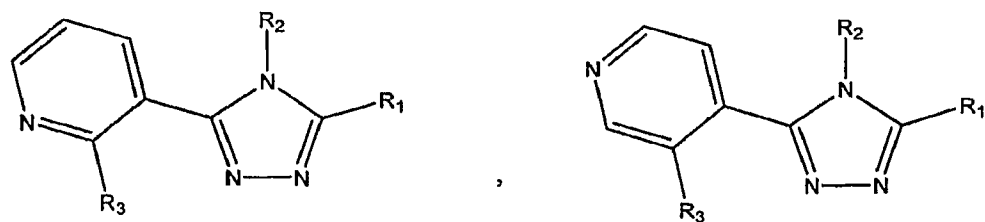
wherein R_1 , R_2 , R_3 , R_6 and R_{25} are defined as above. In a preferred embodiment, R_1 is -SH or -OH; R_3 and R_{25} are -OH; R_{12} is a lower alkyl, lower alkoxy, a lower alkyl sulfanyl, or -NR₁₀R₁₁; and R_9 , for each occurrence, is independently selected from the group consisting of -OH, -SH, halo, a lower haloalkyl, cyano, a lower alkyl, a lower alkoxy, and a lower alkyl sulfanyl.

Compounds represented by formula (II), or any of the embodiments of formula (II) in which particular groups are disclosed, the compound is represented by one of the following structural formulas:

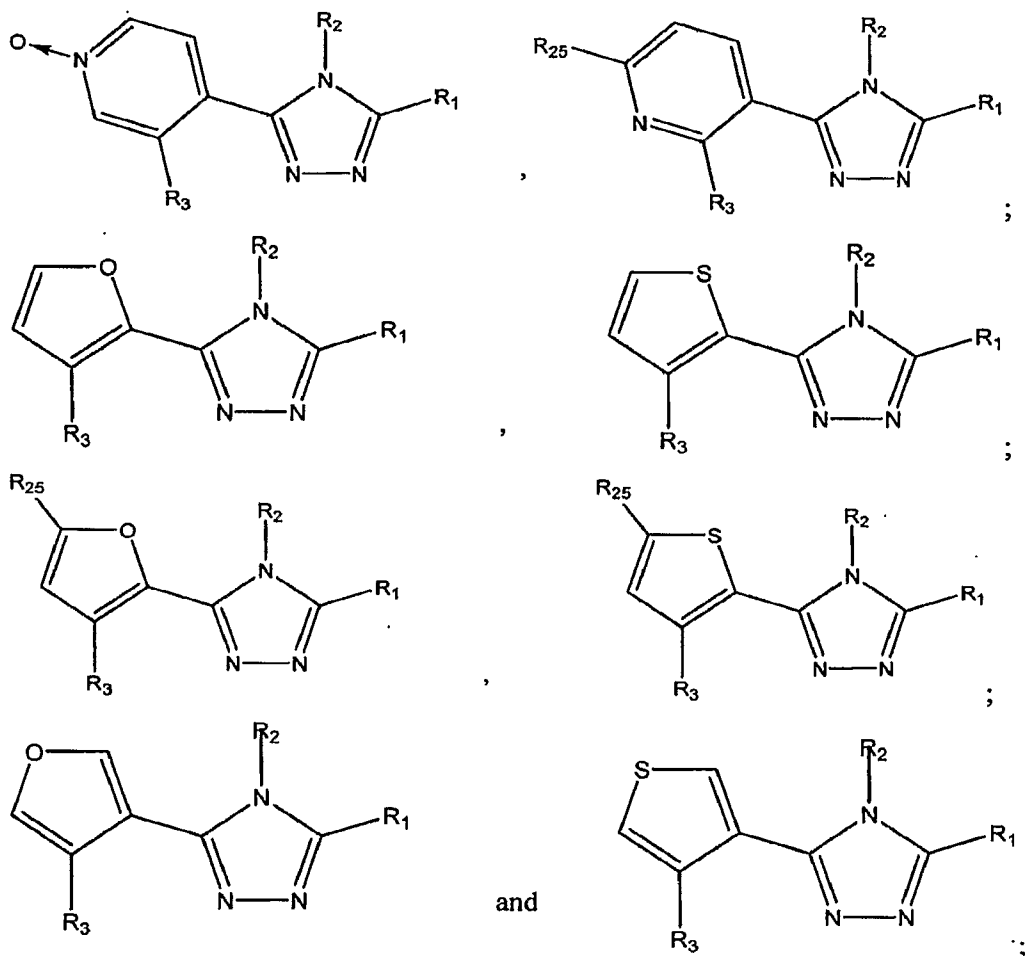


wherein R_1 , R_2 , R_3 , R_6 , X_3 , X_4 , X_5 and n are defined as above.

Compounds represented by formula (II), or any of the embodiments of formula (II) in which particular groups are disclosed, the compound being selected from the group consisting of:

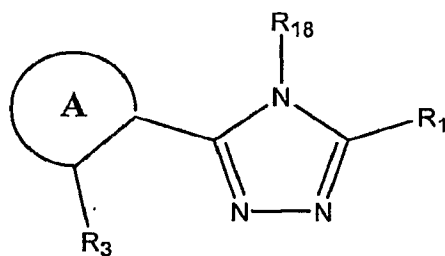


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5 wherein R_1 , R_2 , R_3 , and R_{25} are defined as above.

Compounds of formula (III) as set forth below:



(III)

10 and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs. In formula (III), ring **A**, R_1 , and R_3 are defined as above; and

R_{18} is an optionally substituted cycloalkyl, and optionally substituted cycloalkenyl, or a substituted alkyl, wherein the alkyl group is substituted with one or more substituents independently selected from the group consisting of an optionally substituted alkynyl, an

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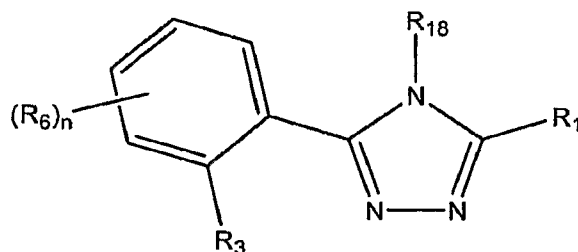
optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, halo, cyano, nitro, guanadino, a haloalkyl, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, or $-S(O)_pNR_{10}R_{11}$, wherein R_7 , R_8 , R_{10} , R_{11} , and p are defined as above.

Compounds of formula (III) inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of formula (III) are particularly useful in treating cancer when given in combination with other anti-cancer agent.

In another embodiment, in formula (III) R_{18} is an optionally substituted cycloalkyl or an optionally substituted cycloalkenyl.

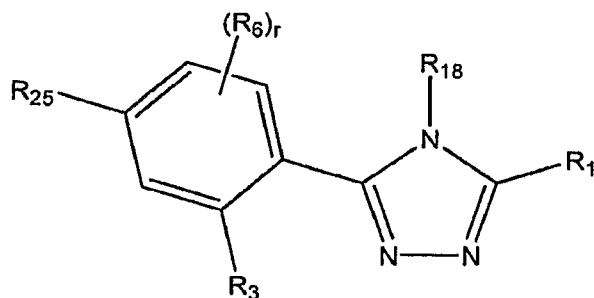
In another embodiment, in formula (III) R_{18} is a substituted alkyl.

Compounds represented by formula (III), or any of the embodiments of formula (III) in which particular groups are disclosed, the compound being represented by the following structural formula:



wherein R_1 , R_3 , R_6 , R_{18} , and n are defined as above.

Compounds represented by formula (III), or any of the embodiments of formula (III) in which particular groups are disclosed, the compound being represented by the following structural formula:

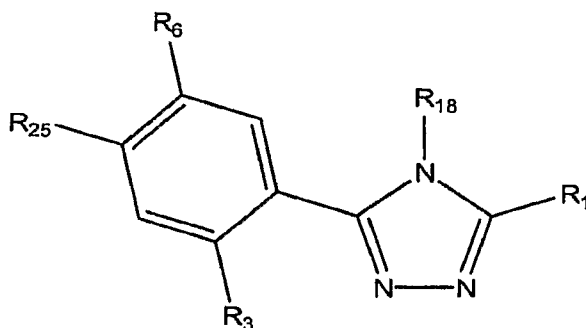


wherein R_1 , R_3 , R_6 , R_{18} , R_{25} and r are defined as above.

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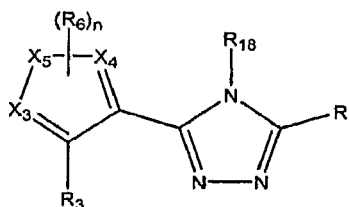
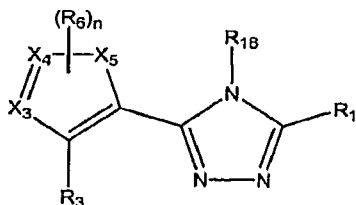
Compounds represented by formula (III), or any of the embodiments of formula (III) in which particular groups are disclosed, R_1 and R_3 are each, independently, -OH, -SH, or -NHR₇.

Compounds represented by formula (III), or any of the embodiments of formula (III) in which particular groups are disclosed, the compound is represented by the following structural formula:



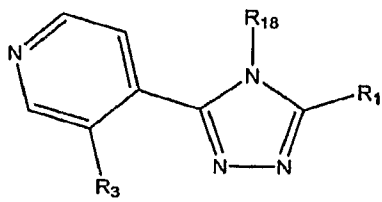
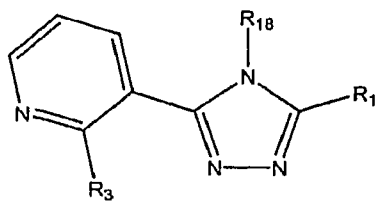
wherein R_1 , R_3 , R_6 , R_{18} , and R_{25} are defined as above. In a preferred embodiment, R_1 is -SH or -OH; R_3 and R_{25} are -OH; and R_{12} is a lower alkyl, lower alkoxy, a lower alkyl sulfanyl, or -NR₁₀R₁₁.

Compounds represented by formula (III), or any of the embodiments of formula (III) in which particular groups are disclosed, the compound being represented by one of the following structural formulas:



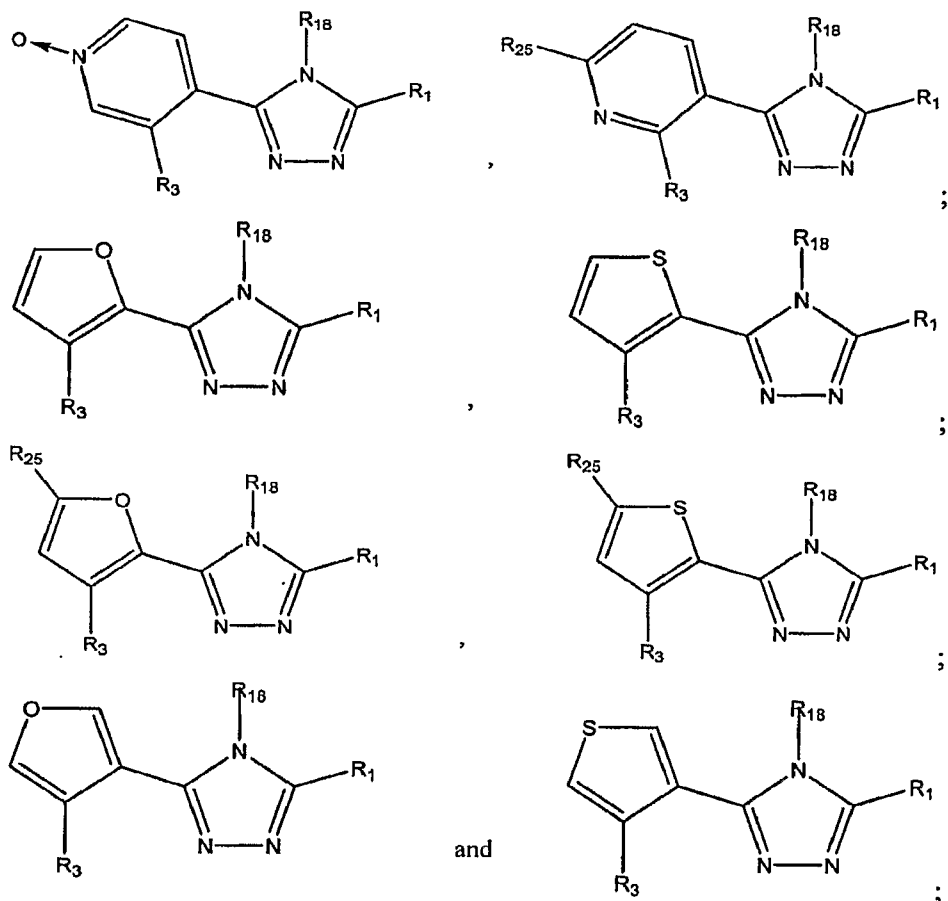
wherein R_1 , R_3 , R_6 , R_{18} , X_3 , X_4 , X_5 , and n are defined as above.

Compounds represented by formula (III), or any of the embodiments of formula (III) in which particular groups are disclosed, the compound being selected from the group consisting of:



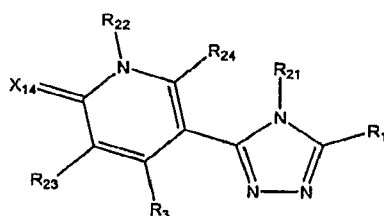
;

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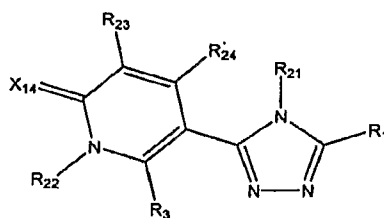


5 wherein R_1 , R_3 , R_{18} , and R_{25} are defined as above.

Compounds of formula (IV) or (V) as set forth below:



(IV)



(V)

and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof.

10 In formulas (IV) and (V), R_1 and R_3 are as defined above; and

X_{14} is O, S, or NR_7 ;

R_{21} is an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an

15 optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl;

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R_{22} , for each occurrence, is independently an -H or is selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, a haloalkyl, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-S(O)_pR_7$, $-S(O)_pOR_7$, or $-S(O)_pNR_{10}R_{11}$; and

R_{23} and R_{24} , for each occurrence, are independently -H or are selected from the group consisting of an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, or an optionally substituted heteraralkyl, halo, cyano, nitro, guanidino, a haloalkyl, a heteroalkyl, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, or $-S(O)_pNR_{10}R_{11}$;

wherein R_7 , R_8 , R_{10} , R_{11} and p are defined as above.

In one embodiment, in formulas (IV) and (V), R_{21} is an optionally substituted alkyl, an optionally substituted cycloalkyl, an optionally substituted aryl or an optionally substituted heteroaryl.

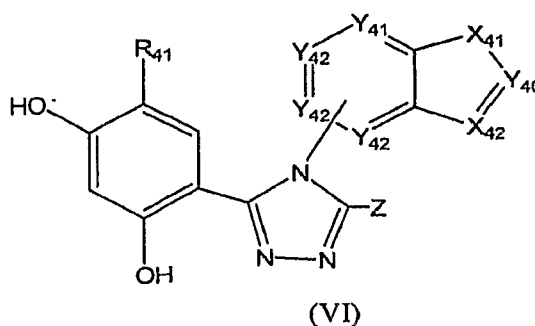
In another embodiment, in the formulas (IV) and (V), R_1 is -OH, -SH, or -NHR₇.

In another embodiment, in the formulas (IV) and (V), R_{22} is -H, an alkyl, an aralkyl, $-C(O)R_7$, $-C(O)OR_7$, or $-C(O)NR_{10}R_{11}$.

In another embodiment, in the formulas (IV) and (V), X_{14} is O.

Compounds of formula (IV) or (V) inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of formula (IV) or (V) are particularly useful in treating cancer when given in combination with other anti-cancer agent.

Compounds represented by formula (VI):



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and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof, wherein:

X_{41} is O, S, or NR_{42} ;

X_{42} is CR_{44} or N;

5 Y_{40} is N or CR_{43} ;

Y_{41} is N or CR_{45} ;

Y_{42} , for each occurrence, is independently N, C or CR_{46} ;

Z is OH, SH, or NHR_7 ;

10 R_{41} is -H, -OH, -SH, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, halo, cyano, nitro, guanidino, a haloalkyl, a heteroalkyl, an alkoxy or cycloalkoxy, a haloalkoxy, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-C(S)R_7$, $-C(O)SR_7$,
 15 $-C(S)SR_7$, $-C(S)OR_7$, $-C(S)NR_{10}R_{11}$, $-C(NR_8)OR_7$, $-C(NR_8)R_7$, $-C(NR_8)NR_{10}R_{11}$, $-C(NR_8)SR_7$, $-OC(O)R_7$, $-OC(O)OR_7$, $-OC(S)OR_7$, $-OC(NR_8)OR_7$, $-SC(O)R_7$, $-SC(O)OR_7$, $-SC(NR_8)OR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-SC(S)OR_7$, $-OC(O)NR_{10}R_{11}$, $-OC(S)NR_{10}R_{11}$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-NR_7C(S)R_7$, $-NR_7C(S)OR_7$, $-NR_7C(NR_8)R_7$,
 20 $-NR_7C(O)OR_7$, $-NR_7C(NR_8)OR_7$, $-NR_7C(O)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-NR_7C(NR_8)NR_{10}R_{11}$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-OS(O)_pOR_7$, $-OS(O)_pNR_{10}R_{11}$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, $-NR_7S(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pOR_7$, $-S(O)_pNR_{10}R_{11}$, $-SS(O)_pR_7$, $-SS(O)_pOR_7$, $-SS(O)_pNR_{10}R_{11}$, $-OP(O)(OR_7)_2$, or $-SP(O)(OR_7)_2$;

25 R_{42} is -H, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, hydroxyalkyl, alkoxyalkyl, a haloalkyl, a heteroalkyl, $-C(O)R_7$, $-(CH_2)_mC(O)OR_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-S(O)_pR_7$, $-S(O)_pOR_7$, or
 30 $-S(O)_pNR_{10}R_{11}$;

R_{43} and R_{44} are, independently, -H, -OH, an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, hydroxyalkyl, alkoxyalkyl, halo, cyano, nitro,

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guanadino, a haloalkyl, a heteroalkyl, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, $-S(O)_pNR_{10}R_{11}$, or R_{43} and R_{44} taken together with the carbon atoms to which they are attached form an optionally substituted cycloalkenyl, an optionally substituted aryl, an optionally substituted heterocyclyl, or an optionally substituted heteroaryl;

R_{45} is $-H$, $-OH$, $-SH$, $-NR_7H$, $-OR_{26}$, $-SR_{26}$, $-NHR_{26}$, $-O(CH_2)_mOH$, $-O(CH_2)_mSH$, $-O(CH_2)_mNR_7H$, $-S(CH_2)_mOH$, $-S(CH_2)_mSH$, $-S(CH_2)_mNR_7H$, $-OC(O)NR_{10}R_{11}$, $-SC(O)NR_{10}R_{11}$, $-NR_7C(O)NR_{10}R_{11}$, $-OC(O)R_7$, $-SC(O)R_7$, $-NR_7C(O)R_7$, $-OC(O)OR_7$, $-SC(O)OR_7$, $-NR_7C(O)OR_7$, $-OCH_2C(O)R_7$, $-SCH_2C(O)R_7$, $-NR_7CH_2C(O)R_7$, $-OCH_2C(O)OR_7$, $-SCH_2C(O)OR_7$, $-NR_7CH_2C(O)OR_7$, $-OCH_2C(O)NR_{10}R_{11}$, $-SCH_2C(O)NR_{10}R_{11}$, $-NR_7CH_2C(O)NR_{10}R_{11}$, $-OS(O)_pR_7$, $-SS(O)_pR_7$, $-NR_7S(O)_pR_7$, $-OS(O)_pNR_{10}R_{11}$, $-SS(O)_pNR_{10}R_{11}$, $-NR_7S(O)_pNR_{10}R_{11}$, $-OS(O)_pOR_7$, $-SS(O)_pOR_7$, $-NR_7S(O)_pOR_7$, $-OC(S)R_7$, $-SC(S)R_7$, $-NR_7C(S)R_7$, $-OC(S)OR_7$, $-SC(S)OR_7$, $-NR_7C(S)OR_7$, $-OC(S)NR_{10}R_{11}$, $-SC(S)NR_{10}R_{11}$, $-NR_7C(S)NR_{10}R_{11}$, $-OC(NR_8)R_7$, $-SC(NR_8)R_7$, $-NR_7C(NR_8)R_7$, $-OC(NR_8)OR_7$, $-SC(NR_8)OR_7$, $-NR_7C(NR_8)OR_7$, $-OC(NR_8)NR_{10}R_{11}$, $-SC(NR_8)NR_{10}R_{11}$, or $-NR_7C(NR_8)NR_{10}R_{11}$;

R_{46} , for each occurrence, is independently selected from the group consisting of H , an optionally substituted alkyl, an optionally substituted alkenyl, an optionally substituted alkynyl, an optionally substituted cycloalkyl, an optionally substituted cycloalkenyl, an optionally substituted heterocyclyl, an optionally substituted aryl, an optionally substituted heteroaryl, an optionally substituted aralkyl, an optionally substituted heteraralkyl, halo, cyano, nitro, guanadino, a haloalkyl, a heteroalkyl, $-NR_{10}R_{11}$, $-OR_7$, $-C(O)R_7$, $-C(O)OR_7$, $-OC(O)R_7$, $-C(O)NR_{10}R_{11}$, $-NR_8C(O)R_7$, $-SR_7$, $-S(O)_pR_7$, $-OS(O)_pR_7$, $-S(O)_pOR_7$, $-NR_8S(O)_pR_7$, or $-S(O)_pNR_{10}R_{11}$;

R_7 , R_8 , R_{10} , R_{11} , R_{26} , p , and m are defined as above.

In one embodiment, in formula (VI), X_{41} is NR_{42} and X_{42} is CR_{44} .

In another embodiment, in formula (VI), X_{41} is NR_{42} and X_{42} is N .

In another embodiment, in formula (VI), R_{41} is selected from the group consisting of $-H$, lower alkyl, lower alkoxy, lower cycloalkyl, and lower cycloalkoxy.

In another embodiment, in formula (VI), R_{41} is selected from the group consisting of $-H$, methyl, ethyl, propyl, isopropyl, cyclopropyl, methoxy, ethoxy, propoxy, and cyclopropoxy.

In another embodiment, in formula (VI), X_{41} is NR_{42} , and R_{42} is selected from the group consisting of $-H$, a lower alkyl, a lower cycloalkyl, $-C(O)N(R_{27})_2$, and $-C(O)OH$, wherein R_{27} is $-H$ or a lower alkyl.

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In another embodiment, in formula (VI), X_{41} is NR_{42} , and R_{42} is selected from the group consisting of -H, methyl, ethyl, n-propyl, isopropyl, cyclopropyl, n-butyl, *sec*-butyl, *tert*-butyl, n-pentyl, n-hexyl, -C(O)OH, $-(CH_2)_mC(O)OH$, $-CH_2OCH_3$, $-CH_2CH_2OCH_3$, and $-C(O)N(CH_3)_2$.

5 In one embodiment, Y_{40} is CR_{43} . Preferably, Y_{40} is CR_{43} and R_{43} is H or a lower alkyl.

In another embodiment, in formula (VI), R_{43} and R_{44} are, independently, selected from the group consisting of -H, methyl, ethyl, propyl, isopropyl, cyclopropyl, methoxy, ethoxy, propoxy, and cyclopropoxy.

10 In another embodiment, in formula (VI), X_{42} is CR_{44} ; Y is CR_{43} ; and R_{43} and R_{44} together with the carbon atoms to which they are attached form a cycloalkenyl, an aryl, heterocyclyl, or heteroaryl ring. In one aspect of this embodiment, R_{43} and R_{44} together with the carbon atoms to which they are attached form a C_5 - C_8 cycloalkenyl or a C_5 - C_8 aryl.

15 In another embodiment, in formula (VI), R_{45} is selected from the group consisting of -H, -OH, -SH, $-NH_2$, a lower alkoxy, a lower alkyl amino, and a lower dialkyl amino.

In another embodiment, in formula (VI), R_{45} is selected from the group consisting of -H, -OH, methoxy and ethoxy.

In another embodiment, in formula (VI), X_{41} is O.

20 In another embodiment, the compound is selected from the group consisting of:
3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(2-methyl-7-methoxy-benzofuran-4-yl)-5-mercapto-[1,2,4]triazole,

3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(benzofuran-5-yl)-5-mercapto-[1,2,4]triazole,

3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(2-methyl-1,3-benzoxaz-5-yl)-5-mercapto-[1,2,4]triazole, and

25 tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof.

In another embodiment, in formula (VI), Z is -OH.

30 In another embodiment, the compound is selected from the group consisting of:
3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1,3-dimethyl-indol-5-yl)-5-hydroxy-[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1,3-dimethyl-indol-5-yl)-5-hydroxy-[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-methyl-indol-5-yl)-5-hydroxy-[1,2,4]triazole,

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3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-isopropyl-indol-4-yl)-5-hydroxy-
[1,2,4]triazole, and

tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof.

5 In another embodiment, Z is -SH.

In another embodiment, the compound is selected from the group consisting of:

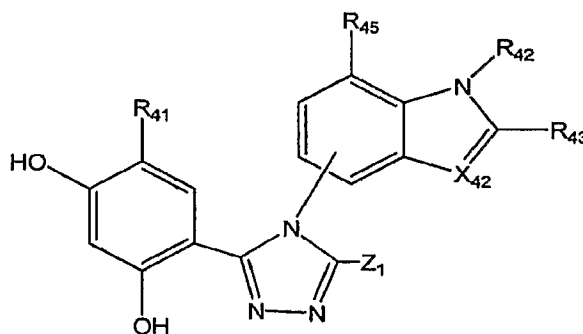
3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-methyl-indazol-5-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-methyl-indazol-6-yl)-5-mercapto-
10 [1,2,4]triazole, and

tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof.

Compounds of formula (VI) inhibit the activity of Hsp90 and are particularly useful
for treating or preventing proliferative disorders, such as cancer. In addition, compounds of
15 formula (VI) are particularly useful in treating cancer when given in combination with other
anti-cancer agent.

Compounds represented by formula (VII):



(VII)

20 and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof, wherein:

Z₁ is -OH or -SH;

X₄₂, R₄₁, R₄₂, R₄₃, and R₄₅ are defined as above.

In one embodiment, in formula (VII), Z₁ is -OH.

25 In another embodiment, in formula (VII), Z₁ is -SH.

In another embodiment, in formula (VII), R₄₁ is selected from the group consisting of -H, lower alkyl, lower alkoxy, lower cycloalkyl, and lower cycloalkoxy.

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In another embodiment, in formula (VII), R_{41} is selected from the group consisting of -H, methyl, ethyl, propyl, isopropyl, cyclopropyl, methoxy, ethoxy, propoxy, and cyclopropoxy.

In another embodiment, in formula (VII), R_{42} is selected from the group consisting of lower alkyl, lower cycloalkyl, $-C(O)N(R_{27})_2$, or $-C(O)OH$, wherein R_{27} is -H or a lower alkyl.

In another embodiment, in formula (VII), R_{42} is selected from the group consisting of -H, methyl, ethyl, n-propyl, isopropyl, cyclopropyl, n-butyl, *sec*-butyl, *tert*-butyl, n-pentyl, n-hexyl, $-C(O)OH$, $-(CH_2)_mC(O)OH$, $-CH_2OCH_3$, $-CH_2CH_2OCH_3$, and $-C(O)N(CH_3)_2$.

In another embodiment, R_{43} is H or a lower alkyl.

In another embodiment, in formula (VII), X_{42} is CR_{44} , and R_{43} and R_{44} are, independently, selected from the group consisting of -H, methyl, ethyl, propyl, isopropyl, cyclopropyl, methoxy, ethoxy, propoxy, and cyclopropoxy.

In another embodiment, in formula (VII), X_{42} is CR_{44} , and R_{43} and R_{44} , taken together with the carbon atoms to which they are attached, form a cycloalkenyl, aryl, heterocyclyl, or heteroaryl ring. Preferably, in this embodiment, R_{43} and R_{44} , taken together with the carbon atoms to which they are attached, form a C_5 - C_8 cycloalkenyl or a C_5 - C_8 aryl.

In another embodiment, in formula (VII), R_{45} is selected from the group consisting of -H, -OH, -SH, -NH₂, a lower alkoxy, a lower alkyl amino, and a lower dialkyl amino.

In another embodiment, in formula (VII), R_{45} is selected from the group consisting of -H, -OH, methoxy, and ethoxy.

In another embodiment, in formula (VII), X_{43} is CR_{44} .

In another embodiment, the compound is selected from the group consisting of:

3-(2,4-dihydroxyphenyl)-4-(1-ethyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,
 3-(2,4-dihydroxyphenyl)-4-(1-isopropyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,
 3-(2,4-dihydroxyphenyl)-4-(indol-4-yl)-5-mercapto-[1,2,4]triazole,
 3-(2,4-dihydroxyphenyl)-4-(1-methoxyethyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,
 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,
 3-(2,4-dihydroxyphenyl)-4-(1-dimethylcarbamoyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,
 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-propyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,

- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1,2,3-trimethyl-indol-5-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(2,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4]triazole,
- 5 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-acetyl-2,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-propyl-2,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4]triazole,
- 10 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(N-methyl-tetrahydrocarbozol-7-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(N-methyl-cyclononan[a]indol-5-yl)-5-mercapto-[1,2,4]triazole,
- 15 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-n-butyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-n-pentyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-n-hexyl-indol-4-yl)-5-mercapto-[1,2,4]triazole,
- 20 3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1-(1-methylcyclopropyl)-indol-4-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4]triazole,
- 25 3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1,2,3-trimethyl-indol-5-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4]triazole disodium salt,
- 3-(2,4-dihydroxy-5-*tert*-butyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4]triazole,
- 30 3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1-propyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4]triazole,
- 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-methyl-3-ethyl-indol-5-yl)-5-mercapto-[1,2,4]triazole,

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3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1,3-dimethyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-
mercapto-[1,2,4]triazole,

5 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-methyl-3-isopropyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(N-ethyl-carbozol-7-yl)-5-mercapto-
[1,2,4]triazole,

10 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-7-hydroxy-indol-4-yl)-5-
mercapto-[1,2,4]triazole,

3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-7-ethoxy-indol-4-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1,2-dimethyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

15 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(N-methyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1,3-dimethyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

20 3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1,3-dimethyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1-methyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1H-indol-5-yl)-5-mercapto-[1,2,4]triazole,

25 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1,2-dimethyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-ethyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-propyl-indol-5-yl)-5-mercapto-
[1,2,4]triazole, and

30 tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs
thereof.

In another embodiment, in formula (VII), X₄₂ is N.

In another embodiment, the compound is selected from the group consisting of

35 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-ethyl-benzimidazol-4-yl)-5-mercapto-
[1,2,4]triazole,

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3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-ethyl-benzimidazol-4-yl)-5-mercapto-[1,2,4]triazole HCL salt,

3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(2-methyl-3-ethyl-benzimidazol-5-yl)-5-mercapto-[1,2,4]triazole,

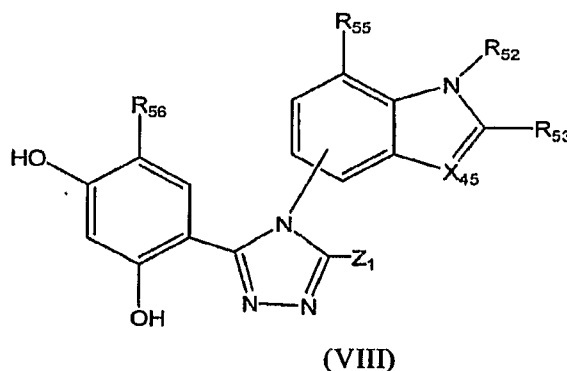
5 3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-ethyl-2-methyl-benzimidazol-5-yl)-5-mercapto-[1,2,4]triazole,

3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-methyl-2-trifluoromethyl-benzimidazol-5-yl)-5-mercapto-[1,2,4]triazole, and

10 tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof.

Compounds of formula (VII) inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of formula (VII) are particularly useful in treating cancer when given in combination with other anti-cancer agent.

15 Compounds represented by formula (VIII):



and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof, wherein:

20 X_{45} is CR_{54} or N;

Z_1 is -OH or -SH;

R_{52} is selected from the group consisting of -H, methyl, ethyl, n-propyl, isopropyl, n-butyl, n-pentyl, n-hexyl, $-(CH_2)_2OCH_3$, $-CH_2C(O)OH$, and $-C(O)N(CH_3)_2$;

25 R_{53} and R_{54} are each, independently, -H, methyl, ethyl, or isopropyl; or R_{53} and R_{54} taken together with the carbon atoms to which they are attached form a phenyl, cyclohexenyl, or cyclooctenyl ring;

R_{55} is selected from the group consisting of -H, -OH, $-OCH_3$, and $-OCH_2CH_3$; and

R_{56} is selected from the group consisting of -H, methyl, ethyl, isopropyl, and cyclopropyl.

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In one embodiment, in formula (VIII), Z_1 is $-\text{OH}$.

In another embodiment, in formula (VIII), Z_1 is $-\text{SH}$.

In another embodiment, in formula (VIII), R_{53} is H or a lower alkyl.

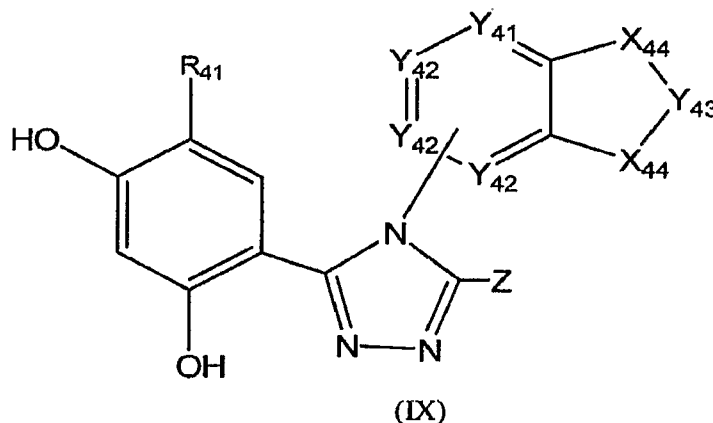
In another embodiment, in formula (VIII), X_{45} is CR_{54} . Preferably, R_{54} is H or a lower alkyl.

In another embodiment, X_{45} is N.

In another embodiment, the compound is 3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(N-methyl-indol-5-yl)-5-mercapto-[1,2,4]triazole.

Compounds of formula (VIII) inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of formula (VIII) are particularly useful in treating cancer when given in combination with other anti-cancer agent.

Compounds represented by formula (IX):



and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof, wherein,

X_{44} , for each occurrence, is independently, O, NR_{42} or $\text{C}(\text{R}_{46})_2$;

Y_{43} is NR_{42} or $\text{C}(\text{R}_{46})_2$;

Y_{41} , Y_{42} , Z , R_{41} , R_{42} , and R_{46} are defined as above.

In one embodiment, in formula (IX), R_{41} is selected from the group consisting of $-\text{H}$, lower alkyl, lower alkoxy, lower cycloalkyl, and lower cycloalkoxy.

In another embodiment, in formula (IX), R_{41} is selected from the group consisting of $-\text{H}$, methyl, ethyl, propyl, isopropyl, cyclopropyl, methoxy, ethoxy, propoxy, and cyclopropoxy.

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In another embodiment, in formula (IX), R_{42} is selected from the group consisting of -H, methyl, ethyl, n-propyl, isopropyl, cyclopropyl, n-butyl, *sec*-butyl, *tert*-butyl, n-pentyl, n-hexyl, $-C(O)OH$, $-(CH_2)_mC(O)OH$, $-CH_2OCH_3$, $-CH_2CH_2OCH_3$, and $-C(O)N(CH_3)_2$.

5 In another embodiment, in formula (IX), Y_{41} is CR_{45} . Preferably, R_{45} is H, a lower alkoxy, or -OH.

In another embodiment, in formula (IX), Y_{42} is CH.

In another embodiment, in formula (IX), Y_{43} is CH_2 .

In another embodiment, in formula (IX), Y_{43} is NR_{42} , wherein R_{42} is H or a lower alkyl.

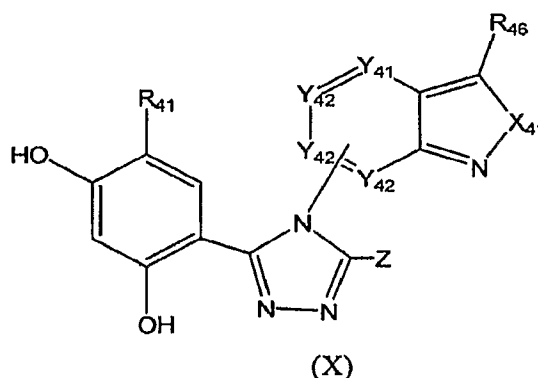
10 In another embodiment, in formula (IX), one of X_{44} is NR_{42} and the other is CH_2 or $C(R_6)_2$. Preferably, one of X_{44} is NR_{42} and the other is CH_2 .

In another embodiment, in formula (VI), Z is -OH.

In another embodiment, Z is -SH.

15 Compounds of formula (IX) inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of formula (IX) are particularly useful in treating cancer when given in combination with other anti-cancer agent.

Compounds represented by formula (X):



20

and tautomers, pharmaceutically acceptable salts, solvates, clathrates, and prodrugs thereof, wherein:

X_{41} , Y_{41} , Y_{42} , Z, R_7 , R_8 , R_{10} , R_{11} , R_{41} , R_{46} , and p are defined as above.

25 In one embodiment, in formula (X), R_{41} is selected from the group consisting of -H, lower alkyl, lower alkoxy, lower cycloalkyl, and lower cycloalkoxy.

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In another embodiment, in formula (X), R_{41} is selected from the group consisting of -H, methyl, ethyl, propyl, isopropyl, cyclopropyl, methoxy, ethoxy, propoxy, and cyclopropoxy.

In another embodiment, in formula (X), X_{41} is NR_{42} . Preferably, R_{42} is selected from the group consisting of -H, methyl, ethyl, n-propyl, isopropyl, cyclopropyl, n-butyl, *sec*-butyl, *tert*-butyl, n-pentyl, n-hexyl, $-C(O)OH$, $-(CH_2)_mC(O)OH$, $-CH_2OCH_3$, $-CH_2CH_2OCH_3$, and $-C(O)N(CH_3)_2$. More preferably, R_{42} is H or a lower alkyl.

In another embodiment, in formula (X), X_{41} is O.

In another embodiment, in formula (X), X_{41} is S.

In another embodiment, in formula (X), Y_{41} is CR_{45} . Preferably, R_{45} is H, a lower alkoxy, or -OH.

In another embodiment, in formula (X), Y_{42} is CH.

In another embodiment, in formula (X), R_{46} is H or a lower alkyl.

In one embodiment, the compound is 3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(2-methyl-indazol-6-yl)-5-mercapto-[1,2,4]triazole.

Compounds of formula (X) inhibit the activity of Hsp90 and are particularly useful for treating or preventing proliferative disorders, such as cancer. In addition, compounds of formula (X) are particularly useful in treating cancer when given in combination with other anti-cancer agent.

i) Exemplary Compounds of the Invention

Exemplary compounds of the invention are depicted in Table 1 below, including tautomers, pharmaceutically acceptable salts, solvates, clathrates, hydrates, polymorphs or prodrugs thereof.

Table 1

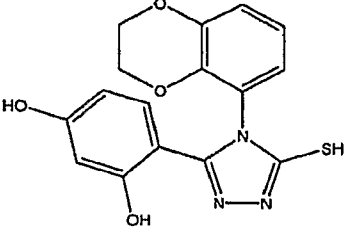
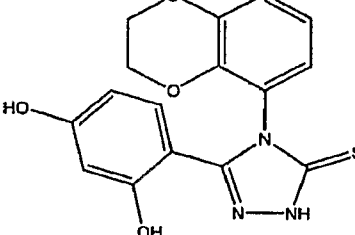
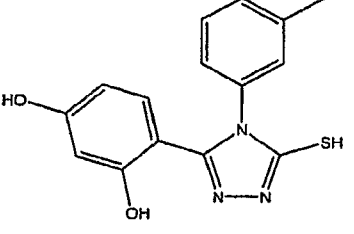
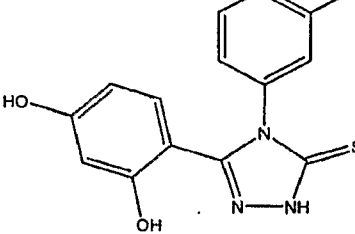
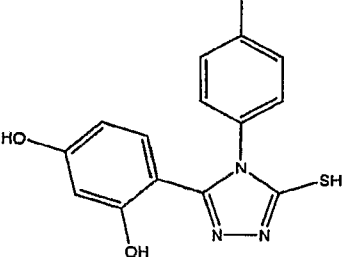
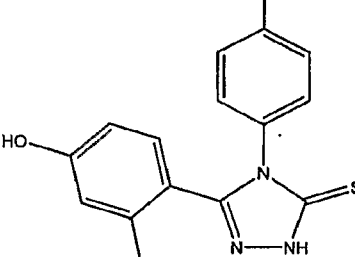
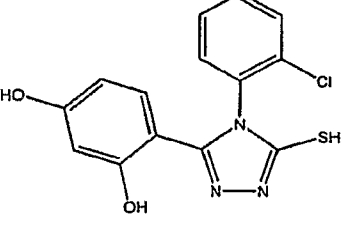
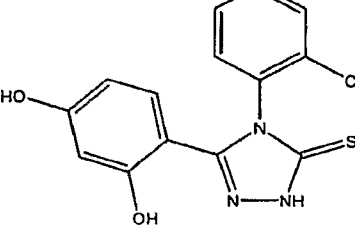
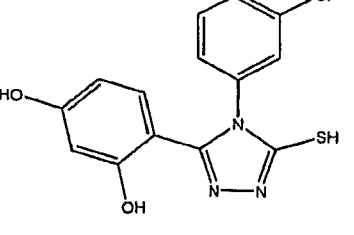
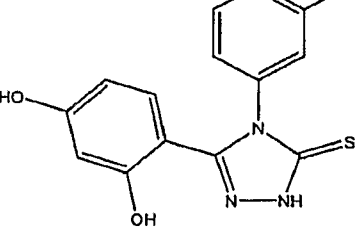
No.	Structure	Tautomeric Structure	Name
1			3-(2-Hydroxyphenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole

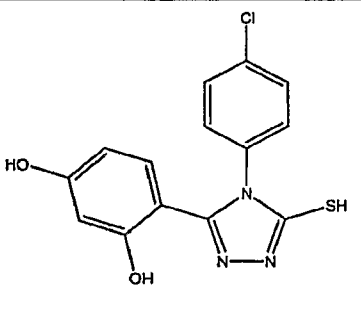
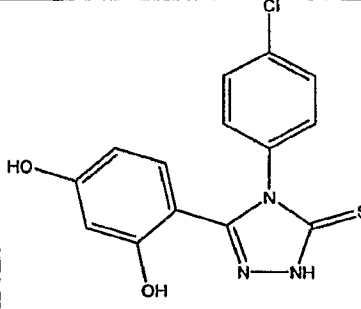
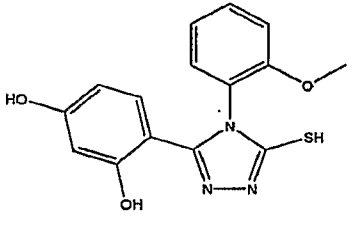
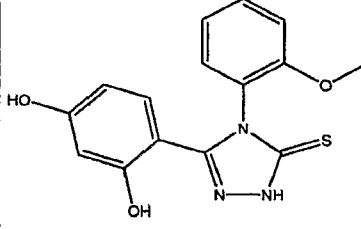
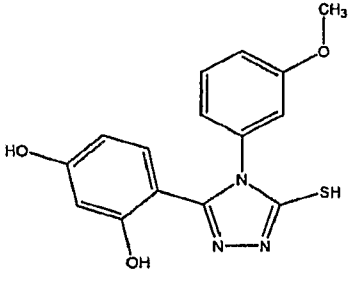
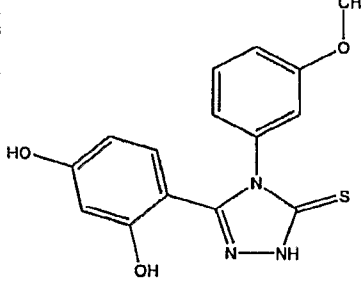
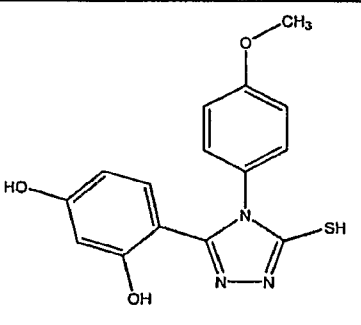
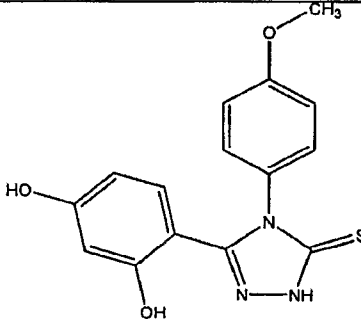
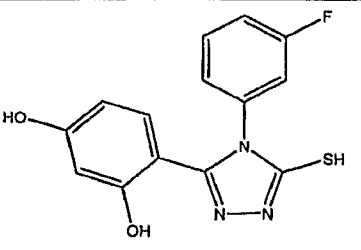
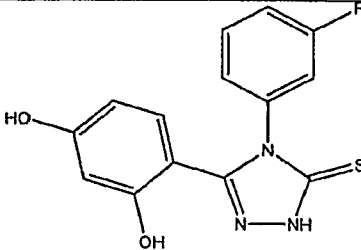
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2			3-(2,4-Dihydroxyphenyl)-4-[4-(2-methoxyethoxy)-naphthalen-1-yl]-5-mercapto-[1,2,4] triazole
3			3-(2,4-Dihydroxyphenyl)-4-(2-methyl-4-bromophenyl)-5-mercapto-[1,2,4] triazole
4			3-(2,4-Dihydroxyphenyl)-4-(4-bromophenyl)-5-mercapto-[1,2,4] triazole
5			3-(3,4-Dihydroxyphenyl)-4-(6-methoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
6			3-(3,4-Dihydroxyphenyl)-4-(6-ethoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
7			3-(3,4-Dihydroxyphenyl)-4-(6-propoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole

8			3-(2,4-Dihydroxy-5-ethylphenyl)-4-(5-methoxynaphthalen-1-yl)-5-mercapto-[1,2,4] triazole
9			3-(3,4-Dihydroxyphenyl)-4-(6-isopropoxynaphthalen-1-yl)-5-mercapto-[1,2,4] triazole
10			3-(2,4-Dihydroxyphenyl)-4-(2,6-diethylphenyl)-5-mercapto-[1,2,4] triazole
11			3-(2,4-Dihydroxyphenyl)-4-(2-methyl-6-ethylphenyl)-5-mercapto-[1,2,4] triazole
12			3-(2,4-Dihydroxyphenyl)-4-(2,6-diisopropylphenyl)-5-mercapto-[1,2,4] triazole
13			3-(2,4-Dihydroxyphenyl)-4-(1-ethylindol-4-yl)-5-mercapto-[1,2,4] triazole

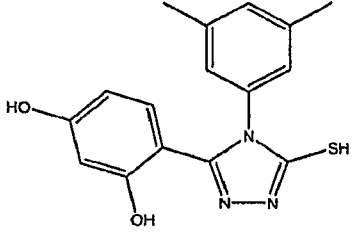
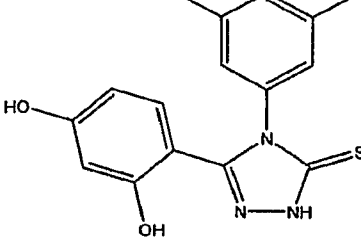
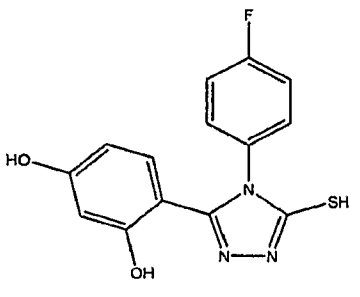
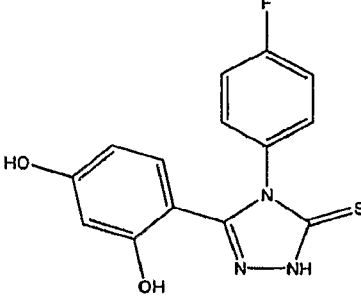
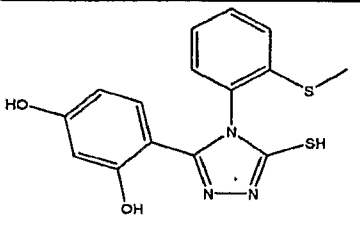
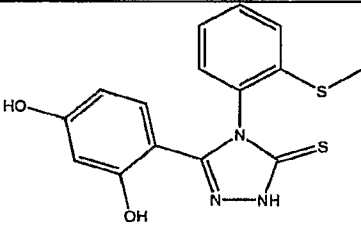
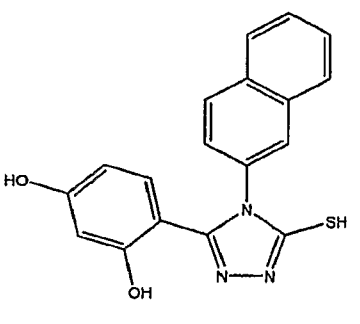
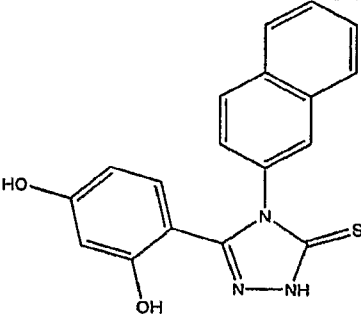
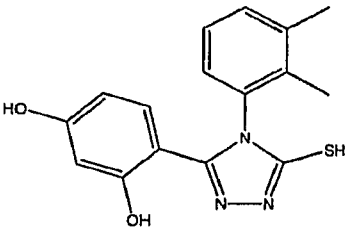
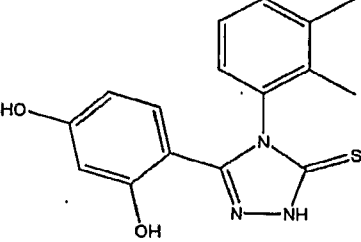
-103-

14			3-(2,4-Dihydroxyphenyl)-4-(2,3-dihydrobenzo[1,4]dioxin-5-yl)-5-mercapto-[1,2,4] triazole
15			3-(2,4-Dihydroxyphenyl)-4-(3-methylphenyl)-5-mercapto-[1,2,4] triazole
16			3-(2,4-Dihydroxyphenyl)-4-(4-methylphenyl)-5-mercapto-[1,2,4] triazole
17			3-(2,4-Dihydroxyphenyl)-4-(2-chlorophenyl)-5-mercapto-[1,2,4] triazole
18			3-(2,4-Dihydroxyphenyl)-4-(3-chlorophenyl)-5-mercapto-[1,2,4] triazole

19			3-(2,4-Dihydroxyphenyl)-4-(4-chlorophenyl)-5-mercapto-[1,2,4] triazole
20			3-(2,4-Dihydroxyphenyl)-4-(2-methoxyphenyl)-5-mercapto-[1,2,4] triazole
21			3-(2,4-Dihydroxyphenyl)-4-(3-methoxyphenyl)-5-mercapto-[1,2,4] triazole
22			3-(2,4-Dihydroxyphenyl)-4-(4-methoxyphenyl)-5-mercapto-[1,2,4] triazole
23			3-(2,4-Dihydroxyphenyl)-4-(3-fluorophenyl)-5-mercapto-[1,2,4] triazole

24		3-(2,4-Dihydroxyphenyl)-4-(2-ethylphenyl)-5-mercapto-[1,2,4] triazole
25		3-(2-Hydroxy-4-fluorophenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
26		3-(2-Hydroxy-4-aminophenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
27		3-(2,4-Dihydroxyphenyl)-4-(2-methyl-4-butyl-phenyl)-5-mercapto-[1,2,4] triazole
28		3-(2,4-Dihydroxyphenyl)-4-(2,4-dimethyl-phenyl)-5-mercapto-[1,2,4] triazole
29		3-(2,4-Dihydroxyphenyl)-4-(2,6-dimethyl-phenyl)-5-mercapto-[1,2,4] triazole

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30			3-(2,4-Dihydroxyphenyl)-4-(2,6-dimethylphenyl)-5-mercapto-[1,2,4] triazole
31			3-(2,4-Dihydroxyphenyl)-4-(4-fluorophenyl)-5-mercapto-[1,2,4] triazole
32			3-(2,4-Dihydroxyphenyl)-4-(2-methylsulfanylphenyl)-5-mercapto-[1,2,4] triazole
33			3-(2,4-Dihydroxyphenyl)-4-(naphthalene-2-yl)-5-mercapto-[1,2,4] triazole
34			3-(2,4-Dihydroxyphenyl)-4-(2,3-dimethylphenyl)-5-mercapto-[1,2,4] triazole

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35			3-(2,4-Dihydroxyphenyl)-4-(2-methyl-4-fluorophenyl)-5-mercapto-[1,2,4] triazole
36			3-(2,4-Dihydroxyphenyl)-4-(acenaphthalen-5-yl)-5-mercapto-[1,2,4] triazole
37			3-(2-Hydroxy-4-methoxyphenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
38			3-(2,4-Dihydroxyphenyl)-4-(2,3-dichlorophenyl)-5-mercapto-[1,2,4] triazole
39			3-(2,4-Dihydroxyphenyl)-4-(5-methoxynaphthalen-1-yl)-5-mercapto-[1,2,4] triazole

40			3-(2,4-Dihydroxyphenyl)-4-(pyren-1-yl)-5-mercapto-[1,2,4] triazole
41			3-(2,4-Dihydroxyphenyl)-4-(quinolin-5-yl)-5-mercapto-[1,2,4] triazole
42			3-(2,4-Dihydroxyphenyl)-4-(1,2,3,4-tetrahydronaphthalen-5-yl)-5-mercapto-[1,2,4] triazole
43			3-(2,4-Dihydroxyphenyl)-4-(anthracen-1-yl)-5-mercapto-[1,2,4] triazole
44			3-(2,4-Dihydroxyphenyl)-4-(biphenyl-2-yl)-5-mercapto-[1,2,4] triazole
45			3-(2,4-Dihydroxy-6-methylphenyl)-4-(naphthalene-1-yl)-5-mercapto-[1,2,4] triazole

46		3-(2,4-Dihydroxyphenyl)-4-(4-pentyloxyphenyl)-5-mercapto-[1,2,4] triazole
47		3-(2,4-Dihydroxyphenyl)-4-(4-octyloxyphenyl)-5-mercapto-[1,2,4] triazole
48		3-(2,4-Dihydroxyphenyl)-4-(4-chloronaphthalen-1-yl)-5-mercapto-[1,2,4] triazole
49		3-(2,4-Dihydroxy-5-ethylphenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
50		3-(2,4-Dihydroxy-5-ethylphenyl)-4-(7-carboxymethoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
51		3-(2,4-Dihydroxyphenyl)-4-(2-methyl-quinolin-4-yl)-5-mercapto-[1,2,4] triazole

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52			3-(3-Hydroxypyridin-4-yl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
53			3-(2-Hydroxy-4-acetylaminophenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
54			3-(2,4-Dihydroxyphenyl)-4-(1,2,3,4-tetrahydronaphthalen-1-yl)-5-mercapto-[1,2,4] triazole
55			3-(2,4-Dihydroxyphenyl)-4-(2,3-dihydrobenzo[1,4]dioxin-5-yl)-5-mercapto-[1,2,4] triazole
56			3-(2,4-Dihydroxyphenyl)-4-(3,5-dimethoxyphenyl)-5-mercapto-[1,2,4] triazole
57			3-(2,4-Dihydroxyphenyl)-4-(2,3-dimethyl-1H-indol-4-yl)-5-mercapto-[1,2,4] triazole

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58			3-(2,4-Dihydroxy-3-propylphenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
59			3-(1-ethyl-4-hydroxy-6-oxo-1,6-dihydro-pyridin-3-yl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
60			3-(4-hydroxy-6-oxo-pyridin-3-yl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
61			3-(2,4-Dihydroxy-phenyl)-4-(3,5-di- <i>tert</i> -butylphenyl)-5-mercapto-[1,2,4] triazole
62			3-(2,6-Dihydroxy-5-fluoropyridin-3-yl) 4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
63			3-(2,4-Dihydroxy-5-methylphenyl)-4-(naphthalene-1-yl)-5-mercapto-[1,2,4] triazole

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64			3-[2,4-Dihydroxy-phenyl]-4-(3-benzoylphenyl)-5-mercapto-[1,2,4] triazole
65			3-(2,4-Dihydroxy-phenyl)-4-(4-carboxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
66			3-(2,4-Dihydroxy-phenyl)-4-[4-(N,N-dimethylcarbamoyl)-naphthalen-1-yl]-5-mercapto-[1,2,4] triazole
67			3-(2,4-Dihydroxy-phenyl)-4-(4-propoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
68			3-(2,4-Dihydroxy-phenyl)-4-(4-isopropoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole

69			3-(2,4-Dihydroxy-phenyl)-4-(5-isopropoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
70			3-(2,4-Dihydroxy-phenyl)-4-(isoquinolin-5-yl)-5-mercapto-[1,2,4] triazole
71			3-(2,4-Dihydroxy-phenyl)-4-(5-propoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
72			3-(2-Hydroxy-4-methanesulfamino-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
73			3-(2,4-Dihydroxy-3,6-dimethyl-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
74			3-(2,4-Dihydroxy-phenyl)-4-[7-(2-methoxyethoxy)-naphthalen-1-yl]-5-mercapto-[1,2,4] triazole

75		3-(2,4-Dihydroxy-5-hexyl-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
76		3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(4-methoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
77		3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(6-methoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
78		3-(2,4-Dihydroxy-3-chloro-5-ethyl-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
79		3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(2,3-dimethoxy-4-methoxy-phenyl)-5-mercapto-[1,2,4] triazole
80		3-(2,4-Dihydroxy-phenyl)-4-(7-isopropoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
81		3-(2,4-Dihydroxy-phenyl)-4-(7-ethoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole

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82			3-(2,4-Dihydroxy-phenyl)-4-(7-propoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
83			3-(2-Hydroxy-4-methoxymethoxy-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
84			3-[2-Hydroxy-4-(2-hydroxyethoxy)-phenyl]-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
85			3-(2,4-Dihydroxyphenyl)-4-(7-methoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
86			3-(2,4-Dihydroxyphenyl)-4-(5-methoxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
87			3-(2,4-Dihydroxyphenyl)-4-(4-hydroxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
88			3-(2,4-Dihydroxyphenyl)-4-(1-isopropyl-indol-4-yl)-5-mercapto-[1,2,4] triazole

89			3-(2,4-Dihydroxy-5-tert-butyl-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
90			3-(2,4-Dihydroxy-5-propyl-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
91			3-(2,4-Dihydroxy-3-methyl-5-ethyl-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
92			3-(2,4-Dihydroxy-5-isobutyl-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
93			3-(2,4-Dihydroxy-phenyl)-4-(2,3-dimethoxy-phenyl)-5-mercapto-[1,2,4] triazole
94			3-(2,4-Dihydroxy-phenyl)-4-(2-methoxy-3-chloro-phenyl)-5-mercapto-[1,2,4] triazole

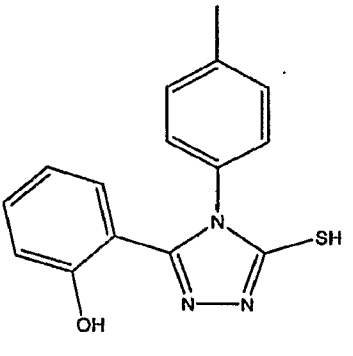
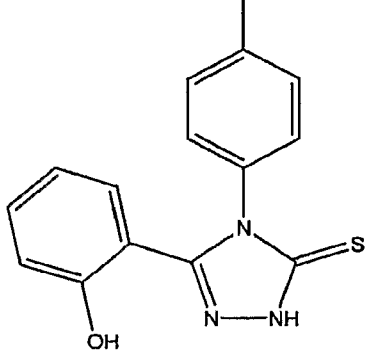
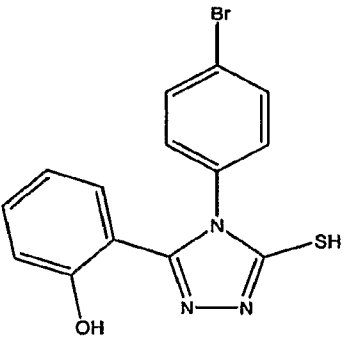
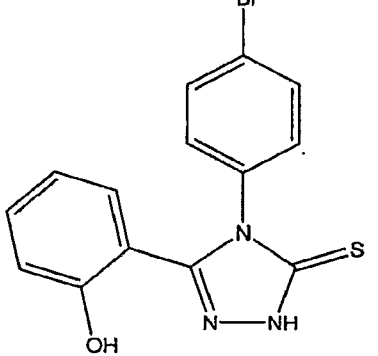
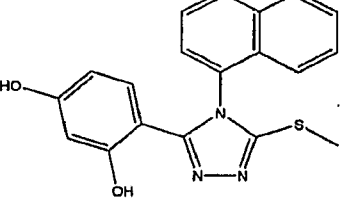
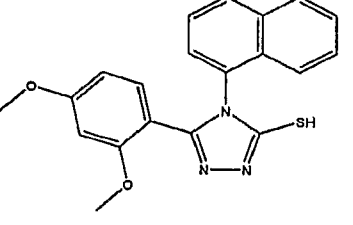
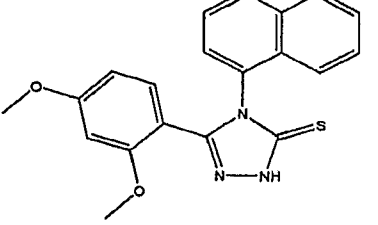
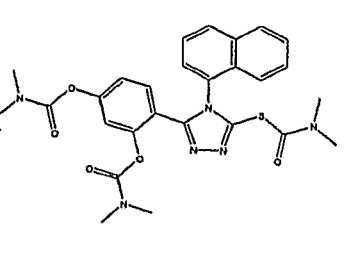
95			3-(2,4-Dihydroxy-phenyl)-4-(indol-4-yl)-5-mercapto-[1,2,4] triazole
96			3-(2,4-Dihydroxy-phenyl)-4-[1-(2-methoxyethoxy)-indol-4-yl]-5-mercapto-[1,2,4] triazole
97			3-(2,4-Dihydroxy-phenyl)-4-(naphthalen-1-yl)-5-hydroxy-[1,2,4] triazole
98			3-(1-Oxo-3-hydroxy-pyridin-4-yl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
99			3-(2,5-Dihydroxy-4-carboxy)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
100			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-indol-4-yl)-5-mercapto-[1,2,4] triazole

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101			3-(2,4-Dihydroxy-5-ethylphenyl)-4-[1-(dimethylcarbamoyl)-indol-4-yl]-5-mercapto-[1,2,4] triazole
102			3-(2,4-Dihydroxy-5-ethylphenyl)-4-(1-ethylbenzoimidazol-4-yl)-5-mercapto-[1,2,4] triazole
103			3-(2,4-Dihydroxy-5-ethylphenyl)-4-(1,2,3-trimethylindol-5-yl)-5-mercapto-[1,2,4] triazole
104			3-(2,5-Dihydroxy-4-hydroxymethylphenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
105			3-(2-Hydroxy-4-amino-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
106			3-(2-Hydroxy-4-acetylamino-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole

107			3-(2,4-Dihydroxy-3-chloro-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
108			3-(2,4-Dihydroxy-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
109			3-(2,4-Dihydroxy-phenyl)-4-(2-methyl-phenyl)-5-mercapto-[1,2,4] triazole
110			3-(2,4-Dihydroxy-phenyl)-4-(2,5-dimethoxy-phenyl)-5-mercapto-[1,2,4] triazole
111			3-(2,4-Dihydroxy-phenyl)-4-phenyl-5-mercapto-[1,2,4] triazole
112			3-(2-Hydroxy-phenyl)-4-(2-methoxy-phenyl)-5-mercapto-[1,2,4] triazole

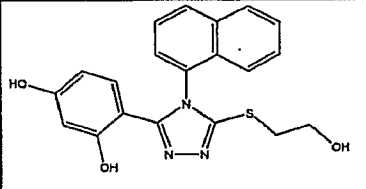
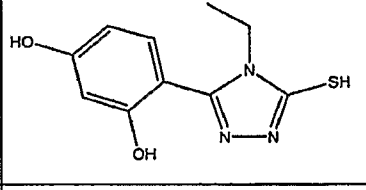
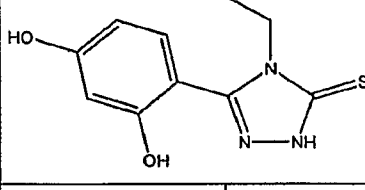
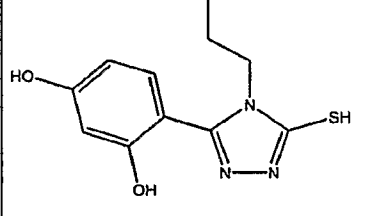
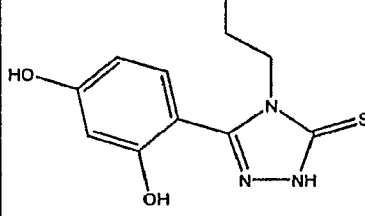
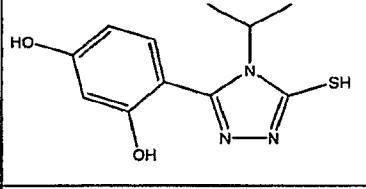
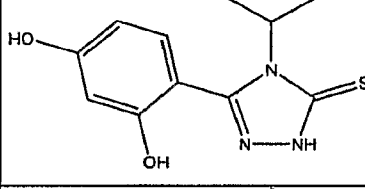
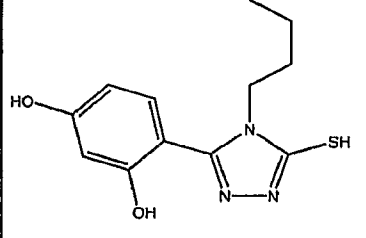
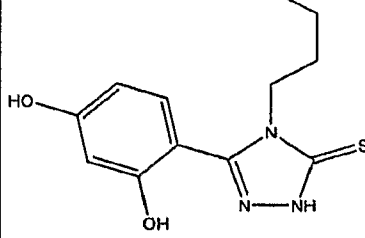
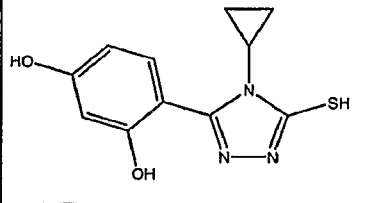
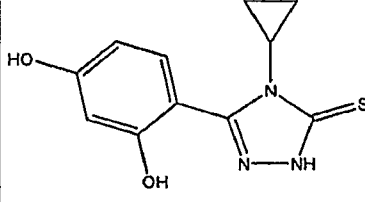
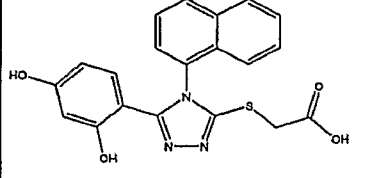
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113			3-(2-Hydroxy-phenyl)-4-(4-methyl-phenyl)-5-mercapto-[1,2,4] triazole
114			3-(2-Hydroxy-phenyl)-4-(4-bromo-phenyl)-5-mercapto-[1,2,4] triazole
115			3-(2,4-Dihydroxy-phenyl)-4-(naphthalen-1-yl)-5-(methyl sulfanyl)- [1,2,4] triazole
116			3-(2,4-Dimethoxy-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
117			3-[2,4-Di-(dimethyl-carbamoyloxy)-phenyl]-4-(naphthalen-1-yl)-5-(dimethyl-carbamoylsulfanyl)- [1,2,4] triazole

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118			3-(2,4-Dihydroxy-phenyl)-4-(naphthalen-1-yl)-5-(dimethylcarbamoylsulfanyl)-[1,2,4] triazole
119			3-(2,4-Diethoxycarbonyloxy-phenyl)-4-(naphthalen-1-yl)-5-(ethoxycarbonylsulfanyl)-[1,2,4] triazole
120			3-(2,4-Di-isobutyryloxy-phenyl)-4-(naphthalen-1-yl)-5-(isobutyrylsulfanyl)-[1,2,4] triazole
121			3-[2,4-Di-(dimethylcarbamoyloxy)-phenyl]-4-(quinolin-5-yl)-5-(dimethylcarbamoylsulfanyl)-[1,2,4] triazole
122			3-(2,4-Diacetoxy-phenyl)-4-(naphthalen-1-yl)-5-(acetylsulfanyl)-[1,2,4] triazole
123			3-(2,4-Diacetoxy-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
124			3-(2,4-Diethylcarbamoyloxy-phenyl)-4-(naphthalen-1-yl)-5-(ethylcarbamoylsulfanyl)-[1,2,4] triazole

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125			3-(2,4-Dihydroxy-phenyl)-4-(naphthalen-1-yl)-5-(2-hydroxyethylsulfanyl)-[1,2,4] triazole
126			3-(2,4-Dihydroxy-phenyl)-4-ethyl-5-mercapto-[1,2,4] triazole
127			3-(2,4-Dihydroxy-phenyl)-4-propyl-5-mercapto-[1,2,4] triazole
128			3-(2,4-Dihydroxy-phenyl)-4-isopropyl-5-mercapto-[1,2,4] triazole
129			3-(2,4-Dihydroxy-phenyl)-4-butyl-5-mercapto-[1,2,4] triazole
130			3-(2,4-Dihydroxy-phenyl)-4-cyclopropyl-5-mercapto-[1,2,4] triazole
131			3-(2,4-Dihydroxy-phenyl)-4-(naphthalen-1-yl)-5-(carboxyethylsulfanyl)-[1,2,4] triazole

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132			3-(2,6-Dimethoxy-5-fluoropyridin-3-yl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
133			3-(2-Methanesulfonyloxy-4-methanesulfonylamino-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
134			3-(2-Methoxy-phenyl)-4-(4-methoxy-phenyl)-5-mercapto-[1,2,4] triazole
135			3-(3-Hydroxy-naphthalen-2-yl)-4-phenyl-5-mercapto-[1,2,4] triazole
136			3-(2-Methoxy-phenyl)-4-(4-methyl-phenyl)-5-mercapto-[1,2,4] triazole

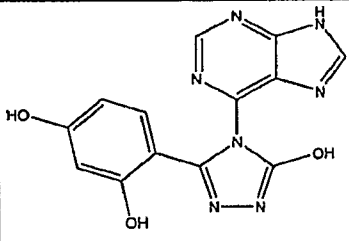
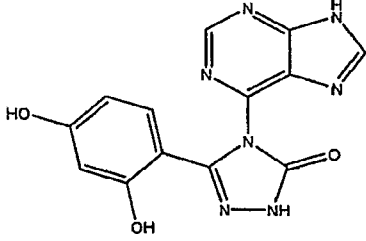
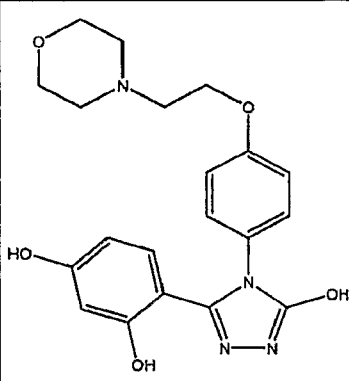
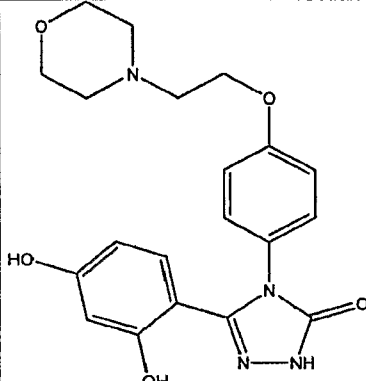
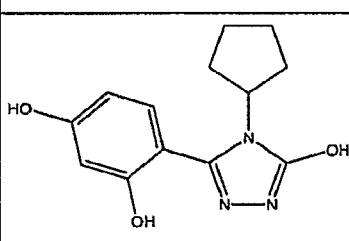
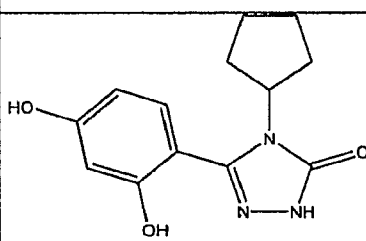
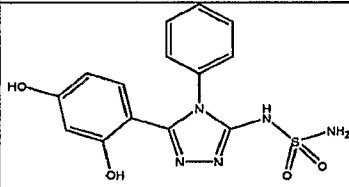
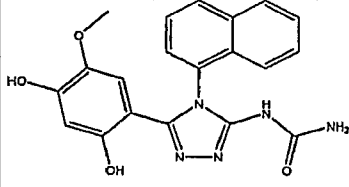
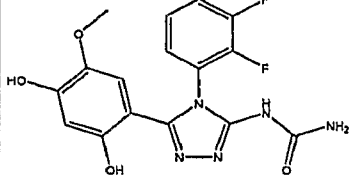
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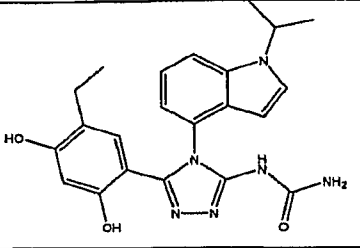
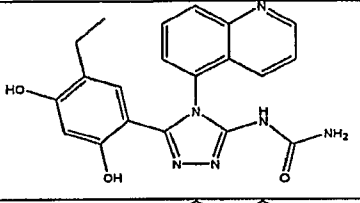
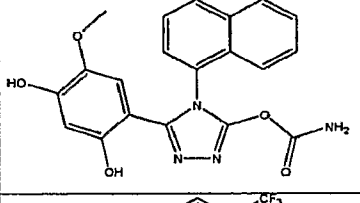
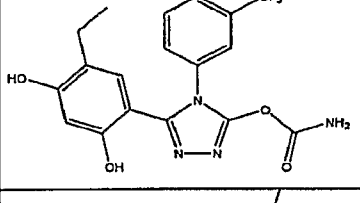
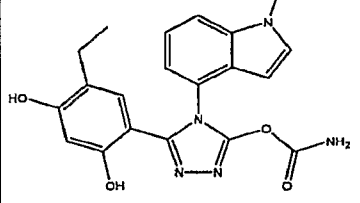
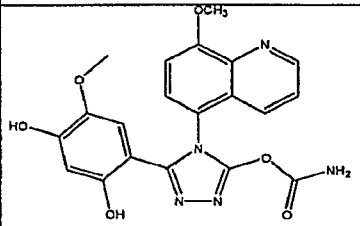
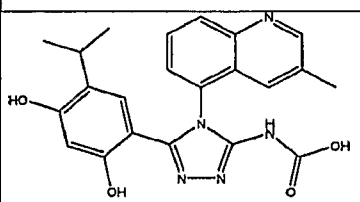
137			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(3-methoxy-phenyl)-5-hydroxy-[1,2,4] triazole
138			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(naphthalen-1-yl)-5-hydroxy-[1,2,4] triazole
139			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-indol-3-yl)-5-hydroxy-[1,2,4] triazole
140			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-indol-4-yl)-5-amino-[1,2,4] triazole
141			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(3-methoxy-phenyl)-5-amino-[1,2,4] triazole
142			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(naphthalen-1-yl)-5-amino-[1,2,4] triazole

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143			3-(2-Hydroxy-5-ethoxy-phenyl)-4-(naphthalen-1-yl)-5-hydroxy-[1,2,4] triazole
144			3-(2-Hydroxy-5-isopropyl-phenyl)-4-(naphthalen-1-yl)-5-hydroxy-[1,2,4] triazole
145			3-(2-Dihydroxy-phenyl)-4-(7-fluoro-naphthalen-1-yl)-5-hydroxy-[1,2,4] triazole
146			3-(2,4-Dihydroxy-phenyl)-4-(2,3-difluorophenyl)-5-hydroxy-[1,2,4] triazole
147			3-(2,4-Dihydroxy-phenyl)-4-[2-(1H-tetrazol-5-yl)-phenyl]-5-hydroxy-[1,2,4] triazole
148			3-(2,4-Dihydroxy-phenyl)-4-(benzothiazol-4-yl)-5-hydroxy-[1,2,4] triazole

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149			3-(2,4-Dihydroxy-phenyl)-4-(9H-purin-6-yl)-5-hydroxy-[1,2,4] triazole
150			3-(2,4-Dihydroxy-phenyl)-4-{4-[2-(morpholin-1-yl)-ethoxy]-phenyl}-5-hydroxy-[1,2,4] triazole
151			3-(2,4-Dihydroxy-phenyl)-4-cyclopentyl-5-hydroxy-[1,2,4] triazole
152			3-(2,4-Dihydroxy-phenyl)-4-phenyl-5-(sulfamoylamino)-[1,2,4] triazole
153			3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(naphthalene-1-yl)-5-ureido-[1,2,4] triazole
154			3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(2,3-difluorophenyl)-5-ureido-[1,2,4] triazole

155			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-indol-4-yl)-5-ureido-[1,2,4] triazole
156			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(quinolin-5-yl)-5-ureido-[1,2,4] triazole
157			3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(naphthalene-1-yl)-5-carbamoyloxy-[1,2,4] triazole
158			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(3-trifluoromethyl-phenyl)-5-carbamoyloxy-[1,2,4] triazole
159			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(1-methyl-indol-4-yl)-5-carbamoyloxy-[1,2,4] triazole
160			3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(8-methoxy-quinolin-5-yl)-5-carbamoyloxy-[1,2,4] triazole
161			3-(2,4-Dihydroxy-5-isopropyl-phenyl)-4-(3-methyl-quinolin-5-yl)-5-carboxyamino-[1,2,4] triazole

162		3-(2,4-Dihydroxy-phenyl)-4-(1-methyl-2-chloro-indol-4-yl)-5-carbamoyloxy-[1,2,4] triazole
163		3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-[3,5-di(trifluoromethyl)-phenyl]-5-carbamoyloxy-[1,2,4] triazole
164		3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(3-trifluoromethyl-phenyl)-5-(sulfamoylamino)-[1,2,4] triazole
165		3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(naphthalene-1-yl)-5-(sulfamoylamino)-[1,2,4] triazole
166		3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(1-isopropyl-benzoimidazol-4-yl)-5-(sulfamoylamino)-[1,2,4] triazole
167		3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(3-isopropylphenyl)-5-(thiocarboxyamino)-[1,2,4] triazole
168		3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(3-isopropoxyphenyl)-5-(sulfamoyloxy)-[1,2,4] triazole

169			3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(naphthalene-1-yl)-5-(sulfamoyloxy)- [1,2,4] triazole
170			3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(1-isopropyl-benzoimidazol-4-yl)-5-(sulfamoyloxy)- [1,2,4] triazole
171			3-(2-Hydroxy-4-ethoxycarbonyoxy-5-methoxy-phenyl)-4-(1-isopropyl-benzoimidazol-4-yl)-5-hydroxy-[1,2,4] triazole
172			3-(2-Hydroxy-4-ethoxycarbonyoxy-5-ethyl-phenyl)-4-(naphthalin-2-yl)-5-hydroxy-[1,2,4] triazole
173			3-[2-Hydroxy-4-(dimethyl-carbamoyoxy)-5-ethyl-phenyl]-4-(naphthalin-2-yl)-5-hydroxy-[1,2,4] triazole
174			3-[2-Hydroxy-4-(dimethyl-carbamoyoxy)-5-chloro-phenyl]-4-(quinolin-5-yl)-5-mercapto-[1,2,4] triazole
175			3-[2-Hydroxy-4-(dimethyl-carbamoyoxy)-5-ethyl-phenyl]-4-(2,3-difluoro-phenyl)-5-mercapto-[1,2,4] triazole

176		3-[2-Hydroxy-4-isobutyryloxy-5-ethyl-phenyl]-4-(1-methyl-benzimidazol-4-yl)-5-hydroxy-[1,2,4] triazole
177		3-(2,4-Dihydroxy-5-methoxy-phenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
178		3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(5-hydroxy-naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
179		3-(2,4-Dihydroxy-phenyl)-4-(naphthalen-1-ylmethyl)-5-mercapto-[1,2,4] triazole
180		3-(2-Hydroxy-4-methoxyphenyl)-4-(naphthalen-1-yl)-5-mercapto-[1,2,4] triazole
181		3-(2,4-Dihydroxy-phenyl)-4-(biphenyl-3-yl)-5-mercapto-[1,2,4] triazole

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182		3-(2,4-Dihydroxy-phenyl)-4-(2-methyl-5-hydroxymethyl-phenyl)-5-mercapto-[1,2,4] triazole
183		3-(2,4-Dihydroxy-phenyl)-4-(1-dimethylcarbamoyl-indol-4-yl)-5-mercapto-[1,2,4] triazole
184		3-(2,4,5-Trihydroxy-phenyl)-4-(naphthalene-1-yl)-5-mercapto-[1,2,4] triazole
185		3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(2,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
186		3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(3-t-butyl-4-methoxy-phenyl)-5-mercapto-[1,2,4] triazole
187		3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(1-ethyl-1H-benzoimidazol-4-yl)-5-mercapto-[1,2,4] triazole, HCl salt

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188			3-(2,4-Dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4] triazole
189			3-(2,4-Dihydroxy-5-cyclopropyl-phenyl)-4-(naphthalene-1-yl)-5-mercapto-[1,2,4] triazole
190			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-propyl-indol-4-yl)-5-mercapto-[1,2,4] triazole
191			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-acetyl-2,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
192			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(2-methyl-3-ethyl-benzimidazol-5-yl)-5-mercapto-[1,2,4] triazole
193			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-ethyl-2-methyl-benzimidazol-5-yl)-5-mercapto-[1,2,4] triazole

194			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-propyl-2,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
195			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(N-methyl-tetrahydrocarbozol-7-yl)-5-mercapto-[1,2,4] triazole
196			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(N-methyl-cyclononan[a]indol-5-yl)-5-mercapto-[1,2,4] triazole
197			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-n-butyl-indol-4-yl)-5-mercapto-[1,2,4] triazole
198			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-n-pentyl-indol-4-yl)-5-mercapto-[1,2,4] triazole

199		3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-n-hexyl-indol-4-yl)-5-mercapto-[1,2,4] triazole
200		3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1-(1-methylcyclopropyl)-indol-4-yl)-5-mercapto-[1,2,4] triazole
201		3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4] triazole
202		3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1,2,3-trimethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
203		3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4] triazole disodium salt
204		3-(2,4-dihydroxy-5-tert-butyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4] triazole

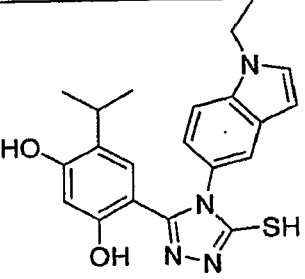
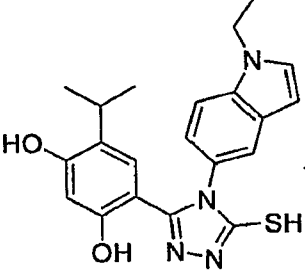
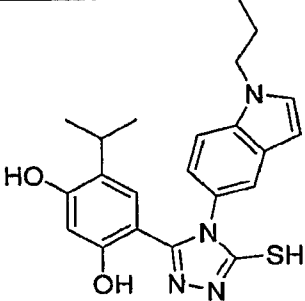
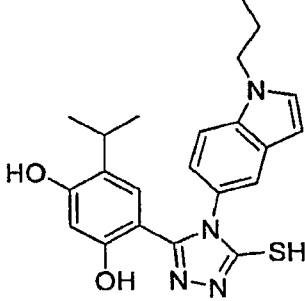
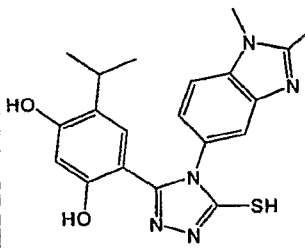
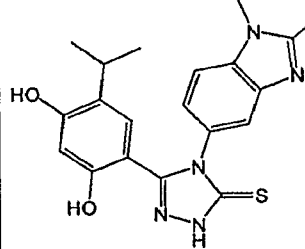
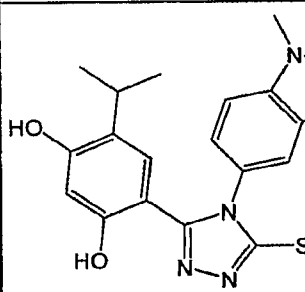
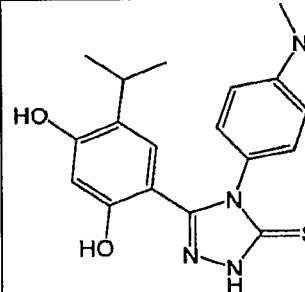
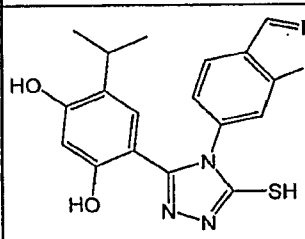
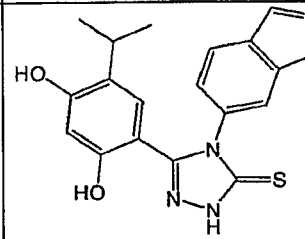
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207		3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
208		3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-isopropyl-7-methoxy-indol-4-yl)-5-mercapto-[1,2,4] triazole
209		3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(1-methyl-3-isopropyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
210		3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(N-ethyl-carbozol-7-yl)-5-mercapto-[1,2,4] triazole

211			3-(2,4-dihydroxy-5-ethylphenyl)-4-(1-isopropyl-7-hydroxyindol-4-yl)-5-mercapto-[1,2,4] triazole
212			3-(2,4-dihydroxy-5-ethylphenyl)-4-(1-isopropyl-7-ethoxyindol-4-yl)-5-mercapto-[1,2,4] triazole
213			3-(2,4-dihydroxy-5-ethylphenyl)-4-(1,2-dimethylindol-5-yl)-5-mercapto-[1,2,4] triazole
214			3-(2,4-dihydroxy-5-ethylphenyl)-4-(N-methylindol-5-yl)-5-mercapto-[1,2,4] triazole
215			3-(2,4-dihydroxy-5-ethylphenyl)-4-(2-methyl-7-methoxybenzofuran-4-yl)-5-mercapto-[1,2,4] triazole

216		3-(2,4-dihydroxy-5-ethylphenyl)-4-(benzofuran-5-yl)-5-mercapto-[1,2,4] triazole
217		3-(2,4-dihydroxy-5-ethylphenyl)-4-(2-methyl-1,3-benzoxaz-5-yl)-5-mercapto-[1,2,4] triazole
218		3-(2,4-dihydroxy-5-isopropylphenyl)-4-(1,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
219		3-(2,4-dihydroxy-5-cyclopropylphenyl)-4-(1,3-dimethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
220		3-(2,4-dihydroxy-5-ethylphenyl)-4-(1,3-dimethyl-indol-5-yl)-5-hydroxy-[1,2,4] triazole
221		3-(2,4-dihydroxy-5-isopropylphenyl)-4-(N-methyl-indol-5-yl)-5-mercapto-[1,2,4] triazole

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222			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1,2-dimethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
223			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1,3-dimethyl-indol-5-yl)-5-hydroxy-[1,2,4] triazole
224			3-(2,4-dihydroxy-5-cyclopropyl-phenyl)-4-(1-methyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
225			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1H-indol-5-yl)-5-mercapto-[1,2,4] triazole
226			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-methyl-indol-5-yl)-5-hydroxy-[1,2,4] triazole

227			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-ethyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
228			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-propyl-indol-5-yl)-5-mercapto-[1,2,4] triazole
229			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-methyl-2-trifluoromethyl-benzimidazol-5-yl)-5-mercapto-[1,2,4] triazole
230			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-methyl-indazol-5-yl)-5-mercapto-[1,2,4] triazole
231			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-methyl-indazol-6-yl)-5-mercapto-[1,2,4] triazole

232			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1-isopropyl-indol-4-yl)-5-hydroxy-[1,2,4] triazole
233			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(1,3-benzodioxol-5-yl)-5-mercapto-[1,2,4] triazole
234			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(indan-5-yl)-5-mercapto-[1,2,4] triazole
235			3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(2-methyl-indazol-6-yl)-5-mercapto-[1,2,4] triazole
236			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(3-oxo-benzo[1,4]oxazin-6-yl)-5-mercapto-[1,2,4] triazole
237			3-(2,4-dihydroxy-5-ethyl-phenyl)-4-(2-oxo-1,3-dihydro-benzimidazol-5-yl)-5-mercapto-[1,2,4] triazole

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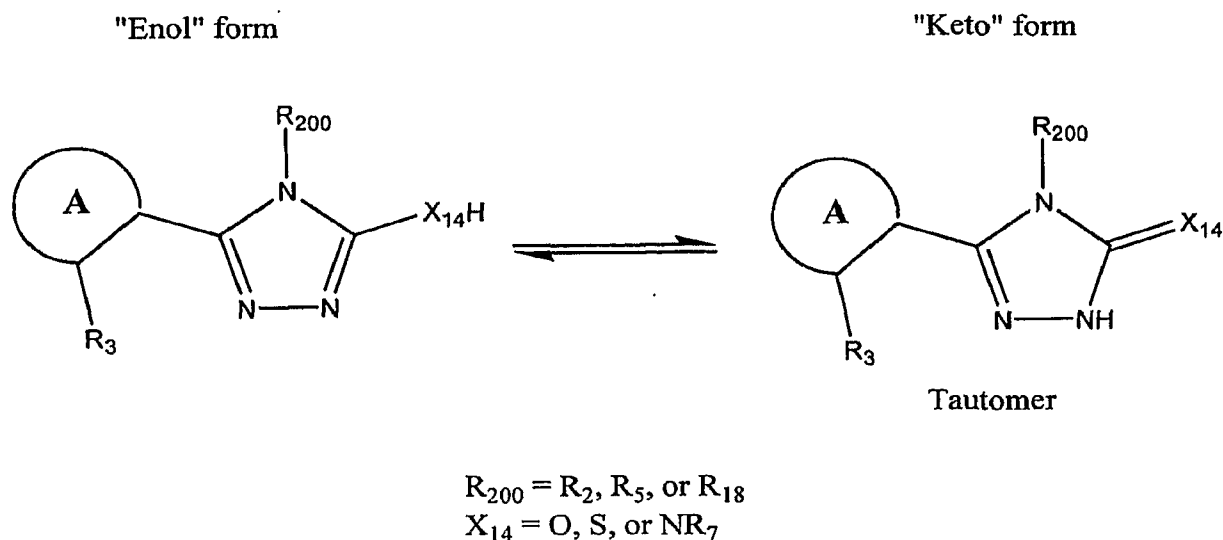
238		3-(2,4-dihydroxy-5-isopropyl-phenyl)-4-(2 <i>H</i> -benzo[1,4]oxazin-6-yl)-5-mercapto-[1,2,4] triazole
239		4-Ethyl-6-[5-mercapto-4-(1-methyl-2,3-dihydro-1 <i>H</i> -indol-5-yl)-4 <i>H</i> -[1,2,4]triazol-3-yl]-benzene-1,3-diol
240		5-(3-(5-ethyl-2,4-dihydroxyphenyl)-5-mercapto-4 <i>H</i> -1,2,4-triazol-4-yl)indolin-2-one
241		5-(3-(5-ethyl-2,4-dihydroxyphenyl)-5-mercapto-4 <i>H</i> -1,2,4-triazol-4-yl)-1 <i>H</i> -benzo[d]imidazol-2(3 <i>H</i>)-one
242		5-(3-(5-ethyl-2,4-dihydroxyphenyl)-5-mercapto-4 <i>H</i> -1,2,4-triazol-4-yl)-1-methylindolin-2-one

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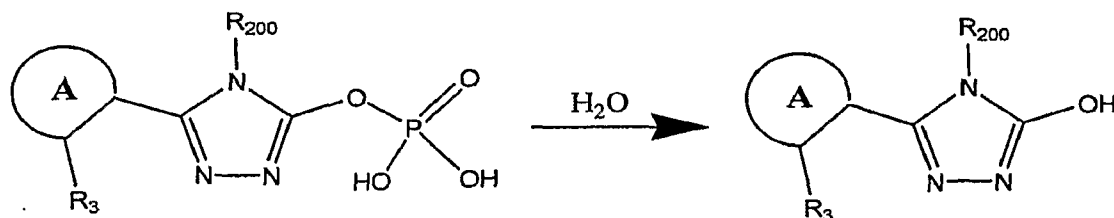
243			4-isopropyl-6-(5-mercapto-4-(4-propyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-6-yl)-4H-1,2,4-triazol-3-yl)benzene-1,3-diol
244			6-(3-(5-ethyl-2,4-dihydroxyphenyl)-5-mercapto-4H-1,2,4-triazol-4-yl)-2H-benzo[b][1,4]oxazin-3(4H)-one
245			6-(3-(5-ethyl-2,4-dihydroxyphenyl)-5-mercapto-4H-1,2,4-triazol-4-yl)-3-methylbenzo[d]thiazol-2(3H)-one
246			6-(3-(5-ethyl-2,4-dihydroxyphenyl)-5-mercapto-4H-1,2,4-triazol-4-yl)benzo[d]thiazol-2(3H)-one
247			3-(2,4-hydroxy-5-isopropylphenyl)-4-[(benzo[1,3]dioxol-5-yl)-methyl]-5-mercapto-4H-[1,2,4]triazole

Compounds listed above can form a tautomeric structure as shown below and as exemplified below:

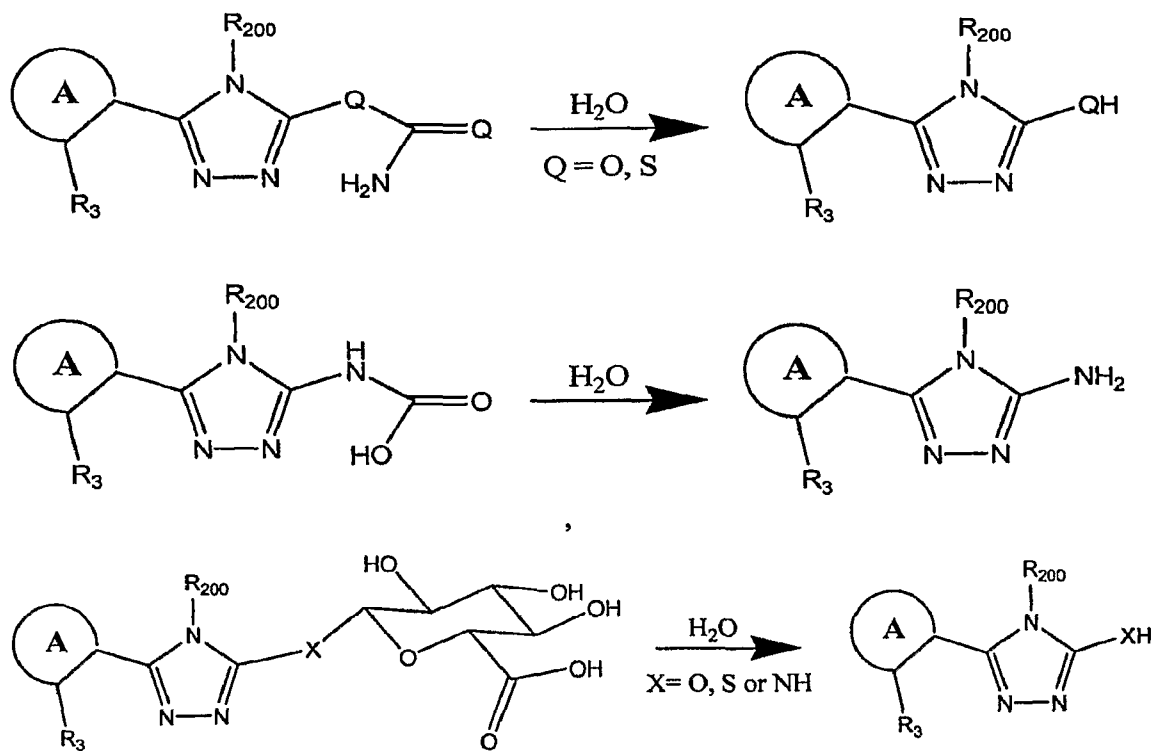
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- Without wishing to be bound by theory, it is believed that, in some cases, the "keto" form of the triazole ring may allow inhibitors as described herein to have additional
- 5 interaction (e.g., may form hydrogen-bonds) with amino acid residues within the binding site of Hsp90, which may contribute to the enhanced potency observed with triazole inhibitors when compared to other similar compounds. The presence of an electron-deficient moiety (e.g., C=O, C=S, C=NR₇) adjacent to the NH at the 1-position of the triazole ring may increase the acidity of the proton of the NH, which forms a hydrogen bond
- 10 with Gly97, and, thus, enhance its ability to act as a hydrogen donor. For example, when X₁₄ is oxygen, the electron-withdrawing ability of the carbonyl group may increase the acidity of the NH group at the 2-position to a greater extent than when X₁₄ is sulfur. In some cases, compounds having more than one resonance structure wherein the predominant resonance structure allows such hydrogen-bonding are preferred. Similarly, prodrugs, *i.e.*
- 15 compounds which can be metabolized or hydrolyzed *in vivo* to a compound of the present invention are encompassed by the present description. For example, the following embodiments of a compound of the present invention can be produced *in vivo* in the following reaction:



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where R_{200} is R_2 , R_5 or R_{18} .

One skilled in the art will understand that other hydrolyzable protecting groups can be employed with the compounds of the present invention to obtain prodrugs encompassed by the present description.

Without wishing to be bound by any theory, it is believed that the compounds of the invention preferentially bind to Hsp90 in the tautomeric form shown above, and thereby inhibit the activity of Hsp90.

C. Uses of Compounds of the Invention

The present invention is directed to therapies which involve administering one or more compounds of the invention, or compositions comprising said compounds to a subject, preferably a human subject, to inhibit the activity of Hsp90 or to prevent, treat, manage, or ameliorate a proliferative disorder, such as cancer, or one or more symptoms thereof. In one embodiment, the present invention is directed to treating cancers in which aberrant expression and/or activation of c-kit has been implicated as contributing to neoplastic pathology by administering one or more compounds of the invention.

In one aspect, the invention provides a method of inhibiting the activity of Hsp90 in a cell, comprising administering to the cell an effective amount of a compound of the present

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invention, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below. In one embodiment, the compound is administered to a cell in a subject, preferably a mammal, and more preferably a human.

5 In another aspect, the invention provides a method of treating or preventing a proliferation disorder in a mammal, comprising administering to the mammal an effective amount of a compound of the present invention, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below.

10 In one embodiment, the compound is administered to a human to treat or prevent a proliferative disorder. In another embodiment, the proliferation disorder is cancer. In another embodiment, the compound is administered with one or more additional therapeutic agents. In a preferred embodiment, the additional therapeutic agent is an anticancer agent.

15 In another aspect, the invention provides a method for treating cancer in a mammal, comprising administering to the mammal an effective amount of a compound of the present invention, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below.

20 In one embodiment, the compound is administered to a human to treat or prevent cancer. In another embodiment, the compound is administered with one or more additional therapeutic agents. In a preferred embodiment, the one or more additional therapeutic agents are anticancer agents.

25 In another aspect, the invention provides a method for treating a c-kit associated cancer in a mammal, comprising administering to the mammal an effective amount of a compound of the present invention, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) as defined below.

30 In one embodiment, the compound is administered to a human to treat or prevent the c-kit associated cancer. In another embodiment, the compound is administered with one or more additional therapeutic agents. In a preferred embodiment, the one or more additional therapeutic agents are anticancer agents.

1. c-Kit Associated Cancers

35 SCF binding to the c-kit protects hematopoietic stem and progenitor cells from apoptosis (Lee, *et al.*, 1997, *J. Immunol.*, 159:3211-3219), thereby contributing to colony formation and hematopoiesis. Expression of c-kit is frequently observed in acute

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myelocytic leukemia (AML) and sometimes observed in acute lymphocytic leukemia (ALL) (for reviews, see Sperling, *et al.*, 1997, *Haemat.*, 82:617-621; Escribano, *et al.*, 1998, *Leuk. Lymph.*, 30:459-466). Although c-kit is expressed in the majority of AML cells, its expression does not appear to be prognostic of disease progression (Sperling, *et al.*, 1997, *Haemat.*, 82:617-621). However, SCF protected AML cells from apoptosis induced by
5 chemotherapeutic agents (Hassan, *et al.*, 1996, *Acta. Hem.*, 95:257-262). Therefore, degradation of c-kit caused by the inhibition of Hsp90 by the compounds of the invention will enhance the efficacy of these agents and may induce apoptosis of AML cells.

The clonal growth of cells from patients with myelodysplastic syndrome (Sawada, *et al.*, 1996, *Blood*, 88:319-327) or chronic myelogenous leukemia (CML) (Sawai, *et al.*, 1996, *Exp. Hem.*, 2:116-122) was found to be significantly enhanced by SCF in combination with other cytokines. CML is characterized by expansion of Philadelphia chromosome positive cells of the marrow (Verfaillie, *et al.*, 1998, *Leuk.*, 12:136-138), which appears to primarily result from inhibition of apoptotic death (Jones, 1997, *Curr. Opin. Onc.*, 9:3-7).
15 The product of the Philadelphia chromosome, p210.sup.BCR-ABL, has been reported to mediate inhibition of apoptosis (Bedi, *et al.*, 1995, *Blood*, 86:1148-1158). Since p210.sup.BCR-ABL and the c-kit RTK both inhibit apoptosis and p62.sup.dok has been suggested as a substrate (Carpino, *et al.*, 1997, *Cell*, 88:197-204), it is possible that clonal expansion mediated by these kinases occurs through a common signaling pathway.
20 However, c-kit has also been reported to interact directly with p210.sup.BCR-ABL (Hallek, *et al.*, 1996, *Brit. J Haem.*, 94:5-16), which suggests that c-kit may have a more causative role in CML pathology. Therefore, degradation of c-kit caused by the inhibition of Hsp90 by the compounds of the invention will prove useful in the treatment of CML.

Normal colorectal mucosa does not express c-kit (Bellone, *et al.*, 1997, *J. Cell Physiol.*, 172:1-11). However, c-kit is frequently expressed in colorectal carcinoma (Bellone, *et al.*, 1997, *J. Cell Physiol.*, 172: 1-11), and autocrine loops of SCF and c-kit have been observed in several colon carcinoma cell lines (Toyota, *et al.*, 1993, *Turn. Biol.*, 14:295-302; Lahm, *et al.*, 1995, *Cell Growth & Differ.*, 6:1111-1118; Bellone, *et al.*, 1997, *J. Cell Physiol.*, 172:1-11). Furthermore, disruption of the autocrine loop by the use of
30 neutralizing antibodies (Lahm, *et al.*, 1995, *Cell Growth & Differ.*, 6:1111-1118) and downregulation of c-kit and/or SCF significantly inhibits cell proliferation (Lahm, *et al.*, 1995, *Cell Growth & Differ.*, 6:1111-1118; Bellone, *et al.*, 1997, *J. Cell Physiol.*, 172:1-11).

SCF/c-kit autocrine loops have been observed in gastric carcinoma cell lines
35 (Turner, *et al.*, 1992, *Blood*, 80:374-381; Hassan, *et al.*, 1998, *Digest. Dis. Science*, 43:8-

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14), and constitutive c-kit activation also appears to be important for gastrointestinal stromal tumors (GISTs). GISTs are the most common mesenchymal tumor of the digestive system. More than 90% of GISTs express c-kit, which is consistent with the putative origin of these tumor cells from interstitial cells of Cajal (ICCs) (Hirota, *et al.*, 1998, *Science*, 279:577-580). The c-kit expressed in GISTs from several different patients was observed to have mutations in the intracellular juxtamembrane domain leading to constitutive activation (Hirota, *et al.*, 1998, *Science* 279:577-580). Therefore, degradation of c-kit caused by the inhibition of Hsp90 by the compounds of the invention will be an efficacious means for the treatment of these cancers.

10 Male germ cell tumors have been histologically categorized into seminomas, which retain germ cell characteristics, and nonseminomas which can display characteristics of embryonal differentiation. Both seminomas and nonseminomas are thought to initiate from a preinvasive stage designated carcinoma in situ (CIS) (Murty, *et al.*, 1998, *Sem. Oncol.*, 25:133-144). Both c-kit and SCF have been reported to be essential for normal gonadal development during embryogenesis (Loveland, *et al.*, 1997, *J. Endocrinol.*, 153:337-344). Loss of either the receptor or the ligand resulted in animals devoid of germ cells. In postnatal testes, c-kit has been found to be expressed in Leydig cells and spermatogonia, while SCF was expressed in Sertoli cells (Loveland, *et al.*, 1997, *J. Endocrinol.*, 153:337-344). Testicular tumors develop from Leydig cells with high frequency in transgenic mice expressing human papilloma virus 16 (HPV16) E6 and E7 oncogenes (Kondoh, *et al.*, 1991, *J. Virol.*, 65:3335-3339; Kondoh, *et al.*, 1994, *J. Urol.*, 152:2151-2154). These tumors express both c-kit and SCF, and an autocrine loop may contribute to the tumorigenesis (Kondoh, *et al.*, 1995, *Oncogene*, 10:341-347) associated with cellular loss of functional p53 and the retinoblastoma gene product by association with E6 and E7 (Dyson, *et al.*, 1989, *Science*, 243:934-937; Werness, *et al.*, 1990, *Science*, 248:76-79; Scheffner, *et al.*, 1990, *Cell*, 63:1129-1136). Defective signaling mutants of SCF (Kondoh, *et al.*, 1995, *Oncogene*, 10:341-347) or c-kit (Li, *et al.*, 1996, *Canc. Res.*, 56:4343-4346) inhibited formation of testicular tumors in mice expressing HPV16 E6 and E7. Since c-kit kinase activation is pivotal to tumorigenesis in these animals, the compounds of the invention which inhibit Hsp90 and thereby cause the degradation of c-kit will be useful for preventing or treating testicular tumors associated with human papilloma virus.

Expression of c-kit on germ cell tumors shows that the receptor is expressed by the majority of carcinomas in situ and seminomas, but c-kit is expressed in only a minority of nonseminomas (Strohmeyer, *et al.*, 1991, *Canc. Res.*, 51:1811-1816; Rajpert-de Meyts, *et al.*, 1994, *Int. J. Androl.*, 17:85-92; Izquierdo, *et al.*, 1995, *J. Pathol.*, 177:253-258;

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Strohmeyer, *et al.*, 1995, *J. Urol.*, 153:511-515; Bokenmeyer, *et al.*, 1996, *J. Cance. Res., Clin. Oncol.*, 122:301-306; Sandlow, *et al.*, 1996, *J. Androl.*, 17:403-408). Therefore, degradation of c-kit caused by the inhibition of Hsp90 by the compounds of the invention will be an efficacious means for the treatment of these cancers.

- 5 SCF and c-kit are expressed throughout the central nervous system of developing rodents, and the pattern of expression suggests a role in growth, migration and differentiation of neuroectodermal cells. Expression of SCF and c-kit have also been reported in the adult brain (Hamel, *et al.*, 1997, *J. Neuro-Onc.*, 35:327-333). Expression of c-kit has also been observed in normal human brain tissue (Tada, *et al.* 1994, *J. Neuro.*, 10 80:1063-1073). Glioblastoma and astrocytoma, which define the majority of intracranial tumors, arise from neoplastic transformation of astrocytes (Levin, *et al.*, 1997, *Principles & Practice of Oncology*, 2022-2082). Expression of c-kit has been observed in glioblastoma cell lines and tissues (Berdel, *et al.*, 1992, *Canc. Res.*, 52:3498-3502; Tada, *et al.*, 1994, *J. Neuro.*, 80:1063-1073; Stanulla, *et al.*, 1995, *Act. Neuropath.*, 89:158-165).
- 15 The association of c-kit with astrocytoma pathology is less clear. Reports of expression of c-kit in normal astrocytes have been made (Natali, *et al.*, 1992, *Int. J. Canc.*, 52:197-201), (Tada, *et al.* 1994, *J. Neuro.*, 80:1063-1073), while others report it is not expressed (Kristt, *et al.*, 1993, *Neuro.*, 33:106-115). In the former case, high levels of c-kit expression in high grade tumors were observed (Kristt, *et al.*, 1993, *Neuro.*, 33:106-115), 20 whereas in the latter case researchers were unable to detect any expression in astrocytomas. In addition, contradictory reports of c-kit and SCF expression in neuroblastomas also exist. One study found that neuroblastoma cell lines often express SCF, but rarely express c-kit. In primary tumors, c-kit was detected in about 8% of neuroblastomas, while SCF was found in 18% of tumors (Beck, *et al.*, 1995, *Blood*, 86:3132-3138). In contrast, other studies 25 (Cohen, *et al.*, 1994, *Blood*, 84:3465-3472) have reported that all 14 neuroblastoma cell lines examined contained c-kit/SCF autocrine loops, and expression of both the receptor and ligand were observed in 45% of tumor samples examined. In two cell lines, anti-c-kit antibodies inhibited cell proliferation, suggesting that the SCF/c-kit autocrine loop contributed to growth (Cohen, *et al.*, 1994, *Blood*, 84:3465-3472). Therefore, degradation of 30 c-kit caused by the inhibition of Hsp90 by the compounds of the invention will be an efficacious means for treating some cancers of the central nervous system.

2. Combination Therapies and Treatment of Refractory Cancers

- 35 The invention also provides methods of preventing, treating, managing, or ameliorating a proliferative disorder, such as cancer, or one or more symptoms thereof, said

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methods comprising administering to a subject in need thereof one or more compounds of the invention and one or more other therapies (*e.g.*, one or more prophylactic or therapeutic agents that are currently being used, have been used, are known to be useful or in development for use in the prevention, treatment or amelioration of a proliferative disorder, such as cancer, or one or more symptoms associated with said proliferative disorder).

5 The prophylactic or therapeutic agents of the combination therapies of the invention can be administered sequentially or concurrently. In a specific embodiment, the combination therapies of the invention comprise one or more compounds and at least one other therapy (*e.g.*, another prophylactic or therapeutic agent) which has the same mechanism of action as said compounds. In another specific embodiment, the combination therapies of the invention comprise one or more compounds of the invention and at least one other therapy (*e.g.*, another prophylactic or therapeutic agent) which has a different mechanism of action than said compounds. In certain embodiments, the combination therapies of the present invention improve the prophylactic or therapeutic effect of one or more compounds of the invention by functioning together with the compounds to have an additive or synergistic effect. In certain embodiments, the combination therapies of the present invention reduce the side effects associated with the therapies (*e.g.*, prophylactic or therapeutic agents). In certain embodiments, the combination therapies of the present invention reduce the effective dosage of one or more of the therapies.

20 The prophylactic or therapeutic agents of the combination therapies can be administered to a subject, preferably a human subject, in the same pharmaceutical composition. In alternative embodiments, the prophylactic or therapeutic agents of the combination therapies can be administered concurrently to a subject in separate pharmaceutical compositions. The prophylactic or therapeutic agents may be administered to a subject by the same or different routes of administration.

25 In a specific embodiment, a pharmaceutical composition comprising one or more compounds of the invention is administered to a subject, preferably a human, to prevent, treat, manage, or ameliorate a proliferative disorder, such as cancer, or one or more symptom thereof. In accordance with the invention, pharmaceutical compositions of the invention may also comprise one or more other agents (*e.g.*, prophylactic or therapeutic agents which are currently being used, have been used, or are known to be useful in the prevention, treatment or amelioration of a proliferative disorder or a symptom thereof).

30 The invention provides methods for preventing, managing, treating or ameliorating a proliferative disorder, such as cancer, or one or more symptoms thereof in a subject refractory (either completely or partially) to existing agent therapies for such a proliferative

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disorder, said methods comprising administering to said subject a dose of an effective amount of one or more compounds of the invention and a dose of an effective amount of one or more therapies (e.g., one or more prophylactic or therapeutic agents useful for the prevention, treatment, management, or amelioration of a proliferative disorder or a symptom thereof). The invention also provides methods for preventing, treating, managing, or ameliorating a proliferative disorder or a symptom thereof by administering one or more compounds of the invention in combination with any other therapy(ies) to patients who have proven refractory to other therapies but are no longer on these therapies.

The compounds of the invention and/or other therapies can be administered to a subject by any route known to one of skill in the art. Examples of routes of administration include, but are not limited to, parenteral, e.g., intravenous, intradermal, subcutaneous, oral (e.g., inhalation), intranasal, transdermal (topical), transmucosal, and rectal administration.

3. Agents Useful In Combination With the Compounds of the Invention

Without wishing to be bound by theory, it is believed that the compounds of the invention can be particularly effective at treating subjects whose cancer has become multi-drug resistant. Although chemotherapeutic agents initially cause tumor regression, most agents that are currently used to treat cancer target only one pathway to tumor progression. Therefore, in many instances, after treatment with one or more chemotherapeutic agents, a tumor develops multidrug resistance and no longer response positively to treatment. One of the advantages of inhibiting Hsp90 activity is that several of its client proteins, which are mostly protein kinases or transcription factors involved in signal transduction, have been shown to be involved in the progression of cancer. Thus, inhibition of Hsp90 provides a method of short circuiting several pathways for tumor progression simultaneously. Therefore, it is believed that treatment of cancer with an Hsp90 inhibitor of the invention either alone, or in combination with other chemotherapeutic agents, is more likely to result in regression or elimination of the tumor, and less likely to result in the development of more aggressive multidrug resistant tumors than other currently available therapies.

Anticancer agents that can be co-administered with the compounds of the invention include TaxolTM, also referred to as "paclitaxel", is a well-known anti-cancer drug which acts by enhancing and stabilizing microtubule formation, and analogs of TaxolTM, such as TaxotereTM. Compounds that have the basic taxane skeleton as a common structure feature, have also been shown to have the ability to arrest cells in the G2-M phases due to stabilization or inhibition of microtubules.

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Other anti-cancer agents that can be employed in combination with the compounds of the invention include Avastin, Adriamycin, Dactinomycin, Bleomycin, Vinblastine, Cisplatin, acivicin; aclarubicin; acodazole hydrochloride; acronine; adozelesin; aldesleukin; altretamine; ambomycin; ametantrone acetate; aminoglutethimide; amsacrine; anastrozole; 5 anthramycin; asparaginase; asperlin; azacitidine; azetepa; azotomycin; batimastat; benzodepa; bicalutamide; bisantrene hydrochloride; bisnafide dimesylate; bizelesin; bleomycin sulfate; brequinar sodium; bropirimine; busulfan; cactinomycin; calusterone; caracemide; carbetimer; carboplatin; carmustine; carubicin hydrochloride; carzelesin; cedefingol; chlorambucil; cirolemycin; cladribine; crisnatol mesylate; cyclophosphamide; 10 cytarabine; dacarbazine; daunorubicin hydrochloride; decitabine; dexormaplatin; dezaguanine; dezaguanine mesylate; diaziquone; doxorubicin; doxorubicin hydrochloride; droloxifene; droloxifene citrate; dromostanolone propionate; duazomycin; edatrexate; eflornithine hydrochloride; elsamitrucin; enloplatin; enpromate; epipropidine; epirubicin hydrochloride; erbulozole; esorubicin hydrochloride; estramustine; estramustine phosphate 15 sodium; etanidazole; etoposide; etoposide phosphate; etoprine; fadrozole hydrochloride; fazarabine; fenretinide; floxuridine; fludarabine phosphate; fluorouracil; flurocitabine; fosquidone; fostriecin sodium; gemcitabine; gemcitabine hydrochloride; hydroxyurea; idarubicin hydrochloride; ifosfamide; ilmofosine; interleukin II (including recombinant interleukin II, or rIL2), interferon alfa-2a; interferon alfa-2b; interferon alfa-n1 ; interferon 20 alfa-n3; interferon beta-I a; interferon gamma-I b; iproplatin; irinotecan hydrochloride; lanreotide acetate; letrozole; leuprolide acetate; liarozole hydrochloride; lometrexol sodium; lomustine; losoxantrone hydrochloride; masoprocol; maytansine; mechlorethamine hydrochloride; megestrol acetate; melengestrol acetate; melphalan; menogaril; mercaptopurine; methotrexate; methotrexate sodium; metoprine; meturedopa; mitindomide; 25 mitocarcin; mitocromin; mitogillin; mitomalcin; mitomycin; mitosper; mitotane; mitoxantrone hydrochloride; mycophenolic acid; nocodazole; nogalamycin; ormaplatin; oxisuran; pegaspargase; peliomycin; pentamustine; peplomycin sulfate; perfosfamide; pipobroman; piposulfan; piroxantrone hydrochloride; plicamycin; plomestane; porfimer sodium; porfiromycin; prednimustine; procarbazine hydrochloride; puromycin; puromycin 30 hydrochloride; pyrazofurin; riboprine; rogletimide; safigol; safigol hydrochloride; semustine; simtrazene; sparfosate sodium; sparsomycin; spirogermanium hydrochloride; spiromustine; spiroplatin; streptonigrin; streptozocin; sulofenur; talisomycin; tecogalan sodium; tegafur; teloxantrone hydrochloride; temoporfin; teniposide; teroxirone; testolactone; thiamiprine; thioguanine; thiotepa; tiazofurin; tirapazamine; toremifene citrate; 35 trestolone acetate; tricitabine phosphate; trimetrexate; trimetrexate glucuronate; triptorelin;

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tubulozole hydrochloride; uracil mustard; uredepa; vapreotide; verteporfin; vinblastine sulfate; vincristine sulfate; vindesine; vindesine sulfate; vinepidine sulfate; vinglycinat sulfate; vinleurosine sulfate; vinorelbine tartrate; vinrosidine sulfate; vinzolidine sulfate; vorozole; zeniplatin; zinostatin; zorubicin hydrochloride.

- 5 Other anti-cancer drugs that can be employed in combination with the compounds of the invention include: 20-epi-1,25 dihydroxyvitamin D3; 5-ethynyluracil; abiraterone; aclarubicin; acylfulvene; adecypenol; adozelesin; aldesleukin; ALL-TK antagonists; altretamine; ambamustine; amidox; amifostine; aminolevulinic acid; amrubicin; amsacrine; anagrelide; anastrozole; andrographolide; angiogenesis inhibitors; antagonist D; antagonist
- 10 G; antarelix; anti-dorsalizing morphogenetic protein-1; antiandrogen, prostatic carcinoma; antiestrogen; antineoplaston; antisense oligonucleotides; aphidicolin glycinate; apoptosis gene modulators; apoptosis regulators; apurinic acid; ara-CDP-DL-PTBA; arginine deaminase; asulacrine; atamestane; atrimustine; axinastatin 1; axinastatin 2; axinastatin 3; azasetron; azatoxin; azatyrosine; baccatin III derivatives; balanol; batimastat; BCR/ABL
- 15 antagonists; benzochlorins; benzoylstauosporine; beta lactam derivatives; beta-alethine; betaclamycin B; betulinic acid; bFGF inhibitor; bicalutamide; bisantrene; bisaziridinylspermine; bisnafide; bistratene A; bizelesin; breflate; broprimine; budotitane; buthionine sulfoximine; calcipotriol; calphostin C; camptothecin derivatives; canarypox IL-
- 20 2; capecitabine; carboxamide-amino-triazole; carboxyamidotriazole; CaRest M3; CARN 700; cartilage derived inhibitor; carzelesin; casein kinase inhibitors (ICOS); castanospermine; cecropin B; cetorelix; chlorIns; chloroquinoxaline sulfonamide; cicaprost; cis-porphyrin; cladribine; clomifene analogues; clotrimazole; collismycin A; collismycin B; combretastatin A4; combretastatin analogue; conagenin; crambescidin 816; crisnatol; cryptophycin 8; cryptophycin A derivatives; curacin A; cyclopentantraquinones;
- 25 cycloplatam; cypemycin; cytarabine ocfosfate; cytolytic factor; cytostatin; dacliximab; decitabine; dehydrodidemnin B; deslorelin; dexamethasone; dexifosfamide; dexrazoxane; dexverapamil; diaziquone; didemnin B; didox; diethylnorspermine; dihydro-5-azacytidine; 9- dioxamycin; diphenyl spiromustine; docosanol; dolasetron; doxifluridine; droloxifene; dronabinol; duocarmycin SA; ebselen; ecomustine; edelfosine; edrecolomab; eflornithine;
- 30 elemene; emitefur; epirubicin; epristeride; estramustine analogue; estrogen agonists; estrogen antagonists; etanidazole; etoposide phosphate; exemestane; fadrozole; fazarabine; fenretinide; filgrastim; finasteride; flavopiridol; flezelastine; fluasterone; fludarabine; fluorodaunorunicin hydrochloride; forfenimex; formestane; fostriecin; fotemustine; gadolinium texaphyrin; gallium nitrate; galocitabine; ganirelix; gelatinase inhibitors;
- 35 gemcitabine; glutathione inhibitors; hepsulfam; heregulin; hexamethylene bisacetamide;

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- hypericin; ibandronic acid; idarubicin; idoxifene; idramantone; ilmofofosine; ilomastat; imidazoacridones; imiquimod; immunostimulant peptides; insulin-like growth factor-1 receptor inhibitor; interferon agonists; interferons; interleukins; iobenguane; iododoxorubicin; ipomeanol, 4-; iroplact; irsogladine; isobengazole; isohomohalicondrin B;
- 5 itasetron; jasplakinolide; kahalalide F; lamellarin-N triacetate; lanreotide; leinamycin; lenograstim; lentinan sulfate; leptolstatin; letrozole; leukemia inhibiting factor; leukocyte alpha interferon; leuprolide+estrogen+progesterone; leuprorelin; levamisole; liarazole; linear polyamine analogue; lipophilic disaccharide peptide; lipophilic platinum compounds; lissoclinamide 7; lobaplatin; lombricine; lometrexol; lonidamine; losoxantrone; lovastatin;
- 10 loxoribine; lurtotecan; lutetium texaphyrin; lysofylline; lytic peptides; maitansine; mannostatin A; marimastat; masoproc; maspin; matrilysin inhibitors; matrix metalloproteinase inhibitors; menogaril; merbarone; meterelin; methioninase; metoclopramide; MIF inhibitor; mifepristone; miltefosine; mirimostim; mismatched double stranded RNA; mitoguazone; mitolactol; mitomycin analogues; mitonafide; mitotoxin
- 15 fibroblast growth factor-saporin; mitoxantrone; mofarotene; molgramostim; monoclonal antibody, human chorionic gonadotrophin; monophosphoryl lipid A+myobacterium cell wall sk; mopidamol; multiple drug resistance gene inhibitor; multiple tumor suppressor 1-based therapy; mustard anticancer agent; mycaperoxide B; mycobacterial cell wall extract; myriaporone; N-acetyldinaline; N-substituted benzamides; nafarelin; nagrestip;
- 20 naloxone+pentazocine; napavin; naphterpin; nartograstim; nedaplatin; nemorubicin; neridronic acid; neutral endopeptidase; nilutamide; nisamycin; nitric oxide modulators; nitroxide antioxidant; nitrullyn; O6-benzylguanine; octreotide; okicenone; oligonucleotides; onapristone; ondansetron; ondansetron; oracin; oral cytokine inducer; ormaplatin; osaterone; oxaliplatin; oxaunomycin; palauamine; palmitoylrhizoxin; pamidronic acid; panaxytriol;
- 25 panomifene; parabactin; pazelliptine; pegaspargase; peldesine; pentosan polysulfate sodium; pentostatin; pentrozole; perflubron; perfosfamide; perillyl alcohol; phenazinomycin; phenylacetate; phosphatase inhibitors; picibanil; pilocarpine hydrochloride; pirarubicin; piritrexim; placetin A; placetin B; plasminogen activator inhibitor; platinum complex; platinum compounds; platinum-triamine complex; porfimer sodium; porfiromycin;
- 30 prednisone; propyl bis-acridone; prostaglandin J2; proteasome inhibitors; protein A-based immune modulator; protein kinase C inhibitor; protein kinase C inhibitors, microalgal; protein tyrosine phosphatase inhibitors; purine nucleoside phosphorylase inhibitors; purpurins; pyrazoloacridine; pyridoxylated hemoglobin polyoxyethylene conjugate; raf antagonists; raltitrexed; ramosetron; ras farnesyl protein transferase inhibitors; ras
- 35 inhibitors; ras-GAP inhibitor; retelliptine demethylated; rhenium Re 186 etidronate;

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rhizoxin; ribozymes; RII retinamide; rogletimide; rohitukine; romurtide; roquinimex; rubiginone B1; ruboxyl; safingol; saintopin; SarCNU; sarcophytol A; sargramostim; Sdi 1 mimetics; semustine; senescence derived inhibitor 1; sense oligonucleotides; signal transduction inhibitors; signal transduction modulators; single chain antigen-binding protein; sizofiran; sobuzoxane; sodium borocaptate; sodium phenylacetate; solverol; 5 somatomedin binding protein; sonermin; sparfosic acid; spicamycin D; spiromustine; splenopentin; spongistatin 1; squalamine; stem cell inhibitor; stem-cell division inhibitors; stipiamide; stromelysin inhibitors; sulfinosine; superactive vasoactive intestinal peptide antagonist; suradista; suramin; swainsonine; synthetic glycosaminoglycans; tallimustine; 10 tamoxifen methiodide; tauromustine; tazarotene; tecogalan sodium; tegafur; tellurapyrylium; telomerase inhibitors; temoporfin; temozolomide; teniposide; tetrachlorodecaoxide; tetrazomine; thaliblastine; thiocoraline; thrombopoietin; thrombopoietin mimetic; thymalfasin; thymopoietin receptor agonist; thymotrinan; thyroid stimulating hormone; tin ethyl etiopurpurin; tirapazamine; titanocene bichloride; topsentin; 15 toremifene; totipotent stem cell factor; translation inhibitors; tretinoin; triacetyluridine; triciribine; trimetrexate; triptorelin; tropisetron; turosteride; tyrosine kinase inhibitors; tyrphostins; UBC inhibitors; ubenimex; urogenital sinus-derived growth inhibitory factor; urokinase receptor antagonists; vapreotide; variolin B; vector system, erythrocyte gene therapy; velaresol; veramine; verdins; verteporfin; vinorelbine; vinxaltine; vitaxin; vorozole; 20 zanoterone; zeniplatin; zilascorb; and zinostatin stimalamer. Preferred anti-cancer drugs are 5-fluorouracil and leucovorin.

Other chemotherapeutic agents that can be employed in combination with the compounds of the invention include but are not limited to alkylating agents, antimetabolites, natural products, or hormones. Examples of alkylating agents useful for the treatment or 25 prevention of T-cell malignancies in the methods and compositions of the invention include but are not limited to, nitrogen mustards (*e.g.*, mechloroethamine, cyclophosphamide, chlorambucil, *etc.*), alkyl sulfonates (*e.g.*, busulfan), nitrosoureas (*e.g.*, carmustine, lomustine, *etc.*), or triazenes (decabazine, *etc.*). Examples of antimetabolites useful for the treatment or prevention of T-cell malignancies in the methods and compositions of the 30 invention include but are not limited to folic acid analog (*e.g.*, methotrexate), or pyrimidine analogs (*e.g.*, Cytarabine), purine analogs (*e.g.*, mercaptopurine, thioguanine, pentostatin). Examples of natural products useful for the treatment or prevention of T-cell malignancies in the methods and compositions of the invention include but are not limited to vinca alkaloids (*e.g.*, vinblastin, vincristine), epipodophyllotoxins (*e.g.*, etoposide), antibiotics

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(*e.g.*, daunorubicin, doxorubicin, bleomycin), enzymes (*e.g.*, L-asparaginase), or biological response modifiers (*e.g.*, interferon alpha).

Examples of alkylating agents that can be employed in combination with the compounds of the invention include but are not limited to, nitrogen mustards (*e.g.*,
5 mechloroethamine, cyclophosphamide, chlorambucil, melphalan, *etc.*), ethylenimine and methylmelamines (*e.g.*, hexamethylmelamine, thiotepa), alkyl sulfonates (*e.g.*, busulfan), nitrosoureas (*e.g.*, carmustine, lomustine, semustine, streptozocin, *etc.*), or triazenes (decarbazine, *etc.*). Examples of antimetabolites useful for the treatment or prevention of cancer in the methods and compositions of the invention include but are not limited to folic
10 acid analog (*e.g.*, methotrexate), or pyrimidine analogs (*e.g.*, fluorouracil, floxouridine, Cytarabine), purine analogs (*e.g.*, mercaptopurine, thioguanine, pentostatin). Examples of natural products useful for the treatment or prevention of cancer in the methods and compositions of the invention include but are not limited to vinca alkaloids (*e.g.*, vinblastin, vincristine), epipodophyllotoxins (*e.g.*, etoposide, teniposide), antibiotics (*e.g.*, actinomycin
15 D, daunorubicin, doxorubicin, bleomycin, plicamycin, mitomycin), enzymes (*e.g.*, L-asparaginase), or biological response modifiers (*e.g.*, interferon alpha). Examples of hormones and antagonists useful for the treatment or prevention of cancer in the methods and compositions of the invention include but are not limited to adrenocorticosteroids (*e.g.*, prednisone), progestins (*e.g.*, hydroxyprogesterone caproate, megestrol acetate,
20 medroxyprogesterone acetate), estrogens (*e.g.*, diethylstilbestrol, ethinyl estradiol), antiestrogen (*e.g.*, tamoxifen), androgens (*e.g.*, testosterone propionate, fluoxymesterone), antiandrogen (*e.g.*, flutamide), gonadotropin releasing hormone analog (*e.g.*, leuprolide). Other agents that can be used in the methods and compositions of the invention for the treatment or prevention of cancer include platinum coordination complexes (*e.g.*, cisplatin,
25 carboblatin), anthracenedione (*e.g.*, mitoxantrone), substituted urea (*e.g.*, hydroxyurea), methyl hydrazine derivative (*e.g.*, procarbazine), adrenocortical suppressant (*e.g.*, mitotane, aminoglutethimide).

Examples of anti-cancer agents which act by arresting cells in the G2-M phases due to stabilization or inhibition of microtubules and which can be used in combination with the
30 compounds of the invention include without limitation the following marketed drugs and drugs in development: Erbulozole (also known as R-55104), Dolastatin 10 (also known as DLS-10 and NSC-376128), Mivobulin isethionate (also known as CI-980), Vincristine, NSC-639829, Discodermolide (also known as NVP-XX-A-296), ABT-751 (Abbott, also known as E-7010), Altorhyrtins (such as Altorhyrtin A and Altorhyrtin C), Spongistatins
35 (such as Spongistatin 1, Spongistatin 2, Spongistatin 3, Spongistatin 4, Spongistatin 5,

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Spongistatin 6, Spongistatin 7, Spongistatin 8, and Spongistatin 9), Cemadotin hydrochloride (also known as LU-103793 and NSC-D-669356), Epothilones (such as Epothilone A, Epothilone B, Epothilone C (also known as desoxyepothilone A or dEpoA), Epothilone D (also referred to as KOS-862, dEpoB, and desoxyepothilone B), Epothilone E, Epothilone F, Epothilone B N-oxide, Epothilone A N-oxide, 16-aza-epothilone B, 21-aminoepothilone B (also known as BMS-310705), 21-hydroxyepothilone D (also known as Desoxyepothilone F and dEpoF), 26-fluoroepothilone), Auristatin PE (also known as NSC-654663), Soblidotin (also known as TZT-1027), LS-4559-P (Pharmacia, also known as LS-4577), LS-4578 (Pharmacia, also known as LS-477-P), LS-4477 (Pharmacia), LS-4559 (Pharmacia), RPR-112378 (Aventis), Vincristine sulfate, DZ-3358 (Daiichi), FR-182877 (Fujisawa, also known as WS-9885B), GS-164 (Takeda), GS-198 (Takeda), KAR-2 (Hungarian Academy of Sciences), BSF-223651 (BASF, also known as ILX-651 and LU-223651), SAH-49960 (Lilly/Novartis), SDZ-268970 (Lilly/Novartis), AM-97 (Armad/Kyowa Hakko), AM-132 (Armad), AM-138 (Armad/Kyowa Hakko), IDN-5005 (Indena), Cryptophycin 52 (also known as LY-355703), AC-7739 (Ajinomoto, also known as AVE-8063A and CS-39.HCl), AC-7700 (Ajinomoto, also known as AVE-8062, AVE-8062A, CS-39-L-Ser.HCl, and RPR-258062A), Vitilevuamide, Tubulysin A, Canadensol, Centaureidin (also known as NSC-106969), T-138067 (Tularik, also known as T-67, TL-138067 and TI-138067), COBRA-1 (Parker Hughes Institute, also known as DDE-261 and WHI-261), H10 (Kansas State University), H16 (Kansas State University), Oncocidin A1 (also known as BTO-956 and DIME), DDE-313 (Parker Hughes Institute), Fijianolide B, Laulimalide, SPA-2 (Parker Hughes Institute), SPA-1 (Parker Hughes Institute, also known as SPIKET-P), 3-IAABU (Cytoskeleton/Mt. Sinai School of Medicine, also known as MF-569), Narcosine (also known as NSC-5366), Nascapine, D-24851 (Asta Medica), A-105972 (Abbott), Hemiasterlin, 3-BAABU (Cytoskeleton/Mt. Sinai School of Medicine, also known as MF-191), TMPN (Arizona State University), Vanadocene acetylacetonate, T-138026 (Tularik), Monsatrol, Inanocine (also known as NSC-698666), 3-IAABE (Cytoskeleton/Mt. Sinai School of Medicine), A-204197 (Abbott), T-607 (Tularik, also known as T-900607), RPR-115781 (Aventis), Eleutherobins (such as Desmethyleleutherobin, Desaetyeleutherobin, Isoeleutherobin A, and Z-Eleutherobin), Caribaeoside, Caribaeolin, Halichondrin B, D-64131 (Asta Medica), D-68144 (Asta Medica), Diazonamide A, A-293620 (Abbott), NPI-2350 (Nereus), Taccalonolide A, TUB-245 (Aventis), A-259754 (Abbott), Diozostatin, (-)-Phenylahistin (also known as NSCL-96F037), D-68838 (Asta Medica), D-68836 (Asta Medica), Myoseverin B, D-43411 (Zentaris, also known as D-81862), A-289099 (Abbott), A-318315 (Abbott), HTI-286 (also known as SPA-110,

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trifluoroacetate salt) (Wyeth), D-82317 (Zentaris), D-82318 (Zentaris), SC-12983 (NCI), Resverastatin phosphate sodium, BPR-0Y-007 (National Health Research Institutes), and SSR-250411 (Sanofi).

5 D. Compositions and Methods for Administering Therapies

The present invention provides compositions for the treatment, prophylaxis, and amelioration of proliferative disorders, such as cancer. In a specific embodiment, a composition comprises one or more compounds of the invention, or a pharmaceutically acceptable salt, solvate, clathrate, hydrate or prodrug thereof. In another embodiment, a
10 composition of the invention comprises one or more prophylactic or therapeutic agents other than a compound of the invention, or a pharmaceutically acceptable salt, solvate, clathrate, hydrate, prodrug thereof. In another embodiment, a composition of the invention comprises one or more compounds of the invention, or a pharmaceutically acceptable salt, solvate, clathrate, hydrate or prodrug thereof, and one or more other prophylactic or therapeutic
15 agents. In another embodiment, the composition comprises a compound of the invention, or a pharmaceutically acceptable salt, solvate, clathrate, hydrate, or prodrug thereof, and a pharmaceutically acceptable carrier, diluent or excipient.

In a preferred embodiment, a composition of the invention is a pharmaceutical composition or a single unit dosage form. Pharmaceutical compositions and dosage forms
20 of the invention comprise one or more active ingredients in relative amounts and formulated in such a way that a given pharmaceutical composition or dosage form can be used to treat or prevent proliferative disorders, such as cancer.

A pharmaceutical composition of the invention is formulated to be compatible with its intended route of administration. Examples of routes of administration include, but are
25 not limited to, parenteral, *e.g.*, intravenous, intradermal, subcutaneous, oral (*e.g.*, inhalation), intranasal, transdermal (topical), transmucosal, and rectal administration. In a specific embodiment, the composition is formulated in accordance with routine procedures as a pharmaceutical composition adapted for intravenous, subcutaneous, intramuscular, oral, intranasal or topical administration to human beings. In a preferred embodiment, a
30 pharmaceutical composition is formulated in accordance with routine procedures for subcutaneous administration to human beings.

Single unit dosage forms of the invention are suitable for oral, mucosal (*e.g.*, nasal, sublingual, vaginal, buccal, or rectal), parenteral (*e.g.*, subcutaneous, intravenous, bolus injection, intramuscular, or intraarterial), or transdermal administration to a patient.
35 Examples of dosage forms include, but are not limited to: tablets; caplets; capsules, such as

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soft elastic gelatin capsules; cachets; troches; lozenges; dispersions; suppositories; ointments; cataplasms (poultices); pastes; powders; dressings; creams; plasters; solutions; patches; aerosols (*e.g.*, nasal sprays or inhalers); gels; liquid dosage forms suitable for oral or mucosal administration to a patient, including suspensions (*e.g.*, aqueous or non-aqueous liquid suspensions, oil-in-water emulsions, or a water-in-oil liquid emulsions), solutions, and elixirs; liquid dosage forms suitable for parenteral administration to a patient; and sterile solids (*e.g.*, crystalline or amorphous solids) that can be reconstituted to provide liquid dosage forms suitable for parenteral administration to a patient.

The composition, shape, and type of dosage forms of the invention will typically vary depending on their use. For example, a dosage form suitable for mucosal administration may contain a smaller amount of active ingredient(s) than an oral dosage form used to treat the same indication. This aspect of the invention will be readily apparent to those skilled in the art. *See, e.g.*, Remington's Pharmaceutical Sciences (1990) 18th ed., Mack Publishing, Easton PA.

Typical pharmaceutical compositions and dosage forms comprise one or more excipients. Suitable excipients are well known to those skilled in the art of pharmacy, and non-limiting examples of suitable excipients are provided herein. Whether a particular excipient is suitable for incorporation into a pharmaceutical composition or dosage form depends on a variety of factors well known in the art including, but not limited to, the way in which the dosage form will be administered to a patient. For example, oral dosage forms such as tablets may contain excipients not suited for use in parenteral dosage forms.

The suitability of a particular excipient may also depend on the specific active ingredients in the dosage form. For example, the decomposition of some active ingredients can be accelerated by some excipients such as lactose, or when exposed to water. Active ingredients that comprise primary or secondary amines (*e.g.*, N-desmethylvenlafaxine and N,N-didesmethylvenlafaxine) are particularly susceptible to such accelerated decomposition. Consequently, this invention encompasses pharmaceutical compositions and dosage forms that contain little, if any, lactose. As used herein, the term "lactose-free" means that the amount of lactose present, if any, is insufficient to substantially increase the degradation rate of an active ingredient. Lactose-free compositions of the invention can comprise excipients that are well known in the art and are listed, for example, in the U.S. Pharmacopia (USP) SP (XXI)/NF (XVI). In general, lactose-free compositions comprise active ingredients, a binder/filler, and a lubricant in pharmaceutically compatible and pharmaceutically acceptable amounts. Preferred lactose-free dosage forms comprise active ingredients, microcrystalline cellulose, pre-gelatinized starch, and magnesium stearate.

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This invention further encompasses anhydrous pharmaceutical compositions and dosage forms comprising active ingredients, since water can facilitate the degradation of some compounds. For example, the addition of water (*e.g.*, 5%) is widely accepted in the pharmaceutical arts as a means of simulating long-term storage in order to determine characteristics such as shelf-life or the stability of formulations over time. *See, e.g.*, Jens T. Carstensen (1995) *Drug Stability: Principles & Practice*, 2d. Ed., Marcel Dekker, NY, NY, 379-80. In effect, water and heat accelerate the decomposition of some compounds. Thus, the effect of water on a formulation can be of great significance since moisture and/or humidity are commonly encountered during manufacture, handling, packaging, storage, shipment, and use of formulations.

Anhydrous pharmaceutical compositions and dosage forms of the invention can be prepared using anhydrous or low moisture containing ingredients and low moisture or low humidity conditions. Pharmaceutical compositions and dosage forms that comprise lactose and at least one active ingredient that comprises a primary or secondary amine are preferably anhydrous if substantial contact with moisture and/or humidity during manufacturing, packaging, and/or storage is expected.

An anhydrous pharmaceutical composition should be prepared and stored such that its anhydrous nature is maintained. Accordingly, anhydrous compositions are preferably packaged using materials known to prevent exposure to water such that they can be included in suitable formulary kits. Examples of suitable packaging include, but are not limited to, hermetically sealed foils, plastics, unit dose containers (*e.g.*, vials), blister packs, and strip packs.

The invention further encompasses pharmaceutical compositions and dosage forms that comprise one or more compounds that reduce the rate by which an active ingredient will decompose. Such compounds, which are referred to herein as "stabilizer" include, but are not limited to, antioxidants such as ascorbic acid, pH buffers, or salt buffers.

1) Oral Dosage Forms

Pharmaceutical compositions of the invention that are suitable for oral administration can be presented as discrete dosage forms, such as, but are not limited to, tablets (*e.g.*, chewable tablets), caplets, capsules, and liquids (*e.g.*, flavored syrups). Such dosage forms contain predetermined amounts of active ingredients, and may be prepared by methods of pharmacy well known to those skilled in the art. *See generally*, Remington's *Pharmaceutical Sciences* (1990) 18th ed., Mack Publishing, Easton PA.

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Typical oral dosage forms of the invention are prepared by combining the active ingredient(s) in an admixture with at least one excipient according to conventional pharmaceutical compounding techniques. Excipients can take a wide variety of forms depending on the form of preparation desired for administration. For example, excipients
5 suitable for use in oral liquid or aerosol dosage forms include, but are not limited to, water, glycols, oils, alcohols, flavoring agents, preservatives, and coloring agents. Examples of excipients suitable for use in solid oral dosage forms (*e.g.*, powders, tablets, capsules, and caplets) include, but are not limited to, starches, sugars, micro-crystalline cellulose, diluents, granulating agents, lubricants, binders, and disintegrating agents.

10 Because of their ease of administration, tablets and capsules represent the most advantageous oral dosage unit forms, in which case solid excipients are employed. If desired, tablets can be coated by standard aqueous or nonaqueous techniques. Such dosage forms can be prepared by any of the methods of pharmacy. In general, pharmaceutical compositions and dosage forms are prepared by uniformly and intimately admixing the
15 active ingredients with liquid carriers, finely divided solid carriers, or both, and then shaping the product into the desired presentation if necessary.

For example, a tablet can be prepared by compression or molding. Compressed tablets can be prepared by compressing in a suitable machine the active ingredients in a free-flowing form such as powder or granules, optionally mixed with an excipient. Molded
20 tablets can be made by molding in a suitable machine a mixture of the powdered compound moistened with an inert liquid diluent.

Examples of excipients that can be used in oral dosage forms of the invention include, but are not limited to, binders, fillers, disintegrants, and lubricants. Binders suitable for use in pharmaceutical compositions and dosage forms include, but are not limited to,
25 corn starch, potato starch, or other starches, gelatin, natural and synthetic gums such as acacia, sodium alginate, alginic acid, other alginates, powdered tragacanth, guar gum, cellulose and its derivatives (*e.g.*, ethyl cellulose, cellulose acetate, carboxymethyl cellulose calcium, sodium carboxymethyl cellulose), polyvinyl pyrrolidone, methyl cellulose, pre-gelatinized starch, hydroxypropyl methyl cellulose, (*e.g.*, Nos. 2208, 2906, 2910),
30 microcrystalline cellulose, and mixtures thereof.

Suitable forms of microcrystalline cellulose include, but are not limited to, the materials sold as AVICEL-PH-101, AVICEL-PH-103 AVICEL RC-581, AVICEL-PH-105 (available from FMC Corporation, American Viscose Division, Avicel Sales, Marcus Hook, PA), and mixtures thereof. One specific binder is a mixture of microcrystalline cellulose

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and sodium carboxymethyl cellulose sold as AVICEL RC-581. Suitable anhydrous or low moisture excipients or additives include AVICEL-PH-103J and Starch 1500 LM.

Examples of fillers suitable for use in the pharmaceutical compositions and dosage forms disclosed herein include, but are not limited to, talc, calcium carbonate (*e.g.*, granules or powder), microcrystalline cellulose, powdered cellulose, dextrates, kaolin, mannitol, silicic acid, sorbitol, starch, pre-gelatinized starch, and mixtures thereof. The binder or filler in pharmaceutical compositions of the invention is typically present in from about 50 to about 99 weight percent of the pharmaceutical composition or dosage form.

Disintegrants are used in the compositions of the invention to provide tablets that disintegrate when exposed to an aqueous environment. Tablets that contain too much disintegrant may disintegrate in storage, while those that contain too little may not disintegrate at a desired rate or under the desired conditions. Thus, a sufficient amount of disintegrant that is neither too much nor too little to detrimentally alter the release of the active ingredients should be used to form solid oral dosage forms of the invention. The amount of disintegrant used varies based upon the type of formulation, and is readily discernible to those of ordinary skill in the art. Typical pharmaceutical compositions comprise from about 0.5 to about 15 weight percent of disintegrant, preferably from about 1 to about 5 weight percent of disintegrant.

Disintegrants that can be used in pharmaceutical compositions and dosage forms of the invention include, but are not limited to, agar-agar, alginic acid, calcium carbonate, microcrystalline cellulose, croscarmellose sodium, crospovidone, polacrillin potassium, sodium starch glycolate, potato or tapioca starch, other starches, pre-gelatinized starch, other starches, clays, other alginates, other celluloses, gums, and mixtures thereof.

Lubricants that can be used in pharmaceutical compositions and dosage forms of the invention include, but are not limited to, calcium stearate, magnesium stearate, mineral oil, light mineral oil, glycerin, sorbitol, mannitol, polyethylene glycol, other glycols, stearic acid, sodium lauryl sulfate, talc, hydrogenated vegetable oil (*e.g.*, peanut oil, cottonseed oil, sunflower oil, sesame oil, olive oil, corn oil, and soybean oil), zinc stearate, ethyl oleate, ethyl laureate, agar, and mixtures thereof. Additional lubricants include, for example, a syloid silica gel (AEROSIL 200, manufactured by W.R. Grace Co. of Baltimore, MD), a coagulated aerosol of synthetic silica (marketed by Degussa Co. of Plano, TX), CAB-O-SIL (a pyrogenic silicon dioxide product sold by Cabot Co. of Boston, MA), and mixtures thereof. If used at all, lubricants are typically used in an amount of less than about 1 weight percent of the pharmaceutical compositions or dosage forms into which they are incorporated.

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2) Controlled Release Dosage Forms

Active ingredients of the invention can be administered by controlled release means or by delivery devices that are well known to those of ordinary skill in the art. Examples include, but are not limited to, those described in U.S. Patent Nos.: 3,845,770; 3,916,899; 5 3,536,809; 3,598,123; and 4,008,719, 5,674,533, 5,059,595, 5,591,767, 5,120,548, 5,073,543, 5,639,476, 5,354,556, and 5,733,566, each of which is incorporated herein by reference. Such dosage forms can be used to provide slow or controlled-release of one or more active ingredients using, for example, hydropropylmethyl cellulose, other polymer matrices, gels, permeable membranes, osmotic systems, multilayer coatings, microparticles, 10 liposomes, microspheres, or a combination thereof to provide the desired release profile in varying proportions. Suitable controlled-release formulations known to those of ordinary skill in the art, including those described herein, can be readily selected for use with the active ingredients of the invention. The invention thus encompasses single unit dosage forms suitable for oral administration such as, but not limited to, tablets, capsules, gelcaps, 15 and caplets that are adapted for controlled-release.

All controlled-release pharmaceutical products have a common goal of improving drug therapy over that achieved by their non-controlled counterparts. Ideally, the use of an optimally designed controlled-release preparation in medical treatment is characterized by a minimum of drug substance being employed to cure or control the condition in a minimum 20 amount of time. Advantages of controlled-release formulations include extended activity of the drug, reduced dosage frequency, and increased patient compliance.

Most controlled-release formulations are designed to initially release an amount of drug (active ingredient) that promptly produces the desired therapeutic effect, and gradually and continually release of other amounts of drug to maintain this level of therapeutic or 25 prophylactic effect over an extended period of time. In order to maintain this constant level of drug in the body, the drug must be released from the dosage form at a rate that will replace the amount of drug being metabolized and excreted from the body. Controlled-release of an active ingredient can be stimulated by various conditions including, but not limited to, pH, temperature, enzymes, water, or other physiological conditions or 30 compounds.

A particular extended release formulation of this invention comprises a therapeutically or prophylactically effective amount of a compound of the present invention, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX) or a pharmaceutically acceptable salt, solvate, hydrate, clathrate, or

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prodrug thereof, in spheroids which further comprise microcrystalline cellulose and, optionally, hydroxypropylmethyl-cellulose coated with a mixture of ethyl cellulose and hydroxypropylmethylcellulose. Such extended release formulations can be prepared according to U.S. Patent No. 6,274,171, the entirety of which is incorporated herein by reference.

A specific controlled-release formulation of this invention comprises from about 6% to about 40% a compound of the present invention, provided that the compound is not represented by structural formulas (I) - (XXXIX) or encompassed within formulas (I) - (XXXIX), or a pharmaceutically acceptable salt, solvate, hydrate, clathrate, or prodrug thereof, by weight, about 50% to about 94% microcrystalline cellulose, NF, by weight, and optionally from about 0.25% to about 1% by weight of hydroxypropyl-methylcellulose, USP, wherein the spheroids are coated with a film coating composition comprised of ethyl cellulose and hydroxypropylmethylcellulose.

3) Parenteral Dosage Forms

Parenteral dosage forms can be administered to patients by various routes including, but not limited to, subcutaneous, intravenous (including bolus injection), intramuscular, and intraarterial. Because their administration typically bypasses patients' natural defenses against contaminants, parenteral dosage forms are preferably sterile or capable of being sterilized prior to administration to a patient. Examples of parenteral dosage forms include, but are not limited to, solutions ready for injection, dry products ready to be dissolved or suspended in a pharmaceutically acceptable vehicle for injection, suspensions ready for injection, and emulsions.

Suitable vehicles that can be used to provide parenteral dosage forms of the invention are well known to those skilled in the art. Examples include, but are not limited to: Water for Injection USP; aqueous vehicles such as, but not limited to, Sodium Chloride Injection, Ringer's Injection, Dextrose Injection, Dextrose and Sodium Chloride Injection, and Lactated Ringer's Injection; water-miscible vehicles such as, but not limited to, ethyl alcohol, polyethylene glycol, and polypropylene glycol; and non-aqueous vehicles such as, but not limited to, corn oil, cottonseed oil, peanut oil, sesame oil, ethyl oleate, isopropyl myristate, and benzyl benzoate.

Compounds that increase the solubility of one or more of the active ingredients disclosed herein can also be incorporated into the parenteral dosage forms of the invention.

4) Transdermal, Topical, and Mucosal Dosage Forms

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Transdermal, topical, and mucosal dosage forms of the invention include, but are not limited to, ophthalmic solutions, sprays, aerosols, creams, lotions, ointments, gels, solutions, emulsions, suspensions, or other forms known to one of skill in the art. *See, e.g.,* Remington's Pharmaceutical Sciences (1980 & 1990) 16th and 18th eds., Mack Publishing, Easton PA and Introduction to Pharmaceutical Dosage Forms (1985) 4th ed., Lea & Febiger, Philadelphia. Dosage forms suitable for treating mucosal tissues within the oral cavity can be formulated as mouthwashes or as oral gels. Further, transdermal dosage forms include "reservoir type" or "matrix type" patches, which can be applied to the skin and worn for a specific period of time to permit the penetration of a desired amount of active ingredients.

Suitable excipients (*e.g.*, carriers and diluents) and other materials that can be used to provide transdermal, topical, and mucosal dosage forms encompassed by this invention are well known to those skilled in the pharmaceutical arts, and depend on the particular tissue to which a given pharmaceutical composition or dosage form will be applied. With that fact in mind, typical excipients include, but are not limited to, water, acetone, ethanol, ethylene glycol, propylene glycol, butane-1,3-diol, isopropyl myristate, isopropyl palmitate, mineral oil, and mixtures thereof to form lotions, tinctures, creams, emulsions, gels or ointments, which are non-toxic and pharmaceutically acceptable. Moisturizers or humectants can also be added to pharmaceutical compositions and dosage forms if desired. Examples of such additional ingredients are well known in the art. *See, e.g.,* Remington's Pharmaceutical Sciences (1980 & 1990) 16th and 18th eds., Mack Publishing, Easton PA.

Depending on the specific tissue to be treated, additional components may be used prior to, in conjunction with, or subsequent to treatment with active ingredients of the invention. For example, penetration enhancers can be used to assist in delivering the active ingredients to the tissue. Suitable penetration enhancers include, but are not limited to: acetone; various alcohols such as ethanol, oleyl, and tetrahydrofuryl; alkyl sulfoxides such as dimethyl sulfoxide; dimethyl acetamide; dimethyl formamide; polyethylene glycol; pyrrolidones such as polyvinylpyrrolidone; Kollidon grades (Povidone, Polyvidone); urea; and various water-soluble or insoluble sugar esters such as Tween 80 (polysorbate 80) and Span 60 (sorbitan monostearate).

The pH of a pharmaceutical composition or dosage form, or of the tissue to which the pharmaceutical composition or dosage form is applied, may also be adjusted to improve delivery of one or more active ingredients. Similarly, the polarity of a solvent carrier, its ionic strength, or tonicity can be adjusted to improve delivery. Compounds such as stearates can also be added to pharmaceutical compositions or dosage forms to advantageously alter the hydrophilicity or lipophilicity of one or more active ingredients so as to improve

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treating physician will know how and when to interrupt, adjust, or terminate therapy in conjunction with individual patient response.

Different therapeutically effective amounts may be applicable for different proliferative disorders, as will be readily known by those of ordinary skill in the art.

5 Similarly, amounts sufficient to prevent, manage, treat or ameliorate such proliferative disorders, but insufficient to cause, or sufficient to reduce, adverse effects associated with the compounds of the invention are also encompassed by the above described dosage amounts and dose frequency schedules. Further, when a patient is administered multiple dosages of a compound of the invention, not all of the dosages need be the same. For
10 example, the dosage administered to the patient may be increased to improve the prophylactic or therapeutic effect of the compound or it may be decreased to reduce one or more side effects that a particular patient is experiencing.

In a specific embodiment, the dosage of the composition of the invention or a compound of the invention administered to prevent, treat, manage, or ameliorate a
15 proliferative disorders, such as cancer, or one or more symptoms thereof in a patient is 150 µg/kg, preferably 250 µg/kg, 500 µg/kg, 1 mg/kg, 5 mg/kg, 10 mg/kg, 25 mg/kg, 50 mg/kg, 75 mg/kg, 100 mg/kg, 125 mg/kg, 150 mg/kg, or 200 mg/kg or more of a patient's body weight. In another embodiment, the dosage of the composition of the invention or a compound of the invention administered to prevent, treat, manage, or ameliorate a
20 proliferative disorders, such as cancer, or one or more symptoms thereof in a patient is a unit dose of 0.1 mg to 20 mg, 0.1 mg to 15 mg, 0.1 mg to 12 mg, 0.1 mg to 10 mg, 0.1 mg to 8 mg, 0.1 mg to 7 mg, 0.1 mg to 5 mg, 0.1 to 2.5 mg, 0.25 mg to 20 mg, 0.25 to 15 mg, 0.25 to 12 mg, 0.25 to 10 mg, 0.25 to 8 mg, 0.25 mg to 7m g, 0.25 mg to 5 mg, 0.5 mg to 2.5 mg, 1 mg to 20 mg, 1 mg to 15 mg, 1 mg to 12 mg, 1 mg to 10 mg, 1 mg to 8 mg, 1 mg to 7 mg,
25 1 mg to 5 mg, or 1 mg to 2.5 mg.

The dosages of prophylactic or therapeutic agents other than compounds of the invention, which have been or are currently being used to prevent, treat, manage, or proliferative disorders, such as cancer, or one or more symptoms thereof can be used in the combination therapies of the invention. Preferably, dosages lower than those which have
30 been or are currently being used to prevent, treat, manage, or ameliorate a proliferative disorders, or one or more symptoms thereof, are used in the combination therapies of the invention. The recommended dosages of agents currently used for the prevention, treatment, management, or amelioration of a proliferative disorders, such as cancer, or one or more symptoms thereof, can obtained from any reference in the art including, but not
35 limited to, Hardman *et al.*, eds., 1996, Goodman & Gilman's The Pharmacological Basis Of

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Basis Of Therapeutics 9th Ed, Mc-Graw-Hill, New York; Physician's Desk Reference (PDR) 57th Ed., 2003, Medical Economics Co., Inc., Montvale, NJ, which are incorporated herein by reference in its entirety.

In certain embodiments, when the compounds of the invention are administered in
5 combination with another therapy, the therapies (*e.g.*, prophylactic or therapeutic agents) are administered less than 5 minutes apart, less than 30 minutes apart, 1 hour apart, at about 1 hour apart, at about 1 to about 2 hours apart, at about 2 hours to about 3 hours apart, at about 3 hours to about 4 hours apart, at about 4 hours to about 5 hours apart, at about 5 hours to about 6 hours apart, at about 6 hours to about 7 hours apart, at about 7 hours to about 8
10 hours apart, at about 8 hours to about 9 hours apart, at about 9 hours to about 10 hours apart, at about 10 hours to about 11 hours apart, at about 11 hours to about 12 hours apart, at about 12 hours to 18 hours apart, 18 hours to 24 hours apart, 24 hours to 36 hours apart, 36 hours to 48 hours apart, 48 hours to 52 hours apart, 52 hours to 60 hours apart, 60 hours to 72 hours apart, 72 hours to 84 hours apart, 84 hours to 96 hours apart, or 96 hours to 120 hours
15 part. In one embodiment, two or more therapies (*e.g.*, prophylactic or therapeutic agents) are administered within the same patent visit.

In certain embodiments, one or more compounds of the invention and one or more other the therapies (*e.g.*, prophylactic or therapeutic agents) are cyclically administered. Cycling therapy involves the administration of a first therapy (*e.g.*, a first prophylactic or
20 therapeutic agents) for a period of time, followed by the administration of a second therapy (*e.g.*, a second prophylactic or therapeutic agents) for a period of time, followed by the administration of a third therapy (*e.g.*, a third prophylactic or therapeutic agents) for a period of time and so forth, and repeating this sequential administration, *i.e.*, the cycle in order to reduce the development of resistance to one of the agents, to avoid or reduce the
25 side effects of one of the agents, and/or to improve the efficacy of the treatment.

In certain embodiments, administration of the same compound of the invention may be repeated and the administrations may be separated by at least 1 day, 2 days, 3 days, 5 days, 10 days, 15 days, 30 days, 45 days, 2 months, 75 days, 3 months, or 6 months. In other embodiments, administration of the same prophylactic or therapeutic agent may be
30 repeated and the administration may be separated by at least at least 1 day, 2 days, 3 days, 5 days, 10 days, 15 days, 30 days, 45 days, 2 months, 75 days, 3 months, or 6 months.

In a specific embodiment, the invention provides a method of preventing, treating, managing, or ameliorating a proliferative disorders, such as cancer, or one or more symptoms thereof, said methods comprising administering to a subject in need thereof a
35 dose of at least 150 µg/kg, preferably at least 250 µg/kg, at least 500 µg/kg, at least 1 mg/kg,

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at least 5 mg/kg, at least 10 mg/kg, at least 25 mg/kg, at least 50 mg/kg, at least 75 mg/kg, at least 100 mg/kg, at least 125 mg/kg, at least 150 mg/kg, or at least 200 mg/kg or more of one or more compounds of the invention once every day, preferably, once every 2 days, once every 3 days, once every 4 days, once every 5 days, once every 6 days, once every 7 days, once every 8 days, once every 10 days, once every two weeks, once every three weeks, or once a month.

F. Other Embodiments

The compounds of the invention may be used as research tools (for example, to evaluate the mechanism of action of new drug agents, to isolate new drug discovery targets using affinity chromatography, as antigens in an ELISA or ELISA-like assay, or as standards in *in vitro* or *in vivo* assays). These and other uses and embodiments of the compounds and compositions of this invention will be apparent to those of ordinary skill in the art.

The invention is further defined by reference to the following examples describing in detail the preparation of compounds of the invention. It will be apparent to those skilled in the art that many modifications, both to materials and methods, may be practiced without departing from the purpose and interest of this invention. The following examples are set forth to assist in understanding the invention and should not be construed as specifically limiting the invention described and claimed herein. Such variations of the invention, including the substitution of all equivalents now known or later developed, which would be within the purview of those skilled in the art, and changes in formulation or minor changes in experimental design, are to be considered to fall within the scope of the invention incorporated herein.

EXAMPLES

Reagents and solvents used below can be obtained from commercial sources such as Aldrich Chemical Co. (Milwaukee, Wisconsin, USA). ¹H-NMR and ¹³C-NMR spectra were recorded on a Varian 300MHz NMR spectrometer. Significant peaks are tabulated in the order: δ (ppm): chemical shift, multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br s, broad singlet), coupling constant(s) in Hertz (Hz) and number of protons.

Example 1: Inhibition of Hsp90

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Hsp90 protein was obtained from Stressgen (Cat#SPP-770). Assay buffer: 100 mM Tris-HCl, pH 7.4, 20 mM KCl, 6 mM MgCl₂. Malachite green (0.0812% w/v) (M9636) and polyvinyl alcohol USP (2.32% w/v) (P1097) were obtained from Sigma. A Malachite Green Assay (see Methods Mol Med, 2003, 85:149 for method details) was used for examination of ATPase activity of Hsp90 protein. Briefly, Hsp90 protein in assay buffer (100 mM Tris-HCl, pH 7.4, 20 mM KCl, 6 mM MgCl₂) was mixed with ATP alone (negative control) or in the presence of Geldanamycin (a positive control) or Compound 108 in a 96-well plate. Malachite green reagent was added to the reaction. The mixtures were incubated at 37°C for 4 hours and sodium citrate buffer (34% w/v sodium citrate) was added to the reaction. The plate was read by an ELISA reader with an absorbance at 620 nm.

As can be seen in Figure 1, 40 µM of geldanamycin, a natural product known to inhibit Hsp90 activity, the ATPase activity of Hsp90 was only slightly higher than background. 40 µM Compound 108 showed an even greater inhibition of ATPase activity of Hsp90 than geldanamycin, and even at 4 µM Compound 108 showed significant inhibition of ATPase activity of Hsp90 protein.

Example 2: Degradation of Hsp90 Client Proteins via Inhibition of Hsp90 Activity

A. Cells and Cell Culture

Human high-Her2 breast carcinoma BT474 (HTB-20), SK-BR-3 (HTB-30) and MCF-7 breast carcinoma (HTB-22) from American Type Culture Collection, VA, USA were grown in Dulbecco's modified Eagle's medium with 4 mM L-glutamine and antibiotics (100 IU/ml penicillin and 100 µg/ml streptomycin; Gibco BRL). To obtain exponential cell growth, cells were trypsinized, counted and seeded at a cell density of 0.5×10^6 cells/ml regularly, every 3 days. All experiments were performed on day 1 after cell passage.

B. Degradation of Her2 in Cells after Treatment with a Compound of the Invention

BT-474 cells were treated with 0.5 µM, 2 µM, or 5 µM of 17AAG (a positive control) or 0.5 µM, 2 µM, or 5 µM of Compound 108 or Compound 49 overnight in DMEM medium. After treatment, each cytoplasmic sample was prepared from 1×10^6 cells by incubation of cell lysis buffer (#9803, Cell Signaling Technology) on ice for 10 minutes. The resulting supernatant used as the cytosol fractions were dissolved with sample buffer for SDS-PAGE and run on a SDS-PAGE gel, blotted onto a nitrocellulose membrane by using semi-dry transfer. Non-specific binding to nitrocellulose was blocked with 5% skim milk in TBS with 0.5% Tween at room temperature for 1 hour, then probed with anti-Her2/ErB2

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mAb (rabbit IgG, #2242, Cell Signaling) and anti-Tubulin (T9026, Sigma) as housekeeping control protein. HRP-conjugated goat anti-rabbit IgG (H+L) and HRP-conjugated horse anti-mouse IgG (H+L) were used as secondary Ab (#7074, #7076, Cell Signaling) and LumiGLO reagent, 20x Peroxide (#7003, Cell Signaling) was used for visualization.

- 5 As can be seen from Figure 2, Her2, an Hsp90 client protein, is almost completely degraded when cells are treated with 5 μ M of Compound 108 and partially degraded when cells are treated with 2 μ M and 0.5 μ M of Compound 108. Compound 49 which is even more active than Compound 108 causes complete degradation of Her2 when cells are treated with 2 μ M and 5 μ M and causes partial degraded when cells are treated with 0.5 μ M
- 10 17AAG is a known Hsp90 inhibitor and is used as a positive control.

C. Fluorescent Staining of Her2 on the Surface of Cells Treated with a Compound of the Invention

- After treatment with a compound of the invention, cells were washed twice with
- 15 1xPBS/1%FBS, and then stained with anti-Her2-FITC (#340553, BD) for 30 min at 4°C. Cells were then washed three times in FACS buffer before the fixation in 0.5 ml 1% paraformaldehyde. Data was acquired on a FACSCalibur system. Isotype-matched controls were used to establish the non-specific staining of samples and to set the fluorescent markers. A total 10,000 events were recorded from each sample. Data were
- 20 analysed by using CellQuest software (BD Biosciences). The IC₅₀ range for Hsp90 inhibition by compounds of the invention are listed below in Table 2.

Table 2: IC₅₀ range of compounds of the invention for inhibition of Hsp90

() IC ₅₀ Range	() Compound Number
() < 3 μ M	() 8, 13, 39, 49, 63, 76, 77, 79, 87, 88, 95, 96, 202, 203, 204, 205, 206, 207, 208, 209, 211, 212, 213, 214,
() 3 μ M to	() 2, 5, 6, 7, 9, 14, 27, 28, 34, 36, 38, 42, 48,
() 10 μ M to	() 21, 22, 30, 51, 59, 60, 61, 62, 94, 98, 99,

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D. Apoptosis analysis

After treatment with the compounds of the invention, cells were washed once with 1xPBS/1%FBS, and then stained in binding buffer with FITC-conjugated Annexin V and Propidium iodide (PI) (all obtained from BD Biosciences) for 30 min at 4°C. Flow
5 cytometric analysis was performed with FACSCalibur (BD Biosciences) and a total 10,000 events were recorded from each sample. Data were analyzed by using CellQuest software (BD Biosciences). The relative fluorescence was calculated after subtraction of the fluorescence of control.

10 E. Degradation of c-Kit in Cells after Treatment with a Compound of the Invention

Two leukemia cell lines, HEL92.1.7 and Kasumi-1, were used for testing c-kit degradation induced by Hsp90 inhibitors of the invention. The cells (3×10^5 per well) were treated with 17AAG ($0.5 \mu\text{M}$), Compound 188 or Compound 221 for about 18 h (see Figs.
15 3 and 4 for concentrations). The cells were collected and centrifuged (SORVALL RT 6000D) at 1200 rpm for 5 min. The supernatants were discarded, and the cells were washed one time with 1X PBS. After centrifugation the cells were stained with FITC conjugated c-kit antibody (MBL International, Cat# K0105-4) in 100 ml 1X PBS at 4°C for 1 h. The samples were read and analyzed with FACSCalibur flow cytometer (Becton Dickinson).
20 c-Kit, a tyrosine kinase receptor and one of the Hsp90 client proteins, was selected and used in a FACS-based degradation assay. The results of the assay showed that Compound 188 and Compound 221, induced c-kit degradation at 0.5 and 0.05 μM in a dose-dependent manner. Surprisingly, 17-AAG, which is a potent Hsp90 inhibitor and is in phase 2 clinical trials, could not induce c-kit degradation at 0.5 μM in two leukemia cell
25 lines, HEL92.1.7 (see Fig. 3) and Kasumi-1 (see Fig. 4). Since the compounds of the invention cause c-kit degradation more efficiently than other Hsp90 inhibitors, the compounds of the invention are expected to be more effective in the treatment of c-kit associated tumors, such as leukemias, mast cell tumors, small cell lung cancer, testicular cancer, some cancers of the gastrointestinal tract (including GIST), and some central
30 nervous system.

The results of the FACS analysis were confirmed with Western blot analysis (see Fig. 5). In Kasumi-1 cells (myelogenous leukemia), Compound 221 (100 nM and 400 nM) induced the degradation of c-Kit. In contrast, 17-AAG had no effect of c-Kit protein levels.

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F. Degradation of c-Met in Cells after Treatment with a Compound of the Invention

We examined the ability of the Hsp90 inhibitors of the invention to induce the degradation of c-Met, an Hsp90 client protein that is expressed at high levels in several types of non-small cell lung cancer. NCI-H1993 (ATCC, cat# CRL-5909) were seeded in 6-well plates at 5×10^5 cells/well. The cells were treated with 17AAG (100 nM or 400 nM) or Compound 221 (100 nM or 400 nM), and cell lysis was prepared 24 h after treatment. Equal amount of proteins were used for Western blot analysis. The compounds of the invention potently induced degradation of c-Met in this cell line due to inhibition of Hsp90 (see Fig. 6).

Example 3: Compound 49 Displays Anti-tumor Activity Against the Human Tumor Cell Line MDA-MB-435S in a *nude* Mouse Xenograft Model

The human tumor cell line, MDA-MB-435S (ATCC #HTB-129; G. Ellison, et al., *Mol. Pathol.* 55:294-299, 2002), was obtained from the American Type Culture Collection (Manassus, Virginia, USA). The cell line was cultured in growth media prepared from 50% Dulbecco's Modified Eagle Medium (high glucose), 50% RPMI Media 1640, 10% fetal bovine serum (FBS), 1% 100X L-glutamine, 1% 100X Penicillin-Streptomycin, 1% 100X sodium pyruvate and 1% 100X MEM non-essential amino acids. FBS was obtained from Sigma-Aldrich Corp. (St. Louis, Missouri, USA), and all other reagents were obtained from Invitrogen Corp. (Carlsbad, California, USA). Approximately $4-5 \times 10^6$ cells that had been cryopreserved in liquid nitrogen were rapidly thawed at 37°C and transferred to a 175 cm² tissue culture flask containing 50 ml of growth media and then incubated at 37°C in a 5% CO₂ incubator. The growth media was replaced every 2-3 days until the flask became 90% confluent, typically in 5-7 days. To passage and expand the cell line, a 90% confluent flask was washed with 10 ml of room temperature phosphate buffered saline (PBS) and the cells were disassociated by adding 5 ml 1X Trypsin-EDTA (Invitrogen) and incubating at 37°C until the cells detached from the surface of the flask. To inactivate the trypsin, 5 ml of growth media was added and then the contents of the flask were centrifuged to pellet the cells. The supernatant was aspirated and the cell pellet was resuspended in 10 ml of growth media and the cell number determined using a hemocytometer. Approximately $1-3 \times 10^6$ cells per flask were seeded into 175 cm² flasks containing 50 ml of growth media and incubated at 37°C in a 5% CO₂ incubator. When the flasks reached 90% confluence, the above passaging process was repeated until sufficient cells had been obtained for implantation into mice.

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Six to eight week old, female Crl:CD-1-*nu*BR (*nude*) mice were obtained from Charles River Laboratories (Wilmington, Massachusetts, USA). Animals were housed 4-5/cage in micro-isolators, with a 12hr/12hr light/dark cycle, acclimated for at least 1 week prior to use and fed normal laboratory chow *ad libitum*. Studies were conducted on
5 animals between 7 and 12 weeks of age at implantation. To implant tumor cells into *nude* mice, the cells were trypsinized as above, washed in PBS and resuspended at a concentration of 50×10^6 cells/ml in PBS. Using a 27 gauge needle and 1 cc syringe, 0.1 ml of the cell suspension was injected into the corpus adiposum of *nude* mice. The corpus
10 adiposum is a fat body located in the ventral abdominal viscera in the right quadrant of the abdomen at the juncture of the os coxae (pelvic bone) and the os femoris (femur). Tumors were then permitted to develop *in vivo* until they reached approximately 150 mm³ in volume, which typically required 2-3 weeks following implantation. Tumor volumes (V) were calculated by caliper measurement of the width (W), length (L) and thickness (T) of tumors using the following formula: $V = 0.5326 \times (L \times W \times T)$. Animals were randomized
15 into treatment groups so that the average tumor volumes of each group were similar at the start of dosing.

Stock solutions of test compounds were prepared by dissolving the appropriate amounts of each compound in dimethyl sulfoxide (DMSO) by sonication in an ultrasonic water bath. Stock solutions were prepared at the start of the study, stored at -20°C and
20 diluted fresh each day for dosing. A solution of 20% Cremophore RH40 (polyoxyl 40 hydrogenated castor oil; BASF Corp., Aktiengesellschaft, Ludwigshafen, Germany) in 80% D5W (5% dextrose in water; Abbott Laboratories, North Chicago, Illinois, USA) was also prepared by first heating 100% Cremophore RH40 at 50-60°C until liquefied and clear, diluting 1:5 with 100% D5W, reheating again until clear and then mixing well. This
25 solution was stored at room temperature for up to 3 months prior to use. To prepare formulations for daily dosing, DMSO stock solutions were diluted 1:10 with 20% Cremophore RH40. The final formulation for dosing contained 10% DMSO, 18% Cremophore RH40, 3.6% dextrose and 68.4% water and the appropriate amount of test article. Animals were intraperitoneal (IP) injected with this solution at 10 ml per kg body
30 weight on a schedule of 5 days per week (Monday thru Friday, with no dosing on Saturday and Sunday) for 3 weeks.

As shown in Figure 7, treatment with 300 mg/kg body weight of Compound 49 decreased the growth rate of MDA-MB-435S cells in *nude* mice to a greater extent than did a dose of 100 mg/kg body weight of the Hsp90 inhibitor 17-AAG. This effect was not

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associated with significant toxicity, as shown by the lack of an effect on body weights (Figure 8).

Example 4: Compound 188 Displays Anti-tumor Activity Against Human

5 Tumor Cells in a *nude* Mouse Xenograft Model

The human squamous non-small cell lung cancer cell line, RERF-LC-AI (RCB0444; S. Kyoizumi, et al., *Cancer. Res.* 45:3274-3281, 1985), was obtained from the Riken Cell Bank (Tsukuba, Ibaraki, Japan). The cell line was cultured in growth media prepared from 50% Dulbecco's Modified Eagle Medium (high glucose), 50% RPMI Media
10 1640, 10% fetal bovine serum (FBS), 1% 100X L-glutamine, 1% 100X penicillin-streptomycin, 1% 100X sodium pyruvate and 1% 100X MEM non-essential amino acids. FBS was obtained from American Type Culture Collection (Manassas, Virginia, USA) and all other reagents were obtained from Invitrogen Corp. (Carlsbad, California, USA). Approximately 4-5 x 10⁶ cells that had been cryopreserved in liquid nitrogen were
15 rapidly thawed at 37°C and transferred to a 175 cm² tissue culture flask containing 50 ml of growth media and then incubated at 37°C in a 5% CO₂ incubator.

The growth media was replaced every 2-3 days until the flask became 90% confluent, typically in 5-7 days. To passage and expand the cell line, a 90% confluent flask was washed with 10 ml of room temperature phosphate buffered saline (PBS) and the cells
20 were disassociated by adding 5 ml 1X trypsin-EDTA (Invitrogen) and incubating at 37°C until the cells detached from the surface of the flask. To inactivate the trypsin, 5 ml of growth media was added and then the contents of the flask were centrifuged to pellet the cells. The supernatant was aspirated and the cell pellet was resuspended in 10 ml of growth media and the cell number determined using a hemocytometer. Approximately 1-3 x 10⁶
25 cells per flask were seeded into 175 cm² flasks containing 50 ml of growth media and incubated at 37°C in a 5% CO₂ incubator. When the flasks reached 90% confluence, the above passaging process was repeated until sufficient cells had been obtained for implantation into mice.

Seven to eight week old, female Crl:CD-1-*nu*BR (*nude*) mice were obtained from
30 Charles River Laboratories (Wilmington, Massachusetts, USA). Animals were housed 4-5/cage in micro-isolators, with a 12hr/12hr light/dark cycle, acclimated for at least 1 week prior to use and fed normal laboratory chow *ad libitum*. Studies were conducted on animals between 8 and 12 weeks of age at implantation. To implant RERF-LC-AI tumor

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cells into nude mice, the cells were trypsinized as above, washed in PBS and resuspended at a concentration of 50×10^6 cells/ml in 50% non-supplemented RPMI Media 1640 and 50% Matrigel Basement Membrane Matrix (#354234; BD Biosciences; Bedford, Massachusetts, USA). Using a 27 gauge needle and 1 cc syringe, 0.1 ml of the cell suspension was injected subcutaneously into the flank of each *nude* mouse. Tumor volumes (V) were calculated by caliper measurement of the width (W), length (L) and thickness (T) of tumors using the following formula: $V = 0.5236 \times (L \times W \times T)$.

In vivo passaged RERF-LC-AI tumor cells (RERF-LC-AI^{IVP}) were isolated to improve the rate of tumor implantation relative to the parental cell line in *nude* mice.

10 RERF-LC-AI tumors were permitted to develop *in vivo* until they reached approximately 250 mm³ in volume, which required approximately 3 weeks following implantation. Mice were euthanized via CO₂ asphyxiation and their exteriors sterilized with 70% ethanol in a laminar flow hood. Using sterile technique, tumors were excised and diced in 50 ml PBS using a scalpel blade. A single cell suspension was prepared using a 55 ml Wheaton Safe-Grind tissue grinder (catalog #62400-358; VWR International, West Chester, Pennsylvania, USA) by plunging the pestle up and down 4-5 times without twisting. The suspension was strained through a 70 µm nylon cell strainer and then centrifuged to pellet the cells. The resulting pellet was resuspended in 0.1 M NH₄Cl to lyse contaminating red blood cells and then immediately centrifuged to pellet the cells. The cell pellet was

20 resuspended in growth media and seeded into 175 cm² flasks containing 50 ml of growth media at 1-3 tumors/flask or approximately 10×10^6 cells/flask. After overnight incubation at 37°C in a 5% CO₂ incubator, non-adherent cells were removed by rinsing two times with PBS and then the cultures were fed with fresh growth media. When the flasks reached 90% confluence, the above passaging process was repeated until sufficient cells

25 had been obtained for implantation into mice.

RERF-LC-AI^{IVP} cells were then implanted as above and tumors were permitted to develop *in vivo* until the majority reached an average of 100-200 mm³ in tumor volume, which typically required 2-3 weeks following implantation. Animals with oblong or very small or large tumors were discarded, and only animals carrying tumors that displayed

30 consistent growth rates were selected for studies. Animals were randomized into treatment groups so that the average tumor volumes of each group were similar at the start of dosing.

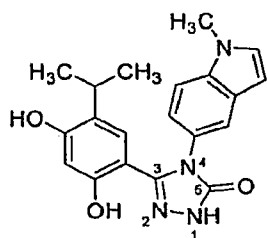
The HSP90 inhibitor, 17-allylamino-17-demethoxygeldanamycin (17-AAG), was employed as a positive control (Albany Molecular Research, Albany, New York, USA). Stock solutions of test articles were prepared by dissolving the appropriate amounts of each

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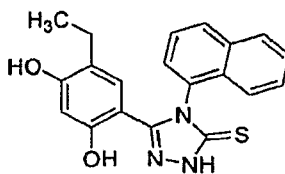
compound in dimethyl sulfoxide (DMSO) by sonication in an ultrasonic water bath. Stock solutions were prepared weekly, stored at -20°C and diluted fresh each day for dosing. A solution of 20% Cremophore RH40 (polyoxyl 40 hydrogenated castor oil; BASF Corp., Aktiengesellschaft, Ludwigshafen, Germany) in 80% D5W (5% dextrose in water; Abbott Laboratories, North Chicago, Illinois, USA) was also prepared by first heating 100% Cremophore RH40 at 50-60°C until liquefied and clear, diluting 1:5 with 100% D5W, reheating again until clear and then mixing well. This solution was stored at room temperature for up to 3 months prior to use. To prepare formulations for daily dosing, DMSO stock solutions were diluted 1:10 with 20% Cremophore RH40. The final formulation for dosing contained 10% DMSO, 18% Cremophore RH40, 3.6% dextrose, 68.4% water and the appropriate amount of test article. Animals were intraperitoneally (i.p.) injected with this solution at 10 ml per kg body weight on a schedule of 5 days per week (Monday, Tuesday, Wednesday, Thursday and Friday, with no dosing on Saturday and Sunday) for a total of 15 doses.

As shown in Figure 9, treatment with 200 mg/kg body weight of Compound 188 decreased the growth rate of RERF-LC-AI^{IVP} human lung tumor cells in *nude* mice, as did a dose of 75 mg/kg body weight of 17-AAG (an unrelated HSP90 inhibitor). This effect was not associated with overt toxicity, as shown by the minimal effect on body weights depicted in Figure 10.

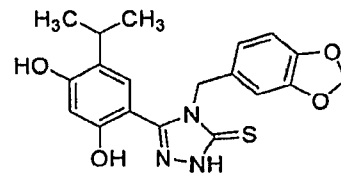
Example 5: Use of X-ray Crystal Structures of Co-crystals of Hsp90:Inhibitor Complexes to Identify Key Binding Interactions between Hsp90 and Hsp Inhibitors



Compound A



Compound B



Compound C

In an illustrative embodiment, co-crystals of Hsp90 were obtained with Compound A (corresponding to Compound 226 of Table 1), Compound B (corresponding to Compound 49 of Table 1), and Compound C (corresponding to Compound 247 of Table 1), as shown below. The X-ray diffraction data for co-crystals of Hsp90 with Compounds A, B, and C are shown in Table 3, Table 4, and Table 5, respectively.

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Compound A was found to have superior activity, relative to Compound B and Compound C, in the inhibition of Hsp90 activity.

From the X-ray diffraction data obtained, compounds A, B, and C were found to interact with several amino acid residues in the binding site of Hsp90, as illustrated in Figure 11a, Figure 11b, and Figure 11c, respectively. For example, the hydroxyl group at the 2'-position of the resorcinol moiety for Compounds A, B, and C was observed to interact (e.g., form a hydrogen bond) with the side-chain carboxylic group of Asp93, wherein the hydroxyl group can act as either a hydrogen-bond donor or acceptor. The hydrogen bond between Asp93 and Hsp90 inhibitors may be considered as an anchor for the binding of ligands to the N-terminal ADP/ATP binding site of Hsp90, including ATP. Another key interaction observed between Hsp90 and Compounds A, B, and C is a hydrogen bond formed between the NH at the 1-position of the triazole ring (e.g., in the "keto" tautomer) and the carbonyl of Gly97, wherein the NH of the triazole ring serves as a hydrogen bond donor and the carbonyl of Gly97 serves as a hydrogen bond acceptor.

Compound A was observed to possess a key interaction wherein a hydrogen bond is formed between the carbonyl group at the 5-position of the triazole ring (e.g., in the "keto" tautomer) and the NH₂ side chain Lys58. In this interaction, the side chain of Lys58 is pulled closer to the inhibitor to form the hydrogen-bond. Without wishing to be bound by theory, the existence of the additional hydrogen bond formed between the Compound A with the NH₂ side chain of Lys58 may be responsible for the superior ability of Compound A, and other inhibitors substituted with carbonyl group at the 5-position of the triazole core, to inhibit Hsp90 activity relative to, for example, similar 3,4-diaryl triazoles substituted with a thione group at the 5-position of the triazine core.

Other interactions may exist between Hsp90 and Compound A, B, and C. For example, a hydrogen bond is formed between the N at the 2-position of the triazole ring and Thr184. Also, water-bridged hydrogen bonds are formed between the hydroxyl group at the 4'-position of resorcinol moiety and the amino acid residues Asn51 and Ser52. Furthermore, the binding site of Hsp90 contains a hydrophobic pocket, formed by amino acid residues including Phe138, Leu107 and Val150, which may contribute to the binding affinity of inhibitors, such the 3,4-diaryl triazoles and related structures described herein, which are substituted with a hydrophobic group at the 5'-position of the resorcinol moiety, including methyl, ethyl, propyl, isopropyl, and the like. In some cases, the strength of the interaction between the inhibitor and the hydrophobic pocket of the Hsp90 binding site may increase with increasing size of the group substituted at the 5'-position of the resorcinol moiety (e.g., Me < Et < i-Pro).

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According to methods of the invention, these observations for the binding interactions for Compounds A, B, and C may be applied to the design inhibitors, and variants of inhibitors, to preserve and/or strengthen the interactions between the binding site and inhibitor as described herein.

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All publications, patent applications, patents, and other documents cited herein are incorporated by reference in their entirety. In case of conflict, the present specification, including definitions, will control. In addition, the materials, methods, and examples are illustrative only and not intended to be limiting.

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While this invention has been particularly shown and described with references to preferred embodiments thereof, it will be understood by those skilled in the art that various changes in form and details may be made therein without departing from the scope of the invention encompassed by the appended claims.

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Table 3. Atomic Coordinates of Hsp90 with Compound 226

		Amino Acid				Temp.		Atom Type
Atom Number	Residue	X	Y	Z	Occ. Factor			
ATOM 1	N GLU A 16	10.154	-11.775	28.593	1.00	24.66		N
20 ATOM 2	CA GLU A 16	11.578	-11.860	29.035	1.00	23.82		C
ATOM 3	CB GLU A 16	12.070	-13.306	28.974	1.00	24.68		C
ATOM 4	CG GLU A 16	13.283	-13.577	29.849	1.00	26.15		C
ATOM 8	C GLU A 16	12.489	-10.946	28.209	1.00	22.90		C
ATOM 9	O GLU A 16	12.699	-11.158	27.003	1.00	23.87		O
25 ATOM 10	N VAL A 17	13.032	-9.930	28.872	1.00	20.89		N
ATOM 11	CA VAL A 17	13.821	-8.904	28.195	1.00	18.83		C
ATOM 12	CB VAL A 17	13.216	-7.492	28.414	1.00	19.45		C
ATOM 13	CG1 VAL A 17	13.994	-6.448	27.633	1.00	19.58		C
ATOM 14	CG2 VAL A 17	11.733	-7.460	28.005	1.00	19.65		C
30 ATOM 15	C VAL A 17	15.270	-8.967	28.698	1.00	17.23		C
ATOM 16	O VAL A 17	15.511	-9.023	29.908	1.00	16.52		O
ATOM 17	N GLU A 18	16.220	-8.986	27.764	1.00	14.92		N
ATOM 18	CA GLU A 18	17.640	-8.931	28.100	1.00	13.95		C
ATOM 19	CB GLU A 18	18.416	-10.022	27.364	1.00	14.25		C
35 ATOM 20	CG GLU A 18	18.102	-11.429	27.854	1.00	15.56		C

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	ATOM	21	CD	GLU A 18	18.893	-12.475	27.106	1.00	18.69	C
	ATOM	22	OE1	GLU A 18	18.743	-12.562	25.875	1.00	18.84	O
	ATOM	23	OE2	GLU A 18	19.673	-13.206	27.748	1.00	20.45	O
	ATOM	24	C	GLU A 18	18.211	-7.559	27.751	1.00	13.37	C
5	ATOM	25	O	GLU A 18	17.957	-7.025	26.660	1.00	12.60	O
	ATOM	26	N	THR A 19	18.953	-6.985	28.696	1.00	12.63	N
	ATOM	27	CA	THR A 19	19.591	-5.691	28.492	1.00	12.33	C
	ATOM	28	CB	THR A 19	19.329	-4.720	29.675	1.00	12.75	C
	ATOM	29	OG1	THR A 19	17.911	-4.589	29.874	1.00	11.87	O
10	ATOM	30	CG2	THR A 19	19.905	-3.337	29.373	1.00	12.02	C
	ATOM	31	C	THR A 19	21.085	-5.884	28.272	1.00	12.45	C
	ATOM	32	O	THR A 19	21.704	-6.738	28.913	1.00	11.80	O
	ATOM	33	N	PHE A 20	21.637	-5.090	27.354	1.00	12.11	N
	ATOM	34	CA	PHE A 20	23.053	-5.153	26.966	1.00	12.65	C
15	ATOM	35	CB	PHE A 20	23.203	-5.736	25.558	1.00	12.41	C
	ATOM	36	CG	PHE A 20	22.578	-7.092	25.371	1.00	13.19	C
	ATOM	37	CD1	PHE A 20	21.224	-7.221	25.064	1.00	13.40	C
	ATOM	38	CE1	PHE A 20	20.647	-8.485	24.876	1.00	13.18	C
	ATOM	39	CZ	PHE A 20	21.435	-9.636	24.998	1.00	13.70	C
20	ATOM	40	CE2	PHE A 20	22.795	-9.512	25.292	1.00	14.13	C
	ATOM	41	CD2	PHE A 20	23.352	-8.238	25.479	1.00	13.58	C
	ATOM	42	C	PHE A 20	23.650	-3.747	26.953	1.00	12.36	C
	ATOM	43	O	PHE A 20	22.927	-2.765	26.734	1.00	12.69	O
	ATOM	44	N	ALA A 21	24.961	-3.653	27.156	1.00	12.01	N
25	ATOM	45	CA	ALA A 21	25.681	-2.391	26.970	1.00	12.42	C
	ATOM	46	CB	ALA A 21	26.763	-2.220	28.041	1.00	12.76	C
	ATOM	47	C	ALA A 21	26.304	-2.359	25.578	1.00	12.05	C
	ATOM	48	O	ALA A 21	26.806	-3.378	25.093	1.00	12.33	O
	ATOM	49	N	PHE A 22	26.267	-1.206	24.917	1.00	11.77	N
30	ATOM	50	CA	PHE A 22	27.073	-1.036	23.705	1.00	11.99	C
	ATOM	51	CB	PHE A 22	26.792	0.314	23.035	1.00	11.54	C
	ATOM	52	CG	PHE A 22	25.426	0.406	22.419	1.00	10.87	C
	ATOM	53	CD1	PHE A 22	25.134	-0.270	21.227	1.00	10.70	C
	ATOM	54	CE1	PHE A 22	23.857	-0.192	20.651	1.00	9.47	C
35	ATOM	55	CZ	PHE A 22	22.864	0.571	21.267	1.00	11.03	C

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	ATOM	56	CE2 PHE A 22	23.148	1.256	22.465	1.00	11.07	C
	ATOM	57	CD2 PHE A 22	24.426	1.163	23.034	1.00	11.83	C
	ATOM	58	C PHE A 22	28.546	-1.076	24.071	1.00	12.59	C
	ATOM	59	O PHE A 22	28.933	-0.584	25.138	1.00	12.77	O
5	ATOM	60	N GLN A 23	29.359	-1.649	23.186	1.00	12.76	N
	ATOM	61	CA GLN A 23	30.806	-1.435	23.243	1.00	14.00	C
	ATOM	62	CB GLN A 23	31.471	-2.067	22.022	1.00	14.46	C
	ATOM	63	CG GLN A 23	32.988	-2.047	22.063	1.00	15.24	C
	ATOM	64	CD GLN A 23	33.624	-2.835	20.931	1.00	16.59	C
10	ATOM	65	OE1 GLN A 23	32.931	-3.496	20.142	1.00	13.78	O
	ATOM	66	NE2 GLN A 23	34.964	-2.781	20.852	1.00	18.56	N
	ATOM	67	C GLN A 23	31.077	0.079	23.306	1.00	13.56	C
	ATOM	68	O GLN A 23	30.369	0.871	22.668	1.00	12.42	O
	ATOM	69	N ALA A 24	32.094	0.476	24.067	1.00	11.94	N
15	ATOM	70	CA ALA A 24	32.370	1.901	24.321	1.00	13.11	C
	ATOM	71	CB ALA A 24	33.676	2.057	25.103	1.00	12.81	C
	ATOM	72	C ALA A 24	32.397	2.773	23.059	1.00	12.75	C
	ATOM	73	O ALA A 24	31.769	3.838	23.021	1.00	13.55	O
	ATOM	74	N GLU A 25	33.123	2.317	22.037	1.00	13.05	N
20	ATOM	75	CA GLU A 25	33.253	3.046	20.770	1.00	13.70	C
	ATOM	76	CB GLU A 25	34.221	2.346	19.805	1.00	14.63	C
	ATOM	77	CG GLU A 25	35.696	2.368	20.243	1.00	16.11	C
	ATOM	78	CD GLU A 25	36.071	1.243	21.220	1.00	19.23	C
	ATOM	79	OE1 GLU A 25	37.284	1.097	21.505	1.00	21.42	O
25	ATOM	80	OE2 GLU A 25	35.185	0.499	21.705	1.00	17.23	O
	ATOM	81	C GLU A 25	31.907	3.270	20.075	1.00	13.18	C
	ATOM	82	O GLU A 25	31.679	4.334	19.502	1.00	12.16	O
	ATOM	83	N ILE A 26	31.029	2.266	20.131	1.00	12.12	N
	ATOM	84	CA ILE A 26	29.673	2.412	19.579	1.00	12.09	C
30	ATOM	85	CB ILE A 26	28.945	1.043	19.448	1.00	12.08	C
	ATOM	86	CG1 ILE A 26	29.732	0.086	18.521	1.00	12.46	C
	ATOM	87	CD1 ILE A 26	29.791	0.485	17.039	1.00	12.62	C
	ATOM	88	CG2 ILE A 26	27.471	1.218	18.999	1.00	11.98	C
	ATOM	89	C ILE A 26	28.851	3.439	20.387	1.00	12.35	C
35	ATOM	90	O ILE A 26	28.147	4.281	19.804	1.00	11.39	O

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	ATOM	91	N	ALA	A	27	28.963	3.388	21.714	1.00	11.65	N
	ATOM	92	CA	ALA	A	27	28.249	4.348	22.557	1.00	12.18	C
	ATOM	93	CB	ALA	A	27	28.438	4.029	24.047	1.00	12.58	C
	ATOM	94	C	ALA	A	27	28.696	5.775	22.218	1.00	12.79	C
5	ATOM	95	O	ALA	A	27	27.868	6.687	22.095	1.00	11.69	O
	ATOM	96	N	GLN	A	28	30.005	5.939	22.022	1.00	13.46	N
	ATOM	97	CA	GLN	A	28	30.594	7.236	21.672	1.00	13.87	C
	ATOM	98	CB	GLN	A	28	32.110	7.151	21.720	1.00	14.20	C
	ATOM	99	CG	GLN	A	28	32.621	7.008	23.145	1.00	17.94	C
10	ATOM	100	CD	GLN	A	28	34.070	6.596	23.224	1.00	21.46	C
	ATOM	101	OE1	GLN	A	28	34.653	6.098	22.257	1.00	21.85	O
	ATOM	102	NE2	GLN	A	28	34.662	6.792	24.396	1.00	25.75	N
	ATOM	103	C	GLN	A	28	30.113	7.733	20.313	1.00	13.42	C
	ATOM	104	O	GLN	A	28	29.774	8.907	20.166	1.00	12.80	O
15	ATOM	105	N	LEU	A	29	30.077	6.831	19.334	1.00	13.08	N
	ATOM	106	CA	LEU	A	29	29.520	7.129	18.010	1.00	12.53	C
	ATOM	107	CB	LEU	A	29	29.653	5.903	17.090	1.00	12.67	C
	ATOM	108	CG	LEU	A	29	29.006	5.989	15.702	1.00	13.86	C
	ATOM	109	CD1	LEU	A	29	29.529	7.207	14.914	1.00	13.82	C
20	ATOM	110	CD2	LEU	A	29	29.207	4.688	14.911	1.00	13.55	C
	ATOM	111	C	LEU	A	29	28.060	7.595	18.103	1.00	12.17	C
	ATOM	112	O	LEU	A	29	27.698	8.639	17.546	1.00	10.96	O
	ATOM	113	N	MET	A	30	27.238	6.835	18.826	1.00	11.28	N
	ATOM	114	CA	MET	A	30	25.814	7.158	18.962	1.00	12.43	C
25	ATOM	115	CB	MET	A	30	25.087	6.078	19.759	1.00	11.52	C
	ATOM	116	CG	MET	A	30	24.980	4.758	18.979	1.00	12.67	C
	ATOM	117	SD	MET	A	30	24.260	3.414	19.945	1.00	12.65	S
	ATOM	118	CE	MET	A	30	22.516	3.862	19.912	1.00	13.83	C
	ATOM	119	C	MET	A	30	25.640	8.520	19.612	1.00	12.51	C
30	ATOM	120	O	MET	A	30	24.825	9.326	19.166	1.00	12.42	O
	ATOM	121	N	SER	A	31	26.423	8.774	20.656	1.00	12.76	N
	ATOM	122	CA	SER	A	31	26.356	10.065	21.344	1.00	14.62	C
	ATOM	123	CB	SER	A	31	27.290	10.092	22.551	1.00	14.46	C
	ATOM	124	OG	BSER	A	31	26.774	9.289	23.602	0.40	13.77	O
35	ATOM	125	OG	ASER	A	31	27.171	11.327	23.231	0.60	15.82	O

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	ATOM	126	C	SER A 31	26.655	11.244	20.409	1.00	15.02	C
	ATOM	127	O	SER A 31	25.954	12.268	20.450	1.00	15.78	O
	ATOM	128	N	LEU A 32	27.688	11.097	19.585	1.00	15.41	N
	ATOM	129	CA	LEU A 32	28.061	12.126	18.622	1.00	16.41	C
5	ATOM	130	CB	LEU A 32	29.373	11.755	17.920	1.00	16.90	C
	ATOM	131	CG	LEU A 32	30.102	12.746	16.996	1.00	17.48	C
	ATOM	132	CD1	LEU A 32	30.144	14.188	17.531	1.00	20.14	C
	ATOM	133	CD2	LEU A 32	31.523	12.246	16.763	1.00	18.46	C
	ATOM	134	C	LEU A 32	26.935	12.342	17.601	1.00	16.41	C
10	ATOM	135	O	LEU A 32	26.582	13.488	17.296	1.00	16.51	O
	ATOM	136	N	ILE A 33	26.382	11.248	17.077	1.00	15.71	N
	ATOM	137	CA	ILE A 33	25.290	11.330	16.086	1.00	16.60	C
	ATOM	138	CB	ILE A 33	24.996	9.952	15.431	1.00	15.98	C
	ATOM	139	CG1	ILE A 33	26.217	9.489	14.629	1.00	15.42	C
15	ATOM	140	CD1	ILE A 33	26.156	8.038	14.184	1.00	17.13	C
	ATOM	141	CG2	ILE A 33	23.694	10.005	14.571	1.00	15.83	C
	ATOM	142	C	ILE A 33	24.005	11.908	16.667	1.00	18.38	C
	ATOM	143	O	ILE A 33	23.393	12.808	16.070	1.00	17.88	O
	ATOM	144	N	ILE A 34	23.603	11.378	17.826	1.00	20.00	N
20	ATOM	145	CA	ILE A 34	22.348	11.742	18.492	1.00	22.93	C
	ATOM	146	CB	ILE A 34	22.183	10.964	19.856	1.00	22.33	C
	ATOM	147	CG1	ILE A 34	21.193	9.803	19.700	1.00	25.36	C
	ATOM	148	CD1	ILE A 34	19.678	10.188	19.687	1.00	25.34	C
	ATOM	149	CG2	ILE A 34	21.771	11.889	21.006	1.00	24.95	C
25	ATOM	150	C	ILE A 34	22.248	13.241	18.718	1.00	22.80	C
	ATOM	151	O	ILE A 34	21.163	13.827	18.591	1.00	24.25	O
	ATOM	152	N	ASN A 35	23.395	13.848	19.004	1.00	22.86	N
	ATOM	153	CA	ASN A 35	23.479	15.215	19.473	1.00	22.91	C
	ATOM	154	CB	ASN A 35	24.401	15.268	20.693	1.00	23.39	C
30	ATOM	155	CG	ASN A 35	23.787	14.592	21.915	1.00	25.30	C
	ATOM	156	OD1	ASN A 35	22.706	14.973	22.364	1.00	27.54	O
	ATOM	157	ND2	ASN A 35	24.465	13.580	22.447	1.00	25.89	N
	ATOM	158	C	ASN A 35	23.937	16.237	18.433	1.00	22.39	C
	ATOM	159	O	ASN A 35	23.873	17.454	18.679	1.00	23.21	O
35	ATOM	160	N	THR A 36	24.400	15.761	17.279	1.00	20.18	N

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	ATOM	161	CA	THR	A	36	24.989	16.670	16.295	1.00	18.37	C
	ATOM	162	CB	THR	A	36	25.798	15.920	15.204	1.00	18.20	C
	ATOM	163	OG1	THR	A	36	26.419	16.872	14.329	1.00	15.96	O
	ATOM	164	CG2	THR	A	36	24.902	14.968	14.397	1.00	16.97	C
5	ATOM	165	C	THR	A	36	23.939	17.593	15.671	1.00	17.57	C
	ATOM	166	O	THR	A	36	22.781	17.208	15.512	1.00	18.15	O
	ATOM	167	N	PHE	A	37	24.351	18.815	15.344	1.00	17.07	N
	ATOM	168	CA	PHE	A	37	23.519	19.729	14.571	1.00	16.71	C
	ATOM	169	CB	PHE	A	37	23.846	21.186	14.914	1.00	17.01	C
10	ATOM	170	CG	PHE	A	37	23.309	21.627	16.241	1.00	17.51	C
	ATOM	171	CD1	PHE	A	37	21.933	21.663	16.477	1.00	17.82	C
	ATOM	172	CE1	PHE	A	37	21.429	22.073	17.716	1.00	18.75	C
	ATOM	173	CZ	PHE	A	37	22.313	22.477	18.719	1.00	17.88	C
	ATOM	174	CE2	PHE	A	37	23.688	22.450	18.482	1.00	18.41	C
15	ATOM	175	CD2	PHE	A	37	24.176	22.028	17.253	1.00	18.38	C
	ATOM	176	C	PHE	A	37	23.683	19.512	13.067	1.00	15.81	C
	ATOM	177	O	PHE	A	37	23.113	20.257	12.268	1.00	15.59	O
	ATOM	178	N	TYR	A	38	24.470	18.502	12.684	1.00	14.95	N
	ATOM	179	CA	TYR	A	38	24.654	18.144	11.264	1.00	13.36	C
20	ATOM	180	CB	TYR	A	38	25.219	16.718	11.151	1.00	13.58	C
	ATOM	181	CG	TYR	A	38	25.567	16.285	9.746	1.00	13.52	C
	ATOM	182	CD1	TYR	A	38	26.753	16.717	9.130	1.00	13.36	C
	ATOM	183	CE1	TYR	A	38	27.085	16.306	7.832	1.00	14.53	C
	ATOM	184	CZ	TYR	A	38	26.217	15.453	7.141	1.00	14.07	C
25	ATOM	185	OH	TYR	A	38	26.521	15.035	5.865	1.00	14.69	O
	ATOM	186	CE2	TYR	A	38	25.039	15.016	7.735	1.00	14.03	C
	ATOM	187	CD2	TYR	A	38	24.723	15.430	9.034	1.00	13.55	C
	ATOM	188	C	TYR	A	38	23.350	18.248	10.468	1.00	13.01	C
	ATOM	189	O	TYR	A	38	22.390	17.543	10.757	1.00	12.63	O
30	ATOM	190	N	SER	A	39	23.330	19.115	9.455	1.00	12.59	N
	ATOM	191	CA	SER	A	39	22.071	19.483	8.795	1.00	12.84	C
	ATOM	192	CB	SER	A	39	22.163	20.910	8.246	1.00	13.21	C
	ATOM	193	OG	SER	A	39	23.134	20.979	7.225	1.00	14.18	O
	ATOM	194	C	SER	A	39	21.616	18.527	7.689	1.00	11.87	C
35	ATOM	195	O	SER	A	39	20.427	18.474	7.372	1.00	11.54	O

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	ATOM	196	N	ASN A 40	22.562	17.791	7.099	1.00	11.96	N
	ATOM	197	CA	ASN A 40	22.309	16.935	5.929	1.00	11.67	C
	ATOM	198	CB	ASN A 40	23.624	16.822	5.122	1.00	12.77	C
	ATOM	199	CG	ASN A 40	23.540	15.887	3.901	1.00	13.17	C
5	ATOM	200	OD1	ASN A 40	24.524	15.196	3.593	1.00	15.81	O
	ATOM	201	ND2	ASN A 40	22.412	15.889	3.190	1.00	9.80	N
	ATOM	202	C	ASN A 40	21.739	15.563	6.371	1.00	11.94	C
	ATOM	203	O	ASN A 40	22.262	14.505	6.023	1.00	12.54	O
	ATOM	204	N	LYS A 41	20.651	15.606	7.141	1.00	10.90	N
10	ATOM	205	CA	LYS A 41	20.140	14.410	7.825	1.00	11.16	C
	ATOM	206	CB	LYS A 41	19.158	14.807	8.933	1.00	11.10	C
	ATOM	207	CG	LYS A 41	19.809	15.591	10.072	1.00	11.04	C
	ATOM	208	CD	LYS A 41	18.828	15.839	11.221	1.00	12.16	C
	ATOM	209	CE	LYS A 41	19.565	16.323	12.479	1.00	14.93	C
15	ATOM	210	NZ	LYS A 41	20.203	17.648	12.297	1.00	16.15	N
	ATOM	211	C	LYS A 41	19.520	13.335	6.915	1.00	11.27	C
	ATOM	212	O	LYS A 41	19.429	12.165	7.320	1.00	10.41	O
	ATOM	213	N	GLU A 42	19.107	13.727	5.713	1.00	10.69	N
	ATOM	214	CA	GLU A 42	18.382	12.827	4.800	1.00	11.37	C
20	ATOM	215	CB	GLU A 42	17.936	13.571	3.532	1.00	11.28	C
	ATOM	216	CG	GLU A 42	19.096	13.998	2.612	1.00	12.32	C
	ATOM	217	CD	GLU A 42	18.637	14.687	1.345	1.00	13.13	C
	ATOM	218	OE1	GLU A 42	17.536	15.267	1.333	1.00	17.31	O
	ATOM	219	OE2	GLU A 42	19.375	14.639	0.345	1.00	14.66	O
25	ATOM	220	C	GLU A 42	19.185	11.578	4.405	1.00	11.07	C
	ATOM	221	O	GLU A 42	18.602	10.578	3.977	1.00	11.48	O
	ATOM	222	N	ILE A 43	20.515	11.645	4.531	1.00	11.27	N
	ATOM	223	CA	ILE A 43	21.387	10.499	4.233	1.00	11.45	C
	ATOM	224	CB	ILE A 43	22.914	10.888	4.238	1.00	12.23	C
30	ATOM	225	CG1	ILE A 43	23.384	11.351	5.624	1.00	12.50	C
	ATOM	226	CD1	ILE A 43	23.795	10.262	6.575	1.00	16.01	C
	ATOM	227	CG2	ILE A 43	23.192	11.989	3.199	1.00	14.01	C
	ATOM	228	C	ILE A 43	21.110	9.240	5.093	1.00	10.99	C
	ATOM	229	O	ILE A 43	21.556	8.144	4.733	1.00	10.35	O
35	ATOM	230	N	PHE A 44	20.374	9.371	6.203	1.00	10.17	N

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	ATOM	231	CA	PHE A 44	20.059	8.180	7.014	1.00	10.22	C
	ATOM	232	CB	PHE A 44	19.202	8.512	8.250	1.00	10.70	C
	ATOM	233	CG	PHE A 44	17.740	8.699	7.929	1.00	10.13	C
	ATOM	234	CD1	PHE A 44	17.252	9.957	7.574	1.00	10.41	C
5	ATOM	235	CE1	PHE A 44	15.907	10.129	7.244	1.00	11.26	C
	ATOM	236	CZ	PHE A 44	15.038	9.042	7.264	1.00	11.92	C
	ATOM	237	CE2	PHE A 44	15.519	7.776	7.604	1.00	11.39	C
	ATOM	238	CD2	PHE A 44	16.863	7.613	7.942	1.00	9.58	C
	ATOM	239	C	PHE A 44	19.321	7.158	6.147	1.00	10.35	C
10	ATOM	240	O	PHE A 44	19.496	5.952	6.315	1.00	9.83	O
	ATOM	241	N	LEU A 45	18.486	7.651	5.231	1.00	10.24	N
	ATOM	242	CA	LEU A 45	17.635	6.757	4.448	1.00	10.63	C
	ATOM	243	CB	LEU A 45	16.483	7.505	3.763	1.00	10.89	C
	ATOM	244	CG	LEU A 45	15.455	6.628	3.027	1.00	11.08	C
15	ATOM	245	CD1	LEU A 45	14.365	7.511	2.425	1.00	11.38	C
	ATOM	246	CD2	LEU A 45	14.843	5.562	3.952	1.00	10.54	C
	ATOM	247	C	LEU A 45	18.436	5.914	3.459	1.00	10.15	C
	ATOM	248	O	LEU A 45	18.206	4.706	3.358	1.00	9.10	O
	ATOM	249	N	ARG A 46	19.356	6.533	2.717	1.00	10.94	N
20	ATOM	250	CA	ARG A 46	20.206	5.733	1.818	1.00	11.17	C
	ATOM	251	CB	ARG A 46	21.093	6.602	0.924	1.00	13.76	C
	ATOM	252	CG	ARG A 46	22.199	7.218	1.656	1.00	15.69	C
	ATOM	253	CD	ARG A 46	23.354	7.647	0.784	1.00	18.16	C
	ATOM	254	NE	ARG A 46	24.360	8.048	1.746	1.00	20.65	N
25	ATOM	255	CZ	ARG A 46	25.298	8.954	1.559	1.00	23.15	C
	ATOM	256	NH1	ARG A 46	25.418	9.583	0.399	1.00	24.96	N
	ATOM	257	NH2	ARG A 46	26.123	9.213	2.559	1.00	25.28	N
	ATOM	258	C	ARG A 46	21.047	4.699	2.585	1.00	10.94	C
	ATOM	259	O	ARG A 46	21.306	3.613	2.063	1.00	10.47	O
30	ATOM	260	N	GLU A 47	21.467	5.027	3.809	1.00	9.90	N
	ATOM	261	CA	GLU A 47	22.270	4.079	4.598	1.00	9.63	C
	ATOM	262	CB	GLU A 47	22.837	4.747	5.861	1.00	10.33	C
	ATOM	263	CG	GLU A 47	23.830	5.912	5.596	1.00	11.04	C
	ATOM	264	CD	GLU A 47	25.023	5.518	4.731	1.00	14.29	C
35	ATOM	265	OE1	GLU A 47	25.408	4.324	4.703	1.00	13.83	O

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	ATOM	266	OE2	GLU A 47	25.591	6.423	4.079	1.00	16.09	O
	ATOM	267	C	GLU A 47	21.468	2.826	4.968	1.00	9.12	C
	ATOM	268	O	GLU A 47	21.980	1.688	4.878	1.00	8.63	O
	ATOM	269	N	LEU A 48	20.216	3.037	5.375	1.00	8.15	N
5	ATOM	270	CA	LEU A 48	19.338	1.921	5.748	1.00	8.83	C
	ATOM	271	CB	LEU A 48	18.108	2.428	6.516	1.00	8.33	C
	ATOM	272	CG	LEU A 48	18.433	3.041	7.888	1.00	8.75	C
	ATOM	273	CD1	LEU A 48	17.187	3.576	8.567	1.00	8.41	C
	ATOM	274	CD2	LEU A 48	19.180	2.072	8.809	1.00	9.71	C
10	ATOM	275	C	LEU A 48	18.937	1.103	4.517	1.00	9.05	C
	ATOM	276	O	LEU A 48	18.915	-0.133	4.560	1.00	9.33	O
	ATOM	277	N	ILE A 49	18.641	1.798	3.420	1.00	8.31	N
	ATOM	278	CA	ILE A 49	18.346	1.138	2.151	1.00	8.96	C
	ATOM	279	CB	ILE A 49	17.836	2.158	1.077	1.00	7.88	C
15	ATOM	280	CG1	ILE A 49	16.427	2.662	1.476	1.00	7.82	C
	ATOM	281	CD1	ILE A 49	15.827	3.705	0.520	1.00	9.70	C
	ATOM	282	CG2	ILE A 49	17.823	1.505	-0.318	1.00	9.43	C
	ATOM	283	C	ILE A 49	19.553	0.304	1.671	1.00	8.82	C
	ATOM	284	O	ILE A 49	19.391	-0.845	1.219	1.00	7.37	O
20	ATOM	285	N	SER A 50	20.754	0.876	1.786	1.00	9.03	N
	ATOM	286	CA	SER A 50	21.989	0.147	1.448	1.00	9.38	C
	ATOM	287	CB	SER A 50	23.211	1.058	1.558	1.00	9.67	C
	ATOM	288	OG	BSER A 50	23.245	1.944	0.448	0.50	7.05	O
	ATOM	289	OG	ASER A 50	24.400	0.363	1.240	0.50	11.71	O
25	ATOM	290	C	SER A 50	22.155	-1.127	2.293	1.00	9.59	C
	ATOM	291	O	SER A 50	22.511	-2.177	1.762	1.00	9.26	O
	ATOM	292	N	ASN A 51	21.880	-1.036	3.594	1.00	8.13	N
	ATOM	293	CA	ASN A 51	21.924	-2.217	4.468	1.00	9.27	C
	ATOM	294	CB	ASN A 51	21.661	-1.842	5.922	1.00	8.16	C
30	ATOM	295	CG	ASN A 51	22.849	-1.142	6.569	1.00	9.44	C
	ATOM	296	OD1	ASN A 51	23.913	-1.001	5.962	1.00	9.93	O
	ATOM	297	ND2	ASN A 51	22.670	-0.704	7.804	1.00	9.45	N
	ATOM	298	C	ASN A 51	20.929	-3.289	4.025	1.00	8.92	C
	ATOM	299	O	ASN A 51	21.264	-4.484	3.984	1.00	9.40	O
35	ATOM	300	N	SER A 52	19.723	-2.851	3.676	1.00	9.04	N

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	ATOM	301	CA	SER A 52	18.685	-3.765	3.166	1.00	8.54	C
	ATOM	302	CB	SER A 52	17.378	-3.013	2.898	1.00	8.30	C
	ATOM	303	OG	SER A 52	16.757	-2.608	4.107	1.00	7.96	O
	ATOM	304	C	SER A 52	19.169	-4.471	1.891	1.00	9.30	C
5	ATOM	305	O	SER A 52	19.005	-5.696	1.739	1.00	8.23	O
	ATOM	306	N	SER A 53	19.752	-3.695	0.975	1.00	9.37	N
	ATOM	307	CA	SER A 53	20.283	-4.246	-0.264	1.00	10.27	C
	ATOM	308	CB	SER A 53	20.812	-3.121	-1.166	1.00	9.48	C
	ATOM	309	OG	SER A 53	21.242	-3.645	-2.406	1.00	10.70	O
10	ATOM	310	C	SER A 53	21.371	-5.295	0.028	1.00	9.91	C
	ATOM	311	O	SER A 53	21.395	-6.369	-0.591	1.00	9.03	O
	ATOM	312	N	ASP A 54	22.257	-4.983	0.973	1.00	9.82	N
	ATOM	313	CA	ASP A 54	23.313	-5.920	1.379	1.00	9.98	C
	ATOM	314	CB	ASP A 54	24.217	-5.291	2.444	1.00	11.45	C
15	ATOM	315	CG	ASP A 54	25.139	-4.197	1.885	1.00	14.35	C
	ATOM	316	OD1	ASP A 54	25.175	-3.969	0.647	1.00	14.41	O
	ATOM	317	OD2	ASP A 54	25.825	-3.563	2.708	1.00	18.20	O
	ATOM	318	C	ASP A 54	22.699	-7.234	1.915	1.00	9.66	C
	ATOM	319	O	ASP A 54	23.137	-8.329	1.553	1.00	9.18	O
20	ATOM	320	N	ALA A 55	21.668	-7.122	2.745	1.00	8.41	N
	ATOM	321	CA	ALA A 55	21.006	-8.313	3.312	1.00	8.65	C
	ATOM	322	CB	ALA A 55	20.043	-7.920	4.426	1.00	8.24	C
	ATOM	323	C	ALA A 55	20.290	-9.138	2.236	1.00	8.83	C
	ATOM	324	O	ALA A 55	20.248	-10.371	2.315	1.00	8.37	O
25	ATOM	325	N	LEU A 56	19.729	-8.444	1.240	1.00	8.74	N
	ATOM	326	CA	LEU A 56	19.135	-9.086	0.064	1.00	8.84	C
	ATOM	327	CB	LEU A 56	18.353	-8.061	-0.770	1.00	9.01	C
	ATOM	328	CG	LEU A 56	17.049	-7.605	-0.090	1.00	9.33	C
	ATOM	329	CD1	LEU A 56	16.555	-6.271	-0.651	1.00	9.62	C
30	ATOM	330	CD2	LEU A 56	15.933	-8.685	-0.134	1.00	8.38	C
	ATOM	331	C	LEU A 56	20.206	-9.808	-0.762	1.00	9.67	C
	ATOM	332	O	LEU A 56	19.999	-10.963	-1.157	1.00	9.76	O
	ATOM	333	N	ASP A 57	21.359	-9.161	-0.967	1.00	8.45	N
	ATOM	334	CA	ASP A 57	22.509	-9.826	-1.601	1.00	9.17	C
35	ATOM	335	CB	ASP A 57	23.744	-8.926	-1.603	1.00	9.62	C

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	ATOM	336	CG	ASP	A	57	23.604	-7.694	-2.504	1.00	10.48	C
	ATOM	337	OD1	ASP	A	57	22.750	-7.642	-3.427	1.00	12.38	O
	ATOM	338	OD2	ASP	A	57	24.405	-6.766	-2.277	1.00	13.17	O
	ATOM	339	C	ASP	A	57	22.846	-11.137	-0.871	1.00	9.84	C
5	ATOM	340	O	ASP	A	57	23.072	-12.177	-1.505	1.00	9.47	O
	ATOM	341	N	LYS	A	58	22.825	-11.085	0.460	1.00	9.77	N
	ATOM	342	CA	LYS	A	58	23.219	-12.236	1.282	1.00	10.66	C
	ATOM	343	CB	LYS	A	58	23.301	-11.851	2.755	1.00	10.60	C
	ATOM	344	CG	LYS	A	58	24.488	-10.931	3.078	1.00	12.51	C
10	ATOM	345	CD	LYS	A	58	24.498	-10.566	4.552	1.00	12.99	C
	ATOM	346	CE	LYS	A	58	25.628	-9.596	4.851	1.00	15.00	C
	ATOM	347	NZ	LYS	A	58	25.695	-9.237	6.291	1.00	16.39	N
	ATOM	348	C	LYS	A	58	22.283	-13.432	1.091	1.00	10.61	C
	ATOM	349	O	LYS	A	58	22.744	-14.557	0.880	1.00	10.34	O
15	ATOM	350	N	ILE	A	59	20.979	-13.201	1.163	1.00	10.07	N
	ATOM	351	CA	ILE	A	59	20.052	-14.318	0.951	1.00	11.71	C
	ATOM	352	CB	ILE	A	59	18.603	-14.046	1.476	1.00	11.61	C
	ATOM	353	CG1	ILE	A	59	17.757	-15.332	1.404	1.00	12.19	C
	ATOM	354	CD1	ILE	A	59	18.137	-16.396	2.452	1.00	13.51	C
20	ATOM	355	CG2	ILE	A	59	17.946	-12.879	0.735	1.00	11.14	C
	ATOM	356	C	ILE	A	59	20.073	-14.825	-0.498	1.00	11.58	C
	ATOM	357	O	ILE	A	59	20.015	-16.040	-0.723	1.00	11.64	O
	ATOM	358	N	ARG	A	60	20.198	-13.909	-1.465	1.00	12.31	N
	ATOM	359	CA	ARG	A	60	20.291	-14.306	-2.875	1.00	14.09	C
25	ATOM	360	CB	ARG	A	60	20.346	-13.086	-3.805	1.00	14.77	C
	ATOM	361	CG	ARG	A	60	20.950	-13.387	-5.181	1.00	19.46	C
	ATOM	362	CD	ARG	A	60	20.246	-12.656	-6.311	1.00	25.11	C
	ATOM	363	NE	ARG	A	60	19.416	-13.586	-7.066	1.00	30.26	N
	ATOM	364	CZ	ARG	A	60	19.804	-14.233	-8.164	1.00	31.43	C
30	ATOM	365	NH1	ARG	A	60	18.971	-15.073	-8.757	1.00	31.76	N
	ATOM	366	NH2	ARG	A	60	21.012	-14.045	-8.676	1.00	31.40	N
	ATOM	367	C	ARG	A	60	21.505	-15.230	-3.093	1.00	13.65	C
	ATOM	368	O	ARG	A	60	21.389	-16.286	-3.731	1.00	12.93	O
	ATOM	369	N	TYR	A	61	22.651	-14.820	-2.552	1.00	12.56	N
35	ATOM	370	CA	TYR	A	61	23.881	-15.609	-2.634	1.00	12.62	C

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	ATOM	371	CB	TYR A 61	25.016	-14.894	-1.910	1.00	12.93	C
	ATOM	372	CG	TYR A 61	26.313	-15.665	-1.909	1.00	13.94	C
	ATOM	373	CD1	TYR A 61	27.117	-15.701	-3.055	1.00	14.11	C
	ATOM	374	CE1	TYR A 61	28.311	-16.398	-3.072	1.00	13.69	C
5	ATOM	375	CZ	TYR A 61	28.713	-17.094	-1.942	1.00	15.14	C
	ATOM	376	OH	TYR A 61	29.901	-17.790	-1.984	1.00	15.85	O
	ATOM	377	CE2	TYR A 61	27.934	-17.088	-0.789	1.00	15.63	C
	ATOM	378	CD2	TYR A 61	26.728	-16.375	-0.781	1.00	14.75	C
	ATOM	379	C	TYR A 61	23.693	-17.033	-2.072	1.00	13.28	C
10	ATOM	380	O	TYR A 61	24.018	-18.023	-2.741	1.00	12.30	O
	ATOM	381	N	GLU A 62	23.166	-17.122	-0.855	1.00	12.98	N
	ATOM	382	CA	GLU A 62	22.969	-18.427	-0.207	1.00	14.42	C
	ATOM	383	CB	GLU A 62	22.552	-18.270	1.255	1.00	14.23	C
	ATOM	384	CG	GLU A 62	23.657	-17.635	2.108	1.00	17.61	C
15	ATOM	385	CD	GLU A 62	23.498	-17.867	3.596	1.00	20.97	C
	ATOM	386	OE1	GLU A 62	22.507	-18.502	4.016	1.00	20.80	O
	ATOM	387	OE2	GLU A 62	24.383	-17.392	4.352	1.00	25.32	O
	ATOM	388	C	GLU A 62	21.986	-19.288	-0.995	1.00	14.17	C
	ATOM	389	O	GLU A 62	22.199	-20.497	-1.139	1.00	15.02	O
20	ATOM	390	N	SER A 63	20.957	-18.651	-1.559	1.00	13.74	N
	ATOM	391	CA	SER A 63	19.922	-19.358	-2.319	1.00	14.64	C
	ATOM	392	CB	SER A 63	18.768	-18.421	-2.694	1.00	14.38	C
	ATOM	393	OG	SER A 63	19.084	-17.652	-3.847	1.00	13.96	O
	ATOM	394	C	SER A 63	20.465	-20.051	-3.569	1.00	15.36	C
25	ATOM	395	O	SER A 63	19.881	-21.026	-4.037	1.00	15.08	O
	ATOM	396	N	LEU A 64	21.571	-19.533	-4.112	1.00	15.34	N
	ATOM	397	CA	LEU A 64	22.193	-20.127	-5.304	1.00	16.91	C
	ATOM	398	CB	LEU A 64	23.420	-19.326	-5.759	1.00	16.24	C
	ATOM	399	CG	LEU A 64	23.135	-17.890	-6.230	1.00	16.83	C
30	ATOM	400	CD1	LEU A 64	24.441	-17.177	-6.534	1.00	18.62	C
	ATOM	401	CD2	LEU A 64	22.209	-17.862	-7.435	1.00	19.26	C
	ATOM	402	C	LEU A 64	22.573	-21.592	-5.088	1.00	18.36	C
	ATOM	403	O	LEU A 64	22.391	-22.418	-5.990	1.00	19.54	O
	ATOM	404	N	THR A 65	23.079	-21.909	-3.902	1.00	19.01	N
35	ATOM	405	CA	THR A 65	23.516	-23.285	-3.599	1.00	20.34	C

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	ATOM	406	CB	THR A 65	24.911	-23.310	-2.964	1.00	20.33	C
	ATOM	407	OG1	THR A 65	24.927	-22.448	-1.824	1.00	22.16	O
	ATOM	408	CG2	THR A 65	25.960	-22.841	-3.972	1.00	21.25	C
	ATOM	409	C	THR A 65	22.523	-24.076	-2.735	1.00	20.39	C
5	ATOM	410	O	THR A 65	22.589	-25.311	-2.675	1.00	20.48	O
	ATOM	411	N	ASP A 66	21.617	-23.361	-2.067	1.00	19.03	N
	ATOM	412	CA	ASP A 66	20.531	-23.982	-1.314	1.00	18.98	C
	ATOM	413	CB	ASP A 66	20.870	-24.060	0.189	1.00	19.22	C
	ATOM	414	CG	ASP A 66	19.814	-24.831	1.006	1.00	20.06	C
10	ATOM	415	OD1	ASP A 66	18.783	-25.260	0.441	1.00	20.59	O
	ATOM	416	OD2	ASP A 66	20.009	-24.989	2.228	1.00	20.04	O
	ATOM	417	C	ASP A 66	19.226	-23.210	-1.576	1.00	18.77	C
	ATOM	418	O	ASP A 66	18.881	-22.296	-0.824	1.00	17.92	O
	ATOM	419	N	PRO A 67	18.497	-23.585	-2.651	1.00	18.69	N
15	ATOM	420	CA	PRO A 67	17.196	-22.990	-2.999	1.00	19.02	C
	ATOM	421	CB	PRO A 67	16.667	-23.906	-4.114	1.00	20.00	C
	ATOM	423	CD	PRO A 67	18.901	-24.625	-3.622	1.00	19.82	C
	ATOM	424	C	PRO A 67	16.188	-22.969	-1.847	1.00	18.41	C
	ATOM	425	O	PRO A 67	15.341	-22.077	-1.802	1.00	17.92	O
20	ATOM	426	N	SER A 68	16.282	-23.938	-0.932	1.00	17.22	N
	ATOM	427	CA	SER A 68	15.319	-24.051	0.170	1.00	17.24	C
	ATOM	428	CB	SER A 68	15.511	-25.362	0.947	1.00	17.85	C
	ATOM	429	OG	SER A 68	16.590	-25.271	1.859	1.00	19.15	O
	ATOM	430	C	SER A 68	15.371	-22.842	1.119	1.00	16.44	C
25	ATOM	431	O	SER A 68	14.437	-22.603	1.870	1.00	16.49	O
	ATOM	432	N	LYS A 69	16.455	-22.072	1.054	1.00	15.92	N
	ATOM	433	CA	LYS A 69	16.578	-20.848	1.859	1.00	16.11	C
	ATOM	434	CB	LYS A 69	17.997	-20.290	1.767	1.00	16.40	C
	ATOM	435	CG	LYS A 69	19.024	-21.272	2.329	1.00	18.47	C
30	ATOM	436	CD	LYS A 69	20.307	-20.612	2.706	1.00	20.20	C
	ATOM	437	CE	LYS A 69	21.174	-21.581	3.494	1.00	20.73	C
	ATOM	438	NZ	LYS A 69	22.569	-21.082	3.633	1.00	22.96	N
	ATOM	439	C	LYS A 69	15.533	-19.783	1.494	1.00	15.43	C
	ATOM	440	O	LYS A 69	15.266	-18.866	2.287	1.00	15.36	O
35	ATOM	441	N	LEU A 70	14.950	-19.910	0.302	1.00	14.65	N

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	ATOM	442	CA	LEU A 70	13.839	-19.048	-0.104	1.00	14.66	C
	ATOM	443	CB	LEU A 70	13.952	-18.641	-1.582	1.00	14.96	C
	ATOM	444	CG	LEU A 70	15.213	-17.868	-1.978	1.00	15.61	C
	ATOM	445	CD1	LEU A 70	15.214	-17.625	-3.487	1.00	16.32	C
5	ATOM	446	CD2	LEU A 70	15.333	-16.560	-1.187	1.00	15.87	C
	ATOM	447	C	LEU A 70	12.456	-19.638	0.186	1.00	14.88	C
	ATOM	448	O	LEU A 70	11.438	-19.068	-0.219	1.00	14.13	O
	ATOM	449	N	ASP A 71	12.403	-20.756	0.908	1.00	15.18	N
	ATOM	450	CA	ASP A 71	11.095	-21.300	1.317	1.00	15.96	C
10	ATOM	451	CB	ASP A 71	11.227	-22.627	2.061	1.00	15.91	C
	ATOM	452	CG	ASP A 71	11.638	-23.773	1.156	1.00	17.35	C
	ATOM	453	OD1	ASP A 71	11.725	-23.601	-0.084	1.00	17.57	O
	ATOM	454	OD2	ASP A 71	11.875	-24.868	1.700	1.00	20.00	O
	ATOM	455	C	ASP A 71	10.345	-20.297	2.192	1.00	15.72	C
15	ATOM	456	O	ASP A 71	9.116	-20.275	2.183	1.00	16.43	O
	ATOM	457	N	SER A 72	11.098	-19.469	2.920	1.00	15.32	N
	ATOM	458	CA	SER A 72	10.543	-18.398	3.761	1.00	15.32	C
	ATOM	459	CB	SER A 72	11.535	-18.030	4.868	1.00	14.99	C
	ATOM	460	OG	SER A 72	12.830	-17.785	4.331	1.00	12.63	O
20	ATOM	461	C	SER A 72	10.146	-17.138	2.974	1.00	15.44	C
	ATOM	462	O	SER A 72	9.716	-16.144	3.564	1.00	16.51	O
	ATOM	463	N	GLY A 73	10.284	-17.184	1.651	1.00	15.34	N
	ATOM	464	CA	GLY A 73	9.813	-16.102	0.776	1.00	15.39	C
	ATOM	465	C	GLY A 73	10.752	-15.879	-0.385	1.00	15.38	C
25	ATOM	466	O	GLY A 73	11.956	-15.703	-0.190	1.00	15.70	O
	ATOM	467	N	LYS A 74	10.215	-15.902	-1.603	1.00	15.14	N
	ATOM	468	CA	LYS A 74	11.054	-15.763	-2.803	1.00	15.98	C
	ATOM	469	CB	LYS A 74	10.460	-16.539	-3.999	1.00	16.34	C
	ATOM	470	CG	LYS A 74	10.512	-18.060	-3.833	1.00	18.03	C
30	ATOM	474	C	LYS A 74	11.314	-14.305	-3.201	1.00	15.20	C
	ATOM	475	O	LYS A 74	12.329	-14.015	-3.834	1.00	16.31	O
	ATOM	476	N	GLU A 75	10.410	-13.403	-2.819	1.00	15.00	N
	ATOM	477	CA	GLU A 75	10.502	-11.982	-3.211	1.00	14.60	C
	ATOM	478	CB	GLU A 75	9.180	-11.248	-2.955	1.00	15.16	C
35	ATOM	479	CG	GLU A 75	7.976	-11.807	-3.725	1.00	17.31	C

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	ATOM	483	C	GLU A 75	11.640 -11.266 -2.478	1.00 13.34	C
	ATOM	484	O	GLU A 75	11.753 -11.370 -1.264	1.00 14.45	O
	ATOM	485	N	LEU A 76	12.465 -10.551 -3.234	1.00 12.22	N
	ATOM	486	CA	LEU A 76	13.585 -9.770 -2.703	1.00 11.63	C
5	ATOM	487	CB	LEU A 76	14.887 -10.146 -3.425	1.00 12.10	C
	ATOM	488	CG	LEU A 76	15.232 -11.639 -3.377	1.00 13.36	C
	ATOM	489	CD1	LEU A 76	16.527 -11.898 -4.133	1.00 14.86	C
	ATOM	490	CD2	LEU A 76	15.289 -12.183 -1.944	1.00 13.05	C
	ATOM	491	C	LEU A 76	13.276 -8.301 -2.932	1.00 11.14	C
10	ATOM	492	O	LEU A 76	13.370 -7.815 -4.061	1.00 11.21	O
	ATOM	493	N	HIS A 77	12.875 -7.607 -1.870	1.00 10.32	N
	ATOM	494	CA	HIS A 77	12.417 -6.227 -2.011	1.00 10.88	C
	ATOM	495	CB	HIS A 77	10.943 -6.162 -2.468	1.00 11.82	C
	ATOM	496	CG	HIS A 77	9.973 -6.777 -1.501	1.00 14.68	C
15	ATOM	497	ND1	HIS A 77	9.105 -7.785 -1.859	1.00 19.40	N
	ATOM	498	CE1	HIS A 77	8.375 -8.133 -0.812	1.00 18.02	C
	ATOM	499	NE2	HIS A 77	8.727 -7.378 0.213	1.00 17.48	N
	ATOM	500	CD2	HIS A 77	9.725 -6.520 -0.192	1.00 18.25	C
	ATOM	501	C	HIS A 77	12.596 -5.419 -0.733	1.00 9.15	C
20	ATOM	502	O	HIS A 77	12.918 -5.962 0.328	1.00 8.68	O
	ATOM	503	N	ILE A 78	12.393 -4.116 -0.877	1.00 8.19	N
	ATOM	504	CA	ILE A 78	12.494 -3.141 0.206	1.00 8.49	C
	ATOM	505	CB	ILE A 78	13.701 -2.211 -0.006	1.00 8.75	C
	ATOM	506	CG1	ILE A 78	15.000 -3.036 -0.113	1.00 7.55	C
25	ATOM	507	CD1	ILE A 78	16.235 -2.249 -0.583	1.00 8.18	C
	ATOM	508	CG2	ILE A 78	13.761 -1.148 1.107	1.00 9.52	C
	ATOM	509	C	ILE A 78	11.219 -2.291 0.209	1.00 9.01	C
	ATOM	510	O	ILE A 78	10.853 -1.725 -0.823	1.00 10.30	O
	ATOM	511	N	ASN A 79	10.559 -2.195 1.357	1.00 9.55	N
30	ATOM	512	CA	ASN A 79	9.359 -1.366 1.474	1.00 9.88	C
	ATOM	513	CB	ASN A 79	8.154 -2.197 1.942	1.00 10.14	C
	ATOM	514	CG	ASN A 79	7.737 -3.298 0.949	1.00 11.81	C
	ATOM	515	OD1	ASN A 79	7.184 -4.326 1.358	1.00 17.52	O
	ATOM	516	ND2	ASN A 79	7.952 -3.074 -0.330	1.00 8.96	N
35	ATOM	517	C	ASN A 79	9.600 -0.221 2.465	1.00 9.12	C

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	ATOM	518	O	ASN A 79	10.211	-0.430	3.511	1.00	9.58	O
	ATOM	519	N	LEU A 80	9.086	0.967	2.143	1.00	9.25	N
	ATOM	520	CA	LEU A 80	9.188	2.132	3.030	1.00	9.20	C
	ATOM	521	CB	LEU A 80	9.846	3.302	2.298	1.00	9.57	C
5	ATOM	522	CG	LEU A 80	11.128	3.007	1.511	1.00	9.11	C
	ATOM	523	CD1	LEU A 80	11.557	4.234	0.722	1.00	9.83	C
	ATOM	524	CD2	LEU A 80	12.255	2.525	2.446	1.00	10.15	C
	ATOM	525	C	LEU A 80	7.794	2.524	3.525	1.00	10.31	C
	ATOM	526	O	LEU A 80	6.881	2.734	2.728	1.00	10.08	O
10	ATOM	527	N	ILE A 81	7.636	2.617	4.841	1.00	11.05	N
	ATOM	528	CA	ILE A 81	6.305	2.763	5.439	1.00	11.69	C
	ATOM	529	CB	ILE A 81	5.814	1.423	6.095	1.00	11.56	C
	ATOM	530	CG1	ILE A 81	5.947	0.250	5.107	1.00	12.92	C
	ATOM	531	CD1	ILE A 81	5.712	-1.134	5.715	1.00	13.72	C
15	ATOM	532	CG2	ILE A 81	4.370	1.574	6.602	1.00	13.12	C
	ATOM	533	C	ILE A 81	6.279	3.916	6.448	1.00	10.83	C
	ATOM	534	O	ILE A 81	6.599	3.727	7.615	1.00	11.67	O
	ATOM	535	N	PRO A 82	5.940	5.134	5.982	1.00	11.20	N
	ATOM	536	CA	PRO A 82	5.703	6.224	6.927	1.00	11.37	C
20	ATOM	537	CB	PRO A 82	5.633	7.469	6.034	1.00	11.26	C
	ATOM	538	CG	PRO A 82	5.234	6.952	4.671	1.00	11.21	C
	ATOM	539	CD	PRO A 82	5.810	5.559	4.577	1.00	10.48	C
	ATOM	540	C	PRO A 82	4.393	6.048	7.699	1.00	12.13	C
	ATOM	541	O	PRO A 82	3.397	5.543	7.146	1.00	11.18	O
25	ATOM	542	N	ASN A 83	4.396	6.487	8.953	1.00	12.14	N
	ATOM	543	CA	ASN A 83	3.208	6.420	9.808	1.00	13.05	C
	ATOM	544	CB	ASN A 83	3.247	5.161	10.703	1.00	13.53	C
	ATOM	545	CG	ASN A 83	1.934	4.919	11.461	1.00	14.37	C
	ATOM	546	OD1	ASN A 83	1.284	5.855	11.919	1.00	15.55	O
30	ATOM	547	ND2	ASN A 83	1.554	3.655	11.601	1.00	16.83	N
	ATOM	548	C	ASN A 83	3.107	7.701	10.638	1.00	14.17	C
	ATOM	549	O	ASN A 83	3.734	7.819	11.691	1.00	14.26	O
	ATOM	550	N	LYS A 84	2.324	8.666	10.157	1.00	14.87	N
	ATOM	551	CA	LYS A 84	2.211	9.952	10.852	1.00	16.41	C
35	ATOM	552	CB	LYS A 84	1.484	10.994	9.999	1.00	16.85	C

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	ATOM	553	CG	LYS	A	84	2.317	11.509	8.844	1.00	19.23	C
	ATOM	554	CD	LYS	A	84	1.566	12.585	8.102	1.00	24.04	C
	ATOM	555	CE	LYS	A	84	2.180	12.857	6.750	1.00	24.07	C
	ATOM	556	NZ	LYS	A	84	1.519	14.058	6.167	1.00	27.57	N
5	ATOM	557	C	LYS	A	84	1.552	9.817	12.222	1.00	17.26	C
	ATOM	558	O	LYS	A	84	1.936	10.512	13.164	1.00	18.64	O
	ATOM	559	N	GLN	A	85	0.583	8.911	12.334	1.00	17.95	N
	ATOM	560	CA	GLN	A	85	-0.106	8.672	13.609	1.00	18.58	C
	ATOM	561	CB	GLN	A	85	-1.200	7.614	13.449	1.00	18.85	C
10	ATOM	566	C	GLN	A	85	0.869	8.262	14.713	1.00	18.57	C
	ATOM	567	O	GLN	A	85	0.795	8.775	15.833	1.00	19.58	O
	ATOM	568	N	ASP	A	86	1.798	7.366	14.375	1.00	17.32	N
	ATOM	569	CA	ASP	A	86	2.750	6.811	15.335	1.00	16.84	C
	ATOM	570	CB	ASP	A	86	3.059	5.348	14.992	1.00	17.52	C
15	ATOM	571	CG	ASP	A	86	1.874	4.425	15.219	1.00	20.96	C
	ATOM	572	OD1	ASP	A	86	0.798	4.901	15.665	1.00	22.85	O
	ATOM	573	OD2	ASP	A	86	2.017	3.216	14.935	1.00	22.91	O
	ATOM	574	C	ASP	A	86	4.057	7.592	15.357	1.00	15.36	C
	ATOM	575	O	ASP	A	86	4.918	7.339	16.204	1.00	14.78	O
20	ATOM	576	N	ARG	A	87	4.184	8.534	14.425	1.00	14.03	N
	ATOM	577	CA	ARG	A	87	5.439	9.244	14.155	1.00	13.23	C
	ATOM	578	CB	ARG	A	87	5.769	10.276	15.238	1.00	13.71	C
	ATOM	579	CG	ARG	A	87	6.627	11.410	14.691	1.00	16.54	C
	ATOM	580	CD	ARG	A	87	7.505	12.017	15.747	1.00	19.57	C
25	ATOM	581	NE	ARG	A	87	6.725	12.723	16.756	1.00	21.61	N
	ATOM	582	CZ	ARG	A	87	7.166	13.023	17.976	1.00	23.57	C
	ATOM	583	NH1	ARG	A	87	8.388	12.672	18.362	1.00	22.38	N
	ATOM	584	NH2	ARG	A	87	6.376	13.681	18.817	1.00	24.20	N
	ATOM	585	C	ARG	A	87	6.599	8.267	13.965	1.00	12.66	C
30	ATOM	586	O	ARG	A	87	7.668	8.411	14.579	1.00	11.75	O
	ATOM	587	N	THR	A	88	6.378	7.261	13.123	1.00	12.02	N
	ATOM	588	CA	THR	A	88	7.432	6.300	12.800	1.00	11.86	C
	ATOM	589	CB	THR	A	88	7.138	4.885	13.369	1.00	12.08	C
	ATOM	590	OG1	THR	A	88	5.886	4.408	12.847	1.00	11.90	O
35	ATOM	591	CG2	THR	A	88	7.091	4.912	14.898	1.00	13.05	C

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	ATOM	592	C	THR	A	88	7.629	6.171	11.289	1.00	11.43	C
	ATOM	593	O	THR	A	88	6.681	6.333	10.496	1.00	10.65	O
	ATOM	594	N	LEU	A	89	8.874	5.907	10.899	1.00	10.52	N
	ATOM	595	CA	LEU	A	89	9.186	5.539	9.527	1.00	10.86	C
5	ATOM	596	CB	LEU	A	89	10.170	6.536	8.881	1.00	11.11	C
	ATOM	597	CG	LEU	A	89	10.648	6.178	7.460	1.00	11.20	C
	ATOM	598	CD1	LEU	A	89	9.479	6.124	6.450	1.00	12.16	C
	ATOM	599	CD2	LEU	A	89	11.755	7.118	6.960	1.00	11.51	C
	ATOM	600	C	LEU	A	89	9.785	4.141	9.599	1.00	10.79	C
10	ATOM	601	O	LEU	A	89	10.767	3.908	10.326	1.00	10.16	O
	ATOM	602	N	THR	A	90	9.189	3.217	8.861	1.00	10.80	N
	ATOM	603	CA	THR	A	90	9.636	1.827	8.883	1.00	10.86	C
	ATOM	604	CB	THR	A	90	8.471	0.867	9.283	1.00	11.11	C
	ATOM	605	OG1	THR	A	90	8.004	1.207	10.600	1.00	11.95	O
15	ATOM	606	CG2	THR	A	90	8.935	-0.591	9.278	1.00	11.85	C
	ATOM	607	C	THR	A	90	10.264	1.427	7.545	1.00	10.94	C
	ATOM	608	O	THR	A	90	9.689	1.679	6.488	1.00	11.30	O
	ATOM	609	N	ILE	A	91	11.458	0.837	7.603	1.00	10.52	N
	ATOM	610	CA	ILE	A	91	12.122	0.280	6.422	1.00	10.67	C
20	ATOM	611	CB	ILE	A	91	13.576	0.806	6.239	1.00	10.77	C
	ATOM	612	CG1	ILE	A	91	13.616	2.347	6.056	1.00	12.35	C
	ATOM	613	CD1	ILE	A	91	13.641	3.150	7.362	1.00	15.33	C
	ATOM	614	CG2	ILE	A	91	14.237	0.118	5.039	1.00	10.35	C
	ATOM	615	C	ILE	A	91	12.111	-1.256	6.566	1.00	10.51	C
25	ATOM	616	O	ILE	A	91	12.669	-1.791	7.523	1.00	11.29	O
	ATOM	617	N	VAL	A	92	11.458	-1.944	5.632	1.00	10.73	N
	ATOM	618	CA	VAL	A	92	11.299	-3.407	5.697	1.00	10.99	C
	ATOM	619	CB	VAL	A	92	9.793	-3.851	5.695	1.00	11.84	C
	ATOM	620	CG1	VAL	A	92	9.678	-5.385	5.801	1.00	13.35	C
30	ATOM	621	CG2	VAL	A	92	9.017	-3.208	6.834	1.00	13.66	C
	ATOM	622	C	VAL	A	92	12.006	-4.045	4.510	1.00	11.05	C
	ATOM	623	O	VAL	A	92	11.892	-3.565	3.384	1.00	10.48	O
	ATOM	624	N	ASP	A	93	12.740	-5.122	4.763	1.00	10.40	N
	ATOM	625	CA	ASP	A	93	13.310	-5.897	3.667	1.00	9.71	C
35	ATOM	626	CB	ASP	A	93	14.787	-5.539	3.453	1.00	9.55	C

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	ATOM	627	CG	ASP	A	93	15.681	-5.981	4.616	1.00	10.76	C
	ATOM	628	OD1	ASP	A	93	15.806	-7.213	4.839	1.00	9.33	O
	ATOM	629	OD2	ASP	A	93	16.274	-5.092	5.281	1.00	9.54	O
	ATOM	630	C	ASP	A	93	13.104	-7.391	3.892	1.00	9.21	C
5	ATOM	631	O	ASP	A	93	12.822	-7.826	5.014	1.00	9.76	O
	ATOM	632	N	THR	A	94	13.235	-8.157	2.811	1.00	9.50	N
	ATOM	633	CA	THR	A	94	13.161	-9.615	2.857	1.00	9.63	C
	ATOM	634	CB	THR	A	94	12.154	-10.127	1.814	1.00	9.66	C
	ATOM	635	OG1	THR	A	94	12.515	-9.614	0.522	1.00	9.37	O
10	ATOM	636	CG2	THR	A	94	10.723	-9.661	2.180	1.00	10.71	C
	ATOM	637	C	THR	A	94	14.558	-10.217	2.628	1.00	9.85	C
	ATOM	638	O	THR	A	94	14.728	-11.230	1.908	1.00	9.56	O
	ATOM	639	N	GLY	A	95	15.562	-9.557	3.214	1.00	9.79	N
	ATOM	640	CA	GLY	A	95	16.942	-10.049	3.176	1.00	9.03	C
15	ATOM	641	C	GLY	A	95	17.144	-11.252	4.095	1.00	8.81	C
	ATOM	642	O	GLY	A	95	16.180	-11.857	4.589	1.00	9.25	O
	ATOM	643	N	ILE	A	96	18.406	-11.596	4.321	1.00	9.49	N
	ATOM	644	CA	ILE	A	96	18.768	-12.795	5.086	1.00	9.45	C
	ATOM	645	CB	ILE	A	96	20.299	-13.093	4.960	1.00	8.65	C
20	ATOM	646	CG1	ILE	A	96	20.602	-14.576	5.275	1.00	10.28	C
	ATOM	647	CD1	ILE	A	96	21.922	-15.058	4.678	1.00	12.46	C
	ATOM	648	CG2	ILE	A	96	21.124	-12.095	5.762	1.00	7.80	C
	ATOM	649	C	ILE	A	96	18.301	-12.761	6.553	1.00	9.50	C
	ATOM	650	O	ILE	A	96	18.125	-13.805	7.176	1.00	10.01	O
25	ATOM	651	N	GLY	A	97	18.063	-11.560	7.079	1.00	9.00	N
	ATOM	652	CA	GLY	A	97	17.724	-11.390	8.484	1.00	9.76	C
	ATOM	653	C	GLY	A	97	18.952	-11.614	9.357	1.00	9.55	C
	ATOM	654	O	GLY	A	97	20.073	-11.755	8.853	1.00	8.93	O
	ATOM	655	N	MET	A	98	18.739	-11.651	10.666	1.00	10.02	N
30	ATOM	656	CA	MET	A	98	19.833	-11.848	11.620	1.00	11.29	C
	ATOM	657	CB	MET	A	98	20.257	-10.510	12.239	1.00	12.22	C
	ATOM	658	CG	MET	A	98	20.915	-9.539	11.254	1.00	10.95	C
	ATOM	659	SD	MET	A	98	21.099	-7.874	11.966	1.00	12.92	S
	ATOM	660	CE	MET	A	98	19.416	-7.273	11.787	1.00	13.18	C
35	ATOM	661	C	MET	A	98	19.402	-12.807	12.724	1.00	11.94	C

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	ATOM	662	O	MET A 98	18.307	-12.677	13.264	1.00	12.18	O
	ATOM	663	N	THR A 99	20.265	-13.766	13.051	1.00	11.17	N
	ATOM	664	CA	THR A 99	20.076	-14.593	14.252	1.00	11.75	C
	ATOM	665	CB	THR A 99	21.130	-15.725	14.332	1.00	11.30	C
5	ATOM	666	OG1	THR A 99	22.426	-15.148	14.525	1.00	11.69	O
	ATOM	667	CG2	THR A 99	21.146	-16.580	13.027	1.00	13.44	C
	ATOM	668	C	THR A 99	20.178	-13.703	15.506	1.00	11.41	C
	ATOM	669	O	THR A 99	20.651	-12.558	15.426	1.00	11.00	O
	ATOM	670	N	LYS A 100	19.739	-14.214	16.657	1.00	11.40	N
10	ATOM	671	CA	LYS A 100	19.914	-13.487	17.914	1.00	11.12	C
	ATOM	672	CB	LYS A 100	19.465	-14.322	19.114	1.00	11.79	C
	ATOM	673	CG	LYS A 100	19.328	-13.509	20.383	1.00	12.71	C
	ATOM	674	CD	LYS A 100	19.140	-14.418	21.602	1.00	15.02	C
	ATOM	675	CE	LYS A 100	19.034	-13.587	22.862	1.00	16.41	C
15	ATOM	676	NZ	LYS A 100	18.973	-14.460	24.083	1.00	17.00	N
	ATOM	677	C	LYS A 100	21.369	-13.045	18.116	1.00	11.28	C
	ATOM	678	O	LYS A 100	21.618	-11.890	18.468	1.00	10.13	O
	ATOM	679	N	ALA A 101	22.314	-13.969	17.907	1.00	11.14	N
	ATOM	680	CA	ALA A 101	23.746	-13.668	18.048	1.00	12.44	C
20	ATOM	681	CB	ALA A 101	24.593	-14.933	17.872	1.00	12.98	C
	ATOM	682	C	ALA A 101	24.200	-12.587	17.067	1.00	12.35	C
	ATOM	683	O	ALA A 101	24.908	-11.664	17.483	1.00	12.09	O
	ATOM	684	N	ASP A 102	23.801	-12.722	15.790	1.00	13.28	N
	ATOM	685	CA	ASP A 102	24.096	-11.742	14.714	1.00	13.41	C
25	ATOM	686	CB	ASP A 102	23.347	-12.051	13.397	1.00	15.35	C
	ATOM	687	CG	ASP A 102	23.854	-13.285	12.621	1.00	18.57	C
	ATOM	688	OD1	ASP A 102	25.034	-13.708	12.735	1.00	16.05	O
	ATOM	689	OD2	ASP A 102	23.011	-13.804	11.824	1.00	20.05	O
	ATOM	690	C	ASP A 102	23.601	-10.348	15.132	1.00	12.87	C
30	ATOM	691	O	ASP A 102	24.301	-9.348	14.972	1.00	11.23	O
	ATOM	692	N	LEU A 103	22.366	-10.295	15.631	1.00	11.78	N
	ATOM	693	CA	LEU A 103	21.713	-9.038	16.001	1.00	11.81	C
	ATOM	694	CB	LEU A 103	20.272	-9.318	16.449	1.00	11.27	C
	ATOM	695	CG	LEU A 103	19.378	-8.142	16.849	1.00	11.19	C
35	ATOM	696	CD1	LEU A 103	19.219	-7.138	15.690	1.00	10.35	C

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	ATOM	697	CD2 LEU A 103	18.033	-8.711	17.282	1.00	11.00	C
	ATOM	698	C LEU A 103	22.472	-8.299	17.101	1.00	11.88	C
	ATOM	699	O LEU A 103	22.764	-7.098	16.987	1.00	11.49	O
	ATOM	700	N ILE A 104	22.771	-9.026	18.174	1.00	10.96	N
5	ATOM	701	CA ILE A 104	23.526	-8.490	19.292	1.00	11.02	C
	ATOM	702	CB ILE A 104	23.602	-9.521	20.455	1.00	10.34	C
	ATOM	703	CG1 ILE A 104	22.189	-9.773	21.007	1.00	10.25	C
	ATOM	704	CD1 ILE A 104	22.069	-11.072	21.835	1.00	11.31	C
	ATOM	705	CG2 ILE A 104	24.592	-9.044	21.548	1.00	11.10	C
10	ATOM	706	C ILE A 104	24.922	-8.016	18.862	1.00	10.88	C
	ATOM	707	O ILE A 104	25.330	-6.902	19.200	1.00	10.35	O
	ATOM	708	N ASN A 105	25.615	-8.832	18.068	1.00	11.26	N
	ATOM	709	CA ASN A 105	26.965	-8.493	17.620	1.00	12.75	C
	ATOM	710	CB ASN A 105	27.652	-9.702	16.975	1.00	13.63	C
15	ATOM	711	CG ASN A 105	29.151	-9.489	16.782	1.00	18.15	C
	ATOM	712	OD1 ASN A 105	29.644	-9.433	15.648	1.00	22.67	O
	ATOM	713	ND2 ASN A 105	29.885	-9.374	17.891	1.00	20.72	N
	ATOM	714	C ASN A 105	26.983	-7.304	16.659	1.00	11.53	C
	ATOM	715	O ASN A 105	27.780	-6.368	16.828	1.00	10.90	O
20	ATOM	716	N ASN A 106	26.091	-7.336	15.674	1.00	11.55	N
	ATOM	717	CA ASN A 106	26.052	-6.308	14.636	1.00	12.20	C
	ATOM	718	CB ASN A 106	25.019	-6.636	13.555	1.00	12.61	C
	ATOM	719	CG ASN A 106	25.440	-7.773	12.659	1.00	12.13	C
	ATOM	720	OD1 ASN A 106	26.610	-8.160	12.618	1.00	14.77	O
25	ATOM	721	ND2 ASN A 106	24.478	-8.323	11.933	1.00	12.05	N
	ATOM	722	C ASN A 106	25.740	-4.933	15.176	1.00	12.88	C
	ATOM	723	O ASN A 106	26.255	-3.935	14.670	1.00	13.74	O
	ATOM	724	N LEU A 107	24.870	-4.878	16.176	1.00	12.36	N
	ATOM	725	CA LEU A 107	24.405	-3.585	16.680	1.00	13.75	C
30	ATOM	726	CB LEU A 107	22.879	-3.561	16.815	1.00	13.90	C
	ATOM	727	CG LEU A 107	22.140	-3.852	15.489	1.00	14.03	C
	ATOM	728	CD1 LEU A 107	20.636	-3.673	15.638	1.00	15.24	C
	ATOM	729	CD2 LEU A 107	22.656	-3.007	14.333	1.00	14.81	C
	ATOM	730	C LEU A 107	25.105	-3.165	17.963	1.00	13.67	C
35	ATOM	731	O LEU A 107	25.244	-1.962	18.241	1.00	14.95	O

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	ATOM	732	N	GLY A 108	25.587	-4.148	18.715	1.00	12.35	N
	ATOM	733	CA	GLY A 108	26.187	-3.882	20.020	1.00	12.11	C
	ATOM	734	C	GLY A 108	27.691	-3.661	20.019	1.00	11.67	C
	ATOM	735	O	GLY A 108	28.236	-3.133	20.988	1.00	11.41	O
5	ATOM	736	N	THR A 109	28.365	-4.075	18.945	1.00	11.40	N
	ATOM	737	CA	THR A 109	29.838	-4.070	18.906	1.00	11.58	C
	ATOM	738	CB	THR A 109	30.414	-5.508	19.044	1.00	11.95	C
	ATOM	739	OG1	THR A 109	30.274	-6.205	17.798	1.00	11.34	O
	ATOM	740	CG2	THR A 109	29.706	-6.291	20.174	1.00	12.09	C
10	ATOM	741	C	THR A 109	30.391	-3.447	17.625	1.00	11.81	C
	ATOM	742	O	THR A 109	29.648	-3.188	16.677	1.00	10.58	O
	ATOM	743	N	ILE A 110	31.709	-3.237	17.594	1.00	11.92	N
	ATOM	744	CA	ILE A 110	32.391	-2.741	16.404	1.00	12.96	C
	ATOM	745	CB	ILE A 110	33.912	-2.511	16.674	1.00	13.50	C
15	ATOM	746	CG1	ILE A 110	34.125	-1.427	17.748	1.00	15.90	C
	ATOM	747	CD1	ILE A 110	33.319	-0.212	17.576	1.00	19.17	C
	ATOM	748	CG2	ILE A 110	34.686	-2.189	15.378	1.00	15.87	C
	ATOM	749	C	ILE A 110	32.192	-3.732	15.257	1.00	12.47	C
	ATOM	750	O	ILE A 110	32.089	-3.331	14.098	1.00	12.92	O
20	ATOM	751	N	ALA A 111	32.144	-5.023	15.593	1.00	11.93	N
	ATOM	752	CA	ALA A 111	31.835	-6.074	14.609	1.00	12.60	C
	ATOM	753	CB	ALA A 111	30.366	-5.996	14.185	1.00	11.98	C
	ATOM	754	C	ALA A 111	32.790	-5.975	13.405	1.00	11.78	C
	ATOM	755	O	ALA A 111	34.008	-5.986	13.610	1.00	11.62	O
25	ATOM	756	N	LYS A 112	32.255	-5.822	12.184	1.00	11.07	N
	ATOM	757	CA	LYS A 112	33.078	-5.815	10.953	1.00	11.50	C
	ATOM	758	CB	LYS A 112	32.358	-6.549	9.802	1.00	11.40	C
	ATOM	759	CG	LYS A 112	31.757	-7.903	10.172	1.00	13.47	C
	ATOM	760	CD	LYS A 112	31.086	-8.568	8.954	1.00	14.40	C
30	ATOM	761	CE	LYS A 112	30.534	-9.955	9.290	1.00	17.15	C
	ATOM	762	NZ	LYS A 112	29.730	-9.975	10.531	1.00	21.43	N
	ATOM	763	C	LYS A 112	33.470	-4.396	10.485	1.00	10.58	C
	ATOM	764	O	LYS A 112	34.102	-4.227	9.437	1.00	10.79	O
	ATOM	765	N	SER A 113	33.106	-3.386	11.272	1.00	10.26	N
35	ATOM	766	CA	SER A 113	33.216	-1.992	10.846	1.00	9.44	C

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	ATOM	767	CB	SER A 113	32.143	-1.154	11.549	1.00	9.90	C
	ATOM	768	OG	SER A 113	32.500	-0.955	12.916	1.00	9.83	O
	ATOM	769	C	SER A 113	34.574	-1.321	11.085	1.00	10.37	C
	ATOM	770	O	SER A 113	35.429	-1.824	11.834	1.00	9.27	O
5	ATOM	771	N	GLY A 114	34.729	-0.149	10.463	1.00	9.42	N
	ATOM	772	CA	GLY A 114	35.862	0.745	10.708	1.00	10.87	C
	ATOM	773	C	GLY A 114	35.468	1.875	11.650	1.00	11.32	C
	ATOM	774	O	GLY A 114	35.811	3.035	11.416	1.00	11.73	O
	ATOM	775	N	THR A 115	34.771	1.523	12.731	1.00	11.87	N
10	ATOM	776	CA	THR A 115	34.291	2.500	13.728	1.00	13.00	C
	ATOM	777	CB	THR A 115	33.544	1.811	14.904	1.00	13.12	C
	ATOM	778	OG1	THR A 115	32.287	1.281	14.450	1.00	11.85	O
	ATOM	779	CG2	THR A 115	33.282	2.797	16.050	1.00	13.11	C
	ATOM	780	C	THR A 115	35.393	3.409	14.290	1.00	14.31	C
15	ATOM	781	O	THR A 115	35.219	4.624	14.334	1.00	14.42	O
	ATOM	782	N	LYS A 116	36.520	2.846	14.718	1.00	14.85	N
	ATOM	783	CA	LYS A 116	37.554	3.731	15.285	1.00	16.59	C
	ATOM	784	CB	LYS A 116	38.674	3.001	16.019	1.00	17.65	C
	ATOM	785	CG	LYS A 116	38.902	1.573	15.670	1.00	21.26	C
20	ATOM	786	CD	LYS A 116	39.608	0.861	16.826	1.00	25.23	C
	ATOM	787	CE	LYS A 116	38.648	0.592	17.977	1.00	25.85	C
	ATOM	788	NZ	LYS A 116	38.969	-0.681	18.664	1.00	27.50	N
	ATOM	789	C	LYS A 116	38.128	4.697	14.255	1.00	15.57	C
	ATOM	790	O	LYS A 116	38.341	5.869	14.563	1.00	15.73	O
25	ATOM	791	N	ALA A 117	38.352	4.213	13.037	1.00	14.60	N
	ATOM	792	CA	ALA A 117	38.818	5.072	11.952	1.00	14.43	C
	ATOM	793	CB	ALA A 117	39.126	4.242	10.695	1.00	14.19	C
	ATOM	794	C	ALA A 117	37.799	6.183	11.646	1.00	14.90	C
	ATOM	795	O	ALA A 117	38.185	7.322	11.349	1.00	14.32	O
30	ATOM	796	N	PHE A 118	36.506	5.867	11.744	1.00	14.68	N
	ATOM	797	CA	PHE A 118	35.455	6.879	11.513	1.00	15.26	C
	ATOM	798	CB	PHE A 118	34.060	6.240	11.465	1.00	15.20	C
	ATOM	799	CG	PHE A 118	32.951	7.204	11.082	1.00	14.53	C
	ATOM	800	CD1	PHE A 118	33.064	8.024	9.957	1.00	15.09	C
35	ATOM	801	CE1	PHE A 118	32.028	8.908	9.592	1.00	15.25	C

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	ATOM	802	CZ	PHE A 118	30.872	8.966	10.362	1.00	14.47	C
	ATOM	803	CE2	PHE A 118	30.737	8.139	11.479	1.00	14.09	C
	ATOM	804	CD2	PHE A 118	31.782	7.267	11.837	1.00	15.16	C
	ATOM	805	C	PHE A 118	35.479	7.983	12.570	1.00	15.99	C
5	ATOM	806	O	PHE A 118	35.370	9.169	12.238	1.00	16.59	O
	ATOM	807	N	MET A 119	35.608	7.580	13.831	1.00	17.24	N
	ATOM	808	CA	MET A 119	35.661	8.527	14.947	1.00	18.91	C
	ATOM	809	CB	MET A 119	35.645	7.798	16.292	1.00	19.59	C
	ATOM	810	CG	MET A 119	34.343	7.023	16.592	1.00	21.27	C
10	ATOM	811	SD	MET A 119	32.865	8.046	16.577	1.00	27.11	S
	ATOM	812	CE	MET A 119	32.989	8.874	18.171	1.00	25.52	C
	ATOM	813	C	MET A 119	36.891	9.429	14.818	1.00	20.34	C
	ATOM	814	O	MET A 119	36.809	10.637	15.048	1.00	20.39	O
	ATOM	815	N	GLU A 120	38.019	8.836	14.432	1.00	21.19	N
15	ATOM	816	CA	GLU A 120	39.230	9.593	14.110	1.00	23.01	C
	ATOM	817	CB	GLU A 120	40.393	8.638	13.789	1.00	23.08	C
	ATOM	818	CG	GLU A 120	40.959	7.951	15.029	1.00	25.62	C
	ATOM	819	CD	GLU A 120	41.977	6.851	14.730	1.00	27.22	C
	ATOM	820	OE1	GLU A 120	42.584	6.342	15.701	1.00	31.70	O
20	ATOM	821	OE2	GLU A 120	42.167	6.478	13.544	1.00	32.30	O
	ATOM	822	C	GLU A 120	38.999	10.572	12.956	1.00	22.36	C
	ATOM	823	O	GLU A 120	39.412	11.738	13.029	1.00	22.25	O
	ATOM	824	N	ALA A 121	38.330	10.107	11.900	1.00	21.71	N
	ATOM	825	CA	ALA A 121	38.014	10.967	10.754	1.00	22.13	C
25	ATOM	826	CB	ALA A 121	37.442	10.148	9.572	1.00	21.35	C
	ATOM	827	C	ALA A 121	37.085	12.123	11.143	1.00	21.97	C
	ATOM	828	O	ALA A 121	37.300	13.252	10.707	1.00	22.09	O
	ATOM	829	N	LEU A 122	36.085	11.845	11.982	1.00	22.68	N
	ATOM	830	CA	LEU A 122	35.171	12.881	12.498	1.00	23.70	C
30	ATOM	831	CB	LEU A 122	34.051	12.252	13.328	1.00	23.60	C
	ATOM	832	CG	LEU A 122	32.652	12.106	12.708	1.00	24.24	C
	ATOM	833	CD1	LEU A 122	32.656	12.058	11.187	1.00	24.39	C
	ATOM	834	CD2	LEU A 122	31.912	10.913	13.326	1.00	24.70	C
	ATOM	835	C	LEU A 122	35.905	13.950	13.312	1.00	24.48	C
35	ATOM	836	O	LEU A 122	35.712	15.147	13.087	1.00	24.33	O

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	ATOM	837	N	GLN A 123	36.756	13.502	14.236	1.00	25.47	N
	ATOM	838	CA	GLN A 123	37.631	14.388	15.017	1.00	26.52	C
	ATOM	839	CB	GLN A 123	38.558	13.554	15.912	1.00	26.51	C
	ATOM	840	CG	GLN A 123	39.410	14.361	16.892	1.00	26.98	C
5	ATOM	841	CD	GLN A 123	40.236	13.474	17.811	1.00	27.22	C
	ATOM	844	C	GLN A 123	38.451	15.304	14.100	1.00	27.01	C
	ATOM	845	O	GLN A 123	38.653	16.485	14.403	1.00	28.00	O
	ATOM	846	N	ALA A 124	38.905	14.747	12.979	1.00	27.12	N
	ATOM	847	CA	ALA A 124	39.687	15.470	11.981	1.00	27.43	C
10	ATOM	848	CB	ALA A 124	40.519	14.489	11.162	1.00	27.08	C
	ATOM	849	C	ALA A 124	38.830	16.352	11.060	1.00	27.36	C
	ATOM	850	O	ALA A 124	39.364	17.022	10.168	1.00	28.48	O
	ATOM	851	N	GLY A 125	37.513	16.331	11.264	1.00	26.55	N
	ATOM	852	CA	GLY A 125	36.586	17.180	10.516	1.00	26.12	C
15	ATOM	853	C	GLY A 125	35.891	16.544	9.317	1.00	25.55	C
	ATOM	854	O	GLY A 125	35.329	17.262	8.481	1.00	25.95	O
	ATOM	855	N	ALA A 126	35.916	15.209	9.222	1.00	24.24	N
	ATOM	856	CA	ALA A 126	35.241	14.509	8.117	1.00	22.89	C
	ATOM	857	CB	ALA A 126	35.559	13.013	8.124	1.00	22.69	C
20	ATOM	858	C	ALA A 126	33.735	14.725	8.158	1.00	21.67	C
	ATOM	859	O	ALA A 126	33.154	15.022	9.214	1.00	21.63	O
	ATOM	860	N	ASP A 127	33.107	14.551	7.000	1.00	20.10	N
	ATOM	861	CA	ASP A 127	31.671	14.731	6.855	1.00	19.48	C
	ATOM	862	CB	ASP A 127	31.371	15.169	5.412	1.00	19.75	C
25	ATOM	863	CG	BASP A 127	29.966	15.734	5.267	0.40	18.87	C
	ATOM	864	CG	AASP A 127	29.922	14.999	4.997	0.60	20.92	C
	ATOM	865	OD1	BASP A 127	29.005	14.943	5.157	0.40	16.92	O
	ATOM	866	OD1A	AASP A 127	29.015	14.949	5.847	0.60	20.45	O
	ATOM	867	OD2	BASP A 127	29.819	16.973	5.283	0.40	18.03	O
30	ATOM	868	OD2A	AASP A 127	29.697	14.943	3.769	0.60	24.13	O
	ATOM	869	C	ASP A 127	30.960	13.432	7.246	1.00	19.41	C
	ATOM	870	O	ASP A 127	31.337	12.342	6.792	1.00	18.31	O
	ATOM	871	N	ILE A 128	29.942	13.534	8.090	1.00	18.30	N
	ATOM	872	CA	ILE A 128	29.323	12.297	8.570	1.00	18.70	C
35	ATOM	873	CB	ILE A 128	28.500	12.452	9.889	1.00	19.93	C

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	ATOM	874	CG1 ILE A 128	27.118	13.001	9.641	1.00	20.42	C
	ATOM	875	CD1 ILE A 128	26.078	11.953	9.834	1.00	22.91	C
	ATOM	876	CG2 ILE A 128	29.274	13.147	10.973	1.00	20.27	C
	ATOM	877	C ILE A 128	28.561	11.536	7.480	1.00	17.07	C
5	ATOM	878	O ILE A 128	28.222	10.370	7.679	1.00	16.42	O
	ATOM	879	N SER A 129	28.345	12.170	6.320	1.00	15.92	N
	ATOM	880	CA SER A 129	27.801	11.470	5.143	1.00	16.11	C
	ATOM	881	CB SER A 129	27.575	12.431	3.966	1.00	16.27	C
	ATOM	882	OG BSER A 129	28.796	12.836	3.369	0.40	14.70	O
10	ATOM	883	OG ASER A 129	27.198	11.724	2.795	0.60	19.71	O
	ATOM	884	C SER A 129	28.694	10.293	4.708	1.00	15.54	C
	ATOM	885	O SER A 129	28.241	9.394	3.984	1.00	14.42	O
	ATOM	886	N MET A 130	29.952	10.299	5.154	1.00	14.64	N
	ATOM	887	CA MET A 130	30.886	9.193	4.855	1.00	16.22	C
15	ATOM	888	CB MET A 130	32.333	9.647	5.046	1.00	16.22	C
	ATOM	889	CG MET A 130	32.769	10.804	4.159	1.00	18.84	C
	ATOM	890	SD MET A 130	34.467	11.251	4.566	1.00	22.79	S
	ATOM	891	CE MET A 130	35.340	9.814	3.938	1.00	22.23	C
	ATOM	892	C MET A 130	30.659	7.938	5.719	1.00	14.67	C
20	ATOM	893	O MET A 130	31.361	6.929	5.558	1.00	14.12	O
	ATOM	894	N ILE A 131	29.692	8.012	6.631	1.00	13.26	N
	ATOM	895	CA ILE A 131	29.492	6.982	7.661	1.00	12.85	C
	ATOM	896	CB ILE A 131	28.254	7.315	8.556	1.00	12.32	C
	ATOM	897	CG1 ILE A 131	28.150	6.340	9.733	1.00	12.52	C
25	ATOM	898	CD1 ILE A 131	27.261	6.845	10.872	1.00	12.64	C
	ATOM	899	CG2 ILE A 131	26.945	7.378	7.721	1.00	12.57	C
	ATOM	900	C ILE A 131	29.420	5.545	7.117	1.00	12.36	C
	ATOM	901	O ILE A 131	30.003	4.622	7.709	1.00	12.11	O
	ATOM	902	N GLY A 132	28.710	5.365	6.003	1.00	12.24	N
30	ATOM	903	CA GLY A 132	28.567	4.039	5.375	1.00	13.42	C
	ATOM	904	C GLY A 132	29.872	3.445	4.845	1.00	12.70	C
	ATOM	905	O GLY A 132	30.041	2.220	4.803	1.00	11.65	O
	ATOM	906	N GLN A 133	30.800	4.317	4.445	1.00	12.69	N
	ATOM	907	CA GLN A 133	32.134	3.900	3.985	1.00	12.26	C
35	ATOM	908	CB GLN A 133	32.902	5.100	3.435	1.00	11.97	C

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	ATOM	909	CG	GLN A 133	32.134	5.822	2.322	1.00	13.70	C
	ATOM	910	CD	GLN A 133	32.812	7.080	1.826	1.00	14.15	C
	ATOM	911	OE1	GLN A 133	32.146	7.998	1.342	1.00	19.35	O
	ATOM	912	NE2	GLN A 133	34.128	7.119	1.903	1.00	15.15	N
5	ATOM	913	C	GLN A 133	32.945	3.236	5.113	1.00	11.81	C
	ATOM	914	O	GLN A 133	33.920	2.538	4.858	1.00	11.22	O
	ATOM	915	N	PHE A 134	32.530	3.473	6.353	1.00	10.82	N
	ATOM	916	CA	PHE A 134	33.162	2.879	7.534	1.00	10.65	C
	ATOM	917	CB	PHE A 134	33.387	3.948	8.602	1.00	10.61	C
10	ATOM	918	CG	PHE A 134	34.386	5.001	8.204	1.00	10.76	C
	ATOM	919	CD1	PHE A 134	35.725	4.893	8.588	1.00	11.50	C
	ATOM	920	CE1	PHE A 134	36.650	5.877	8.228	1.00	11.47	C
	ATOM	921	CZ	PHE A 134	36.237	6.983	7.465	1.00	12.01	C
	ATOM	922	CE2	PHE A 134	34.901	7.099	7.080	1.00	12.13	C
15	ATOM	923	CD2	PHE A 134	33.984	6.103	7.445	1.00	11.38	C
	ATOM	924	C	PHE A 134	32.326	1.725	8.117	1.00	11.05	C
	ATOM	925	O	PHE A 134	32.651	1.191	9.177	1.00	12.11	O
	ATOM	926	N	GLY A 135	31.261	1.348	7.415	1.00	11.64	N
	ATOM	927	CA	GLY A 135	30.467	0.173	7.771	1.00	11.16	C
20	ATOM	928	C	GLY A 135	29.539	0.338	8.963	1.00	11.22	C
	ATOM	929	O	GLY A 135	29.079	-0.658	9.525	1.00	11.52	O
	ATOM	930	N	VAL A 136	29.246	1.592	9.334	1.00	10.51	N
	ATOM	931	CA	VAL A 136	28.355	1.889	10.462	1.00	11.27	C
	ATOM	932	CB	VAL A 136	29.138	2.449	11.701	1.00	10.79	C
25	ATOM	933	CG1	VAL A 136	29.846	1.309	12.447	1.00	12.74	C
	ATOM	934	CG2	VAL A 136	30.154	3.534	11.290	1.00	11.70	C
	ATOM	935	C	VAL A 136	27.190	2.828	10.090	1.00	10.53	C
	ATOM	936	O	VAL A 136	26.682	3.573	10.940	1.00	10.31	O
	ATOM	937	N	GLY A 137	26.767	2.768	8.826	1.00	9.86	N
30	ATOM	938	CA	GLY A 137	25.681	3.600	8.312	1.00	9.88	C
	ATOM	939	C	GLY A 137	24.386	3.497	9.112	1.00	9.66	C
	ATOM	940	O	GLY A 137	23.653	4.482	9.252	1.00	9.71	O
	ATOM	941	N	PHE A 138	24.106	2.314	9.661	1.00	9.74	N
	ATOM	942	CA	PHE A 138	22.920	2.136	10.515	1.00	9.74	C
35	ATOM	943	CB	PHE A 138	22.926	0.771	11.238	1.00	9.33	C

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	ATOM	944	CG	PHE A 138	21.906	0.673	12.343	1.00	10.52	C
	ATOM	945	CD1	PHE A 138	20.548	0.569	12.040	1.00	10.16	C
	ATOM	946	CE1	PHE A 138	19.585	0.483	13.055	1.00	11.64	C
	ATOM	947	CZ	PHE A 138	19.976	0.543	14.405	1.00	10.51	C
5	ATOM	948	CE2	PHE A 138	21.342	0.672	14.725	1.00	11.27	C
	ATOM	949	CD2	PHE A 138	22.298	0.734	13.689	1.00	10.91	C
	ATOM	950	C	PHE A 138	22.752	3.260	11.559	1.00	9.80	C
	ATOM	951	O	PHE A 138	21.646	3.764	11.749	1.00	10.15	O
	ATOM	952	N	TYR A 139	23.836	3.640	12.236	1.00	9.55	N
10	ATOM	953	CA	TYR A 139	23.731	4.598	13.341	1.00	10.29	C
	ATOM	954	CB	TYR A 139	24.997	4.612	14.208	1.00	10.76	C
	ATOM	955	CG	TYR A 139	25.270	3.244	14.797	1.00	11.25	C
	ATOM	956	CD1	TYR A 139	24.544	2.778	15.908	1.00	11.38	C
	ATOM	957	CE1	TYR A 139	24.781	1.477	16.438	1.00	12.99	C
15	ATOM	958	CZ	TYR A 139	25.740	0.672	15.832	1.00	12.57	C
	ATOM	959	OH	TYR A 139	26.022	-0.602	16.298	1.00	14.94	O
	ATOM	960	CE2	TYR A 139	26.438	1.112	14.727	1.00	13.72	C
	ATOM	961	CD2	TYR A 139	26.208	2.397	14.212	1.00	12.04	C
	ATOM	962	C	TYR A 139	23.339	6.007	12.908	1.00	9.77	C
20	ATOM	963	O	TYR A 139	22.935	6.806	13.749	1.00	9.74	O
	ATOM	964	N	SER A 140	23.438	6.301	11.611	1.00	10.33	N
	ATOM	965	CA	SER A 140	22.917	7.574	11.087	1.00	11.02	C
	ATOM	966	CB	SER A 140	23.267	7.771	9.603	1.00	11.70	C
	ATOM	967	OG	SER A 140	22.493	6.954	8.751	1.00	12.12	O
25	ATOM	968	C	SER A 140	21.397	7.711	11.315	1.00	10.92	C
	ATOM	969	O	SER A 140	20.853	8.808	11.199	1.00	10.40	O
	ATOM	970	N	ALA A 141	20.724	6.601	11.631	1.00	10.37	N
	ATOM	971	CA	ALA A 141	19.299	6.646	11.991	1.00	10.41	C
	ATOM	972	CB	ALA A 141	18.792	5.270	12.365	1.00	10.84	C
30	ATOM	973	C	ALA A 141	19.046	7.629	13.135	1.00	10.50	C
	ATOM	974	O	ALA A 141	17.994	8.289	13.179	1.00	10.15	O
	ATOM	975	N	TYR A 142	20.015	7.726	14.045	1.00	9.88	N
	ATOM	976	CA	TYR A 142	19.882	8.600	15.223	1.00	10.45	C
	ATOM	977	CB	TYR A 142	20.825	8.154	16.352	1.00	10.43	C
35	ATOM	978	CG	TYR A 142	20.369	6.840	16.940	1.00	11.00	C

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	ATOM	979	CD1 TYR A 142	19.367	6.804	17.911	1.00	9.34	C
	ATOM	980	CE1 TYR A 142	18.910	5.585	18.435	1.00	11.39	C
	ATOM	981	CZ TYR A 142	19.454	4.398	17.965	1.00	10.59	C
	ATOM	982	OH TYR A 142	19.032	3.195	18.452	1.00	10.88	O
5	ATOM	983	CE2 TYR A 142	20.440	4.413	16.986	1.00	10.40	C
	ATOM	984	CD2 TYR A 142	20.886	5.631	16.475	1.00	10.15	C
	ATOM	985	C TYR A 142	20.006	10.096	14.913	1.00	10.48	C
	ATOM	986	O TYR A 142	19.819	10.922	15.797	1.00	11.07	O
	ATOM	987	N LEU A 143	20.320	10.440	13.661	1.00	11.63	N
10	ATOM	988	CA LEU A 143	20.181	11.836	13.207	1.00	11.63	C
	ATOM	989	CB LEU A 143	20.698	12.007	11.773	1.00	11.64	C
	ATOM	990	CG LEU A 143	22.204	11.887	11.507	1.00	12.47	C
	ATOM	991	CD1 LEU A 143	22.476	11.872	9.999	1.00	14.95	C
	ATOM	992	CD2 LEU A 143	22.996	12.996	12.208	1.00	12.89	C
15	ATOM	993	C LEU A 143	18.712	12.261	13.279	1.00	11.85	C
	ATOM	994	O LEU A 143	18.393	13.410	13.603	1.00	11.79	O
	ATOM	995	N VAL A 144	17.817	11.318	12.997	1.00	11.34	N
	ATOM	996	CA VAL A 144	16.390	11.641	12.856	1.00	11.17	C
	ATOM	997	CB VAL A 144	15.861	11.384	11.398	1.00	10.85	C
20	ATOM	998	CG1 VAL A 144	16.613	12.236	10.375	1.00	11.54	C
	ATOM	999	CG2 VAL A 144	15.910	9.879	11.011	1.00	10.78	C
	ATOM	1000	C VAL A 144	15.498	10.959	13.895	1.00	11.24	C
	ATOM	1001	O VAL A 144	14.380	11.411	14.144	1.00	10.50	O
	ATOM	1002	N ALA A 145	16.007	9.885	14.505	1.00	11.51	N
25	ATOM	1003	CA ALA A 145	15.226	9.082	15.450	1.00	11.34	C
	ATOM	1004	CB ALA A 145	15.240	7.598	15.049	1.00	11.21	C
	ATOM	1005	C ALA A 145	15.721	9.243	16.878	1.00	11.84	C
	ATOM	1006	O ALA A 145	16.939	9.276	17.131	1.00	11.59	O
	ATOM	1007	N GLU A 146	14.766	9.345	17.802	1.00	12.21	N
30	ATOM	1008	CA GLU A 146	15.038	9.310	19.242	1.00	13.73	C
	ATOM	1009	CB GLU A 146	13.945	10.058	20.026	1.00	13.11	C
	ATOM	1010	CG GLU A 146	12.529	9.477	19.907	1.00	16.23	C
	ATOM	1011	CD GLU A 146	11.458	10.297	20.632	1.00	18.07	C
	ATOM	1012	OE1 GLU A 146	11.746	11.436	21.067	1.00	22.71	O
35	ATOM	1013	OE2 GLU A 146	10.316	9.796	20.749	1.00	20.80	O

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	ATOM	1014	C	GLU A 146	15.169	7.874	19.762	1.00	12.68	C
	ATOM	1015	O	GLU A 146	15.790	7.623	20.806	1.00	12.55	O
	ATOM	1016	N	LYS A 147	14.556	6.946	19.035	1.00	11.49	N
	ATOM	1017	CA	LYS A 147	14.573	5.527	19.380	1.00	11.46	C
5	ATOM	1018	CB	LYS A 147	13.386	5.162	20.284	1.00	11.45	C
	ATOM	1019	CG	LYS A 147	13.323	3.691	20.711	1.00	13.05	C
	ATOM	1020	CD	LYS A 147	12.185	3.422	21.709	1.00	13.29	C
	ATOM	1021	CE	LYS A 147	12.008	1.914	21.927	1.00	15.92	C
	ATOM	1022	NZ	LYS A 147	10.722	1.581	22.617	1.00	17.75	N
10	ATOM	1023	C	LYS A 147	14.502	4.755	18.071	1.00	10.29	C
	ATOM	1024	O	LYS A 147	13.808	5.170	17.141	1.00	9.22	O
	ATOM	1025	N	VAL A 148	15.228	3.640	18.013	1.00	8.62	N
	ATOM	1026	CA	VAL A 148	15.166	2.743	16.868	1.00	9.25	C
	ATOM	1027	CB	VAL A 148	16.483	2.738	16.048	1.00	8.81	C
15	ATOM	1028	CG1	VAL A 148	16.361	1.797	14.824	1.00	9.26	C
	ATOM	1029	CG2	VAL A 148	16.879	4.173	15.590	1.00	9.55	C
	ATOM	1030	C	VAL A 148	14.843	1.337	17.366	1.00	9.58	C
	ATOM	1031	O	VAL A 148	15.420	0.869	18.357	1.00	10.42	O
	ATOM	1032	N	THR A 149	13.905	0.688	16.687	1.00	10.55	N
20	ATOM	1033	CA	THR A 149	13.573	-0.705	16.942	1.00	10.52	C
	ATOM	1034	CB	THR A 149	12.070	-0.880	17.285	1.00	11.46	C
	ATOM	1035	OG1	THR A 149	11.730	-0.088	18.434	1.00	11.99	O
	ATOM	1036	CG2	THR A 149	11.741	-2.356	17.574	1.00	11.50	C
	ATOM	1037	C	THR A 149	13.932	-1.511	15.684	1.00	10.47	C
25	ATOM	1038	O	THR A 149	13.616	-1.108	14.559	1.00	10.92	O
	ATOM	1039	N	VAL A 150	14.597	-2.641	15.876	1.00	9.28	N
	ATOM	1040	CA	VAL A 150	14.968	-3.501	14.761	1.00	9.73	C
	ATOM	1041	CB	VAL A 150	16.519	-3.594	14.579	1.00	9.45	C
	ATOM	1042	CG1	VAL A 150	16.886	-4.620	13.488	1.00	9.41	C
30	ATOM	1043	CG2	VAL A 150	17.144	-2.200	14.287	1.00	10.22	C
	ATOM	1044	C	VAL A 150	14.370	-4.878	15.040	1.00	10.40	C
	ATOM	1045	O	VAL A 150	14.708	-5.501	16.045	1.00	9.84	O
	ATOM	1046	N	ILE A 151	13.449	-5.298	14.168	1.00	10.59	N
	ATOM	1047	CA	ILE A 151	12.799	-6.608	14.245	1.00	11.07	C
35	ATOM	1048	CB	ILE A 151	11.269	-6.505	13.982	1.00	11.91	C

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	ATOM	1049	CG1 ILE A 151	10.617	-5.352	14.765	1.00	14.73	C
	ATOM	1050	CD1 ILE A 151	10.424	-5.587	16.223	1.00	16.38	C
	ATOM	1051	CG2 ILE A 151	10.586	-7.874	14.170	1.00	11.87	C
	ATOM	1052	C ILE A 151	13.415	-7.454	13.128	1.00	10.32	C
5	ATOM	1053	O ILE A 151	13.531	-6.993	11.988	1.00	11.10	O
	ATOM	1054	N THR A 152	13.808	-8.681	13.437	1.00	9.11	N
	ATOM	1055	CA THR A 152	14.515	-9.485	12.444	1.00	8.95	C
	ATOM	1056	CB THR A 152	16.062	-9.207	12.478	1.00	8.55	C
	ATOM	1057	OG1 THR A 152	16.686	-9.719	11.297	1.00	9.56	O
10	ATOM	1058	CG2 THR A 152	16.747	-9.800	13.725	1.00	8.97	C
	ATOM	1059	C THR A 152	14.165	-10.964	12.557	1.00	8.98	C
	ATOM	1060	O THR A 152	13.842	-11.450	13.651	1.00	9.10	O
	ATOM	1061	N LYS A 153	14.171	-11.636	11.406	1.00	9.20	N
	ATOM	1062	CA LYS A 153	13.889	-13.071	11.313	1.00	9.40	C
15	ATOM	1063	CB LYS A 153	12.436	-13.318	10.894	1.00	9.84	C
	ATOM	1064	CG LYS A 153	12.059	-14.801	10.722	1.00	10.54	C
	ATOM	1065	CD LYS A 153	12.136	-15.558	12.059	1.00	11.68	C
	ATOM	1066	CE LYS A 153	11.639	-17.006	11.891	1.00	11.69	C
	ATOM	1067	NZ LYS A 153	12.614	-17.830	11.127	1.00	11.25	N
20	ATOM	1068	C LYS A 153	14.841	-13.699	10.299	1.00	10.10	C
	ATOM	1069	O LYS A 153	14.795	-13.378	9.105	1.00	9.31	O
	ATOM	1070	N HIS A 154	15.702	-14.579	10.808	1.00	10.30	N
	ATOM	1071	CA HIS A 154	16.634	-15.367	10.007	1.00	11.27	C
	ATOM	1072	CB HIS A 154	18.017	-15.363	10.685	1.00	10.97	C
25	ATOM	1073	CG HIS A 154	19.098	-16.034	9.888	1.00	13.07	C
	ATOM	1074	ND1 HIS A 154	19.237	-17.405	9.828	1.00	13.64	N
	ATOM	1075	CE1 HIS A 154	20.279	-17.709	9.072	1.00	15.54	C
	ATOM	1076	NE2 HIS A 154	20.830	-16.583	8.649	1.00	14.99	N
	ATOM	1077	CD2 HIS A 154	20.114	-15.521	9.153	1.00	14.07	C
30	ATOM	1078	C HIS A 154	16.062	-16.795	9.912	1.00	11.34	C
	ATOM	1079	O HIS A 154	15.387	-17.262	10.833	1.00	11.23	O
	ATOM	1080	N ASN A 155	16.323	-17.473	8.802	1.00	11.83	N
	ATOM	1081	CA ASN A 155	15.835	-18.850	8.611	1.00	12.98	C
	ATOM	1082	CB ASN A 155	16.387	-19.453	7.311	1.00	12.71	C
35	ATOM	1083	CG ASN A 155	15.650	-18.960	6.083	1.00	13.41	C

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	ATOM	1084	OD1 ASN A 155	14.481 -18.559	6.162	1.00	16.73	O
	ATOM	1085	ND2 ASN A 155	16.328 -18.971	4.941	1.00	13.18	N
	ATOM	1086	C ASN A 155	16.155 -19.769	9.788	1.00	13.60	C
	ATOM	1087	O ASN A 155	15.345 -20.627	10.132	1.00	14.49	O
5	ATOM	1088	N ASP A 156	17.311 -19.562	10.415	1.00	13.89	N
	ATOM	1089	CA ASP A 156	17.801 -20.470	11.460	1.00	14.80	C
	ATOM	1090	CB ASP A 156	19.306 -20.687	11.291	1.00	15.32	C
	ATOM	1091	CG ASP A 156	19.665 -21.330	9.959	1.00	14.91	C
	ATOM	1092	OD1 ASP A 156	18.810 -21.984	9.331	1.00	18.04	O
10	ATOM	1093	OD2 ASP A 156	20.815 -21.157	9.536	1.00	17.59	O
	ATOM	1094	C ASP A 156	17.507 -20.060	12.917	1.00	15.22	C
	ATOM	1095	O ASP A 156	18.048 -20.663	13.848	1.00	15.48	O
	ATOM	1096	N ASP A 157	16.664 -19.046	13.119	1.00	14.01	N
	ATOM	1097	CA ASP A 157	16.352 -18.569	14.469	1.00	13.75	C
15	ATOM	1098	CB ASP A 157	17.393 -17.515	14.918	1.00	14.14	C
	ATOM	1099	CG ASP A 157	17.612 -17.488	16.436	1.00	15.04	C
	ATOM	1100	OD1 ASP A 157	16.817 -18.089	17.197	1.00	14.44	O
	ATOM	1101	OD2 ASP A 157	18.598 -16.847	16.872	1.00	15.17	O
	ATOM	1102	C ASP A 157	14.918 -18.022	14.542	1.00	13.95	C
20	ATOM	1103	O ASP A 157	14.215 -17.995	13.529	1.00	13.29	O
	ATOM	1104	N GLU A 158	14.501 -17.622	15.744	1.00	13.92	N
	ATOM	1105	CA GLU A 158	13.188 -17.043	16.020	1.00	16.01	C
	ATOM	1106	CB GLU A 158	12.895 -17.117	17.520	1.00	16.63	C
	ATOM	1107	CG GLU A 158	12.503 -18.458	18.109	1.00	21.65	C
25	ATOM	1108	CD GLU A 158	11.867 -18.273	19.497	1.00	22.79	C
	ATOM	1109	OE1 GLU A 158	12.509 -17.645	20.375	1.00	28.71	O
	ATOM	1110	OE2 GLU A 158	10.711 -18.720	19.701	1.00	28.30	O
	ATOM	1111	C GLU A 158	13.179 -15.560	15.638	1.00	13.84	C
	ATOM	1112	O GLU A 158	14.223 -14.989	15.321	1.00	13.41	O
30	ATOM	1113	N GLN A 159	12.007 -14.937	15.705	1.00	12.73	N
	ATOM	1114	CA GLN A 159	11.908 -13.501	15.430	1.00	12.21	C
	ATOM	1115	CB GLN A 159	10.512 -13.162	14.919	1.00	12.18	C
	ATOM	1116	CG GLN A 159	10.346 -11.740	14.394	1.00	12.50	C
	ATOM	1117	CD GLN A 159	9.083 -11.606	13.562	1.00	15.28	C
35	ATOM	1118	OE1 GLN A 159	8.911 -12.312	12.561	1.00	16.38	O

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	ATOM	1119	NE2	GLN A 159	8.190	-10.711	13.973	1.00	13.95	N
	ATOM	1120	C	GLN A 159	12.240	-12.717	16.698	1.00	11.76	C
	ATOM	1121	O	GLN A 159	11.682	-13.006	17.773	1.00	12.26	O
	ATOM	1122	N	TYR A 160	13.155	-11.748	16.570	1.00	11.87	N
5	ATOM	1123	CA	TYR A 160	13.639	-10.933	17.705	1.00	12.58	C
	ATOM	1124	CB	TYR A 160	15.136	-11.172	17.945	1.00	14.94	C
	ATOM	1125	CG	TYR A 160	15.446	-12.550	18.460	1.00	17.46	C
	ATOM	1126	CD1	TYR A 160	15.331	-12.852	19.818	1.00	18.82	C
	ATOM	1127	CE1	TYR A 160	15.610	-14.141	20.291	1.00	21.20	C
10	ATOM	1128	CZ	TYR A 160	15.993	-15.128	19.397	1.00	20.51	C
	ATOM	1129	OH	TYR A 160	16.277	-16.408	19.843	1.00	23.99	O
	ATOM	1130	CE2	TYR A 160	16.109	-14.848	18.045	1.00	20.45	C
	ATOM	1131	CD2	TYR A 160	15.838	-13.559	17.587	1.00	18.88	C
	ATOM	1132	C	TYR A 160	13.429	-9.443	17.477	1.00	11.58	C
15	ATOM	1133	O	TYR A 160	13.427	-8.992	16.329	1.00	11.28	O
	ATOM	1134	N	ALA A 161	13.268	-8.698	18.577	1.00	10.77	N
	ATOM	1135	CA	ALA A 161	13.157	-7.247	18.557	1.00	10.80	C
	ATOM	1136	CB	ALA A 161	11.821	-6.791	19.146	1.00	11.47	C
	ATOM	1137	C	ALA A 161	14.303	-6.661	19.365	1.00	10.52	C
20	ATOM	1138	O	ALA A 161	14.448	-6.955	20.559	1.00	10.91	O
	ATOM	1139	N	TRP A 162	15.122	-5.858	18.696	1.00	10.98	N
	ATOM	1140	CA	TRP A 162	16.177	-5.058	19.322	1.00	10.73	C
	ATOM	1141	CB	TRP A 162	17.430	-5.118	18.448	1.00	11.62	C
	ATOM	1142	CG	TRP A 162	18.612	-4.242	18.828	1.00	10.55	C
25	ATOM	1143	CD1	TRP A 162	19.754	-4.657	19.457	1.00	12.03	C
	ATOM	1144	NE1	TRP A 162	20.638	-3.605	19.584	1.00	11.19	N
	ATOM	1145	CE2	TRP A 162	20.080	-2.482	19.031	1.00	11.05	C
	ATOM	1146	CD2	TRP A 162	18.808	-2.844	18.525	1.00	11.28	C
	ATOM	1147	CE3	TRP A 162	18.026	-1.860	17.889	1.00	11.22	C
30	ATOM	1148	CZ3	TRP A 162	18.539	-0.553	17.783	1.00	11.18	C
	ATOM	1149	CH2	TRP A 162	19.812	-0.225	18.284	1.00	11.37	C
	ATOM	1150	CZ2	TRP A 162	20.599	-1.169	18.920	1.00	12.10	C
	ATOM	1151	C	TRP A 162	15.656	-3.622	19.396	1.00	11.36	C
	ATOM	1152	O	TRP A 162	14.927	-3.180	18.500	1.00	11.02	O
35	ATOM	1153	N	GLU A 163	16.012	-2.905	20.462	1.00	11.35	N

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	ATOM	1154	CA	GLU A 163	15.690	-1.468	20.559	1.00	11.13	C
	ATOM	1155	CB	GLU A 163	14.270	-1.219	21.129	1.00	12.20	C
	ATOM	1156	CG	GLU A 163	14.051	-1.631	22.596	1.00	13.42	C
	ATOM	1157	CD	GLU A 163	14.629	-0.635	23.619	1.00	16.75	C
5	ATOM	1158	OE1	GLU A 163	14.753	0.571	23.303	1.00	17.28	O
	ATOM	1159	OE2	GLU A 163	14.955	-1.069	24.748	1.00	16.61	O
	ATOM	1160	C	GLU A 163	16.715	-0.698	21.370	1.00	10.86	C
	ATOM	1161	O	GLU A 163	17.289	-1.220	22.335	1.00	9.07	O
	ATOM	1162	N	SER A 164	16.906	0.567	21.002	1.00	10.37	N
10	ATOM	1163	CA	SER A 164	17.723	1.464	21.806	1.00	10.24	C
	ATOM	1164	CB	SER A 164	19.219	1.324	21.479	1.00	9.55	C
	ATOM	1165	OG	SER A 164	19.995	2.116	22.372	1.00	10.11	O
	ATOM	1166	C	SER A 164	17.294	2.905	21.620	1.00	10.37	C
	ATOM	1167	O	SER A 164	17.034	3.352	20.493	1.00	10.35	O
15	ATOM	1168	N	SER A 165	17.252	3.624	22.738	1.00	11.39	N
	ATOM	1169	CA	SER A 165	17.134	5.083	22.723	1.00	13.13	C
	ATOM	1170	CB	SER A 165	16.111	5.544	23.765	1.00	13.33	C
	ATOM	1171	OG	SER A 165	14.833	5.039	23.455	1.00	13.43	O
	ATOM	1172	C	SER A 165	18.493	5.704	23.008	1.00	14.47	C
20	ATOM	1173	O	SER A 165	18.577	6.821	23.530	1.00	15.31	O
	ATOM	1174	N	ALA A 166	19.555	4.970	22.668	1.00	14.85	N
	ATOM	1175	CA	ALA A 166	20.933	5.363	22.959	1.00	16.58	C
	ATOM	1176	CB	ALA A 166	21.283	6.694	22.267	1.00	17.04	C
	ATOM	1177	C	ALA A 166	21.158	5.398	24.487	1.00	17.21	C
25	ATOM	1178	O	ALA A 166	20.555	4.604	25.210	1.00	18.47	O
	ATOM	1179	N	GLY A 167	21.991	6.301	24.990	1.00	17.88	N
	ATOM	1180	CA	GLY A 167	22.276	6.316	26.434	1.00	16.86	C
	ATOM	1181	C	GLY A 167	23.073	5.121	26.966	1.00	16.62	C
	ATOM	1182	O	GLY A 167	23.164	4.923	28.189	1.00	16.60	O
30	ATOM	1183	N	GLY A 168	23.642	4.319	26.058	1.00	15.44	N
	ATOM	1184	CA	GLY A 168	24.625	3.294	26.428	1.00	14.73	C
	ATOM	1185	C	GLY A 168	24.139	1.856	26.489	1.00	14.07	C
	ATOM	1186	O	GLY A 168	24.940	0.931	26.669	1.00	14.23	O
	ATOM	1187	N	SER A 169	22.829	1.658	26.372	1.00	13.27	N
35	ATOM	1188	CA	SER A 169	22.264	0.318	26.462	1.00	13.07	C

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	ATOM	1189	CB	SER A 169	21.659	0.070	27.856	1.00	14.10	C
	ATOM	1190	OG	SER A 169	20.510	0.866	28.070	1.00	16.96	O
	ATOM	1191	C	SER A 169	21.228	0.054	25.374	1.00	12.83	C
	ATOM	1192	O	SER A 169	20.690	0.996	24.762	1.00	10.83	O
5	ATOM	1193	N	PHE A 170	20.988	-1.235	25.135	1.00	11.59	N
	ATOM	1194	CA	PHE A 170	19.923	-1.694	24.255	1.00	11.75	C
	ATOM	1195	CB	PHE A 170	20.432	-1.942	22.828	1.00	11.47	C
	ATOM	1196	CG	PHE A 170	21.494	-3.029	22.694	1.00	11.29	C
	ATOM	1197	CD1	PHE A 170	21.132	-4.355	22.400	1.00	11.19	C
10	ATOM	1198	CE1	PHE A 170	22.103	-5.356	22.211	1.00	10.29	C
	ATOM	1199	CZ	PHE A 170	23.473	-5.030	22.308	1.00	9.75	C
	ATOM	1200	CE2	PHE A 170	23.850	-3.709	22.602	1.00	12.18	C
	ATOM	1201	CD2	PHE A 170	22.853	-2.709	22.781	1.00	10.29	C
	ATOM	1202	C	PHE A 170	19.277	-2.939	24.843	1.00	11.98	C
15	ATOM	1203	O	PHE A 170	19.836	-3.562	25.763	1.00	12.71	O
	ATOM	1204	N	THR A 171	18.096	-3.289	24.336	1.00	11.64	N
	ATOM	1205	CA	THR A 171	17.434	-4.527	24.773	1.00	11.18	C
	ATOM	1206	CB	THR A 171	16.094	-4.308	25.523	1.00	11.31	C
	ATOM	1207	OG1	THR A 171	15.109	-3.743	24.638	1.00	11.89	O
20	ATOM	1208	CG2	THR A 171	16.279	-3.437	26.776	1.00	12.93	C
	ATOM	1209	C	THR A 171	17.155	-5.437	23.597	1.00	10.95	C
	ATOM	1210	O	THR A 171	17.031	-4.980	22.458	1.00	11.07	O
	ATOM	1211	N	VAL A 172	17.076	-6.730	23.889	1.00	10.13	N
	ATOM	1212	CA	VAL A 172	16.631	-7.731	22.921	1.00	11.59	C
25	ATOM	1213	CB	VAL A 172	17.809	-8.606	22.405	1.00	11.02	C
	ATOM	1214	CG1	VAL A 172	17.310	-9.712	21.471	1.00	11.80	C
	ATOM	1215	CG2	VAL A 172	18.850	-7.739	21.689	1.00	12.26	C
	ATOM	1216	C	VAL A 172	15.590	-8.627	23.591	1.00	11.68	C
	ATOM	1217	O	VAL A 172	15.752	-9.041	24.749	1.00	11.80	O
30	ATOM	1218	N	ARG A 173	14.523	-8.919	22.859	1.00	11.81	N
	ATOM	1219	CA	ARG A 173	13.484	-9.823	23.335	1.00	13.39	C
	ATOM	1220	CB	ARG A 173	12.373	-9.036	24.048	1.00	12.89	C
	ATOM	1221	CG	ARG A 173	11.553	-8.107	23.133	1.00	13.96	C
	ATOM	1222	CD	ARG A 173	10.809	-7.045	23.930	1.00	14.00	C
35	ATOM	1223	NE	ARG A 173	11.700	-5.968	24.360	1.00	16.47	N

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	ATOM	1224	CZ	ARG A 173	11.410	-5.078	25.306	1.00	17.96	C
	ATOM	1225	NH1	ARG A 173	10.238	-5.119	25.943	1.00	18.39	N
	ATOM	1226	NH2	ARG A 173	12.289	-4.135	25.608	1.00	17.76	N
	ATOM	1227	C	ARG A 173	12.915	-10.597	22.151	1.00	13.93	C
5	ATOM	1228	O	ARG A 173	13.009	-10.152	21.007	1.00	13.76	O
	ATOM	1229	N	THR A 174	12.330	-11.758	22.421	1.00	15.43	N
	ATOM	1230	CA	THR A 174	11.591	-12.461	21.382	1.00	17.74	C
	ATOM	1231	CB	THR A 174	11.168	-13.874	21.835	1.00	18.33	C
	ATOM	1232	OG1	THR A 174	12.330	-14.588	22.273	1.00	21.25	O
10	ATOM	1233	CG2	THR A 174	10.557	-14.631	20.682	1.00	19.79	C
	ATOM	1234	C	THR A 174	10.391	-11.592	20.987	1.00	18.44	C
	ATOM	1235	O	THR A 174	9.717	-11.016	21.851	1.00	18.68	O
	ATOM	1236	N	ASP A 175	10.169	-11.444	19.685	1.00	19.37	N
	ATOM	1237	CA	ASP A 175	9.144	-10.533	19.189	1.00	21.33	C
15	ATOM	1238	CB	ASP A 175	9.489	-10.041	17.781	1.00	20.85	C
	ATOM	1239	CG	ASP A 175	8.539	-8.973	17.283	1.00	20.54	C
	ATOM	1240	OD1	ASP A 175	8.089	-8.139	18.097	1.00	21.95	O
	ATOM	1241	OD2	ASP A 175	8.257	-8.955	16.068	1.00	19.10	O
	ATOM	1242	C	ASP A 175	7.781	-11.217	19.186	1.00	23.16	C
20	ATOM	1243	O	ASP A 175	7.624	-12.275	18.581	1.00	23.49	O
	ATOM	1244	N	THR A 176	6.813	-10.595	19.859	1.00	25.66	N
	ATOM	1245	CA	THR A 176	5.419	-11.071	19.883	1.00	27.51	C
	ATOM	1246	CB	THR A 176	4.774	-10.921	21.290	1.00	27.91	C
	ATOM	1247	OG1	THR A 176	4.951	-9.580	21.762	1.00	29.60	O
25	ATOM	1248	CG2	THR A 176	5.397	-11.898	22.286	1.00	28.18	C
	ATOM	1249	C	THR A 176	4.545	-10.347	18.858	1.00	27.98	C
	ATOM	1251	N	GLY A 177	5.175	-9.538	18.008	1.00	28.08	N
	ATOM	1252	CA	GLY A 177	4.473	-8.834	16.943	1.00	28.03	C
	ATOM	1253	C	GLY A 177	4.140	-9.732	15.764	1.00	27.90	C
30	ATOM	1254	O	GLY A 177	4.293	-10.955	15.829	1.00	27.98	O
	ATOM	1255	N	GLU A 178	3.674	-9.115	14.683	1.00	27.63	N
	ATOM	1256	CA	GLU A 178	3.318	-9.830	13.468	1.00	27.87	C
	ATOM	1257	CB	GLU A 178	2.781	-8.840	12.437	1.00	27.83	C
	ATOM	1258	CG	GLU A 178	2.438	-9.441	11.092	1.00	30.92	C
35	ATOM	1259	CD	GLU A 178	2.044	-8.387	10.073	1.00	31.91	C

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	ATOM	1260	OE1	GLU A 178	1.702	-7.252	10.484	1.00	34.87	O
	ATOM	1261	OE2	GLU A 178	2.080	-8.698	8.857	1.00	36.63	O
	ATOM	1262	C	GLU A 178	4.529	-10.598	12.916	1.00	25.85	C
	ATOM	1263	O	GLU A 178	5.592	-10.010	12.717	1.00	24.55	O
5	ATOM	1264	N	PRO A 179	4.372	-11.920	12.693	1.00	24.96	N
	ATOM	1265	CA	PRO A 179	5.471	-12.729	12.151	1.00	24.42	C
	ATOM	1266	CB	PRO A 179	4.887	-14.146	12.097	1.00	24.55	C
	ATOM	1267	CG	PRO A 179	3.718	-14.123	13.030	1.00	24.93	C
	ATOM	1268	CD	PRO A 179	3.170	-12.735	12.955	1.00	25.26	C
10	ATOM	1269	C	PRO A 179	5.878	-12.280	10.756	1.00	23.98	C
	ATOM	1270	O	PRO A 179	5.021	-12.011	9.912	1.00	23.84	O
	ATOM	1271	N	MET A 180	7.185	-12.174	10.541	1.00	22.51	N
	ATOM	1272	CA	MET A 180	7.745	-11.933	9.220	1.00	22.89	C
	ATOM	1273	CB	MET A 180	8.931	-10.969	9.312	1.00	22.66	C
15	ATOM	1274	CG	MET A 180	8.693	-9.708	10.133	1.00	24.51	C
	ATOM	1275	SD	MET A 180	10.273	-8.936	10.605	1.00	27.14	S
	ATOM	1276	CE	MET A 180	10.936	-8.538	9.003	1.00	25.48	C
	ATOM	1277	C	MET A 180	8.243	-13.284	8.716	1.00	21.09	C
	ATOM	1278	O	MET A 180	8.714	-14.103	9.502	1.00	22.18	O
20	ATOM	1279	N	GLY A 181	8.150	-13.525	7.417	1.00	19.67	N
	ATOM	1280	CA	GLY A 181	8.694	-14.760	6.850	1.00	17.12	C
	ATOM	1281	C	GLY A 181	10.205	-14.819	7.047	1.00	15.63	C
	ATOM	1282	O	GLY A 181	10.737	-15.800	7.565	1.00	15.01	O
	ATOM	1283	N	ARG A 182	10.879	-13.738	6.656	1.00	13.97	N
25	ATOM	1284	CA	ARG A 182	12.336	-13.617	6.740	1.00	12.99	C
	ATOM	1285	CB	ARG A 182	13.009	-14.558	5.728	1.00	12.45	C
	ATOM	1286	CG	ARG A 182	14.542	-14.508	5.724	1.00	11.41	C
	ATOM	1287	CD	ARG A 182	15.126	-15.018	4.408	1.00	10.49	C
	ATOM	1288	NE	ARG A 182	14.769	-14.181	3.253	1.00	10.39	N
30	ATOM	1289	CZ	ARG A 182	13.960	-14.572	2.264	1.00	11.57	C
	ATOM	1290	NH1	ARG A 182	13.417	-15.793	2.289	1.00	11.61	N
	ATOM	1291	NH2	ARG A 182	13.697	-13.761	1.241	1.00	10.55	N
	ATOM	1292	C	ARG A 182	12.696	-12.173	6.398	1.00	11.93	C
	ATOM	1293	O	ARG A 182	12.121	-11.593	5.469	1.00	12.50	O
35	ATOM	1294	N	GLY A 183	13.641	-11.602	7.134	1.00	10.42	N

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	ATOM	1295	CA	GLY A 183	14.153	-10.277	6.792	1.00	11.40	C
	ATOM	1296	C	GLY A 183	14.280	-9.389	8.005	1.00	10.58	C
	ATOM	1297	O	GLY A 183	14.363	-9.878	9.138	1.00	10.37	O
	ATOM	1298	N	THR A 184	14.289	-8.081	7.760	1.00	9.48	N
5	ATOM	1299	CA	THR A 184	14.528	-7.103	8.807	1.00	10.26	C
	ATOM	1300	CB	THR A 184	16.016	-6.668	8.833	1.00	10.53	C
	ATOM	1301	OG1	THR A 184	16.825	-7.818	9.124	1.00	9.97	O
	ATOM	1302	CG2	THR A 184	16.292	-5.602	9.912	1.00	10.37	C
	ATOM	1303	C	THR A 184	13.611	-5.909	8.601	1.00	10.75	C
10	ATOM	1304	O	THR A 184	13.383	-5.477	7.468	1.00	10.74	O
	ATOM	1305	N	LYS A 185	13.102	-5.397	9.716	1.00	11.15	N
	ATOM	1306	CA	LYS A 185	12.307	-4.185	9.754	1.00	13.04	C
	ATOM	1307	CB	LYS A 185	10.860	-4.553	10.125	1.00	13.59	C
	ATOM	1308	CG	LYS A 185	10.046	-3.576	10.940	1.00	17.50	C
15	ATOM	1309	CD	LYS A 185	8.559	-4.019	11.003	1.00	16.69	C
	ATOM	1310	CE	LYS A 185	8.363	-5.334	11.768	1.00	18.37	C
	ATOM	1311	NZ	LYS A 185	6.901	-5.713	11.882	1.00	21.06	N
	ATOM	1312	C	LYS A 185	12.972	-3.213	10.730	1.00	11.63	C
	ATOM	1313	O	LYS A 185	13.212	-3.543	11.897	1.00	11.71	O
20	ATOM	1314	N	VAL A 186	13.307	-2.030	10.231	1.00	10.59	N
	ATOM	1315	CA	VAL A 186	13.909	-0.990	11.056	1.00	10.63	C
	ATOM	1316	CB	VAL A 186	15.173	-0.374	10.387	1.00	10.82	C
	ATOM	1317	CG1	VAL A 186	15.732	0.780	11.225	1.00	10.86	C
	ATOM	1318	CG2	VAL A 186	16.250	-1.447	10.173	1.00	10.03	C
25	ATOM	1319	C	VAL A 186	12.840	0.065	11.276	1.00	11.03	C
	ATOM	1320	O	VAL A 186	12.369	0.668	10.309	1.00	11.26	O
	ATOM	1321	N	ILE A 187	12.446	0.253	12.535	1.00	10.67	N
	ATOM	1322	CA	ILE A 187	11.423	1.244	12.894	1.00	11.58	C
	ATOM	1323	CB	ILE A 187	10.346	0.650	13.847	1.00	11.48	C
30	ATOM	1324	CG1	ILE A 187	9.783	-0.663	13.273	1.00	12.22	C
	ATOM	1325	CD1	ILE A 187	9.076	-1.552	14.297	1.00	13.63	C
	ATOM	1326	CG2	ILE A 187	9.232	1.681	14.119	1.00	11.02	C
	ATOM	1327	C	ILE A 187	12.090	2.462	13.531	1.00	10.60	C
	ATOM	1328	O	ILE A 187	12.677	2.365	14.606	1.00	11.36	O
35	ATOM	1329	N	LEU A 188	12.028	3.590	12.830	1.00	9.56	N

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	ATOM	1330	CA	LEU A 188	12.581	4.840	13.325	1.00	10.37	C
	ATOM	1331	CB	LEU A 188	13.113	5.680	12.147	1.00	10.23	C
	ATOM	1332	CG	LEU A 188	14.095	4.953	11.221	1.00	12.23	C
	ATOM	1333	CD1	LEU A 188	14.506	5.827	10.037	1.00	14.59	C
5	ATOM	1334	CD2	LEU A 188	15.320	4.494	12.001	1.00	12.81	C
	ATOM	1335	C	LEU A 188	11.478	5.590	14.047	1.00	10.14	C
	ATOM	1336	O	LEU A 188	10.500	6.005	13.415	1.00	10.10	O
	ATOM	1337	N	HIS A 189	11.624	5.742	15.363	1.00	9.90	N
	ATOM	1338	CA	HIS A 189	10.713	6.552	16.168	1.00	10.60	C
10	ATOM	1339	CB	HIS A 189	10.635	6.029	17.616	1.00	10.71	C
	ATOM	1340	CG	HIS A 189	10.318	4.564	17.719	1.00	11.39	C
	ATOM	1341	ND1	HIS A 189	9.045	4.091	17.960	1.00	13.91	N
	ATOM	1342	CE1	HIS A 189	9.066	2.767	17.990	1.00	13.48	C
	ATOM	1343	NE2	HIS A 189	10.309	2.365	17.793	1.00	12.97	N
15	ATOM	1344	CD2	HIS A 189	11.113	3.469	17.622	1.00	13.81	C
	ATOM	1345	C	HIS A 189	11.275	7.980	16.115	1.00	10.37	C
	ATOM	1346	O	HIS A 189	12.247	8.314	16.804	1.00	10.38	O
	ATOM	1347	N	LEU A 190	10.673	8.810	15.267	1.00	10.34	N
	ATOM	1348	CA	LEU A 190	11.276	10.091	14.909	1.00	10.85	C
20	ATOM	1349	CB	LEU A 190	10.615	10.682	13.650	1.00	10.38	C
	ATOM	1350	CG	LEU A 190	10.736	9.867	12.345	1.00	9.48	C
	ATOM	1351	CD1	LEU A 190	10.020	10.603	11.222	1.00	11.29	C
	ATOM	1352	CD2	LEU A 190	12.203	9.613	11.960	1.00	10.36	C
	ATOM	1353	C	LEU A 190	11.283	11.120	16.036	1.00	11.22	C
25	ATOM	1354	O	LEU A 190	10.366	11.174	16.856	1.00	11.82	O
	ATOM	1355	N	LYS A 191	12.349	11.916	16.056	1.00	11.72	N
	ATOM	1356	CA	LYS A 191	12.440	13.147	16.858	1.00	12.95	C
	ATOM	1357	CB	LYS A 191	13.795	13.829	16.604	1.00	11.94	C
	ATOM	1358	CG	LYS A 191	15.021	13.087	17.152	1.00	12.55	C
30	ATOM	1359	CD	LYS A 191	16.326	13.744	16.638	1.00	13.79	C
	ATOM	1360	CE	LYS A 191	17.559	12.908	16.986	1.00	13.32	C
	ATOM	1361	NZ	LYS A 191	18.830	13.580	16.544	1.00	15.56	N
	ATOM	1362	C	LYS A 191	11.301	14.099	16.473	1.00	13.03	C
	ATOM	1363	O	LYS A 191	10.861	14.119	15.326	1.00	12.73	O
35	ATOM	1364	N	GLU A 192	10.822	14.893	17.426	1.00	14.54	N

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	ATOM	1365	CA	GLU A 192	9.643	15.720	17.171	1.00	16.07	C
	ATOM	1366	CB	GLU A 192	9.139	16.409	18.455	1.00	17.37	C
	ATOM	1367	CG	GLU A 192	10.169	17.254	19.188	1.00	20.84	C
	ATOM	1368	CD	GLU A 192	9.592	17.955	20.427	1.00	21.85	C
5	ATOM	1369	OE1	GLU A 192	10.319	18.769	21.036	1.00	27.95	O
	ATOM	1370	OE2	GLU A 192	8.420	17.693	20.790	1.00	25.80	O
	ATOM	1371	C	GLU A 192	9.838	16.746	16.049	1.00	14.93	C
	ATOM	1372	O	GLU A 192	8.877	17.099	15.380	1.00	14.27	O
	ATOM	1373	N	ASP A 193	11.079	17.200	15.862	1.00	14.09	N
10	ATOM	1374	CA	ASP A 193	11.433	18.183	14.823	1.00	15.11	C
	ATOM	1375	CB	ASP A 193	12.650	19.008	15.260	1.00	15.74	C
	ATOM	1376	CG	ASP A 193	12.336	19.999	16.373	1.00	20.16	C
	ATOM	1377	OD1	ASP A 193	11.153	20.163	16.727	1.00	22.70	O
	ATOM	1378	OD2	ASP A 193	13.285	20.631	16.895	1.00	23.53	O
15	ATOM	1379	C	ASP A 193	11.752	17.539	13.470	1.00	14.05	C
	ATOM	1380	O	ASP A 193	12.113	18.241	12.515	1.00	13.15	O
	ATOM	1381	N	GLN A 194	11.627	16.214	13.381	1.00	13.72	N
	ATOM	1382	CA	GLN A 194	12.070	15.492	12.178	1.00	13.95	C
	ATOM	1383	CB	GLN A 194	13.199	14.500	12.526	1.00	14.01	C
20	ATOM	1384	CG	GLN A 194	14.459	15.154	13.140	1.00	14.25	C
	ATOM	1385	CD	GLN A 194	15.177	16.110	12.195	1.00	13.90	C
	ATOM	1386	OE1	GLN A 194	15.169	15.928	10.980	1.00	14.83	O
	ATOM	1387	NE2	GLN A 194	15.821	17.137	12.762	1.00	14.34	N
	ATOM	1388	C	GLN A 194	10.942	14.791	11.411	1.00	14.39	C
25	ATOM	1389	O	GLN A 194	11.178	13.811	10.682	1.00	13.72	O
	ATOM	1390	N	THR A 195	9.720	15.308	11.537	1.00	13.86	N
	ATOM	1391	CA	THR A 195	8.571	14.641	10.920	1.00	13.85	C
	ATOM	1392	CB	THR A 195	7.220	15.021	11.586	1.00	14.24	C
	ATOM	1393	OG1	THR A 195	6.963	16.409	11.367	1.00	15.88	O
30	ATOM	1394	CG2	THR A 195	7.255	14.739	13.076	1.00	15.87	C
	ATOM	1395	C	THR A 195	8.482	14.847	9.404	1.00	12.80	C
	ATOM	1396	O	THR A 195	7.632	14.246	8.764	1.00	12.11	O
	ATOM	1397	N	GLU A 196	9.368	15.664	8.828	1.00	13.07	N
	ATOM	1398	CA	GLU A 196	9.402	15.800	7.358	1.00	13.91	C
35	ATOM	1399	CB	GLU A 196	10.447	16.822	6.900	1.00	14.36	C

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	ATOM	1400	CG	GLU A 196	11.896	16.352	7.015	1.00	15.40	C
	ATOM	1401	CD	GLU A 196	12.883	17.489	6.866	1.00	16.02	C
	ATOM	1402	OE1	GLU A 196	13.014	18.275	7.826	1.00	18.52	O
	ATOM	1403	OE2	GLU A 196	13.519	17.600	5.796	1.00	17.58	O
5	ATOM	1404	C	GLU A 196	9.627	14.452	6.644	1.00	13.50	C
	ATOM	1405	O	GLU A 196	9.210	14.284	5.480	1.00	12.54	O
	ATOM	1406	N	TYR A 197	10.281	13.511	7.336	1.00	12.53	N
	ATOM	1407	CA	TYR A 197	10.589	12.174	6.769	1.00	12.92	C
	ATOM	1408	CB	TYR A 197	11.857	11.584	7.420	1.00	12.71	C
10	ATOM	1409	CG	TYR A 197	13.015	12.540	7.269	1.00	12.60	C
	ATOM	1410	CD1	TYR A 197	13.610	12.756	6.012	1.00	12.65	C
	ATOM	1411	CE1	TYR A 197	14.655	13.673	5.856	1.00	12.73	C
	ATOM	1412	CZ	TYR A 197	15.097	14.400	6.954	1.00	13.17	C
	ATOM	1413	OH	TYR A 197	16.132	15.293	6.786	1.00	14.00	O
15	ATOM	1414	CE2	TYR A 197	14.524	14.213	8.206	1.00	12.58	C
	ATOM	1415	CD2	TYR A 197	13.478	13.291	8.359	1.00	12.58	C
	ATOM	1416	C	TYR A 197	9.398	11.210	6.796	1.00	13.42	C
	ATOM	1417	O	TYR A 197	9.530	10.025	6.462	1.00	14.72	O
	ATOM	1418	N	LEU A 198	8.237	11.732	7.193	1.00	13.22	N
20	ATOM	1419	CA	LEU A 198	6.958	11.029	7.061	1.00	13.56	C
	ATOM	1420	CB	LEU A 198	6.122	11.217	8.329	1.00	13.49	C
	ATOM	1421	CG	LEU A 198	6.844	10.766	9.600	1.00	14.54	C
	ATOM	1422	CD1	LEU A 198	6.027	11.101	10.840	1.00	17.77	C
	ATOM	1423	CD2	LEU A 198	7.165	9.282	9.511	1.00	16.57	C
25	ATOM	1424	C	LEU A 198	6.175	11.517	5.839	1.00	14.29	C
	ATOM	1425	O	LEU A 198	5.130	10.961	5.494	1.00	14.16	O
	ATOM	1426	N	GLU A 199	6.672	12.575	5.206	1.00	14.37	N
	ATOM	1427	CA	GLU A 199	6.041	13.109	3.999	1.00	15.37	C
	ATOM	1428	CB	GLU A 199	6.374	14.590	3.811	1.00	15.72	C
30	ATOM	1429	CG	GLU A 199	5.860	15.491	4.907	1.00	19.31	C
	ATOM	1430	CD	GLU A 199	4.349	15.432	5.061	1.00	24.17	C
	ATOM	1431	OE1	GLU A 199	3.624	15.315	4.042	1.00	26.25	O
	ATOM	1432	OE2	GLU A 199	3.887	15.511	6.215	1.00	26.37	O
	ATOM	1433	C	GLU A 199	6.445	12.316	2.762	1.00	14.22	C
35	ATOM	1434	O	GLU A 199	7.634	12.214	2.432	1.00	13.04	O

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	ATOM	1435	N	GLU A 200	5.455	11.745	2.076	1.00	14.20	N
	ATOM	1436	CA	GLU A 200	5.753	10.974	0.863	1.00	14.43	C
	ATOM	1437	CB	GLU A 200	4.498	10.320	0.257	1.00	14.82	C
	ATOM	1438	CG	GLU A 200	3.413	11.281	-0.179	1.00	17.91	C
5	ATOM	1442	C	GLU A 200	6.563	11.763	-0.187	1.00	14.44	C
	ATOM	1443	O	GLU A 200	7.494	11.215	-0.769	1.00	13.21	O
	ATOM	1444	N	ARG A 201	6.255	13.043	-0.401	1.00	13.78	N
	ATOM	1445	CA	ARG A 201	7.043	13.810	-1.376	1.00	14.78	C
	ATOM	1446	CB	ARG A 201	6.435	15.183	-1.674	1.00	16.40	C
10	ATOM	1447	CG	ARG A 201	6.565	16.222	-0.592	1.00	19.05	C
	ATOM	1448	CD	ARG A 201	5.701	17.426	-0.965	1.00	25.37	C
	ATOM	1449	NE	ARG A 201	5.816	18.537	-0.023	1.00	27.93	N
	ATOM	1450	CZ	ARG A 201	5.316	18.542	1.211	1.00	29.56	C
	ATOM	1451	NH1	ARG A 201	4.677	17.477	1.691	1.00	29.55	N
15	ATOM	1452	NH2	ARG A 201	5.475	19.617	1.977	1.00	29.79	N
	ATOM	1453	C	ARG A 201	8.516	13.917	-0.970	1.00	13.84	C
	ATOM	1454	O	ARG A 201	9.403	13.897	-1.824	1.00	13.54	O
	ATOM	1455	N	ARG A 202	8.762	14.039	0.335	1.00	12.69	N
	ATOM	1456	CA	ARG A 202	10.124	14.100	0.850	1.00	12.51	C
20	ATOM	1457	CB	ARG A 202	10.105	14.513	2.323	1.00	12.44	C
	ATOM	1458	CG	ARG A 202	11.486	14.690	2.974	1.00	13.80	C
	ATOM	1459	CD	ARG A 202	12.154	15.980	2.535	1.00	14.85	C
	ATOM	1460	NE	ARG A 202	13.319	16.285	3.362	1.00	15.02	N
	ATOM	1461	CZ	ARG A 202	14.583	16.146	2.970	1.00	13.59	C
25	ATOM	1462	NH1	ARG A 202	14.872	15.729	1.748	1.00	16.55	N
	ATOM	1463	NH2	ARG A 202	15.568	16.448	3.801	1.00	13.67	N
	ATOM	1464	C	ARG A 202	10.827	12.750	0.664	1.00	11.92	C
	ATOM	1465	O	ARG A 202	11.970	12.692	0.196	1.00	11.88	O
	ATOM	1466	N	ILE A 203	10.142	11.666	1.026	1.00	11.79	N
30	ATOM	1467	CA	ILE A 203	10.743	10.325	0.901	1.00	11.05	C
	ATOM	1468	CB	ILE A 203	9.843	9.213	1.488	1.00	11.47	C
	ATOM	1469	CG1	ILE A 203	9.597	9.465	2.980	1.00	10.38	C
	ATOM	1470	CD1	ILE A 203	8.418	8.702	3.568	1.00	12.56	C
	ATOM	1471	CG2	ILE A 203	10.498	7.839	1.285	1.00	10.79	C
35	ATOM	1472	C	ILE A 203	11.101	10.038	-0.566	1.00	11.67	C

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	ATOM	1473	O	ILE A 203	12.222	9.633	-0.877	1.00	11.27	O
	ATOM	1474	N	LYS A 204	10.141	10.273	-1.455	1.00	12.75	N
	ATOM	1475	CA	LYS A 204	10.313	10.035	-2.889	1.00	14.14	C
	ATOM	1476	CB	LYS A 204	9.111	10.578	-3.653	1.00	15.63	C
5	ATOM	1477	CG	LYS A 204	7.880	9.717	-3.636	1.00	19.18	C
	ATOM	1478	CD	LYS A 204	6.949	10.131	-4.796	1.00	22.73	C
	ATOM	1479	CE	LYS A 204	7.761	10.313	-6.080	1.00	24.17	C
	ATOM	1480	NZ	LYS A 204	7.112	9.813	-7.333	1.00	27.93	N
	ATOM	1481	C	LYS A 204	11.566	10.709	-3.434	1.00	14.06	C
10	ATOM	1482	O	LYS A 204	12.349	10.093	-4.165	1.00	13.72	O
	ATOM	1483	N	GLU A 205	11.756	11.975	-3.077	1.00	14.44	N
	ATOM	1484	CA	GLU A 205	12.909	12.729	-3.562	1.00	14.83	C
	ATOM	1485	CB	GLU A 205	12.749	14.235	-3.287	1.00	16.41	C
	ATOM	1486	CG	GLU A 205	13.870	15.094	-3.902	1.00	20.56	C
15	ATOM	1487	CD	GLU A 205	14.046	14.846	-5.407	1.00	25.90	C
	ATOM	1488	OE1	GLU A 205	15.207	14.654	-5.845	1.00	28.47	O
	ATOM	1489	OE2	GLU A 205	13.025	14.817	-6.149	1.00	27.03	O
	ATOM	1490	C	GLU A 205	14.240	12.202	-3.011	1.00	13.53	C
	ATOM	1491	O	GLU A 205	15.234	12.174	-3.736	1.00	12.53	O
20	ATOM	1492	N	ILE A 206	14.244	11.787	-1.744	1.00	11.97	N
	ATOM	1493	CA	ILE A 206	15.452	11.245	-1.100	1.00	11.36	C
	ATOM	1494	CB	ILE A 206	15.240	11.017	0.408	1.00	12.48	C
	ATOM	1495	CG1	ILE A 206	15.046	12.368	1.115	1.00	12.08	C
	ATOM	1496	CD1	ILE A 206	14.484	12.250	2.518	1.00	11.77	C
25	ATOM	1497	CG2	ILE A 206	16.433	10.266	1.044	1.00	12.39	C
	ATOM	1498	C	ILE A 206	15.863	9.953	-1.820	1.00	11.08	C
	ATOM	1499	O	ILE A 206	17.029	9.768	-2.147	1.00	9.36	O
	ATOM	1500	N	VAL A 207	14.883	9.093	-2.085	1.00	10.41	N
	ATOM	1501	CA	VAL A 207	15.124	7.837	-2.821	1.00	11.45	C
30	ATOM	1502	CB	VAL A 207	13.855	6.931	-2.834	1.00	11.10	C
	ATOM	1503	CG1	VAL A 207	14.000	5.775	-3.829	1.00	11.62	C
	ATOM	1504	CG2	VAL A 207	13.553	6.408	-1.442	1.00	11.82	C
	ATOM	1505	C	VAL A 207	15.680	8.103	-4.235	1.00	11.45	C
	ATOM	1506	O	VAL A 207	16.626	7.445	-4.664	1.00	11.63	O
35	ATOM	1507	N	LYS A 208	15.106	9.085	-4.935	1.00	11.78	N

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	ATOM	1508	CA	LYS A 208	15.554	9.459	-6.276	1.00	12.60	C
	ATOM	1509	CB	LYS A 208	14.585	10.486	-6.896	1.00	13.13	C
	ATOM	1510	CG	LYS A 208	14.925	10.864	-8.340	1.00	16.12	C
	ATOM	1513	NZ	LYS A 208	18.079	13.211	-8.901	1.00	42.08	N
5	ATOM	1514	C	LYS A 208	16.985	10.017	-6.252	1.00	12.84	C
	ATOM	1515	O	LYS A 208	17.788	9.711	-7.135	1.00	13.30	O
	ATOM	1516	N	LYS A 209	17.295	10.827	-5.242	1.00	11.91	N
	ATOM	1517	CA	LYS A 209	18.629	11.397	-5.107	1.00	12.80	C
	ATOM	1518	CB	LYS A 209	18.667	12.429	-3.977	1.00	13.37	C
10	ATOM	1519	CG	LYS A 209	18.132	13.802	-4.386	1.00	15.76	C
	ATOM	1520	CD	LYS A 209	18.016	14.706	-3.164	1.00	19.09	C
	ATOM	1521	CE	LYS A 209	19.306	15.443	-2.847	1.00	21.27	C
	ATOM	1522	NZ	LYS A 209	19.128	16.445	-1.725	1.00	22.04	N
	ATOM	1523	C	LYS A 209	19.708	10.345	-4.864	1.00	12.17	C
15	ATOM	1524	O	LYS A 209	20.710	10.327	-5.569	1.00	11.21	O
	ATOM	1525	N	HIS A 210	19.479	9.465	-3.887	1.00	10.88	N
	ATOM	1526	CA	HIS A 210	20.560	8.661	-3.295	1.00	11.55	C
	ATOM	1527	CB	HIS A 210	20.672	8.939	-1.788	1.00	11.51	C
	ATOM	1528	CG	HIS A 210	20.848	10.386	-1.446	1.00	12.48	C
20	ATOM	1529	ND1	HIS A 210	21.908	11.141	-1.908	1.00	13.86	N
	ATOM	1530	CE1	HIS A 210	21.797	12.377	-1.448	1.00	14.84	C
	ATOM	1531	NE2	HIS A 210	20.708	12.447	-0.701	1.00	14.09	N
	ATOM	1532	CD2	HIS A 210	20.092	11.218	-0.692	1.00	13.95	C
	ATOM	1533	C	HIS A 210	20.448	7.148	-3.471	1.00	11.80	C
25	ATOM	1534	O	HIS A 210	21.417	6.424	-3.200	1.00	12.26	O
	ATOM	1535	N	SER A 211	19.273	6.672	-3.873	1.00	11.26	N
	ATOM	1536	CA	SER A 211	19.023	5.225	-3.970	1.00	11.56	C
	ATOM	1537	CB	SER A 211	18.069	4.784	-2.846	1.00	10.69	C
	ATOM	1538	OG	SER A 211	18.613	5.057	-1.565	1.00	11.83	O
30	ATOM	1539	C	SER A 211	18.501	4.783	-5.347	1.00	11.39	C
	ATOM	1540	O	SER A 211	17.955	3.680	-5.494	1.00	11.31	O
	ATOM	1541	N	GLN A 212	18.676	5.623	-6.364	1.00	11.79	N
	ATOM	1542	CA	GLN A 212	18.100	5.309	-7.675	1.00	13.03	C
	ATOM	1543	CB	GLN A 212	18.066	6.532	-8.592	1.00	13.79	C
35	ATOM	1544	CG	GLN A 212	19.397	7.071	-8.950	1.00	16.37	C

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	ATOM	1548	C	GLN A 212	18.747	4.112	-8.375	1.00	11.98	C
	ATOM	1549	O	GLN A 212	18.131	3.513	-9.259	1.00	12.09	O
	ATOM	1550	N	PHE A 213	19.966	3.758	-7.960	1.00	10.91	N
	ATOM	1551	CA	PHE A 213	20.704	2.649	-8.573	1.00	11.14	C
5	ATOM	1552	CB	PHE A 213	22.069	3.137	-9.063	1.00	11.46	C
	ATOM	1553	CG	PHE A 213	21.965	4.143	-10.166	1.00	12.07	C
	ATOM	1554	CD1	PHE A 213	21.768	3.723	-11.481	1.00	13.51	C
	ATOM	1555	CE1	PHE A 213	21.646	4.653	-12.518	1.00	15.33	C
	ATOM	1556	CZ	PHE A 213	21.707	6.011	-12.237	1.00	14.78	C
10	ATOM	1557	CE2	PHE A 213	21.899	6.446	-10.925	1.00	14.00	C
	ATOM	1558	CD2	PHE A 213	22.020	5.507	-9.891	1.00	13.65	C
	ATOM	1559	C	PHE A 213	20.806	1.390	-7.706	1.00	11.15	C
	ATOM	1560	O	PHE A 213	21.578	0.471	-8.005	1.00	10.89	O
	ATOM	1561	N	ILE A 214	20.003	1.350	-6.642	1.00	11.08	N
15	ATOM	1562	CA	ILE A 214	19.702	0.098	-5.935	1.00	10.73	C
	ATOM	1563	CB	ILE A 214	18.911	0.363	-4.611	1.00	10.03	C
	ATOM	1564	CG1	ILE A 214	19.753	1.162	-3.591	1.00	10.42	C
	ATOM	1565	CD1	ILE A 214	20.918	0.389	-2.947	1.00	11.66	C
	ATOM	1566	CG2	ILE A 214	18.361	-0.941	-3.968	1.00	9.49	C
20	ATOM	1567	C	ILE A 214	18.853	-0.739	-6.907	1.00	10.72	C
	ATOM	1568	O	ILE A 214	17.882	-0.236	-7.470	1.00	11.92	O
	ATOM	1569	N	GLY A 215	19.214	-2.004	-7.103	1.00	10.20	N
	ATOM	1570	CA	GLY A 215	18.536	-2.833	-8.107	1.00	10.91	C
	ATOM	1571	C	GLY A 215	17.286	-3.536	-7.600	1.00	11.01	C
25	ATOM	1572	O	GLY A 215	16.409	-3.880	-8.387	1.00	11.64	O
	ATOM	1573	N	TYR A 216	17.216	-3.780	-6.292	1.00	10.67	N
	ATOM	1574	CA	TYR A 216	16.004	-4.356	-5.692	1.00	10.14	C
	ATOM	1575	CB	TYR A 216	16.274	-4.846	-4.258	1.00	10.19	C
	ATOM	1576	CG	TYR A 216	17.395	-5.851	-4.200	1.00	10.22	C
30	ATOM	1577	CD1	TYR A 216	17.169	-7.183	-4.571	1.00	10.45	C
	ATOM	1578	CE1	TYR A 216	18.178	-8.126	-4.520	1.00	11.09	C
	ATOM	1579	CZ	TYR A 216	19.443	-7.748	-4.107	1.00	10.58	C
	ATOM	1580	OH	TYR A 216	20.432	-8.700	-4.075	1.00	11.72	O
	ATOM	1581	CE2	TYR A 216	19.717	-6.431	-3.727	1.00	11.01	C
35	ATOM	1582	CD2	TYR A 216	18.673	-5.483	-3.768	1.00	10.70	C

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	ATOM	1583	C	TYR A 216	14.873	-3.341	-5.710	1.00	10.46	C
	ATOM	1584	O	TYR A 216	15.116	-2.135	-5.533	1.00	9.63	O
	ATOM	1585	N	PRO A 217	13.631	-3.811	-5.936	1.00	10.49	N
	ATOM	1586	CA	PRO A 217	12.485	-2.888	-5.937	1.00	11.31	C
5	ATOM	1587	CB	PRO A 217	11.272	-3.802	-6.192	1.00	11.58	C
	ATOM	1588	CG	PRO A 217	11.832	-5.102	-6.672	1.00	12.36	C
	ATOM	1589	CD	PRO A 217	13.235	-5.211	-6.190	1.00	11.02	C
	ATOM	1590	C	PRO A 217	12.327	-2.195	-4.583	1.00	11.27	C
	ATOM	1591	O	PRO A 217	12.338	-2.858	-3.551	1.00	11.96	O
10	ATOM	1592	N	ILE A 218	12.200	-0.871	-4.607	1.00	10.81	N
	ATOM	1593	CA	ILE A 218	11.895	-0.090	-3.416	1.00	10.93	C
	ATOM	1594	CB	ILE A 218	12.889	1.081	-3.207	1.00	10.90	C
	ATOM	1595	CG1	ILE A 218	14.333	0.568	-3.117	1.00	11.10	C
	ATOM	1596	CD1	ILE A 218	15.377	1.693	-3.291	1.00	10.36	C
15	ATOM	1597	CG2	ILE A 218	12.494	1.936	-1.966	1.00	11.21	C
	ATOM	1598	C	ILE A 218	10.495	0.481	-3.589	1.00	11.42	C
	ATOM	1599	O	ILE A 218	10.230	1.240	-4.539	1.00	10.98	O
	ATOM	1600	N	THR A 219	9.604	0.114	-2.678	1.00	10.40	N
	ATOM	1601	CA	THR A 219	8.221	0.572	-2.755	1.00	10.66	C
20	ATOM	1602	CB	THR A 219	7.247	-0.607	-2.810	1.00	10.69	C
	ATOM	1603	OG1	THR A 219	7.584	-1.434	-3.932	1.00	10.53	O
	ATOM	1604	CG2	THR A 219	5.803	-0.093	-2.954	1.00	12.51	C
	ATOM	1605	C	THR A 219	7.876	1.478	-1.576	1.00	10.65	C
	ATOM	1606	O	THR A 219	8.003	1.083	-0.410	1.00	10.99	O
25	ATOM	1607	N	LEU A 220	7.440	2.693	-1.890	1.00	10.68	N
	ATOM	1608	CA	LEU A 220	6.968	3.614	-0.881	1.00	11.02	C
	ATOM	1609	CB	LEU A 220	7.228	5.070	-1.309	1.00	10.66	C
	ATOM	1610	CG	LEU A 220	6.600	6.170	-0.438	1.00	12.15	C
	ATOM	1611	CD1	LEU A 220	7.049	6.073	1.045	1.00	12.01	C
30	ATOM	1612	CD2	LEU A 220	6.919	7.555	-1.015	1.00	12.23	C
	ATOM	1613	C	LEU A 220	5.470	3.375	-0.677	1.00	11.28	C
	ATOM	1614	O	LEU A 220	4.686	3.474	-1.618	1.00	11.31	O
	ATOM	1615	N	PHE A 221	5.090	3.057	0.555	1.00	11.30	N
	ATOM	1616	CA	PHE A 221	3.682	2.903	0.886	1.00	12.28	C
35	ATOM	1617	CB	PHE A 221	3.480	1.792	1.912	1.00	12.49	C

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	ATOM	1618	CG	PHE A 221	3.632	0.431	1.316	1.00	13.56	C
	ATOM	1619	CD1	PHE A 221	2.511	-0.293	0.934	1.00	14.75	C
	ATOM	1620	CE1	PHE A 221	2.644	-1.556	0.343	1.00	15.14	C
	ATOM	1621	CZ	PHE A 221	3.903	-2.082	0.110	1.00	14.37	C
5	ATOM	1622	CE2	PHE A 221	5.044	-1.352	0.467	1.00	14.87	C
	ATOM	1623	CD2	PHE A 221	4.905	-0.100	1.059	1.00	14.91	C
	ATOM	1624	C	PHE A 221	3.108	4.239	1.338	1.00	12.77	C
	ATOM	1625	O	PHE A 221	3.438	4.743	2.413	1.00	13.03	O
	ATOM	1626	N	VAL A 222	2.277	4.815	0.474	1.00	12.47	N
10	ATOM	1627	CA	VAL A 222	1.660	6.122	0.731	1.00	12.48	C
	ATOM	1628	CB	VAL A 222	1.066	6.742	-0.571	1.00	12.73	C
	ATOM	1629	CG1	VAL A 222	0.377	8.101	-0.293	1.00	12.52	C
	ATOM	1630	CG2	VAL A 222	2.147	6.888	-1.658	1.00	11.86	C
	ATOM	1631	C	VAL A 222	0.563	5.932	1.769	1.00	13.22	C
15	ATOM	1632	O	VAL A 222	-0.222	4.991	1.688	1.00	12.44	O
	ATOM	1633	N	GLU A 223	0.514	6.825	2.752	1.00	14.12	N
	ATOM	1634	CA	GLU A 223	-0.502	6.724	3.791	1.00	15.31	C
	ATOM	1635	CB	GLU A 223	-0.136	7.585	4.986	1.00	16.38	C
	ATOM	1636	CG	GLU A 223	0.931	6.958	5.823	1.00	17.54	C
20	ATOM	1637	CD	GLU A 223	0.878	7.428	7.244	1.00	19.35	C
	ATOM	1638	OE1	GLU A 223	0.281	6.707	8.072	1.00	22.23	O
	ATOM	1639	OE2	GLU A 223	1.432	8.510	7.530	1.00	19.89	O
	ATOM	1640	C	GLU A 223	-1.908	7.070	3.308	1.00	16.31	C
	ATOM	1641	O	GLU A 223	-2.106	7.992	2.508	1.00	15.79	O
25	ATOM	1642	N	LYS A 224	-2.865	6.295	3.802	1.00	16.73	N
	ATOM	1643	CA	LYS A 224	-4.282	6.510	3.541	1.00	17.86	C
	ATOM	1644	CB	LYS A 224	-5.045	5.182	3.664	1.00	17.19	C
	ATOM	1645	CG	LYS A 224	-4.503	4.070	2.735	1.00	16.08	C
	ATOM	1646	CD	LYS A 224	-5.240	2.730	2.911	1.00	16.22	C
30	ATOM	1647	CE	LYS A 224	-4.997	2.103	4.293	1.00	14.75	C
	ATOM	1648	NZ	LYS A 224	-3.537	1.925	4.603	1.00	14.02	N
	ATOM	1649	C	LYS A 224	-4.805	7.557	4.536	1.00	19.73	C
	ATOM	1650	O	LYS A 224	-6.002	7.859	4.569	1.00	23.75	O
	ATOM	1651	N	VAL B 17	-2.761	50.990	10.227	1.00	17.66	N
35	ATOM	1652	CA	VAL B 17	-1.947	49.908	9.567	1.00	16.47	C

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	ATOM	1653	CB	VAL B 17	-2.302	48.494	10.110	1.00	17.08	C
	ATOM	1654	CG1	VAL B 17	-1.424	47.428	9.454	1.00	16.70	C
	ATOM	1655	CG2	VAL B 17	-2.159	48.429	11.634	1.00	17.19	C
	ATOM	1656	C	VAL B 17	-2.180	49.960	8.054	1.00	15.67	C
5	ATOM	1657	O	VAL B 17	-3.329	49.986	7.597	1.00	15.50	O
	ATOM	1658	N	GLU B 18	-1.095	49.970	7.282	1.00	13.83	N
	ATOM	1659	CA	GLU B 18	-1.194	49.888	5.827	1.00	13.23	C
	ATOM	1660	CB	GLU B 18	-0.361	50.977	5.158	1.00	13.87	C
	ATOM	1661	CG	GLU B 18	-0.926	52.383	5.356	1.00	15.74	C
10	ATOM	1662	CD	GLU B 18	-0.063	53.429	4.699	1.00	19.52	C
	ATOM	1663	OE1	GLU B 18	1.104	53.573	5.113	1.00	18.68	O
	ATOM	1664	OE2	GLU B 18	-0.551	54.099	3.764	1.00	21.12	O
	ATOM	1665	C	GLU B 18	-0.752	48.516	5.340	1.00	12.63	C
	ATOM	1666	O	GLU B 18	0.268	47.970	5.812	1.00	11.95	O
15	ATOM	1667	N	THR B 19	-1.539	47.964	4.417	1.00	11.63	N
	ATOM	1668	CA	THR B 19	-1.257	46.666	3.821	1.00	11.34	C
	ATOM	1669	CB	THR B 19	-2.501	45.726	3.890	1.00	11.32	C
	ATOM	1670	OG1	THR B 19	-2.894	45.579	5.264	1.00	11.56	O
	ATOM	1671	CG2	THR B 19	-2.168	44.351	3.322	1.00	11.20	C
20	ATOM	1672	C	THR B 19	-0.794	46.854	2.385	1.00	11.33	C
	ATOM	1673	O	THR B 19	-1.327	47.706	1.667	1.00	11.18	O
	ATOM	1674	N	PHE B 20	0.198	46.054	1.994	1.00	11.20	N
	ATOM	1675	CA	PHE B 20	0.836	46.116	0.673	1.00	11.09	C
	ATOM	1676	CB	PHE B 20	2.255	46.680	0.782	1.00	10.83	C
25	ATOM	1677	CG	PHE B 20	2.331	48.045	1.398	1.00	10.48	C
	ATOM	1678	CD1	PHE B 20	2.343	48.202	2.788	1.00	10.76	C
	ATOM	1679	CE1	PHE B 20	2.410	49.465	3.363	1.00	10.60	C
	ATOM	1680	CZ	PHE B 20	2.466	50.594	2.543	1.00	11.76	C
	ATOM	1681	CE2	PHE B 20	2.461	50.441	1.156	1.00	12.38	C
30	ATOM	1682	CD2	PHE B 20	2.391	49.165	0.596	1.00	10.44	C
	ATOM	1683	C	PHE B 20	0.936	44.712	0.083	1.00	11.20	C
	ATOM	1684	O	PHE B 20	1.027	43.724	0.824	1.00	12.26	O
	ATOM	1685	N	ALA B 21	0.946	44.628	-1.243	1.00	10.92	N
	ATOM	1686	CA	ALA B 21	1.243	43.375	-1.937	1.00	11.90	C
35	ATOM	1687	CB	ALA B 21	0.339	43.211	-3.164	1.00	12.32	C

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	ATOM	1688	C	ALA B 21	2.716	43.337	-2.353	1.00	11.93	C
	ATOM	1689	O	ALA B 21	3.269	44.349	-2.805	1.00	11.51	O
	ATOM	1690	N	PHE B 22	3.358	42.182	-2.197	1.00	11.67	N
	ATOM	1691	CA	PHE B 22	4.683	41.985	-2.787	1.00	12.51	C
5	ATOM	1692	CB	PHE B 22	5.292	40.628	-2.382	1.00	11.68	C
	ATOM	1693	CG	PHE B 22	5.663	40.540	-0.926	1.00	12.08	C
	ATOM	1694	CD1	PHE B 22	6.777	41.239	-0.429	1.00	11.68	C
	ATOM	1695	CE1	PHE B 22	7.127	41.164	0.921	1.00	10.44	C
	ATOM	1696	CZ	PHE B 22	6.368	40.382	1.798	1.00	11.24	C
10	ATOM	1697	CE2	PHE B 22	5.243	39.679	1.314	1.00	11.52	C
	ATOM	1698	CD2	PHE B 22	4.901	39.764	-0.046	1.00	12.55	C
	ATOM	1699	C	PHE B 22	4.551	42.023	-4.295	1.00	12.90	C
	ATOM	1700	O	PHE B 22	3.545	41.547	-4.844	1.00	12.61	O
	ATOM	1701	N	GLN B 23	5.550	42.600	-4.960	1.00	12.81	N
15	ATOM	1702	CA	GLN B 23	5.729	42.395	-6.390	1.00	13.96	C
	ATOM	1703	CB	GLN B 23	7.043	43.028	-6.857	1.00	14.49	C
	ATOM	1704	CG	GLN B 23	7.250	43.013	-8.366	1.00	15.32	C
	ATOM	1705	CD	GLN B 23	8.449	43.838	-8.817	1.00	16.47	C
	ATOM	1706	OE1	GLN B 23	9.113	44.493	-8.004	1.00	14.85	O
20	ATOM	1707	NE2	GLN B 23	8.729	43.814	-10.127	1.00	18.47	N
	ATOM	1708	C	GLN B 23	5.710	40.885	-6.664	1.00	13.31	C
	ATOM	1709	O	GLN B 23	6.191	40.095	-5.847	1.00	11.91	O
	ATOM	1710	N	ALA B 24	5.149	40.489	-7.802	1.00	12.35	N
	ATOM	1711	CA	ALA B 24	4.916	39.069	-8.089	1.00	13.25	C
25	ATOM	1712	CB	ALA B 24	4.303	38.906	-9.480	1.00	13.15	C
	ATOM	1713	C	ALA B 24	6.171	38.194	-7.931	1.00	12.67	C
	ATOM	1714	O	ALA B 24	6.115	37.102	-7.347	1.00	13.77	O
	ATOM	1715	N	GLU B 25	7.297	38.675	-8.446	1.00	13.41	N
	ATOM	1716	CA	GLU B 25	8.563	37.935	-8.374	1.00	13.51	C
30	ATOM	1717	CB	GLU B 25	9.673	38.648	-9.166	1.00	14.23	C
	ATOM	1718	CG	GLU B 25	9.483	38.647	-10.691	1.00	16.96	C
	ATOM	1719	CD	GLU B 25	8.518	39.730	-11.207	1.00	19.13	C
	ATOM	1720	OE1	GLU B 25	7.888	40.468	-10.407	1.00	18.11	O
	ATOM	1721	OE2	GLU B 25	8.391	39.841	-12.445	1.00	20.86	O
35	ATOM	1722	C	GLU B 25	9.011	37.696	-6.925	1.00	12.45	C

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	ATOM	1723	O	GLU B 25	9.505	36.619	-6.588	1.00	10.84	O
	ATOM	1724	N	ILE B 26	8.830	38.699	-6.071	1.00	11.70	N
	ATOM	1725	CA	ILE B 26	9.169	38.549	-4.647	1.00	11.40	C
	ATOM	1726	CB	ILE B 26	9.195	39.920	-3.912	1.00	11.61	C
5	ATOM	1727	CG1	ILE B 26	10.233	40.867	-4.559	1.00	12.42	C
	ATOM	1728	CD1	ILE B 26	11.711	40.437	-4.410	1.00	13.28	C
	ATOM	1729	CG2	ILE B 26	9.446	39.746	-2.387	1.00	11.11	C
	ATOM	1730	C	ILE B 26	8.232	37.526	-3.970	1.00	12.23	C
	ATOM	1731	O	ILE B 26	8.683	36.680	-3.194	1.00	10.55	O
10	ATOM	1732	N	ALA B 27	6.942	37.576	-4.296	1.00	11.03	N
	ATOM	1733	CA	ALA B 27	6.003	36.604	-3.729	1.00	11.49	C
	ATOM	1734	CB	ALA B 27	4.574	36.932	-4.128	1.00	11.49	C
	ATOM	1735	C	ALA B 27	6.388	35.171	-4.133	1.00	12.10	C
	ATOM	1736	O	ALA B 27	6.362	34.250	-3.309	1.00	11.34	O
15	ATOM	1737	N	GLN B 28	6.783	35.011	-5.391	1.00	12.36	N
	ATOM	1738	CA	GLN B 28	7.213	33.718	-5.929	1.00	13.59	C
	ATOM	1739	CB	GLN B 28	7.442	33.827	-7.426	1.00	14.37	C
	ATOM	1740	CG	GLN B 28	6.139	33.916	-8.221	1.00	18.84	C
	ATOM	1741	CD	GLN B 28	6.318	34.458	-9.623	1.00	22.24	C
20	ATOM	1742	OE1	GLN B 28	7.406	34.879	-10.018	1.00	24.59	O
	ATOM	1743	NE2	GLN B 28	5.230	34.466	-10.383	1.00	26.35	N
	ATOM	1744	C	GLN B 28	8.474	33.214	-5.229	1.00	13.26	C
	ATOM	1745	O	GLN B 28	8.542	32.050	-4.830	1.00	12.36	O
	ATOM	1746	N	LEU B 29	9.452	34.107	-5.069	1.00	12.66	N
25	ATOM	1747	CA	LEU B 29	10.671	33.812	-4.302	1.00	12.38	C
	ATOM	1748	CB	LEU B 29	11.593	35.042	-4.278	1.00	12.09	C
	ATOM	1749	CG	LEU B 29	12.840	34.967	-3.384	1.00	13.79	C
	ATOM	1750	CD1	LEU B 29	13.711	33.742	-3.755	1.00	13.31	C
	ATOM	1751	CD2	LEU B 29	13.657	36.264	-3.439	1.00	13.39	C
30	ATOM	1752	C	LEU B 29	10.341	33.365	-2.872	1.00	12.08	C
	ATOM	1753	O	LEU B 29	10.855	32.343	-2.396	1.00	10.57	O
	ATOM	1754	N	MET B 30	9.490	34.134	-2.189	1.00	12.47	N
	ATOM	1755	CA	MET B 30	9.131	33.816	-0.802	1.00	13.22	C
	ATOM	1756	CB	MET B 30	8.235	34.901	-0.204	1.00	13.38	C
35	ATOM	1757	CG	MET B 30	8.978	36.218	0.025	1.00	13.12	C

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	ATOM	1758	SD	MET B	30	7.900	37.536	0.612	1.00	12.78	S
	ATOM	1759	CE	MET B	30	7.636	37.059	2.325	1.00	12.90	C
	ATOM	1760	C	MET B	30	8.450	32.459	-0.707	1.00	13.94	C
	ATOM	1761	O	MET B	30	8.753	31.671	0.192	1.00	13.45	O
5	ATOM	1762	N	SER B	31	7.536	32.193	-1.639	1.00	14.15	N
	ATOM	1763	CA	SER B	31	6.848	30.900	-1.681	1.00	15.96	C
	ATOM	1764	CB	SER B	31	5.769	30.886	-2.774	1.00	16.46	C
	ATOM	1765	OG	SER B	31	5.076	29.647	-2.778	1.00	19.91	O
	ATOM	1766	C	SER B	31	7.828	29.724	-1.839	1.00	15.82	C
10	ATOM	1767	O	SER B	31	7.695	28.703	-1.142	1.00	15.94	O
	ATOM	1768	N	LEU B	32	8.810	29.880	-2.726	1.00	15.33	N
	ATOM	1769	CA	LEU B	32	9.833	28.862	-2.938	1.00	16.08	C
	ATOM	1770	CB	LEU B	32	10.757	29.265	-4.097	1.00	16.81	C
	ATOM	1771	CG	LEU B	32	11.875	28.332	-4.586	1.00	17.64	C
15	ATOM	1772	CD1	LEU B	32	12.249	28.677	-6.030	1.00	20.08	C
	ATOM	1773	CD2	LEU B	32	13.102	28.392	-3.665	1.00	19.81	C
	ATOM	1774	C	LEU B	32	10.622	28.632	-1.640	1.00	16.25	C
	ATOM	1775	O	LEU B	32	10.805	27.480	-1.217	1.00	16.44	O
	ATOM	1776	N	ILE B	33	11.069	29.721	-1.011	1.00	15.43	N
20	ATOM	1777	CA	ILE B	33	11.893	29.636	0.207	1.00	16.38	C
	ATOM	1778	CB	ILE B	33	12.488	31.015	0.602	1.00	16.24	C
	ATOM	1779	CG1	ILE B	33	13.474	31.485	-0.469	1.00	15.84	C
	ATOM	1780	CD1	ILE B	33	13.901	32.935	-0.330	1.00	18.37	C
	ATOM	1781	CG2	ILE B	33	13.139	30.958	2.016	1.00	15.87	C
25	ATOM	1782	C	ILE B	33	11.148	29.050	1.402	1.00	17.43	C
	ATOM	1783	O	ILE B	33	11.647	28.150	2.082	1.00	16.70	O
	ATOM	1784	N	ILE B	34	9.950	29.567	1.658	1.00	18.74	N
	ATOM	1785	CA	ILE B	34	9.238	29.253	2.890	1.00	21.29	C
	ATOM	1786	CB	ILE B	34	8.038	30.242	3.116	1.00	21.07	C
30	ATOM	1787	CG1	ILE B	34	7.765	30.463	4.617	1.00	23.15	C
	ATOM	1788	CD1	ILE B	34	6.832	29.455	5.275	1.00	27.93	C
	ATOM	1789	CG2	ILE B	34	6.821	29.846	2.277	1.00	21.41	C
	ATOM	1790	C	ILE B	34	8.818	27.783	2.898	1.00	21.49	C
	ATOM	1791	O	ILE B	34	8.647	27.186	3.969	1.00	22.63	O
35	ATOM	1792	N	ASN B	35	8.718	27.204	1.702	1.00	21.66	N

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	ATOM	1793	CA	ASN B 35	8.253	25.839	1.510	1.00	21.95	C
	ATOM	1794	CB	ASN B 35	7.198	25.811	0.404	1.00	22.49	C
	ATOM	1795	CG	ASN B 35	5.891	26.483	0.825	1.00	24.17	C
	ATOM	1796	OD1	ASN B 35	5.288	26.118	1.837	1.00	25.21	O
5	ATOM	1797	ND2	ASN B 35	5.450	27.464	0.047	1.00	24.26	N
	ATOM	1798	C	ASN B 35	9.327	24.778	1.222	1.00	21.56	C
	ATOM	1799	O	ASN B 35	9.038	23.567	1.253	1.00	22.35	O
	ATOM	1800	N	THR B 36	10.550	25.214	0.939	1.00	19.55	N
	ATOM	1801	CA	THR B 36	11.597	24.285	0.507	1.00	18.52	C
10	ATOM	1802	CB	THR B 36	12.812	25.016	-0.138	1.00	18.51	C
	ATOM	1803	OG1	THR B 36	13.757	24.049	-0.619	1.00	16.88	O
	ATOM	1804	CG2	THR B 36	13.500	25.957	0.867	1.00	17.81	C
	ATOM	1805	C	THR B 36	12.060	23.370	1.642	1.00	17.30	C
	ATOM	1806	O	THR B 36	12.025	23.753	2.813	1.00	17.72	O
15	ATOM	1807	N	PHE B 37	12.482	22.161	1.279	1.00	17.05	N
	ATOM	1808	CA	PHE B 37	13.124	21.246	2.221	1.00	17.07	C
	ATOM	1809	CB	PHE B 37	12.817	19.787	1.860	1.00	17.71	C
	ATOM	1810	CG	PHE B 37	11.412	19.361	2.198	1.00	18.60	C
	ATOM	1811	CD1	PHE B 37	10.547	18.938	1.197	1.00	19.37	C
20	ATOM	1812	CE1	PHE B 37	9.247	18.531	1.500	1.00	20.04	C
	ATOM	1813	CZ	PHE B 37	8.802	18.544	2.826	1.00	20.07	C
	ATOM	1814	CE2	PHE B 37	9.665	18.975	3.841	1.00	20.96	C
	ATOM	1815	CD2	PHE B 37	10.964	19.367	3.521	1.00	19.98	C
	ATOM	1816	C	PHE B 37	14.641	21.450	2.288	1.00	16.49	C
25	ATOM	1817	O	PHE B 37	15.354	20.675	2.942	1.00	16.34	O
	ATOM	1818	N	TYR B 38	15.133	22.473	1.591	1.00	14.99	N
	ATOM	1819	CA	TYR B 38	16.564	22.821	1.626	1.00	14.06	C
	ATOM	1820	CB	TYR B 38	16.769	24.231	1.050	1.00	14.04	C
	ATOM	1821	CG	TYR B 38	18.214	24.658	0.942	1.00	14.40	C
30	ATOM	1822	CD1	TYR B 38	19.016	24.232	-0.128	1.00	14.20	C
	ATOM	1823	CE1	TYR B 38	20.359	24.644	-0.235	1.00	14.70	C
	ATOM	1824	CZ	TYR B 38	20.890	25.481	0.753	1.00	14.35	C
	ATOM	1825	OH	TYR B 38	22.201	25.895	0.686	1.00	15.68	O
	ATOM	1826	CE2	TYR B 38	20.105	25.911	1.810	1.00	15.11	C
35	ATOM	1827	CD2	TYR B 38	18.778	25.500	1.902	1.00	15.09	C

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	ATOM	1828	C	TYR B 38	17.098	22.735	3.058	1.00	13.19	C
	ATOM	1829	O	TYR B 38	16.634	23.460	3.944	1.00	12.94	O
	ATOM	1830	N	SER B 39	18.053	21.831	3.282	1.00	12.61	N
	ATOM	1831	CA	SER B 39	18.509	21.501	4.638	1.00	12.55	C
5	ATOM	1832	CB	SER B 39	19.068	20.073	4.678	1.00	13.57	C
	ATOM	1833	OG	SER B 39	20.190	19.972	3.829	1.00	14.92	O
	ATOM	1834	C	SER B 39	19.551	22.440	5.245	1.00	11.90	C
	ATOM	1835	O	SER B 39	19.729	22.455	6.466	1.00	10.94	O
	ATOM	1836	N	ASN B 40	20.245	23.200	4.400	1.00	10.85	N
10	ATOM	1837	CA	ASN B 40	21.370	24.050	4.834	1.00	11.73	C
	ATOM	1838	CB	ASN B 40	22.370	24.170	3.666	1.00	12.65	C
	ATOM	1839	CG	ASN B 40	23.568	25.092	3.958	1.00	13.03	C
	ATOM	1840	OD1	ASN B 40	24.028	25.805	3.050	1.00	15.23	O
	ATOM	1841	ND2	ASN B 40	24.080	25.072	5.190	1.00	8.86	N
15	ATOM	1842	C	ASN B 40	20.848	25.421	5.321	1.00	11.97	C
	ATOM	1843	O	ASN B 40	21.254	26.480	4.836	1.00	12.14	O
	ATOM	1844	N	LYS B 41	19.937	25.374	6.291	1.00	11.69	N
	ATOM	1845	CA	LYS B 41	19.176	26.552	6.694	1.00	11.84	C
	ATOM	1846	CB	LYS B 41	17.935	26.144	7.497	1.00	12.11	C
20	ATOM	1847	CG	LYS B 41	16.904	25.374	6.674	1.00	11.99	C
	ATOM	1848	CD	LYS B 41	15.583	25.232	7.439	1.00	12.21	C
	ATOM	1849	CE	LYS B 41	14.476	24.691	6.536	1.00	15.55	C
	ATOM	1850	NZ	LYS B 41	14.766	23.336	6.013	1.00	17.47	N
	ATOM	1851	C	LYS B 41	19.974	27.618	7.454	1.00	11.68	C
25	ATOM	1852	O	LYS B 41	19.572	28.787	7.469	1.00	10.77	O
	ATOM	1853	N	GLU B 42	21.092	27.227	8.061	1.00	11.00	N
	ATOM	1854	CA	GLU B 42	21.862	28.144	8.917	1.00	11.52	C
	ATOM	1855	CB	GLU B 42	23.047	27.416	9.566	1.00	11.86	C
	ATOM	1856	CG	GLU B 42	24.148	27.004	8.570	1.00	12.77	C
30	ATOM	1857	CD	GLU B 42	25.326	26.300	9.235	1.00	13.77	C
	ATOM	1858	OE1	GLU B 42	25.156	25.710	10.317	1.00	17.45	O
	ATOM	1859	OE2	GLU B 42	26.432	26.341	8.673	1.00	16.41	O
	ATOM	1860	C	GLU B 42	22.365	29.398	8.175	1.00	11.33	C
	ATOM	1861	O	GLU B 42	22.688	30.404	8.813	1.00	11.12	O
35	ATOM	1862	N	ILE B 43	22.435	29.326	6.843	1.00	10.97	N

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	ATOM	1863	CA	ILE B 43	22.900	30.460	6.019	1.00	11.52	C
	ATOM	1864	CB	ILE B 43	23.196	30.050	4.523	1.00	12.58	C
	ATOM	1865	CG1	ILE B 43	21.932	29.571	3.788	1.00	12.53	C
	ATOM	1866	CD1	ILE B 43	21.054	30.651	3.235	1.00	15.70	C
5	ATOM	1867	CG2	ILE B 43	24.283	28.955	4.456	1.00	13.87	C
	ATOM	1868	C	ILE B 43	22.014	31.724	6.133	1.00	11.55	C
	ATOM	1869	O	ILE B 43	22.453	32.828	5.769	1.00	10.16	O
	ATOM	1870	N	PHE B 44	20.797	31.584	6.678	1.00	11.18	N
	ATOM	1871	CA	PHE B 44	19.945	32.770	6.891	1.00	11.16	C
10	ATOM	1872	CB	PHE B 44	18.585	32.413	7.533	1.00	11.50	C
	ATOM	1873	CG	PHE B 44	18.655	32.239	9.034	1.00	11.24	C
	ATOM	1874	CD1	PHE B 44	18.944	30.990	9.592	1.00	11.06	C
	ATOM	1875	CE1	PHE B 44	19.040	30.833	10.972	1.00	11.00	C
	ATOM	1876	CZ	PHE B 44	18.868	31.933	11.814	1.00	10.89	C
15	ATOM	1877	CE2	PHE B 44	18.589	33.183	11.271	1.00	10.99	C
	ATOM	1878	CD2	PHE B 44	18.480	33.331	9.888	1.00	10.50	C
	ATOM	1879	C	PHE B 44	20.683	33.800	7.760	1.00	11.50	C
	ATOM	1880	O	PHE B 44	20.567	35.004	7.537	1.00	10.97	O
	ATOM	1881	N	LEU B 45	21.455	33.320	8.739	1.00	10.61	N
20	ATOM	1882	CA	LEU B 45	22.049	34.232	9.714	1.00	10.46	C
	ATOM	1883	CB	LEU B 45	22.529	33.489	10.968	1.00	10.85	C
	ATOM	1884	CG	LEU B 45	23.122	34.378	12.075	1.00	11.15	C
	ATOM	1885	CD1	LEU B 45	23.642	33.504	13.207	1.00	11.72	C
	ATOM	1886	CD2	LEU B 45	22.075	35.393	12.584	1.00	9.11	C
25	ATOM	1887	C	LEU B 45	23.172	35.058	9.094	1.00	10.20	C
	ATOM	1888	O	LEU B 45	23.269	36.267	9.363	1.00	8.73	O
	ATOM	1889	N	ARG B 46	24.015	34.427	8.271	1.00	10.72	N
	ATOM	1890	CA	ARG B 46	25.063	35.204	7.585	1.00	11.15	C
	ATOM	1891	CB	ARG B 46	26.083	34.317	6.857	1.00	13.56	C
30	ATOM	1892	CG	ARG B 46	25.541	33.693	5.638	1.00	15.63	C
	ATOM	1893	CD	ARG B 46	26.603	33.262	4.626	1.00	18.21	C
	ATOM	1894	NE	ARG B 46	25.815	32.883	3.476	1.00	21.01	N
	ATOM	1895	CZ	ARG B 46	26.148	32.010	2.544	1.00	23.85	C
	ATOM	1896	NH1	ARG B 46	27.322	31.399	2.560	1.00	25.43	N
35	ATOM	1897	NH2	ARG B 46	25.274	31.773	1.578	1.00	25.50	N

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	ATOM	1898	C	ARG B 46	24.460	36.242	6.625	1.00	11.24	C
	ATOM	1899	O	ARG B 46	25.024	37.317	6.456	1.00	11.02	O
	ATOM	1900	N	GLU B 47	23.321	35.931	6.004	1.00	9.68	N
	ATOM	1901	CA	GLU B 47	22.688	36.895	5.089	1.00	9.93	C
5	ATOM	1902	CB	GLU B 47	21.524	36.248	4.313	1.00	10.17	C
	ATOM	1903	CG	GLU B 47	21.938	35.091	3.386	1.00	11.66	C
	ATOM	1904	CD	GLU B 47	22.983	35.477	2.350	1.00	13.86	C
	ATOM	1905	OE1	GLU B 47	23.085	36.667	1.971	1.00	12.59	O
	ATOM	1906	OE2	GLU B 47	23.708	34.565	1.904	1.00	15.31	O
10	ATOM	1907	C	GLU B 47	22.210	38.161	5.814	1.00	9.34	C
	ATOM	1908	O	GLU B 47	22.421	39.290	5.315	1.00	9.15	O
	ATOM	1909	N	LEU B 48	21.584	37.965	6.976	1.00	8.65	N
	ATOM	1910	CA	LEU B 48	21.081	39.070	7.815	1.00	8.74	C
	ATOM	1911	CB	LEU B 48	20.142	38.543	8.908	1.00	9.00	C
15	ATOM	1912	CG	LEU B 48	18.859	37.891	8.360	1.00	8.55	C
	ATOM	1913	CD1	LEU B 48	17.941	37.433	9.472	1.00	10.01	C
	ATOM	1914	CD2	LEU B 48	18.123	38.827	7.390	1.00	8.72	C
	ATOM	1915	C	LEU B 48	22.227	39.885	8.422	1.00	8.81	C
	ATOM	1916	O	LEU B 48	22.191	41.121	8.447	1.00	8.96	O
20	ATOM	1917	N	ILE B 49	23.256	39.182	8.878	1.00	7.31	N
	ATOM	1918	CA	ILE B 49	24.461	39.840	9.381	1.00	7.93	C
	ATOM	1919	CB	ILE B 49	25.424	38.817	10.064	1.00	7.04	C
	ATOM	1920	CG1	ILE B 49	24.798	38.329	11.391	1.00	7.45	C
	ATOM	1921	CD1	ILE B 49	25.598	37.232	12.112	1.00	8.45	C
25	ATOM	1922	CG2	ILE B 49	26.798	39.472	10.312	1.00	8.80	C
	ATOM	1923	C	ILE B 49	25.140	40.661	8.279	1.00	8.29	C
	ATOM	1924	O	ILE B 49	25.570	41.803	8.517	1.00	7.65	O
	ATOM	1925	N	SER B 50	25.216	40.095	7.075	1.00	8.07	N
	ATOM	1926	CA	SER B 50	25.754	40.816	5.923	1.00	9.28	C
30	ATOM	1927	CB	SER B 50	25.852	39.893	4.709	1.00	9.93	C
	ATOM	1928	OG	BSER B 50	26.915	38.970	4.909	0.50	5.34	O
	ATOM	1929	OG	ASER B 50	26.362	40.580	3.587	0.50	11.67	O
	ATOM	1930	C	SER B 50	24.956	42.095	5.605	1.00	9.40	C
	ATOM	1931	O	SER B 50	25.545	43.146	5.344	1.00	8.82	O
35	ATOM	1932	N	ASN B 51	23.628	42.004	5.652	1.00	7.90	N

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	ATOM	1933	CA	ASN B 51	22.780	43.180	5.457	1.00	8.66	C
	ATOM	1934	CB	ASN B 51	21.292	42.794	5.474	1.00	8.66	C
	ATOM	1935	CG	ASN B 51	20.850	42.118	4.174	1.00	9.10	C
	ATOM	1936	OD1	ASN B 51	21.634	41.983	3.234	1.00	10.28	O
5	ATOM	1937	ND2	ASN B 51	19.575	41.718	4.112	1.00	8.64	N
	ATOM	1938	C	ASN B 51	23.054	44.251	6.510	1.00	8.71	C
	ATOM	1939	O	ASN B 51	23.152	45.440	6.187	1.00	8.58	O
	ATOM	1940	N	SER B 52	23.170	43.814	7.761	1.00	8.32	N
	ATOM	1941	CA	SER B 52	23.508	44.710	8.878	1.00	8.43	C
10	ATOM	1942	CB	SER B 52	23.532	43.943	10.201	1.00	8.33	C
	ATOM	1943	OG	SER B 52	22.216	43.572	10.583	1.00	7.70	O
	ATOM	1944	C	SER B 52	24.850	45.417	8.645	1.00	9.26	C
	ATOM	1945	O	SER B 52	24.953	46.636	8.854	1.00	8.07	O
	ATOM	1946	N	SER B 53	25.857	44.648	8.220	1.00	8.89	N
15	ATOM	1947	CA	SER B 53	27.162	45.203	7.853	1.00	9.75	C
	ATOM	1948	CB	SER B 53	28.153	44.087	7.479	1.00	9.31	C
	ATOM	1949	OG	SER B 53	29.443	44.638	7.234	1.00	10.33	O
	ATOM	1950	C	SER B 53	27.049	46.239	6.721	1.00	9.52	C
	ATOM	1951	O	SER B 53	27.674	47.311	6.791	1.00	8.35	O
20	ATOM	1952	N	ASP B 54	26.243	45.930	5.700	1.00	9.08	N
	ATOM	1953	CA	ASP B 54	26.013	46.863	4.587	1.00	9.55	C
	ATOM	1954	CB	ASP B 54	25.129	46.231	3.500	1.00	10.51	C
	ATOM	1955	CG	ASP B 54	25.852	45.151	2.665	1.00	13.73	C
	ATOM	1956	OD1	ASP B 54	27.078	44.924	2.838	1.00	14.06	O
25	ATOM	1957	OD2	ASP B 54	25.171	44.528	1.820	1.00	18.68	O
	ATOM	1958	C	ASP B 54	25.386	48.176	5.109	1.00	9.40	C
	ATOM	1959	O	ASP B 54	25.819	49.270	4.730	1.00	9.40	O
	ATOM	1960	N	ALA B 55	24.405	48.074	6.007	1.00	8.74	N
	ATOM	1961	CA	ALA B 55	23.746	49.276	6.565	1.00	8.60	C
30	ATOM	1962	CB	ALA B 55	22.497	48.893	7.351	1.00	8.28	C
	ATOM	1963	C	ALA B 55	24.695	50.112	7.433	1.00	8.96	C
	ATOM	1964	O	ALA B 55	24.602	51.347	7.457	1.00	7.94	O
	ATOM	1965	N	LEU B 56	25.589	49.424	8.150	1.00	8.41	N
	ATOM	1966	CA	LEU B 56	26.637	50.065	8.947	1.00	8.92	C
35	ATOM	1967	CB	LEU B 56	27.309	49.047	9.894	1.00	8.77	C

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	ATOM	1968	CG	LEU	B	56	26.406	48.580	11.057	1.00	8.97	C
	ATOM	1969	CD1	LEU	B	56	26.839	47.228	11.643	1.00	9.98	C
	ATOM	1970	CD2	LEU	B	56	26.295	49.649	12.166	1.00	7.49	C
	ATOM	1971	C	LEU	B	56	27.645	50.780	8.034	1.00	9.38	C
5	ATOM	1972	O	LEU	B	56	28.015	51.923	8.317	1.00	9.81	O
	ATOM	1973	N	ASP	B	57	28.034	50.138	6.925	1.00	8.32	N
	ATOM	1974	CA	ASP	B	57	28.831	50.799	5.872	1.00	8.80	C
	ATOM	1975	CB	ASP	B	57	29.005	49.881	4.663	1.00	9.38	C
	ATOM	1976	CG	ASP	B	57	29.898	48.675	4.939	1.00	9.66	C
10	ATOM	1977	OD1	ASP	B	57	30.623	48.629	5.964	1.00	10.96	O
	ATOM	1978	OD2	ASP	B	57	29.865	47.769	4.081	1.00	13.14	O
	ATOM	1979	C	ASP	B	57	28.189	52.116	5.404	1.00	9.32	C
	ATOM	1980	O	ASP	B	57	28.870	53.152	5.281	1.00	8.55	O
	ATOM	1981	N	LYS	B	58	26.874	52.076	5.201	1.00	8.67	N
15	ATOM	1982	CA	LYS	B	58	26.136	53.227	4.675	1.00	10.46	C
	ATOM	1983	CB	LYS	B	58	24.694	52.833	4.363	1.00	9.79	C
	ATOM	1984	CG	LYS	B	58	24.578	51.845	3.201	1.00	12.21	C
	ATOM	1985	CD	LYS	B	58	23.116	51.474	2.949	1.00	12.90	C
	ATOM	1986	CE	LYS	B	58	22.987	50.663	1.664	1.00	13.75	C
20	ATOM	1987	NZ	LYS	B	58	21.585	50.251	1.395	1.00	15.87	N
	ATOM	1988	C	LYS	B	58	26.185	54.425	5.633	1.00	10.18	C
	ATOM	1989	O	LYS	B	58	26.493	55.541	5.213	1.00	10.56	O
	ATOM	1990	N	ILE	B	59	25.898	54.193	6.912	1.00	10.08	N
	ATOM	1991	CA	ILE	B	59	25.951	55.289	7.895	1.00	11.09	C
25	ATOM	1992	CB	ILE	B	59	25.190	54.983	9.230	1.00	11.33	C
	ATOM	1993	CG1	ILE	B	59	25.089	56.246	10.119	1.00	11.48	C
	ATOM	1994	CD1	ILE	B	59	24.169	57.369	9.553	1.00	11.01	C
	ATOM	1995	CG2	ILE	B	59	25.824	53.809	9.987	1.00	11.02	C
	ATOM	1996	C	ILE	B	59	27.380	55.797	8.135	1.00	11.53	C
30	ATOM	1997	O	ILE	B	59	27.586	57.015	8.250	1.00	11.19	O
	ATOM	1998	N	ARG	B	60	28.351	54.881	8.182	1.00	11.64	N
	ATOM	1999	CA	ARG	B	60	29.765	55.284	8.280	1.00	13.47	C
	ATOM	2000	CB	ARG	B	60	30.704	54.072	8.351	1.00	12.95	C
	ATOM	2001	CG	ARG	B	60	32.187	54.455	8.125	1.00	15.90	C
35	ATOM	2002	CD	ARG	B	60	33.144	53.822	9.106	1.00	19.69	C

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	ATOM	2003	NE	ARG B 60	34.524	54.161	8.740	1.00	21.30	N
	ATOM	2004	CZ	ARG B 60	35.171	55.263	9.111	1.00	22.75	C
	ATOM	2005	NH1	ARG B 60	36.419	55.455	8.702	1.00	21.94	N
	ATOM	2006	NH2	ARG B 60	34.591	56.171	9.894	1.00	23.78	N
5	ATOM	2007	C	ARG B 60	30.139	56.200	7.102	1.00	13.28	C
	ATOM	2008	O	ARG B 60	30.739	57.268	7.304	1.00	13.17	O
	ATOM	2009	N	TYR B 61	29.791	55.773	5.883	1.00	12.57	N
	ATOM	2010	CA	TYR B 61	30.057	56.566	4.673	1.00	12.58	C
	ATOM	2011	CB	TYR B 61	29.542	55.848	3.419	1.00	12.58	C
10	ATOM	2012	CG	TYR B 61	29.769	56.615	2.145	1.00	14.43	C
	ATOM	2013	CD1	TYR B 61	28.732	57.337	1.544	1.00	16.13	C
	ATOM	2014	CE1	TYR B 61	28.951	58.053	0.351	1.00	15.77	C
	ATOM	2015	CZ	TYR B 61	30.216	58.044	-0.229	1.00	15.21	C
	ATOM	2016	OH	TYR B 61	30.459	58.738	-1.394	1.00	16.18	O
15	ATOM	2017	CE2	TYR B 61	31.256	57.336	0.350	1.00	14.71	C
	ATOM	2018	CD2	TYR B 61	31.030	56.627	1.535	1.00	13.92	C
	ATOM	2019	C	TYR B 61	29.467	57.985	4.758	1.00	12.77	C
	ATOM	2020	O	TYR B 61	30.176	58.976	4.525	1.00	11.74	O
	ATOM	2021	N	GLU B 62	28.182	58.074	5.083	1.00	12.77	N
20	ATOM	2022	CA	GLU B 62	27.512	59.386	5.205	1.00	14.04	C
	ATOM	2023	CB	GLU B 62	25.998	59.229	5.398	1.00	13.60	C
	ATOM	2024	CG	GLU B 62	25.327	58.554	4.188	1.00	15.84	C
	ATOM	2025	CD	GLU B 62	23.828	58.803	4.066	1.00	19.03	C
	ATOM	2026	OE1	GLU B 62	23.237	59.450	4.950	1.00	18.80	O
25	ATOM	2027	OE2	GLU B 62	23.246	58.322	3.063	1.00	22.67	O
	ATOM	2028	C	GLU B 62	28.147	60.263	6.294	1.00	13.88	C
	ATOM	2029	O	GLU B 62	28.301	61.472	6.101	1.00	14.92	O
	ATOM	2030	N	SER B 63	28.556	59.642	7.402	1.00	13.81	N
	ATOM	2031	CA	SER B 63	29.146	60.358	8.533	1.00	14.87	C
30	ATOM	2032	CB	SER B 63	29.309	59.435	9.743	1.00	14.65	C
	ATOM	2033	OG	SER B 63	30.485	58.637	9.627	1.00	14.83	O
	ATOM	2034	C	SER B 63	30.485	61.032	8.211	1.00	15.85	C
	ATOM	2035	O	SER B 63	30.885	61.957	8.914	1.00	15.70	O
	ATOM	2036	N	LEU B 64	31.175	60.552	7.171	1.00	16.10	N
35	ATOM	2037	CA	LEU B 64	32.463	61.136	6.758	1.00	17.65	C

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	ATOM	2038	CB	LEU B 64	33.110	60.335	5.622	1.00	17.24	C
	ATOM	2039	CG	LEU B 64	33.501	58.887	5.969	1.00	18.25	C
	ATOM	2040	CD1	LEU B 64	34.104	58.188	4.769	1.00	20.49	C
	ATOM	2041	CD2	LEU B 64	34.454	58.834	7.157	1.00	20.54	C
5	ATOM	2042	C	LEU B 64	32.316	62.602	6.349	1.00	18.84	C
	ATOM	2043	O	LEU B 64	33.202	63.416	6.623	1.00	19.60	O
	ATOM	2044	N	THR B 65	31.196	62.924	5.708	1.00	19.73	N
	ATOM	2045	CA	THR B 65	30.952	64.274	5.184	1.00	20.99	C
	ATOM	2046	CB	THR B 65	30.538	64.235	3.703	1.00	21.03	C
10	ATOM	2047	OG1	THR B 65	29.396	63.383	3.550	1.00	23.16	O
	ATOM	2048	CG2	THR B 65	31.682	63.717	2.832	1.00	22.36	C
	ATOM	2049	C	THR B 65	29.894	65.037	5.988	1.00	20.83	C
	ATOM	2050	O	THR B 65	29.739	66.250	5.824	1.00	21.19	O
	ATOM	2051	N	ASP B 66	29.160	64.316	6.836	1.00	19.80	N
15	ATOM	2052	CA	ASP B 66	28.221	64.923	7.782	1.00	19.41	C
	ATOM	2053	CB	ASP B 66	26.792	64.982	7.201	1.00	19.32	C
	ATOM	2054	CG	ASP B 66	25.805	65.752	8.102	1.00	19.86	C
	ATOM	2055	OD1	ASP B 66	26.185	66.177	9.212	1.00	17.96	O
	ATOM	2056	OD2	ASP B 66	24.629	65.911	7.703	1.00	20.42	O
20	ATOM	2057	C	ASP B 66	28.271	64.156	9.110	1.00	19.31	C
	ATOM	2058	O	ASP B 66	27.479	63.240	9.335	1.00	18.78	O
	ATOM	2059	N	PRO B 67	29.208	64.538	10.000	1.00	19.27	N
	ATOM	2060	CA	PRO B 67	29.344	63.917	11.331	1.00	19.02	C
	ATOM	2061	CB	PRO B 67	30.435	64.758	12.008	1.00	19.71	C
25	ATOM	2063	CD	PRO B 67	30.223	65.590	9.771	1.00	20.13	C
	ATOM	2064	C	PRO B 67	28.072	63.943	12.185	1.00	18.05	C
	ATOM	2065	O	PRO B 67	27.916	63.089	13.067	1.00	17.62	O
	ATOM	2066	N	SER B 68	27.175	64.900	11.927	1.00	16.76	N
	ATOM	2067	CA	SER B 68	25.927	65.019	12.698	1.00	16.96	C
30	ATOM	2068	CB	SER B 68	25.181	66.327	12.379	1.00	16.90	C
	ATOM	2069	OG	SER B 68	24.480	66.235	11.148	1.00	18.03	O
	ATOM	2070	C	SER B 68	25.002	63.811	12.486	1.00	16.18	C
	ATOM	2071	O	SER B 68	24.093	63.569	13.277	1.00	15.99	O
	ATOM	2072	N	LYS B 69	25.262	63.043	11.433	1.00	15.95	N
35	ATOM	2073	CA	LYS B 69	24.480	61.830	11.166	1.00	16.00	C

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	ATOM	2074	CB	LYS	B	69	24.782	61.287	9.772	1.00	16.10	C
	ATOM	2075	CG	LYS	B	69	24.187	62.195	8.705	1.00	18.54	C
	ATOM	2076	CD	LYS	B	69	24.206	61.595	7.349	1.00	19.69	C
	ATOM	2077	CE	LYS	B	69	23.505	62.530	6.387	1.00	20.47	C
5	ATOM	2078	NZ	LYS	B	69	23.564	62.038	4.991	1.00	23.43	N
	ATOM	2079	C	LYS	B	69	24.651	60.759	12.247	1.00	15.56	C
	ATOM	2080	O	LYS	B	69	23.810	59.853	12.380	1.00	15.56	O
	ATOM	2081	N	LEU	B	70	25.726	60.882	13.024	1.00	14.33	N
	ATOM	2082	CA	LEU	B	70	25.947	60.025	14.188	1.00	14.29	C
10	ATOM	2083	CB	LEU	B	70	27.434	59.645	14.345	1.00	14.59	C
	ATOM	2084	CG	LEU	B	70	28.068	58.905	13.157	1.00	15.48	C
	ATOM	2085	CD1	LEU	B	70	29.577	58.700	13.383	1.00	16.58	C
	ATOM	2086	CD2	LEU	B	70	27.358	57.583	12.889	1.00	16.24	C
	ATOM	2087	C	LEU	B	70	25.412	60.595	15.500	1.00	14.45	C
15	ATOM	2088	O	LEU	B	70	25.648	60.013	16.560	1.00	13.38	O
	ATOM	2089	N	ASP	B	71	24.692	61.719	15.444	1.00	14.26	N
	ATOM	2090	CA	ASP	B	71	24.075	62.258	16.671	1.00	15.68	C
	ATOM	2091	CB	ASP	B	71	23.362	63.597	16.429	1.00	16.11	C
	ATOM	2092	CG	ASP	B	71	24.330	64.747	16.168	1.00	18.36	C
20	ATOM	2093	OD1	ASP	B	71	25.566	64.570	16.277	1.00	18.90	O
	ATOM	2094	OD2	ASP	B	71	23.837	65.845	15.844	1.00	20.99	O
	ATOM	2095	C	ASP	B	71	23.095	61.256	17.272	1.00	15.46	C
	ATOM	2096	O	ASP	B	71	22.908	61.225	18.489	1.00	16.26	O
	ATOM	2097	N	SER	B	72	22.492	60.433	16.413	1.00	14.92	N
25	ATOM	2098	CA	SER	B	72	21.588	59.356	16.838	1.00	15.08	C
	ATOM	2099	CB	SER	B	72	20.664	58.964	15.678	1.00	14.69	C
	ATOM	2100	OG	SER	B	72	21.413	58.766	14.491	1.00	12.21	O
	ATOM	2101	C	SER	B	72	22.319	58.109	17.370	1.00	15.01	C
	ATOM	2102	O	SER	B	72	21.686	57.110	17.709	1.00	16.13	O
30	ATOM	2103	N	GLY	B	73	23.647	58.166	17.438	1.00	14.63	N
	ATOM	2104	CA	GLY	B	73	24.434	57.100	18.070	1.00	15.12	C
	ATOM	2105	C	GLY	B	73	25.720	56.836	17.327	1.00	14.99	C
	ATOM	2106	O	GLY	B	73	25.711	56.611	16.120	1.00	14.93	O
	ATOM	2107	N	LYS	B	74	26.840	56.878	18.042	1.00	14.93	N
35	ATOM	2108	CA	LYS	B	74	28.145	56.732	17.402	1.00	15.77	C

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	ATOM	2109	CB	LYS	B	74	29.221	57.532	18.158	1.00	16.29	C
	ATOM	2110	CG	LYS	B	74	29.089	59.051	17.996	1.00	18.09	C
	ATOM	2114	C	LYS	B	74	28.578	55.270	17.235	1.00	15.08	C
	ATOM	2115	O	LYS	B	74	29.393	54.970	16.366	1.00	15.42	O
5	ATOM	2116	N	GLU	B	75	28.012	54.372	18.044	1.00	14.66	N
	ATOM	2117	CA	GLU	B	75	28.415	52.953	18.023	1.00	14.98	C
	ATOM	2118	CB	GLU	B	75	27.904	52.206	19.263	1.00	15.33	C
	ATOM	2119	CG	GLU	B	75	28.455	52.724	20.598	1.00	17.48	C
	ATOM	2123	C	GLU	B	75	27.912	52.261	16.753	1.00	13.47	C
10	ATOM	2124	O	GLU	B	75	26.754	52.401	16.389	1.00	14.40	O
	ATOM	2125	N	LEU	B	76	28.803	51.544	16.082	1.00	12.42	N
	ATOM	2126	CA	LEU	B	76	28.459	50.752	14.899	1.00	11.65	C
	ATOM	2127	CB	LEU	B	76	29.355	51.138	13.711	1.00	12.62	C
	ATOM	2128	CG	LEU	B	76	29.313	52.627	13.346	1.00	12.73	C
15	ATOM	2129	CD1	LEU	B	76	30.294	52.900	12.226	1.00	15.35	C
	ATOM	2130	CD2	LEU	B	76	27.887	53.121	13.014	1.00	14.09	C
	ATOM	2131	C	LEU	B	76	28.643	49.281	15.228	1.00	11.56	C
	ATOM	2132	O	LEU	B	76	29.775	48.797	15.297	1.00	10.47	O
	ATOM	2133	N	HIS	B	77	27.529	48.579	15.433	1.00	10.80	N
20	ATOM	2134	CA	HIS	B	77	27.597	47.203	15.900	1.00	11.69	C
	ATOM	2135	CB	HIS	B	77	27.798	47.139	17.421	1.00	12.95	C
	ATOM	2136	CG	HIS	B	77	26.680	47.747	18.212	1.00	15.54	C
	ATOM	2137	ND1	HIS	B	77	26.877	48.786	19.094	1.00	19.44	N
	ATOM	2138	CE1	HIS	B	77	25.723	49.122	19.644	1.00	16.59	C
25	ATOM	2139	NE2	HIS	B	77	24.785	48.326	19.167	1.00	17.20	N
	ATOM	2140	CD2	HIS	B	77	25.357	47.454	18.269	1.00	17.77	C
	ATOM	2141	C	HIS	B	77	26.372	46.392	15.508	1.00	10.68	C
	ATOM	2142	O	HIS	B	77	25.380	46.935	14.992	1.00	9.70	O
	ATOM	2143	N	ILE	B	78	26.472	45.093	15.770	1.00	9.55	N
30	ATOM	2144	CA	ILE	B	78	25.430	44.112	15.479	1.00	8.64	C
	ATOM	2145	CB	ILE	B	78	25.860	43.181	14.328	1.00	8.82	C
	ATOM	2146	CG1	ILE	B	78	26.231	44.007	13.079	1.00	7.92	C
	ATOM	2147	CD1	ILE	B	78	26.856	43.206	11.946	1.00	8.28	C
	ATOM	2148	CG2	ILE	B	78	24.777	42.089	14.087	1.00	9.82	C
35	ATOM	2149	C	ILE	B	78	25.226	43.255	16.725	1.00	8.52	C

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	ATOM	2150	O	ILE B 78	26.190	42.683	17.240	1.00	10.19	O
	ATOM	2151	N	ASN B 79	23.985	43.164	17.195	1.00	9.07	N
	ATOM	2152	CA	ASN B 79	23.647	42.346	18.354	1.00	9.70	C
	ATOM	2153	CB	ASN B 79	22.973	43.190	19.454	1.00	9.67	C
5	ATOM	2154	CG	ASN B 79	23.881	44.296	20.049	1.00	11.62	C
	ATOM	2155	OD1	ASN B 79	23.377	45.305	20.546	1.00	16.97	O
	ATOM	2156	ND2	ASN B 79	25.177	44.091	20.043	1.00	9.04	N
	ATOM	2157	C	ASN B 79	22.705	41.192	17.949	1.00	8.81	C
	ATOM	2158	O	ASN B 79	21.762	41.396	17.162	1.00	9.17	O
10	ATOM	2159	N	LEU B 80	22.947	40.004	18.505	1.00	8.70	N
	ATOM	2160	CA	LEU B 80	22.099	38.830	18.268	1.00	8.96	C
	ATOM	2161	CB	LEU B 80	22.931	37.649	17.755	1.00	9.68	C
	ATOM	2162	CG	LEU B 80	23.902	37.932	16.596	1.00	9.97	C
	ATOM	2163	CD1	LEU B 80	24.764	36.709	16.285	1.00	10.27	C
15	ATOM	2164	CD2	LEU B 80	23.191	38.454	15.332	1.00	10.59	C
	ATOM	2165	C	LEU B 80	21.367	38.449	19.554	1.00	9.62	C
	ATOM	2166	O	LEU B 80	21.987	38.262	20.599	1.00	8.37	O
	ATOM	2167	N	ILE B 81	20.044	38.351	19.483	1.00	10.49	N
	ATOM	2168	CA	ILE B 81	19.252	38.216	20.703	1.00	12.08	C
20	ATOM	2169	CB	ILE B 81	18.535	39.553	21.087	1.00	12.15	C
	ATOM	2170	CG1	ILE B 81	19.536	40.728	21.091	1.00	13.69	C
	ATOM	2171	CD1	ILE B 81	18.919	42.104	21.253	1.00	14.69	C
	ATOM	2172	CG2	ILE B 81	17.796	39.401	22.448	1.00	13.91	C
	ATOM	2173	C	ILE B 81	18.259	37.054	20.581	1.00	11.47	C
25	ATOM	2174	O	ILE B 81	17.154	37.227	20.059	1.00	11.55	O
	ATOM	2175	N	PRO B 82	18.669	35.854	21.026	1.00	11.57	N
	ATOM	2176	CA	PRO B 82	17.696	34.768	21.106	1.00	11.94	C
	ATOM	2177	CB	PRO B 82	18.570	33.523	21.328	1.00	12.27	C
	ATOM	2178	CG	PRO B 82	19.809	34.059	22.034	1.00	11.35	C
30	ATOM	2179	CD	PRO B 82	20.026	35.431	21.433	1.00	10.61	C
	ATOM	2180	C	PRO B 82	16.714	34.966	22.268	1.00	12.69	C
	ATOM	2181	O	PRO B 82	17.079	35.522	23.327	1.00	11.28	O
	ATOM	2182	N	ASN B 83	15.486	34.494	22.075	1.00	12.31	N
	ATOM	2183	CA	ASN B 83	14.461	34.566	23.112	1.00	13.05	C
35	ATOM	2184	CB	ASN B 83	13.601	35.832	22.929	1.00	13.56	C

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	ATOM	2185	CG	ASN B 83	12.595	36.050	24.064	1.00	15.17	C
	ATOM	2186	OD1	ASN B 83	12.049	35.105	24.632	1.00	17.41	O
	ATOM	2187	ND2	ASN B 83	12.335	37.315	24.379	1.00	18.74	N
	ATOM	2188	C	ASN B 83	13.612	33.298	23.066	1.00	13.68	C
5	ATOM	2189	O	ASN B 83	12.694	33.198	22.267	1.00	13.70	O
	ATOM	2190	N	LYS B 84	13.933	32.330	23.918	1.00	14.66	N
	ATOM	2191	CA	LYS B 84	13.225	31.044	23.899	1.00	16.65	C
	ATOM	2192	CB	LYS B 84	13.943	30.001	24.762	1.00	17.00	C
	ATOM	2193	CG	LYS B 84	15.203	29.455	24.110	1.00	19.70	C
10	ATOM	2194	CD	LYS B 84	15.797	28.346	24.954	1.00	23.56	C
	ATOM	2195	CE	LYS B 84	17.221	28.041	24.540	1.00	24.98	C
	ATOM	2196	NZ	LYS B 84	17.656	26.772	25.174	1.00	28.06	N
	ATOM	2197	C	LYS B 84	11.762	31.175	24.309	1.00	17.21	C
	ATOM	2198	O	LYS B 84	10.903	30.480	23.762	1.00	18.30	O
15	ATOM	2199	N	GLN B 85	11.480	32.076	25.248	1.00	17.84	N
	ATOM	2200	CA	GLN B 85	10.114	32.278	25.745	1.00	18.77	C
	ATOM	2201	CB	GLN B 85	10.091	33.278	26.908	1.00	18.82	C
	ATOM	2202	CG	GLN B 85	8.699	33.542	27.504	1.00	21.35	C
	ATOM	2206	C	GLN B 85	9.185	32.725	24.620	1.00	18.60	C
20	ATOM	2207	O	GLN B 85	8.047	32.246	24.526	1.00	19.12	O
	ATOM	2208	N	ASP B 86	9.688	33.613	23.759	1.00	16.83	N
	ATOM	2209	CA	ASP B 86	8.917	34.171	22.648	1.00	16.83	C
	ATOM	2210	CB	ASP B 86	9.319	35.635	22.416	1.00	17.59	C
	ATOM	2211	CG	ASP B 86	8.863	36.555	23.537	1.00	21.22	C
25	ATOM	2212	OD1	ASP B 86	8.177	36.084	24.480	1.00	23.25	O
	ATOM	2213	OD2	ASP B 86	9.200	37.756	23.473	1.00	22.85	O
	ATOM	2214	C	ASP B 86	9.102	33.391	21.348	1.00	15.30	C
	ATOM	2215	O	ASP B 86	8.405	33.647	20.362	1.00	15.05	O
	ATOM	2216	N	ARG B 87	10.043	32.446	21.366	1.00	14.04	N
30	ATOM	2217	CA	ARG B 87	10.515	31.735	20.168	1.00	13.05	C
	ATOM	2218	CB	ARG B 87	9.494	30.705	19.674	1.00	13.55	C
	ATOM	2219	CG	ARG B 87	10.145	29.568	18.895	1.00	15.88	C
	ATOM	2220	CD	ARG B 87	9.201	29.006	17.865	1.00	18.49	C
	ATOM	2221	NE	ARG B 87	8.114	28.265	18.483	1.00	19.71	N
35	ATOM	2222	CZ	ARG B 87	6.977	27.933	17.875	1.00	21.56	C

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	ATOM	2223	NH1	ARG B 87	6.749	28.277	16.610	1.00	21.35	N
	ATOM	2224	NH2	ARG B 87	6.060	27.244	18.542	1.00	22.11	N
	ATOM	2225	C	ARG B 87	10.897	32.710	19.048	1.00	12.61	C
	ATOM	2226	O	ARG B 87	10.458	32.571	17.901	1.00	11.93	O
5	ATOM	2227	N	THR B 88	11.700	33.712	19.400	1.00	11.51	N
	ATOM	2228	CA	THR B 88	12.195	34.683	18.429	1.00	11.41	C
	ATOM	2229	CB	THR B 88	11.593	36.096	18.659	1.00	11.38	C
	ATOM	2230	OG1	THR B 88	11.928	36.554	19.981	1.00	12.01	O
	ATOM	2231	CG2	THR B 88	10.068	36.086	18.468	1.00	12.79	C
10	ATOM	2232	C	THR B 88	13.721	34.812	18.482	1.00	10.48	C
	ATOM	2233	O	THR B 88	14.351	34.633	19.542	1.00	9.97	O
	ATOM	2234	N	LEU B 89	14.306	35.101	17.322	1.00	10.27	N
	ATOM	2235	CA	LEU B 89	15.720	35.458	17.231	1.00	10.26	C
	ATOM	2236	CB	LEU B 89	16.501	34.459	16.364	1.00	10.60	C
15	ATOM	2237	CG	LEU B 89	17.979	34.793	16.099	1.00	10.61	C
	ATOM	2238	CD1	LEU B 89	18.769	34.876	17.423	1.00	10.72	C
	ATOM	2239	CD2	LEU B 89	18.636	33.793	15.122	1.00	11.10	C
	ATOM	2240	C	LEU B 89	15.740	36.836	16.604	1.00	10.12	C
	ATOM	2241	O	LEU B 89	15.188	37.039	15.515	1.00	10.11	O
20	ATOM	2242	N	THR B 90	16.325	37.780	17.319	1.00	10.47	N
	ATOM	2243	CA	THR B 90	16.370	39.166	16.865	1.00	10.42	C
	ATOM	2244	CB	THR B 90	15.811	40.114	17.958	1.00	11.60	C
	ATOM	2245	OG1	THR B 90	14.437	39.777	18.222	1.00	12.03	O
	ATOM	2246	CG2	THR B 90	15.892	41.576	17.516	1.00	12.15	C
25	ATOM	2247	C	THR B 90	17.797	39.547	16.489	1.00	10.48	C
	ATOM	2248	O	THR B 90	18.731	39.262	17.235	1.00	10.58	O
	ATOM	2249	N	ILE B 91	17.946	40.170	15.323	1.00	9.88	N
	ATOM	2250	CA	ILE B 91	19.232	40.683	14.844	1.00	11.15	C
	ATOM	2251	CB	ILE B 91	19.611	40.131	13.439	1.00	11.04	C
30	ATOM	2252	CG1	ILE B 91	19.782	38.590	13.441	1.00	12.21	C
	ATOM	2253	CD1	ILE B 91	18.498	37.802	13.183	1.00	14.45	C
	ATOM	2254	CG2	ILE B 91	20.896	40.792	12.929	1.00	11.69	C
	ATOM	2255	C	ILE B 91	19.096	42.213	14.798	1.00	11.09	C
	ATOM	2256	O	ILE B 91	18.280	42.745	14.027	1.00	12.02	O
35	ATOM	2257	N	VAL B 92	19.888	42.901	15.619	1.00	11.03	N

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	ATOM	2258	CA	VAL B 92	19.812	44.371	15.746	1.00	11.16	C
	ATOM	2259	CB	VAL B 92	19.568	44.819	17.224	1.00	11.49	C
	ATOM	2260	CG1	VAL B 92	19.487	46.345	17.327	1.00	13.18	C
	ATOM	2261	CG2	VAL B 92	18.298	44.190	17.803	1.00	13.87	C
5	ATOM	2262	C	VAL B 92	21.107	45.013	15.256	1.00	11.18	C
	ATOM	2263	O	VAL B 92	22.201	44.579	15.620	1.00	10.36	O
	ATOM	2264	N	ASP B 93	20.982	46.059	14.447	1.00	10.16	N
	ATOM	2265	CA	ASP B 93	22.147	46.850	14.089	1.00	9.56	C
	ATOM	2266	CB	ASP B 93	22.608	46.513	12.673	1.00	9.40	C
10	ATOM	2267	CG	ASP B 93	21.610	46.957	11.606	1.00	11.15	C
	ATOM	2268	OD1	ASP B 93	21.424	48.190	11.441	1.00	10.36	O
	ATOM	2269	OD2	ASP B 93	21.055	46.068	10.912	1.00	9.41	O
	ATOM	2270	C	ASP B 93	21.891	48.352	14.284	1.00	9.25	C
	ATOM	2271	O	ASP B 93	20.738	48.789	14.387	1.00	8.87	O
15	ATOM	2272	N	THR B 94	22.983	49.109	14.346	1.00	9.13	N
	ATOM	2273	CA	THR B 94	22.935	50.569	14.437	1.00	9.87	C
	ATOM	2274	CB	THR B 94	23.827	51.056	15.591	1.00	9.67	C
	ATOM	2275	OG1	THR B 94	25.146	50.512	15.433	1.00	10.19	O
	ATOM	2276	CG2	THR B 94	23.250	50.599	16.940	1.00	11.25	C
20	ATOM	2277	C	THR B 94	23.352	51.193	13.094	1.00	9.38	C
	ATOM	2278	O	THR B 94	24.035	52.236	13.037	1.00	9.00	O
	ATOM	2279	N	GLY B 95	22.955	50.522	12.006	1.00	9.80	N
	ATOM	2280	CA	GLY B 95	23.202	51.011	10.644	1.00	8.66	C
	ATOM	2281	C	GLY B 95	22.340	52.218	10.266	1.00	8.47	C
25	ATOM	2282	O	GLY B 95	21.678	52.823	11.113	1.00	8.26	O
	ATOM	2283	N	ILE B 96	22.356	52.564	8.984	1.00	9.05	N
	ATOM	2284	CA	ILE B 96	21.666	53.761	8.484	1.00	9.68	C
	ATOM	2285	CB	ILE B 96	22.040	54.053	7.002	1.00	9.25	C
	ATOM	2286	CG1	ILE B 96	21.739	55.522	6.652	1.00	10.76	C
30	ATOM	2287	CD1	ILE B 96	22.414	55.985	5.357	1.00	12.53	C
	ATOM	2288	CG2	ILE B 96	21.378	53.047	6.030	1.00	8.89	C
	ATOM	2289	C	ILE B 96	20.134	53.731	8.689	1.00	10.00	C
	ATOM	2290	O	ILE B 96	19.490	54.776	8.759	1.00	10.29	O
	ATOM	2291	N	GLY B 97	19.575	52.534	8.834	1.00	10.39	N
35	ATOM	2292	CA	GLY B 97	18.125	52.366	8.932	1.00	10.58	C

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	ATOM	2293	C	GLY B 97	17.444	52.575	7.592	1.00	10.12	C
	ATOM	2294	O	GLY B 97	18.103	52.704	6.555	1.00	10.50	O
	ATOM	2295	N	MET B 98	16.116	52.612	7.609	1.00	10.28	N
	ATOM	2296	CA	MET B 98	15.347	52.803	6.386	1.00	10.83	C
5	ATOM	2297	CB	MET B 98	14.812	51.459	5.866	1.00	11.30	C
	ATOM	2298	CG	MET B 98	15.890	50.513	5.354	1.00	11.71	C
	ATOM	2299	SD	MET B 98	15.260	48.837	5.048	1.00	12.32	S
	ATOM	2300	CE	MET B 98	15.151	48.200	6.718	1.00	13.42	C
	ATOM	2301	C	MET B 98	14.196	53.766	6.628	1.00	11.25	C
10	ATOM	2302	O	MET B 98	13.467	53.630	7.606	1.00	10.64	O
	ATOM	2303	N	THR B 99	14.040	54.740	5.734	1.00	10.92	N
	ATOM	2304	CA	THR B 99	12.825	55.569	5.724	1.00	11.28	C
	ATOM	2305	CB	THR B 99	12.927	56.718	4.693	1.00	11.52	C
	ATOM	2306	OG1	THR B 99	12.913	56.172	3.371	1.00	11.66	O
15	ATOM	2307	CG2	THR B 99	14.237	57.527	4.891	1.00	13.20	C
	ATOM	2308	C	THR B 99	11.615	54.687	5.390	1.00	10.72	C
	ATOM	2309	O	THR B 99	11.776	53.554	4.917	1.00	10.74	O
	ATOM	2310	N	LYS B 100	10.405	55.192	5.626	1.00	10.72	N
	ATOM	2311	CA	LYS B 100	9.204	54.452	5.252	1.00	10.26	C
20	ATOM	2312	CB	LYS B 100	7.944	55.289	5.484	1.00	10.75	C
	ATOM	2313	CG	LYS B 100	6.663	54.478	5.435	1.00	12.02	C
	ATOM	2314	CD	LYS B 100	5.434	55.389	5.453	1.00	14.27	C
	ATOM	2315	CE	LYS B 100	4.157	54.560	5.425	1.00	15.35	C
	ATOM	2316	NZ	LYS B 100	2.969	55.453	5.244	1.00	14.51	N
25	ATOM	2317	C	LYS B 100	9.258	54.015	3.784	1.00	10.80	C
	ATOM	2318	O	LYS B 100	8.975	52.857	3.471	1.00	9.84	O
	ATOM	2319	N	ALA B 101	9.602	54.945	2.893	1.00	10.92	N
	ATOM	2320	CA	ALA B 101	9.686	54.644	1.457	1.00	12.27	C
	ATOM	2321	CB	ALA B 101	9.983	55.909	0.637	1.00	13.49	C
30	ATOM	2322	C	ALA B 101	10.715	53.554	1.158	1.00	12.15	C
	ATOM	2323	O	ALA B 101	10.385	52.608	0.438	1.00	11.81	O
	ATOM	2324	N	ASP B 102	11.936	53.705	1.701	1.00	12.46	N
	ATOM	2325	CA	ASP B 102	13.021	52.704	1.610	1.00	13.14	C
	ATOM	2326	CB	ASP B 102	14.219	53.028	2.544	1.00	14.41	C
35	ATOM	2327	CG	ASP B 102	15.044	54.273	2.145	1.00	18.61	C

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	ATOM	2328	OD1 ASP B 102	15.077	54.680	0.958	1.00	17.26	O
	ATOM	2329	OD2 ASP B 102	15.729	54.813	3.073	1.00	20.87	O
	ATOM	2330	C ASP B 102	12.517	51.318	2.045	1.00	12.42	C
	ATOM	2331	O ASP B 102	12.764	50.309	1.373	1.00	11.45	O
5	ATOM	2332	N LEU B 103	11.859	51.272	3.202	1.00	11.21	N
	ATOM	2333	CA LEU B 103	11.373	50.020	3.784	1.00	10.98	C
	ATOM	2334	CB LEU B 103	10.667	50.307	5.109	1.00	10.47	C
	ATOM	2335	CG LEU B 103	10.110	49.151	5.947	1.00	10.41	C
	ATOM	2336	CD1 LEU B 103	11.184	48.104	6.286	1.00	12.09	C
10	ATOM	2337	CD2 LEU B 103	9.507	49.736	7.211	1.00	10.86	C
	ATOM	2338	C LEU B 103	10.437	49.275	2.831	1.00	11.37	C
	ATOM	2339	O LEU B 103	10.623	48.081	2.548	1.00	11.04	O
	ATOM	2340	N ILE B 104	9.423	49.998	2.356	1.00	10.33	N
	ATOM	2341	CA ILE B 104	8.425	49.459	1.446	1.00	10.87	C
15	ATOM	2342	CB ILE B 104	7.307	50.503	1.165	1.00	10.24	C
	ATOM	2343	CG1 ILE B 104	6.520	50.795	2.453	1.00	10.13	C
	ATOM	2344	CD1 ILE B 104	5.647	52.067	2.370	1.00	11.29	C
	ATOM	2345	CG2 ILE B 104	6.383	50.019	0.032	1.00	10.89	C
	ATOM	2346	C ILE B 104	9.066	48.974	0.146	1.00	10.81	C
20	ATOM	2347	O ILE B 104	8.801	47.850	-0.288	1.00	10.59	O
	ATOM	2348	N ASN B 105	9.947	49.799	-0.427	1.00	11.11	N
	ATOM	2349	CA ASN B 105	10.627	49.476	-1.672	1.00	12.61	C
	ATOM	2350	CB ASN B 105	11.402	50.691	-2.211	1.00	14.17	C
	ATOM	2351	CG ASN B 105	11.827	50.515	-3.667	1.00	19.12	C
25	ATOM	2352	OD1 ASN B 105	13.028	50.509	-3.990	1.00	23.95	O
	ATOM	2353	ND2 ASN B 105	10.845	50.380	-4.555	1.00	22.29	N
	ATOM	2354	C ASN B 105	11.575	48.283	-1.527	1.00	11.46	C
	ATOM	2355	O ASN B 105	11.542	47.361	-2.343	1.00	10.66	O
	ATOM	2356	N ASN B 106	12.382	48.303	-0.468	1.00	11.43	N
30	ATOM	2357	CA ASN B 106	13.403	47.281	-0.247	1.00	12.17	C
	ATOM	2358	CB ASN B 106	14.282	47.625	0.958	1.00	12.09	C
	ATOM	2359	CG ASN B 106	15.265	48.747	0.676	1.00	12.64	C
	ATOM	2360	OD1 ASN B 106	15.497	49.114	-0.475	1.00	14.20	O
	ATOM	2361	ND2 ASN B 106	15.851	49.293	1.733	1.00	11.98	N
35	ATOM	2362	C ASN B 106	12.811	45.905	-0.016	1.00	12.58	C

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	ATOM	2363	O	ASN B 106	13.389	44.901	-0.433	1.00	13.10	O
	ATOM	2364	N	LEU B 107	11.691	45.852	0.696	1.00	12.32	N
	ATOM	2365	CA	LEU B 107	11.124	44.559	1.081	1.00	13.50	C
	ATOM	2366	CB	LEU B 107	10.756	44.546	2.575	1.00	13.77	C
5	ATOM	2367	CG	LEU B 107	11.949	44.839	3.512	1.00	14.54	C
	ATOM	2368	CD1	LEU B 107	11.599	44.684	4.988	1.00	15.61	C
	ATOM	2369	CD2	LEU B 107	13.150	43.962	3.166	1.00	14.99	C
	ATOM	2370	C	LEU B 107	9.960	44.143	0.179	1.00	14.10	C
	ATOM	2371	O	LEU B 107	9.667	42.945	0.044	1.00	15.12	O
10	ATOM	2372	N	GLY B 108	9.351	45.123	-0.488	1.00	12.73	N
	ATOM	2373	CA	GLY B 108	8.166	44.879	-1.322	1.00	12.48	C
	ATOM	2374	C	GLY B 108	8.397	44.628	-2.809	1.00	11.82	C
	ATOM	2375	O	GLY B 108	7.514	44.110	-3.493	1.00	11.98	O
	ATOM	2376	N	THR B 109	9.576	44.995	-3.311	1.00	11.03	N
15	ATOM	2377	CA	THR B 109	9.845	44.987	-4.751	1.00	11.34	C
	ATOM	2378	CB	THR B 109	9.826	46.434	-5.328	1.00	11.34	C
	ATOM	2379	OG1	THR B 109	11.027	47.123	-4.950	1.00	10.87	O
	ATOM	2380	CG2	THR B 109	8.592	47.225	-4.836	1.00	11.84	C
	ATOM	2381	C	THR B 109	11.206	44.377	-5.086	1.00	11.64	C
20	ATOM	2382	O	THR B 109	12.026	44.154	-4.196	1.00	11.31	O
	ATOM	2383	N	ILE B 110	11.451	44.147	-6.378	1.00	11.50	N
	ATOM	2384	CA	ILE B 110	12.756	43.690	-6.864	1.00	12.39	C
	ATOM	2385	CB	ILE B 110	12.758	43.501	-8.416	1.00	13.03	C
	ATOM	2386	CG1	ILE B 110	11.743	42.430	-8.847	1.00	15.47	C
25	ATOM	2387	CD1	ILE B 110	11.779	41.200	-8.036	1.00	19.29	C
	ATOM	2388	CG2	ILE B 110	14.168	43.169	-8.967	1.00	15.31	C
	ATOM	2389	C	ILE B 110	13.838	44.682	-6.455	1.00	11.89	C
	ATOM	2390	O	ILE B 110	14.955	44.280	-6.128	1.00	11.08	O
	ATOM	2391	N	ALA B 111	13.495	45.972	-6.478	1.00	11.48	N
30	ATOM	2392	CA	ALA B 111	14.401	47.034	-6.024	1.00	12.24	C
	ATOM	2393	CB	ALA B 111	14.580	46.969	-4.507	1.00	11.97	C
	ATOM	2394	C	ALA B 111	15.744	46.944	-6.776	1.00	11.78	C
	ATOM	2395	O	ALA B 111	15.737	46.972	-8.009	1.00	11.31	O
	ATOM	2396	N	LYS B 112	16.862	46.794	-6.052	1.00	11.60	N
35	ATOM	2397	CA	LYS B 112	18.208	46.793	-6.662	1.00	11.54	C

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	ATOM	2398	CB	LYS B 112	19.218	47.516	-5.753	1.00	11.65	C
	ATOM	2399	CG	LYS B 112	18.738	48.863	-5.216	1.00	13.09	C
	ATOM	2400	CD	LYS B 112	19.779	49.509	-4.304	1.00	14.03	C
	ATOM	2401	CE	LYS B 112	19.397	50.941	-3.944	1.00	17.67	C
5	ATOM	2402	NZ	LYS B 112	18.012	51.089	-3.439	1.00	22.15	N
	ATOM	2403	C	LYS B 112	18.735	45.378	-6.966	1.00	10.78	C
	ATOM	2404	O	LYS B 112	19.892	45.212	-7.376	1.00	10.71	O
	ATOM	2405	N	SER B 113	17.888	44.367	-6.757	1.00	9.77	N
	ATOM	2406	CA	SER B 113	18.338	42.978	-6.756	1.00	9.75	C
10	ATOM	2407	CB	SER B 113	17.464	42.155	-5.806	1.00	9.64	C
	ATOM	2408	OG	SER B 113	16.186	41.943	-6.390	1.00	9.47	O
	ATOM	2409	C	SER B 113	18.337	42.299	-8.126	1.00	10.24	C
	ATOM	2410	O	SER B 113	17.764	42.809	-9.098	1.00	10.22	O
	ATOM	2411	N	GLY B 114	18.953	41.118	-8.174	1.00	9.25	N
15	ATOM	2412	CA	GLY B 114	18.883	40.251	-9.348	1.00	10.20	C
	ATOM	2413	C	GLY B 114	17.901	39.114	-9.094	1.00	10.89	C
	ATOM	2414	O	GLY B 114	18.194	37.952	-9.381	1.00	11.54	O
	ATOM	2415	N	THR B 115	16.716	39.461	-8.583	1.00	10.89	N
	ATOM	2416	CA	THR B 115	15.683	38.465	-8.233	1.00	12.31	C
20	ATOM	2417	CB	THR B 115	14.395	39.131	-7.684	1.00	11.47	C
	ATOM	2418	OG1	THR B 115	14.635	39.693	-6.384	1.00	12.16	O
	ATOM	2419	CG2	THR B 115	13.239	38.107	-7.582	1.00	12.42	C
	ATOM	2420	C	THR B 115	15.301	37.560	-9.406	1.00	12.84	C
	ATOM	2421	O	THR B 115	15.215	36.348	-9.239	1.00	13.59	O
25	ATOM	2422	N	LYS B 116	15.093	38.133	-10.590	1.00	13.78	N
	ATOM	2423	CA	LYS B 116	14.664	37.294	-11.721	1.00	14.96	C
	ATOM	2424	CB	LYS B 116	14.140	38.109	-12.909	1.00	15.59	C
	ATOM	2425	CG	LYS B 116	15.034	39.199	-13.413	1.00	17.17	C
	ATOM	2429	C	LYS B 116	15.756	36.295	-12.137	1.00	15.15	C
30	ATOM	2430	O	LYS B 116	15.468	35.120	-12.378	1.00	15.08	O
	ATOM	2431	N	ALA B 117	17.004	36.758	-12.162	1.00	14.14	N
	ATOM	2432	CA	ALA B 117	18.144	35.884	-12.447	1.00	14.58	C
	ATOM	2433	CB	ALA B 117	19.442	36.704	-12.527	1.00	14.19	C
	ATOM	2434	C	ALA B 117	18.275	34.770	-11.389	1.00	14.69	C
35	ATOM	2435	O	ALA B 117	18.647	33.638	-11.716	1.00	14.36	O

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	ATOM	2436	N	PHE B 118	17.970	35.085	-10.130	1.00	14.18	N
	ATOM	2437	CA	PHE B 118	18.048	34.082	-9.046	1.00	15.51	C
	ATOM	2438	CB	PHE B 118	17.855	34.726	-7.667	1.00	15.22	C
	ATOM	2439	CG	PHE B 118	18.054	33.769	-6.503	1.00	15.12	C
5	ATOM	2440	CD1	PHE B 118	19.164	32.918	-6.451	1.00	16.65	C
	ATOM	2441	CE1	PHE B 118	19.358	32.037	-5.361	1.00	16.93	C
	ATOM	2442	CZ	PHE B 118	18.437	32.015	-4.321	1.00	16.15	C
	ATOM	2443	CE2	PHE B 118	17.323	32.863	-4.358	1.00	14.86	C
	ATOM	2444	CD2	PHE B 118	17.140	33.738	-5.453	1.00	16.03	C
10	ATOM	2445	C	PHE B 118	17.020	32.973	-9.243	1.00	16.54	C
	ATOM	2446	O	PHE B 118	17.340	31.786	-9.122	1.00	17.31	O
	ATOM	2447	N	MET B 119	15.791	33.374	-9.550	1.00	17.77	N
	ATOM	2448	CA	MET B 119	14.707	32.417	-9.786	1.00	19.97	C
	ATOM	2449	CB	MET B 119	13.381	33.147	-9.943	1.00	19.55	C
15	ATOM	2450	CG	MET B 119	12.996	33.954	-8.693	1.00	19.55	C
	ATOM	2451	SD	BMET B 119	12.610	32.915	-7.287	0.40	15.80	S
	ATOM	2452	SD	AMET B 119	11.291	33.787	-8.167	0.60	24.26	S
	ATOM	2453	CE	BMET B 119	11.070	32.157	-7.814	0.40	17.84	C
	ATOM	2454	CE	AMET B 119	11.185	32.030	-7.811	0.60	23.93	C
20	ATOM	2455	C	MET B 119	15.006	31.529	-11.000	1.00	20.67	C
	ATOM	2456	O	MET B 119	14.746	30.322	-10.974	1.00	20.63	O
	ATOM	2457	N	GLU B 120	15.563	32.128	-12.049	1.00	21.68	N
	ATOM	2458	CA	GLU B 120	16.069	31.371	-13.199	1.00	23.30	C
	ATOM	2459	CB	GLU B 120	16.575	32.321	-14.297	1.00	23.40	C
25	ATOM	2460	CG	GLU B 120	15.464	33.002	-15.097	1.00	25.60	C
	ATOM	2461	CD	GLU B 120	15.918	34.252	-15.856	1.00	27.39	C
	ATOM	2462	OE1	GLU B 120	15.067	34.848	-16.561	1.00	31.87	O
	ATOM	2463	OE2	GLU B 120	17.104	34.662	-15.747	1.00	31.51	O
	ATOM	2464	C	GLU B 120	17.175	30.394	-12.781	1.00	23.02	C
30	ATOM	2465	O	GLU B 120	17.163	29.222	-13.188	1.00	22.88	O
	ATOM	2466	N	ALA B 121	18.119	30.866	-11.962	1.00	22.39	N
	ATOM	2467	CA	ALA B 121	19.199	30.008	-11.448	1.00	22.92	C
	ATOM	2468	CB	ALA B 121	20.234	30.831	-10.651	1.00	22.37	C
	ATOM	2469	C	ALA B 121	18.663	28.834	-10.617	1.00	22.64	C
35	ATOM	2470	O	ALA B 121	19.109	27.702	-10.795	1.00	22.59	O

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	ATOM	2471	N	LEU B 122	17.700	29.112	-9.735	1.00	23.31	N
	ATOM	2472	CA	LEU B 122	17.017	28.085	-8.923	1.00	24.34	C
	ATOM	2473	CB	LEU B 122	16.009	28.743	-7.975	1.00	24.22	C
	ATOM	2474	CG	LEU B 122	16.367	28.925	-6.490	1.00	24.43	C
5	ATOM	2475	CD1	LEU B 122	17.862	28.924	-6.190	1.00	24.87	C
	ATOM	2476	CD2	LEU B 122	15.664	30.143	-5.902	1.00	24.60	C
	ATOM	2477	C	LEU B 122	16.313	27.029	-9.776	1.00	25.22	C
	ATOM	2478	O	LEU B 122	16.468	25.828	-9.536	1.00	25.54	O
	ATOM	2479	N	GLN B 123	15.544	27.489	-10.764	1.00	26.34	N
10	ATOM	2480	CA	GLN B 123	14.898	26.616	-11.746	1.00	27.25	C
	ATOM	2481	CB	GLN B 123	14.178	27.457	-12.810	1.00	27.47	C
	ATOM	2482	CG	GLN B 123	13.373	26.654	-13.831	1.00	28.37	C
	ATOM	2486	C	GLN B 123	15.932	25.696	-12.398	1.00	27.90	C
	ATOM	2487	O	GLN B 123	15.670	24.508	-12.616	1.00	29.05	O
15	ATOM	2488	N	ALA B 124	17.108	26.253	-12.681	1.00	27.87	N
	ATOM	2489	CA	ALA B 124	18.210	25.538	-13.311	1.00	28.08	C
	ATOM	2490	CB	ALA B 124	19.162	26.528	-13.969	1.00	27.86	C
	ATOM	2491	C	ALA B 124	18.968	24.624	-12.342	1.00	28.19	C
	ATOM	2492	O	ALA B 124	19.856	23.878	-12.761	1.00	28.97	O
20	ATOM	2493	N	GLY B 125	18.630	24.699	-11.055	1.00	27.34	N
	ATOM	2494	CA	GLY B 125	19.189	23.804	-10.046	1.00	27.07	C
	ATOM	2495	C	GLY B 125	20.219	24.415	-9.106	1.00	26.27	C
	ATOM	2496	O	GLY B 125	20.858	23.686	-8.339	1.00	26.91	O
	ATOM	2497	N	ALA B 126	20.379	25.743	-9.151	1.00	24.87	N
25	ATOM	2498	CA	ALA B 126	21.362	26.431	-8.299	1.00	23.36	C
	ATOM	2499	CB	ALA B 126	21.425	27.920	-8.622	1.00	23.59	C
	ATOM	2500	C	ALA B 126	21.056	26.230	-6.824	1.00	22.11	C
	ATOM	2501	O	ALA B 126	19.913	25.936	-6.438	1.00	22.05	O
	ATOM	2502	N	ASP B 127	22.081	26.409	-5.999	1.00	20.64	N
30	ATOM	2503	CA	ASP B 127	21.934	26.249	-4.563	1.00	19.65	C
	ATOM	2504	CB	ASP B 127	23.264	25.840	-3.938	1.00	20.09	C
	ATOM	2505	CG	ASP B 127	23.090	25.277	-2.548	1.00	22.48	C
	ATOM	2506	OD1	ASP B 127	23.168	26.061	-1.592	1.00	21.34	O
	ATOM	2507	OD2	ASP B 127	22.842	24.053	-2.416	1.00	25.00	O
35	ATOM	2508	C	ASP B 127	21.420	27.540	-3.918	1.00	18.62	C

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	ATOM	2509	O	ASP B 127	21.894	28.636	-4.248	1.00	17.48	O
	ATOM	2510	N	ILE B 128	20.466	27.395	-3.001	1.00	17.56	N
	ATOM	2511	CA	ILE B 128	19.860	28.534	-2.288	1.00	17.66	C
	ATOM	2512	CB	ILE B 128	18.692	28.067	-1.363	1.00	17.16	C
5	ATOM	2513	CG1	ILE B 128	17.452	27.759	-2.218	1.00	17.26	C
	ATOM	2514	CD1	ILE B 128	16.271	27.148	-1.439	1.00	18.50	C
	ATOM	2515	CG2	ILE B 128	18.364	29.110	-0.293	1.00	17.60	C
	ATOM	2516	C	ILE B 128	20.881	29.379	-1.516	1.00	16.75	C
	ATOM	2517	O	ILE B 128	20.651	30.576	-1.292	1.00	16.01	O
10	ATOM	2518	N	SER B 129	22.012	28.772	-1.137	1.00	15.92	N
	ATOM	2519	CA	SER B 129	23.075	29.495	-0.425	1.00	16.37	C
	ATOM	2520	CB	SER B 129	24.221	28.551	-0.007	1.00	16.53	C
	ATOM	2521	OG	SER B 129	24.950	28.095	-1.141	1.00	18.99	O
	ATOM	2522	C	SER B 129	23.641	30.666	-1.241	1.00	15.62	C
15	ATOM	2523	O	SER B 129	24.311	31.549	-0.684	1.00	14.98	O
	ATOM	2524	N	MET B 130	23.384	30.666	-2.553	1.00	14.78	N
	ATOM	2525	CA	MET B 130	23.838	31.755	-3.438	1.00	16.26	C
	ATOM	2526	CB	MET B 130	23.858	31.291	-4.898	1.00	16.39	C
	ATOM	2527	CG	MET B 130	24.835	30.160	-5.200	1.00	18.99	C
20	ATOM	2528	SD	MET B 130	24.735	29.710	-6.942	1.00	22.71	S
	ATOM	2529	CE	MET B 130	25.497	31.147	-7.703	1.00	21.45	C
	ATOM	2530	C	MET B 130	22.971	33.018	-3.359	1.00	14.88	C
	ATOM	2531	O	MET B 130	23.272	34.021	-4.020	1.00	14.41	O
	ATOM	2532	N	ILE B 131	21.892	32.946	-2.579	1.00	14.05	N
25	ATOM	2533	CA	ILE B 131	20.848	33.981	-2.541	1.00	13.43	C
	ATOM	2534	CB	ILE B 131	19.773	33.656	-1.443	1.00	12.78	C
	ATOM	2535	CG1	ILE B 131	18.581	34.620	-1.533	1.00	13.63	C
	ATOM	2536	CD1	ILE B 131	17.343	34.097	-0.849	1.00	11.96	C
	ATOM	2537	CG2	ILE B 131	20.403	33.598	-0.024	1.00	13.47	C
30	ATOM	2538	C	ILE B 131	21.383	35.416	-2.404	1.00	12.91	C
	ATOM	2539	O	ILE B 131	20.910	36.323	-3.105	1.00	12.66	O
	ATOM	2540	N	GLY B 132	22.362	35.601	-1.513	1.00	12.50	N
	ATOM	2541	CA	GLY B 132	22.972	36.914	-1.259	1.00	13.58	C
	ATOM	2542	C	GLY B 132	23.706	37.502	-2.455	1.00	13.16	C
35	ATOM	2543	O	GLY B 132	23.771	38.720	-2.617	1.00	12.97	O

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	ATOM	2544	N	GLN B 133	24.256	36.632	-3.298	1.00	12.51	N
	ATOM	2545	CA	GLN B 133	24.915	37.055	-4.539	1.00	12.12	C
	ATOM	2546	CB	GLN B 133	25.596	35.862	-5.208	1.00	11.88	C
	ATOM	2547	CG	GLN B 133	26.502	35.093	-4.250	1.00	12.64	C
5	ATOM	2548	CD	GLN B 133	27.145	33.862	-4.872	1.00	13.69	C
	ATOM	2549	OE1	GLN B 133	27.532	32.933	-4.164	1.00	18.72	O
	ATOM	2550	NE2	GLN B 133	27.294	33.866	-6.184	1.00	15.31	N
	ATOM	2551	C	GLN B 133	23.938	37.725	-5.511	1.00	11.66	C
	ATOM	2552	O	GLN B 133	24.354	38.444	-6.414	1.00	10.92	O
10	ATOM	2553	N	PHE B 134	22.642	37.486	-5.309	1.00	10.93	N
	ATOM	2554	CA	PHE B 134	21.595	38.078	-6.138	1.00	10.84	C
	ATOM	2555	CB	PHE B 134	20.584	37.003	-6.551	1.00	11.19	C
	ATOM	2556	CG	PHE B 134	21.155	35.952	-7.474	1.00	11.26	C
	ATOM	2557	CD1	PHE B 134	21.029	36.077	-8.861	1.00	13.21	C
15	ATOM	2558	CE1	PHE B 134	21.544	35.096	-9.721	1.00	11.94	C
	ATOM	2559	CZ	PHE B 134	22.214	33.973	-9.182	1.00	12.38	C
	ATOM	2560	CE2	PHE B 134	22.347	33.843	-7.790	1.00	11.75	C
	ATOM	2561	CD2	PHE B 134	21.829	34.836	-6.948	1.00	12.54	C
	ATOM	2562	C	PHE B 134	20.881	39.242	-5.418	1.00	10.66	C
20	ATOM	2563	O	PHE B 134	19.890	39.785	-5.915	1.00	11.47	O
	ATOM	2564	N	GLY B 135	21.398	39.623	-4.254	1.00	11.40	N
	ATOM	2565	CA	GLY B 135	20.908	40.803	-3.536	1.00	10.73	C
	ATOM	2566	C	GLY B 135	19.592	40.611	-2.797	1.00	11.22	C
	ATOM	2567	O	GLY B 135	18.938	41.591	-2.432	1.00	11.40	O
25	ATOM	2568	N	VAL B 136	19.203	39.355	-2.562	1.00	10.71	N
	ATOM	2569	CA	VAL B 136	17.939	39.058	-1.880	1.00	10.78	C
	ATOM	2570	CB	VAL B 136	16.846	38.503	-2.864	1.00	10.93	C
	ATOM	2571	CG1	VAL B 136	16.165	39.658	-3.585	1.00	12.69	C
	ATOM	2572	CG2	VAL B 136	17.448	37.496	-3.869	1.00	11.50	C
30	ATOM	2573	C	VAL B 136	18.103	38.130	-0.671	1.00	10.31	C
	ATOM	2574	O	VAL B 136	17.177	37.393	-0.317	1.00	9.76	O
	ATOM	2575	N	GLY B 137	19.277	38.196	-0.038	1.00	10.08	N
	ATOM	2576	CA	GLY B 137	19.606	37.373	1.118	1.00	9.49	C
	ATOM	2577	C	GLY B 137	18.590	37.461	2.253	1.00	9.24	C
35	ATOM	2578	O	GLY B 137	18.335	36.475	2.948	1.00	9.16	O

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	ATOM	2579	N	PHE B 138	17.987	38.641	2.430	1.00	9.01	N
	ATOM	2580	CA	PHE B 138	16.968	38.824	3.471	1.00	9.58	C
	ATOM	2581	CB	PHE B 138	16.242	40.179	3.329	1.00	9.42	C
	ATOM	2582	CG	PHE B 138	14.998	40.280	4.173	1.00	8.90	C
5	ATOM	2583	CD1	PHE B 138	15.086	40.424	5.557	1.00	9.30	C
	ATOM	2584	CE1	PHE B 138	13.931	40.511	6.348	1.00	10.15	C
	ATOM	2585	CZ	PHE B 138	12.665	40.441	5.743	1.00	9.52	C
	ATOM	2586	CE2	PHE B 138	12.571	40.278	4.361	1.00	10.04	C
	ATOM	2587	CD2	PHE B 138	13.728	40.204	3.582	1.00	10.56	C
10	ATOM	2588	C	PHE B 138	15.911	37.704	3.483	1.00	9.80	C
	ATOM	2589	O	PHE B 138	15.523	37.234	4.558	1.00	10.11	O
	ATOM	2590	N	TYR B 139	15.442	37.300	2.302	1.00	10.28	N
	ATOM	2591	CA	TYR B 139	14.323	36.354	2.222	1.00	11.37	C
	ATOM	2592	CB	TYR B 139	13.669	36.346	0.830	1.00	12.03	C
15	ATOM	2593	CG	TYR B 139	13.138	37.715	0.458	1.00	13.29	C
	ATOM	2594	CD1	TYR B 139	11.933	38.194	0.997	1.00	13.53	C
	ATOM	2595	CE1	TYR B 139	11.458	39.485	0.668	1.00	14.75	C
	ATOM	2596	CZ	TYR B 139	12.205	40.281	-0.194	1.00	14.16	C
	ATOM	2597	OH	TYR B 139	11.776	41.543	-0.552	1.00	15.84	O
20	ATOM	2598	CE2	TYR B 139	13.406	39.830	-0.714	1.00	14.55	C
	ATOM	2599	CD2	TYR B 139	13.869	38.550	-0.383	1.00	12.99	C
	ATOM	2600	C	TYR B 139	14.676	34.947	2.683	1.00	10.97	C
	ATOM	2601	O	TYR B 139	13.775	34.160	2.967	1.00	10.54	O
	ATOM	2602	N	SER B 140	15.975	34.650	2.787	1.00	10.42	N
25	ATOM	2603	CA	SER B 140	16.400	33.392	3.395	1.00	10.81	C
	ATOM	2604	CB	SER B 140	17.926	33.191	3.308	1.00	11.04	C
	ATOM	2605	OG	SER B 140	18.617	34.058	4.172	1.00	11.85	O
	ATOM	2606	C	SER B 140	15.919	33.269	4.851	1.00	10.30	C
	ATOM	2607	O	SER B 140	15.911	32.172	5.398	1.00	9.90	O
30	ATOM	2608	N	ALA B 141	15.547	34.391	5.479	1.00	9.58	N
	ATOM	2609	CA	ALA B 141	14.917	34.351	6.806	1.00	10.51	C
	ATOM	2610	CB	ALA B 141	14.423	35.735	7.209	1.00	10.77	C
	ATOM	2611	C	ALA B 141	13.758	33.344	6.862	1.00	10.16	C
	ATOM	2612	O	ALA B 141	13.552	32.673	7.881	1.00	9.74	O
35	ATOM	2613	N	TYR B 142	13.006	33.254	5.769	1.00	9.97	N

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	ATOM	2614	CA	TYR B 142	11.823	32.370	5.715	1.00	10.24	C
	ATOM	2615	CB	TYR B 142	10.853	32.816	4.604	1.00	10.35	C
	ATOM	2616	CG	TYR B 142	10.201	34.128	4.968	1.00	10.87	C
	ATOM	2617	CD1	TYR B 142	9.090	34.160	5.822	1.00	10.67	C
5	ATOM	2618	CE1	TYR B 142	8.496	35.376	6.202	1.00	11.64	C
	ATOM	2619	CZ	TYR B 142	9.032	36.567	5.736	1.00	11.04	C
	ATOM	2620	OH	TYR B 142	8.463	37.760	6.105	1.00	10.76	O
	ATOM	2621	CE2	TYR B 142	10.151	36.562	4.898	1.00	10.04	C
	ATOM	2622	CD2	TYR B 142	10.730	35.340	4.522	1.00	9.84	C
10	ATOM	2623	C	TYR B 142	12.140	30.861	5.652	1.00	10.52	C
	ATOM	2624	O	TYR B 142	11.233	30.040	5.677	1.00	11.08	O
	ATOM	2625	N	LEU B 143	13.423	30.506	5.574	1.00	11.77	N
	ATOM	2626	CA	LEU B 143	13.848	29.108	5.791	1.00	11.73	C
	ATOM	2627	CB	LEU B 143	15.359	28.947	5.518	1.00	12.04	C
15	ATOM	2628	CG	LEU B 143	15.851	29.086	4.068	1.00	12.85	C
	ATOM	2629	CD1	LEU B 143	17.383	29.129	3.984	1.00	14.59	C
	ATOM	2630	CD2	LEU B 143	15.292	27.967	3.178	1.00	14.59	C
	ATOM	2631	C	LEU B 143	13.529	28.683	7.224	1.00	12.13	C
	ATOM	2632	O	LEU B 143	13.136	27.542	7.489	1.00	12.33	O
20	ATOM	2633	N	VAL B 144	13.690	29.622	8.150	1.00	11.31	N
	ATOM	2634	CA	VAL B 144	13.603	29.312	9.575	1.00	11.38	C
	ATOM	2635	CB	VAL B 144	14.944	29.600	10.308	1.00	11.41	C
	ATOM	2636	CG1	VAL B 144	16.101	28.759	9.708	1.00	11.08	C
	ATOM	2637	CG2	VAL B 144	15.291	31.104	10.288	1.00	11.15	C
25	ATOM	2638	C	VAL B 144	12.435	29.999	10.281	1.00	11.35	C
	ATOM	2639	O	VAL B 144	12.031	29.574	11.378	1.00	10.67	O
	ATOM	2640	N	ALA B 145	11.900	31.050	9.651	1.00	11.06	N
	ATOM	2641	CA	ALA B 145	10.838	31.864	10.247	1.00	11.09	C
	ATOM	2642	CB	ALA B 145	11.254	33.349	10.293	1.00	10.88	C
30	ATOM	2643	C	ALA B 145	9.506	31.707	9.513	1.00	11.24	C
	ATOM	2644	O	ALA B 145	9.465	31.673	8.272	1.00	11.73	O
	ATOM	2645	N	GLU B 146	8.433	31.605	10.293	1.00	11.96	N
	ATOM	2646	CA	GLU B 146	7.056	31.655	9.789	1.00	13.41	C
	ATOM	2647	CB	GLU B 146	6.105	30.891	10.732	1.00	13.69	C
35	ATOM	2648	CG	GLU B 146	6.012	31.449	12.164	1.00	15.49	C

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	ATOM	2649	CD	GLU B 146	5.089	30.648	13.084	1.00	17.54	C
	ATOM	2650	OE1	GLU B 146	4.671	29.532	12.705	1.00	21.48	O
	ATOM	2651	OE2	GLU B 146	4.795	31.139	14.201	1.00	20.82	O
	ATOM	2652	C	GLU B 146	6.569	33.102	9.598	1.00	12.85	C
5	ATOM	2653	O	GLU B 146	5.625	33.372	8.842	1.00	13.22	O
	ATOM	2654	N	LYS B 147	7.204	34.020	10.315	1.00	11.72	N
	ATOM	2655	CA	LYS B 147	6.874	35.437	10.251	1.00	11.66	C
	ATOM	2656	CB	LYS B 147	5.782	35.790	11.270	1.00	11.53	C
	ATOM	2657	CG	LYS B 147	5.430	37.276	11.328	1.00	12.49	C
10	ATOM	2658	CD	LYS B 147	4.227	37.540	12.228	1.00	13.86	C
	ATOM	2659	CE	LYS B 147	3.968	39.042	12.342	1.00	16.91	C
	ATOM	2660	NZ	LYS B 147	3.038	39.358	13.466	1.00	19.48	N
	ATOM	2661	C	LYS B 147	8.147	36.213	10.555	1.00	10.98	C
	ATOM	2662	O	LYS B 147	8.953	35.798	11.397	1.00	9.60	O
15	ATOM	2663	N	VAL B 148	8.327	37.324	9.848	1.00	9.46	N
	ATOM	2664	CA	VAL B 148	9.440	38.218	10.106	1.00	9.52	C
	ATOM	2665	CB	VAL B 148	10.467	38.233	8.941	1.00	9.45	C
	ATOM	2666	CG1	VAL B 148	11.635	39.195	9.267	1.00	8.81	C
	ATOM	2667	CG2	VAL B 148	10.999	36.803	8.616	1.00	8.93	C
20	ATOM	2668	C	VAL B 148	8.894	39.623	10.352	1.00	9.90	C
	ATOM	2669	O	VAL B 148	7.997	40.096	9.629	1.00	10.08	O
	ATOM	2670	N	THR B 149	9.422	40.272	11.384	1.00	9.41	N
	ATOM	2671	CA	THR B 149	9.106	41.677	11.672	1.00	9.72	C
	ATOM	2672	CB	THR B 149	8.536	41.854	13.105	1.00	10.09	C
25	ATOM	2673	OG1	THR B 149	7.347	41.066	13.259	1.00	10.89	O
	ATOM	2674	CG2	THR B 149	8.196	43.335	13.396	1.00	9.16	C
	ATOM	2675	C	THR B 149	10.404	42.481	11.519	1.00	9.95	C
	ATOM	2676	O	THR B 149	11.455	42.070	12.022	1.00	9.89	O
	ATOM	2677	N	VAL B 150	10.337	43.601	10.809	1.00	8.89	N
30	ATOM	2678	CA	VAL B 150	11.511	44.460	10.615	1.00	9.09	C
	ATOM	2679	CB	VAL B 150	11.936	44.573	9.110	1.00	9.27	C
	ATOM	2680	CG1	VAL B 150	13.073	45.597	8.934	1.00	9.17	C
	ATOM	2681	CG2	VAL B 150	12.337	43.191	8.521	1.00	9.29	C
	ATOM	2682	C	VAL B 150	11.141	45.830	11.199	1.00	10.10	C
35	ATOM	2683	O	VAL B 150	10.200	46.463	10.717	1.00	9.81	O

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	ATOM	2684	N	ILE B 151	11.834	46.227	12.274	1.00	10.19	N
	ATOM	2685	CA	ILE B 151	11.662	47.545	12.906	1.00	10.93	C
	ATOM	2686	CB	ILE B 151	11.651	47.451	14.458	1.00	12.11	C
	ATOM	2687	CG1	ILE B 151	10.780	46.291	14.968	1.00	15.13	C
5	ATOM	2688	CD1	ILE B 151	9.311	46.518	14.910	1.00	16.98	C
	ATOM	2689	CG2	ILE B 151	11.303	48.819	15.094	1.00	11.44	C
	ATOM	2690	C	ILE B 151	12.857	48.412	12.482	1.00	10.82	C
	ATOM	2691	O	ILE B 151	14.017	47.977	12.587	1.00	10.97	O
	ATOM	2692	N	THR B 152	12.596	49.622	11.996	1.00	9.34	N
10	ATOM	2693	CA	THR B 152	13.693	50.439	11.473	1.00	9.91	C
	ATOM	2694	CB	THR B 152	13.926	50.171	9.948	1.00	9.49	C
	ATOM	2695	OG1	THR B 152	15.192	50.699	9.536	1.00	10.66	O
	ATOM	2696	CG2	THR B 152	12.798	50.764	9.075	1.00	10.02	C
	ATOM	2697	C	THR B 152	13.507	51.922	11.765	1.00	9.70	C
15	ATOM	2698	O	THR B 152	12.367	52.414	11.856	1.00	9.88	O
	ATOM	2699	N	LYS B 153	14.637	52.606	11.935	1.00	9.28	N
	ATOM	2700	CA	LYS B 153	14.672	54.039	12.230	1.00	9.00	C
	ATOM	2701	CB	LYS B 153	14.852	54.283	13.734	1.00	8.69	C
	ATOM	2702	CG	LYS B 153	15.030	55.766	14.127	1.00	9.37	C
20	ATOM	2703	CD	LYS B 153	13.721	56.536	13.901	1.00	11.36	C
	ATOM	2704	CE	LYS B 153	13.819	57.974	14.425	1.00	11.03	C
	ATOM	2705	NZ	LYS B 153	14.652	58.814	13.531	1.00	10.38	N
	ATOM	2706	C	LYS B 153	15.833	54.658	11.469	1.00	9.49	C
	ATOM	2707	O	LYS B 153	17.004	54.356	11.745	1.00	9.30	O
25	ATOM	2708	N	HIS B 154	15.486	55.517	10.516	1.00	9.69	N
	ATOM	2709	CA	HIS B 154	16.450	56.300	9.741	1.00	10.74	C
	ATOM	2710	CB	HIS B 154	16.010	56.301	8.269	1.00	10.21	C
	ATOM	2711	CG	HIS B 154	16.972	56.972	7.333	1.00	12.18	C
	ATOM	2712	ND1	HIS B 154	17.025	58.340	7.171	1.00	13.78	N
30	ATOM	2713	CE1	HIS B 154	17.950	58.643	6.275	1.00	14.49	C
	ATOM	2714	NE2	HIS B 154	18.495	57.517	5.844	1.00	13.99	N
	ATOM	2715	CD2	HIS B 154	17.892	56.459	6.481	1.00	13.00	C
	ATOM	2716	C	HIS B 154	16.447	57.723	10.327	1.00	10.90	C
	ATOM	2717	O	HIS B 154	15.420	58.193	10.813	1.00	11.36	O
35	ATOM	2718	N	ASN B 155	17.584	58.402	10.272	1.00	10.48	N

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	ATOM	2719	CA	ASN B 155	17.689	59.780	10.770	1.00	12.04	C
	ATOM	2720	CB	ASN B 155	19.071	60.371	10.444	1.00	12.02	C
	ATOM	2721	CG	ASN B 155	20.152	59.895	11.398	1.00	12.82	C
	ATOM	2722	OD1	ASN B 155	19.868	59.476	12.525	1.00	15.20	O
5	ATOM	2723	ND2	ASN B 155	21.407	59.949	10.946	1.00	12.40	N
	ATOM	2724	C	ASN B 155	16.599	60.718	10.246	1.00	12.57	C
	ATOM	2725	O	ASN B 155	16.165	61.618	10.964	1.00	13.74	O
	ATOM	2726	N	ASP B 156	16.166	60.500	9.008	1.00	12.45	N
	ATOM	2727	CA	ASP B 156	15.228	61.412	8.343	1.00	14.13	C
10	ATOM	2728	CB	ASP B 156	15.632	61.591	6.876	1.00	14.60	C
	ATOM	2729	CG	ASP B 156	17.001	62.251	6.712	1.00	14.75	C
	ATOM	2730	OD1	ASP B 156	17.484	62.909	7.649	1.00	17.11	O
	ATOM	2731	OD2	ASP B 156	17.588	62.087	5.633	1.00	17.15	O
	ATOM	2732	C	ASP B 156	13.741	61.024	8.432	1.00	14.25	C
15	ATOM	2733	O	ASP B 156	12.900	61.653	7.783	1.00	14.42	O
	ATOM	2734	N	ASP B 157	13.409	60.005	9.225	1.00	13.49	N
	ATOM	2735	CA	ASP B 157	12.020	59.537	9.330	1.00	13.42	C
	ATOM	2736	CB	ASP B 157	11.734	58.497	8.229	1.00	13.56	C
	ATOM	2737	CG	ASP B 157	10.265	58.467	7.791	1.00	14.77	C
20	ATOM	2738	OD1	ASP B 157	9.384	59.062	8.458	1.00	12.54	O
	ATOM	2739	OD2	ASP B 157	9.994	57.813	6.768	1.00	14.93	O
	ATOM	2740	C	ASP B 157	11.719	58.976	10.734	1.00	13.47	C
	ATOM	2741	O	ASP B 157	12.605	58.938	11.590	1.00	12.69	O
	ATOM	2742	N	GLU B 158	10.467	58.567	10.957	1.00	13.05	N
25	ATOM	2743	CA	GLU B 158	9.999	57.997	12.216	1.00	15.11	C
	ATOM	2744	CB	GLU B 158	8.475	58.134	12.326	1.00	15.08	C
	ATOM	2745	CG	GLU B 158	7.911	59.551	12.280	1.00	19.72	C
	ATOM	2746	CD	GLU B 158	6.386	59.567	12.450	1.00	21.03	C
	ATOM	2747	OE1	GLU B 158	5.682	59.920	11.474	1.00	27.44	O
30	ATOM	2748	OE2	GLU B 158	5.886	59.193	13.546	1.00	27.33	O
	ATOM	2749	C	GLU B 158	10.340	56.499	12.267	1.00	13.20	C
	ATOM	2750	O	GLU B 158	10.816	55.934	11.287	1.00	12.95	O
	ATOM	2751	N	GLN B 159	10.085	55.877	13.412	1.00	12.68	N
	ATOM	2752	CA	GLN B 159	10.321	54.445	13.572	1.00	11.99	C
35	ATOM	2753	CB	GLN B 159	10.556	54.120	15.042	1.00	12.56	C

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	ATOM	2754	CG	GLN B 159	11.091	52.714	15.301	1.00	13.60	C
	ATOM	2755	CD	GLN B 159	11.720	52.600	16.669	1.00	16.11	C
	ATOM	2756	OE1	GLN B 159	12.644	53.350	17.006	1.00	17.31	O
	ATOM	2757	NE2	GLN B 159	11.228	51.658	17.471	1.00	16.10	N
5	ATOM	2758	C	GLN B 159	9.128	53.666	13.012	1.00	11.80	C
	ATOM	2759	O	GLN B 159	7.970	53.979	13.338	1.00	11.93	O
	ATOM	2760	N	TYR B 160	9.420	52.693	12.146	1.00	11.91	N
	ATOM	2761	CA	TYR B 160	8.390	51.875	11.484	1.00	12.35	C
	ATOM	2762	CB	TYR B 160	8.385	52.103	9.969	1.00	14.75	C
10	ATOM	2763	CG	TYR B 160	7.920	53.483	9.579	1.00	17.28	C
	ATOM	2764	CD1	TYR B 160	6.559	53.782	9.465	1.00	19.74	C
	ATOM	2765	CE1	TYR B 160	6.136	55.074	9.114	1.00	21.83	C
	ATOM	2766	CZ	TYR B 160	7.091	56.059	8.896	1.00	20.85	C
	ATOM	2767	OH	TYR B 160	6.716	57.344	8.548	1.00	23.57	O
15	ATOM	2768	CE2	TYR B 160	8.441	55.775	9.016	1.00	21.53	C
	ATOM	2769	CD2	TYR B 160	8.844	54.494	9.348	1.00	19.76	C
	ATOM	2770	C	TYR B 160	8.574	50.392	11.734	1.00	11.44	C
	ATOM	2771	O	TYR B 160	9.700	49.928	11.946	1.00	10.39	O
	ATOM	2772	N	ALA B 161	7.456	49.664	11.679	1.00	10.22	N
20	ATOM	2773	CA	ALA B 161	7.450	48.220	11.819	1.00	10.52	C
	ATOM	2774	CB	ALA B 161	6.677	47.806	13.065	1.00	10.96	C
	ATOM	2775	C	ALA B 161	6.814	47.638	10.564	1.00	10.67	C
	ATOM	2776	O	ALA B 161	5.666	47.966	10.215	1.00	10.84	O
	ATOM	2777	N	TRP B 162	7.595	46.823	9.868	1.00	10.71	N
25	ATOM	2778	CA	TRP B 162	7.167	46.045	8.706	1.00	10.73	C
	ATOM	2779	CB	TRP B 162	8.271	46.089	7.646	1.00	11.24	C
	ATOM	2780	CG	TRP B 162	8.104	45.226	6.405	1.00	9.84	C
	ATOM	2781	CD1	TRP B 162	7.680	45.651	5.170	1.00	11.34	C
	ATOM	2782	NE1	TRP B 162	7.712	44.607	4.272	1.00	10.95	N
30	ATOM	2783	CE2	TRP B 162	8.159	43.480	4.906	1.00	10.71	C
	ATOM	2784	CD2	TRP B 162	8.432	43.831	6.253	1.00	11.38	C
	ATOM	2785	CE3	TRP B 162	8.928	42.842	7.123	1.00	10.92	C
	ATOM	2786	CZ3	TRP B 162	9.118	41.536	6.624	1.00	10.80	C
	ATOM	2787	CH2	TRP B 162	8.839	41.220	5.282	1.00	11.08	C
35	ATOM	2788	CZ2	TRP B 162	8.363	42.173	4.401	1.00	12.14	C

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	ATOM	2789	C	TRP B 162	6.999	44.616	9.207	1.00	10.71	C
	ATOM	2790	O	TRP B 162	7.761	44.172	10.077	1.00	10.30	O
	ATOM	2791	N	GLU B 163	6.004	43.896	8.681	1.00	10.64	N
	ATOM	2792	CA	GLU B 163	5.895	42.453	8.983	1.00	10.72	C
5	ATOM	2793	CB	GLU B 163	5.126	42.186	10.303	1.00	11.79	C
	ATOM	2794	CG	GLU B 163	3.631	42.586	10.302	1.00	13.47	C
	ATOM	2795	CD	GLU B 163	2.723	41.626	9.526	1.00	15.61	C
	ATOM	2796	OE1	GLU B 163	1.669	42.090	9.025	1.00	15.13	O
	ATOM	2797	OE2	GLU B 163	3.040	40.414	9.429	1.00	16.25	O
10	ATOM	2798	C	GLU B 163	5.273	41.679	7.836	1.00	10.62	C
	ATOM	2799	O	GLU B 163	4.416	42.206	7.105	1.00	8.34	O
	ATOM	2800	N	SER B 164	5.680	40.419	7.697	1.00	10.80	N
	ATOM	2801	CA	SER B 164	5.003	39.521	6.773	1.00	11.08	C
	ATOM	2802	CB	SER B 164	5.569	39.644	5.355	1.00	10.42	C
15	ATOM	2803	OG	SER B 164	4.788	38.893	4.447	1.00	11.92	O
	ATOM	2804	C	SER B 164	5.099	38.080	7.233	1.00	11.29	C
	ATOM	2805	O	SER B 164	6.155	37.627	7.685	1.00	11.09	O
	ATOM	2806	N	SER B 165	3.983	37.372	7.093	1.00	11.47	N
	ATOM	2807	CA	SER B 165	3.974	35.915	7.221	1.00	13.04	C
20	ATOM	2808	CB	SER B 165	2.768	35.463	8.049	1.00	13.39	C
	ATOM	2809	OG	SER B 165	2.882	35.934	9.373	1.00	13.35	O
	ATOM	2810	C	SER B 165	3.948	35.267	5.847	1.00	13.82	C
	ATOM	2811	O	SER B 165	3.500	34.127	5.700	1.00	15.00	O
	ATOM	2812	N	ALA B 166	4.443	36.001	4.846	1.00	13.99	N
25	ATOM	2813	CA	ALA B 166	4.378	35.612	3.441	1.00	15.36	C
	ATOM	2814	CB	ALA B 166	5.110	34.289	3.205	1.00	15.61	C
	ATOM	2815	C	ALA B 166	2.909	35.579	2.953	1.00	15.94	C
	ATOM	2816	O	ALA B 166	2.089	36.354	3.431	1.00	16.59	O
	ATOM	2817	N	GLY B 167	2.578	34.706	2.007	1.00	16.74	N
30	ATOM	2818	CA	GLY B 167	1.205	34.660	1.481	1.00	16.16	C
	ATOM	2819	C	GLY B 167	0.805	35.863	0.632	1.00	16.39	C
	ATOM	2820	O	GLY B 167	-0.386	36.062	0.352	1.00	16.97	O
	ATOM	2821	N	GLY B 168	1.790	36.666	0.221	1.00	14.83	N
	ATOM	2822	CA	GLY B 168	1.590	37.696	-0.801	1.00	14.12	C
35	ATOM	2823	C	GLY B 168	1.438	39.129	-0.317	1.00	13.20	C

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	ATOM	2824	O	GLY B 168	1.402	40.056	-1.133	1.00	13.20	O
	ATOM	2825	N	SER B 169	1.315	39.314	0.994	1.00	12.68	N
	ATOM	2826	CA	SER B 169	1.162	40.654	1.564	1.00	12.74	C
	ATOM	2827	CB	SER B 169	-0.301	40.926	1.964	1.00	13.58	C
5	ATOM	2828	OG	SER B 169	-0.689	40.108	3.051	1.00	15.23	O
	ATOM	2829	C	SER B 169	2.079	40.911	2.757	1.00	12.47	C
	ATOM	2830	O	SER B 169	2.611	39.970	3.387	1.00	10.92	O
	ATOM	2831	N	PHE B 170	2.248	42.199	3.048	1.00	11.05	N
	ATOM	2832	CA	PHE B 170	2.933	42.661	4.238	1.00	10.99	C
10	ATOM	2833	CB	PHE B 170	4.429	42.906	3.975	1.00	10.88	C
	ATOM	2834	CG	PHE B 170	4.731	43.993	2.950	1.00	10.30	C
	ATOM	2835	CD1	PHE B 170	4.957	45.315	3.356	1.00	10.62	C
	ATOM	2836	CE1	PHE B 170	5.286	46.316	2.427	1.00	9.70	C
	ATOM	2837	CZ	PHE B 170	5.408	45.988	1.054	1.00	9.19	C
15	ATOM	2838	CE2	PHE B 170	5.186	44.672	0.633	1.00	10.97	C
	ATOM	2839	CD2	PHE B 170	4.855	43.675	1.594	1.00	9.70	C
	ATOM	2840	C	PHE B 170	2.249	43.915	4.748	1.00	11.35	C
	ATOM	2841	O	PHE B 170	1.460	44.551	4.019	1.00	12.11	O
	ATOM	2842	N	THR B 171	2.540	44.266	5.994	1.00	11.35	N
20	ATOM	2843	CA	THR B 171	2.019	45.508	6.569	1.00	10.66	C
	ATOM	2844	CB	THR B 171	1.087	45.284	7.783	1.00	11.09	C
	ATOM	2845	OG1	THR B 171	1.819	44.688	8.865	1.00	11.67	O
	ATOM	2846	CG2	THR B 171	-0.123	44.426	7.412	1.00	11.71	C
	ATOM	2847	C	THR B 171	3.147	46.416	7.018	1.00	11.09	C
25	ATOM	2848	O	THR B 171	4.262	45.948	7.309	1.00	10.66	O
	ATOM	2849	N	VAL B 172	2.843	47.709	7.067	1.00	10.21	N
	ATOM	2850	CA	VAL B 172	3.718	48.722	7.664	1.00	11.51	C
	ATOM	2851	CB	VAL B 172	4.413	49.607	6.583	1.00	10.87	C
	ATOM	2852	CG1	VAL B 172	5.313	50.684	7.231	1.00	11.34	C
30	ATOM	2853	CG2	VAL B 172	5.227	48.736	5.599	1.00	11.94	C
	ATOM	2854	C	VAL B 172	2.880	49.606	8.587	1.00	11.81	C
	ATOM	2855	O	VAL B 172	1.760	50.010	8.242	1.00	11.57	O
	ATOM	2856	N	ARG B 173	3.431	49.906	9.755	1.00	12.59	N
	ATOM	2857	CA	ARG B 173	2.785	50.793	10.722	1.00	13.69	C
35	ATOM	2858	CB	ARG B 173	1.929	49.988	11.717	1.00	13.14	C

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	ATOM	2859	CG	ARG B 173	2.719	49.088	12.692	1.00	13.91	C
	ATOM	2860	CD	ARG B 173	1.840	47.995	13.304	1.00	14.71	C
	ATOM	2861	NE	ARG B 173	1.527	46.944	12.336	1.00	17.30	N
	ATOM	2862	CZ	ARG B 173	0.535	46.063	12.463	1.00	17.88	C
5	ATOM	2863	NH1	ARG B 173	0.343	45.148	11.522	1.00	18.88	N
	ATOM	2864	NH2	ARG B 173	-0.258	46.082	13.534	1.00	17.26	N
	ATOM	2865	C	ARG B 173	3.866	51.566	11.458	1.00	14.59	C
	ATOM	2866	O	ARG B 173	5.012	51.133	11.513	1.00	13.16	O
	ATOM	2867	N	THR B 174	3.501	52.720	12.006	1.00	15.20	N
10	ATOM	2868	CA	THR B 174	4.393	53.419	12.916	1.00	17.75	C
	ATOM	2869	CB	THR B 174	3.810	54.785	13.315	1.00	18.26	C
	ATOM	2870	OG1	THR B 174	3.631	55.568	12.131	1.00	20.03	O
	ATOM	2871	CG2	THR B 174	4.760	55.514	14.262	1.00	20.24	C
	ATOM	2872	C	THR B 174	4.608	52.524	14.136	1.00	18.09	C
15	ATOM	2873	O	THR B 174	3.661	51.930	14.652	1.00	18.09	O
	ATOM	2874	N	ASP B 175	5.857	52.393	14.572	1.00	19.25	N
	ATOM	2875	CA	ASP B 175	6.178	51.482	15.668	1.00	21.37	C
	ATOM	2876	CB	ASP B 175	7.635	51.013	15.579	1.00	21.08	C
	ATOM	2877	CG	ASP B 175	7.970	49.942	16.600	1.00	21.23	C
20	ATOM	2878	OD1	ASP B 175	7.111	49.079	16.882	1.00	22.97	O
	ATOM	2879	OD2	ASP B 175	9.103	49.952	17.116	1.00	20.61	O
	ATOM	2880	C	ASP B 175	5.917	52.155	17.012	1.00	23.11	C
	ATOM	2881	O	ASP B 175	6.375	53.273	17.240	1.00	23.74	O
	ATOM	2882	N	THR B 176	5.197	51.451	17.887	1.00	25.56	N
25	ATOM	2883	CA	THR B 176	4.895	51.908	19.252	1.00	27.48	C
	ATOM	2884	CB	THR B 176	3.462	51.513	19.678	1.00	27.76	C
	ATOM	2885	OG1	THR B 176	3.330	50.085	19.645	1.00	30.12	O
	ATOM	2886	CG2	THR B 176	2.421	52.145	18.745	1.00	28.79	C
	ATOM	2887	C	THR B 176	5.867	51.332	20.283	1.00	27.31	C
30	ATOM	2889	N	GLY B 177	6.731	50.421	19.838	1.00	27.14	N
	ATOM	2890	CA	GLY B 177	7.709	49.778	20.709	1.00	26.27	C
	ATOM	2891	C	GLY B 177	8.804	50.701	21.213	1.00	25.77	C
	ATOM	2892	O	GLY B 177	8.752	51.922	21.011	1.00	26.22	O
	ATOM	2893	N	GLU B 178	9.792	50.111	21.886	1.00	24.88	N
35	ATOM	2894	CA	GLU B 178	10.927	50.852	22.416	1.00	24.07	C

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	ATOM	2895	CB	GLU B 178	11.927	49.895	23.075	1.00	23.89	C
	ATOM	2900	C	GLU B 178	11.606	51.631	21.288	1.00	23.48	C
	ATOM	2901	O	GLU B 178	11.927	51.050	20.251	1.00	22.45	O
	ATOM	2902	N	PRO B 179	11.801	52.949	21.477	1.00	23.46	N
5	ATOM	2903	CA	PRO B 179	12.518	53.743	20.472	1.00	23.30	C
	ATOM	2904	CB	PRO B 179	12.520	55.157	21.062	1.00	23.57	C
	ATOM	2905	CG	PRO B 179	11.436	55.159	22.082	1.00	23.96	C
	ATOM	2906	CD	PRO B 179	11.371	53.772	22.623	1.00	23.67	C
	ATOM	2907	C	PRO B 179	13.952	53.254	20.307	1.00	23.28	C
10	ATOM	2908	O	PRO B 179	14.624	52.956	21.301	1.00	23.27	O
	ATOM	2909	N	MET B 180	14.383	53.129	19.055	1.00	22.11	N
	ATOM	2910	CA	MET B 180	15.778	52.884	18.704	1.00	22.96	C
	ATOM	2911	CB	MET B 180	15.868	51.940	17.498	1.00	22.10	C
	ATOM	2912	CG	MET B 180	15.067	50.653	17.603	1.00	24.84	C
15	ATOM	2913	SD	MET B 180	14.733	49.936	15.967	1.00	27.87	S
	ATOM	2914	CE	MET B 180	16.387	49.549	15.432	1.00	24.75	C
	ATOM	2915	C	MET B 180	16.355	54.238	18.302	1.00	21.14	C
	ATOM	2916	O	MET B 180	15.655	55.051	17.711	1.00	22.43	O
	ATOM	2917	N	GLY B 181	17.624	54.483	18.593	1.00	20.43	N
20	ATOM	2918	CA	GLY B 181	18.267	55.714	18.117	1.00	17.37	C
	ATOM	2919	C	GLY B 181	18.316	55.773	16.593	1.00	15.93	C
	ATOM	2920	O	GLY B 181	17.909	56.765	15.983	1.00	15.19	O
	ATOM	2921	N	ARG B 182	18.789	54.684	15.988	1.00	13.89	N
	ATOM	2922	CA	ARG B 182	18.950	54.571	14.539	1.00	12.69	C
25	ATOM	2923	CB	ARG B 182	20.047	55.529	14.039	1.00	12.08	C
	ATOM	2924	CG	ARG B 182	20.332	55.463	12.545	1.00	10.98	C
	ATOM	2925	CD	ARG B 182	21.729	55.986	12.198	1.00	10.31	C
	ATOM	2926	NE	ARG B 182	22.813	55.157	12.759	1.00	9.66	N
	ATOM	2927	CZ	ARG B 182	23.660	55.552	13.715	1.00	11.41	C
30	ATOM	2928	NH1	ARG B 182	23.569	56.783	14.235	1.00	9.75	N
	ATOM	2929	NH2	ARG B 182	24.618	54.729	14.144	1.00	8.46	N
	ATOM	2930	C	ARG B 182	19.365	53.132	14.244	1.00	11.74	C
	ATOM	2931	O	ARG B 182	20.187	52.553	14.974	1.00	12.36	O
	ATOM	2932	N	GLY B 183	18.807	52.567	13.181	1.00	10.29	N
35	ATOM	2933	CA	GLY B 183	19.233	51.251	12.721	1.00	10.39	C

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	ATOM	2934	C	GLY B 183	18.058	50.369	12.397	1.00	9.99	C
	ATOM	2935	O	GLY B 183	16.956	50.867	12.101	1.00	10.10	O
	ATOM	2936	N	THR B 184	18.289	49.055	12.468	1.00	9.45	N
	ATOM	2937	CA	THR B 184	17.291	48.079	12.049	1.00	10.55	C
5	ATOM	2938	CB	THR B 184	17.500	47.655	10.569	1.00	11.11	C
	ATOM	2939	OG1	THR B 184	17.361	48.810	9.724	1.00	10.57	O
	ATOM	2940	CG2	THR B 184	16.468	46.587	10.115	1.00	10.08	C
	ATOM	2941	C	THR B 184	17.337	46.876	12.984	1.00	11.07	C
	ATOM	2942	O	THR B 184	18.423	46.411	13.369	1.00	10.83	O
10	ATOM	2943	N	LYS B 185	16.146	46.386	13.319	1.00	10.84	N
	ATOM	2944	CA	LYS B 185	15.956	45.186	14.105	1.00	12.69	C
	ATOM	2945	CB	LYS B 185	15.204	45.586	15.375	1.00	13.68	C
	ATOM	2946	CG	LYS B 185	14.760	44.490	16.308	1.00	16.64	C
	ATOM	2947	CD	LYS B 185	14.441	45.056	17.711	1.00	17.16	C
15	ATOM	2948	CE	LYS B 185	13.468	46.244	17.655	1.00	20.18	C
	ATOM	2949	NZ	LYS B 185	13.018	46.654	19.025	1.00	23.03	N
	ATOM	2950	C	LYS B 185	15.139	44.197	13.262	1.00	12.17	C
	ATOM	2951	O	LYS B 185	14.030	44.521	12.826	1.00	11.69	O
	ATOM	2952	N	VAL B 186	15.697	43.011	13.017	1.00	11.09	N
20	ATOM	2953	CA	VAL B 186	14.988	41.950	12.304	1.00	10.44	C
	ATOM	2954	CB	VAL B 186	15.840	41.334	11.147	1.00	10.96	C
	ATOM	2955	CG1	VAL B 186	15.060	40.219	10.442	1.00	10.70	C
	ATOM	2956	CG2	VAL B 186	16.234	42.411	10.125	1.00	9.32	C
	ATOM	2957	C	VAL B 186	14.590	40.888	13.330	1.00	11.17	C
25	ATOM	2958	O	VAL B 186	15.455	40.276	13.961	1.00	10.77	O
	ATOM	2959	N	ILE B 187	13.282	40.725	13.530	1.00	10.34	N
	ATOM	2960	CA	ILE B 187	12.747	39.740	14.471	1.00	11.11	C
	ATOM	2961	CB	ILE B 187	11.617	40.344	15.371	1.00	11.23	C
	ATOM	2962	CG1	ILE B 187	12.107	41.632	16.052	1.00	10.77	C
30	ATOM	2963	CD1	ILE B 187	11.001	42.537	16.577	1.00	13.02	C
	ATOM	2964	CG2	ILE B 187	11.114	39.299	16.404	1.00	11.12	C
	ATOM	2965	C	ILE B 187	12.228	38.522	13.697	1.00	10.36	C
	ATOM	2966	O	ILE B 187	11.261	38.620	12.929	1.00	10.73	O
	ATOM	2967	N	LEU B 188	12.889	37.387	13.894	1.00	9.53	N
35	ATOM	2968	CA	LEU B 188	12.489	36.122	13.275	1.00	9.20	C

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	ATOM	2969	CB	LEU B 188	13.736	35.290	12.911	1.00	10.04	C
	ATOM	2970	CG	LEU B 188	14.792	36.002	12.049	1.00	10.85	C
	ATOM	2971	CD1	LEU B 188	15.966	35.082	11.763	1.00	13.88	C
	ATOM	2972	CD2	LEU B 188	14.188	36.505	10.756	1.00	11.93	C
5	ATOM	2973	C	LEU B 188	11.596	35.350	14.243	1.00	9.40	C
	ATOM	2974	O	LEU B 188	12.052	34.913	15.303	1.00	9.29	O
	ATOM	2975	N	HIS B 189	10.320	35.223	13.888	1.00	9.24	N
	ATOM	2976	CA	HIS B 189	9.372	34.394	14.614	1.00	9.68	C
	ATOM	2977	CB	HIS B 189	7.950	34.924	14.392	1.00	10.33	C
10	ATOM	2978	CG	HIS B 189	7.809	36.388	14.688	1.00	11.77	C
	ATOM	2979	ND1	HIS B 189	7.364	36.861	15.902	1.00	14.37	N
	ATOM	2980	CE1	HIS B 189	7.354	38.184	15.882	1.00	14.33	C
	ATOM	2981	NE2	HIS B 189	7.782	38.586	14.699	1.00	12.61	N
	ATOM	2982	CD2	HIS B 189	8.074	37.483	13.932	1.00	13.86	C
15	ATOM	2983	C	HIS B 189	9.532	32.967	14.074	1.00	9.89	C
	ATOM	2984	O	HIS B 189	9.037	32.635	12.990	1.00	10.06	O
	ATOM	2985	N	LEU B 190	10.259	32.138	14.819	1.00	10.05	N
	ATOM	2986	CA	LEU B 190	10.742	30.869	14.268	1.00	10.63	C
	ATOM	2987	CB	LEU B 190	11.848	30.274	15.150	1.00	10.68	C
20	ATOM	2988	CG	LEU B 190	13.150	31.095	15.232	1.00	9.86	C
	ATOM	2989	CD1	LEU B 190	14.126	30.384	16.144	1.00	11.34	C
	ATOM	2990	CD2	LEU B 190	13.785	31.347	13.855	1.00	10.12	C
	ATOM	2991	C	LEU B 190	9.642	29.842	14.067	1.00	11.33	C
	ATOM	2992	O	LEU B 190	8.693	29.782	14.848	1.00	11.27	O
25	ATOM	2993	N	LYS B 191	9.787	29.063	12.995	1.00	11.61	N
	ATOM	2994	CA	LYS B 191	9.015	27.827	12.771	1.00	13.04	C
	ATOM	2995	CB	LYS B 191	9.515	27.135	11.498	1.00	12.25	C
	ATOM	2996	CG	LYS B 191	9.185	27.849	10.193	1.00	13.77	C
	ATOM	2997	CD	LYS B 191	9.970	27.228	9.012	1.00	14.18	C
30	ATOM	2998	CE	LYS B 191	9.670	27.955	7.712	1.00	15.99	C
	ATOM	2999	NZ	LYS B 191	10.412	27.358	6.547	1.00	17.87	N
	ATOM	3000	C	LYS B 191	9.206	26.892	13.975	1.00	13.40	C
	ATOM	3001	O	LYS B 191	10.271	26.882	14.589	1.00	12.69	O
	ATOM	3002	N	GLU B 192	8.186	26.104	14.313	1.00	14.41	N
35	ATOM	3003	CA	GLU B 192	8.260	25.280	15.522	1.00	16.14	C

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	ATOM	3004	CB	GLU B 192	6.918	24.593	15.832	1.00	17.26	C
	ATOM	3005	CG	GLU B 192	6.423	23.662	14.744	1.00	20.52	C
	ATOM	3006	CD	GLU B 192	5.117	22.946	15.114	1.00	21.47	C
	ATOM	3007	OE1	GLU B 192	4.701	22.067	14.330	1.00	26.91	O
5	ATOM	3008	OE2	GLU B 192	4.513	23.263	16.170	1.00	24.43	O
	ATOM	3009	C	GLU B 192	9.398	24.254	15.501	1.00	14.99	C
	ATOM	3010	O	GLU B 192	9.901	23.891	16.551	1.00	14.76	O
	ATOM	3011	N	ASP B 193	9.785	23.805	14.304	1.00	14.38	N
	ATOM	3012	CA	ASP B 193	10.861	22.819	14.126	1.00	15.21	C
10	ATOM	3013	CB	ASP B 193	10.619	21.978	12.863	1.00	15.62	C
	ATOM	3014	CG	ASP B 193	9.505	20.960	13.031	1.00	20.17	C
	ATOM	3015	OD1	ASP B 193	9.129	20.321	12.019	1.00	23.53	O
	ATOM	3016	OD2	ASP B 193	9.010	20.779	14.163	1.00	22.34	O
	ATOM	3017	C	ASP B 193	12.250	23.459	14.024	1.00	14.03	C
15	ATOM	3018	O	ASP B 193	13.238	22.757	13.831	1.00	12.51	O
	ATOM	3019	N	GLN B 194	12.318	24.785	14.159	1.00	13.55	N
	ATOM	3020	CA	GLN B 194	13.574	25.520	13.920	1.00	13.70	C
	ATOM	3021	CB	GLN B 194	13.390	26.521	12.763	1.00	13.22	C
	ATOM	3022	CG	GLN B 194	12.996	25.866	11.419	1.00	13.42	C
20	ATOM	3023	CD	GLN B 194	14.027	24.863	10.904	1.00	12.66	C
	ATOM	3024	OE1	GLN B 194	15.221	25.041	11.094	1.00	14.03	O
	ATOM	3025	NE2	GLN B 194	13.558	23.806	10.241	1.00	14.39	N
	ATOM	3026	C	GLN B 194	14.143	26.209	15.168	1.00	13.89	C
	ATOM	3027	O	GLN B 194	14.905	27.186	15.064	1.00	13.21	O
25	ATOM	3028	N	THR B 195	13.817	25.677	16.350	1.00	13.98	N
	ATOM	3029	CA	THR B 195	14.237	26.318	17.603	1.00	14.00	C
	ATOM	3030	CB	THR B 195	13.369	25.905	18.828	1.00	14.63	C
	ATOM	3031	OG1	THR B 195	13.553	24.514	19.104	1.00	16.33	O
	ATOM	3032	CG2	THR B 195	11.886	26.202	18.584	1.00	15.78	C
30	ATOM	3033	C	THR B 195	15.726	26.135	17.930	1.00	13.18	C
	ATOM	3034	O	THR B 195	16.225	26.756	18.862	1.00	12.04	O
	ATOM	3035	N	GLU B 196	16.435	25.310	17.160	1.00	12.80	N
	ATOM	3036	CA	GLU B 196	17.891	25.181	17.360	1.00	13.71	C
	ATOM	3037	CB	GLU B 196	18.517	24.176	16.391	1.00	13.89	C
35	ATOM	3038	CG	GLU B 196	18.568	24.614	14.941	1.00	15.69	C

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	ATOM	3039	CD	GLU B 196	18.897	23.467	14.017	1.00	16.57	C
	ATOM	3040	OE1	GLU B 196	17.984	22.671	13.729	1.00	17.96	O
	ATOM	3041	OE2	GLU B 196	20.064	23.353	13.596	1.00	17.78	O
	ATOM	3042	C	GLU B 196	18.617	26.533	17.263	1.00	13.38	C
5	ATOM	3043	O	GLU B 196	19.680	26.710	17.875	1.00	12.70	O
	ATOM	3044	N	TYR B 197	18.041	27.469	16.498	1.00	13.04	N
	ATOM	3045	CA	TYR B 197	18.648	28.793	16.285	1.00	13.33	C
	ATOM	3046	CB	TYR B 197	18.214	29.379	14.921	1.00	12.97	C
	ATOM	3047	CG	TYR B 197	18.548	28.416	13.797	1.00	13.32	C
10	ATOM	3048	CD1	TYR B 197	19.881	28.193	13.420	1.00	13.84	C
	ATOM	3049	CE1	TYR B 197	20.208	27.283	12.424	1.00	12.88	C
	ATOM	3050	CZ	TYR B 197	19.203	26.563	11.800	1.00	13.31	C
	ATOM	3051	OH	TYR B 197	19.551	25.677	10.816	1.00	13.73	O
	ATOM	3052	CE2	TYR B 197	17.867	26.750	12.149	1.00	13.30	C
15	ATOM	3053	CD2	TYR B 197	17.544	27.670	13.158	1.00	11.99	C
	ATOM	3054	C	TYR B 197	18.419	29.752	17.465	1.00	14.02	C
	ATOM	3055	O	TYR B 197	18.778	30.937	17.394	1.00	15.44	O
	ATOM	3056	N	LEU B 198	17.839	29.225	18.548	1.00	12.89	N
	ATOM	3057	CA	LEU B 198	17.779	29.928	19.838	1.00	13.38	C
20	ATOM	3058	CB	LEU B 198	16.389	29.781	20.470	1.00	13.35	C
	ATOM	3059	CG	LEU B 198	15.234	30.198	19.553	1.00	14.39	C
	ATOM	3060	CD1	LEU B 198	13.889	29.900	20.186	1.00	17.18	C
	ATOM	3061	CD2	LEU B 198	15.372	31.666	19.176	1.00	16.46	C
	ATOM	3062	C	LEU B 198	18.853	29.422	20.811	1.00	13.56	C
25	ATOM	3063	O	LEU B 198	19.047	29.989	21.887	1.00	13.00	O
	ATOM	3064	N	GLU B 199	19.545	28.348	20.435	1.00	13.80	N
	ATOM	3065	CA	GLU B 199	20.635	27.832	21.269	1.00	15.20	C
	ATOM	3066	CB	GLU B 199	20.874	26.343	21.008	1.00	15.31	C
	ATOM	3067	CG	GLU B 199	19.656	25.470	21.242	1.00	19.42	C
30	ATOM	3068	CD	GLU B 199	19.250	25.405	22.706	1.00	24.59	C
	ATOM	3069	OE1	GLU B 199	20.133	25.496	23.592	1.00	26.66	O
	ATOM	3070	OE2	GLU B 199	18.039	25.259	22.968	1.00	27.47	O
	ATOM	3071	C	GLU B 199	21.916	28.630	21.046	1.00	14.18	C
	ATOM	3072	O	GLU B 199	22.393	28.758	19.914	1.00	13.42	O
35	ATOM	3073	N	GLU B 200	22.462	29.173	22.132	1.00	14.68	N

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	ATOM	3074	CA	GLU B 200	23.682	29.975	22.051	1.00	15.09	C
	ATOM	3075	CB	GLU B 200	24.065	30.539	23.424	1.00	16.14	C
	ATOM	3076	CG	GLU B 200	23.105	31.623	23.933	1.00	19.21	C
	ATOM	3077	CD	GLU B 200	21.856	31.079	24.641	1.00	21.31	C
5	ATOM	3078	OE1	GLU B 200	21.680	29.825	24.728	1.00	22.57	O
	ATOM	3079	OE2	GLU B 200	21.051	31.913	25.125	1.00	17.77	O
	ATOM	3080	C	GLU B 200	24.842	29.196	21.405	1.00	15.44	C
	ATOM	3081	O	GLU B 200	25.548	29.742	20.566	1.00	13.79	O
	ATOM	3082	N	ARG B 201	25.009	27.920	21.759	1.00	14.94	N
10	ATOM	3083	CA	ARG B 201	26.069	27.096	21.144	1.00	17.52	C
	ATOM	3084	CB	ARG B 201	26.080	25.696	21.772	1.00	17.71	C
	ATOM	3085	CG	ARG B 201	26.939	24.657	21.074	1.00	23.10	C
	ATOM	3086	CD	ARG B 201	26.663	23.247	21.620	1.00	23.49	C
	ATOM	3087	NE	ARG B 201	25.296	23.125	22.138	1.00	30.24	N
15	ATOM	3088	CZ	ARG B 201	24.522	22.052	22.003	1.00	32.05	C
	ATOM	3089	NH1	ARG B 201	24.958	20.979	21.348	1.00	33.73	N
	ATOM	3090	NH2	ARG B 201	23.296	22.059	22.514	1.00	34.35	N
	ATOM	3091	C	ARG B 201	25.920	27.035	19.613	1.00	15.33	C
	ATOM	3092	O	ARG B 201	26.912	27.092	18.862	1.00	14.79	O
20	ATOM	3093	N	ARG B 202	24.672	26.928	19.156	1.00	13.83	N
	ATOM	3094	CA	ARG B 202	24.379	26.877	17.733	1.00	12.65	C
	ATOM	3095	CB	ARG B 202	22.926	26.440	17.505	1.00	12.63	C
	ATOM	3096	CG	ARG B 202	22.513	26.301	16.033	1.00	14.85	C
	ATOM	3097	CD	ARG B 202	23.045	25.007	15.441	1.00	16.63	C
25	ATOM	3098	NE	ARG B 202	22.432	24.684	14.152	1.00	15.56	N
	ATOM	3099	CZ	ARG B 202	23.037	24.805	12.972	1.00	14.32	C
	ATOM	3100	NH1	ARG B 202	24.287	25.230	12.885	1.00	15.81	N
	ATOM	3101	NH2	ARG B 202	22.388	24.482	11.867	1.00	14.68	N
	ATOM	3102	C	ARG B 202	24.660	28.228	17.065	1.00	12.29	C
30	ATOM	3103	O	ARG B 202	25.311	28.281	16.026	1.00	11.41	O
	ATOM	3104	N	ILE B 203	24.176	29.314	17.673	1.00	11.54	N
	ATOM	3105	CA	ILE B 203	24.396	30.652	17.107	1.00	10.71	C
	ATOM	3106	CB	ILE B 203	23.689	31.757	17.918	1.00	10.70	C
	ATOM	3107	CG1	ILE B 203	22.164	31.514	17.944	1.00	9.39	C
35	ATOM	3108	CD1	ILE B 203	21.411	32.305	18.996	1.00	11.61	C

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	ATOM	3109	CG2 ILE B 203	24.022	33.142	17.332	1.00	9.16	C
	ATOM	3110	C ILE B 203	25.910	30.936	16.998	1.00	10.68	C
	ATOM	3111	O ILE B 203	26.397	31.347	15.950	1.00	10.32	O
	ATOM	3112	N LYS B 204	26.641	30.678	18.077	1.00	12.05	N
5	ATOM	3113	CA LYS B 204	28.082	30.968	18.114	1.00	12.89	C
	ATOM	3114	CB LYS B 204	28.685	30.591	19.462	1.00	13.62	C
	ATOM	3115	CG LYS B 204	28.220	31.467	20.590	1.00	15.10	C
	ATOM	3119	C LYS B 204	28.843	30.272	16.993	1.00	13.05	C
	ATOM	3120	O LYS B 204	29.707	30.875	16.368	1.00	12.57	O
10	ATOM	3121	N GLU B 205	28.515	29.009	16.740	1.00	13.76	N
	ATOM	3122	CA GLU B 205	29.197	28.251	15.699	1.00	14.35	C
	ATOM	3123	CB GLU B 205	28.908	26.750	15.815	1.00	16.41	C
	ATOM	3124	CG GLU B 205	29.796	25.902	14.879	1.00	20.59	C
	ATOM	3125	CD GLU B 205	31.282	26.302	14.951	1.00	25.71	C
15	ATOM	3126	OE1 GLU B 205	31.865	26.640	13.890	1.00	27.65	O
	ATOM	3127	OE2 GLU B 205	31.863	26.300	16.068	1.00	26.16	O
	ATOM	3128	C GLU B 205	28.886	28.770	14.292	1.00	13.01	C
	ATOM	3129	O GLU B 205	29.772	28.811	13.431	1.00	12.82	O
	ATOM	3130	N ILE B 206	27.639	29.180	14.076	1.00	11.60	N
20	ATOM	3131	CA ILE B 206	27.207	29.720	12.787	1.00	10.56	C
	ATOM	3132	CB ILE B 206	25.673	29.930	12.743	1.00	11.37	C
	ATOM	3133	CG1 ILE B 206	24.953	28.573	12.796	1.00	10.70	C
	ATOM	3134	CD1 ILE B 206	23.435	28.683	13.040	1.00	11.02	C
	ATOM	3135	CG2 ILE B 206	25.262	30.678	11.463	1.00	10.59	C
25	ATOM	3136	C ILE B 206	27.953	31.027	12.478	1.00	10.47	C
	ATOM	3137	O ILE B 206	28.422	31.225	11.358	1.00	9.63	O
	ATOM	3138	N VAL B 207	28.061	31.893	13.484	1.00	10.29	N
	ATOM	3139	CA VAL B 207	28.820	33.147	13.367	1.00	11.41	C
	ATOM	3140	CB VAL B 207	28.658	34.042	14.631	1.00	10.85	C
30	ATOM	3141	CG1 VAL B 207	29.576	35.256	14.560	1.00	11.39	C
	ATOM	3142	CG2 VAL B 207	27.208	34.475	14.795	1.00	11.21	C
	ATOM	3143	C VAL B 207	30.298	32.866	13.052	1.00	11.17	C
	ATOM	3144	O VAL B 207	30.865	33.487	12.156	1.00	11.41	O
	ATOM	3145	N LYS B 208	30.887	31.900	13.757	1.00	11.92	N
35	ATOM	3146	CA LYS B 208	32.281	31.499	13.536	1.00	12.76	C

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	ATOM	3147	CB	LYS B 208	32.709	30.458	14.587	1.00	12.96	C
	ATOM	3148	CG	LYS B 208	34.138	29.933	14.410	1.00	16.62	C
	ATOM	3151	NZ	LYS B 208	35.458	28.214	11.104	1.00	35.31	N
	ATOM	3152	C	LYS B 208	32.510	30.958	12.114	1.00	13.18	C
5	ATOM	3153	O	LYS B 208	33.514	31.277	11.477	1.00	12.90	O
	ATOM	3154	N	LYS B 209	31.573	30.144	11.631	1.00	11.95	N
	ATOM	3155	CA	LYS B 209	31.655	29.576	10.291	1.00	13.22	C
	ATOM	3156	CB	LYS B 209	30.533	28.558	10.080	1.00	13.56	C
	ATOM	3157	CG	LYS B 209	30.836	27.185	10.659	1.00	16.16	C
10	ATOM	3158	CD	LYS B 209	29.629	26.272	10.547	1.00	18.92	C
	ATOM	3159	CE	LYS B 209	29.562	25.528	9.220	1.00	21.66	C
	ATOM	3160	NZ	LYS B 209	28.390	24.570	9.203	1.00	22.16	N
	ATOM	3161	C	LYS B 209	31.599	30.619	9.172	1.00	12.47	C
	ATOM	3162	O	LYS B 209	32.455	30.625	8.291	1.00	12.16	O
15	ATOM	3163	N	HIS B 210	30.608	31.508	9.236	1.00	11.68	N
	ATOM	3164	CA	HIS B 210	30.218	32.314	8.070	1.00	11.96	C
	ATOM	3165	CB	HIS B 210	28.754	32.042	7.682	1.00	12.39	C
	ATOM	3166	CG	HIS B 210	28.434	30.591	7.469	1.00	13.13	C
	ATOM	3167	ND1	HIS B 210	29.074	29.813	6.526	1.00	15.13	N
20	ATOM	3168	CE1	HIS B 210	28.583	28.585	6.564	1.00	15.70	C
	ATOM	3169	NE2	HIS B 210	27.652	28.538	7.500	1.00	13.89	N
	ATOM	3170	CD2	HIS B 210	27.541	29.779	8.083	1.00	14.34	C
	ATOM	3171	C	HIS B 210	30.398	33.822	8.218	1.00	11.85	C
	ATOM	3172	O	HIS B 210	30.341	34.549	7.219	1.00	12.65	O
25	ATOM	3173	N	SER B 211	30.584	34.295	9.446	1.00	11.08	N
	ATOM	3174	CA	SER B 211	30.625	35.743	9.693	1.00	11.01	C
	ATOM	3175	CB	SER B 211	29.358	36.165	10.446	1.00	10.29	C
	ATOM	3176	OG	SER B 211	28.210	35.885	9.669	1.00	11.06	O
	ATOM	3177	C	SER B 211	31.881	36.196	10.438	1.00	10.88	C
30	ATOM	3178	O	SER B 211	31.932	37.298	10.990	1.00	10.88	O
	ATOM	3179	N	GLN B 212	32.907	35.357	10.443	1.00	11.64	N
	ATOM	3180	CA	GLN B 212	34.099	35.668	11.222	1.00	12.36	C
	ATOM	3181	CB	GLN B 212	34.967	34.426	11.406	1.00	13.78	C
	ATOM	3182	CG	GLN B 212	35.574	33.920	10.156	1.00	16.26	C
35	ATOM	3186	C	GLN B 212	34.909	36.845	10.672	1.00	11.18	C

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	ATOM	3187	O	GLN B 212	35.717	37.440	11.398	1.00	11.65	O
	ATOM	3188	N	PHE B 213	34.667	37.204	9.411	1.00	10.25	N
	ATOM	3189	CA	PHE B 213	35.376	38.310	8.777	1.00	10.50	C
	ATOM	3190	CB	PHE B 213	36.078	37.824	7.511	1.00	10.68	C
5	ATOM	3191	CG	PHE B 213	37.142	36.813	7.794	1.00	11.78	C
	ATOM	3192	CD1	PHE B 213	38.401	37.228	8.227	1.00	13.00	C
	ATOM	3193	CE1	PHE B 213	39.407	36.290	8.516	1.00	14.60	C
	ATOM	3194	CZ	PHE B 213	39.135	34.931	8.387	1.00	14.07	C
	ATOM	3195	CE2	PHE B 213	37.878	34.504	7.967	1.00	13.87	C
10	ATOM	3196	CD2	PHE B 213	36.877	35.451	7.682	1.00	12.62	C
	ATOM	3197	C	PHE B 213	34.537	39.573	8.542	1.00	10.92	C
	ATOM	3198	O	PHE B 213	34.956	40.497	7.817	1.00	10.41	O
	ATOM	3199	N	ILE B 214	33.363	39.609	9.169	1.00	10.41	N
	ATOM	3200	CA	ILE B 214	32.629	40.865	9.357	1.00	10.35	C
15	ATOM	3201	CB	ILE B 214	31.188	40.610	9.905	1.00	9.32	C
	ATOM	3202	CG1	ILE B 214	30.342	39.776	8.915	1.00	9.69	C
	ATOM	3203	CD1	ILE B 214	30.009	40.450	7.560	1.00	10.60	C
	ATOM	3204	CG2	ILE B 214	30.479	41.912	10.288	1.00	9.53	C
	ATOM	3205	C	ILE B 214	33.449	41.706	10.343	1.00	10.49	C
20	ATOM	3206	O	ILE B 214	33.854	41.211	11.392	1.00	11.30	O
	ATOM	3207	N	GLY B 215	33.702	42.966	10.003	1.00	10.35	N
	ATOM	3208	CA	GLY B 215	34.581	43.802	10.822	1.00	11.05	C
	ATOM	3209	C	GLY B 215	33.904	44.495	11.997	1.00	10.77	C
	ATOM	3210	O	GLY B 215	34.563	44.851	12.970	1.00	11.43	O
25	ATOM	3211	N	TYR B 216	32.598	44.725	11.888	1.00	10.60	N
	ATOM	3212	CA	TYR B 216	31.824	45.323	12.980	1.00	10.69	C
	ATOM	3213	CB	TYR B 216	30.458	45.809	12.475	1.00	10.22	C
	ATOM	3214	CG	TYR B 216	30.582	46.821	11.361	1.00	9.88	C
	ATOM	3215	CD1	TYR B 216	30.928	48.142	11.645	1.00	10.80	C
30	ATOM	3216	CE1	TYR B 216	31.042	49.092	10.639	1.00	10.81	C
	ATOM	3217	CZ	TYR B 216	30.823	48.725	9.323	1.00	10.60	C
	ATOM	3218	OH	TYR B 216	30.960	49.671	8.335	1.00	11.42	O
	ATOM	3219	CE2	TYR B 216	30.485	47.409	8.993	1.00	10.65	C
	ATOM	3220	CD2	TYR B 216	30.350	46.463	10.029	1.00	10.38	C
35	ATOM	3221	C	TYR B 216	31.655	44.304	14.101	1.00	10.98	C

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	ATOM	3222	O	TYR B 216	31.523	43.101	13.822	1.00	10.61	O
	ATOM	3223	N	PRO B 217	31.652	44.769	15.364	1.00	10.95	N
	ATOM	3224	CA	PRO B 217	31.502	43.839	16.491	1.00	11.56	C
	ATOM	3225	CB	PRO B 217	31.584	44.747	17.726	1.00	12.00	C
5	ATOM	3226	CG	PRO B 217	32.150	46.038	17.233	1.00	13.16	C
	ATOM	3227	CD	PRO B 217	31.762	46.168	15.816	1.00	11.46	C
	ATOM	3228	C	PRO B 217	30.132	43.163	16.430	1.00	11.28	C
	ATOM	3229	O	PRO B 217	29.124	43.838	16.222	1.00	11.95	O
	ATOM	3230	N	ILE B 218	30.127	41.840	16.567	1.00	11.39	N
10	ATOM	3231	CA	ILE B 218	28.898	41.053	16.674	1.00	10.96	C
	ATOM	3232	CB	ILE B 218	28.853	39.879	15.645	1.00	11.01	C
	ATOM	3233	CG1	ILE B 218	28.984	40.402	14.204	1.00	11.12	C
	ATOM	3234	CD1	ILE B 218	29.332	39.306	13.152	1.00	10.22	C
	ATOM	3235	CG2	ILE B 218	27.572	39.029	15.826	1.00	11.10	C
15	ATOM	3236	C	ILE B 218	28.837	40.500	18.097	1.00	11.26	C
	ATOM	3237	O	ILE B 218	29.740	39.762	18.539	1.00	10.94	O
	ATOM	3238	N	THR B 219	27.794	40.873	18.826	1.00	10.17	N
	ATOM	3239	CA	THR B 219	27.649	40.404	20.203	1.00	10.64	C
	ATOM	3240	CB	THR B 219	27.559	41.580	21.200	1.00	11.14	C
20	ATOM	3241	OG1	THR B 219	28.719	42.419	21.041	1.00	10.88	O
	ATOM	3242	CG2	THR B 219	27.506	41.056	22.623	1.00	12.36	C
	ATOM	3243	C	THR B 219	26.437	39.496	20.333	1.00	11.09	C
	ATOM	3244	O	THR B 219	25.316	39.874	19.977	1.00	10.74	O
	ATOM	3245	N	LEU B 220	26.678	38.284	20.831	1.00	11.08	N
25	ATOM	3246	CA	LEU B 220	25.600	37.363	21.123	1.00	11.81	C
	ATOM	3247	CB	LEU B 220	26.039	35.902	20.918	1.00	11.11	C
	ATOM	3248	CG	LEU B 220	25.057	34.839	21.454	1.00	12.11	C
	ATOM	3249	CD1	LEU B 220	23.655	34.931	20.798	1.00	12.61	C
	ATOM	3250	CD2	LEU B 220	25.646	33.437	21.300	1.00	13.65	C
30	ATOM	3251	C	LEU B 220	25.148	37.589	22.560	1.00	11.80	C
	ATOM	3252	O	LEU B 220	25.945	37.489	23.495	1.00	12.01	O
	ATOM	3253	N	PHE B 221	23.870	37.901	22.733	1.00	11.65	N
	ATOM	3254	CA	PHE B 221	23.322	38.064	24.076	1.00	12.06	C
	ATOM	3255	CB	PHE B 221	22.284	39.183	24.118	1.00	12.66	C
35	ATOM	3256	CG	PHE B 221	22.902	40.543	24.086	1.00	13.56	C

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	ATOM	3257	CD1 PHE B 221	23.091	41.256	25.263	1.00	14.55	C
	ATOM	3258	CE1 PHE B 221	23.704	42.515	25.240	1.00	15.16	C
	ATOM	3259	CZ PHE B 221	24.160	43.045	24.040	1.00	14.61	C
	ATOM	3260	CE2 PHE B 221	24.003	42.325	22.855	1.00	15.78	C
5	ATOM	3261	CD2 PHE B 221	23.375	41.078	22.885	1.00	15.44	C
	ATOM	3262	C PHE B 221	22.765	36.743	24.568	1.00	12.87	C
	ATOM	3263	O PHE B 221	21.744	36.263	24.069	1.00	13.05	O
	ATOM	3264	N VAL B 222	23.472	36.156	25.531	1.00	11.87	N
	ATOM	3265	CA VAL B 222	23.098	34.859	26.106	1.00	12.23	C
10	ATOM	3266	CB VAL B 222	24.265	34.213	26.908	1.00	12.80	C
	ATOM	3267	CG1 VAL B 222	23.858	32.834	27.488	1.00	11.49	C
	ATOM	3268	CG2 VAL B 222	25.519	34.086	26.042	1.00	11.58	C
	ATOM	3269	C VAL B 222	21.902	35.053	27.022	1.00	13.31	C
	ATOM	3270	O VAL B 222	21.867	35.980	27.829	1.00	12.84	O
15	ATOM	3271	N GLU B 223	20.925	34.162	26.897	1.00	13.99	N
	ATOM	3272	CA GLU B 223	19.729	34.237	27.729	1.00	15.65	C
	ATOM	3273	CB GLU B 223	18.639	33.340	27.165	1.00	16.10	C
	ATOM	3274	CG GLU B 223	18.005	33.941	25.951	1.00	17.67	C
	ATOM	3275	CD GLU B 223	16.583	33.490	25.776	1.00	19.19	C
20	ATOM	3276	OE1 GLU B 223	16.367	32.416	25.170	1.00	18.98	O
	ATOM	3277	OE2 GLU B 223	15.686	34.223	26.238	1.00	21.75	O
	ATOM	3278	C GLU B 223	19.986	33.903	29.195	1.00	16.44	C
	ATOM	3279	O GLU B 223	20.747	32.982	29.521	1.00	16.16	O
	ATOM	3280	N LYS B 224	19.353	34.680	30.065	1.00	17.02	N
25	ATOM	3281	CA LYS B 224	19.389	34.436	31.494	1.00	18.20	C
	ATOM	3282	CB LYS B 224	19.168	35.751	32.262	1.00	17.99	C
	ATOM	3283	CG LYS B 224	20.133	36.879	31.830	1.00	16.19	C
	ATOM	3284	CD LYS B 224	19.833	38.227	32.504	1.00	17.07	C
	ATOM	3285	CE LYS B 224	18.507	38.824	32.036	1.00	15.71	C
30	ATOM	3286	NZ LYS B 224	18.454	39.053	30.568	1.00	15.35	N
	ATOM	3287	C LYS B 224	18.312	33.384	31.813	1.00	20.26	C
	ATOM	3288	O LYS B 224	18.125	33.004	32.968	1.00	24.00	O
	ATOM	3289	C1 LIG Y 1	19.373	-3.022	8.311	1.00	9.23	C
	ATOM	3290	C2 LIG Y 1	20.357	-3.590	9.127	1.00	9.69	C
35	ATOM	3291	C3 LIG Y 1	20.709	-4.929	9.009	1.00	10.15	C

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	ATOM	3292	C4	LIG Y	1	20.117	-5.793	8.081	1.00	10.31	C
	ATOM	3293	C5	LIG Y	1	19.135	-5.233	7.258	1.00	10.61	C
	ATOM	3294	C6	LIG Y	1	18.774	-3.878	7.366	1.00	10.34	C
	ATOM	3295	C7	LIG Y	1	20.593	-7.191	7.958	1.00	10.24	C
5	ATOM	3296	N8	LIG Y	1	21.906	-7.487	7.753	1.00	12.35	N
	ATOM	3297	C9	LIG Y	1	21.928	-8.832	7.644	1.00	12.30	C
	ATOM	3298	N10	LIG Y	1	20.679	-9.336	7.730	1.00	9.49	N
	ATOM	3299	N11	LIG Y	1	19.840	-8.311	7.912	1.00	9.08	N
	ATOM	3300	C12	LIG Y	1	22.961	-6.616	7.713	1.00	13.09	C
10	ATOM	3301	C13	LIG Y	1	23.120	-5.721	6.640	1.00	12.86	C
	ATOM	3302	C14	LIG Y	1	23.880	-6.549	8.774	1.00	13.51	C
	ATOM	3303	C15	LIG Y	1	24.157	-4.781	6.551	1.00	13.97	C
	ATOM	3304	C16	LIG Y	1	25.075	-4.737	7.624	1.00	13.12	C
	ATOM	3305	C17	LIG Y	1	24.921	-5.613	8.710	1.00	12.73	C
15	ATOM	3306	C18	LIG Y	1	25.977	-5.329	9.580	1.00	14.21	C
	ATOM	3307	N19	LIG Y	1	26.168	-3.954	7.839	1.00	12.86	N
	ATOM	3308	C20	LIG Y	1	26.727	-4.298	9.024	1.00	12.85	C
	ATOM	3309	C21	LIG Y	1	26.687	-2.907	6.957	1.00	13.42	C
	ATOM	3310	C22	LIG Y	1	21.042	-2.753	10.200	1.00	9.53	C
20	ATOM	3311	C23	LIG Y	1	20.142	-2.827	11.455	1.00	9.87	C
	ATOM	3312	C24	LIG Y	1	22.502	-3.121	10.562	1.00	10.85	C
	ATOM	3313	O25	LIG Y	1	19.015	-1.741	8.379	1.00	9.75	O
	ATOM	3314	O26	LIG Y	1	18.549	-6.032	6.357	1.00	10.14	O
	ATOM	3315	O27	LIG Y	1	23.061	-9.495	7.475	1.00	11.66	O
25	ATOM	3316	C1	LIG Y	2	18.575	43.978	7.333	1.00	9.88	C
	ATOM	3317	C2	LIG Y	2	17.937	44.550	6.221	1.00	9.66	C
	ATOM	3318	C3	LIG Y	2	18.113	45.895	5.903	1.00	10.30	C
	ATOM	3319	C4	LIG Y	2	18.934	46.751	6.645	1.00	10.48	C
	ATOM	3320	C5	LIG Y	2	19.569	46.184	7.755	1.00	10.62	C
30	ATOM	3321	C6	LIG Y	2	19.384	44.835	8.098	1.00	8.83	C
	ATOM	3322	C7	LIG Y	2	19.134	48.150	6.195	1.00	9.83	C
	ATOM	3323	N8	LIG Y	2	19.535	48.447	4.928	1.00	11.90	N
	ATOM	3324	C9	LIG Y	2	19.643	49.794	4.912	1.00	11.20	C
	ATOM	3325	N10	LIG Y	2	19.368	50.305	6.131	1.00	9.06	N
35	ATOM	3326	N11	LIG Y	2	19.066	49.279	6.941	1.00	9.19	N

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	ATOM	3327	C12	LIG	Y	2	19.739	47.582	3.897	1.00	12.67	C
	ATOM	3328	C13	LIG	Y	2	20.858	46.726	3.895	1.00	13.25	C
	ATOM	3329	C14	LIG	Y	2	18.821	47.490	2.845	1.00	13.04	C
	ATOM	3330	C15	LIG	Y	2	21.121	45.788	2.885	1.00	13.24	C
5	ATOM	3331	C16	LIG	Y	2	20.177	45.714	1.837	1.00	12.38	C
	ATOM	3332	C17	LIG	Y	2	19.055	46.558	1.832	1.00	12.70	C
	ATOM	3333	C18	LIG	Y	2	18.336	46.253	0.675	1.00	14.02	C
	ATOM	3334	N19	LIG	Y	2	20.140	44.935	0.727	1.00	12.43	N
	ATOM	3335	C20	LIG	Y	2	19.027	45.240	0.014	1.00	13.31	C
10	ATOM	3336	C21	LIG	Y	2	21.117	43.912	0.337	1.00	12.59	C
	ATOM	3337	C22	LIG	Y	2	16.987	43.722	5.360	1.00	8.97	C
	ATOM	3338	C23	LIG	Y	2	15.623	43.782	6.080	1.00	10.49	C
	ATOM	3339	C24	LIG	Y	2	16.838	44.119	3.873	1.00	10.08	C
	ATOM	3340	O25	LIG	Y	2	18.446	42.700	7.686	1.00	10.28	O
15	ATOM	3341	O26	LIG	Y	2	20.354	46.986	8.493	1.00	10.56	O
	ATOM	3342	O27	LIG	Y	2	19.974	50.453	3.818	1.00	12.26	O
	ATOM	3343	O	HOH	X	2	26.962	0.672	6.846	1.00	9.73	O
	ATOM	3344	O	HOH	X	3	21.266	40.286	0.082	1.00	9.98	O
	ATOM	3345	O	HOH	X	4	16.338	-14.613	13.588	1.00	11.84	O
20	ATOM	3346	O	HOH	X	5	17.172	-0.985	6.744	1.00	10.88	O
	ATOM	3347	O	HOH	X	6	18.540	16.515	4.805	1.00	13.31	O
	ATOM	3348	O	HOH	X	7	15.238	-2.969	7.021	1.00	9.09	O
	ATOM	3349	O	HOH	X	8	36.007	-4.421	12.531	1.00	12.65	O
	ATOM	3350	O	HOH	X	9	23.899	-4.285	-1.878	1.00	12.62	O
25	ATOM	3351	O	HOH	X	10	17.515	23.756	10.599	1.00	16.78	O
	ATOM	3352	O	HOH	X	11	4.724	36.507	0.160	1.00	12.69	O
	ATOM	3353	O	HOH	X	12	16.020	17.223	8.801	1.00	15.46	O
	ATOM	3354	O	HOH	X	13	21.893	24.440	8.766	1.00	14.13	O
	ATOM	3355	O	HOH	X	14	1.498	38.206	9.451	1.00	13.69	O
30	ATOM	3356	O	HOH	X	15	9.278	-3.283	-2.876	1.00	13.98	O
	ATOM	3357	O	HOH	X	16	1.624	38.220	5.811	1.00	13.67	O
	ATOM	3358	O	HOH	X	17	20.697	3.478	-0.837	1.00	9.81	O
	ATOM	3359	O	HOH	X	18	6.066	3.147	10.306	1.00	13.56	O
	ATOM	3360	O	HOH	X	19	24.901	1.786	5.419	1.00	14.27	O
35	ATOM	3361	O	HOH	X	20	25.338	-0.154	9.028	1.00	10.45	O

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	ATOM	3362	O	HOH X 21	19.470	44.086	-3.575	1.00	11.92	O
	ATOM	3363	O	HOH X 22	22.743	20.494	4.630	1.00	20.36	O
	ATOM	3364	O	HOH X 23	4.033	4.799	-3.863	1.00	11.82	O
	ATOM	3365	O	HOH X 24	20.617	38.460	28.222	1.00	12.80	O
5	ATOM	3366	O	HOH X 25	28.066	36.162	24.508	1.00	12.44	O
	ATOM	3367	O	HOH X 26	32.745	36.748	7.242	1.00	11.05	O
	ATOM	3368	O	HOH X 27	15.544	23.104	15.324	1.00	13.45	O
	ATOM	3369	O	HOH X 28	28.561	-0.711	5.052	1.00	17.81	O
	ATOM	3370	O	HOH X 29	3.894	42.354	-9.635	1.00	18.77	O
10	ATOM	3371	O	HOH X 30	24.143	4.409	23.126	1.00	12.36	O
	ATOM	3372	O	HOH X 31	17.741	-16.414	6.636	1.00	11.34	O
	ATOM	3373	O	HOH X 32	33.736	-1.391	25.588	1.00	16.54	O
	ATOM	3374	O	HOH X 33	10.577	-13.137	3.354	1.00	17.44	O
	ATOM	3375	O	HOH X 34	3.558	46.162	10.486	1.00	12.42	O
15	ATOM	3376	O	HOH X 35	17.386	-8.825	6.429	1.00	11.03	O
	ATOM	3377	O	HOH X 36	-0.833	2.493	2.904	1.00	14.09	O
	ATOM	3378	O	HOH X 37	13.838	-5.177	22.599	1.00	14.19	O
	ATOM	3379	O	HOH X 38	21.790	4.261	-5.716	1.00	10.30	O
	ATOM	3380	O	HOH X 39	17.853	7.388	-0.219	1.00	13.98	O
20	ATOM	3381	O	HOH X 40	12.997	-17.068	8.289	1.00	18.97	O
	ATOM	3382	O	HOH X 41	2.841	4.112	4.888	1.00	16.77	O
	ATOM	3383	O	HOH X 42	30.282	-3.093	9.303	1.00	11.75	O
	ATOM	3384	O	HOH X 43	11.088	17.893	9.940	1.00	13.46	O
	ATOM	3385	O	HOH X 44	28.499	-7.457	10.739	1.00	18.38	O
25	ATOM	3386	O	HOH X 45	3.681	1.562	10.424	1.00	15.87	O
	ATOM	3387	O	HOH X 46	4.441	34.274	-1.506	1.00	13.77	O
	ATOM	3388	O	HOH X 47	14.442	2.789	24.857	1.00	15.21	O
	ATOM	3389	O	HOH X 48	2.341	34.204	11.189	1.00	20.04	O
	ATOM	3390	O	HOH X 49	18.127	2.784	25.293	1.00	14.37	O
30	ATOM	3391	O	HOH X 50	19.060	24.839	-3.579	1.00	19.87	O
	ATOM	3392	O	HOH X 51	23.373	41.626	-1.187	1.00	17.98	O
	ATOM	3393	O	HOH X 52	4.143	44.667	12.981	1.00	21.12	O
	ATOM	3394	O	HOH X 53	30.212	16.108	9.482	1.00	18.86	O
	ATOM	3395	O	HOH X 54	25.043	-10.419	9.954	1.00	18.51	O
35	ATOM	3396	O	HOH X 55	31.103	33.035	17.287	1.00	16.64	O

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	ATOM	3397	O	HOH X 56	25.701	6.709	23.770	1.00	15.06	O
	ATOM	3398	O	HOH X 57	14.239	20.492	12.037	1.00	32.40	O
	ATOM	3399	O	HOH X 58	12.800	6.736	23.773	1.00	20.49	O
	ATOM	3400	O	HOH X 59	36.274	31.813	11.989	1.00	21.35	O
5	ATOM	3401	O	HOH X 60	15.910	44.311	-1.633	1.00	19.07	O
	ATOM	3402	O	HOH X 61	28.633	33.549	23.689	1.00	13.95	O
	ATOM	3403	O	HOH X 62	4.958	7.402	-4.300	1.00	17.87	O
	ATOM	3404	O	HOH X 63	2.299	9.031	2.802	1.00	16.03	O
	ATOM	3405	O	HOH X 64	29.476	26.792	19.754	1.00	19.96	O
10	ATOM	3406	O	HOH X 65	0.948	40.811	6.499	1.00	19.95	O
	ATOM	3407	O	HOH X 66	8.863	14.109	-4.568	1.00	20.51	O
	ATOM	3408	O	HOH X 67	23.699	-21.616	0.896	1.00	16.61	O
	ATOM	3409	O	HOH X 68	11.628	7.934	-5.732	1.00	16.87	O
	ATOM	3410	O	HOH X 69	26.497	-1.463	11.094	1.00	24.44	O
15	ATOM	3411	O	HOH X 70	17.392	45.849	-3.245	1.00	12.26	O
	ATOM	3412	O	HOH X 71	4.073	31.732	7.600	1.00	18.65	O
	ATOM	3413	O	HOH X 72	29.595	-4.903	11.158	1.00	11.71	O
	ATOM	3414	O	HOH X 73	0.637	2.560	5.266	1.00	18.34	O
	ATOM	3415	O	HOH X 74	26.584	62.584	4.281	1.00	18.86	O
20	ATOM	3416	O	HOH X 75	28.173	6.684	3.385	1.00	20.96	O
	ATOM	3417	O	HOH X 76	7.014	31.777	15.712	1.00	20.29	O
	ATOM	3418	O	HOH X 77	22.996	-5.799	-5.408	1.00	20.30	O
	ATOM	3419	O	HOH X 78	26.545	26.057	5.767	1.00	17.80	O
	ATOM	3420	O	HOH X 79	21.140	-3.217	-5.112	1.00	10.67	O
25	ATOM	3421	O	HOH X 80	20.416	33.143	-13.642	1.00	20.61	O
	ATOM	3422	O	HOH X 81	40.306	7.769	9.794	1.00	18.70	O
	ATOM	3423	O	HOH X 82	1.836	34.607	-2.595	1.00	24.47	O
	ATOM	3424	O	HOH X 83	12.560	23.104	17.220	1.00	19.39	O
	ATOM	3425	O	HOH X 84	16.757	-2.164	30.137	1.00	16.32	O
30	ATOM	3426	O	HOH X 85	16.860	42.485	0.000	1.00	26.73	O
	ATOM	3427	O	HOH X 86	12.009	26.296	4.163	1.00	18.44	O
	ATOM	3428	O	HOH X 87	15.774	26.234	21.638	1.00	19.03	O
	ATOM	3429	O	HOH X 88	36.596	40.258	11.578	1.00	31.02	O
	ATOM	3430	O	HOH X 89	17.345	0.108	25.879	1.00	19.58	O
35	ATOM	3431	O	HOH X 90	27.633	1.470	26.487	1.00	25.38	O

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	ATOM	3432	O	HOH X 91	26.470	3.274	2.509	1.00	24.22	O
	ATOM	3433	O	HOH X 92	-4.561	52.497	6.882	1.00	23.23	O
	ATOM	3434	O	HOH X 93	13.685	-8.622	-6.592	1.00	22.43	O
	ATOM	3435	O	HOH X 94	4.026	14.501	0.657	1.00	17.64	O
5	ATOM	3436	O	HOH X 95	7.346	30.050	-6.052	1.00	21.12	O
	ATOM	3437	O	HOH X 96	16.022	-11.446	31.216	1.00	21.83	O
	ATOM	3438	O	HOH X 97	16.846	9.212	22.543	1.00	18.70	O
	ATOM	3439	O	HOH X 98	7.492	33.329	17.665	1.00	26.70	O
	ATOM	3440	O	HOH X 99	9.220	9.246	18.301	1.00	20.95	O
10	ATOM	3441	O	HOH X 100	29.216	45.500	0.709	1.00	17.93	O
	ATOM	3442	O	HOH X 101	7.462	7.671	17.556	1.00	26.59	O
	ATOM	3443	O	HOH X 102	17.654	48.362	-2.030	1.00	17.97	O
	ATOM	3444	O	HOH X 103	-4.538	47.564	6.123	1.00	15.83	O
	ATOM	3445	O	HOH X 104	8.729	17.859	12.684	1.00	21.28	O
15	ATOM	3446	O	HOH X 105	16.117	17.170	15.771	1.00	26.03	O
	ATOM	3447	O	HOH X 106	13.656	47.591	-9.510	1.00	22.16	O
	ATOM	3448	O	HOH X 107	26.074	-19.812	-2.558	1.00	20.59	O
	ATOM	3449	O	HOH X 108	30.820	10.884	21.530	1.00	19.78	O
	ATOM	3450	O	HOH X 109	16.802	-6.573	31.348	1.00	15.23	O
20	ATOM	3451	O	HOH X 110	27.739	-3.326	12.418	1.00	19.00	O
	ATOM	3452	O	HOH X 111	17.602	9.199	-9.901	1.00	25.37	O
	ATOM	3453	O	HOH X 112	6.159	17.049	15.655	1.00	29.35	O
	ATOM	3454	O	HOH X 113	24.705	34.233	-0.444	1.00	25.32	O
	ATOM	3455	O	HOH X 114	8.637	-15.191	12.093	1.00	19.07	O
25	ATOM	3456	O	HOH X 115	15.771	2.677	-6.791	1.00	23.05	O
	ATOM	3457	O	HOH X 116	9.655	57.834	3.483	1.00	17.50	O
	ATOM	3458	O	HOH X 117	4.538	2.319	14.063	1.00	23.35	O
	ATOM	3459	O	HOH X 118	23.540	26.409	23.773	1.00	21.17	O
	ATOM	3460	O	HOH X 119	3.516	-6.141	14.422	1.00	35.10	O
30	ATOM	3461	O	HOH X 120	10.357	-8.950	5.982	1.00	18.97	O
	ATOM	3462	O	HOH X 121	30.315	60.842	2.523	1.00	20.02	O
	ATOM	3463	O	HOH X 122	25.510	-1.142	3.694	1.00	23.00	O
	ATOM	3464	O	HOH X 123	19.524	-18.479	5.666	1.00	19.90	O
	ATOM	3465	O	HOH X 124	22.882	-12.228	9.081	1.00	23.83	O
35	ATOM	3466	O	HOH X 125	1.871	39.563	-3.942	1.00	30.48	O

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	ATOM	3467	O	HOH X 126	29.673	34.762	21.361	1.00	14.99	O
	ATOM	3468	O	HOH X 127	7.491	6.256	-4.854	1.00	14.67	O
	ATOM	3469	O	HOH X 128	13.188	26.640	22.654	1.00	23.64	O
	ATOM	3470	O	HOH X 129	9.419	-17.948	8.618	1.00	25.88	O
5	ATOM	3471	O	HOH X 130	13.086	-7.493	-9.000	1.00	19.39	O
	ATOM	3472	O	HOH X 131	33.947	-2.996	6.922	1.00	18.68	O
	ATOM	3473	O	HOH X 132	6.881	3.389	-4.626	1.00	15.46	O
	ATOM	3474	O	HOH X 133	-3.367	43.123	6.315	1.00	18.17	O
	ATOM	3475	O	HOH X 134	32.416	31.457	21.807	1.00	36.84	O
10	ATOM	3476	O	HOH X 135	22.172	14.903	0.751	1.00	17.76	O
	ATOM	3477	O	HOH X 136	24.349	0.244	-4.035	1.00	16.93	O
	ATOM	3478	O	HOH X 137	4.484	48.438	15.647	1.00	29.06	O
	ATOM	3479	O	HOH X 138	26.532	-6.833	-0.673	1.00	19.38	O
	ATOM	3480	O	HOH X 139	27.847	15.811	2.165	1.00	20.56	O
15	ATOM	3481	O	HOH X 140	24.446	0.354	-1.406	1.00	16.66	O
	ATOM	3482	O	HOH X 141	9.031	23.881	19.137	1.00	33.62	O
	ATOM	3483	O	HOH X 142	8.309	-5.183	-4.683	1.00	21.71	O
	ATOM	3484	O	HOH X 143	0.993	52.414	14.821	1.00	30.22	O
	ATOM	3485	O	HOH X 144	8.470	-8.177	-4.351	1.00	21.29	O
20	ATOM	3486	O	HOH X 145	25.521	37.695	1.233	1.00	21.13	O
	ATOM	3487	O	HOH X 146	11.275	28.641	21.941	1.00	23.76	O
	ATOM	3488	O	HOH X 147	17.692	39.584	-12.497	1.00	11.39	O
	ATOM	3489	O	HOH X 148	3.784	12.354	12.972	1.00	23.30	O
	ATOM	3490	O	HOH X 149	18.235	0.782	-10.162	1.00	29.56	O
25	ATOM	3491	O	HOH X 150	10.090	-12.750	0.509	1.00	14.09	O
	ATOM	3492	O	HOH X 151	21.436	14.644	15.243	1.00	18.92	O
	ATOM	3493	O	HOH X 152	6.699	-13.034	16.122	1.00	29.54	O
	ATOM	3494	O	HOH X 153	10.868	23.607	9.312	1.00	25.98	O
	ATOM	3495	O	HOH X 154	20.280	17.532	2.928	1.00	23.01	O
30	ATOM	3496	O	HOH X 155	19.422	9.132	1.753	1.00	21.26	O
	ATOM	3497	O	HOH X 156	39.134	6.308	17.145	1.00	28.98	O
	ATOM	3498	O	HOH X 157	24.041	23.485	7.324	1.00	22.33	O
	ATOM	3499	O	HOH X 158	30.424	-19.389	0.071	1.00	23.01	O
	ATOM	3500	O	HOH X 159	4.854	14.682	8.606	1.00	19.00	O
35	ATOM	3501	O	HOH X 160	0.650	36.461	-4.245	1.00	32.95	O

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	ATOM	3502	O	HOH X 161	10.816	3.843	-5.217	1.00	26.81	O
	ATOM	3503	O	HOH X 162	19.864	22.686	9.846	1.00	26.22	O
	ATOM	3504	O	HOH X 163	11.469	-3.741	21.656	1.00	19.17	O
	ATOM	3505	O	HOH X 164	6.406	-0.829	11.693	1.00	25.58	O
5	ATOM	3506	O	HOH X 165	26.498	-8.199	1.484	1.00	28.56	O
	ATOM	3507	O	HOH X 166	31.567	27.864	18.176	1.00	21.06	O
	ATOM	3508	O	HOH X 167	17.891	7.671	-11.672	1.00	31.69	O
	ATOM	3509	O	HOH X 168	-0.764	41.530	9.987	1.00	27.06	O
	ATOM	3510	O	HOH X 169	16.062	36.893	26.899	1.00	35.45	O
10	ATOM	3511	O	HOH X 170	-3.567	54.075	3.519	1.00	23.25	O
	ATOM	3512	O	HOH X 171	22.682	3.836	-2.615	1.00	23.08	O
	ATOM	3513	O	HOH X 172	27.692	-4.533	-1.164	1.00	16.16	O
	ATOM	3514	O	HOH X 173	13.057	34.668	-13.511	1.00	26.18	O
	ATOM	3515	O	HOH X 174	25.752	20.519	9.037	1.00	34.09	O
15	ATOM	3516	O	HOH X 175	13.519	33.265	26.935	1.00	32.99	O
	ATOM	3517	O	HOH X 176	24.711	26.357	-7.160	1.00	24.75	O
	ATOM	3518	O	HOH X 177	19.530	-13.231	30.903	1.00	27.54	O
	ATOM	3519	O	HOH X 178	8.899	-11.371	24.542	1.00	36.18	O
	ATOM	3520	O	HOH X 179	6.079	-4.628	-1.852	1.00	32.75	O
20	ATOM	3521	O	HOH X 180	-1.922	38.397	0.143	1.00	30.61	O
	ATOM	3522	O	HOH X 181	1.542	42.753	-6.655	1.00	34.54	O
	ATOM	3523	O	HOH X 182	35.224	-6.649	15.877	1.00	20.68	O
	ATOM	3524	O	HOH X 183	17.098	18.315	6.644	1.00	28.33	O
	ATOM	3525	O	HOH X 184	23.691	-22.837	5.216	1.00	26.86	O
25	ATOM	3526	O	HOH X 185	9.502	57.442	15.674	1.00	26.09	O
	ATOM	3527	O	HOH X 186	27.178	25.782	12.426	1.00	33.68	O
	ATOM	3528	O	HOH X 187	4.296	45.872	15.278	1.00	29.84	O
	ATOM	3529	O	HOH X 188	18.511	16.493	16.681	1.00	24.59	O
	ATOM	3530	O	HOH X 189	26.416	6.505	26.416	1.00	28.40	O
30	ATOM	3531	O	HOH X 190	7.968	-7.000	25.830	1.00	43.92	O
	ATOM	3532	O	HOH X 191	6.362	-4.660	4.283	1.00	27.82	O
	ATOM	3533	O	HOH X 192	17.231	45.384	-9.836	1.00	13.17	O
	ATOM	3534	O	HOH X 193	33.537	33.219	8.234	1.00	16.22	O
	ATOM	3535	O	HOH X 194	20.910	7.686	-6.656	1.00	14.25	O
35	ATOM	3536	O	HOH X 195	38.787	1.422	12.464	1.00	12.83	O

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	ATOM	3537	O	HOH X 196	23.974	-11.734	-4.208	1.00	12.27	O
	ATOM	3538	O	HOH X 197	-2.271	4.137	5.547	1.00	15.57	O
	ATOM	3539	O	HOH X 198	23.390	10.503	-4.286	1.00	16.54	O
	ATOM	3540	O	HOH X 199	22.478	-9.979	-5.765	1.00	12.80	O
5	ATOM	3541	O	HOH X 200	15.053	19.741	5.740	1.00	18.72	O
	ATOM	3542	O	HOH X 201	17.701	36.848	29.259	1.00	15.92	O
	ATOM	3543	O	HOH X 202	31.651	30.465	5.426	1.00	18.52	O
	ATOM	3544	O	HOH X 203	20.522	21.266	11.950	1.00	18.55	O
	ATOM	3545	O	HOH X 204	37.100	-0.302	13.880	1.00	18.77	O
10	ATOM	3546	O	HOH X 205	15.952	41.225	-11.092	1.00	19.96	O
	ATOM	3547	O	HOH X 206	33.674	-6.091	18.123	1.00	19.27	O
	ATOM	3548	O	HOH X 207	9.892	25.262	-2.247	1.00	24.66	O
	ATOM	3549	O	HOH X 208	11.182	47.071	-8.437	1.00	22.79	O
	ATOM	3550	O	HOH X 209	22.301	44.033	-6.817	1.00	20.95	O
15	ATOM	3551	O	HOH X 210	38.448	-1.788	15.784	1.00	24.40	O
	ATOM	3552	O	HOH X 211	3.437	14.432	11.037	1.00	25.25	O
	ATOM	3553	O	HOH X 212	27.293	15.702	18.532	1.00	23.78	O
	ATOM	3554	O	HOH X 213	26.386	-12.122	19.916	1.00	26.81	O
	ATOM	3555	O	HOH X 214	21.124	22.000	1.634	1.00	31.99	O
20	ATOM	3556	O	HOH X 215	15.002	51.289	-2.014	1.00	25.98	O
	ATOM	3557	O	HOH X 216	27.598	-7.068	6.494	1.00	31.88	O
	ATOM	3558	O	HOH X 217	35.528	8.284	-0.019	1.00	23.55	O
	ATOM	3559	O	HOH X 218	25.075	31.817	8.395	1.00	21.59	O
	ATOM	3560	O	HOH X 219	7.169	58.056	2.688	1.00	30.98	O
25	ATOM	3561	O	HOH X 220	10.134	6.272	-3.994	1.00	22.56	O
	ATOM	3562	O	HOH X 221	33.219	60.532	1.659	1.00	28.73	O
	ATOM	3563	O	HOH X 222	21.614	-16.895	17.658	1.00	21.37	O
	ATOM	3564	O	HOH X 223	-3.082	52.487	13.042	1.00	40.44	O
	ATOM	3565	O	HOH X 224	0.789	53.700	11.722	1.00	25.22	O
30	ATOM	3566	O	HOH X 225	-3.720	8.987	0.360	1.00	31.72	O
	ATOM	3567	O	HOH X 226	21.740	62.078	13.762	1.00	23.09	O
	ATOM	3568	O	HOH X 227	3.890	32.377	0.350	1.00	27.57	O
	ATOM	3569	O	HOH X 228	10.735	13.012	-6.219	1.00	28.63	O
	ATOM	3570	O	HOH X 229	10.428	38.577	20.988	1.00	23.48	O
35	ATOM	3571	O	HOH X 230	24.433	4.297	1.080	1.00	21.74	O

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	ATOM	3572	O	HOH X 231	22.298	-24.983	3.520	1.00	27.46	O
	ATOM	3573	O	HOH X 232	0.702	38.357	12.349	1.00	36.82	O
	ATOM	3574	O	HOH X 233	-3.048	0.396	6.843	1.00	33.06	O
	ATOM	3575	O	HOH X 234	16.574	-11.650	24.686	1.00	27.12	O
5	ATOM	3576	O	HOH X 235	14.937	0.115	-6.894	1.00	21.77	O
	ATOM	3577	O	HOH X 236	8.882	-7.394	20.735	1.00	32.98	O
	ATOM	3578	O	HOH X 237	29.309	8.035	24.923	1.00	30.39	O
	ATOM	3579	O	HOH X 238	8.622	23.958	11.359	1.00	29.61	O
	ATOM	3580	O	HOH X 239	34.670	14.671	4.574	1.00	27.01	O
10	ATOM	3581	O	HOH X 240	28.047	-10.315	13.209	1.00	27.49	O
	ATOM	3582	O	HOH X 241	27.333	-5.477	4.372	1.00	26.78	O
	ATOM	3583	O	HOH X 242	26.769	0.678	2.315	1.00	25.24	O
	ATOM	3584	O	HOH X 243	5.478	-2.795	9.322	1.00	32.81	O
	ATOM	3585	O	HOH X 244	20.909	30.451	28.037	1.00	30.30	O
15	ATOM	3586	O	HOH X 245	19.691	49.441	-0.526	1.00	32.13	O
	ATOM	3587	O	HOH X 246	5.470	-2.577	-5.252	1.00	25.11	O
	ATOM	3588	O	HOH X 247	2.670	9.877	5.620	1.00	25.73	O
	ATOM	3589	O	HOH X 248	8.921	54.002	18.743	1.00	32.69	O
	ATOM	3590	O	HOH X 249	9.182	-4.869	21.259	1.00	27.40	O
20	ATOM	3591	O	HOH X 250	16.293	-15.792	23.687	1.00	22.01	O
	ATOM	3592	O	HOH X 251	27.156	30.207	-0.205	1.00	31.47	O
	ATOM	3593	O	HOH X 252	27.577	-19.791	-5.131	1.00	31.21	O
	ATOM	3594	O	HOH X 253	21.407	17.909	-2.453	1.00	30.34	O
	ATOM	3595	O	HOH X 254	38.030	33.240	12.114	1.00	27.48	O
25	ATOM	3596	O	HOH X 255	35.546	37.717	14.131	1.00	25.16	O
	ATOM	3597	O	HOH X 256	13.389	57.845	1.422	1.00	25.56	O
	ATOM	3598	O	HOH X 257	23.616	-16.418	10.340	1.00	27.67	O
	ATOM	3599	O	HOH X 258	13.559	-21.019	4.178	1.00	26.69	O
	ATOM	3600	O	HOH X 259	1.893	52.563	7.448	1.00	27.61	O
30	ATOM	3601	O	HOH X 260	21.934	-23.453	8.581	1.00	23.87	O
	ATOM	3602	O	HOH X 261	17.345	18.756	2.019	1.00	38.99	O
	ATOM	3603	O	HOH X 262	4.996	42.109	13.870	1.00	20.53	O
	ATOM	3604	O	HOH X 263	18.498	31.081	24.328	1.00	26.91	O
	ATOM	3605	O	HOH X 264	29.413	32.718	-7.311	1.00	24.26	O
35	ATOM	3606	O	HOH X 265	29.985	18.290	7.884	1.00	32.46	O

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	ATOM	3607	O	HOH X 266	37.359	4.870	18.588	1.00	39.84	O
	ATOM	3608	O	HOH X 267	23.264	2.431	29.751	1.00	38.11	O
	ATOM	3609	O	HOH X 268	14.432	-14.902	-5.515	1.00	39.99	O
	ATOM	3610	O	HOH X 269	3.770	32.894	-5.168	1.00	30.85	O
5	ATOM	3611	O	HOH X 270	11.270	36.183	-12.106	1.00	43.56	O
	ATOM	3612	O	HOH X 271	14.360	-21.469	12.995	1.00	35.33	O
	ATOM	3613	O	HOH X 272	18.673	64.404	4.807	1.00	25.32	O
	ATOM	3614	O	HOH X 273	6.139	55.681	1.906	1.00	27.13	O
	ATOM	3615	O	HOH X 274	29.338	22.927	7.096	1.00	32.89	O
10	ATOM	3616	O	HOH X 275	-0.977	52.016	11.157	1.00	30.11	O
	ATOM	3617	O	HOH X 276	16.234	18.658	-0.275	1.00	35.03	O
	ATOM	3618	O	HOH X 277	9.693	-16.391	15.815	1.00	27.91	O
	ATOM	3619	O	HOH X 278	6.696	-7.692	14.108	1.00	24.93	O
	ATOM	3620	O	HOH X 279	-0.629	10.534	2.654	1.00	33.85	O
15	ATOM	3621	O	HOH X 280	2.623	11.523	2.679	1.00	32.72	O
	ATOM	3622	O	HOH X 281	28.584	-1.676	14.662	1.00	26.74	O
	ATOM	3623	O	HOH X 282	28.808	13.206	22.241	1.00	33.97	O
	ATOM	3624	O	HOH X 283	23.705	8.542	24.055	1.00	31.66	O
	ATOM	3625	O	HOH X 284	28.328	34.007	-1.428	1.00	36.23	O
20	ATOM	3626	O	HOH X 285	13.838	42.632	-2.813	1.00	26.90	O
	ATOM	3627	O	HOH X 286	13.621	-0.566	26.945	1.00	27.12	O
	ATOM	3628	O	HOH X 287	35.045	11.666	16.964	1.00	34.98	O
	ATOM	3629	O	HOH X 288	6.689	-5.999	17.337	1.00	38.28	O
	ATOM	3630	O	HOH X 289	23.820	6.998	-2.547	1.00	30.14	O
25	ATOM	3631	O	HOH X 290	21.718	65.962	14.371	1.00	27.86	O
	ATOM	3632	O	HOH X 291	24.360	-16.911	14.462	1.00	24.22	O
	ATOM	3633	O	HOH X 292	5.495	59.202	5.147	1.00	31.69	O
	ATOM	3634	O	HOH X 293	8.790	20.473	16.465	1.00	32.50	O
	ATOM	3635	O	HOH X 294	30.172	33.986	4.642	1.00	32.64	O
30	ATOM	3636	O	HOH X 295	30.216	67.758	3.506	1.00	37.23	O
	ATOM	3637	O	HOH X 296	35.972	-1.404	23.402	1.00	35.26	O
	ATOM	3638	O	HOH X 297	10.010	24.435	6.851	1.00	27.42	O
	ATOM	3639	O	HOH X 298	20.651	22.718	-3.249	1.00	39.83	O
	ATOM	3640	O	HOH X 299	2.945	56.767	7.799	1.00	19.84	O
35	ATOM	3641	O	HOH X 300	11.728	0.250	-7.378	1.00	32.76	O

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	ATOM	3642	O	HOH X 301	6.462	27.814	-4.371	1.00	39.06	O
	ATOM	3643	O	HOH X 302	-4.324	11.010	4.749	1.00	46.11	O
	ATOM	3644	O	HOH X 303	1.879	42.246	13.444	1.00	41.36	O
	ATOM	3645	O	HOH X 304	20.106	18.335	15.017	1.00	31.55	O
5	ATOM	3646	O	HOH X 305	29.028	3.878	27.269	1.00	40.60	O
	ATOM	3647	O	HOH X 306	27.038	39.158	-7.293	1.00	35.52	O
	ATOM	3648	O	HOH X 307	6.460	54.889	-0.649	1.00	37.40	O
	ATOM	3649	O	HOH X 308	17.656	-0.197	28.376	1.00	29.94	O
	ATOM	3650	O	HOH X 309	13.821	61.384	14.253	1.00	33.25	O
10	ATOM	3651	O	HOH X 310	17.519	24.856	-7.035	1.00	30.39	O
	ATOM	3652	O	HOH X 311	24.581	22.354	10.446	1.00	37.79	O
	ATOM	3653	O	HOH X 312	12.142	22.572	5.561	1.00	27.80	O
	ATOM	3654	O	HOH X 313	5.824	26.504	12.995	1.00	26.66	O
	ATOM	3655	O	HOH X 314	-3.483	53.824	10.800	1.00	41.11	O
15	ATOM	3656	O	HOH X 315	17.036	57.270	2.698	1.00	25.36	O
	ATOM	3657	O	HOH X 316	6.398	42.402	-11.578	1.00	41.05	O
	ATOM	3658	O	HOH X 317	11.710	2.697	25.132	1.00	35.98	O
	ATOM	3659	O	HOH X 318	9.012	61.728	8.832	1.00	32.83	O
	ATOM	3660	O	HOH X 319	11.969	23.881	-3.207	1.00	46.24	O
20	ATOM	3661	O	HOH X 320	17.490	11.398	-11.407	1.00	35.77	O
	ATOM	3662	O	HOH X 321	8.902	27.453	21.251	1.00	33.77	O
	ATOM	3663	O	HOH X 322	18.982	20.452	1.004	1.00	35.97	O
	ATOM	3664	O	HOH X 323	33.324	10.501	0.513	1.00	31.43	O
	ATOM	3665	O	HOH X 324	26.312	21.960	12.145	1.00	37.69	O
25	ATOM	3666	O	HOH X 325	21.022	63.357	10.876	1.00	36.83	O
	ATOM	3667	O	HOH X 326	8.540	52.953	-1.661	1.00	29.05	O
	ATOM	3668	O	HOH X 327	29.353	6.925	-0.002	1.00	36.84	O
	ATOM	3669	O	HOH X 328	28.518	30.568	-5.207	1.00	30.45	O
	ATOM	3670	O	HOH X 329	12.936	-9.664	31.771	1.00	40.11	O
30	ATOM	3671	O	HOH X 330	20.154	-27.894	3.148	1.00	37.38	O
	ATOM	3672	O	HOH X 331	29.615	-3.382	29.829	1.00	28.54	O
	ATOM	3673	O	HOH X 332	19.961	56.865	3.222	1.00	28.16	O
	ATOM	3674	O	HOH X 333	4.281	33.880	13.839	1.00	31.22	O
	ATOM	3675	O	HOH X 334	5.854	-4.993	14.999	1.00	36.15	O
35	ATOM	3676	O	HOH X 335	-5.722	50.631	9.826	1.00	39.80	O

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	ATOM	3677	O	HOH X 336	-6.183	9.820	6.236	1.00	48.74	O
	ATOM	3678	O	HOH X 337	-0.168	3.972	7.580	1.00	32.15	O
	ATOM	3679	O	HOH X 338	15.951	15.064	-0.861	1.00	37.80	O
	ATOM	3680	O	HOH X 339	42.182	33.074	7.482	1.00	34.40	O
5	ATOM	3681	O	HOH X 340	33.200	34.197	15.429	1.00	31.96	O
	ATOM	3682	O	HOH X 341	4.059	0.050	12.564	1.00	33.18	O
	ATOM	3683	O	HOH X 342	30.356	-1.693	27.284	1.00	35.82	O
	ATOM	3684	O	HOH X 343	15.826	35.114	30.190	1.00	41.63	O
	ATOM	3685	O	HOH X 344	18.044	-15.920	27.269	1.00	54.99	O
10	ATOM	3686	O	HOH X 345	14.821	-9.913	34.103	1.00	31.59	O
	ATOM	3687	O	HOH X 346	11.754	21.272	-1.324	1.00	30.46	O
	ATOM	3688	O	HOH X 347	32.129	18.674	6.252	1.00	40.34	O
	ATOM	3689	O	HOH X 348	9.113	-19.973	-1.520	1.00	34.07	O
	ATOM	3690	O	HOH X 349	25.405	18.979	6.869	1.00	29.43	O
15	ATOM	3691	O	HOH X 350	-2.490	44.519	13.779	1.00	38.29	O
	ATOM	3692	O	HOH X 351	37.667	29.537	12.478	1.00	30.89	O
	ATOM	3693	O	HOH X 352	17.907	21.716	8.192	1.00	32.52	O
	ATOM	3694	O	HOH X 353	9.617	17.310	-1.552	1.00	50.74	O
	ATOM	3695	O	HOH X 354	-3.676	40.508	2.917	1.00	48.87	O
20	ATOM	3696	O	HOH X 355	31.415	-9.737	20.701	1.00	42.73	O
	ATOM	3697	O	HOH X 356	5.976	1.323	16.278	1.00	40.76	O
	ATOM	3698	O	HOH X 357	7.438	46.907	18.430	1.00	30.60	O
	ATOM	3699	O	HOH X 358	28.701	17.100	16.646	1.00	46.24	O
	ATOM	3700	O	HOH X 359	38.773	37.665	12.226	1.00	34.92	O
25	ATOM	3701	O	HOH X 360	27.172	21.483	14.696	1.00	35.33	O
	ATOM	3702	O	HOH X 361	25.201	-13.726	21.779	1.00	38.49	O
	ATOM	3703	O	HOH X 362	33.682	-9.596	13.520	1.00	42.79	O
	ATOM	3704	O	HOH X 363	10.813	62.079	11.215	1.00	36.38	O
	ATOM	3705	O	HOH X 364	23.460	-15.987	7.574	1.00	30.76	O
30	ATOM	3706	O	HOH X 365	27.829	53.278	1.454	1.00	44.50	O
	ATOM	3707	O	HOH X 366	-0.087	37.651	3.084	1.00	35.94	O
	ATOM	3708	O	HOH X 367	6.631	20.016	14.233	1.00	39.91	O
	ATOM	3709	O	HOH X 368	17.698	20.990	-1.689	1.00	28.55	O
	ATOM	3710	O	HOH X 369	16.347	61.019	3.495	1.00	34.40	O
35	ATOM	3711	O	HOH X 370	3.664	26.177	17.150	1.00	38.62	O

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	ATOM	3712	O	HOH X 371	7.706	-7.402	3.082	1.00	30.39	O
	ATOM	3713	O	HOH X 372	33.548	11.066	21.111	1.00	41.14	O
	ATOM	3714	O	HOH X 373	40.181	6.664	6.850	1.00	42.91	O
	ATOM	3715	O	HOH X 374	6.244	-3.082	13.120	1.00	43.05	O
5	ATOM	3716	O	HOH X 375	26.622	-11.863	-0.082	1.00	33.84	O
	ATOM	3717	O	HOH X 376	-0.741	7.702	10.071	1.00	30.92	O
	ATOM	3718	O	HOH X 377	26.341	40.545	-1.839	1.00	37.21	O
	ATOM	3719	O	HOH X 378	21.067	-20.150	14.558	1.00	32.45	O
	ATOM	3720	O	HOH X 379	24.905	68.309	15.590	1.00	37.72	O
10	ATOM	3721	O	HOH X 380	16.365	-20.789	17.524	1.00	33.02	O
	ATOM	3722	O	HOH X 381	7.920	-8.923	22.546	1.00	33.21	O
	ATOM	3723	O	HOH X 382	24.525	-21.887	-8.458	1.00	34.35	O
	ATOM	3724	O	HOH X 383	29.952	0.273	2.949	1.00	32.61	O
	ATOM	3725	O	HOH X 384	34.784	1.315	2.726	1.00	34.58	O
15	ATOM	3726	O	HOH X 385	2.334	54.555	1.698	1.00	32.68	O
	ATOM	3727	O	HOH X 386	-3.293	43.140	8.963	1.00	34.13	O
	ATOM	3728	O	HOH X 387	30.202	-2.629	5.016	1.00	33.34	O
	ATOM	3729	O	HOH X 388	17.829	-15.144	-5.300	1.00	31.59	O
	ATOM	3730	O	HOH X 389	22.234	-17.065	20.238	1.00	33.88	O
20	ATOM	3731	O	HOH X 390	18.729	63.865	12.110	1.00	48.05	O
	ATOM	3732	O	HOH X 391	18.183	3.284	-12.516	1.00	34.37	O
	ATOM	3733	O	HOH X 392	26.602	65.099	3.176	1.00	33.84	O
	ATOM	3734	O	HOH X 393	16.815	-13.076	-10.405	1.00	40.40	O
	ATOM	3735	O	HOH X 394	7.473	2.137	-6.862	1.00	39.09	O
25	ATOM	3736	O	HOH X 395	36.728	-4.577	19.159	1.00	32.88	O
	ATOM	3737	O	HOH X 396	10.771	-1.026	20.628	1.00	19.65	O
	ATOM	3738	O	HOH X 397	16.877	-23.887	9.723	1.00	25.15	O
	ATOM	3739	O	HOH X 398	22.698	-14.768	21.513	1.00	28.01	O
	ATOM	3740	O	HOH X 399	13.654	16.975	17.382	1.00	26.51	O
30	ATOM	3741	O	HOH X 400	19.808	18.006	0.464	1.00	28.59	O
	ATOM	3742	O	HOH X 401	12.067	-12.700	25.179	1.00	26.48	O
	ATOM	3743	O	HOH X 402	22.483	32.028	31.385	1.00	32.34	O
	ATOM	3744	O	HOH X 403	19.514	-18.195	20.997	1.00	34.58	O
	ATOM	3745	O	HOH X 404	27.073	61.201	1.958	1.00	39.57	O
35	ATOM	3746	O	HOH X 405	27.209	-8.305	-3.480	1.00	38.80	O

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	ATOM	3747	O	HOH X 406	9.001	-11.722	5.054	1.00	27.54	O
	ATOM	3748	O	HOH X 407	-0.862	44.323	-6.321	1.00	27.07	O
	ATOM	3749	O	HOH X 408	26.680	19.678	16.534	1.00	35.35	O
	ATOM	3750	O	HOH X 409	-3.622	6.021	7.131	1.00	41.44	O
5	ATOM	3751	O	HOH X 410	13.344	-21.861	-3.830	1.00	33.37	O
	ATOM	3752	O	HOH X 411	15.478	3.273	-9.489	1.00	28.89	O
	ATOM	3753	O	HOH X 412	11.936	-10.771	-6.132	1.00	27.97	O
	ATOM	3754	O	HOH X 413	18.768	-21.997	6.450	1.00	32.95	O
	ATOM	3755	O	HOH X 414	10.541	56.036	18.117	1.00	37.14	O
10	ATOM	3756	O	HOH X 415	-0.433	36.586	5.810	1.00	37.45	O
	ATOM	3757	O	HOH X 416	16.354	-13.075	-7.715	1.00	37.39	O
	ATOM	3758	O	HOH X 417	15.179	25.600	-4.982	1.00	39.90	O
	ATOM	3759	O	HOH X 418	33.561	16.007	11.714	1.00	35.73	O
	ATOM	3760	O	HOH X 419	23.675	43.708	-2.784	1.00	41.63	O
15	ATOM	3761	O	HOH X 420	36.027	62.877	4.954	1.00	43.55	O
	ATOM	3762	O	HOH X 421	13.607	19.466	-1.331	1.00	36.54	O
	ATOM	3763	O	HOH X 422	6.190	35.478	18.018	1.00	41.24	O
	ATOM	3764	O	HOH X 423	10.500	7.083	21.334	1.00	29.61	O
	ATOM	3765	O	HOH X 424	17.891	30.401	32.745	1.00	39.73	O
20	ATOM	3766	O	HOH X 425	25.451	-14.667	2.460	1.00	32.13	O
	ATOM	3767	O	HOH X 426	28.136	20.013	10.617	1.00	30.49	O
	ATOM	3768	O	HOH X 427	6.400	-11.474	5.834	1.00	40.58	O
	ATOM	3769	O	HOH X 428	39.060	2.983	20.492	1.00	48.86	O
	ATOM	3770	O	HOH X 429	16.230	-22.426	5.356	1.00	37.19	O
25	ATOM	3771	O	HOH X 430	9.871	20.913	9.573	1.00	38.83	O
	ATOM	3772	O	HOH X 431	30.618	2.813	0.998	1.00	29.58	O
	ATOM	3773	O	HOH X 432	18.678	-17.837	-9.009	1.00	43.26	O
	ATOM	3774	O	HOH X 433	7.259	14.878	21.456	1.00	40.96	O
	ATOM	3775	O	HOH X 434	16.028	40.543	30.142	1.00	31.02	O
30	ATOM	3776	O	HOH X 435	24.449	-13.503	7.338	1.00	32.70	O
	ATOM	3777	O	HOH X 436	0.731	14.713	10.722	1.00	34.26	O
	ATOM	3778	O	HOH X 437	-2.423	34.094	0.349	1.00	34.23	O
	ATOM	3779	O	HOH X 438	15.531	31.501	32.460	1.00	52.92	O
	ATOM	3780	O	HOH X 439	17.144	39.219	-15.537	1.00	41.84	O
35	ATOM	3781	O	HOH X 440	8.389	39.654	19.139	1.00	34.75	O

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	ATOM	3782	O	HOH X 441	26.202	-20.131	1.023	1.00	39.22	O
	ATOM	3783	O	HOH X 442	4.124	28.098	15.026	1.00	38.25	O
	ATOM	3784	O	HOH X 443	13.873	6.764	-7.409	1.00	34.54	O
	ATOM	3785	O	HOH X 444	8.192	50.260	-6.749	1.00	50.64	O
5	ATOM	3786	O	HOH X 445	-1.404	41.177	5.663	1.00	34.47	O
	ATOM	3787	O	HOH X 446	36.545	18.130	15.521	1.00	40.53	O
	ATOM	3788	O	HOH X 447	9.677	-3.524	28.097	1.00	36.47	O
	ATOM	3789	O	HOH X 448	3.969	13.622	15.444	1.00	32.60	O
	ATOM	3790	O	HOH X 449	24.505	10.855	24.325	1.00	44.56	O
10	ATOM	3791	O	HOH X 450	27.108	17.686	4.311	1.00	34.90	O
	ATOM	3792	O	HOH X 451	13.174	-2.839	-9.311	1.00	42.97	O
	ATOM	3793	O	HOH X 452	25.103	27.637	-9.621	1.00	34.91	O
	ATOM	3794	O	HOH X 453	2.179	31.848	10.016	1.00	45.36	O
	ATOM	3795	O	HOH X 454	19.567	62.470	14.852	1.00	35.66	O
15	ATOM	3796	O	HOH X 455	29.723	62.605	15.052	1.00	32.68	O
	ATOM	3797	O	HOH X 456	29.588	-22.066	-4.554	1.00	44.32	O
	ATOM	3798	O	HOH X 457	22.108	-13.444	25.261	1.00	34.34	O
	ATOM	3799	O	HOH X 458	26.546	22.882	8.129	1.00	29.07	O
	ATOM	3800	O	HOH X 459	14.305	-5.212	-9.627	1.00	31.44	O
20	ATOM	3801	O	HOH X 460	32.309	-5.366	22.258	1.00	52.60	O
	ATOM	3802	O	HOH X 461	17.133	22.293	-6.195	1.00	36.72	O
	ATOM	3803	O	HOH X 462	19.872	0.374	31.120	1.00	40.73	O
	ATOM	3804	O	HOH X 463	8.542	2.774	21.733	1.00	30.72	O
	ATOM	3805	O	HOH X 464	10.665	-14.720	26.241	1.00	44.61	O
25	ATOM	3806	O	HOH X 465	25.659	58.425	0.614	1.00	42.76	O
	ATOM	3807	O	HOH X 466	26.966	23.822	17.007	1.00	44.50	O
	ATOM	3808	O	HOH X 467	7.406	-14.866	3.311	1.00	42.46	O
	ATOM	3809	O	HOH X 468	21.784	65.581	11.774	1.00	40.12	O
	ATOM	3810	O	HOH X 469	15.747	20.075	16.519	1.00	40.42	O
30	ATOM	3811	O	HOH X 470	6.918	21.884	1.071	1.00	44.57	O
	ATOM	3812	O	HOH X 471	13.056	-21.124	8.929	1.00	31.98	O
	ATOM	3813	O	HOH X 472	10.673	45.443	-11.681	1.00	32.27	O
	ATOM	3814	O	HOH X 473	23.733	23.237	0.570	1.00	36.57	O
	ATOM	3815	O	HOH X 474	16.028	28.355	-15.727	1.00	35.64	O
35	ATOM	3816	O	HOH X 475	14.540	-22.859	7.403	1.00	31.65	O

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	ATOM	3817	O	HOH X 476	13.357	62.441	11.777	1.00	42.22	O
	ATOM	3818	O	HOH X 477	31.311	15.256	14.077	1.00	38.46	O
	ATOM	3819	O	HOH X 478	29.924	11.224	1.546	1.00	39.57	O
	ATOM	3820	O	HOH X 479	12.987	-25.068	4.010	1.00	28.31	O
5	ATOM	3821	O	HOH X 480	2.169	-2.135	5.661	1.00	43.39	O
	ATOM	3822	O	HOH X 481	26.878	-12.932	13.881	1.00	38.69	O
	ATOM	3823	O	HOH X 482	11.690	14.393	20.025	1.00	33.36	O
	ATOM	3824	O	HOH X 483	-5.967	4.051	7.315	1.00	40.18	O
	ATOM	3825	O	HOH X 484	20.549	21.077	-0.959	1.00	46.78	O
10	ATOM	3826	O	HOH X 485	11.047	49.383	-6.813	1.00	35.98	O
	ATOM	3827	O	HOH X 486	16.157	22.144	18.450	1.00	48.18	O
	ATOM	3828	O	HOH X 487	27.126	-17.756	2.476	1.00	33.11	O
	ATOM	3829	O	HOH X 488	25.438	55.625	2.192	1.00	36.14	O
	ATOM	3830	O	HOH X 489	26.547	20.094	19.338	1.00	54.49	O
15	ATOM	3831	O	HOH X 490	29.389	33.064	2.631	1.00	29.64	O
	ATOM	3832	O	HOH X 491	19.782	62.302	17.521	1.00	42.99	O
	ATOM	3833	O	HOH X 492	26.540	26.901	-5.470	1.00	34.39	O
	ATOM	3834	O	HOH X 493	9.876	-19.207	14.367	1.00	36.31	O
	ATOM	3835	O	HOH X 494	26.485	60.850	19.236	1.00	48.03	O
20	ATOM	3836	O	HOH X 495	3.008	35.263	-8.647	1.00	44.32	O
	ATOM	3837	O	HOH X 496	8.259	29.796	-8.836	1.00	38.04	O
	ATOM	3838	O	HOH X 497	-3.105	54.871	6.704	1.00	42.38	O
	ATOM	3839	O	HOH X 498	13.153	3.929	-6.667	1.00	39.53	O
	ATOM	3840	O	HOH X 499	20.158	61.998	7.426	1.00	37.13	O
25	ATOM	3841	O	HOH X 500	18.995	16.814	-6.499	1.00	37.42	O
	ATOM	3842	O	HOH X 501	5.635	-4.873	6.742	1.00	35.72	O
	ATOM	3843	O	HOH X 502	29.039	15.357	20.615	1.00	36.70	O
	ATOM	3844	O	HOH X 503	3.192	-2.982	3.358	1.00	43.86	O
	ATOM	3845	O	HOH X 504	31.416	49.326	1.525	1.00	39.05	O
30	ATOM	3846	O	HOH X 505	27.241	-8.630	8.734	1.00	28.53	O
	ATOM	3847	O	HOH X 506	-2.038	43.868	11.060	1.00	33.74	O
	ATOM	3848	O	HOH X 507	21.075	-24.002	6.026	1.00	42.33	O
	ATOM	3849	O	HOH X 508	12.573	61.141	4.735	1.00	37.51	O
	ATOM	3850	O	HOH X 509	10.549	-1.363	23.816	1.00	42.06	O
35	ATOM	3851	O	HOH X 510	11.784	-20.394	12.120	1.00	36.90	O

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	ATOM	3852	O	HOH X 511	5.009	-6.064	0.061	1.00	40.49	O
	ATOM	3853	O	HOH X 512	2.093	37.053	-6.928	1.00	45.12	O
	ATOM	3854	O	HOH X 513	7.505	-16.294	-2.215	1.00	40.60	O
	ATOM	3855	O	HOH X 514	26.391	36.275	-0.955	1.00	42.99	O
5	ATOM	3856	O	HOH X 515	22.657	-20.029	10.934	1.00	37.46	O
	ATOM	3857	O	HOH X 516	26.576	67.669	4.256	1.00	39.17	O
	ATOM	3858	O	HOH X 517	7.572	-15.092	14.537	1.00	38.78	O
	ATOM	3859	O	HOH X 518	13.416	45.353	-11.725	1.00	37.17	O
	ATOM	3860	O	HOH X 519	28.725	-1.282	30.830	1.00	40.70	O
10	ATOM	3861	O	HOH X 520	9.839	37.535	26.461	1.00	39.83	O
	ATOM	3862	O	HOH X 521	1.935	0.209	8.808	1.00	44.86	O
	ATOM	3863	O	HOH X 522	5.992	17.455	8.703	1.00	44.85	O
	ATOM	3864	O	HOH X 523	27.525	62.803	16.939	1.00	36.48	O
	ATOM	3865	O	HOH X 524	20.547	3.303	27.259	1.00	33.67	O
15	ATOM	3866	O	HOH X 525	28.557	4.793	1.700	1.00	41.52	O
	ATOM	3867	O	HOH X 526	22.161	-18.531	6.634	1.00	50.61	O
	ATOM	3868	O	HOH X 527	21.615	-14.790	27.311	1.00	39.16	O
	ATOM	3869	O	HOH X 528	-0.938	3.577	13.852	1.00	40.56	O
	ATOM	3870	O	HOH X 529	6.715	5.458	18.813	1.00	34.49	O
20	ATOM	3871	O	HOH X 530	5.961	28.490	8.210	1.00	32.08	O
	ATOM	3872	O	HOH X 531	19.706	21.555	22.391	1.00	45.13	O
	ATOM	3873	O	HOH X 532	8.352	-19.184	6.382	1.00	46.23	O
	ATOM	3874	O	HOH X 533	25.837	1.702	30.399	1.00	61.60	O
	ATOM	3875	O	HOH X 534	10.864	20.788	19.249	1.00	45.68	O
25	ATOM	3876	O	HOH X 535	7.287	-6.917	8.052	1.00	56.96	O
	ATOM	3877	O	HOH X 536	32.508	58.594	11.482	1.00	37.48	O
	ATOM	3878	O	HOH X 537	12.498	29.324	-9.729	1.00	43.52	O
	ATOM	3879	O	HOH X 538	-0.042	33.131	8.349	1.00	46.00	O
	ATOM	3880	O	HOH X 539	-1.973	4.638	11.384	1.00	35.82	O
30	ATOM	3881	O	HOH X 540	7.741	-3.676	18.583	1.00	43.68	O
	ATOM	3882	O	HOH X 541	13.281	14.998	-0.279	1.00	28.68	O
	ATOM	3883	O	HOH X 542	14.269	42.603	-12.724	1.00	25.85	O
	ATOM	3884	O	HOH X 543	26.072	25.929	14.808	1.00	33.77	O
	ATOM	3885	O	HOH X 544	3.619	38.146	15.894	1.00	33.88	O
35	ATOM	3886	O	HOH X 545	23.739	-26.742	0.946	1.00	36.27	O

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	ATOM	3887	O	HOH X 546	16.540	-13.802	30.038	1.00	41.65	O
	ATOM	3888	O	HOH X 547	15.715	-14.664	27.748	1.00	45.45	O
	ATOM	3889	O	HOH X 548	41.680	12.657	14.180	1.00	29.05	O
	ATOM	3890	O	HOH X 549	12.110	17.115	-1.609	1.00	38.16	O
5	ATOM	3891	O	HOH X 550	14.370	-21.236	15.618	1.00	40.11	O
	ATOM	3892	O	HOH X 551	19.500	4.550	29.377	1.00	45.88	O
	ATOM	3893	O	HOH X 552	2.304	13.593	-1.982	1.00	43.18	O
	ATOM	3894	O	HOH X 553	3.458	-5.440	11.153	1.00	50.27	O
	ATOM	3895	O	HOH X 554	4.562	30.738	-6.553	1.00	38.03	O
10	ATOM	3896	O	HOH X 555	5.122	-8.603	0.405	1.00	48.85	O
	ATOM	3897	O	HOH X 556	41.558	1.627	13.759	1.00	34.58	O
	ATOM	3898	O	HOH X 557	18.769	14.604	20.135	1.00	45.72	O
	ATOM	3899	O	HOH X 558	6.230	21.440	12.094	1.00	45.77	O
	ATOM	3900	O	HOH X 559	-0.864	48.371	15.399	1.00	48.97	O
15	ATOM	3901	O	HOH X 560	24.988	-26.930	-2.839	1.00	43.72	O
	ATOM	3902	O	HOH X 561	5.398	31.364	19.226	1.00	41.87	O
	ATOM	3903	O	HOH X 562	11.280	-21.941	-2.131	1.00	36.15	O
	ATOM	3904	O	HOH X 563	31.212	-9.508	13.468	1.00	42.29	O
	ATOM	3905	O	HOH X 564	22.610	22.325	-5.052	1.00	39.71	O
20	ATOM	3906	O	HOH X 565	18.015	5.604	-13.383	1.00	45.71	O
	ATOM	3907	O	HOH X 566	12.503	31.847	-14.202	1.00	40.02	O
	ATOM	3908	O	HOH X 567	6.210	14.009	-5.092	1.00	33.62	O
	ATOM	3909	O	HOH X 568	18.073	19.163	11.247	1.00	34.82	O
	ATOM	3910	O	HOH X 569	20.784	59.592	5.081	1.00	39.69	O
25	ATOM	3911	O	HOH X 570	23.737	62.907	20.249	1.00	34.53	O
	ATOM	3912	O	HOH X 571	17.941	29.770	27.369	1.00	55.94	O
	ATOM	3913	O	HOH X 572	24.345	8.947	27.829	1.00	51.60	O
	ATOM	3914	O	HOH X 573	12.734	-19.703	-5.836	1.00	44.58	O
	ATOM	3915	O	HOH X 574	17.085	62.161	13.337	1.00	35.94	O
30	ATOM	3916	O	HOH X 575	27.799	20.129	7.421	1.00	46.94	O
	ATOM	3917	O	HOH X 576	18.332	19.084	8.794	1.00	36.05	O
	ATOM	3918	O	HOH X 577	39.797	35.254	12.393	1.00	43.61	O
	ATOM	3919	O	HOH X 578	16.339	12.460	20.686	1.00	31.72	O
	ATOM	3920	O	HOH X 579	11.942	36.337	27.982	1.00	39.63	O
35	ATOM	3921	O	HOH X 580	8.069	19.007	8.903	1.00	39.37	O

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	ATOM	3922	O	HOH X 581	25.956	-1.507	-0.207	1.00	35.57	O
	ATOM	3923	O	HOH X 582	1.406	54.309	9.150	1.00	41.74	O
	ATOM	3924	O	HOH X 583	16.819	23.415	-2.945	1.00	47.30	O
	ATOM	3925	O	HOH X 584	-2.199	39.177	-2.462	1.00	50.28	O
5	ATOM	3926	O	HOH X 585	21.229	-27.134	-4.941	1.00	43.81	O
	ATOM	3927	O	HOH X 586	12.105	40.759	-13.457	1.00	44.57	O
	ATOM	3928	O	HOH X 587	41.921	15.361	14.579	1.00	43.54	O
	ATOM	3929	O	HOH X 588	37.420	13.462	4.544	1.00	34.79	O
	ATOM	3930	O	HOH X 589	3.829	31.360	-9.100	1.00	36.24	O
10	ATOM	3931	O	HOH X 590	17.552	20.012	18.354	1.00	34.34	O
	ATOM	3932	O	HOH X 591	25.857	7.911	-1.594	1.00	32.71	O
	ATOM	3933	O	HOH X 592	14.737	-13.473	24.728	1.00	38.88	O
	ATOM	3934	O	HOH X 593	8.932	21.361	-1.493	1.00	40.09	O
	ATOM	3935	O	HOH X 594	9.134	55.593	-3.632	1.00	55.79	O
15	ATOM	3936	O	HOH X 595	37.069	-4.500	16.476	1.00	38.53	O
	ATOM	3937	O	HOH X 596	34.304	25.970	11.805	1.00	45.38	O
	ATOM	3938	O	HOH X 597	27.736	-2.394	1.417	1.00	34.18	O
	ATOM	3939	O	HOH X 598	22.936	6.854	30.249	1.00	38.47	O
	ATOM	3940	O	HOH X 599	21.500	18.840	20.088	1.00	55.06	O
20	ATOM	3941	O	HOH X 600	24.191	-24.001	2.024	1.00	41.54	O
	ATOM	3942	O	HOH X 601	28.000	-20.762	-0.753	1.00	47.24	O
	ATOM	3943	O	HOH X 602	18.707	22.511	19.748	1.00	47.93	O
	ATOM	3944	O	HOH X 603	27.384	28.707	-2.360	1.00	47.84	O
	ATOM	3945	O	HOH X 604	27.491	38.146	-2.513	1.00	38.67	O
25	ATOM	3946	O	HOH X 605	8.148	-0.579	18.593	1.00	53.03	O
	ATOM	3947	O	HOH X 606	7.124	-18.469	2.414	1.00	36.55	O
	ATOM	3948	O	HOH X 607	6.564	37.827	19.692	1.00	45.17	O
	ATOM	3949	O	HOH X 608	10.972	60.141	15.692	1.00	42.98	O
	ATOM	3950	O	HOH X 609	-0.856	56.922	5.762	1.00	54.80	O
30	ATOM	3951	O	HOH X 610	4.863	-5.779	19.446	1.00	42.44	O
	ATOM	3952	O	HOH X 611	20.802	30.523	-14.474	1.00	40.34	O
	ATOM	3953	O	HOH X 612	8.340	51.021	-3.467	1.00	27.86	O
	ATOM	3954	O	HOH X 613	28.253	-10.115	20.217	1.00	29.26	O
	ATOM	3955	O	HOH X 614	41.651	11.106	16.577	1.00	56.70	O
35	ATOM	3956	O	HOH X 615	21.319	27.389	24.932	1.00	41.67	O

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	ATOM	3957	O	HOH X 616	12.242	-2.786	28.046	1.00	36.76	O
	ATOM	3958	O	HOH X 617	26.624	25.628	-2.584	1.00	44.90	O
	ATOM	3959	O	HOH X 618	27.493	-11.813	9.983	1.00	40.71	O
	ATOM	3960	O	HOH X 619	2.879	31.540	5.069	1.00	48.83	O
5	ATOM	3961	O	HOH X 620	5.769	34.875	24.712	1.00	40.93	O
	ATOM	3962	O	HOH X 621	9.705	-21.359	5.481	1.00	37.46	O
	ATOM	3963	O	HOH X 622	9.945	-8.901	-6.295	1.00	44.58	O
	ATOM	3964	O	HOH X 623	8.006	-8.778	5.401	1.00	36.15	O
	ATOM	3965	O	HOH X 624	34.538	14.538	17.036	1.00	42.77	O
10	ATOM	3966	O	HOH X 625	13.143	26.232	25.423	1.00	44.73	O
	ATOM	3967	O	HOH X 626	36.057	33.431	15.698	1.00	49.47	O
	ATOM	3968	O	HOH X 627	3.808	45.418	-9.327	1.00	43.24	O
	ATOM	3969	O	HOH X 628	33.305	14.078	2.456	1.00	37.03	O
	ATOM	3970	O	HOH X 629	19.770	-17.178	24.445	1.00	54.59	O
15	ATOM	3971	O	HOH X 630	7.364	-11.245	0.395	1.00	48.07	O
	ATOM	3972	O	HOH X 631	39.022	13.531	7.932	1.00	47.59	O
	ATOM	3973	O	HOH X 632	7.803	-13.704	-1.049	1.00	55.16	O
	ATOM	3974	O	HOH X 633	15.466	21.828	8.291	1.00	36.98	O
	ATOM	3975	O	HOH X 634	5.366	-8.449	9.549	1.00	59.26	O
20	ATOM	3976	O	HOH X 635	14.221	-2.170	29.685	1.00	42.40	O
	ATOM	3977	O	HOH X 636	4.023	35.440	15.909	1.00	46.45	O
	ATOM	3978	O	HOH X 637	17.651	-17.784	-6.143	1.00	40.26	O
	ATOM	3979	O	HOH X 638	15.936	25.682	-15.884	1.00	50.30	O
	ATOM	3980	O	HOH X 639	17.384	-23.983	14.148	1.00	55.57	O
25	ATOM	3981	O	HOH X 640	19.880	35.024	-15.923	1.00	46.67	O
	ATOM	3982	O	HOH X 641	-0.599	37.441	8.075	1.00	38.85	O
	ATOM	3983	O	HOH X 642	7.881	58.950	5.495	1.00	33.75	O
	ATOM	3984	O	HOH X 643	26.844	-16.321	15.291	1.00	37.00	O
	ATOM	3985	O	HOH X 644	10.575	-2.200	-9.221	1.00	50.73	O
30	ATOM	3986	O	HOH X 645	13.048	56.869	-1.055	1.00	41.25	O
	ATOM	3987	O	HOH X 646	14.206	19.947	9.630	1.00	42.32	O
	ATOM	3988	O	HOH X 647	15.441	36.764	32.447	1.00	43.82	O
	ATOM	3989	O	HOH X 648	19.956	57.325	9.182	1.00	11.30	O
	ATOM	3990	O	HOH X 649	19.784	41.986	9.781	1.00	11.87	O
35	ATOM	3991	O	HOH X 650	19.165	43.938	11.636	1.00	9.17	O

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	ATOM	3992	O	HOH X 651	18.788	41.093	1.366	1.00	9.27	O
	ATOM	3993	O	HOH X 652	20.091	49.801	9.650	1.00	9.72	O
	ATOM	3994	O	HOH X 653	14.476	37.819	20.257	1.00	11.58	O
	ATOM	3995	O	HOH X 654	32.041	44.186	7.737	1.00	10.97	O
5	ATOM	3996	O	HOH X 655	32.934	42.678	5.602	1.00	13.68	O
	ATOM	3997	O	HOH X 656	27.766	37.486	7.570	1.00	9.19	O
	ATOM	3998	O	HOH X 657	29.333	45.222	4.578	1.00	12.84	O
	ATOM	3999	O	HOH X 658	27.963	44.231	19.201	1.00	12.47	O
	ATOM	4000	O	HOH X 659	12.874	55.544	9.418	1.00	12.24	O
10	ATOM	4001	O	HOH X 660	26.586	33.635	10.270	1.00	14.53	O
	ATOM	4002	O	HOH X 661	22.366	39.160	2.384	1.00	13.02	O
	ATOM	4003	O	HOH X 662	32.956	51.008	6.591	1.00	12.60	O
	ATOM	4004	O	HOH X 663	24.776	53.719	17.822	1.00	13.62	O
	ATOM	4005	O	HOH X 664	31.595	52.682	4.804	1.00	13.49	O
15	ATOM	4006	O	HOH X 665	13.876	39.397	22.516	1.00	17.99	O
	ATOM	4007	O	HOH X 666	19.180	36.886	24.304	1.00	17.71	O
	ATOM	4008	O	HOH X 667	32.626	46.730	6.086	1.00	18.16	O
	ATOM	4009	O	HOH X 668	29.306	37.585	21.732	1.00	16.92	O
	ATOM	4010	O	HOH X 669	18.543	38.415	26.403	1.00	18.68	O
20	ATOM	4011	O	HOH X 670	21.215	59.443	7.682	1.00	18.59	O
	ATOM	4012	O	HOH X 671	17.584	58.042	13.664	1.00	18.75	O
	ATOM	4013	O	HOH X 672	19.430	49.924	16.512	1.00	19.93	O
	ATOM	4014	O	HOH X 673	26.507	36.670	3.510	1.00	21.63	O
	ATOM	4015	O	HOH X 674	24.091	42.086	2.046	1.00	20.08	O
25	ATOM	4016	O	HOH X 675	28.968	40.560	3.867	1.00	18.47	O
	ATOM	4017	O	HOH X 676	22.113	54.060	16.791	1.00	18.69	O
	ATOM	4018	O	HOH X 677	25.705	40.380	1.075	1.00	23.03	O
	ATOM	4019	O	HOH X 678	17.873	51.360	1.500	1.00	18.27	O
	ATOM	4020	O	HOH X 679	29.326	49.127	20.185	1.00	22.52	O
30	ATOM	4021	O	HOH X 680	28.612	47.817	1.700	1.00	21.61	O
	ATOM	4022	O	HOH X 681	29.276	34.761	18.480	1.00	25.51	O
	ATOM	4023	O	HOH X 682	32.940	38.350	13.251	1.00	24.08	O
	ATOM	4024	O	HOH X 683	13.129	56.092	17.318	1.00	21.15	O
	ATOM	4025	O	HOH X 684	32.358	49.548	15.429	1.00	22.69	O
35	ATOM	4026	O	HOH X 685	32.714	40.849	14.244	1.00	24.66	O

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	ATOM	4027	O	HOH X 686	29.873	37.133	5.944	1.00	22.13	O
	ATOM	4028	O	HOH X 687	31.525	40.714	4.435	1.00	17.87	O
	ATOM	4029	O	HOH X 688	18.391	53.135	3.706	1.00	23.32	O
	ATOM	4030	O	HOH X 689	16.673	58.883	17.099	1.00	22.55	O
5	ATOM	4031	O	HOH X 690	21.948	48.006	-0.411	1.00	31.39	O
	ATOM	4032	O	HOH X 691	13.055	41.692	19.644	1.00	26.03	O
	ATOM	4033	O	HOH X 692	20.366	45.622	20.849	1.00	28.21	O
	ATOM	4034	O	HOH X 693	31.536	51.730	17.146	1.00	27.97	O
	ATOM	4035	O	HOH X 694	32.756	40.610	17.091	1.00	30.80	O
10	ATOM	4036	O	HOH X 695	30.273	37.161	17.932	1.00	31.52	O
	ATOM	4037	O	HOH X 696	10.730	48.648	18.903	1.00	27.96	O
	ATOM	4038	O	HOH X 697	27.998	42.502	2.206	1.00	30.36	O
	ATOM	4039	O	HOH X 698	35.366	46.140	15.499	1.00	28.36	O
	ATOM	4040	O	HOH X 699	29.747	43.506	23.313	1.00	29.41	O
15	ATOM	4041	O	HOH X 700	32.478	37.004	16.071	1.00	33.87	O
	ATOM	4042	O	HOH X 701	26.381	49.100	1.307	1.00	30.51	O
	ATOM	4043	O	HOH X 702	31.462	38.877	21.855	1.00	32.31	O
	ATOM	4044	O	HOH X 703	20.391	54.311	2.653	1.00	35.11	O
	ATOM	4045	O	HOH X 704	20.190	52.761	18.136	1.00	28.04	O
20	ATOM	4046	O	HOH X 705	26.524	45.643	22.142	1.00	36.85	O
	ATOM	4047	O	HOH X 706	9.913	47.152	22.009	1.00	31.18	O
	ATOM	4048	O	HOH X 707	23.815	46.388	0.278	1.00	31.73	O
	ATOM	4049	O	HOH X 708	30.314	29.883	22.483	1.00	92.11	O
	ATOM	4050	O	HOH X 709	27.538	14.807	12.496	1.00	72.06	O
25	ATOM	4051	O	HOH X 710	31.854	56.101	11.223	1.00	33.44	O
	ATOM	4052	O	HOH X 711	31.468	55.841	14.563	1.00	36.46	O
	ATOM	4053	O	HOH X 712	29.552	46.090	20.444	1.00	23.02	O
	ATOM	4054	O	HOH X 713	3.638	29.070	4.171	1.00	54.83	O
	ATOM	4055	O	HOH X 714	5.829	45.923	-7.530	1.00	83.83	O
30	ATOM	4056	O	HOH X 715	14.120	13.888	-9.517	1.00	106.80	O
	ATOM	4057	O	HOH X 716	26.672	43.381	0.130	1.00	35.76	O
	ATOM	4058	O	HOH X 717	11.785	44.098	19.438	1.00	34.10	O
	ATOM	4059	O	HOH X 718	16.273	56.171	21.641	1.00	42.06	O
	ATOM	4060	O	HOH X 719	29.411	31.328	4.449	1.00	47.99	O
35	ATOM	4061	O	HOH X 720	21.804	48.437	19.617	1.00	33.01	O

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ATOM 4062 O HOH X 721 31.283 41.892 21.786 1.00 44.77 O

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Table 4. Atomic Coordinates of Hsp90 with Compound 49

		Amino Acid		Temp.				Atom Type
Atom Number	Residue	X	Y	Z	Occ. Factor			
5								
ATOM	1 N PRO A 11	10.302	-4.689	46.665	1.00	41.85		N
ATOM	2 CA PRO A 11	9.400	-5.749	46.217	1.00	41.57		C
ATOM	3 CB PRO A 11	7.999	-5.164	46.472	1.00	42.11		C
ATOM	4 CG PRO A 11	8.217	-3.921	47.308	1.00	41.96		C
10	ATOM	5 CD PRO A 11	9.580	-3.438	46.945	1.00	42.23	C
ATOM	6 C PRO A 11	9.571	-6.055	44.733	1.00	40.87		C
ATOM	7 O PRO A 11	9.902	-5.169	43.939	1.00	41.04		O
ATOM	8 N MET A 12	9.349	-7.311	44.369	1.00	39.94		N
ATOM	9 CA MET A 12	9.366	-7.719	42.975	1.00	38.66		C
15	ATOM	10 CB MET A 12	9.105	-9.220	42.871	1.00	38.47	C
ATOM	11 CG MET A 12	9.066	-9.761	41.453	1.00	36.99		C
ATOM	12 SD MET A 12	9.200	-11.555	41.445	1.00	37.39		S
ATOM	13 CE MET A 12	7.632	-12.050	42.175	1.00	36.61		C
ATOM	14 C MET A 12	8.316	-6.945	42.179	1.00	38.44		C
20	ATOM	15 O MET A 12	7.189	-6.764	42.634	1.00	38.50	O
ATOM	16 N GLU A 13	8.712	-6.479	41.003	1.00	37.96		N
ATOM	17 CA GLU A 13	7.800	-5.836	40.063	1.00	38.09		C
ATOM	18 CB GLU A 13	8.550	-4.808	39.216	1.00	38.18		C
ATOM	19 CG GLU A 13	8.658	-4.385	38.609	0.00	37.42		C
25	ATOM	20 CD GLU A 13	10.085	-3.907	38.220	0.00	39.00	C
ATOM	21 OE1 GLU A 13	11.082	-4.144	38.789	0.00	53.13		O
ATOM	22 OE2 GLU A 13	10.207	-3.392	37.121	0.00	49.88		O
ATOM	23 C GLU A 13	7.139	-6.874	39.162	1.00	38.14		C
ATOM	24 O GLU A 13	7.627	-7.996	39.015	1.00	37.58		O
30	ATOM	25 N GLU A 14	6.027	-6.488	38.553	1.00	38.59	N
ATOM	26 CA GLU A 14	5.231	-7.389	37.748	1.00	39.38		C
ATOM	27 CB GLU A 14	4.004	-7.815	38.551	1.00	39.49		C
ATOM	28 CG GLU A 14	3.321	-9.098	38.112	1.00	40.34		C
ATOM	29 CD GLU A 14	2.071	-9.394	38.943	1.00	41.37		C
35	ATOM	30 OE1 GLU A 14	1.324	-10.332	38.580	1.00	44.46	O

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	ATOM	31	OE2	GLU A 14	1.829	-8.687	39.960	1.00	42.38	O
	ATOM	32	C	GLU A 14	4.820	-6.668	36.468	1.00	39.22	C
	ATOM	33	O	GLU A 14	4.428	-5.491	36.503	1.00	39.16	O
	ATOM	34	N	GLU A 15	4.924	-7.371	35.344	1.00	39.01	N
5	ATOM	35	CA	GLU A 15	4.618	-6.804	34.024	1.00	39.17	C
	ATOM	36	CB	GLU A 15	5.908	-6.473	33.267	1.00	39.03	C
	ATOM	37	CG	GLU A 15	6.728	-5.317	33.844	1.00	40.10	C
	ATOM	38	CD	GLU A 15	7.778	-4.793	32.874	1.00	40.47	C
	ATOM	39	OE1	GLU A 15	8.873	-4.388	33.335	1.00	43.64	O
10	ATOM	40	OE2	GLU A 15	7.520	-4.787	31.650	1.00	41.21	O
	ATOM	41	C	GLU A 15	3.783	-7.768	33.185	1.00	38.70	C
	ATOM	42	O	GLU A 15	4.051	-8.975	33.158	1.00	38.45	O
	ATOM	43	N	GLU A 16	2.776	-7.232	32.499	1.00	38.28	N
	ATOM	44	CA	GLU A 16	1.999	-8.019	31.559	1.00	38.59	C
15	ATOM	45	CB	GLU A 16	0.574	-7.475	31.409	1.00	38.61	C
	ATOM	46	CG	GLU A 16	-0.271	-8.265	30.417	1.00	40.02	C
	ATOM	47	CD	GLU A 16	-1.713	-7.788	30.339	1.00	40.90	C
	ATOM	48	OE1	GLU A 16	-2.617	-8.616	30.601	1.00	43.96	O
	ATOM	49	OE2	GLU A 16	-1.939	-6.596	30.017	1.00	42.66	O
20	ATOM	50	C	GLU A 16	2.690	-8.033	30.203	1.00	37.66	C
	ATOM	51	O	GLU A 16	3.226	-7.019	29.761	1.00	37.44	O
	ATOM	52	N	VAL A 17	2.674	-9.194	29.559	1.00	36.77	N
	ATOM	53	CA	VAL A 17	3.149	-9.329	28.183	1.00	36.47	C
	ATOM	54	CB	VAL A 17	4.581	-9.963	28.143	1.00	36.41	C
25	ATOM	55	CG1	VAL A 17	4.596	-11.344	28.809	1.00	37.40	C
	ATOM	56	CG2	VAL A 17	5.137	-10.030	26.715	1.00	36.65	C
	ATOM	57	C	VAL A 17	2.111	-10.108	27.354	1.00	36.01	C
	ATOM	58	O	VAL A 17	1.389	-10.969	27.878	1.00	36.08	O
	ATOM	59	N	GLU A 18	2.012	-9.775	26.074	1.00	35.20	N
30	ATOM	60	CA	GLU A 18	1.114	-10.461	25.154	1.00	35.21	C
	ATOM	61	CB	GLU A 18	0.013	-9.522	24.655	1.00	35.34	C
	ATOM	62	CG	GLU A 18	-0.901	-9.000	25.748	1.00	37.35	C
	ATOM	63	CD	GLU A 18	-1.938	-8.041	25.209	1.00	38.71	C
	ATOM	64	OE1	GLU A 18	-1.923	-6.867	25.616	1.00	39.82	O
35	ATOM	65	OE2	GLU A 18	-2.761	-8.459	24.373	1.00	41.10	O

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	ATOM	66	C	GLU	A	18	1.909	-10.976	23.973	1.00	34.66	C
	ATOM	67	O	GLU	A	18	2.534	-10.198	23.257	1.00	34.31	O
	ATOM	68	N	THR	A	19	1.893	-12.291	23.788	1.00	34.21	N
	ATOM	69	CA	THR	A	19	2.589	-12.917	22.674	1.00	34.02	C
5	ATOM	70	CB	THR	A	19	3.264	-14.220	23.117	1.00	34.20	C
	ATOM	71	OG1	THR	A	19	4.113	-13.947	24.237	1.00	34.24	O
	ATOM	72	CG2	THR	A	19	4.079	-14.830	21.969	1.00	33.72	C
	ATOM	73	C	THR	A	19	1.628	-13.210	21.534	1.00	34.25	C
	ATOM	74	O	THR	A	19	0.543	-13.745	21.760	1.00	34.79	O
10	ATOM	75	N	PHE	A	20	2.040	-12.880	20.311	1.00	34.04	N
	ATOM	76	CA	PHE	A	20	1.218	-13.103	19.110	1.00	34.25	C
	ATOM	77	CB	PHE	A	20	0.836	-11.769	18.477	1.00	34.31	C
	ATOM	78	CG	PHE	A	20	-0.044	-10.920	19.343	1.00	34.36	C
	ATOM	79	CD1	PHE	A	20	0.504	-9.957	20.179	1.00	35.59	C
15	ATOM	80	CE1	PHE	A	20	-0.310	-9.172	20.992	1.00	36.08	C
	ATOM	81	CZ	PHE	A	20	-1.691	-9.358	20.972	1.00	35.31	C
	ATOM	82	CE2	PHE	A	20	-2.246	-10.319	20.146	1.00	34.78	C
	ATOM	83	CD2	PHE	A	20	-1.423	-11.100	19.339	1.00	35.28	C
	ATOM	84	C	PHE	A	20	1.894	-13.982	18.050	1.00	34.54	C
20	ATOM	85	O	PHE	A	20	3.102	-13.898	17.838	1.00	34.46	O
	ATOM	86	N	ALA	A	21	1.098	-14.793	17.360	1.00	34.71	N
	ATOM	87	CA	ALA	A	21	1.591	-15.589	16.231	1.00	34.75	C
	ATOM	88	CB	ALA	A	21	0.733	-16.841	16.045	1.00	35.13	C
	ATOM	89	C	ALA	A	21	1.567	-14.729	14.977	1.00	34.52	C
25	ATOM	90	O	ALA	A	21	0.566	-14.068	14.699	1.00	34.72	O
	ATOM	91	N	PHE	A	22	2.663	-14.708	14.225	1.00	34.13	N
	ATOM	92	CA	PHE	A	22	2.646	-14.036	12.923	1.00	34.13	C
	ATOM	93	CB	PHE	A	22	4.035	-14.022	12.278	1.00	33.94	C
	ATOM	94	CG	PHE	A	22	4.946	-12.922	12.783	1.00	33.13	C
30	ATOM	95	CD1	PHE	A	22	4.667	-11.590	12.509	1.00	33.06	C
	ATOM	96	CE1	PHE	A	22	5.504	-10.571	12.955	1.00	32.66	C
	ATOM	97	CZ	PHE	A	22	6.649	-10.885	13.693	1.00	33.56	C
	ATOM	98	CE2	PHE	A	22	6.946	-12.221	13.969	1.00	33.25	C
	ATOM	99	CD2	PHE	A	22	6.099	-13.229	13.513	1.00	33.06	C
35	ATOM	100	C	PHE	A	22	1.640	-14.753	12.013	1.00	34.20	C

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	ATOM	101	O	PHE A 22	1.505	-15.982	12.076	1.00	33.33	O
	ATOM	102	N	GLN A 23	0.923	-13.977	11.203	1.00	34.90	N
	ATOM	103	CA	GLN A 23	0.067	-14.504	10.125	1.00	35.11	C
	ATOM	104	CB	GLN A 23	-0.541	-13.337	9.332	1.00	35.37	C
5	ATOM	105	CG	GLN A 23	-1.692	-13.688	8.362	1.00	36.40	C
	ATOM	106	CD	GLN A 23	-1.217	-14.123	6.975	1.00	38.17	C
	ATOM	107	OE1	GLN A 23	-0.044	-13.988	6.635	1.00	39.14	O
	ATOM	108	NE2	GLN A 23	-2.140	-14.640	6.166	1.00	38.31	N
	ATOM	109	C	GLN A 23	0.930	-15.393	9.215	1.00	35.20	C
10	ATOM	110	O	GLN A 23	2.103	-15.087	8.984	1.00	34.53	O
	ATOM	111	N	ALA A 24	0.354	-16.494	8.729	1.00	35.40	N
	ATOM	112	CA	ALA A 24	1.123	-17.558	8.050	1.00	35.95	C
	ATOM	113	CB	ALA A 24	0.195	-18.660	7.525	1.00	36.19	C
	ATOM	114	C	ALA A 24	2.049	-17.077	6.938	1.00	35.97	C
15	ATOM	115	O	ALA A 24	3.229	-17.455	6.913	1.00	36.65	O
	ATOM	116	N	GLU A 25	1.522	-16.251	6.032	1.00	36.01	N
	ATOM	117	CA	GLU A 25	2.313	-15.763	4.892	1.00	36.09	C
	ATOM	118	CB	GLU A 25	1.448	-15.135	3.803	1.00	36.55	C
	ATOM	119	CG	GLU A 25	0.833	-16.152	2.863	1.00	39.20	C
20	ATOM	120	CD	GLU A 25	-0.486	-16.665	3.371	1.00	42.27	C
	ATOM	121	OE1	GLU A 25	-1.439	-15.858	3.477	1.00	42.48	O
	ATOM	122	OE2	GLU A 25	-0.568	-17.879	3.659	1.00	44.61	O
	ATOM	123	C	GLU A 25	3.400	-14.803	5.319	1.00	35.09	C
	ATOM	124	O	GLU A 25	4.495	-14.842	4.764	1.00	34.33	O
25	ATOM	125	N	ILE A 26	3.088	-13.947	6.297	1.00	34.82	N
	ATOM	126	CA	ILE A 26	4.083	-13.068	6.913	1.00	34.48	C
	ATOM	127	CB	ILE A 26	3.456	-12.105	7.964	1.00	34.53	C
	ATOM	128	CG1	ILE A 26	2.537	-11.082	7.282	1.00	34.54	C
	ATOM	129	CD1	ILE A 26	1.741	-10.225	8.258	1.00	34.59	C
30	ATOM	130	CG2	ILE A 26	4.544	-11.382	8.763	1.00	35.23	C
	ATOM	131	C	ILE A 26	5.212	-13.892	7.550	1.00	34.14	C
	ATOM	132	O	ILE A 26	6.389	-13.576	7.367	1.00	33.92	O
	ATOM	133	N	ALA A 27	4.856	-14.938	8.295	1.00	33.87	N
	ATOM	134	CA	ALA A 27	5.869	-15.827	8.875	1.00	34.05	C
35	ATOM	135	CB	ALA A 27	5.223	-16.883	9.778	1.00	33.90	C

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	ATOM	136	C	ALA A 27	6.763	-16.479	7.792	1.00	34.32	C
	ATOM	137	O	ALA A 27	7.986	-16.557	7.956	1.00	34.50	O
	ATOM	138	N	GLN A 28	6.140	-16.923	6.699	1.00	34.42	N
	ATOM	139	CA	GLN A 28	6.827	-17.475	5.527	1.00	35.28	C
5	ATOM	140	CB	GLN A 28	5.815	-17.884	4.447	1.00	35.20	C
	ATOM	141	CG	GLN A 28	5.078	-19.196	4.693	1.00	38.23	C
	ATOM	142	CD	GLN A 28	3.989	-19.479	3.651	1.00	37.46	C
	ATOM	143	OE1	GLN A 28	2.944	-20.056	3.966	1.00	42.73	O
	ATOM	144	NE2	GLN A 28	4.232	-19.078	2.413	1.00	41.10	N
10	ATOM	145	C	GLN A 28	7.786	-16.444	4.930	1.00	34.25	C
	ATOM	146	O	GLN A 28	8.925	-16.765	4.597	1.00	34.19	O
	ATOM	147	N	LEU A 29	7.308	-15.210	4.801	1.00	33.30	N
	ATOM	148	CA	LEU A 29	8.111	-14.101	4.282	1.00	32.95	C
	ATOM	149	CB	LEU A 29	7.254	-12.828	4.190	1.00	32.83	C
15	ATOM	150	CG	LEU A 29	7.977	-11.521	3.848	1.00	33.78	C
	ATOM	151	CD1	LEU A 29	8.594	-11.584	2.458	1.00	35.08	C
	ATOM	152	CD2	LEU A 29	7.038	-10.320	3.987	1.00	33.53	C
	ATOM	153	C	LEU A 29	9.371	-13.852	5.129	1.00	32.60	C
	ATOM	154	O	LEU A 29	10.483	-13.715	4.587	1.00	32.31	O
20	ATOM	155	N	MET A 30	9.190	-13.819	6.451	1.00	32.32	N
	ATOM	156	CA	MET A 30	10.281	-13.557	7.390	1.00	31.83	C
	ATOM	157	CB	MET A 30	9.735	-13.381	8.813	1.00	31.96	C
	ATOM	158	CG	MET A 30	8.985	-12.054	9.018	1.00	30.68	C
	ATOM	159	SD	MET A 30	8.245	-11.892	10.647	1.00	29.50	S
25	ATOM	160	CE	MET A 30	9.685	-11.562	11.663	1.00	30.10	C
	ATOM	161	C	MET A 30	11.325	-14.659	7.332	1.00	32.70	C
	ATOM	162	O	MET A 30	12.534	-14.385	7.296	1.00	33.46	O
	ATOM	163	N	SER A 31	10.869	-15.907	7.306	1.00	33.16	N
	ATOM	164	CA	SER A 31	11.782	-17.029	7.074	1.00	33.86	C
30	ATOM	165	CB	SER A 31	11.043	-18.364	7.138	1.00	34.02	C
	ATOM	166	OG	SER A 31	11.986	-19.418	7.137	1.00	35.71	O
	ATOM	167	C	SER A 31	12.550	-16.907	5.749	1.00	34.12	C
	ATOM	168	O	SER A 31	13.754	-17.151	5.707	1.00	34.17	O
	ATOM	169	N	LEU A 32	11.847	-16.542	4.674	1.00	34.86	N
35	ATOM	170	CA	LEU A 32	12.473	-16.303	3.369	1.00	35.70	C

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	ATOM	171	CB	LEU A 32	11.424	-15.914	2.319	1.00	35.79	C
	ATOM	172	CG	LEU A 32	10.981	-16.948	1.280	1.00	36.96	C
	ATOM	173	CD1	LEU A 32	10.452	-18.235	1.895	1.00	39.28	C
	ATOM	174	CD2	LEU A 32	9.932	-16.335	0.351	1.00	37.31	C
5	ATOM	175	C	LEU A 32	13.558	-15.232	3.435	1.00	35.62	C
	ATOM	176	O	LEU A 32	14.674	-15.446	2.962	1.00	35.71	O
	ATOM	177	N	ILE A 33	13.226	-14.095	4.042	1.00	35.59	N
	ATOM	178	CA	ILE A 33	14.159	-12.976	4.175	1.00	36.11	C
	ATOM	179	CB	ILE A 33	13.483	-11.722	4.830	1.00	35.85	C
10	ATOM	180	CG1	ILE A 33	12.428	-11.129	3.879	1.00	35.90	C
	ATOM	181	CD1	ILE A 33	11.482	-10.098	4.527	1.00	35.62	C
	ATOM	182	CG2	ILE A 33	14.521	-10.665	5.246	1.00	35.67	C
	ATOM	183	C	ILE A 33	15.400	-13.416	4.945	1.00	36.41	C
	ATOM	184	O	ILE A 33	16.518	-13.130	4.516	1.00	36.50	O
15	ATOM	185	N	ILE A 34	15.195	-14.148	6.040	1.00	36.87	N
	ATOM	186	CA	ILE A 34	16.285	-14.546	6.945	1.00	37.69	C
	ATOM	187	CB	ILE A 34	15.747	-14.969	8.342	1.00	37.70	C
	ATOM	188	CG1	ILE A 34	15.186	-13.749	9.075	1.00	37.66	C
	ATOM	189	CD1	ILE A 34	14.247	-14.088	10.201	1.00	37.40	C
20	ATOM	190	CG2	ILE A 34	16.854	-15.579	9.203	1.00	38.21	C
	ATOM	191	C	ILE A 34	17.201	-15.638	6.385	1.00	38.36	C
	ATOM	192	O	ILE A 34	18.415	-15.562	6.546	1.00	38.94	O
	ATOM	193	N	ASN A 35	16.615	-16.627	5.715	1.00	38.83	N
	ATOM	194	CA	ASN A 35	17.334	-17.841	5.320	1.00	39.66	C
25	ATOM	195	CB	ASN A 35	16.503	-19.064	5.708	1.00	39.41	C
	ATOM	196	CG	ASN A 35	16.297	-19.167	7.197	1.00	39.99	C
	ATOM	197	OD1	ASN A 35	17.258	-19.295	7.958	1.00	40.62	O
	ATOM	198	ND2	ASN A 35	15.038	-19.108	7.630	1.00	40.24	N
	ATOM	199	C	ASN A 35	17.753	-17.908	3.844	1.00	39.79	C
30	ATOM	200	O	ASN A 35	18.194	-18.952	3.359	1.00	40.31	O
	ATOM	201	N	THR A 36	17.618	-16.786	3.142	1.00	39.96	N
	ATOM	202	CA	THR A 36	18.002	-16.679	1.742	1.00	39.79	C
	ATOM	203	CB	THR A 36	16.773	-16.405	0.840	1.00	40.31	C
	ATOM	204	OG1	THR A 36	15.803	-17.453	1.003	1.00	41.29	O
35	ATOM	205	CG2	THR A 36	17.169	-16.293	-0.645	1.00	40.28	C

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	ATOM	206	C	THR	A	36	19.013	-15.545	1.606	1.00	39.57	C
	ATOM	207	O	THR	A	36	18.860	-14.482	2.222	1.00	38.78	O
	ATOM	208	N	PHE	A	37	20.049	-15.772	0.803	1.00	39.16	N
	ATOM	209	CA	PHE	A	37	21.033	-14.728	0.545	1.00	38.98	C
5	ATOM	210	CB	PHE	A	37	22.363	-15.309	0.037	1.00	38.99	C
	ATOM	211	CG	PHE	A	37	23.381	-14.254	-0.285	1.00	38.33	C
	ATOM	212	CD1	PHE	A	37	23.517	-13.769	-1.585	1.00	38.27	C
	ATOM	213	CE1	PHE	A	37	24.439	-12.767	-1.875	1.00	37.19	C
	ATOM	214	CZ	PHE	A	37	25.235	-12.241	-0.861	1.00	36.80	C
10	ATOM	215	CE2	PHE	A	37	25.098	-12.708	0.438	1.00	38.40	C
	ATOM	216	CD2	PHE	A	37	24.171	-13.711	0.720	1.00	37.88	C
	ATOM	217	C	PHE	A	37	20.531	-13.662	-0.433	1.00	39.17	C
	ATOM	218	O	PHE	A	37	20.070	-13.977	-1.530	1.00	38.92	O
	ATOM	219	N	TYR	A	38	20.666	-12.399	-0.034	1.00	39.49	N
15	ATOM	220	CA	TYR	A	38	20.353	-11.258	-0.898	1.00	39.73	C
	ATOM	221	CB	TYR	A	38	19.067	-10.556	-0.444	1.00	39.95	C
	ATOM	222	CG	TYR	A	38	17.863	-11.465	-0.444	1.00	40.02	C
	ATOM	223	CD1	TYR	A	38	17.331	-11.950	0.753	1.00	40.64	C
	ATOM	224	CE1	TYR	A	38	16.228	-12.801	0.757	1.00	40.36	C
20	ATOM	225	CZ	TYR	A	38	15.643	-13.166	-0.448	1.00	40.35	C
	ATOM	226	OH	TYR	A	38	14.558	-14.009	-0.459	1.00	40.88	O
	ATOM	227	CE2	TYR	A	38	16.153	-12.703	-1.650	1.00	41.20	C
	ATOM	228	CD2	TYR	A	38	17.258	-11.852	-1.643	1.00	40.46	C
	ATOM	229	C	TYR	A	38	21.510	-10.286	-0.881	1.00	39.66	C
25	ATOM	230	O	TYR	A	38	21.999	-9.917	0.193	1.00	40.15	O
	ATOM	231	N	SER	A	39	21.948	-9.874	-2.066	1.00	39.13	N
	ATOM	232	CA	SER	A	39	23.133	-9.033	-2.201	1.00	39.15	C
	ATOM	233	CB	SER	A	39	23.678	-9.108	-3.632	1.00	39.28	C
	ATOM	234	OG	SER	A	39	22.750	-8.591	-4.573	1.00	39.69	O
30	ATOM	235	C	SER	A	39	22.908	-7.567	-1.802	1.00	38.78	C
	ATOM	236	O	SER	A	39	23.855	-6.860	-1.449	1.00	39.71	O
	ATOM	237	N	ASN	A	40	21.659	-7.125	-1.864	1.00	37.82	N
	ATOM	238	CA	ASN	A	40	21.322	-5.703	-1.784	1.00	36.94	C
	ATOM	239	CB	ASN	A	40	20.435	-5.363	-3.001	1.00	37.28	C
35	ATOM	240	CG	ASN	A	40	20.311	-3.861	-3.276	1.00	39.13	C

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	ATOM	241	OD1 ASN A 40	19.286	-3.399	-3.798	1.00	42.21	O
	ATOM	242	ND2 ASN A 40	21.353	-3.106	-2.969	1.00	40.86	N
	ATOM	243	C ASN A 40	20.620	-5.388	-0.445	1.00	35.52	C
	ATOM	244	O ASN A 40	19.548	-4.769	-0.427	1.00	35.02	O
5	ATOM	245	N LYS A 41	21.242	-5.808	0.665	1.00	33.98	N
	ATOM	246	CA LYS A 41	20.636	-5.750	2.015	1.00	33.28	C
	ATOM	247	CB LYS A 41	21.491	-6.518	3.043	1.00	33.10	C
	ATOM	248	CG LYS A 41	21.486	-8.040	2.879	1.00	33.38	C
	ATOM	249	CD LYS A 41	22.308	-8.719	3.961	1.00	33.30	C
10	ATOM	250	CE LYS A 41	22.090	-10.221	3.962	1.00	33.89	C
	ATOM	251	NZ LYS A 41	22.734	-10.832	2.779	1.00	32.88	N
	ATOM	252	C LYS A 41	20.400	-4.329	2.526	1.00	32.94	C
	ATOM	253	O LYS A 41	19.471	-4.085	3.312	1.00	32.53	O
	ATOM	254	N GLU A 42	21.233	-3.399	2.059	1.00	32.64	N
15	ATOM	255	CA GLU A 42	21.228	-2.013	2.536	1.00	32.85	C
	ATOM	256	CB GLU A 42	22.357	-1.233	1.854	1.00	33.32	C
	ATOM	257	CG GLU A 42	22.025	-0.784	0.426	1.00	35.99	C
	ATOM	258	CD GLU A 42	23.162	-1.044	-0.534	1.00	40.84	C
	ATOM	259	OE1 GLU A 42	24.246	-0.453	-0.349	1.00	41.77	O
20	ATOM	260	OE2 GLU A 42	22.970	-1.851	-1.470	1.00	42.63	O
	ATOM	261	C GLU A 42	19.889	-1.277	2.354	1.00	32.49	C
	ATOM	262	O GLU A 42	19.641	-0.251	3.007	1.00	32.80	O
	ATOM	263	N ILE A 43	19.037	-1.787	1.461	1.00	31.78	N
	ATOM	264	CA ILE A 43	17.719	-1.188	1.215	1.00	31.07	C
25	ATOM	265	CB ILE A 43	17.021	-1.772	-0.063	1.00	31.36	C
	ATOM	266	CG1 ILE A 43	16.719	-3.273	0.076	1.00	30.47	C
	ATOM	267	CD1 ILE A 43	15.466	-3.606	0.904	1.00	31.94	C
	ATOM	268	CG2 ILE A 43	17.872	-1.514	-1.308	1.00	31.59	C
	ATOM	269	C ILE A 43	16.793	-1.244	2.439	1.00	30.64	C
30	ATOM	270	O ILE A 43	15.735	-0.595	2.447	1.00	30.31	O
	ATOM	271	N PHE A 44	17.196	-2.000	3.468	1.00	29.88	N
	ATOM	272	CA PHE A 44	16.435	-2.053	4.730	1.00	29.65	C
	ATOM	273	CB PHE A 44	17.109	-2.964	5.765	1.00	29.57	C
	ATOM	274	CG PHE A 44	18.201	-2.280	6.539	1.00	28.64	C
35	ATOM	275	CD1 PHE A 44	19.511	-2.304	6.074	1.00	28.07	C

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	ATOM	276	CE1 PHE A 44	20.535	-1.645	6.769	1.00	30.55	C
	ATOM	277	CZ PHE A 44	20.232	-0.933	7.922	1.00	30.51	C
	ATOM	278	CE2 PHE A 44	18.917	-0.895	8.391	1.00	29.64	C
	ATOM	279	CD2 PHE A 44	17.911	-1.561	7.703	1.00	28.59	C
5	ATOM	280	C PHE A 44	16.275	-0.635	5.301	1.00	29.73	C
	ATOM	281	O PHE A 44	15.210	-0.283	5.787	1.00	29.24	O
	ATOM	282	N LEU A 45	17.337	0.171	5.224	1.00	29.99	N
	ATOM	283	CA LEU A 45	17.294	1.537	5.751	1.00	30.30	C
	ATOM	284	CB LEU A 45	18.696	2.184	5.808	1.00	30.20	C
10	ATOM	285	CG LEU A 45	18.775	3.548	6.541	1.00	30.51	C
	ATOM	286	CD1 LEU A 45	20.215	4.054	6.605	1.00	30.04	C
	ATOM	287	CD2 LEU A 45	18.202	3.492	7.958	1.00	31.74	C
	ATOM	288	C LEU A 45	16.304	2.422	4.997	1.00	30.36	C
	ATOM	289	O LEU A 45	15.522	3.142	5.628	1.00	30.99	O
15	ATOM	290	N ARG A 46	16.310	2.377	3.668	1.00	30.40	N
	ATOM	291	CA ARG A 46	15.373	3.241	2.940	1.00	30.73	C
	ATOM	292	CB ARG A 46	15.684	3.394	1.451	1.00	31.44	C
	ATOM	293	CG ARG A 46	15.485	2.189	0.592	1.00	33.71	C
	ATOM	294	CD ARG A 46	14.563	2.501	-0.623	1.00	35.60	C
20	ATOM	295	NE ARG A 46	13.916	1.239	-0.983	1.00	38.29	N
	ATOM	296	CZ ARG A 46	14.318	0.403	-1.938	1.00	37.74	C
	ATOM	297	NH1 ARG A 46	15.329	0.706	-2.746	1.00	35.32	N
	ATOM	298	NH2 ARG A 46	13.668	-0.739	-2.104	1.00	39.20	N
	ATOM	299	C ARG A 46	13.919	2.858	3.205	1.00	29.67	C
25	ATOM	300	O ARG A 46	13.063	3.724	3.232	1.00	29.33	O
	ATOM	301	N GLU A 47	13.660	1.574	3.448	1.00	28.84	N
	ATOM	302	CA GLU A 47	12.316	1.135	3.836	1.00	28.27	C
	ATOM	303	CB GLU A 47	12.197	-0.403	3.824	1.00	28.22	C
	ATOM	304	CG GLU A 47	12.390	-1.028	2.433	1.00	29.86	C
30	ATOM	305	CD GLU A 47	11.386	-0.511	1.409	1.00	32.56	C
	ATOM	306	OE1 GLU A 47	10.214	-0.297	1.774	1.00	32.86	O
	ATOM	307	OE2 GLU A 47	11.780	-0.297	0.245	1.00	34.22	O
	ATOM	308	C GLU A 47	11.883	1.716	5.181	1.00	27.70	C
	ATOM	309	O GLU A 47	10.748	2.179	5.328	1.00	27.69	O
35	ATOM	310	N LEU A 48	12.787	1.699	6.160	1.00	27.02	N

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	ATOM	311	CA	LEU A 48	12.497	2.252	7.473	1.00	26.62	C
	ATOM	312	CB	LEU A 48	13.586	1.855	8.481	1.00	26.57	C
	ATOM	313	CG	LEU A 48	13.737	0.328	8.653	1.00	27.20	C
	ATOM	314	CD1	LEU A 48	14.872	0.015	9.613	1.00	28.44	C
5	ATOM	315	CD2	LEU A 48	12.422	-0.345	9.110	1.00	29.09	C
	ATOM	316	C	LEU A 48	12.336	3.762	7.398	1.00	26.05	C
	ATOM	317	O	LEU A 48	11.424	4.315	7.998	1.00	25.77	O
	ATOM	318	N	ILE A 49	13.202	4.423	6.638	1.00	25.56	N
	ATOM	319	CA	ILE A 49	13.084	5.880	6.475	1.00	26.05	C
10	ATOM	320	CB	ILE A 49	14.337	6.483	5.798	1.00	25.67	C
	ATOM	321	CG1	ILE A 49	15.547	6.342	6.748	1.00	25.74	C
	ATOM	322	CD1	ILE A 49	16.880	6.646	6.108	1.00	26.55	C
	ATOM	323	CG2	ILE A 49	14.086	7.960	5.403	1.00	25.58	C
	ATOM	324	C	ILE A 49	11.784	6.251	5.730	1.00	26.07	C
15	ATOM	325	O	ILE A 49	11.106	7.235	6.084	1.00	26.64	O
	ATOM	326	N	SER A 50	11.421	5.442	4.743	1.00	26.25	N
	ATOM	327	CA	SER A 50	10.184	5.664	3.976	1.00	26.45	C
	ATOM	328	CB	BSER A 50	10.077	4.684	2.803	0.35	26.42	C
	ATOM	329	CB	ASER A 50	10.101	4.687	2.799	0.65	26.77	C
20	ATOM	330	OG	BSER A 50	10.871	5.091	1.700	0.35	25.24	O
	ATOM	331	OG	ASER A 50	8.864	4.797	2.112	0.65	27.82	O
	ATOM	332	C	SER A 50	8.933	5.564	4.874	1.00	26.60	C
	ATOM	333	O	SER A 50	7.993	6.369	4.742	1.00	26.09	O
	ATOM	334	N	ASN A 51	8.941	4.582	5.780	1.00	26.69	N
25	ATOM	335	CA	ASN A 51	7.869	4.417	6.763	1.00	27.29	C
	ATOM	336	CB	ASN A 51	8.053	3.111	7.534	1.00	26.99	C
	ATOM	337	CG	ASN A 51	7.655	1.867	6.721	1.00	29.57	C
	ATOM	338	OD1	ASN A 51	7.219	1.949	5.571	1.00	29.73	O
	ATOM	339	ND2	ASN A 51	7.776	0.707	7.353	1.00	32.63	N
30	ATOM	340	C	ASN A 51	7.760	5.609	7.728	1.00	27.04	C
	ATOM	341	O	ASN A 51	6.656	6.094	7.990	1.00	26.69	O
	ATOM	342	N	SER A 52	8.906	6.053	8.267	1.00	27.06	N
	ATOM	343	CA	SER A 52	8.996	7.274	9.075	1.00	27.27	C
	ATOM	344	CB	SER A 52	10.454	7.578	9.467	1.00	27.37	C
35	ATOM	345	OG	SER A 52	11.034	6.540	10.234	1.00	24.92	O

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	ATOM	346	C	SER A 52	8.425	8.492	8.340	1.00	28.09	C
	ATOM	347	O	SER A 52	7.678	9.284	8.938	1.00	27.24	O
	ATOM	348	N	SER A 53	8.806	8.642	7.070	1.00	28.74	N
	ATOM	349	CA	SER A 53	8.360	9.753	6.229	1.00	29.76	C
5	ATOM	350	CB	SER A 53	9.017	9.717	4.847	1.00	29.86	C
	ATOM	351	OG	SER A 53	8.615	10.845	4.077	1.00	31.82	O
	ATOM	352	C	SER A 53	6.837	9.710	6.109	1.00	29.65	C
	ATOM	353	O	SER A 53	6.175	10.719	6.357	1.00	28.97	O
	ATOM	354	N	ASP A 54	6.295	8.524	5.803	1.00	29.81	N
10	ATOM	355	CA	ASP A 54	4.830	8.308	5.759	1.00	30.09	C
	ATOM	356	CB	ASP A 54	4.483	6.840	5.422	1.00	30.70	C
	ATOM	357	CG	ASP A 54	4.771	6.453	3.953	1.00	31.87	C
	ATOM	358	OD1	ASP A 54	5.103	7.313	3.099	1.00	31.39	O
	ATOM	359	OD2	ASP A 54	4.651	5.248	3.652	1.00	33.44	O
15	ATOM	360	C	ASP A 54	4.147	8.716	7.087	1.00	29.58	C
	ATOM	361	O	ASP A 54	3.109	9.390	7.067	1.00	29.17	O
	ATOM	362	N	ALA A 55	4.723	8.297	8.226	1.00	28.46	N
	ATOM	363	CA	ALA A 55	4.198	8.620	9.563	1.00	27.67	C
	ATOM	364	CB	ALA A 55	4.875	7.792	10.642	1.00	27.00	C
20	ATOM	365	C	ALA A 55	4.296	10.108	9.912	1.00	27.84	C
	ATOM	366	O	ALA A 55	3.438	10.633	10.609	1.00	28.01	O
	ATOM	367	N	LEU A 56	5.352	10.758	9.430	1.00	27.75	N
	ATOM	368	CA	LEU A 56	5.529	12.193	9.575	1.00	28.28	C
	ATOM	369	CB	LEU A 56	6.958	12.595	9.211	1.00	28.49	C
25	ATOM	370	CG	LEU A 56	7.984	12.244	10.304	1.00	28.25	C
	ATOM	371	CD1	LEU A 56	9.422	12.312	9.770	1.00	29.38	C
	ATOM	372	CD2	LEU A 56	7.818	13.096	11.568	1.00	28.46	C
	ATOM	373	C	LEU A 56	4.500	12.962	8.739	1.00	28.99	C
	ATOM	374	O	LEU A 56	3.895	13.908	9.236	1.00	28.94	O
30	ATOM	375	N	ASP A 57	4.315	12.547	7.484	1.00	28.95	N
	ATOM	376	CA	ASP A 57	3.233	13.054	6.616	1.00	29.80	C
	ATOM	377	CB	ASP A 57	3.136	12.235	5.329	1.00	29.76	C
	ATOM	378	CG	ASP A 57	4.184	12.617	4.280	1.00	30.58	C
	ATOM	379	OD1	ASP A 57	4.841	13.677	4.381	1.00	30.64	O
35	ATOM	380	OD2	ASP A 57	4.329	11.833	3.330	1.00	32.81	O

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	ATOM	381	C	ASP	A	57	1.879	12.989	7.325	1.00	29.47	C
	ATOM	382	O	ASP	A	57	1.144	13.978	7.366	1.00	29.79	O
	ATOM	383	N	LYS	A	58	1.558	11.818	7.878	1.00	29.45	N
	ATOM	384	CA	LYS	A	58	0.303	11.638	8.605	1.00	29.82	C
5	ATOM	385	CB	LYS	A	58	0.177	10.219	9.169	1.00	29.43	C
	ATOM	386	CG	LYS	A	58	-0.086	9.158	8.084	1.00	29.59	C
	ATOM	387	CD	LYS	A	58	-0.133	7.738	8.663	1.00	29.94	C
	ATOM	388	CE	LYS	A	58	-1.427	7.490	9.433	1.00	32.27	C
	ATOM	389	NZ	LYS	A	58	-2.619	7.556	8.534	1.00	32.56	N
10	ATOM	390	C	LYS	A	58	0.086	12.693	9.686	1.00	30.04	C
	ATOM	391	O	LYS	A	58	-0.951	13.348	9.685	1.00	30.14	O
	ATOM	392	N	ILE	A	59	1.061	12.888	10.583	1.00	29.85	N
	ATOM	393	CA	ILE	A	59	0.875	13.859	11.666	1.00	30.37	C
	ATOM	394	CB	ILE	A	59	1.881	13.686	12.877	1.00	29.73	C
15	ATOM	395	CG1	ILE	A	59	1.539	14.626	14.054	1.00	30.08	C
	ATOM	396	CD1	ILE	A	59	0.228	14.309	14.810	1.00	27.13	C
	ATOM	397	CG2	ILE	A	59	3.325	13.895	12.448	1.00	29.77	C
	ATOM	398	C	ILE	A	59	0.847	15.282	11.133	1.00	30.81	C
	ATOM	399	O	ILE	A	59	0.071	16.104	11.628	1.00	31.51	O
20	ATOM	400	N	ARG	A	60	1.671	15.561	10.126	1.00	31.58	N
	ATOM	401	CA	ARG	A	60	1.709	16.893	9.510	1.00	33.64	C
	ATOM	402	CB	ARG	A	60	2.766	16.964	8.396	1.00	32.96	C
	ATOM	403	CG	ARG	A	60	2.950	18.374	7.806	1.00	35.01	C
	ATOM	404	CD	ARG	A	60	4.244	18.513	7.005	1.00	35.16	C
25	ATOM	405	NE	ARG	A	60	4.318	17.600	5.862	1.00	40.04	N
	ATOM	406	CZ	ARG	A	60	3.717	17.786	4.686	1.00	41.19	C
	ATOM	407	NH1	ARG	A	60	2.967	18.863	4.460	1.00	41.10	N
	ATOM	408	NH2	ARG	A	60	3.866	16.880	3.727	1.00	41.55	N
	ATOM	409	C	ARG	A	60	0.326	17.317	8.988	1.00	33.83	C
30	ATOM	410	O	ARG	A	60	-0.195	18.362	9.389	1.00	34.47	O
	ATOM	411	N	TYR	A	61	-0.263	16.495	8.125	1.00	34.29	N
	ATOM	412	CA	TYR	A	61	-1.559	16.814	7.516	1.00	35.17	C
	ATOM	413	CB	TYR	A	61	-1.854	15.916	6.307	1.00	34.96	C
	ATOM	414	CG	TYR	A	61	-1.035	16.313	5.109	1.00	35.16	C
35	ATOM	415	CD1	TYR	A	61	0.025	15.521	4.669	1.00	34.31	C

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	ATOM	416	CE1 TYR A 61	0.788	15.895	3.586	1.00	35.13	C
	ATOM	417	CZ TYR A 61	0.516	17.092	2.938	1.00	35.41	C
	ATOM	418	OH TYR A 61	1.273	17.475	1.871	1.00	36.35	O
	ATOM	419	CE2 TYR A 61	-0.519	17.903	3.353	1.00	35.19	C
5	ATOM	420	CD2 TYR A 61	-1.286	17.513	4.440	1.00	35.51	C
	ATOM	421	C TYR A 61	-2.721	16.827	8.500	1.00	35.53	C
	ATOM	422	O TYR A 61	-3.610	17.670	8.390	1.00	36.00	O
	ATOM	423	N GLU A 62	-2.696	15.923	9.474	1.00	36.28	N
	ATOM	424	CA GLU A 62	-3.728	15.896	10.515	1.00	37.39	C
10	ATOM	425	CB GLU A 62	-3.691	14.579	11.292	1.00	37.09	C
	ATOM	426	CG GLU A 62	-4.179	13.398	10.470	1.00	39.82	C
	ATOM	427	CD GLU A 62	-4.429	12.160	11.303	1.00	42.89	C
	ATOM	428	OE1 GLU A 62	-4.257	12.212	12.544	1.00	45.96	O
	ATOM	429	OE2 GLU A 62	-4.803	11.131	10.710	1.00	45.34	O
15	ATOM	430	C GLU A 62	-3.658	17.083	11.470	1.00	37.78	C
	ATOM	431	O GLU A 62	-4.692	17.547	11.962	1.00	37.87	O
	ATOM	432	N SER A 63	-2.447	17.578	11.722	1.00	38.21	N
	ATOM	433	CA SER A 63	-2.251	18.727	12.606	1.00	39.02	C
	ATOM	434	CB SER A 63	-0.778	18.867	13.006	1.00	38.72	C
20	ATOM	435	OG SER A 63	0.015	19.357	11.930	1.00	39.01	O
	ATOM	436	C SER A 63	-2.758	20.050	12.009	1.00	39.69	C
	ATOM	437	O SER A 63	-2.998	21.012	12.748	1.00	39.78	O
	ATOM	438	N LEU A 64	-2.905	20.091	10.683	1.00	40.52	N
	ATOM	439	CA LEU A 64	-3.378	21.289	9.967	1.00	41.64	C
25	ATOM	440	CB LEU A 64	-3.356	21.070	8.451	1.00	41.28	C
	ATOM	441	CG LEU A 64	-1.982	21.013	7.779	1.00	42.00	C
	ATOM	442	CD1 LEU A 64	-2.111	20.911	6.265	1.00	40.56	C
	ATOM	443	CD2 LEU A 64	-1.319	22.449	8.180	0.00	41.12	C
	ATOM	444	C LEU A 64	-4.781	21.674	10.401	1.00	42.38	C
30	ATOM	445	O LEU A 64	-5.109	22.855	10.488	1.00	42.65	O
	ATOM	446	N THR A 65	-5.597	20.663	10.672	1.00	43.47	N
	ATOM	447	CA THR A 65	-6.971	20.866	11.120	1.00	44.62	C
	ATOM	448	CB THR A 65	-7.968	19.989	10.324	1.00	44.74	C
	ATOM	449	OG1 THR A 65	-7.371	18.718	10.030	1.00	45.78	O
35	ATOM	450	CG2 THR A 65	-8.325	20.680	9.013	1.00	45.57	C

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	ATOM	451	C	THR A 65	-7.147	20.678	12.632	1.00	44.81	C
	ATOM	452	O	THR A 65	-8.117	21.173	13.207	1.00	44.94	O
	ATOM	453	N	ASP A 66	-6.211	19.977	13.271	1.00	44.89	N
	ATOM	454	CA	ASP A 66	-6.199	19.876	14.733	1.00	45.00	C
5	ATOM	455	CB	ASP A 66	-6.743	18.523	15.219	1.00	45.05	C
	ATOM	456	CG	ASP A 66	-6.934	18.469	16.742	1.00	45.50	C
	ATOM	457	OD1	ASP A 66	-6.522	19.412	17.457	1.00	46.26	O
	ATOM	458	OD2	ASP A 66	-7.497	17.466	17.232	1.00	46.33	O
	ATOM	459	C	ASP A 66	-4.797	20.126	15.285	1.00	44.74	C
10	ATOM	460	O	ASP A 66	-4.019	19.182	15.445	1.00	44.77	O
	ATOM	461	N	PRO A 67	-4.487	21.397	15.607	1.00	44.50	N
	ATOM	462	CA	PRO A 67	-3.146	21.796	16.069	1.00	44.24	C
	ATOM	463	CB	PRO A 67	-3.262	23.313	16.273	1.00	44.24	C
	ATOM	464	CG	PRO A 67	-4.419	23.823	15.346	0.00	46.99	C
15	ATOM	465	CD	PRO A 67	-5.434	22.531	15.555	1.00	44.48	C
	ATOM	466	C	PRO A 67	-2.729	21.117	17.373	1.00	44.11	C
	ATOM	467	O	PRO A 67	-1.537	20.875	17.580	1.00	44.15	O
	ATOM	468	N	SER A 68	-3.704	20.793	18.225	1.00	43.62	N
	ATOM	469	CA	SER A 68	-3.434	20.144	19.514	1.00	43.37	C
20	ATOM	470	CB	SER A 68	-4.719	20.000	20.339	1.00	43.37	C
	ATOM	471	OG	SER A 68	-5.498	18.901	19.896	1.00	43.34	O
	ATOM	472	C	SER A 68	-2.751	18.778	19.379	1.00	42.92	C
	ATOM	473	O	SER A 68	-2.226	18.253	20.360	1.00	43.23	O
	ATOM	474	N	LYS A 69	-2.768	18.208	18.175	1.00	42.15	N
25	ATOM	475	CA	LYS A 69	-2.106	16.920	17.923	1.00	41.78	C
	ATOM	476	CB	LYS A 69	-2.534	16.344	16.572	1.00	41.49	C
	ATOM	477	CG	LYS A 69	-3.913	15.699	16.590	1.00	41.65	C
	ATOM	478	CD	LYS A 69	-4.292	15.148	15.227	1.00	40.96	C
	ATOM	479	CE	LYS A 69	-5.674	14.516	15.254	1.00	41.18	C
30	ATOM	480	NZ	LYS A 69	-6.024	13.983	13.909	1.00	42.42	N
	ATOM	481	C	LYS A 69	-0.577	17.027	18.006	1.00	41.72	C
	ATOM	482	O	LYS A 69	0.119	16.013	18.166	1.00	41.27	O
	ATOM	483	N	LEU A 70	-0.071	18.256	17.898	1.00	41.37	N
	ATOM	484	CA	LEU A 70	1.365	18.536	18.028	1.00	41.62	C
35	ATOM	485	CB	LEU A 70	1.817	19.623	17.038	1.00	41.38	C

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	ATOM	486	CG	LEU A 70	1.721	19.329	15.537	1.00	41.39	C
	ATOM	487	CD1	LEU A 70	2.190	20.526	14.708	1.00	41.22	C
	ATOM	488	CD2	LEU A 70	2.480	18.064	15.131	1.00	41.35	C
	ATOM	489	C	LEU A 70	1.780	18.920	19.446	1.00	41.56	C
5	ATOM	490	O	LEU A 70	2.954	19.221	19.678	1.00	42.14	O
	ATOM	491	N	ASP A 71	0.831	18.913	20.387	1.00	41.56	N
	ATOM	492	CA	ASP A 71	1.146	19.155	21.808	1.00	41.37	C
	ATOM	493	CB	ASP A 71	-0.095	18.972	22.690	1.00	41.34	C
	ATOM	494	CG	ASP A 71	-1.065	20.146	22.614	1.00	42.37	C
10	ATOM	495	OD1	ASP A 71	-0.784	21.140	21.905	1.00	40.81	O
	ATOM	496	OD2	ASP A 71	-2.128	20.061	23.273	1.00	43.30	O
	ATOM	497	C	ASP A 71	2.242	18.205	22.286	1.00	41.01	C
	ATOM	498	O	ASP A 71	3.108	18.582	23.090	1.00	41.27	O
	ATOM	499	N	SER A 72	2.197	16.970	21.779	1.00	40.32	N
15	ATOM	500	CA	SER A 72	3.201	15.943	22.067	1.00	39.32	C
	ATOM	501	CB	SER A 72	2.657	14.570	21.664	1.00	39.56	C
	ATOM	502	OG	SER A 72	2.117	14.620	20.347	1.00	37.10	O
	ATOM	503	C	SER A 72	4.555	16.187	21.383	1.00	39.48	C
	ATOM	504	O	SER A 72	5.459	15.340	21.458	1.00	39.10	O
20	ATOM	505	N	GLY A 73	4.695	17.332	20.719	1.00	38.99	N
	ATOM	506	CA	GLY A 73	5.978	17.734	20.128	1.00	39.59	C
	ATOM	507	C	GLY A 73	5.841	18.262	18.716	1.00	39.08	C
	ATOM	508	O	GLY A 73	5.214	17.622	17.870	1.00	39.49	O
	ATOM	509	N	LYS A 74	6.445	19.421	18.458	1.00	38.66	N
25	ATOM	510	CA	LYS A 74	6.259	20.123	17.185	1.00	38.41	C
	ATOM	511	CB	LYS A 74	6.284	21.643	17.397	1.00	38.45	C
	ATOM	512	CG	LYS A 74	5.052	22.183	18.132	1.00	39.15	C
	ATOM	513	CD	LYS A 74	5.125	23.029	18.987	0.00	51.18	C
	ATOM	514	CE	LYS A 74	4.418	22.457	20.350	0.00	53.91	C
30	ATOM	515	NZ	LYS A 74	3.113	22.248	20.148	0.00	50.42	N
	ATOM	516	C	LYS A 74	7.246	19.719	16.087	1.00	37.82	C
	ATOM	517	O	LYS A 74	6.897	19.747	14.905	1.00	38.24	O
	ATOM	518	N	GLU A 75	8.465	19.349	16.481	1.00	37.17	N
	ATOM	519	CA	GLU A 75	9.531	19.014	15.533	1.00	36.22	C
35	ATOM	520	CB	GLU A 75	10.887	18.955	16.250	1.00	36.04	C

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	ATOM	521	CG	GLU A 75	11.397	20.309	16.743	1.00	37.08	C
	ATOM	522	CD	GLU A 75	12.756	20.229	17.428	0.30	36.44	C
	ATOM	523	OE1	GLU A 75	13.339	21.299	17.707	0.30	36.68	O
	ATOM	524	OE2	GLU A 75	13.243	19.105	17.689	0.30	36.62	O
5	ATOM	525	C	GLU A 75	9.240	17.696	14.817	1.00	35.57	C
	ATOM	526	O	GLU A 75	8.982	16.680	15.461	1.00	35.54	O
	ATOM	527	N	LEU A 76	9.237	17.736	13.487	1.00	34.75	N
	ATOM	528	CA	LEU A 76	8.989	16.555	12.661	1.00	34.00	C
	ATOM	529	CB	LEU A 76	7.893	16.837	11.621	1.00	34.11	C
10	ATOM	530	CG	LEU A 76	6.508	17.229	12.149	1.00	34.20	C
	ATOM	531	CD1	LEU A 76	5.497	17.200	11.027	1.00	35.60	C
	ATOM	532	CD2	LEU A 76	6.061	16.318	13.269	1.00	35.28	C
	ATOM	533	C	LEU A 76	10.289	16.158	11.975	1.00	33.25	C
	ATOM	534	O	LEU A 76	10.750	16.842	11.062	1.00	32.94	O
15	ATOM	535	N	HIS A 77	10.895	15.068	12.437	1.00	32.66	N
	ATOM	536	CA	HIS A 77	12.246	14.708	11.988	1.00	31.87	C
	ATOM	537	CB	HIS A 77	13.299	15.585	12.685	1.00	32.60	C
	ATOM	538	CG	HIS A 77	13.301	15.461	14.179	1.00	35.67	C
	ATOM	539	ND1	HIS A 77	13.038	16.524	15.013	1.00	39.46	N
20	ATOM	540	CE1	HIS A 77	13.118	16.124	16.271	1.00	39.61	C
	ATOM	541	NE2	HIS A 77	13.417	14.838	16.281	1.00	39.78	N
	ATOM	542	CD2	HIS A 77	13.534	14.399	14.987	1.00	37.66	C
	ATOM	543	C	HIS A 77	12.570	13.243	12.226	1.00	30.34	C
	ATOM	544	O	HIS A 77	11.818	12.526	12.893	1.00	29.57	O
25	ATOM	545	N	ILE A 78	13.703	12.822	11.673	1.00	29.01	N
	ATOM	546	CA	ILE A 78	14.213	11.460	11.825	1.00	28.36	C
	ATOM	547	CB	ILE A 78	14.282	10.746	10.461	1.00	27.61	C
	ATOM	548	CG1	ILE A 78	12.877	10.686	9.807	1.00	27.52	C
	ATOM	549	CD1	ILE A 78	12.866	10.349	8.347	1.00	28.83	C
30	ATOM	550	CG2	ILE A 78	14.962	9.376	10.594	1.00	27.01	C
	ATOM	551	C	ILE A 78	15.621	11.513	12.438	1.00	28.25	C
	ATOM	552	O	ILE A 78	16.466	12.281	11.971	1.00	28.93	O
	ATOM	553	N	ASN A 79	15.866	10.711	13.473	1.00	28.07	N
	ATOM	554	CA	ASN A 79	17.221	10.538	14.012	1.00	27.88	C
35	ATOM	555	CB	ASN A 79	17.303	10.867	15.506	1.00	28.35	C

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	ATOM	556	CG	ASN A 79	16.952	12.307	15.832	1.00	28.55	C
	ATOM	557	OD1	ASN A 79	16.474	12.588	16.929	1.00	32.79	O
	ATOM	558	ND2	ASN A 79	17.204	13.218	14.912	1.00	29.53	N
	ATOM	559	C	ASN A 79	17.756	9.129	13.792	1.00	27.76	C
5	ATOM	560	O	ASN A 79	17.036	8.139	13.968	1.00	27.50	O
	ATOM	561	N	LEU A 80	19.030	9.046	13.416	1.00	27.82	N
	ATOM	562	CA	LEU A 80	19.726	7.765	13.338	1.00	27.47	C
	ATOM	563	CB	LEU A 80	20.319	7.576	11.942	1.00	27.83	C
	ATOM	564	CG	LEU A 80	19.394	7.718	10.730	1.00	27.37	C
10	ATOM	565	CD1	LEU A 80	20.198	7.472	9.451	1.00	29.41	C
	ATOM	566	CD2	LEU A 80	18.176	6.785	10.827	1.00	26.78	C
	ATOM	567	C	LEU A 80	20.825	7.687	14.407	1.00	27.78	C
	ATOM	568	O	LEU A 80	21.653	8.605	14.505	1.00	27.90	O
	ATOM	569	N	ILE A 81	20.831	6.597	15.185	1.00	27.41	N
15	ATOM	570	CA	ILE A 81	21.753	6.419	16.329	1.00	27.96	C
	ATOM	571	CB	ILE A 81	21.035	6.631	17.703	1.00	27.79	C
	ATOM	572	CG1	ILE A 81	20.171	7.904	17.687	1.00	29.25	C
	ATOM	573	CD1	ILE A 81	18.964	7.849	18.636	1.00	32.80	C
	ATOM	574	CG2	ILE A 81	22.067	6.697	18.866	1.00	28.16	C
20	ATOM	575	C	ILE A 81	22.434	5.035	16.314	1.00	28.40	C
	ATOM	576	O	ILE A 81	21.879	4.064	16.814	1.00	27.99	O
	ATOM	577	N	PRO A 82	23.634	4.947	15.721	1.00	28.95	N
	ATOM	578	CA	PRO A 82	24.413	3.707	15.765	1.00	29.91	C
	ATOM	579	CB	PRO A 82	25.415	3.875	14.607	1.00	29.51	C
25	ATOM	580	CG	PRO A 82	25.550	5.346	14.394	1.00	29.63	C
	ATOM	581	CD	PRO A 82	24.310	6.021	14.969	1.00	28.84	C
	ATOM	582	C	PRO A 82	25.115	3.555	17.129	1.00	30.16	C
	ATOM	583	O	PRO A 82	25.633	4.548	17.650	1.00	30.91	O
	ATOM	584	N	ASN A 83	25.089	2.348	17.704	1.00	31.05	N
30	ATOM	585	CA	ASN A 83	25.733	2.039	19.008	1.00	31.54	C
	ATOM	586	CB	ASN A 83	24.686	1.842	20.123	1.00	31.83	C
	ATOM	587	CG	ASN A 83	25.311	1.691	21.530	1.00	32.31	C
	ATOM	588	OD1	ASN A 83	26.383	1.111	21.703	1.00	32.08	O
	ATOM	589	ND2	ASN A 83	24.617	2.203	22.530	1.00	33.27	N
35	ATOM	590	C	ASN A 83	26.628	0.810	18.896	1.00	32.25	C

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	ATOM	591	O	ASN A 83	26.153	-0.340	18.921	1.00	31.50	O
	ATOM	592	N	LYS A 84	27.926	1.059	18.772	1.00	33.10	N
	ATOM	593	CA	LYS A 84	28.899	-0.007	18.546	1.00	34.55	C
	ATOM	594	CB	LYS A 84	30.240	0.579	18.092	1.00	34.53	C
5	ATOM	595	CG	LYS A 84	30.221	1.103	16.668	1.00	35.46	C
	ATOM	596	CD	LYS A 84	31.548	1.721	16.288	1.00	37.36	C
	ATOM	597	CE	LYS A 84	31.564	2.077	14.810	1.00	39.49	C
	ATOM	598	NZ	LYS A 84	32.797	2.817	14.434	1.00	39.33	N
	ATOM	599	C	LYS A 84	29.082	-0.874	19.788	1.00	35.11	C
10	ATOM	600	O	LYS A 84	29.432	-2.043	19.686	1.00	35.72	O
	ATOM	601	N	GLN A 85	28.849	-0.285	20.955	1.00	35.72	N
	ATOM	602	CA	GLN A 85	28.874	-1.015	22.215	1.00	36.60	C
	ATOM	603	CB	GLN A 85	28.799	-0.027	23.377	1.00	36.88	C
	ATOM	604	CG	GLN A 85	29.619	-0.417	24.581	1.00	39.44	C
15	ATOM	605	CD	GLN A 85	29.584	0.634	25.659	1.00	42.55	C
	ATOM	606	OE1	GLN A 85	28.945	0.452	26.695	1.00	44.46	O
	ATOM	607	NE2	GLN A 85	30.258	1.756	25.419	1.00	43.80	N
	ATOM	608	C	GLN A 85	27.720	-2.030	22.292	1.00	36.55	C
	ATOM	609	O	GLN A 85	27.934	-3.181	22.679	1.00	36.76	O
20	ATOM	610	N	ASP A 86	26.519	-1.593	21.893	1.00	36.11	N
	ATOM	611	CA	ASP A 86	25.285	-2.396	21.925	1.00	36.14	C
	ATOM	612	CB	ASP A 86	24.050	-1.474	21.917	1.00	36.98	C
	ATOM	613	CG	ASP A 86	23.607	-1.052	23.299	1.00	40.60	C
	ATOM	614	OD1	ASP A 86	24.265	-1.431	24.302	1.00	44.27	O
25	ATOM	615	OD2	ASP A 86	22.586	-0.326	23.380	1.00	43.70	O
	ATOM	616	C	ASP A 86	25.131	-3.289	20.707	1.00	34.60	C
	ATOM	617	O	ASP A 86	24.341	-4.236	20.731	1.00	34.24	O
	ATOM	618	N	ARG A 87	25.869	-2.950	19.646	1.00	32.56	N
	ATOM	619	CA	ARG A 87	25.642	-3.431	18.284	1.00	31.17	C
30	ATOM	620	CB	ARG A 87	26.072	-4.890	18.098	1.00	31.06	C
	ATOM	621	CG	ARG A 87	26.476	-5.187	16.655	1.00	32.65	C
	ATOM	622	CD	ARG A 87	26.249	-6.643	16.296	1.00	37.41	C
	ATOM	623	NE	ARG A 87	27.155	-7.536	17.013	1.00	39.24	N
	ATOM	624	CZ	ARG A 87	26.946	-8.841	17.181	1.00	39.02	C
35	ATOM	625	NH1	ARG A 87	25.846	-9.426	16.699	1.00	37.25	N

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	ATOM	626	NH2 ARG A 87	27.839	-9.560	17.842	1.00	38.26	N
	ATOM	627	C ARG A 87	24.193	-3.196	17.817	1.00	30.43	C
	ATOM	628	O ARG A 87	23.535	-4.096	17.258	1.00	29.35	O
	ATOM	629	N THR A 88	23.688	-1.996	18.071	1.00	28.50	N
5	ATOM	630	CA THR A 88	22.349	-1.649	17.604	1.00	28.62	C
	ATOM	631	CB THR A 88	21.373	-1.363	18.775	1.00	28.64	C
	ATOM	632	OG1 THR A 88	21.855	-0.254	19.537	1.00	27.22	O
	ATOM	633	CG2 THR A 88	21.216	-2.580	19.674	1.00	28.29	C
	ATOM	634	C THR A 88	22.396	-0.407	16.747	1.00	28.50	C
10	ATOM	635	O THR A 88	23.202	0.496	16.988	1.00	28.64	O
	ATOM	636	N LEU A 89	21.533	-0.369	15.741	1.00	28.96	N
	ATOM	637	CA LEU A 89	21.251	0.850	15.017	1.00	29.07	C
	ATOM	638	CB LEU A 89	21.504	0.668	13.509	1.00	29.79	C
	ATOM	639	CG BLEU A 89	21.461	1.864	12.545	0.35	29.32	C
15	ATOM	640	CG ALEU A 89	21.050	1.752	12.517	0.65	29.90	C
	ATOM	641	CD1 BLEU A 89	20.089	1.997	11.910	0.35	28.70	C
	ATOM	642	CD1 ALEU A 89	21.804	3.062	12.737	0.65	30.70	C
	ATOM	643	CD2 BLEU A 89	21.893	3.174	13.203	0.35	29.28	C
	ATOM	644	CD2 ALEU A 89	21.204	1.280	11.067	0.65	29.34	C
20	ATOM	645	C LEU A 89	19.793	1.198	15.317	1.00	28.94	C
	ATOM	646	O LEU A 89	18.887	0.372	15.140	1.00	27.51	O
	ATOM	647	N THR A 90	19.591	2.416	15.803	1.00	28.32	N
	ATOM	648	CA THR A 90	18.277	2.859	16.211	1.00	28.59	C
	ATOM	649	CB THR A 90	18.311	3.355	17.666	1.00	28.69	C
25	ATOM	650	OG1 THR A 90	18.658	2.269	18.538	1.00	29.61	O
	ATOM	651	CG2 THR A 90	16.945	3.947	18.083	1.00	27.28	C
	ATOM	652	C THR A 90	17.793	3.954	15.263	1.00	28.77	C
	ATOM	653	O THR A 90	18.542	4.882	14.937	1.00	29.03	O
	ATOM	654	N ILE A 91	16.551	3.827	14.804	1.00	28.60	N
30	ATOM	655	CA ILE A 91	15.929	4.835	13.966	1.00	29.21	C
	ATOM	656	CB ILE A 91	15.480	4.268	12.580	1.00	29.13	C
	ATOM	657	CG1 ILE A 91	16.656	3.631	11.830	1.00	29.99	C
	ATOM	658	CD1 ILE A 91	16.719	2.134	12.011	1.00	30.52	C
	ATOM	659	CG2 ILE A 91	14.805	5.342	11.744	1.00	29.94	C
35	ATOM	660	C ILE A 91	14.718	5.411	14.692	1.00	29.13	C

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	ATOM	661	O	ILE A 91	13.780	4.670	15.043	1.00	29.24	O
	ATOM	662	N	VAL A 92	14.735	6.727	14.893	1.00	28.69	N
	ATOM	663	CA	VAL A 92	13.678	7.400	15.653	1.00	29.28	C
	ATOM	664	CB	VAL A 92	14.217	8.069	16.954	1.00	29.38	C
5	ATOM	665	CG1	VAL A 92	13.062	8.704	17.753	1.00	29.81	C
	ATOM	666	CG2	VAL A 92	14.966	7.073	17.821	1.00	30.79	C
	ATOM	667	C	VAL A 92	12.991	8.461	14.805	1.00	28.64	C
	ATOM	668	O	VAL A 92	13.659	9.266	14.147	1.00	28.05	O
	ATOM	669	N	ASP A 93	11.658	8.465	14.821	1.00	28.15	N
10	ATOM	670	CA	ASP A 93	10.901	9.566	14.216	1.00	27.71	C
	ATOM	671	CB	ASP A 93	10.233	9.150	12.894	1.00	27.75	C
	ATOM	672	CG	ASP A 93	9.122	8.125	13.092	1.00	28.69	C
	ATOM	673	OD1	ASP A 93	8.059	8.490	13.657	1.00	29.17	O
	ATOM	674	OD2	ASP A 93	9.322	6.955	12.696	1.00	27.08	O
15	ATOM	675	C	ASP A 93	9.880	10.169	15.181	1.00	27.32	C
	ATOM	676	O	ASP A 93	9.477	9.533	16.155	1.00	26.69	O
	ATOM	677	N	THR A 94	9.473	11.398	14.881	1.00	27.20	N
	ATOM	678	CA	THR A 94	8.408	12.083	15.618	1.00	27.14	C
	ATOM	679	CB	THR A 94	8.827	13.517	15.964	1.00	26.93	C
20	ATOM	680	OG1	THR A 94	9.435	14.114	14.824	1.00	26.39	O
	ATOM	681	CG2	THR A 94	9.865	13.504	17.095	1.00	27.85	C
	ATOM	682	C	THR A 94	7.102	12.052	14.802	1.00	27.06	C
	ATOM	683	O	THR A 94	6.334	13.018	14.777	1.00	26.77	O
	ATOM	684	N	GLY A 95	6.852	10.913	14.149	1.00	27.21	N
25	ATOM	685	CA	GLY A 95	5.655	10.736	13.317	1.00	27.35	C
	ATOM	686	C	GLY A 95	4.415	10.513	14.168	1.00	27.82	C
	ATOM	687	O	GLY A 95	4.440	10.703	15.388	1.00	27.81	O
	ATOM	688	N	ILE A 96	3.331	10.103	13.524	1.00	28.39	N
	ATOM	689	CA	ILE A 96	2.052	9.908	14.218	1.00	28.93	C
30	ATOM	690	CB	ILE A 96	0.856	9.802	13.213	1.00	28.61	C
	ATOM	691	CG1	ILE A 96	-0.475	10.081	13.938	1.00	28.31	C
	ATOM	692	CD1	ILE A 96	-1.681	10.181	13.024	1.00	29.05	C
	ATOM	693	CG2	ILE A 96	0.851	8.429	12.468	1.00	28.30	C
	ATOM	694	C	ILE A 96	2.076	8.735	15.212	1.00	29.32	C
35	ATOM	695	O	ILE A 96	1.285	8.688	16.158	1.00	30.02	O

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	ATOM	696	N	GLY A 97	3.004	7.803	15.013	1.00	29.58	N
	ATOM	697	CA	GLY A 97	3.132	6.662	15.903	1.00	29.90	C
	ATOM	698	C	GLY A 97	2.015	5.659	15.700	1.00	29.68	C
	ATOM	699	O	GLY A 97	1.217	5.785	14.761	1.00	30.39	O
5	ATOM	700	N	MET A 98	1.973	4.649	16.563	1.00	29.88	N
	ATOM	701	CA	MET A 98	0.982	3.574	16.451	1.00	29.68	C
	ATOM	702	CB	MET A 98	1.628	2.291	15.922	1.00	29.10	C
	ATOM	703	CG	MET A 98	2.173	2.385	14.503	1.00	30.48	C
	ATOM	704	SD	MET A 98	3.167	0.942	14.032	1.00	29.57	S
10	ATOM	705	CE	MET A 98	4.726	1.289	14.874	1.00	29.66	C
	ATOM	706	C	MET A 98	0.291	3.265	17.770	1.00	29.77	C
	ATOM	707	O	MET A 98	0.935	3.201	18.819	1.00	29.32	O
	ATOM	708	N	THR A 99	-1.024	3.054	17.695	1.00	29.87	N
	ATOM	709	CA	THR A 99	-1.807	2.584	18.825	1.00	31.29	C
15	ATOM	710	CB	THR A 99	-3.343	2.771	18.592	1.00	31.39	C
	ATOM	711	OG1	THR A 99	-3.775	1.955	17.502	1.00	31.39	O
	ATOM	712	CG2	THR A 99	-3.694	4.227	18.283	1.00	31.49	C
	ATOM	713	C	THR A 99	-1.493	1.101	19.058	1.00	32.17	C
	ATOM	714	O	THR A 99	-0.905	0.434	18.189	1.00	32.63	O
20	ATOM	715	N	LYS A 100	-1.886	0.579	20.213	1.00	33.14	N
	ATOM	716	CA	LYS A 100	-1.749	-0.846	20.471	1.00	33.45	C
	ATOM	717	CB	LYS A 100	-2.354	-1.215	21.826	1.00	33.71	C
	ATOM	718	CG	LYS A 100	-1.884	-2.562	22.340	1.00	34.64	C
	ATOM	719	CD	LYS A 100	-2.576	-2.915	23.647	1.00	36.44	C
25	ATOM	720	CE	LYS A 100	-2.504	-4.396	23.892	1.00	37.65	C
	ATOM	721	NZ	LYS A 100	-3.349	-4.780	25.058	1.00	38.04	N
	ATOM	722	C	LYS A 100	-2.385	-1.682	19.343	1.00	33.64	C
	ATOM	723	O	LYS A 100	-1.772	-2.633	18.844	1.00	33.95	O
	ATOM	724	N	ALA A 101	-3.599	-1.315	18.933	1.00	34.20	N
30	ATOM	725	CA	ALA A 101	-4.295	-2.029	17.854	1.00	34.02	C
	ATOM	726	CB	ALA A 101	-5.699	-1.500	17.670	1.00	34.75	C
	ATOM	727	C	ALA A 101	-3.526	-1.974	16.534	1.00	34.10	C
	ATOM	728	O	ALA A 101	-3.382	-3.000	15.859	1.00	33.46	O
	ATOM	729	N	ASP A 102	-3.021	-0.786	16.183	1.00	33.84	N
35	ATOM	730	CA	ASP A 102	-2.173	-0.626	14.996	1.00	34.40	C

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	ATOM	731	CB	ASP	A 102	-1.604	0.796	14.890	1.00	35.03	C
	ATOM	732	CG	ASP	A 102	-2.669	1.854	14.637	1.00	37.26	C
	ATOM	733	OD1	ASP	A 102	-3.749	1.524	14.087	1.00	39.89	O
	ATOM	734	OD2	ASP	A 102	-2.419	3.037	14.986	1.00	39.91	O
5	ATOM	735	C	ASP	A 102	-1.021	-1.627	14.987	1.00	33.64	C
	ATOM	736	O	ASP	A 102	-0.793	-2.302	13.983	1.00	34.05	O
	ATOM	737	N	LEU	A 103	-0.290	-1.712	16.099	1.00	33.47	N
	ATOM	738	CA	LEU	A 103	0.849	-2.623	16.210	1.00	32.76	C
	ATOM	739	CB	LEU	A 103	1.484	-2.551	17.602	1.00	32.94	C
10	ATOM	740	CG	LEU	A 103	2.519	-1.491	17.958	1.00	33.26	C
	ATOM	741	CD1	LEU	A 103	2.913	-1.669	19.408	1.00	31.65	C
	ATOM	742	CD2	LEU	A 103	3.752	-1.575	17.027	1.00	32.89	C
	ATOM	743	C	LEU	A 103	0.460	-4.062	15.951	1.00	32.49	C
	ATOM	744	O	LEU	A 103	1.053	-4.733	15.114	1.00	32.15	O
15	ATOM	745	N	ILE	A 104	-0.538	-4.530	16.695	1.00	31.99	N
	ATOM	746	CA	ILE	A 104	-0.843	-5.950	16.760	1.00	32.33	C
	ATOM	747	CB	ILE	A 104	-1.873	-6.255	17.857	1.00	32.32	C
	ATOM	748	CG1	ILE	A 104	-1.211	-6.168	19.241	1.00	32.19	C
	ATOM	749	CD1	ILE	A 104	-2.185	-5.772	20.354	1.00	33.24	C
20	ATOM	750	CG2	ILE	A 104	-2.504	-7.612	17.614	1.00	32.02	C
	ATOM	751	C	ILE	A 104	-1.666	-6.022	15.194	0.00	51.96	C
	ATOM	752	O	ILE	A 104	-0.983	-7.298	14.558	1.00	32.67	O
	ATOM	753	N	ASN	A 105	-2.418	-5.497	14.597	1.00	34.09	N
	ATOM	754	CA	ASN	A 105	-3.072	-5.607	13.293	1.00	34.53	C
25	ATOM	755	CB	ASN	A 105	-4.209	-4.591	13.149	1.00	34.19	C
	ATOM	756	CG	ASN	A 105	-5.352	-4.845	14.125	1.00	35.65	C
	ATOM	757	OD1	ASN	A 105	-5.578	-5.974	14.549	1.00	35.75	O
	ATOM	758	ND2	ASN	A 105	-6.071	-3.787	14.486	1.00	36.00	N
	ATOM	759	C	ASN	A 105	-2.079	-5.454	12.151	1.00	34.17	C
30	ATOM	760	O	ASN	A 105	-1.988	-6.327	11.293	1.00	34.30	O
	ATOM	761	N	ASN	A 106	-1.327	-4.355	12.164	1.00	34.55	N
	ATOM	762	CA	ASN	A 106	-0.477	-3.969	11.027	1.00	34.78	C
	ATOM	763	CB	ASN	A 106	-0.492	-2.436	10.819	1.00	35.15	C
	ATOM	764	CG	ASN	A 106	-1.905	-1.877	10.664	1.00	37.59	C
35	ATOM	765	OD1	ASN	A 106	-2.790	-2.545	10.126	1.00	39.75	O

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	ATOM	766	ND2 ASN A 106	-2.122	-0.647	11.144	1.00	38.59	N
	ATOM	767	C ASN A 106	0.959	-4.484	11.050	1.00	34.81	C
	ATOM	768	O ASN A 106	1.626	-4.462	10.013	1.00	34.39	O
	ATOM	769	N LEU A 107	1.450	-4.911	12.216	1.00	34.86	N
5	ATOM	770	CA LEU A 107	2.799	-5.496	12.306	1.00	35.14	C
	ATOM	771	CB LEU A 107	3.707	-4.702	13.255	1.00	35.39	C
	ATOM	772	CG LEU A 107	4.462	-3.469	12.764	1.00	36.19	C
	ATOM	773	CD1 LEU A 107	5.613	-3.190	13.710	1.00	36.39	C
	ATOM	774	CD2 LEU A 107	4.965	-3.616	11.325	1.00	36.39	C
10	ATOM	775	C LEU A 107	2.820	-6.975	12.700	1.00	35.01	C
	ATOM	776	O LEU A 107	3.649	-7.402	13.509	1.00	34.99	O
	ATOM	777	N GLY A 108	1.931	-7.768	12.119	1.00	34.87	N
	ATOM	778	CA GLY A 108	2.060	-9.210	12.279	1.00	34.73	C
	ATOM	779	C GLY A 108	0.850	-10.099	12.086	1.00	35.02	C
15	ATOM	780	O GLY A 108	0.954	-11.136	11.442	1.00	34.38	O
	ATOM	781	N THR A 109	-0.288	-9.718	12.664	1.00	35.05	N
	ATOM	782	CA THR A 109	-1.428	-10.634	12.734	1.00	35.55	C
	ATOM	783	CB THR A 109	-2.311	-10.369	13.979	1.00	35.30	C
	ATOM	784	OG1 THR A 109	-2.809	-9.027	13.918	1.00	35.34	O
20	ATOM	785	CG2 THR A 109	-1.504	-10.566	15.284	1.00	35.62	C
	ATOM	786	C THR A 109	-2.312	-10.666	11.479	1.00	36.20	C
	ATOM	787	O THR A 109	-2.903	-11.702	11.180	1.00	36.21	O
	ATOM	788	N ILE A 110	-2.417	-9.544	10.770	1.00	37.06	N
	ATOM	789	CA ILE A 110	-3.319	-9.449	9.610	1.00	38.28	C
25	ATOM	790	CB ILE A 110	-4.135	-8.120	9.606	1.00	38.52	C
	ATOM	791	CG1 ILE A 110	-5.010	-8.000	10.870	1.00	38.57	C
	ATOM	792	CD1 ILE A 110	-6.051	-9.116	11.059	1.00	38.96	C
	ATOM	793	CG2 ILE A 110	-4.981	-7.982	8.321	1.00	37.90	C
	ATOM	794	C ILE A 110	-2.561	-9.595	8.292	1.00	39.19	C
30	ATOM	795	O ILE A 110	-1.549	-8.914	8.061	1.00	38.85	O
	ATOM	796	N ALA A 111	-3.069	-10.477	7.432	1.00	40.36	N
	ATOM	797	CA ALA A 111	-2.472	-10.735	6.113	1.00	41.70	C
	ATOM	798	CB ALA A 111	-2.251	-12.195	5.650	0.00	38.32	C
	ATOM	799	C ALA A 111	-2.447	-9.483	5.231	1.00	42.48	C
35	ATOM	800	O ALA A 111	-3.356	-8.648	5.281	1.00	43.00	O

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	ATOM	801	N	LYS A 112	-1.390	-9.352	4.438	1.00	43.20	N
	ATOM	802	CA	LYS A 112	-1.258	-8.239	3.504	1.00	43.76	C
	ATOM	803	CB	LYS A 112	0.088	-7.523	3.698	1.00	44.16	C
	ATOM	804	CG	LYS A 112	0.252	-6.856	5.080	1.00	44.54	C
5	ATOM	805	CD	LYS A 112	-0.764	-5.729	5.271	1.00	45.67	C
	ATOM	806	CE	LYS A 112	-1.229	-5.621	6.711	1.00	46.86	C
	ATOM	807	NZ	LYS A 112	-2.686	-5.290	6.805	1.00	47.23	N
	ATOM	808	C	LYS A 112	-1.415	-8.732	2.070	1.00	44.03	C
	ATOM	809	O	LYS A 112	-0.933	-9.817	1.726	1.00	43.64	O
10	ATOM	810	N	SER A 113	-2.088	-7.926	1.243	1.00	44.20	N
	ATOM	811	CA	SER A 113	-2.378	-8.275	-0.156	1.00	44.53	C
	ATOM	812	CB	SER A 113	-3.149	-7.148	-0.853	1.00	44.59	C
	ATOM	813	OG	SER A 113	-4.460	-7.020	-0.334	1.00	45.38	O
	ATOM	814	C	SER A 113	-1.134	-8.629	-0.977	1.00	44.45	C
15	ATOM	815	O	SER A 113	-1.185	-9.492	-1.860	1.00	44.03	O
	ATOM	816	N	GLY A 114	-0.021	-7.968	-0.672	1.00	44.33	N
	ATOM	817	CA	GLY A 114	1.204	-8.138	-1.438	1.00	44.07	C
	ATOM	818	C	GLY A 114	2.136	-9.252	-1.001	1.00	43.78	C
	ATOM	819	O	GLY A 114	3.114	-9.531	-1.691	1.00	43.67	O
20	ATOM	820	N	THR A 115	1.838	-9.901	0.123	1.00	43.92	N
	ATOM	821	CA	THR A 115	2.774	-10.876	0.715	1.00	43.94	C
	ATOM	822	CB	THR A 115	2.319	-11.354	2.114	1.00	43.98	C
	ATOM	823	OG1	THR A 115	1.869	-10.232	2.883	1.00	42.24	O
	ATOM	824	CG2	THR A 115	3.476	-12.023	2.849	1.00	43.97	C
25	ATOM	825	C	THR A 115	3.111	-12.070	-0.195	1.00	44.30	C
	ATOM	826	O	THR A 115	4.264	-12.236	-0.591	1.00	44.25	O
	ATOM	827	N	LYS A 116	2.114	-12.887	-0.535	1.00	44.90	N
	ATOM	828	CA	LYS A 116	2.350	-14.048	-1.398	1.00	45.27	C
	ATOM	829	CB	LYS A 116	1.182	-15.065	-1.381	1.00	45.64	C
30	ATOM	830	CG	LYS A 116	-0.201	-14.500	-1.074	1.00	46.73	C
	ATOM	831	CD	LYS A 116	-0.323	-14.077	0.396	1.00	48.47	C
	ATOM	832	CE	LYS A 116	-1.198	-12.846	0.568	1.00	48.28	C
	ATOM	833	NZ	LYS A 116	-0.737	-11.730	-0.293	1.00	48.89	N
	ATOM	834	C	LYS A 116	2.746	-13.631	-2.812	1.00	45.18	C
35	ATOM	835	O	LYS A 116	3.545	-14.306	-3.462	1.00	45.39	O

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	ATOM	836	N	ALA A 117	2.220 -12.498 -3.269	1.00 45.39	N
	ATOM	837	CA	ALA A 117	2.650 -11.906 -4.531	1.00 45.30	C
	ATOM	838	CB	ALA A 117	1.849 -10.641 -4.835	1.00 45.42	C
	ATOM	839	C	ALA A 117	4.150 -11.608 -4.517	1.00 45.32	C
5	ATOM	840	O	ALA A 117	4.850 -11.891 -5.493	1.00 45.43	O
	ATOM	841	N	PHE A 118	4.641 -11.048 -3.411	1.00 45.21	N
	ATOM	842	CA	PHE A 118	6.063 -10.711 -3.298	1.00 45.11	C
	ATOM	843	CB	PHE A 118	6.328 -9.749 -2.134	1.00 44.92	C
	ATOM	844	CG	PHE A 118	7.766 -9.328 -2.027	1.00 44.19	C
10	ATOM	845	CD1	PHE A 118	8.407 -8.722 -3.108	1.00 44.15	C
	ATOM	846	CE1	PHE A 118	9.737 -8.349 -3.031	1.00 43.52	C
	ATOM	847	CZ	PHE A 118	10.446 -8.572 -1.853	1.00 44.51	C
	ATOM	848	CE2	PHE A 118	9.814 -9.173 -0.759	1.00 43.89	C
	ATOM	849	CD2	PHE A 118	8.483 -9.552 -0.857	1.00 44.29	C
15	ATOM	850	C	PHE A 118	6.970 -11.938 -3.196	1.00 45.32	C
	ATOM	851	O	PHE A 118	7.993 -12.012 -3.878	1.00 45.17	O
	ATOM	852	N	MET A 119	6.593 -12.883 -2.339	1.00 45.52	N
	ATOM	853	CA	MET A 119	7.329 -14.142 -2.193	1.00 46.27	C
	ATOM	854	CB	MET A 119	6.647 -15.051 -1.170	1.00 46.14	C
20	ATOM	855	CG	MET A 119	6.626 -14.490 0.244	1.00 46.40	C
	ATOM	856	SD	MET A 119	6.307 -15.740 1.505	1.00 45.93	S
	ATOM	857	CE	MET A 119	4.522 -15.941 1.394	1.00 47.28	C
	ATOM	858	C	MET A 119	7.479 -14.883 -3.524	1.00 46.80	C
	ATOM	859	O	MET A 119	8.548 -15.417 -3.832	1.00 46.83	O
25	ATOM	860	N	GLU A 120	6.404 -14.913 -4.310	1.00 47.08	N
	ATOM	861	CA	GLU A 120	6.438 -15.586 -5.598	1.00 47.78	C
	ATOM	862	CB	GLU A 120	5.021 -15.789 -6.149	1.00 47.57	C
	ATOM	863	CG	GLU A 120	4.224 -16.838 -5.366	1.00 48.06	C
	ATOM	864	CD	GLU A 120	2.726 -16.851 -5.670	1.00 48.20	C
30	ATOM	865	OE1	GLU A 120	2.018 -17.686 -5.070	1.00 48.94	O
	ATOM	866	OE2	GLU A 120	2.251 -16.044 -6.495	1.00 48.80	O
	ATOM	867	C	GLU A 120	7.325 -14.807 -6.563	1.00 48.12	C
	ATOM	868	O	GLU A 120	8.020 -15.399 -7.391	1.00 47.92	O
	ATOM	869	N	ALA A 121	7.325 -13.481 -6.422	1.00 48.84	N
35	ATOM	870	CA	ALA A 121	8.172 -12.616 -7.248	1.00 49.44	C

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	ATOM	871	CB	ALA A 121	7.817 -11.147 -7.036	1.00 49.29	C
	ATOM	872	C	ALA A 121	9.667 -12.864 -7.014	1.00 50.11	C
	ATOM	873	O	ALA A 121	10.429 -12.983 -7.974	1.00 50.23	O
	ATOM	874	N	LEU A 122	10.086 -12.952 -5.751	1.00 50.87	N
5	ATOM	875	CA	LEU A 122	11.506 -13.177 -5.450	1.00 51.79	C
	ATOM	876	CB	LEU A 122	11.906 -12.657 -4.055	1.00 51.84	C
	ATOM	877	CG	LEU A 122	11.111 -12.912 -2.768	1.00 52.44	C
	ATOM	878	CD1	LEU A 122	11.103 -14.379 -2.384	1.00 52.68	C
	ATOM	879	CD2	LEU A 122	11.710 -12.084 -1.641	1.00 51.81	C
10	ATOM	880	C	LEU A 122	11.963 -14.622 -5.685	1.00 52.22	C
	ATOM	881	O	LEU A 122	13.157 -14.872 -5.866	1.00 52.50	O
	ATOM	882	N	GLN A 123	11.012 -15.559 -5.684	1.00 52.63	N
	ATOM	883	CA	GLN A 123	11.277 -16.939 -6.102	1.00 53.08	C
	ATOM	884	CB	GLN A 123	10.157 -17.881 -5.648	1.00 53.07	C
15	ATOM	885	CG	GLN A 123	10.270 -18.281 -4.170	1.00 54.04	C
	ATOM	886	CD	GLN A 123	8.935 -18.572 -3.497	1.00 55.17	C
	ATOM	887	OE1	GLN A 123	8.863 -18.688 -2.271	1.00 55.84	O
	ATOM	888	NE2	GLN A 123	7.873 -18.694 -4.290	1.00 55.96	N
	ATOM	889	C	GLN A 123	11.482 -16.996 -7.615	1.00 53.07	C
20	ATOM	890	O	GLN A 123	12.207 -17.852 -8.119	1.00 53.26	O
	ATOM	891	N	ALA A 124	10.852 -16.064 -8.328	1.00 53.11	N
	ATOM	892	CA	ALA A 124	11.128 -15.851 -9.748	1.00 53.08	C
	ATOM	893	CB	ALA A 124	9.972 -15.119 -10.416	1.00 52.93	C
	ATOM	894	C	ALA A 124	12.447 -15.091 -9.946	1.00 53.00	C
25	ATOM	895	O	ALA A 124	12.854 -14.830 -11.078	1.00 53.47	O
	ATOM	896	N	GLY A 125	13.109 -14.748 -8.838	1.00 52.76	N
	ATOM	897	CA	GLY A 125	14.425 -14.108 -8.866	1.00 52.08	C
	ATOM	898	C	GLY A 125	14.417 -12.589 -8.867	1.00 51.55	C
	ATOM	899	O	GLY A 125	15.377 -11.966 -9.327	1.00 51.83	O
30	ATOM	900	N	ALA A 126	13.344 -11.992 -8.348	1.00 50.92	N
	ATOM	901	CA	ALA A 126	13.216 -10.529 -8.295	1.00 49.84	C
	ATOM	902	CB	ALA A 126	12.547 -9.767 -9.042	0.00 49.51	C
	ATOM	903	C	ALA A 126	14.141 -9.946 -7.227	1.00 49.17	C
	ATOM	904	O	ALA A 126	14.495 -10.634 -6.271	1.00 49.12	O
35	ATOM	905	N	ASP A 127	14.532 -8.683 -7.410	1.00 48.27	N

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	ATOM	906	CA	ASP A 127	15.357	-7.948	-6.444	1.00	47.43	C
	ATOM	907	CB	ASP A 127	15.745	-6.581	-7.029	1.00	47.65	C
	ATOM	908	CG	ASP A 127	16.938	-5.940	-6.325	1.00	48.70	C
	ATOM	909	OD1	ASP A 127	16.952	-5.851	-5.075	1.00	47.44	O
5	ATOM	910	OD2	ASP A 127	17.862	-5.488	-7.043	1.00	50.36	O
	ATOM	911	C	ASP A 127	14.581	-7.752	-5.136	1.00	46.46	C
	ATOM	912	O	ASP A 127	13.386	-7.442	-5.162	1.00	46.18	O
	ATOM	913	N	ILE A 128	15.265	-7.925	-4.002	1.00	45.18	N
	ATOM	914	CA	ILE A 128	14.665	-7.688	-2.680	1.00	43.86	C
10	ATOM	915	CB	ILE A 128	15.650	-8.054	-1.519	1.00	43.88	C
	ATOM	916	CG1	ILE A 128	14.913	-8.211	-0.188	1.00	43.59	C
	ATOM	917	CD1	ILE A 128	14.265	-9.563	0.002	1.00	43.20	C
	ATOM	918	CG2	ILE A 128	16.798	-7.050	-1.406	1.00	43.57	C
	ATOM	919	C	ILE A 128	14.177	-6.241	-2.543	1.00	43.17	C
15	ATOM	920	O	ILE A 128	13.284	-5.949	-1.744	1.00	42.05	O
	ATOM	921	N	SER A 129	14.766	-5.357	-3.349	1.00	42.70	N
	ATOM	922	CA	SER A 129	14.446	-3.925	-3.357	1.00	42.66	C
	ATOM	923	CB	SER A 129	15.337	-3.187	-4.369	1.00	42.83	C
	ATOM	924	OG	SER A 129	15.118	-1.784	-4.329	1.00	43.38	O
20	ATOM	925	C	SER A 129	12.973	-3.633	-3.654	1.00	42.27	C
	ATOM	926	O	SER A 129	12.485	-2.559	-3.311	1.00	41.98	O
	ATOM	927	N	MET A 130	12.277	-4.587	-4.280	1.00	42.04	N
	ATOM	928	CA	MET A 130	10.864	-4.416	-4.657	1.00	42.39	C
	ATOM	929	CB	MET A 130	10.491	-5.367	-5.809	1.00	42.75	C
25	ATOM	930	CG	MET A 130	11.008	-4.908	-7.187	1.00	43.40	C
	ATOM	931	SD	MET A 130	10.915	-6.187	-8.464	1.00	47.04	S
	ATOM	932	CE	MET A 130	9.112	-6.220	-8.631	0.00	58.42	C
	ATOM	933	C	MET A 130	9.889	-4.568	-3.477	1.00	40.81	C
	ATOM	934	O	MET A 130	8.695	-4.271	-3.609	1.00	40.15	O
30	ATOM	935	N	ILE A 131	10.418	-5.001	-2.328	1.00	39.11	N
	ATOM	936	CA	ILE A 131	9.636	-5.249	-1.097	1.00	38.04	C
	ATOM	937	CB	ILE A 131	10.581	-5.612	0.108	1.00	37.59	C
	ATOM	938	CG1	ILE A 131	9.794	-6.242	1.266	1.00	37.62	C
	ATOM	939	CD1	ILE A 131	10.665	-6.980	2.283	1.00	37.99	C
35	ATOM	940	CG2	ILE A 131	11.427	-4.403	0.554	1.00	36.63	C

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	ATOM	941	C	ILE A 131	8.642	-4.131	-0.715	1.00	37.50	C
	ATOM	942	O	ILE A 131	7.500	-4.408	-0.346	1.00	37.48	O
	ATOM	943	N	GLY A 132	9.081	-2.881	-0.825	1.00	37.08	N
	ATOM	944	CA	GLY A 132	8.275	-1.733	-0.415	1.00	37.22	C
5	ATOM	945	C	GLY A 132	7.019	-1.588	-1.254	1.00	36.97	C
	ATOM	946	O	GLY A 132	5.941	-1.304	-0.726	1.00	36.39	O
	ATOM	947	N	GLN A 133	7.171	-1.797	-2.562	1.00	36.95	N
	ATOM	948	CA	GLN A 133	6.050	-1.750	-3.518	1.00	37.59	C
	ATOM	949	CB	GLN A 133	6.556	-1.962	-4.943	1.00	37.62	C
10	ATOM	950	CG	GLN A 133	7.394	-0.808	-5.483	1.00	41.28	C
	ATOM	951	CD	GLN A 133	6.577	0.453	-5.694	1.00	45.04	C
	ATOM	952	OE1	GLN A 133	5.733	0.519	-6.592	1.00	47.25	O
	ATOM	953	NE2	GLN A 133	6.821	1.462	-4.863	1.00	47.27	N
	ATOM	954	C	GLN A 133	4.936	-2.762	-3.187	1.00	37.00	C
15	ATOM	955	O	GLN A 133	3.784	-2.576	-3.585	1.00	36.97	O
	ATOM	956	N	PHE A 134	5.289	-3.811	-2.445	1.00	36.43	N
	ATOM	957	CA	PHE A 134	4.341	-4.857	-2.060	1.00	36.10	C
	ATOM	958	CB	PHE A 134	5.000	-6.238	-2.166	1.00	36.34	C
	ATOM	959	CG	PHE A 134	5.225	-6.705	-3.589	1.00	37.37	C
20	ATOM	960	CD1	PHE A 134	4.423	-7.706	-4.144	1.00	38.29	C
	ATOM	961	CE1	PHE A 134	4.636	-8.156	-5.461	1.00	37.66	C
	ATOM	962	CZ	PHE A 134	5.639	-7.592	-6.231	1.00	38.10	C
	ATOM	963	CE2	PHE A 134	6.446	-6.582	-5.688	1.00	39.39	C
	ATOM	964	CD2	PHE A 134	6.237	-6.152	-4.372	1.00	37.89	C
25	ATOM	965	C	PHE A 134	3.744	-4.623	-0.667	1.00	35.73	C
	ATOM	966	O	PHE A 134	2.983	-5.459	-0.149	1.00	35.45	O
	ATOM	967	N	GLY A 135	4.079	-3.475	-0.074	1.00	34.96	N
	ATOM	968	CA	GLY A 135	3.519	-3.060	1.207	1.00	34.64	C
	ATOM	969	C	GLY A 135	4.003	-3.823	2.434	1.00	34.31	C
30	ATOM	970	O	GLY A 135	3.306	-3.847	3.455	1.00	34.79	O
	ATOM	971	N	VAL A 136	5.190	-4.430	2.340	1.00	33.10	N
	ATOM	972	CA	VAL A 136	5.792	-5.222	3.434	1.00	32.78	C
	ATOM	973	CB	VAL A 136	5.590	-6.748	3.221	1.00	32.35	C
	ATOM	974	CG1	VAL A 136	4.092	-7.119	3.340	1.00	32.83	C
35	ATOM	975	CG2	VAL A 136	6.166	-7.193	1.868	1.00	32.59	C

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	ATOM	976	C	VAL A 136	7.281	-4.901	3.678	1.00	32.17	C
	ATOM	977	O	VAL A 136	8.068	-5.755	4.148	1.00	31.82	O
	ATOM	978	N	GLY A 137	7.642	-3.656	3.371	1.00	31.77	N
	ATOM	979	CA	GLY A 137	8.989	-3.133	3.558	1.00	30.81	C
5	ATOM	980	C	GLY A 137	9.584	-3.272	4.947	1.00	30.08	C
	ATOM	981	O	GLY A 137	10.792	-3.491	5.072	1.00	30.15	O
	ATOM	982	N	PHE A 138	8.765	-3.143	5.998	1.00	29.38	N
	ATOM	983	CA	PHE A 138	9.274	-3.254	7.380	1.00	28.69	C
	ATOM	984	CB	PHE A 138	8.137	-3.266	8.420	1.00	29.35	C
10	ATOM	985	CG	PHE A 138	8.578	-3.726	9.790	1.00	29.01	C
	ATOM	986	CD1	PHE A 138	9.391	-2.909	10.588	1.00	28.46	C
	ATOM	987	CE1	PHE A 138	9.806	-3.321	11.848	1.00	29.49	C
	ATOM	988	CZ	PHE A 138	9.430	-4.576	12.329	1.00	30.52	C
	ATOM	989	CE2	PHE A 138	8.624	-5.408	11.548	1.00	28.81	C
15	ATOM	990	CD2	PHE A 138	8.206	-4.981	10.278	1.00	29.75	C
	ATOM	991	C	PHE A 138	10.123	-4.509	7.581	1.00	28.49	C
	ATOM	992	O	PHE A 138	11.146	-4.479	8.265	1.00	28.36	O
	ATOM	993	N	TYR A 139	9.678	-5.608	6.994	1.00	28.40	N
	ATOM	994	CA	TYR A 139	10.298	-6.907	7.238	1.00	27.90	C
20	ATOM	995	CB	TYR A 139	9.349	-8.042	6.844	1.00	27.81	C
	ATOM	996	CG	TYR A 139	8.058	-8.004	7.647	1.00	28.66	C
	ATOM	997	CD1	TYR A 139	8.017	-8.466	8.969	1.00	28.64	C
	ATOM	998	CE1	TYR A 139	6.826	-8.407	9.725	1.00	27.93	C
	ATOM	999	CZ	TYR A 139	5.675	-7.898	9.139	1.00	28.15	C
25	ATOM	1000	OH	TYR A 139	4.505	-7.828	9.881	1.00	28.76	O
	ATOM	1001	CE2	TYR A 139	5.701	-7.423	7.841	1.00	29.50	C
	ATOM	1002	CD2	TYR A 139	6.891	-7.481	7.095	1.00	29.05	C
	ATOM	1003	C	TYR A 139	11.702	-7.063	6.649	1.00	27.12	C
	ATOM	1004	O	TYR A 139	12.428	-8.004	7.011	1.00	27.71	O
30	ATOM	1005	N	SER A 140	12.099	-6.113	5.803	1.00	26.82	N
	ATOM	1006	CA	SER A 140	13.451	-6.055	5.265	1.00	25.92	C
	ATOM	1007	CB	SER A 140	13.592	-4.947	4.213	1.00	26.52	C
	ATOM	1008	OG	SER A 140	13.437	-3.663	4.803	1.00	26.60	O
	ATOM	1009	C	SER A 140	14.476	-5.823	6.386	1.00	25.21	C
35	ATOM	1010	O	SER A 140	15.668	-6.103	6.194	1.00	23.69	O

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	ATOM	1011	N	ALA A 141	14.009	-5.297	7.527	1.00	24.15	N
	ATOM	1012	CA	ALA A 141	14.848	-5.152	8.734	1.00	24.84	C
	ATOM	1013	CB	ALA A 141	14.014	-4.712	9.943	1.00	24.40	C
	ATOM	1014	C	ALA A 141	15.582	-6.447	9.056	1.00	24.84	C
5	ATOM	1015	O	ALA A 141	16.739	-6.428	9.519	1.00	25.56	O
	ATOM	1016	N	TYR A 142	14.896	-7.560	8.827	1.00	25.40	N
	ATOM	1017	CA	TYR A 142	15.438	-8.889	9.127	1.00	26.22	C
	ATOM	1018	CB	TYR A 142	14.304	-9.892	9.313	1.00	26.36	C
	ATOM	1019	CG	TYR A 142	13.560	-9.614	10.601	1.00	26.52	C
10	ATOM	1020	CD1	TYR A 142	14.077	-10.041	11.833	1.00	25.71	C
	ATOM	1021	CE1	TYR A 142	13.417	-9.760	13.030	1.00	28.68	C
	ATOM	1022	CZ	TYR A 142	12.235	-9.022	12.996	1.00	27.28	C
	ATOM	1023	OH	TYR A 142	11.580	-8.726	14.171	1.00	28.15	O
	ATOM	1024	CE2	TYR A 142	11.715	-8.564	11.784	1.00	28.03	C
15	ATOM	1025	CD2	TYR A 142	12.384	-8.849	10.598	1.00	26.82	C
	ATOM	1026	C	TYR A 142	16.520	-9.371	8.157	1.00	26.51	C
	ATOM	1027	O	TYR A 142	17.102	-10.459	8.353	1.00	26.58	O
	ATOM	1028	N	LEU A 143	16.796	-8.558	7.130	1.00	26.41	N
	ATOM	1029	CA	LEU A 143	17.965	-8.791	6.277	1.00	26.70	C
20	ATOM	1030	CB	LEU A 143	17.973	-7.895	5.036	1.00	26.52	C
	ATOM	1031	CG	LEU A 143	16.924	-8.098	3.933	1.00	27.28	C
	ATOM	1032	CD1	LEU A 143	16.860	-6.860	3.047	1.00	29.63	C
	ATOM	1033	CD2	LEU A 143	17.258	-9.338	3.128	1.00	26.97	C
	ATOM	1034	C	LEU A 143	19.265	-8.554	7.059	1.00	26.70	C
25	ATOM	1035	O	LEU A 143	20.256	-9.219	6.801	1.00	26.72	O
	ATOM	1036	N	VAL A 144	19.256	-7.571	7.957	1.00	26.32	N
	ATOM	1037	CA	VAL A 144	20.458	-7.198	8.730	1.00	27.09	C
	ATOM	1038	CB	VAL A 144	20.916	-5.717	8.467	1.00	26.91	C
	ATOM	1039	CG1	VAL A 144	21.195	-5.479	7.000	1.00	28.34	C
30	ATOM	1040	CG2	VAL A 144	19.902	-4.709	9.019	1.00	26.79	C
	ATOM	1041	C	VAL A 144	20.352	-7.401	10.249	1.00	26.57	C
	ATOM	1042	O	VAL A 144	21.384	-7.399	10.941	1.00	26.83	O
	ATOM	1043	N	ALA A 145	19.129	-7.540	10.775	1.00	26.99	N
	ATOM	1044	CA	ALA A 145	18.910	-7.682	12.216	1.00	26.55	C
35	ATOM	1045	CB	ALA A 145	17.953	-6.610	12.740	1.00	27.10	C

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	ATOM	1046	C	ALA A 145	18.411	-9.066	12.646	1.00	27.35	C
	ATOM	1047	O	ALA A 145	17.540	-9.649	12.001	1.00	27.36	O
	ATOM	1048	N	GLU A 146	18.959	-9.556	13.758	1.00	27.19	N
	ATOM	1049	CA	GLU A 146	18.526	-10.802	14.385	1.00	28.26	C
5	ATOM	1050	CB	GLU A 146	19.672	-11.459	15.179	1.00	28.19	C
	ATOM	1051	CG	GLU A 146	20.196	-10.685	16.395	1.00	29.84	C
	ATOM	1052	CD	GLU A 146	21.498	-11.256	16.941	1.00	30.32	C
	ATOM	1053	OE1	GLU A 146	22.068	-12.181	16.313	1.00	34.74	O
	ATOM	1054	OE2	GLU A 146	21.945	-10.793	18.014	1.00	33.23	O
10	ATOM	1055	C	GLU A 146	17.287	-10.616	15.262	1.00	28.15	C
	ATOM	1056	O	GLU A 146	16.551	-11.553	15.502	1.00	28.68	O
	ATOM	1057	N	LYS A 147	17.068	-9.387	15.714	1.00	28.34	N
	ATOM	1058	CA	LYS A 147	15.969	-9.047	16.609	1.00	28.46	C
	ATOM	1059	CB	LYS A 147	16.363	-9.281	18.081	1.00	28.31	C
15	ATOM	1060	CG	LYS A 147	15.272	-8.873	19.109	1.00	30.17	C
	ATOM	1061	CD	LYS A 147	15.583	-9.331	20.547	1.00	30.58	C
	ATOM	1062	CE	LYS A 147	16.629	-8.462	21.232	1.00	34.58	C
	ATOM	1063	NZ	LYS A 147	17.139	-9.076	22.489	1.00	35.40	N
	ATOM	1064	C	LYS A 147	15.667	-7.583	16.380	1.00	27.65	C
20	ATOM	1065	O	LYS A 147	16.586	-6.775	16.224	1.00	27.43	O
	ATOM	1066	N	VAL A 148	14.383	-7.249	16.324	1.00	26.61	N
	ATOM	1067	CA	VAL A 148	13.966	-5.869	16.131	1.00	25.71	C
	ATOM	1068	CB	VAL A 148	13.237	-5.675	14.770	1.00	25.09	C
	ATOM	1069	CG1	VAL A 148	12.698	-4.219	14.633	1.00	25.51	C
25	ATOM	1070	CG2	VAL A 148	14.168	-6.060	13.574	1.00	24.67	C
	ATOM	1071	C	VAL A 148	13.020	-5.522	17.271	1.00	26.05	C
	ATOM	1072	O	VAL A 148	12.141	-6.328	17.607	1.00	25.45	O
	ATOM	1073	N	THR A 149	13.211	-4.341	17.853	1.00	25.83	N
	ATOM	1074	CA	THR A 149	12.342	-3.828	18.906	1.00	27.09	C
30	ATOM	1075	CB	THR A 149	13.110	-3.534	20.225	1.00	26.79	C
	ATOM	1076	OG1	THR A 149	13.885	-4.673	20.598	1.00	27.90	O
	ATOM	1077	CG2	THR A 149	12.138	-3.168	21.384	1.00	27.27	C
	ATOM	1078	C	THR A 149	11.760	-2.542	18.358	1.00	27.31	C
	ATOM	1079	O	THR A 149	12.497	-1.695	17.828	1.00	27.69	O
35	ATOM	1080	N	VAL A 150	10.438	-2.431	18.419	1.00	27.37	N

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	ATOM	1081	CA	VAL A 150	9.748	-1.222	17.961	1.00	26.72	C
	ATOM	1082	CB	VAL A 150	8.745	-1.489	16.785	1.00	26.55	C
	ATOM	1083	CG1	VAL A 150	7.995	-0.206	16.408	1.00	27.71	C
	ATOM	1084	CG2	VAL A 150	9.449	-2.059	15.521	1.00	26.10	C
5	ATOM	1085	C	VAL A 150	9.055	-0.591	19.178	1.00	27.01	C
	ATOM	1086	O	VAL A 150	8.192	-1.214	19.809	1.00	26.78	O
	ATOM	1087	N	ILE A 151	9.454	0.642	19.477	1.00	27.32	N
	ATOM	1088	CA	ILE A 151	8.931	1.450	20.579	1.00	28.18	C
	ATOM	1089	CB	ILE A 151	10.074	2.124	21.388	1.00	29.01	C
10	ATOM	1090	CG1	ILE A 151	11.146	1.116	21.841	1.00	30.34	C
	ATOM	1091	CD1	ILE A 151	10.686	0.075	22.852	1.00	31.44	C
	ATOM	1092	CG2	ILE A 151	9.516	2.986	22.557	1.00	29.63	C
	ATOM	1093	C	ILE A 151	8.079	2.542	19.943	1.00	28.29	C
	ATOM	1094	O	ILE A 151	8.537	3.236	19.028	1.00	27.18	O
15	ATOM	1095	N	THR A 152	6.832	2.679	20.399	1.00	28.16	N
	ATOM	1096	CA	THR A 152	5.909	3.576	19.731	1.00	27.72	C
	ATOM	1097	CB	THR A 152	5.157	2.853	18.589	1.00	27.91	C
	ATOM	1098	OG1	THR A 152	4.632	3.813	17.658	1.00	26.57	O
	ATOM	1099	CG2	THR A 152	4.040	1.916	19.133	1.00	27.78	C
20	ATOM	1100	C	THR A 152	4.960	4.283	20.693	1.00	28.11	C
	ATOM	1101	O	THR A 152	4.540	3.712	21.710	1.00	27.07	O
	ATOM	1102	N	LYS A 153	4.669	5.540	20.364	1.00	28.33	N
	ATOM	1103	CA	LYS A 153	3.797	6.405	21.162	1.00	28.85	C
	ATOM	1104	CB	LYS A 153	4.628	7.323	22.063	1.00	29.04	C
25	ATOM	1105	CG	LYS A 153	3.823	8.295	22.920	1.00	28.59	C
	ATOM	1106	CD	LYS A 153	2.865	7.597	23.874	1.00	30.02	C
	ATOM	1107	CE	LYS A 153	2.164	8.607	24.806	1.00	30.10	C
	ATOM	1108	NZ	LYS A 153	1.058	9.290	24.082	1.00	30.22	N
	ATOM	1109	C	LYS A 153	2.900	7.219	20.238	1.00	29.47	C
30	ATOM	1110	O	LYS A 153	3.377	8.027	19.420	1.00	29.17	O
	ATOM	1111	N	HIS A 154	1.598	6.983	20.367	1.00	30.27	N
	ATOM	1112	CA	HIS A 154	0.577	7.663	19.580	1.00	31.15	C
	ATOM	1113	CB	HIS A 154	-0.318	6.609	18.919	1.00	31.37	C
	ATOM	1114	CG	HIS A 154	-1.300	7.155	17.923	1.00	32.22	C
35	ATOM	1115	ND1	HIS A 154	-2.381	7.931	18.284	1.00	33.83	N

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	ATOM	1116	CE1 HIS A 154	-3.090	8.226	17.209	1.00	33.88	C
	ATOM	1117	NE2 HIS A 154	-2.515	7.659	16.164	1.00	33.20	N
	ATOM	1118	CD2 HIS A 154	-1.401	6.974	16.585	1.00	33.06	C
	ATOM	1119	C HIS A 154	-0.219	8.544	20.554	1.00	31.83	C
5	ATOM	1120	O HIS A 154	-0.481	8.125	21.686	1.00	31.92	O
	ATOM	1121	N ASN A 155	-0.568	9.763	20.138	1.00	32.76	N
	ATOM	1122	CA ASN A 155	-1.453	10.624	20.930	1.00	33.65	C
	ATOM	1123	CB ASN A 155	-1.960	11.803	20.099	1.00	34.00	C
	ATOM	1124	CG ASN A 155	-0.881	12.826	19.797	1.00	33.98	C
10	ATOM	1125	OD1 ASN A 155	0.067	12.989	20.557	1.00	34.18	O
	ATOM	1126	ND2 ASN A 155	-1.036	13.537	18.680	1.00	35.71	N
	ATOM	1127	C ASN A 155	-2.651	9.816	21.457	1.00	34.57	C
	ATOM	1128	O ASN A 155	-3.206	8.972	20.738	1.00	34.26	O
	ATOM	1129	N ASP A 156	-3.026	10.065	22.714	1.00	35.71	N
15	ATOM	1130	CA ASP A 156	-4.207	9.437	23.332	1.00	37.07	C
	ATOM	1131	CB ASP A 156	-5.484	9.837	22.581	1.00	37.75	C
	ATOM	1132	CG ASP A 156	-5.571	11.333	22.342	1.00	39.40	C
	ATOM	1133	OD1 ASP A 156	-5.615	12.092	23.333	1.00	41.76	O
	ATOM	1134	OD2 ASP A 156	-5.579	11.747	21.162	1.00	41.89	O
20	ATOM	1135	C ASP A 156	-4.128	7.910	23.485	1.00	37.03	C
	ATOM	1136	O ASP A 156	-5.157	7.243	23.637	1.00	37.75	O
	ATOM	1137	N ASP A 157	-2.914	7.360	23.422	1.00	36.90	N
	ATOM	1138	CA ASP A 157	-2.655	5.979	23.840	1.00	36.34	C
	ATOM	1139	CB ASP A 157	-2.672	5.000	22.654	1.00	36.88	C
25	ATOM	1140	CG ASP A 157	-3.005	3.564	23.082	1.00	37.68	C
	ATOM	1141	OD1 ASP A 157	-3.066	3.296	24.302	1.00	39.18	O
	ATOM	1142	OD2 ASP A 157	-3.209	2.694	22.213	1.00	39.79	O
	ATOM	1143	C ASP A 157	-1.317	5.929	24.595	1.00	35.60	C
	ATOM	1144	O ASP A 157	-0.561	6.886	24.558	1.00	35.38	O
30	ATOM	1145	N GLU A 158	-1.047	4.828	25.286	1.00	34.73	N
	ATOM	1146	CA GLU A 158	0.198	4.665	26.033	1.00	34.34	C
	ATOM	1147	CB GLU A 158	0.037	3.576	27.091	1.00	34.93	C
	ATOM	1148	CG GLU A 158	-0.770	3.994	28.314	1.00	38.56	C
	ATOM	1149	CD GLU A 158	-0.782	2.917	29.377	1.00	43.25	C
35	ATOM	1150	OE1 GLU A 158	-1.095	1.748	29.044	1.00	45.50	O

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	ATOM	1151	OE2	GLU A 158	-0.467	3.242	30.542	1.00	46.13	O
	ATOM	1152	C	GLU A 158	1.350	4.293	25.101	1.00	32.90	C
	ATOM	1153	O	GLU A 158	1.128	3.986	23.932	1.00	32.55	O
	ATOM	1154	N	GLN A 159	2.572	4.319	25.634	1.00	31.93	N
5	ATOM	1155	CA	GLN A 159	3.761	3.873	24.904	1.00	31.46	C
	ATOM	1156	CB	GLN A 159	5.017	4.512	25.510	1.00	31.56	C
	ATOM	1157	CG	GLN A 159	6.346	4.134	24.858	1.00	32.00	C
	ATOM	1158	CD	GLN A 159	7.433	5.168	25.120	1.00	33.39	C
	ATOM	1159	OE1	GLN A 159	7.223	6.372	24.931	1.00	35.51	O
10	ATOM	1160	NE2	GLN A 159	8.606	4.702	25.555	1.00	34.51	N
	ATOM	1161	C	GLN A 159	3.848	2.344	24.961	1.00	31.27	C
	ATOM	1162	O	GLN A 159	3.716	1.747	26.034	1.00	31.28	O
	ATOM	1163	N	TYR A 160	4.069	1.720	23.809	1.00	30.96	N
	ATOM	1164	CA	TYR A 160	4.155	0.254	23.736	1.00	30.68	C
15	ATOM	1165	CB	TYR A 160	3.026	-0.296	22.868	1.00	31.99	C
	ATOM	1166	CG	TYR A 160	1.639	0.017	23.362	1.00	33.65	C
	ATOM	1167	CD1	TYR A 160	1.069	-0.713	24.405	1.00	35.91	C
	ATOM	1168	CE1	TYR A 160	-0.218	-0.428	24.862	1.00	37.04	C
	ATOM	1169	CZ	TYR A 160	-0.945	0.587	24.261	1.00	36.38	C
20	ATOM	1170	OH	TYR A 160	-2.216	0.861	24.702	1.00	37.56	O
	ATOM	1171	CE2	TYR A 160	-0.408	1.319	23.210	1.00	37.02	C
	ATOM	1172	CD2	TYR A 160	0.887	1.030	22.769	1.00	35.87	C
	ATOM	1173	C	TYR A 160	5.478	-0.184	23.120	1.00	29.62	C
	ATOM	1174	O	TYR A 160	6.092	0.573	22.356	1.00	28.60	O
25	ATOM	1175	N	ALA A 161	5.881	-1.412	23.438	1.00	28.18	N
	ATOM	1176	CA	ALA A 161	7.056	-2.040	22.850	1.00	27.70	C
	ATOM	1177	CB	ALA A 161	8.159	-2.245	23.893	1.00	27.60	C
	ATOM	1178	C	ALA A 161	6.674	-3.357	22.201	1.00	27.57	C
	ATOM	1179	O	ALA A 161	6.059	-4.231	22.835	1.00	27.86	O
30	ATOM	1180	N	TRP A 162	7.011	-3.456	20.917	1.00	28.05	N
	ATOM	1181	CA	TRP A 162	6.817	-4.649	20.081	1.00	27.44	C
	ATOM	1182	CB	TRP A 162	6.237	-4.192	18.745	1.00	27.93	C
	ATOM	1183	CG	TRP A 162	6.042	-5.181	17.592	1.00	27.84	C
	ATOM	1184	CD1	TRP A 162	4.839	-5.603	17.088	1.00	27.84	C
35	ATOM	1185	NE1	TRP A 162	5.031	-6.431	16.010	1.00	28.26	N

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	ATOM	1186	CE2 TRP A 162	6.377	-6.550	15.774	1.00	27.26	C
	ATOM	1187	CD2 TRP A 162	7.052	-5.759	16.740	1.00	26.98	C
	ATOM	1188	CE3 TRP A 162	8.455	-5.707	16.709	1.00	27.23	C
	ATOM	1189	CZ3 TRP A 162	9.133	-6.453	15.726	1.00	27.86	C
5	ATOM	1190	CH2 TRP A 162	8.430	-7.215	14.778	1.00	27.90	C
	ATOM	1191	CZ2 TRP A 162	7.055	-7.287	14.793	1.00	28.17	C
	ATOM	1192	C TRP A 162	8.214	-5.213	19.889	1.00	27.54	C
	ATOM	1193	O TRP A 162	9.170	-4.458	19.688	1.00	26.66	O
	ATOM	1194	N GLU A 163	8.342	-6.535	19.933	1.00	27.83	N
10	ATOM	1195	CA GLU A 163	9.649	-7.153	19.706	1.00	28.70	C
	ATOM	1196	CB GLU A 163	10.405	-7.277	21.037	1.00	28.27	C
	ATOM	1197	CG GLU A 163	11.920	-7.297	20.921	1.00	30.89	C
	ATOM	1198	CD GLU A 163	12.590	-7.306	22.294	1.00	31.37	C
	ATOM	1199	OE1 GLU A 163	12.373	-8.268	23.063	1.00	32.13	O
15	ATOM	1200	OE2 GLU A 163	13.312	-6.333	22.610	1.00	36.39	O
	ATOM	1201	C GLU A 163	9.507	-8.528	19.080	1.00	28.10	C
	ATOM	1202	O GLU A 163	8.610	-9.304	19.451	1.00	26.93	O
	ATOM	1203	N SER A 164	10.403	-8.828	18.138	1.00	27.57	N
	ATOM	1204	CA SER A 164	10.490	-10.169	17.599	1.00	27.69	C
20	ATOM	1205	CB SER A 164	9.523	-10.337	16.420	1.00	27.13	C
	ATOM	1206	OG SER A 164	9.640	-11.629	15.874	1.00	27.12	O
	ATOM	1207	C SER A 164	11.902	-10.538	17.163	1.00	28.17	C
	ATOM	1208	O SER A 164	12.611	-9.721	16.583	1.00	27.22	O
	ATOM	1209	N SER A 165	12.284	-11.785	17.437	1.00	29.64	N
25	ATOM	1210	CA SER A 165	13.483	-12.382	16.841	1.00	31.09	C
	ATOM	1211	CB SER A 165	14.275	-13.156	17.895	1.00	31.67	C
	ATOM	1212	OG SER A 165	14.737	-12.288	18.906	1.00	30.68	O
	ATOM	1213	C SER A 165	13.085	-13.302	15.687	1.00	32.42	C
	ATOM	1214	O SER A 165	13.847	-14.196	15.285	1.00	33.00	O
30	ATOM	1215	N ALA A 166	11.896	-13.051	15.138	1.00	33.23	N
	ATOM	1216	CA ALA A 166	11.252	-13.923	14.165	1.00	34.21	C
	ATOM	1217	CB ALA A 166	12.115	-14.095	12.888	1.00	34.20	C
	ATOM	1218	C ALA A 166	10.890	-15.268	14.805	1.00	34.66	C
	ATOM	1219	O ALA A 166	10.346	-15.302	15.910	1.00	35.13	O
35	ATOM	1220	N GLY A 167	11.171	-16.377	14.131	1.00	35.13	N

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	ATOM	1221	CA	GLY A 167	10.784	-17.679	14.692	1.00	35.14	C
	ATOM	1222	C	GLY A 167	9.281	-17.846	14.888	1.00	35.11	C
	ATOM	1223	O	GLY A 167	8.834	-18.763	15.595	1.00	35.44	O
	ATOM	1224	N	GLY A 168	8.505	-16.956	14.272	1.00	34.43	N
5	ATOM	1225	CA	GLY A 168	7.062	-17.139	14.133	1.00	34.21	C
	ATOM	1226	C	GLY A 168	6.175	-16.362	15.087	1.00	33.60	C
	ATOM	1227	O	GLY A 168	4.945	-16.399	14.955	1.00	34.26	O
	ATOM	1228	N	SER A 169	6.775	-15.651	16.042	1.00	32.91	N
	ATOM	1229	CA	SER A 169	5.978	-14.834	16.963	1.00	32.63	C
10	ATOM	1230	CB	SER A 169	5.655	-15.618	18.239	1.00	32.34	C
	ATOM	1231	OG	SER A 169	6.770	-15.628	19.104	1.00	33.90	O
	ATOM	1232	C	SER A 169	6.570	-13.472	17.322	1.00	32.01	C
	ATOM	1233	O	SER A 169	7.756	-13.202	17.085	1.00	31.49	O
	ATOM	1234	N	PHE A 170	5.725	-12.628	17.914	1.00	31.27	N
15	ATOM	1235	CA	PHE A 170	6.150	-11.339	18.454	1.00	31.02	C
	ATOM	1236	CB	PHE A 170	5.984	-10.216	17.421	1.00	30.32	C
	ATOM	1237	CG	PHE A 170	4.543	-9.870	17.076	1.00	30.26	C
	ATOM	1238	CD1	PHE A 170	3.875	-8.834	17.743	1.00	29.35	C
	ATOM	1239	CE1	PHE A 170	2.550	-8.481	17.402	1.00	29.70	C
20	ATOM	1240	CZ	PHE A 170	1.890	-9.168	16.382	1.00	30.10	C
	ATOM	1241	CE2	PHE A 170	2.551	-10.208	15.710	1.00	30.88	C
	ATOM	1242	CD2	PHE A 170	3.877	-10.542	16.061	1.00	30.03	C
	ATOM	1243	C	PHE A 170	5.454	-11.015	19.777	1.00	30.91	C
	ATOM	1244	O	PHE A 170	4.374	-11.550	20.059	1.00	31.61	O
25	ATOM	1245	N	THR A 171	6.092	-10.185	20.606	1.00	30.24	N
	ATOM	1246	CA	THR A 171	5.468	-9.737	21.852	1.00	29.86	C
	ATOM	1247	CB	THR A 171	6.370	-9.950	23.109	1.00	29.61	C
	ATOM	1248	OG1	THR A 171	7.585	-9.200	22.963	1.00	29.43	O
	ATOM	1249	CG2	THR A 171	6.678	-11.436	23.318	1.00	29.32	C
30	ATOM	1250	C	THR A 171	5.082	-8.272	21.785	1.00	29.69	C
	ATOM	1251	O	THR A 171	5.656	-7.491	21.025	1.00	28.91	O
	ATOM	1252	N	VAL A 172	4.084	-7.919	22.582	1.00	29.84	N
	ATOM	1253	CA	VAL A 172	3.710	-6.532	22.786	1.00	30.09	C
	ATOM	1254	CB	VAL A 172	2.417	-6.136	22.005	1.00	30.13	C
35	ATOM	1255	CG1	VAL A 172	2.038	-4.671	22.295	1.00	29.67	C

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	ATOM	1256	CG2 VAL A 172	2.569	-6.360	20.484	1.00	30.36	C
	ATOM	1257	C VAL A 172	3.493	-6.334	24.287	1.00	30.62	C
	ATOM	1258	O VAL A 172	2.876	-7.181	24.950	1.00	29.83	O
	ATOM	1259	N ARG A 173	4.028	-5.236	24.817	1.00	30.99	N
5	ATOM	1260	CA ARG A 173	3.822	-4.855	26.217	1.00	32.30	C
	ATOM	1261	CB ARG A 173	4.932	-5.419	27.121	1.00	32.21	C
	ATOM	1262	CG ARG A 173	6.318	-4.773	26.920	1.00	34.06	C
	ATOM	1263	CD ARG A 173	7.443	-5.659	27.475	1.00	33.74	C
	ATOM	1264	NE ARG A 173	7.720	-6.786	26.585	1.00	37.12	N
10	ATOM	1265	CZ ARG A 173	8.162	-7.972	26.995	1.00	38.47	C
	ATOM	1266	NH1 ARG A 173	8.310	-8.184	28.294	0.00	48.77	N
	ATOM	1267	NH2 ARG A 173	8.383	-8.941	26.117	1.00	38.16	N
	ATOM	1268	C ARG A 173	3.768	-3.339	26.339	1.00	32.34	C
	ATOM	1269	O ARG A 173	4.153	-2.628	25.409	1.00	31.89	O
15	ATOM	1270	N THR A 174	3.283	-2.855	27.482	1.00	32.84	N
	ATOM	1271	CA THR A 174	3.404	-1.447	27.848	1.00	34.10	C
	ATOM	1272	CB THR A 174	2.489	-1.111	29.056	1.00	34.04	C
	ATOM	1273	OG1 THR A 174	1.121	-1.278	28.664	1.00	35.00	O
	ATOM	1274	CG2 THR A 174	2.699	0.327	29.531	1.00	34.35	C
20	ATOM	1275	C THR A 174	4.879	-1.178	28.170	1.00	34.78	C
	ATOM	1276	O THR A 174	5.496	-1.909	28.946	1.00	34.50	O
	ATOM	1277	N ASP A 175	5.449	-0.158	27.534	1.00	36.06	N
	ATOM	1278	CA ASP A 175	6.875	0.149	27.707	1.00	37.59	C
	ATOM	1279	CB ASP A 175	7.407	0.979	26.530	1.00	37.29	C
25	ATOM	1280	CG ASP A 175	8.917	1.217	26.608	1.00	38.09	C
	ATOM	1281	OD1 ASP A 175	9.612	0.465	27.323	1.00	39.42	O
	ATOM	1282	OD2 ASP A 175	9.409	2.157	25.955	1.00	37.68	O
	ATOM	1283	C ASP A 175	7.173	0.847	29.036	1.00	38.28	C
	ATOM	1284	O ASP A 175	6.682	1.950	29.294	1.00	38.38	O
30	ATOM	1285	N THR A 176	7.995	0.209	29.869	1.00	39.80	N
	ATOM	1286	CA THR A 176	8.443	0.835	31.128	1.00	40.53	C
	ATOM	1287	CB THR A 176	8.460	-0.165	32.308	1.00	40.83	C
	ATOM	1288	OG1 THR A 176	9.342	-1.245	32.004	1.00	41.42	O
	ATOM	1289	CG2 THR A 176	7.061	-0.718	32.591	1.00	41.14	C
35	ATOM	1290	C THR A 176	9.825	1.500	30.990	1.00	41.03	C

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	ATOM	1291	O	THR A 176	10.674	1.703	31.765	0.00	46.33	O
	ATOM	1292	N	GLY A 177	10.207	1.785	29.747	1.00	41.17	N
	ATOM	1293	CA	GLY A 177	11.446	2.484	29.442	1.00	41.31	C
	ATOM	1294	C	GLY A 177	11.245	3.986	29.306	1.00	41.27	C
5	ATOM	1295	O	GLY A 177	10.210	4.517	29.709	1.00	41.44	O
	ATOM	1296	N	GLU A 178	12.241	4.656	28.727	1.00	41.16	N
	ATOM	1297	CA	GLU A 178	12.255	6.115	28.581	1.00	41.66	C
	ATOM	1298	CB	GLU A 178	13.566	6.580	27.938	1.00	41.27	C
	ATOM	1299	CG	GLU A 178	14.784	6.620	28.872	1.00	43.27	C
10	ATOM	1300	CD	GLU A 178	16.038	7.134	28.176	1.00	43.52	C
	ATOM	1301	OE1	GLU A 178	17.154	6.720	28.567	1.00	47.34	O
	ATOM	1302	OE2	GLU A 178	15.915	7.949	27.229	1.00	47.09	O
	ATOM	1303	C	GLU A 178	11.087	6.608	27.734	1.00	40.91	C
	ATOM	1304	O	GLU A 178	10.977	6.231	26.575	1.00	40.82	O
15	ATOM	1305	N	PRO A 179	10.212	7.456	28.312	1.00	40.80	N
	ATOM	1306	CA	PRO A 179	9.094	8.001	27.548	1.00	40.65	C
	ATOM	1307	CB	PRO A 179	8.433	8.965	28.538	1.00	40.44	C
	ATOM	1308	CG	PRO A 179	8.778	8.409	29.864	1.00	40.17	C
	ATOM	1309	CD	PRO A 179	10.195	7.945	29.700	1.00	40.69	C
20	ATOM	1310	C	PRO A 179	9.594	8.751	26.321	1.00	40.65	C
	ATOM	1311	O	PRO A 179	10.684	9.342	26.359	1.00	39.89	O
	ATOM	1312	N	MET A 180	8.802	8.715	25.251	1.00	40.74	N
	ATOM	1313	CA	MET A 180	9.204	9.266	23.952	1.00	41.88	C
	ATOM	1314	CB	MET A 180	8.760	8.341	22.813	1.00	41.69	C
25	ATOM	1315	CG	MET A 180	9.767	7.282	22.397	1.00	42.85	C
	ATOM	1316	SD	MET A 180	9.111	6.321	21.013	1.00	45.10	S
	ATOM	1317	CE	MET A 180	7.448	6.693	21.094	0.00	38.78	C
	ATOM	1318	C	MET A 180	8.677	10.670	23.678	1.00	40.97	C
	ATOM	1319	O	MET A 180	9.449	11.584	23.341	1.00	42.19	O
30	ATOM	1320	N	GLY A 181	7.366	10.834	23.804	1.00	39.76	N
	ATOM	1321	CA	GLY A 181	6.706	12.064	23.382	1.00	37.60	C
	ATOM	1322	C	GLY A 181	5.621	11.740	22.365	1.00	36.05	C
	ATOM	1323	O	GLY A 181	4.431	11.812	22.675	1.00	35.72	O
	ATOM	1324	N	ARG A 182	6.056	11.383	21.155	1.00	34.36	N
35	ATOM	1325	CA	ARG A 182	5.190	10.913	20.055	1.00	32.98	C

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	ATOM	1326	CB	ARG A 182	4.255	12.020	19.546	1.00	32.83	C
	ATOM	1327	CG	ARG A 182	3.240	11.555	18.504	1.00	32.33	C
	ATOM	1328	CD	ARG A 182	2.717	12.701	17.645	1.00	32.03	C
	ATOM	1329	NE	ARG A 182	3.764	13.343	16.849	1.00	32.41	N
5	ATOM	1330	CZ	ARG A 182	4.201	14.585	17.042	1.00	32.65	C
	ATOM	1331	NH1	ARG A 182	3.694	15.332	18.023	1.00	32.21	N
	ATOM	1332	NH2	ARG A 182	5.158	15.082	16.267	1.00	31.24	N
	ATOM	1333	C	ARG A 182	6.088	10.437	18.912	1.00	32.20	C
	ATOM	1334	O	ARG A 182	7.038	11.124	18.535	1.00	32.08	O
10	ATOM	1335	N	GLY A 183	5.792	9.255	18.380	1.00	30.74	N
	ATOM	1336	CA	GLY A 183	6.509	8.754	17.215	1.00	29.51	C
	ATOM	1337	C	GLY A 183	6.840	7.288	17.364	1.00	28.92	C
	ATOM	1338	O	GLY A 183	6.177	6.562	18.114	1.00	28.29	O
	ATOM	1339	N	THR A 184	7.885	6.867	16.662	1.00	28.14	N
15	ATOM	1340	CA	THR A 184	8.254	5.465	16.603	1.00	28.49	C
	ATOM	1341	CB	THR A 184	7.687	4.784	15.335	1.00	28.06	C
	ATOM	1342	OG1	THR A 184	6.259	4.761	15.411	1.00	29.30	O
	ATOM	1343	CG2	THR A 184	8.212	3.324	15.197	1.00	28.16	C
	ATOM	1344	C	THR A 184	9.770	5.366	16.629	1.00	28.46	C
20	ATOM	1345	O	THR A 184	10.457	6.100	15.895	1.00	28.19	O
	ATOM	1346	N	LYS A 185	10.273	4.506	17.514	1.00	28.66	N
	ATOM	1347	CA	LYS A 185	11.698	4.174	17.595	1.00	28.78	C
	ATOM	1348	CB	LYS A 185	12.247	4.510	18.987	1.00	29.06	C
	ATOM	1349	CG	LYS A 185	13.567	3.826	19.353	1.00	30.15	C
25	ATOM	1350	CD	LYS A 185	14.266	4.520	20.529	1.00	30.82	C
	ATOM	1351	CE	LYS A 185	13.465	4.410	21.833	1.00	33.90	C
	ATOM	1352	NZ	LYS A 185	14.198	5.105	22.929	1.00	35.33	N
	ATOM	1353	C	LYS A 185	11.911	2.691	17.236	1.00	28.30	C
	ATOM	1354	O	LYS A 185	11.379	1.795	17.906	1.00	27.65	O
30	ATOM	1355	N	VAL A 186	12.666	2.445	16.164	1.00	27.36	N
	ATOM	1356	CA	VAL A 186	12.973	1.078	15.742	1.00	27.27	C
	ATOM	1357	CB	VAL A 186	12.770	0.861	14.232	1.00	27.32	C
	ATOM	1358	CG1	VAL A 186	13.124	-0.594	13.822	1.00	26.62	C
	ATOM	1359	CG2	VAL A 186	11.339	1.216	13.815	1.00	27.76	C
35	ATOM	1360	C	VAL A 186	14.420	0.762	16.104	1.00	27.65	C

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	ATOM	1361	O	VAL A 186	15.346	1.432	15.628	1.00	27.82	O
	ATOM	1362	N	ILE A 187	14.594	-0.254	16.940	1.00	27.25	N
	ATOM	1363	CA	ILE A 187	15.918	-0.670	17.394	1.00	27.77	C
	ATOM	1364	CB	ILE A 187	15.974	-0.850	18.920	1.00	28.08	C
5	ATOM	1365	CG1	ILE A 187	15.424	0.394	19.639	1.00	28.85	C
	ATOM	1366	CD1	ILE A 187	15.178	0.180	21.129	1.00	28.95	C
	ATOM	1367	CG2	ILE A 187	17.413	-1.158	19.370	1.00	28.95	C
	ATOM	1368	C	ILE A 187	16.333	-1.961	16.702	1.00	27.13	C
	ATOM	1369	O	ILE A 187	15.758	-3.023	16.957	1.00	27.27	O
10	ATOM	1370	N	LEU A 188	17.317	-1.855	15.815	1.00	26.81	N
	ATOM	1371	CA	LEU A 188	17.864	-3.016	15.112	1.00	27.58	C
	ATOM	1372	CB	LEU A 188	18.271	-2.623	13.695	1.00	27.90	C
	ATOM	1373	CG	LEU A 188	17.209	-1.994	12.789	1.00	28.79	C
	ATOM	1374	CD1	LEU A 188	17.848	-1.570	11.482	1.00	30.86	C
15	ATOM	1375	CD2	LEU A 188	16.041	-2.949	12.547	1.00	29.46	C
	ATOM	1376	C	LEU A 188	19.063	-3.639	15.837	1.00	27.67	C
	ATOM	1377	O	LEU A 188	20.145	-3.034	15.888	1.00	26.52	O
	ATOM	1378	N	HIS A 189	18.864	-4.853	16.365	1.00	27.38	N
	ATOM	1379	CA	HIS A 189	19.939	-5.640	16.969	1.00	28.58	C
20	ATOM	1380	CB	HIS A 189	19.401	-6.590	18.055	1.00	28.84	C
	ATOM	1381	CG	HIS A 189	18.768	-5.883	19.217	1.00	30.67	C
	ATOM	1382	ND1	HIS A 189	19.457	-5.584	20.374	1.00	33.29	N
	ATOM	1383	CE1	HIS A 189	18.653	-4.953	21.212	1.00	33.82	C
	ATOM	1384	NE2	HIS A 189	17.471	-4.827	20.639	1.00	34.18	N
25	ATOM	1385	CD2	HIS A 189	17.516	-5.402	19.392	1.00	32.40	C
	ATOM	1386	C	HIS A 189	20.616	-6.416	15.838	1.00	28.32	C
	ATOM	1387	O	HIS A 189	20.111	-7.452	15.371	1.00	28.38	O
	ATOM	1388	N	LEU A 190	21.733	-5.873	15.360	1.00	27.84	N
	ATOM	1389	CA	LEU A 190	22.363	-6.383	14.146	1.00	28.33	C
30	ATOM	1390	CB	LEU A 190	23.401	-5.391	13.602	1.00	27.55	C
	ATOM	1391	CG	LEU A 190	22.987	-3.955	13.249	1.00	26.79	C
	ATOM	1392	CD1	LEU A 190	24.216	-3.167	12.806	1.00	25.42	C
	ATOM	1393	CD2	LEU A 190	21.910	-3.883	12.161	1.00	25.49	C
	ATOM	1394	C	LEU A 190	23.020	-7.748	14.302	1.00	29.38	C
35	ATOM	1395	O	LEU A 190	23.589	-8.071	15.357	1.00	29.27	O

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	ATOM	1396	N	LYS A 191	22.933	-8.524	13.225	1.00	30.71	N
	ATOM	1397	CA	LYS A 191	23.681	-9.753	13.075	1.00	32.42	C
	ATOM	1398	CB	LYS A 191	23.315	-10.434	11.762	1.00	32.55	C
	ATOM	1399	CG	LYS A 191	21.958	-11.100	11.776	1.00	33.98	C
5	ATOM	1400	CD	LYS A 191	21.645	-11.789	10.450	1.00	37.30	C
	ATOM	1401	CE	LYS A 191	20.848	-10.885	9.536	1.00	39.73	C
	ATOM	1402	NZ	LYS A 191	20.547	-11.536	8.229	1.00	42.49	N
	ATOM	1403	C	LYS A 191	25.176	-9.427	13.106	1.00	33.16	C
	ATOM	1404	O	LYS A 191	25.605	-8.367	12.632	1.00	32.99	O
10	ATOM	1405	N	GLU A 192	25.954	-10.341	13.676	1.00	34.20	N
	ATOM	1406	CA	GLU A 192	27.410	-10.174	13.800	1.00	35.49	C
	ATOM	1407	CB	GLU A 192	28.056	-11.432	14.401	1.00	36.00	C
	ATOM	1408	CG	GLU A 192	27.910	-12.685	13.536	1.00	39.52	C
	ATOM	1409	CD	GLU A 192	29.164	-13.537	13.513	1.00	44.39	C
15	ATOM	1410	OE1	GLU A 192	29.594	-13.930	12.400	1.00	47.65	O
	ATOM	1411	OE2	GLU A 192	29.723	-13.813	14.597	1.00	46.22	O
	ATOM	1412	C	GLU A 192	28.124	-9.779	12.491	1.00	35.10	C
	ATOM	1413	O	GLU A 192	29.139	-9.081	12.534	1.00	35.34	O
	ATOM	1414	N	ASP A 193	27.591	-10.208	11.345	1.00	34.82	N
20	ATOM	1415	CA	ASP A 193	28.228	-9.929	10.048	1.00	35.37	C
	ATOM	1416	CB	ASP A 193	28.199	-11.164	9.147	1.00	35.59	C
	ATOM	1417	CG	ASP A 193	26.834	-11.410	8.529	1.00	36.99	C
	ATOM	1418	OD1	ASP A 193	25.805	-11.228	9.212	1.00	37.83	O
	ATOM	1419	OD2	ASP A 193	26.798	-11.803	7.350	1.00	41.42	O
25	ATOM	1420	C	ASP A 193	27.640	-8.714	9.313	1.00	34.74	C
	ATOM	1421	O	ASP A 193	27.948	-8.467	8.140	1.00	34.84	O
	ATOM	1422	N	GLN A 194	26.800	-7.961	10.009	1.00	33.94	N
	ATOM	1423	CA	GLN A 194	26.169	-6.788	9.419	1.00	33.46	C
	ATOM	1424	CB	GLN A 194	24.640	-6.987	9.338	1.00	33.02	C
30	ATOM	1425	CG	GLN A 194	24.179	-8.167	8.461	1.00	33.77	C
	ATOM	1426	CD	GLN A 194	24.615	-8.063	7.002	1.00	33.21	C
	ATOM	1427	OE1	GLN A 194	24.547	-6.998	6.389	1.00	33.22	O
	ATOM	1428	NE2	GLN A 194	25.068	-9.177	6.445	1.00	33.76	N
	ATOM	1429	C	GLN A 194	26.541	-5.499	10.165	1.00	33.23	C
35	ATOM	1430	O	GLN A 194	25.819	-4.503	10.089	1.00	32.66	O

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	ATOM	1431	N	THR A 195	27.692	-5.509	10.853	1.00	32.84	N
	ATOM	1432	CA	THR A 195	28.110	-4.358	11.664	1.00	33.29	C
	ATOM	1433	CB	THR A 195	29.256	-4.718	12.646	1.00	33.18	C
	ATOM	1434	OG1	THR A 195	30.429	-5.060	11.899	1.00	34.92	O
5	ATOM	1435	CG2	THR A 195	28.845	-5.884	13.565	1.00	33.45	C
	ATOM	1436	C	THR A 195	28.526	-3.111	10.875	1.00	32.90	C
	ATOM	1437	O	THR A 195	28.686	-2.044	11.461	1.00	32.84	O
	ATOM	1438	N	GLU A 196	28.689	-3.242	9.559	1.00	33.17	N
	ATOM	1439	CA	GLU A 196	29.018	-2.084	8.696	1.00	33.16	C
10	ATOM	1440	CB	GLU A 196	29.165	-2.497	7.225	1.00	33.09	C
	ATOM	1441	CG	GLU A 196	27.866	-2.939	6.517	1.00	33.24	C
	ATOM	1442	CD	GLU A 196	28.128	-3.639	5.190	1.00	34.07	C
	ATOM	1443	OE1	GLU A 196	28.614	-4.792	5.219	1.00	34.96	O
	ATOM	1444	OE2	GLU A 196	27.839	-3.049	4.119	1.00	34.41	O
15	ATOM	1445	C	GLU A 196	27.989	-0.963	8.843	1.00	32.92	C
	ATOM	1446	O	GLU A 196	28.316	0.210	8.673	1.00	32.68	O
	ATOM	1447	N	TYR A 197	26.757	-1.331	9.196	1.00	32.70	N
	ATOM	1448	CA	TYR A 197	25.665	-0.356	9.315	1.00	32.74	C
	ATOM	1449	CB	TYR A 197	24.304	-1.014	8.999	1.00	32.66	C
20	ATOM	1450	CG	TYR A 197	24.294	-1.655	7.622	1.00	32.91	C
	ATOM	1451	CD1	TYR A 197	24.356	-0.868	6.464	1.00	32.78	C
	ATOM	1452	CE1	TYR A 197	24.363	-1.441	5.204	1.00	33.52	C
	ATOM	1453	CZ	TYR A 197	24.315	-2.823	5.070	1.00	32.89	C
	ATOM	1454	OH	TYR A 197	24.336	-3.374	3.815	1.00	33.75	O
25	ATOM	1455	CE2	TYR A 197	24.260	-3.635	6.194	1.00	32.97	C
	ATOM	1456	CD2	TYR A 197	24.252	-3.043	7.471	1.00	33.13	C
	ATOM	1457	C	TYR A 197	25.678	0.422	10.641	1.00	32.75	C
	ATOM	1458	O	TYR A 197	24.717	1.116	10.975	1.00	32.99	O
	ATOM	1459	N	LEU A 198	26.791	0.315	11.371	1.00	32.52	N
30	ATOM	1460	CA	LEU A 198	27.070	1.142	12.545	1.00	32.63	C
	ATOM	1461	CB	LEU A 198	27.575	0.275	13.700	1.00	32.66	C
	ATOM	1462	CG	LEU A 198	26.624	-0.849	14.132	1.00	31.93	C
	ATOM	1463	CD1	LEU A 198	27.259	-1.683	15.208	1.00	34.24	C
	ATOM	1464	CD2	LEU A 198	25.302	-0.276	14.600	1.00	33.95	C
35	ATOM	1465	C	LEU A 198	28.122	2.200	12.217	1.00	32.82	C

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	ATOM	1466	O	LEU A 198	28.444	3.059	13.055	1.00	32.54	O
	ATOM	1467	N	GLU A 199	28.668	2.116	11.003	1.00	32.57	N
	ATOM	1468	CA	GLU A 199	29.716	3.032	10.561	1.00	33.05	C
	ATOM	1469	CB	GLU A 199	30.664	2.353	9.567	1.00	33.53	C
5	ATOM	1470	CG	BGLU A 199	31.409	1.127	10.109	0.35	32.97	C
	ATOM	1471	CG	AGLU A 199	31.661	1.429	10.224	0.65	35.11	C
	ATOM	1472	CD	BGLU A 199	32.417	1.458	11.207	0.35	32.81	C
	ATOM	1473	CD	AGLU A 199	32.285	0.458	9.254	0.65	37.30	C
	ATOM	1474	OE1	BGLU A 199	32.896	2.609	11.271	0.35	32.66	O
10	ATOM	1475	OE1	AGLU A 199	32.365	0.778	8.044	0.65	39.31	O
	ATOM	1476	OE2	BGLU A 199	32.733	0.553	12.007	0.35	33.09	O
	ATOM	1477	OE2	AGLU A 199	32.699	-0.628	9.707	0.65	39.16	O
	ATOM	1478	C	GLU A 199	29.120	4.286	9.939	1.00	33.16	C
	ATOM	1479	O	GLU A 199	28.233	4.208	9.074	1.00	31.89	O
15	ATOM	1480	N	GLU A 200	29.606	5.440	10.394	1.00	33.73	N
	ATOM	1481	CA	GLU A 200	29.108	6.728	9.907	1.00	34.13	C
	ATOM	1482	CB	GLU A 200	29.813	7.900	10.607	1.00	35.00	C
	ATOM	1483	CG	GLU A 200	31.319	7.916	10.453	1.00	37.21	C
	ATOM	1484	CD	GLU A 200	32.010	8.763	11.494	1.00	42.16	C
20	ATOM	1485	OE1	GLU A 200	31.819	10.003	11.482	1.00	44.10	O
	ATOM	1486	OE2	GLU A 200	32.754	8.186	12.322	1.00	44.06	O
	ATOM	1487	C	GLU A 200	29.187	6.852	8.378	1.00	33.88	C
	ATOM	1488	O	GLU A 200	28.207	7.258	7.734	1.00	33.42	O
	ATOM	1489	N	ARG A 201	30.333	6.485	7.799	1.00	33.52	N
25	ATOM	1490	CA	ARG A 201	30.505	6.556	6.346	1.00	33.58	C
	ATOM	1491	CB	ARG A 201	31.904	6.109	5.910	1.00	33.49	C
	ATOM	1492	CG	ARG A 201	32.163	6.376	4.416	1.00	33.97	C
	ATOM	1493	CD	ARG A 201	33.497	5.821	3.936	1.00	35.61	C
	ATOM	1494	NE	ARG A 201	34.615	6.214	4.797	1.00	39.50	N
30	ATOM	1495	CZ	ARG A 201	35.115	7.443	4.887	1.00	41.01	C
	ATOM	1496	NH1	ARG A 201	36.136	7.673	5.707	1.00	41.80	N
	ATOM	1497	NH2	ARG A 201	34.599	8.440	4.173	1.00	41.85	N
	ATOM	1498	C	ARG A 201	29.455	5.737	5.599	1.00	32.68	C
	ATOM	1499	O	ARG A 201	28.842	6.228	4.656	1.00	31.95	O
35	ATOM	1500	N	ARG A 202	29.254	4.490	6.032	1.00	32.36	N

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	ATOM	1501	CA	ARG A 202	28.346	3.577	5.337	1.00	32.22	C
	ATOM	1502	CB	ARG A 202	28.439	2.166	5.923	1.00	32.29	C
	ATOM	1503	CG	ARG A 202	27.527	1.126	5.252	1.00	33.26	C
	ATOM	1504	CD	ARG A 202	28.140	0.581	3.956	1.00	34.34	C
5	ATOM	1505	NE	ARG A 202	27.351	-0.526	3.420	1.00	35.76	N
	ATOM	1506	CZ	ARG A 202	26.673	-0.488	2.275	1.00	34.90	C
	ATOM	1507	NH1	ARG A 202	26.708	0.596	1.505	1.00	36.15	N
	ATOM	1508	NH2	ARG A 202	25.975	-1.544	1.888	1.00	33.98	N
	ATOM	1509	C	ARG A 202	26.904	4.083	5.405	1.00	31.78	C
10	ATOM	1510	O	ARG A 202	26.173	4.023	4.413	1.00	31.68	O
	ATOM	1511	N	ILE A 203	26.512	4.581	6.577	1.00	31.51	N
	ATOM	1512	CA	ILE A 203	25.158	5.079	6.789	1.00	30.78	C
	ATOM	1513	CB	ILE A 203	24.910	5.462	8.273	1.00	31.22	C
	ATOM	1514	CG1A	ILE A 203	24.983	4.219	9.171	0.50	29.42	C
15	ATOM	1515	CD1A	ILE A 203	25.173	4.522	10.660	0.50	30.11	C
	ATOM	1516	CG2A	ILE A 203	23.555	6.146	8.437	0.50	29.46	C
	ATOM	1517	C	ILE A 203	24.933	6.263	5.847	1.00	31.37	C
	ATOM	1518	O	ILE A 203	23.938	6.310	5.108	1.00	30.52	O
	ATOM	1519	N	LYS A 204	25.879	7.201	5.868	1.00	31.72	N
20	ATOM	1520	CA	LYS A 204	25.847	8.352	4.964	1.00	32.90	C
	ATOM	1521	CB	LYS A 204	27.062	9.270	5.199	1.00	32.95	C
	ATOM	1522	CG	LYS A 204	26.970	10.077	6.500	1.00	33.53	C
	ATOM	1523	CD	LYS A 204	27.990	11.214	6.568	1.00	34.16	C
	ATOM	1524	CE	LYS A 204	29.283	10.795	7.236	1.00	36.76	C
25	ATOM	1525	NZ	LYS A 204	30.300	11.902	7.232	1.00	37.69	N
	ATOM	1526	C	LYS A 204	25.731	7.927	3.497	1.00	32.59	C
	ATOM	1527	O	LYS A 204	24.895	8.463	2.760	1.00	32.52	O
	ATOM	1528	N	GLU A 205	26.533	6.941	3.089	1.00	32.69	N
	ATOM	1529	CA	GLU A 205	26.453	6.411	1.724	1.00	32.96	C
30	ATOM	1530	CB	GLU A 205	27.388	5.223	1.528	1.00	32.73	C
	ATOM	1531	CG	GLU A 205	27.480	4.732	0.075	1.00	33.10	C
	ATOM	1532	CD	GLU A 205	28.402	3.531	-0.078	1.00	33.76	C
	ATOM	1533	OE1	GLU A 205	28.626	2.809	0.919	1.00	36.06	O
	ATOM	1534	OE2	GLU A 205	28.915	3.314	-1.199	1.00	36.34	O
35	ATOM	1535	C	GLU A 205	25.036	6.005	1.335	1.00	32.77	C

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	ATOM	1536	O	GLU A 205	24.542	6.412	0.285	1.00	31.84	O
	ATOM	1537	N	ILE A 206	24.397	5.196	2.181	1.00	33.03	N
	ATOM	1538	CA	ILE A 206	23.096	4.630	1.834	1.00	33.53	C
	ATOM	1539	CB	ILE A 206	22.795	3.275	2.564	1.00	33.20	C
5	ATOM	1540	CG1	ILE A 206	22.776	3.428	4.082	1.00	33.66	C
	ATOM	1541	CD1	ILE A 206	22.472	2.111	4.851	1.00	33.15	C
	ATOM	1542	CG2	ILE A 206	23.811	2.201	2.140	1.00	33.96	C
	ATOM	1543	C	ILE A 206	21.939	5.634	1.928	1.00	33.44	C
	ATOM	1544	O	ILE A 206	20.979	5.554	1.149	1.00	33.60	O
10	ATOM	1545	N	VAL A 207	22.036	6.587	2.847	1.00	34.07	N
	ATOM	1546	CA	VAL A 207	21.021	7.632	2.927	1.00	34.17	C
	ATOM	1547	CB	VAL A 207	21.154	8.495	4.216	1.00	34.26	C
	ATOM	1548	CG1	VAL A 207	20.276	9.748	4.142	1.00	33.45	C
	ATOM	1549	CG2	VAL A 207	20.805	7.659	5.461	1.00	32.95	C
15	ATOM	1550	C	VAL A 207	21.051	8.453	1.624	1.00	35.00	C
	ATOM	1551	O	VAL A 207	20.017	8.640	0.974	1.00	34.41	O
	ATOM	1552	N	LYS A 208	22.247	8.876	1.213	1.00	35.44	N
	ATOM	1553	CA	LYS A 208	22.415	9.661	-0.014	1.00	36.29	C
	ATOM	1554	CB	LYS A 208	23.876	10.121	-0.158	1.00	36.41	C
20	ATOM	1555	CG	LYS A 208	24.075	11.216	-1.213	1.00	37.26	C
	ATOM	1556	CD	LYS A 208	25.552	11.162	-1.685	0.00	41.16	C
	ATOM	1557	CE	LYS A 208	25.937	11.576	-3.174	0.00	41.17	C
	ATOM	1558	NZ	LYS A 208	24.636	10.283	-5.096	1.00	59.20	N
	ATOM	1559	C	LYS A 208	21.969	8.914	-1.279	1.00	36.78	C
25	ATOM	1560	O	LYS A 208	21.352	9.504	-2.168	1.00	36.86	O
	ATOM	1561	N	LYS A 209	22.287	7.622	-1.352	1.00	37.69	N
	ATOM	1562	CA	LYS A 209	21.959	6.794	-2.515	1.00	38.72	C
	ATOM	1563	CB	LYS A 209	22.720	5.464	-2.452	1.00	38.70	C
	ATOM	1564	CG	LYS A 209	22.416	4.499	-3.597	1.00	39.52	C
30	ATOM	1565	CD	LYS A 209	23.168	3.186	-3.439	1.00	39.42	C
	ATOM	1566	CE	LYS A 209	22.904	2.291	-4.470	0.00	47.76	C
	ATOM	1567	NZ	LYS A 209	23.811	1.060	-4.498	0.00	48.91	N
	ATOM	1568	C	LYS A 209	20.455	6.532	-2.635	1.00	38.88	C
	ATOM	1569	O	LYS A 209	19.873	6.713	-3.709	1.00	38.70	O
35	ATOM	1570	N	HIS A 210	19.837	6.135	-1.521	1.00	39.10	N

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	ATOM	1571	CA	HIS A 210	18.473	5.604	-1.516	1.00	39.58	C
	ATOM	1572	CB	HIS A 210	18.442	4.260	-0.789	1.00	39.47	C
	ATOM	1573	CG	HIS A 210	19.247	3.189	-1.452	1.00	40.55	C
	ATOM	1574	ND1	HIS A 210	18.897	2.636	-2.668	1.00	40.98	N
5	ATOM	1575	CE1	HIS A 210	19.775	1.702	-2.992	1.00	40.42	C
	ATOM	1576	NE2	HIS A 210	20.684	1.633	-2.034	1.00	41.07	N
	ATOM	1577	CD2	HIS A 210	20.375	2.550	-1.057	1.00	40.50	C
	ATOM	1578	C	HIS A 210	17.388	6.500	-0.911	1.00	39.59	C
	ATOM	1579	O	HIS A 210	16.203	6.293	-1.191	1.00	39.69	O
10	ATOM	1580	N	SER A 211	17.782	7.467	-0.081	1.00	39.76	N
	ATOM	1581	CA	SER A 211	16.829	8.290	0.676	1.00	40.33	C
	ATOM	1582	CB	SER A 211	16.854	7.912	2.165	1.00	39.93	C
	ATOM	1583	OG	SER A 211	16.581	6.540	2.370	1.00	37.36	O
	ATOM	1584	C	SER A 211	17.105	9.786	0.537	1.00	41.37	C
15	ATOM	1585	O	SER A 211	17.052	10.529	1.521	1.00	41.76	O
	ATOM	1586	N	GLN A 212	17.388	10.229	-0.679	1.00	42.52	N
	ATOM	1587	CA	GLN A 212	17.775	11.624	-0.910	1.00	43.65	C
	ATOM	1588	CB	GLN A 212	18.625	11.748	-2.182	1.00	43.73	C
	ATOM	1589	CG	GLN A 212	18.007	11.090	-3.409	1.00	43.48	C
20	ATOM	1590	CD	GLN A 212	18.611	9.580	-3.792	0.00	53.94	C
	ATOM	1591	OE1	GLN A 212	18.175	8.708	-3.172	0.00	60.77	O
	ATOM	1592	NE2	GLN A 212	19.723	9.194	-4.890	0.00	57.21	N
	ATOM	1593	C	GLN A 212	16.608	12.616	-0.954	1.00	44.26	C
	ATOM	1594	O	GLN A 212	16.817	13.813	-0.740	1.00	44.84	O
25	ATOM	1595	N	PHE A 213	15.393	12.130	-1.223	1.00	44.94	N
	ATOM	1596	CA	PHE A 213	14.232	13.020	-1.418	1.00	45.35	C
	ATOM	1597	CB	PHE A 213	13.552	12.751	-2.771	1.00	45.91	C
	ATOM	1598	CG	PHE A 213	14.449	12.980	-3.952	1.00	47.49	C
	ATOM	1599	CD1	PHE A 213	14.947	14.254	-4.228	1.00	48.59	C
30	ATOM	1600	CE1	PHE A 213	15.791	14.473	-5.321	1.00	48.87	C
	ATOM	1601	CZ	PHE A 213	16.142	13.406	-6.147	1.00	48.94	C
	ATOM	1602	CE2	PHE A 213	15.644	12.127	-5.880	1.00	49.33	C
	ATOM	1603	CD2	PHE A 213	14.806	11.922	-4.785	1.00	48.09	C
	ATOM	1604	C	PHE A 213	13.203	12.993	-0.281	1.00	44.83	C
35	ATOM	1605	O	PHE A 213	12.009	13.236	-0.497	1.00	45.34	O

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	ATOM	1606	N	ILE A 214	13.673	12.709	0.929	1.00	43.67	N
	ATOM	1607	CA	ILE A 214	12.820	12.711	2.111	1.00	42.62	C
	ATOM	1608	CB	ILE A 214	13.462	11.892	3.267	1.00	42.51	C
	ATOM	1609	CG1	ILE A 214	13.661	10.430	2.840	1.00	42.77	C
5	ATOM	1610	CD1	ILE A 214	12.396	9.684	2.389	1.00	41.61	C
	ATOM	1611	CG2	ILE A 214	12.660	12.018	4.574	1.00	42.60	C
	ATOM	1612	C	ILE A 214	12.586	14.163	2.515	1.00	41.72	C
	ATOM	1613	O	ILE A 214	13.527	14.958	2.553	1.00	42.39	O
	ATOM	1614	N	GLY A 215	11.329	14.503	2.785	1.00	40.67	N
10	ATOM	1615	CA	GLY A 215	10.928	15.885	3.053	1.00	39.29	C
	ATOM	1616	C	GLY A 215	10.931	16.263	4.520	1.00	38.35	C
	ATOM	1617	O	GLY A 215	10.148	17.115	4.953	1.00	38.25	O
	ATOM	1618	N	TYR A 216	11.813	15.618	5.280	1.00	37.37	N
	ATOM	1619	CA	TYR A 216	11.981	15.873	6.702	1.00	36.51	C
15	ATOM	1620	CB	TYR A 216	11.165	14.868	7.537	1.00	36.25	C
	ATOM	1621	CG	TYR A 216	9.682	14.937	7.227	1.00	36.13	C
	ATOM	1622	CD1	TYR A 216	8.879	15.924	7.807	1.00	36.08	C
	ATOM	1623	CE1	TYR A 216	7.526	16.020	7.502	1.00	36.88	C
	ATOM	1624	CZ	TYR A 216	6.963	15.123	6.607	1.00	36.02	C
20	ATOM	1625	OH	TYR A 216	5.629	15.225	6.318	1.00	36.16	O
	ATOM	1626	CE2	TYR A 216	7.738	14.134	6.013	1.00	35.22	C
	ATOM	1627	CD2	TYR A 216	9.094	14.050	6.323	1.00	35.59	C
	ATOM	1628	C	TYR A 216	13.466	15.788	7.032	1.00	36.04	C
	ATOM	1629	O	TYR A 216	14.186	14.987	6.415	1.00	36.05	O
25	ATOM	1630	N	PRO A 217	13.928	16.601	8.005	1.00	35.48	N
	ATOM	1631	CA	PRO A 217	15.331	16.572	8.416	1.00	35.17	C
	ATOM	1632	CB	PRO A 217	15.399	17.606	9.543	1.00	35.23	C
	ATOM	1633	CG	PRO A 217	14.169	18.428	9.425	1.00	35.14	C
	ATOM	1634	CD	PRO A 217	13.137	17.564	8.796	1.00	35.40	C
30	ATOM	1635	C	PRO A 217	15.701	15.200	8.971	1.00	34.82	C
	ATOM	1636	O	PRO A 217	14.912	14.593	9.700	1.00	34.91	O
	ATOM	1637	N	ILE A 218	16.885	14.719	8.610	1.00	34.27	N
	ATOM	1638	CA	ILE A 218	17.425	13.476	9.147	1.00	33.70	C
	ATOM	1639	CB	ILE A 218	17.619	12.399	8.057	1.00	33.40	C
35	ATOM	1640	CG1	ILE A 218	16.352	12.238	7.205	1.00	33.71	C

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	ATOM	1641	CD1 ILE A 218	16.544	11.376	5.967	1.00	34.66	C
	ATOM	1642	CG2 ILE A 218	18.021	11.065	8.681	1.00	33.88	C
	ATOM	1643	C ILE A 218	18.769	13.823	9.774	1.00	32.99	C
	ATOM	1644	O ILE A 218	19.570	14.542	9.167	1.00	33.27	O
5	ATOM	1645	N THR A 219	19.002	13.336	10.988	1.00	32.19	N
	ATOM	1646	CA THR A 219	20.240	13.630	11.716	1.00	32.00	C
	ATOM	1647	CB THR A 219	19.985	14.598	12.891	1.00	31.70	C
	ATOM	1648	OG1 THR A 219	19.352	15.787	12.393	1.00	31.36	O
	ATOM	1649	CG2 THR A 219	21.300	14.980	13.595	1.00	32.13	C
10	ATOM	1650	C THR A 219	20.917	12.352	12.203	1.00	31.90	C
	ATOM	1651	O THR A 219	20.288	11.499	12.852	1.00	30.92	O
	ATOM	1652	N LEU A 220	22.203	12.232	11.878	1.00	32.21	N
	ATOM	1653	CA LEU A 220	23.004	11.090	12.286	1.00	31.88	C
	ATOM	1654	CB LEU A 220	23.874	10.615	11.117	1.00	31.86	C
15	ATOM	1655	CG LEU A 220	24.831	9.474	11.445	1.00	31.68	C
	ATOM	1656	CD1 LEU A 220	24.066	8.183	11.763	1.00	31.98	C
	ATOM	1657	CD2 LEU A 220	25.818	9.259	10.309	1.00	31.98	C
	ATOM	1658	C LEU A 220	23.866	11.414	13.513	1.00	31.94	C
	ATOM	1659	O LEU A 220	24.681	12.332	13.479	1.00	31.83	O
20	ATOM	1660	N PHE A 221	23.678	10.659	14.588	1.00	31.93	N
	ATOM	1661	CA PHE A 221	24.413	10.891	15.837	1.00	32.94	C
	ATOM	1662	CB PHE A 221	23.467	10.880	17.043	1.00	32.79	C
	ATOM	1663	CG PHE A 221	22.511	12.031	17.059	1.00	32.82	C
	ATOM	1664	CD1 PHE A 221	22.859	13.229	17.657	1.00	32.14	C
25	ATOM	1665	CE1 PHE A 221	21.977	14.317	17.654	1.00	32.77	C
	ATOM	1666	CZ PHE A 221	20.738	14.202	17.033	1.00	33.08	C
	ATOM	1667	CE2 PHE A 221	20.384	13.008	16.418	1.00	33.72	C
	ATOM	1668	CD2 PHE A 221	21.273	11.931	16.428	1.00	33.97	C
	ATOM	1669	C PHE A 221	25.554	9.904	16.026	1.00	33.27	C
30	ATOM	1670	O PHE A 221	25.327	8.694	16.135	1.00	33.46	O
	ATOM	1671	N VAL A 222	26.779	10.432	16.069	1.00	34.06	N
	ATOM	1672	CA VAL A 222	27.985	9.598	16.142	1.00	34.67	C
	ATOM	1673	CB VAL A 222	28.931	9.879	14.939	1.00	34.49	C
	ATOM	1674	CG1 VAL A 222	30.224	9.042	15.034	1.00	34.43	C
35	ATOM	1675	CG2 VAL A 222	28.207	9.602	13.633	1.00	34.68	C

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	ATOM	1676	C	VAL A 222	28.736	9.743	17.471	1.00	35.32	C
	ATOM	1677	O	VAL A 222	29.126	10.845	17.868	1.00	35.25	O
	ATOM	1678	N	GLU A 223	28.948	8.613	18.140	1.00	35.85	N
	ATOM	1679	CA	GLU A 223	29.640	8.569	19.426	1.00	37.08	C
5	ATOM	1680	CB	GLU A 223	29.455	7.186	20.068	1.00	36.87	C
	ATOM	1681	CG	GLU A 223	30.082	7.007	21.464	1.00	37.21	C
	ATOM	1682	CD	GLU A 223	29.403	7.841	22.547	1.00	37.63	C
	ATOM	1683	OE1	GLU A 223	30.110	8.294	23.476	1.00	34.91	O
	ATOM	1684	OE2	GLU A 223	28.169	8.051	22.461	1.00	38.54	O
10	ATOM	1685	C	GLU A 223	31.132	8.902	19.282	1.00	38.21	C
	ATOM	1686	O	GLU A 223	31.799	8.392	18.381	1.00	37.71	O
	ATOM	1687	N	LYS A 224	31.619	9.781	20.161	1.00	39.84	N
	ATOM	1688	CA	LYS A 224	33.062	10.012	20.419	1.00	41.71	C
	ATOM	1689	CB	LYS A 224	33.541	9.095	21.554	1.00	41.90	C
15	ATOM	1690	CG	LYS A 224	33.027	9.494	22.935	1.00	42.64	C
	ATOM	1691	CD	LYS A 224	33.303	8.403	23.968	1.00	42.89	C
	ATOM	1692	CE	LYS A 224	32.867	8.828	25.374	1.00	45.38	C
	ATOM	1693	NZ	LYS A 224	33.829	9.791	26.008	1.00	47.56	N
	ATOM	1694	C	LYS A 224	34.004	9.870	19.223	1.00	42.41	C
20	ATOM	1695	O	LYS A 224	34.786	8.907	19.126	1.00	43.49	O
	ATOM	1696	S26	LIG A 225	0.932	4.745	10.503	1.00	31.03	S
	ATOM	1697	C9	LIG A 225	2.481	4.700	11.339	1.00	29.52	C
	ATOM	1698	N10	LIG A 225	2.741	5.259	12.535	1.00	30.13	N
	ATOM	1699	N11	LIG A 225	4.102	4.939	12.782	1.00	29.19	N
25	ATOM	1700	C7	LIG A 225	4.563	4.224	11.721	1.00	29.16	C
	ATOM	1701	C1	LIG A 225	5.921	3.671	11.520	1.00	29.44	C
	ATOM	1702	C6	LIG A 225	6.010	2.318	11.204	1.00	28.21	C
	ATOM	1703	C5	LIG A 225	7.235	1.716	10.987	1.00	27.89	C
	ATOM	1704	C24	LIG A 225	7.271	0.232	10.661	1.00	27.88	C
30	ATOM	1705	C25	LIG A 225	7.521	-0.448	11.993	1.00	33.06	C
	ATOM	1706	C4	LIG A 225	8.480	2.529	11.106	1.00	29.22	C
	ATOM	1707	O22	LIG A 225	9.691	1.944	10.890	1.00	29.03	O
	ATOM	1708	C3	LIG A 225	8.400	3.898	11.442	1.00	27.72	C
	ATOM	1709	C2	LIG A 225	7.152	4.497	11.662	1.00	27.73	C
35	ATOM	1710	O23	LIG A 225	7.045	5.831	11.977	1.00	27.58	O

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	ATOM	1711	N8	LIG A 225	3.530	4.087	10.853	1.00	30.38	N
	ATOM	1712	C12	LIG A 225	3.636	3.467	9.651	1.00	29.85	C
	ATOM	1713	C17	LIG A 225	3.241	2.027	9.517	1.00	30.69	C
	ATOM	1714	C18	LIG A 225	2.730	1.310	10.595	1.00	31.16	C
5	ATOM	1715	C19	LIG A 225	2.387	-0.034	10.434	1.00	30.75	C
	ATOM	1716	C20	LIG A 225	2.535	-0.680	9.204	1.00	31.06	C
	ATOM	1717	C21	LIG A 225	3.039	-0.011	8.087	1.00	31.20	C
	ATOM	1718	C16	LIG A 225	3.410	1.330	8.201	1.00	31.51	C
	ATOM	1719	C15	LIG A 225	3.930	2.017	7.103	1.00	30.57	C
10	ATOM	1720	C14	LIG A 225	4.289	3.364	7.251	1.00	31.20	C
	ATOM	1721	C13	LIG A 225	4.156	4.050	8.475	1.00	30.30	C
	ATOM	1722	O	HOH A 226	-2.926	11.994	16.430	1.00	23.78	O
	ATOM	1723	O	HOH A 227	7.624	-6.521	23.675	1.00	29.38	O
	ATOM	1724	O	HOH A 228	13.817	6.336	2.008	1.00	28.00	O
15	ATOM	1725	O	HOH A 229	16.341	10.485	19.389	1.00	35.55	O
	ATOM	1726	O	HOH A 230	16.478	-14.115	14.739	1.00	35.78	O
	ATOM	1727	O	HOH A 231	32.810	5.291	9.188	1.00	30.64	O
	ATOM	1728	O	HOH A 232	29.090	-5.851	7.975	1.00	35.24	O
	ATOM	1729	O	HOH A 233	25.117	-5.956	3.762	1.00	32.99	O
20	ATOM	1730	O	HOH A 234	18.757	4.728	2.761	1.00	32.33	O
	ATOM	1731	O	HOH A 235	8.741	-14.939	12.359	1.00	31.82	O
	ATOM	1732	O	HOH A 236	21.357	2.356	18.894	1.00	28.10	O
	ATOM	1733	O	HOH A 237	28.782	5.613	16.861	1.00	35.20	O
	ATOM	1734	O	HOH A 238	16.706	15.219	12.524	1.00	33.28	O
25	ATOM	1735	O	HOH A 239	21.819	3.360	21.629	1.00	49.03	O
	ATOM	1736	O	HOH A 240	1.530	8.816	4.640	1.00	30.48	O
	ATOM	1737	O	HOH A 241	22.615	-7.876	17.877	1.00	33.84	O
	ATOM	1738	O	HOH A 242	0.533	4.688	21.359	1.00	35.93	O
	ATOM	1739	O	HOH A 243	13.127	-12.150	20.913	1.00	36.61	O
30	ATOM	1740	O	HOH A 244	6.102	-1.332	2.296	1.00	31.28	O
	ATOM	1741	O	HOH A 245	2.124	-4.676	29.228	1.00	34.96	O
	ATOM	1742	O	HOH A 246	18.884	-8.789	-3.797	1.00	40.47	O
	ATOM	1743	O	HOH A 247	6.251	10.113	2.759	1.00	32.42	O
	ATOM	1744	O	HOH A 248	5.332	8.411	30.641	1.00	38.22	O
35	ATOM	1745	O	HOH A 249	24.705	-10.128	20.947	1.00	41.28	O

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	ATOM	1746	O	HOH A 250	-1.707	-15.022	18.012	1.00	39.35	O
	ATOM	1747	O	HOH A 251	1.712	11.191	22.084	1.00	33.35	O
	ATOM	1748	O	HOH A 252	-0.184	-18.059	12.907	1.00	47.63	O
	ATOM	1749	O	HOH A 253	9.273	20.194	12.046	1.00	38.97	O
5	ATOM	1750	O	HOH A 254	13.435	-4.921	48.730	1.00	46.07	O
	ATOM	1751	O	HOH A 255	15.751	13.083	22.390	1.00	49.56	O
	ATOM	1752	O	HOH A 256	-4.254	-17.035	2.181	1.00	48.94	O
	ATOM	1753	O	HOH A 257	0.451	-5.603	0.610	1.00	48.91	O
	ATOM	1754	O	HOH A 258	25.850	7.170	18.289	1.00	39.33	O
10	ATOM	1755	O	HOH A 259	-5.430	-9.543	14.591	1.00	48.23	O
	ATOM	1756	O	HOH A 260	-0.183	22.554	11.847	1.00	51.84	O
	ATOM	1757	O	HOH A 261	8.834	-9.330	46.716	1.00	41.33	O
	ATOM	1758	O	HOH A 262	26.958	-9.522	-3.917	1.00	38.48	O
	ATOM	1759	O	HOH A 263	7.922	-19.333	11.325	1.00	39.24	O
15	ATOM	1760	O	HOH A 264	-0.326	10.608	17.407	1.00	34.44	O
	ATOM	1761	O	HOH A 265	3.489	12.282	25.129	1.00	42.17	O
	ATOM	1762	O	HOH A 266	15.392	5.390	-3.654	1.00	43.08	O
	ATOM	1763	O	HOH A 267	11.897	-17.183	10.749	1.00	37.15	O
	ATOM	1764	O	HOH A 268	16.194	15.246	18.337	1.00	50.58	O
20	ATOM	1765	O	HOH A 269	8.167	-14.946	22.395	1.00	43.51	O
	ATOM	1766	O	HOH A 270	24.467	-12.587	14.924	1.00	39.56	O
	ATOM	1767	O	HOH A 271	13.473	12.086	18.725	1.00	39.98	O
	ATOM	1768	O	HOH A 272	-6.913	5.489	16.802	1.00	61.42	O
	ATOM	1769	O	HOH A 273	-7.909	-8.458	14.260	1.00	82.05	O
25	ATOM	1770	O	HOH A 274	28.512	-4.006	1.448	1.00	44.87	O
	ATOM	1771	O	HOH A 275	29.513	-3.503	17.254	1.00	38.64	O
	ATOM	1772	O	HOH A 276	-6.214	-9.563	3.077	1.00	67.24	O
	ATOM	1773	O	HOH A 277	-5.592	-4.268	21.101	1.00	43.16	O
	ATOM	1774	O	HOH A 278	30.753	3.611	2.527	1.00	40.37	O
30	ATOM	1775	O	HOH A 279	-1.858	-14.361	15.105	1.00	50.25	O
	ATOM	1776	O	HOH A 280	12.699	-19.974	4.554	1.00	42.27	O
	ATOM	1777	O	HOH A 281	25.517	1.253	25.129	1.00	43.95	O
	ATOM	1778	O	HOH A 282	-6.806	15.912	12.161	1.00	49.15	O
	ATOM	1779	O	HOH A 283	-2.970	7.084	13.181	1.00	42.59	O
35	ATOM	1780	O	HOH A 284	-3.352	-17.230	21.442	1.00	54.52	O

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	ATOM	1781	O	HOH A 285	15.963	-3.277	22.900	1.00	47.17	O
	ATOM	1782	O	HOH A 286	-4.214	-5.646	28.995	1.00	52.24	O
	ATOM	1783	O	HOH A 287	12.986	6.189	-7.947	1.00	65.53	O
	ATOM	1784	O	HOH A 288	-5.395	0.425	20.325	1.00	44.56	O
5	ATOM	1785	O	HOH A 289	7.276	14.177	19.269	1.00	39.91	O
	ATOM	1786	O	HOH A 290	23.146	-13.403	4.216	1.00	44.08	O
	ATOM	1787	O	HOH A 291	6.635	3.498	3.365	1.00	36.00	O
	ATOM	1788	O	HOH A 292	10.653	6.618	-4.580	1.00	63.63	O
	ATOM	1789	O	HOH A 293	32.485	0.750	21.406	1.00	54.36	O
10	ATOM	1790	O	HOH A 294	0.184	19.197	0.065	1.00	54.75	O
	ATOM	1791	O	HOH A 295	0.046	-7.325	9.756	1.00	40.06	O
	ATOM	1792	O	HOH A 296	17.415	9.299	24.640	1.00	52.56	O
	ATOM	1793	O	HOH A 297	15.336	16.375	23.489	1.00	50.96	O
	ATOM	1794	O	HOH A 298	20.133	-9.655	19.791	1.00	37.94	O
15	ATOM	1795	O	HOH A 299	-0.723	15.870	21.615	1.00	50.61	O
	ATOM	1796	O	HOH A 300	-1.616	12.139	24.098	1.00	47.73	O
	ATOM	1797	O	HOH A 301	19.031	-12.486	4.447	1.00	40.33	O
	ATOM	1798	O	HOH A 302	5.207	21.387	13.008	1.00	55.85	O
	ATOM	1799	O	HOH A 303	-5.786	-18.840	-2.485	1.00	46.35	O
20	ATOM	1800	O	HOH A 304	9.526	7.236	0.601	1.00	54.32	O
	ATOM	1801	O	HOH A 305	-6.051	-13.150	14.311	1.00	60.94	O
	ATOM	1802	O	HOH A 306	9.869	10.079	18.997	1.00	36.35	O
	ATOM	1803	O	HOH A 307	19.932	-14.226	8.448	1.00	45.96	O
	ATOM	1804	O	HOH A 308	10.989	2.661	-0.114	1.00	46.74	O
25	ATOM	1805	O	HOH A 309	33.525	-0.901	19.562	1.00	61.64	O
	ATOM	1806	O	HOH A 310	30.961	-5.173	4.547	1.00	46.99	O
	ATOM	1807	O	HOH A 311	13.900	9.740	-1.263	1.00	51.41	O
	ATOM	1808	O	HOH A 312	8.441	-8.792	-11.008	1.00	62.61	O
	ATOM	1809	O	HOH A 313	10.708	20.197	22.860	1.00	64.41	O
30	ATOM	1810	O	HOH A 314	-0.617	-19.337	18.621	1.00	39.71	O
	ATOM	1811	O	HOH A 315	12.530	-19.486	-10.879	1.00	56.60	O
	ATOM	1812	O	HOH A 316	5.354	-23.472	1.081	1.00	60.56	O
	ATOM	1813	O	HOH A 317	-7.706	-15.992	2.435	1.00	52.56	O
	ATOM	1814	O	HOH A 318	30.114	0.592	0.329	1.00	53.04	O
35	ATOM	1815	O	HOH A 319	28.639	-9.010	5.736	1.00	46.06	O

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	ATOM	1816	O	HOH A 320	3.868	24.395	8.425	1.00	40.64	O
	ATOM	1817	O	HOH A 321	2.009	4.490	5.067	1.00	40.13	O
	ATOM	1818	O	HOH A 322	25.056	-13.498	10.238	1.00	49.63	O
	ATOM	1819	O	HOH A 323	7.544	17.475	4.028	1.00	48.11	O
5	ATOM	1820	O	HOH A 324	3.058	5.665	28.312	1.00	36.70	O
	ATOM	1821	O	HOH A 325	10.621	-21.209	8.798	1.00	50.92	O
	ATOM	1822	O	HOH A 326	-2.508	-3.160	27.410	1.00	49.43	O
	ATOM	1823	O	HOH A 327	6.035	-2.023	5.693	1.00	45.33	O
	ATOM	1824	O	HOH A 328	-4.140	21.875	24.411	1.00	66.09	O
10	ATOM	1825	O	HOH A 329	7.204	-20.403	7.832	1.00	51.82	O
	ATOM	1826	O	HOH A 330	20.065	-18.683	7.680	1.00	54.31	O
	ATOM	1827	O	HOH A 331	24.222	3.651	26.969	1.00	57.60	O
	ATOM	1828	O	HOH A 332	19.728	-13.691	12.521	1.00	61.14	O
	ATOM	1829	O	HOH A 333	9.145	-10.788	28.651	1.00	56.09	O
15	ATOM	1830	O	HOH A 334	7.986	15.720	23.264	1.00	55.52	O
	ATOM	1831	O	HOH A 335	-4.799	14.683	20.179	1.00	52.49	O
	ATOM	1832	O	HOH A 336	10.476	15.868	-0.380	1.00	51.21	O
	ATOM	1833	O	HOH A 337	-1.059	-7.021	39.088	1.00	60.61	O
	ATOM	1834	O	HOH A 338	-7.539	1.550	18.329	1.00	62.68	O
20	ATOM	1835	O	HOH A 339	16.143	3.042	23.384	1.00	46.56	O
	ATOM	1836	O	HOH A 340	11.160	24.175	23.525	1.00	57.97	O
	ATOM	1837	O	HOH A 341	12.357	-22.347	0.538	1.00	54.88	O
	ATOM	1838	O	HOH A 342	11.941	2.004	25.550	1.00	42.66	O
	ATOM	1839	O	HOH A 343	7.905	-13.010	27.159	1.00	53.55	O
25	ATOM	1840	O	HOH A 344	-6.082	3.085	15.462	1.00	58.16	O
	ATOM	1841	O	HOH A 345	22.142	0.837	26.024	1.00	53.78	O
	ATOM	1842	O	HOH A 346	23.771	-17.057	12.641	1.00	71.14	O
	ATOM	1843	O	HOH A 347	32.585	-4.908	14.552	1.00	47.05	O
	ATOM	1844	O	HOH A 348	19.347	3.138	-6.132	1.00	61.85	O
30	ATOM	1845	O	HOH A 349	1.065	-1.907	3.753	1.00	50.31	O
	ATOM	1846	O	HOH A 350	14.439	1.353	24.589	1.00	52.71	O
	ATOM	1847	O	HOH A 351	12.012	16.177	23.105	1.00	53.75	O
	ATOM	1848	O	HOH A 352	15.294	-19.813	-0.870	1.00	59.96	O
	ATOM	1849	O	HOH A 353	14.076	-6.632	-9.756	1.00	51.74	O
35	ATOM	1850	O	HOH A 354	-8.841	-9.292	4.686	1.00	55.08	O

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	ATOM	1851	O	HOH A 355	26.268	-1.415	-1.766	1.00	61.08	O
	ATOM	1852	O	HOH A 356	-5.474	-4.898	1.359	1.00	69.00	O
	ATOM	1853	O	HOH A 357	-8.241	-17.528	4.628	1.00	70.83	O
	ATOM	1854	O	HOH A 358	11.216	-3.525	32.584	1.00	56.70	O
5	ATOM	1855	O	HOH A 359	14.709	22.108	10.753	1.00	50.11	O
	ATOM	1856	O	HOH A 360	4.453	1.909	-1.652	1.00	60.04	O
	ATOM	1857	O	HOH A 361	-8.728	10.843	21.793	1.00	66.37	O
	ATOM	1858	O	HOH A 362	7.570	4.727	29.051	1.00	45.94	O
	ATOM	1859	O	HOH A 363	4.235	15.532	26.428	1.00	52.42	O
10	ATOM	1860	O	HOH A 364	31.741	6.249	16.573	1.00	43.63	O
	ATOM	1861	O	HOH A 365	15.351	-2.566	-7.631	1.00	75.74	O
	ATOM	1862	O	HOH A 366	37.693	-5.753	11.952	1.00	53.92	O
	ATOM	1863	O	HOH A 367	30.299	-9.293	19.630	1.00	69.31	O
	ATOM	1864	O	HOH A 368	28.008	-12.519	18.950	1.00	58.71	O
15	ATOM	1865	O	HOH A 369	-9.315	16.796	13.340	1.00	54.98	O
	ATOM	1866	O	HOH A 370	-3.012	-5.500	2.158	1.00	55.26	O
	ATOM	1867	O	HOH A 371	-3.476	3.089	8.685	1.00	57.30	O
	ATOM	1868	O	HOH A 372	16.084	18.253	12.987	1.00	50.64	O
	ATOM	1869	O	HOH A 373	20.311	0.081	22.050	1.00	50.33	O
20	ATOM	1870	O	HOH A 374	17.876	-23.028	-1.642	1.00	53.63	O
	ATOM	1871	O	HOH A 375	-5.304	-10.657	17.680	1.00	67.83	O
	ATOM	1872	O	HOH A 376	2.158	-0.349	-2.981	1.00	56.23	O
	ATOM	1873	O	HOH A 377	14.007	24.740	13.054	1.00	73.66	O
	ATOM	1874	O	HOH A 378	13.742	17.699	2.975	1.00	70.71	O
25	ATOM	1875	O	HOH A 379	16.495	-22.536	-3.870	1.00	74.58	O
	ATOM	1876	O	HOH A 380	-11.841	-7.606	14.987	1.00	60.60	O
	ATOM	1877	O	HOH A 381	9.237	13.539	25.412	1.00	55.57	O
	ATOM	1878	O	HOH A 382	7.824	19.503	8.543	1.00	55.74	O
	ATOM	1879	O	HOH A 383	4.346	-3.433	7.215	1.00	55.62	O
30	ATOM	1880	O	HOH A 384	-13.812	14.182	19.483	1.00	64.83	O
	ATOM	1881	O	HOH A 385	-12.578	-8.808	17.485	1.00	62.68	O
	ATOM	1882	O	HOH A 386	-16.566	-10.700	19.943	1.00	64.24	O
	ATOM	1883	O	HOH A 387	33.372	10.108	16.177	1.00	72.34	O
	ATOM	1884	O	HOH A 388	27.798	-6.645	3.473	1.00	49.37	O
35	ATOM	1885	O	HOH A 389	14.340	-22.872	-11.849	1.00	70.54	O

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	ATOM	1886	O	HOH A 390	16.037	-3.040	-13.123	1.00	62.94	O
	ATOM	1887	O	HOH A 391	-3.871	-16.219	11.035	1.00	52.50	O
	ATOM	1888	O	HOH A 392	-5.523	25.172	26.712	1.00	52.78	O
	ATOM	1889	O	HOH A 393	-18.175	-7.777	18.448	1.00	70.80	O
5	ATOM	1890	O	HOH A 394	17.085	26.042	11.178	1.00	61.57	O
	ATOM	1891	O	HOH A 395	11.400	4.967	13.511	1.00	28.22	O
	ATOM	1892	O	HOH A 396	11.710	3.549	10.726	1.00	26.84	O
	ATOM	1893	O	HOH A 397	5.680	7.230	13.921	1.00	27.89	O
	ATOM	1894	O	HOH A 398	18.635	2.168	2.031	1.00	32.31	O
10	ATOM	1895	O	HOH A 399	28.969	5.546	14.059	1.00	35.00	O
	ATOM	1896	O	HOH A 400	31.679	5.761	12.673	1.00	44.67	O
	ATOM	1897	O	HOH A 401	2.491	-6.526	8.480	1.00	34.22	O
	ATOM	1898	O	HOH A 402	10.520	-13.909	18.050	1.00	32.67	O
	ATOM	1899	O	HOH A 403	9.063	-16.960	10.565	1.00	34.63	O
15	ATOM	1900	O	HOH A 404	20.344	-18.312	-0.828	1.00	40.32	O
	ATOM	1901	O	HOH A 405	2.647	9.940	2.468	1.00	36.86	O
	ATOM	1902	O	HOH A 406	0.395	6.716	5.573	1.00	50.97	O
	ATOM	1903	O	HOH A 407	17.155	15.707	15.829	1.00	49.51	O
	ATOM	1904	O	HOH A 408	29.061	3.869	19.219	1.00	42.07	O
20	ATOM	1905	O	HOH A 409	29.473	-6.627	17.611	1.00	43.21	O
	ATOM	1906	O	HOH A 410	-5.599	-1.061	14.033	1.00	41.40	O
	ATOM	1907	O	HOH A 411	17.665	-12.026	10.578	1.00	65.08	O
	ATOM	1908	O	HOH A 412	10.382	-5.541	24.229	1.00	53.11	O
	ATOM	1909	O	HOH A 413	8.431	-13.214	20.405	1.00	36.78	O
25	ATOM	1910	O	HOH A 414	30.083	-7.282	10.580	1.00	46.01	O
	ATOM	1911	O	HOH A 415	25.613	-10.213	3.464	1.00	34.49	O
	ATOM	1912	O	HOH A 416	30.839	-1.206	13.063	1.00	37.28	O

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Table 5. Atomic Coordinates of Hsp90 with Compound 247

		Atom Amino Acid				Temp.	
	Atom Number	Type	Residue	X	Y	Z	Occ. Factor
5	ATOM	1	N PRO A 11	10.769	-4.028	46.831	1.00 37.92
	ATOM	2	CA PRO A 11	9.647	-4.915	46.529	1.00 37.68
	ATOM	3	CB PRO A 11	8.418	-4.094	46.946	1.00 37.48
	ATOM	4	CG PRO A 11	8.935	-3.037	47.847	1.00 37.97
	ATOM	5	CD PRO A 11	10.320	-2.730	47.363	1.00 38.10
10	ATOM	6	C PRO A 11	9.600	-5.218	45.038	1.00 36.91
	ATOM	7	O PRO A 11	9.899	-4.345	44.230	1.00 37.31
	ATOM	8	N MET A 12	9.226	-6.444	44.683	1.00 36.11
	ATOM	9	CA MET A 12	9.239	-6.871	43.289	1.00 35.08
	ATOM	10	CB MET A 12	8.876	-8.357	43.175	1.00 34.98
15	ATOM	11	CG MET A 12	8.948	-8.891	41.755	1.00 34.64
	ATOM	12	SD MET A 12	9.093	-10.675	41.681	1.00 33.41
	ATOM	13	CE MET A 12	7.554	-11.177	42.452	1.00 33.57
	ATOM	14	C MET A 12	8.304	-6.034	42.419	1.00 35.13
	ATOM	15	O MET A 12	7.152	-5.791	42.784	1.00 35.57
20	ATOM	16	N GLU A 13	8.814	-5.597	41.273	1.00 34.77
	ATOM	17	CA GLU A 13	8.008	-4.902	40.280	1.00 34.77
	ATOM	18	CB GLU A 13	8.895	-4.038	39.381	1.00 34.89
	ATOM	19	C GLU A 13	7.227	-5.901	39.432	1.00 34.77
	ATOM	20	O GLU A 13	7.597	-7.072	39.323	1.00 34.20
25	ATOM	21	N GLU A 14	6.149	-5.425	38.825	1.00 34.87
	ATOM	22	CA GLU A 14	5.292	-6.273	38.013	1.00 35.32
	ATOM	23	CB GLU A 14	4.064	-6.669	38.823	1.00 35.59
	ATOM	24	CG GLU A 14	3.182	-7.685	38.167	1.00 38.06
	ATOM	25	CD GLU A 14	2.468	-8.533	39.183	1.00 41.49
30	ATOM	26	OE1 GLU A 14	2.513	-9.768	39.030	1.00 44.03
	ATOM	27	OE2 GLU A 14	1.884	-7.981	40.148	1.00 42.96
	ATOM	28	C GLU A 14	4.888	-5.542	36.744	1.00 35.04
	ATOM	29	O GLU A 14	4.415	-4.405	36.805	1.00 35.38
	ATOM	30	N GLU A 15	5.087	-6.195	35.600	1.00 34.60
35	ATOM	31	CA GLU A 15	4.757	-5.621	34.301	1.00 34.46

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	ATOM	32	CB	GLU A 15	6.023	-5.262	33.524	1.00	34.75
	ATOM	33	CG	GLU A 15	6.858	-4.147	34.135	1.00	37.04
	ATOM	34	CD	GLU A 15	7.832	-3.556	33.141	1.00	40.06
	ATOM	35	OE1	GLU A 15	8.934	-3.133	33.565	1.00	42.15
5	ATOM	36	OE2	GLU A 15	7.497	-3.517	31.932	1.00	40.77
	ATOM	37	C	GLU A 15	3.915	-6.578	33.468	1.00	33.96
	ATOM	38	O	GLU A 15	4.235	-7.766	33.355	1.00	33.50
	ATOM	39	N	GLU A 16	2.844	-6.050	32.882	1.00	33.44
	ATOM	40	CA	GLU A 16	1.989	-6.818	31.982	1.00	33.23
10	ATOM	41	CB	GLU A 16	0.588	-6.198	31.936	1.00	33.46
	ATOM	42	CG	GLU A 16	-0.445	-6.985	31.152	1.00	35.03
	ATOM	43	CD	GLU A 16	-1.757	-6.225	30.970	1.00	36.04
	ATOM	44	OE1	GLU A 16	-2.450	-6.476	29.954	1.00	39.67
	ATOM	45	OE2	GLU A 16	-2.088	-5.374	31.832	1.00	39.21
15	ATOM	46	C	GLU A 16	2.603	-6.867	30.582	1.00	32.11
	ATOM	47	O	GLU A 16	3.156	-5.876	30.103	1.00	32.06
	ATOM	48	N	VAL A 17	2.513	-8.034	29.949	1.00	30.97
	ATOM	49	CA	VAL A 17	2.967	-8.230	28.569	1.00	30.25
	ATOM	50	CB	VAL A 17	4.373	-8.919	28.500	1.00	30.19
20	ATOM	51	CG1	VAL A 17	4.335	-10.336	29.053	1.00	30.77
	ATOM	52	CG2	VAL A 17	4.909	-8.929	27.072	1.00	30.19
	ATOM	53	C	VAL A 17	1.924	-9.023	27.782	1.00	29.58
	ATOM	54	O	VAL A 17	1.278	-9.926	28.323	1.00	29.34
	ATOM	55	N	GLU A 18	1.753	-8.667	26.512	1.00	28.31
25	ATOM	56	CA	GLU A 18	0.876	-9.397	25.614	1.00	28.20
	ATOM	57	CB	GLU A 18	-0.179	-8.473	25.012	1.00	28.38
	ATOM	58	CG	GLU A 18	-1.227	-8.021	26.022	1.00	31.04
	ATOM	59	CD	GLU A 18	-2.287	-7.140	25.405	1.00	34.79
	ATOM	60	OE1	GLU A 18	-2.238	-5.917	25.645	1.00	36.86
30	ATOM	61	OE2	GLU A 18	-3.169	-7.669	24.692	1.00	36.80
	ATOM	62	C	GLU A 18	1.716	-10.033	24.517	1.00	27.48
	ATOM	63	O	GLU A 18	2.417	-9.336	23.790	1.00	26.61
	ATOM	64	N	THR A 19	1.664	-11.354	24.423	1.00	26.94
	ATOM	65	CA	THR A 19	2.419	-12.059	23.392	1.00	26.95
35	ATOM	66	CB	THR A 19	3.217	-13.239	23.981	1.00	27.43

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	ATOM	67	OG1 THR A 19	4.112 -12.741 24.986 1.00 27.25
	ATOM	68	CG2 THR A 19	4.017 -13.972 22.879 1.00 27.05
	ATOM	69	C THR A 19	1.482 -12.499 22.282 1.00 26.79
	ATOM	70	O THR A 19	0.448 -13.125 22.539 1.00 26.53
5	ATOM	71	N PHE A 20	1.847 -12.152 21.046 1.00 26.49
	ATOM	72	CA PHE A 20	1.058 -12.473 19.856 1.00 26.37
	ATOM	73	CB PHE A 20	0.653 -11.193 19.120 1.00 26.31
	ATOM	74	CG PHE A 20	-0.306 -10.327 19.883 1.00 26.72
	ATOM	75	CD1 PHE A 20	0.160 -9.395 20.807 1.00 25.39
10	ATOM	76	CE1 PHE A 20	-0.726 -8.595 21.517 1.00 27.79
	ATOM	77	CZ PHE A 20	-2.096 -8.728 21.312 1.00 27.64
	ATOM	78	CE2 PHE A 20	-2.573 -9.649 20.395 1.00 28.43
	ATOM	79	CD2 PHE A 20	-1.670 -10.447 19.680 1.00 27.46
	ATOM	80	C PHE A 20	1.842 -13.338 18.880 1.00 26.56
15	ATOM	81	O PHE A 20	3.036 -13.108 18.672 1.00 26.62
	ATOM	82	N ALA A 21	1.148 -14.302 18.269 1.00 26.30
	ATOM	83	CA ALA A 21	1.650 -15.039 17.107 1.00 26.08
	ATOM	84	CB ALA A 21	0.862 -16.343 16.927 1.00 26.19
	ATOM	85	C ALA A 21	1.533 -14.187 15.844 1.00 25.61
20	ATOM	86	O ALA A 21	0.505 -13.554 15.610 1.00 25.25
	ATOM	87	N PHE A 22	2.573 -14.172 15.014 1.00 25.33
	ATOM	88	CA PHE A 22	2.429 -13.558 13.695 1.00 25.22
	ATOM	89	CB PHE A 22	3.762 -13.492 12.940 1.00 24.61
	ATOM	90	CG PHE A 22	4.682 -12.405 13.421 1.00 23.85
25	ATOM	91	CD1 PHE A 22	4.432 -11.060 13.104 1.00 23.23
	ATOM	92	CE1 PHE A 22	5.290 -10.051 13.548 1.00 21.32
	ATOM	93	CZ PHE A 22	6.415 -10.379 14.305 1.00 22.72
	ATOM	94	CE2 PHE A 22	6.674 -11.712 14.619 1.00 23.40
	ATOM	95	CD2 PHE A 22	5.807 -12.718 14.174 1.00 23.08
30	ATOM	96	C PHE A 22	1.428 -14.360 12.872 1.00 25.50
	ATOM	97	O PHE A 22	1.401 -15.594 12.940 1.00 25.97
	ATOM	98	N GLN A 23	0.604 -13.656 12.103 1.00 25.56
	ATOM	99	CA GLN A 23	-0.209 -14.274 11.062 1.00 25.83
	ATOM	100	CB GLN A 23	-0.873 -13.177 10.230 1.00 26.11
35	ATOM	101	CG GLN A 23	-2.051 -13.629 9.377 1.00 27.76

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	ATOM	102	CD	GLN A 23	-1.616	-14.164	8.036	1.00	29.20
	ATOM	103	OE1	GLN A 23	-0.522	-13.853	7.556	1.00	31.90
	ATOM	104	NE2	GLN A 23	-2.462	-14.972	7.420	1.00	30.87
	ATOM	105	C	GLN A 23	0.737	-15.123	10.207	1.00	25.82
5	ATOM	106	O	GLN A 23	1.884	-14.729	9.990	1.00	25.38
	ATOM	107	N	ALA A 24	0.271	-16.293	9.755	1.00	25.61
	ATOM	108	CA	ALA A 24	1.150	-17.288	9.123	1.00	25.99
	ATOM	109	CB	ALA A 24	0.370	-18.571	8.790	1.00	25.81
	ATOM	110	C	ALA A 24	1.937	-16.800	7.904	1.00	25.86
10	ATOM	111	O	ALA A 24	3.107	-17.155	7.743	1.00	26.80
	ATOM	112	N	GLU A 25	1.310	-15.996	7.051	1.00	25.87
	ATOM	113	CA	GLU A 25	1.990	-15.466	5.864	1.00	26.20
	ATOM	114	CB	GLU A 25	0.992	-14.859	4.880	1.00	26.32
	ATOM	115	CG	GLU A 25	0.167	-15.907	4.106	1.00	28.81
15	ATOM	116	CD	GLU A 25	-1.134	-15.350	3.530	1.00	29.67
	ATOM	117	OE1	GLU A 25	-1.500	-14.199	3.855	1.00	34.74
	ATOM	118	OE2	GLU A 25	-1.796	-16.069	2.740	1.00	35.19
	ATOM	119	C	GLU A 25	3.076	-14.460	6.243	1.00	24.66
	ATOM	120	O	GLU A 25	4.148	-14.419	5.632	1.00	23.79
20	ATOM	121	N	ILE A 26	2.794	-13.655	7.261	1.00	23.65
	ATOM	122	CA	ILE A 26	3.799	-12.746	7.806	1.00	23.27
	ATOM	123	CB	ILE A 26	3.181	-11.750	8.827	1.00	23.42
	ATOM	124	CG1	ILE A 26	2.183	-10.831	8.098	1.00	23.14
	ATOM	125	CD1	ILE A 26	1.375	-9.916	9.010	1.00	23.56
25	ATOM	126	CG2	ILE A 26	4.285	-10.945	9.519	1.00	23.48
	ATOM	127	C	ILE A 26	4.970	-13.520	8.414	1.00	23.20
	ATOM	128	O	ILE A 26	6.131	-13.146	8.230	1.00	22.65
	ATOM	129	N	ALA A 27	4.667	-14.595	9.142	1.00	22.87
	ATOM	130	CA	ALA A 27	5.716	-15.436	9.694	1.00	23.56
30	ATOM	131	CB	ALA A 27	5.121	-16.524	10.609	1.00	23.76
	ATOM	132	C	ALA A 27	6.560	-16.045	8.561	1.00	24.19
	ATOM	133	O	ALA A 27	7.779	-16.074	8.651	1.00	24.02
	ATOM	134	N	GLN A 28	5.907	-16.494	7.492	1.00	25.09
	ATOM	135	CA	GLN A 28	6.617	-17.039	6.332	1.00	26.99
35	ATOM	136	CB	GLN A 28	5.651	-17.629	5.305	1.00	26.76

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	ATOM	137	CG	GLN A 28	4.839	-18.829	5.783	1.00	29.97
	ATOM	138	CD	GLN A 28	3.771	-19.251	4.785	1.00	30.38
	ATOM	139	OE1	GLN A 28	2.576	-19.302	5.113	1.00	36.86
	ATOM	140	NE2	GLN A 28	4.193	-19.558	3.562	1.00	35.08
5	ATOM	141	C	GLN A 28	7.480	-15.968	5.661	1.00	26.11
	ATOM	142	O	GLN A 28	8.620	-16.224	5.300	1.00	26.69
	ATOM	143	N	LEU A 29	6.930	-14.770	5.490	1.00	25.91
	ATOM	144	CA	LEU A 29	7.697	-13.656	4.920	1.00	25.57
	ATOM	145	CB	LEU A 29	6.808	-12.407	4.786	1.00	25.81
10	ATOM	146	CG	LEU A 29	7.439	-11.094	4.300	1.00	26.82
	ATOM	147	CD1	LEU A 29	7.859	-11.218	2.845	1.00	27.12
	ATOM	148	CD2	LEU A 29	6.454	-9.933	4.477	1.00	25.31
	ATOM	149	C	LEU A 29	8.979	-13.346	5.718	1.00	25.14
	ATOM	150	O	LEU A 29	10.060	-13.194	5.129	1.00	25.22
15	ATOM	151	N	MET A 30	8.859	-13.247	7.045	1.00	24.24
	ATOM	152	CA	MET A 30	10.008	-12.966	7.916	1.00	24.24
	ATOM	153	CB	MET A 30	9.573	-12.777	9.382	1.00	24.06
	ATOM	154	CG	MET A 30	8.789	-11.493	9.608	1.00	23.00
	ATOM	155	SD	MET A 30	8.046	-11.328	11.259	1.00	22.79
20	ATOM	156	CE	MET A 30	9.456	-10.800	12.218	1.00	23.09
	ATOM	157	C	MET A 30	11.094	-14.036	7.797	1.00	24.91
	ATOM	158	O	MET A 30	12.275	-13.713	7.670	1.00	25.28
	ATOM	159	N	SER A 31	10.685	-15.302	7.798	1.00	25.69
	ATOM	160	CA	SER A 31	11.612	-16.420	7.566	1.00	26.14
25	ATOM	161	CB	SER A 31	10.872	-17.759	7.647	1.00	26.45
	ATOM	162	OG	SER A 31	11.765	-18.836	7.399	1.00	29.22
	ATOM	163	C	SER A 31	12.373	-16.287	6.240	1.00	25.84
	ATOM	164	O	SER A 31	13.602	-16.436	6.208	1.00	26.37
	ATOM	165	N	LEU A 32	11.653	-16.005	5.154	1.00	25.95
30	ATOM	166	CA	LEU A 32	12.288	-15.795	3.846	1.00	25.82
	ATOM	167	CB	LEU A 32	11.250	-15.608	2.732	1.00	26.10
	ATOM	168	CG	LEU A 32	10.413	-16.839	2.334	1.00	26.60
	ATOM	169	CD1	LEU A 32	9.105	-16.420	1.694	1.00	28.36
	ATOM	170	CD2	LEU A 32	11.186	-17.805	1.429	1.00	28.91
35	ATOM	171	C	LEU A 32	13.266	-14.619	3.877	1.00	25.80

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	ATOM	172	O	LEU A 32	14.381	-14.731	3.366	1.00	25.45
	ATOM	173	N	ILE A 33	12.858	-13.509	4.493	1.00	24.93
	ATOM	174	CA	ILE A 33	13.737	-12.341	4.641	1.00	25.65
	ATOM	175	CB	ILE A 33	12.994	-11.114	5.269	1.00	25.34
5	ATOM	176	CG1	ILE A 33	11.980	-10.533	4.276	1.00	24.10
	ATOM	177	CD1	ILE A 33	10.921	-9.639	4.924	1.00	24.70
	ATOM	178	CG2	ILE A 33	13.983	-10.017	5.700	1.00	25.40
	ATOM	179	C	ILE A 33	15.003	-12.666	5.435	1.00	26.63
	ATOM	180	O	ILE A 33	16.108	-12.245	5.061	1.00	26.76
10	ATOM	181	N	ILE A 34	14.838	-13.424	6.516	1.00	27.71
	ATOM	182	CA	ILE A 34	15.937	-13.723	7.440	1.00	28.84
	ATOM	183	CB	ILE A 34	15.411	-14.112	8.859	1.00	28.54
	ATOM	184	CG1	ILE A 34	14.760	-12.891	9.519	1.00	29.20
	ATOM	185	CD1	ILE A 34	14.047	-13.187	10.825	1.00	28.57
15	ATOM	186	CG2	ILE A 34	16.547	-14.619	9.772	1.00	28.74
	ATOM	187	C	ILE A 34	16.896	-14.781	6.901	1.00	29.53
	ATOM	188	O	ILE A 34	18.103	-14.671	7.089	1.00	30.52
	ATOM	189	N	ASN A 35	16.364	-15.785	6.217	1.00	30.42
	ATOM	190	CA	ASN A 35	17.145	-16.978	5.864	1.00	31.23
20	ATOM	191	CB	ASN A 35	16.366	-18.233	6.258	1.00	31.75
	ATOM	192	CG	ASN A 35	16.105	-18.297	7.740	1.00	32.69
	ATOM	193	OD1	ASN A 35	17.036	-18.382	8.540	1.00	35.15
	ATOM	194	ND2	ASN A 35	14.838	-18.235	8.122	1.00	34.21
	ATOM	195	C	ASN A 35	17.616	-17.075	4.411	1.00	31.29
25	ATOM	196	O	ASN A 35	18.334	-18.011	4.043	1.00	32.28
	ATOM	197	N	THR A 36	17.233	-16.103	3.594	1.00	30.82
	ATOM	198	CA	THR A 36	17.638	-16.062	2.200	1.00	29.86
	ATOM	199	CB	THR A 36	16.429	-15.803	1.283	1.00	30.20
	ATOM	200	OG1	THR A 36	15.357	-16.694	1.634	1.00	30.53
30	ATOM	201	CG2	THR A 36	16.792	-16.001	-0.194	1.00	30.65
	ATOM	202	C	THR A 36	18.676	-14.962	2.022	1.00	29.58
	ATOM	203	O	THR A 36	18.584	-13.907	2.649	1.00	28.80
	ATOM	204	N	PHE A 37	19.658	-15.200	1.156	1.00	28.68
	ATOM	205	CA	PHE A 37	20.631	-14.157	0.840	1.00	28.43
35	ATOM	206	CB	PHE A 37	21.926	-14.739	0.259	1.00	28.28

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	ATOM	207	CG	PHE A 37	22.933	-13.694	-0.105	1.00	27.33
	ATOM	208	CD1	PHE A 37	23.025	-13.226	-1.408	1.00	27.01
	ATOM	209	CE1	PHE A 37	23.950	-12.230	-1.750	1.00	27.16
	ATOM	210	CZ	PHE A 37	24.783	-11.697	-0.774	1.00	26.78
5	ATOM	211	CE2	PHE A 37	24.694	-12.155	0.539	1.00	26.93
	ATOM	212	CD2	PHE A 37	23.769	-13.153	0.865	1.00	26.86
	ATOM	213	C	PHE A 37	20.056	-13.091	-0.096	1.00	28.38
	ATOM	214	O	PHE A 37	19.507	-13.403	-1.150	1.00	28.37
	ATOM	215	N	TYR A 38	20.211	-11.830	0.301	1.00	28.56
10	ATOM	216	CA	TYR A 38	19.830	-10.685	-0.527	1.00	29.11
	ATOM	217	CB	TYR A 38	18.560	-10.013	0.021	1.00	29.69
	ATOM	218	CG	TYR A 38	17.362	-10.934	0.005	1.00	30.12
	ATOM	219	CD1	TYR A 38	16.860	-11.481	1.184	1.00	30.36
	ATOM	220	CE1	TYR A 38	15.774	-12.342	1.166	1.00	29.75
15	ATOM	221	CZ	TYR A 38	15.178	-12.668	-0.039	1.00	30.60
	ATOM	222	OH	TYR A 38	14.111	-13.537	-0.068	1.00	31.59
	ATOM	223	CE2	TYR A 38	15.663	-12.151	-1.229	1.00	30.54
	ATOM	224	CD2	TYR A 38	16.745	-11.281	-1.199	1.00	30.27
	ATOM	225	C	TYR A 38	20.999	-9.724	-0.545	1.00	29.28
20	ATOM	226	O	TYR A 38	21.570	-9.433	0.504	1.00	28.98
	ATOM	227	N	SER A 39	21.387	-9.262	-1.730	1.00	29.45
	ATOM	228	CA	SER A 39	22.581	-8.421	-1.851	1.00	30.25
	ATOM	229	CB	SER A 39	23.194	-8.531	-3.252	1.00	30.06
	ATOM	230	OG	SER A 39	22.312	-8.023	-4.231	1.00	30.81
25	ATOM	231	C	SER A 39	22.340	-6.950	-1.500	1.00	30.53
	ATOM	232	O	SER A 39	23.271	-6.248	-1.098	1.00	32.07
	ATOM	233	N	ASN A 40	21.103	-6.489	-1.633	1.00	30.08
	ATOM	234	CA	ASN A 40	20.816	-5.049	-1.535	1.00	29.70
	ATOM	235	CB	ASN A 40	19.926	-4.633	-2.716	1.00	30.33
30	ATOM	236	CG	ASN A 40	19.927	-3.121	-2.976	1.00	32.63
	ATOM	237	OD1	ASN A 40	19.011	-2.595	-3.622	1.00	37.58
	ATOM	238	ND2	ASN A 40	20.949	-2.428	-2.499	1.00	34.60
	ATOM	239	C	ASN A 40	20.153	-4.693	-0.197	1.00	28.49
	ATOM	240	O	ASN A 40	19.101	-4.051	-0.167	1.00	27.69
35	ATOM	241	N	LYS A 41	20.788	-5.095	0.904	1.00	27.03

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	ATOM	242	CA	LYS A 41	20.153	-4.986	2.240	1.00	26.64
	ATOM	243	CB	LYS A 41	20.901	-5.837	3.273	1.00	26.24
	ATOM	244	CG	LYS A 41	20.878	-7.346	2.990	1.00	27.75
	ATOM	245	CD	LYS A 41	21.629	-8.109	4.068	1.00	27.63
5	ATOM	246	CE	LYS A 41	21.431	-9.619	3.949	1.00	31.59
	ATOM	247	NZ	LYS A 41	22.381	-10.216	2.964	1.00	32.45
	ATOM	248	C	LYS A 41	20.012	-3.543	2.736	1.00	25.88
	ATOM	249	O	LYS A 41	19.197	-3.265	3.616	1.00	24.74
	ATOM	250	N	GLU A 42	20.783	-2.626	2.151	1.00	24.94
10	ATOM	251	CA	GLU A 42	20.755	-1.217	2.564	1.00	25.61
	ATOM	252	CB	GLU A 42	21.824	-0.404	1.820	1.00	24.93
	ATOM	253	CG	GLU A 42	21.464	-0.081	0.366	1.00	26.92
	ATOM	254	CD	GLU A 42	22.634	0.444	-0.440	1.00	28.94
	ATOM	255	OE1	GLU A 42	22.390	1.049	-1.507	1.00	33.85
15	ATOM	256	OE2	GLU A 42	23.798	0.251	-0.022	1.00	34.00
	ATOM	257	C	GLU A 42	19.386	-0.538	2.405	1.00	24.60
	ATOM	258	O	GLU A 42	19.140	0.503	3.019	1.00	24.97
	ATOM	259	N	ILE A 43	18.511	-1.115	1.584	1.00	23.83
	ATOM	260	CA	ILE A 43	17.157	-0.574	1.376	1.00	23.41
20	ATOM	261	CB	ILE A 43	16.393	-1.303	0.226	1.00	24.13
	ATOM	262	CG1	ILE A 43	16.101	-2.766	0.572	1.00	24.73
	ATOM	263	CD1	ILE A 43	14.802	-3.013	1.313	1.00	27.64
	ATOM	264	CG2	ILE A 43	17.179	-1.199	-1.103	1.00	25.23
	ATOM	265	C	ILE A 43	16.300	-0.586	2.652	1.00	21.82
25	ATOM	266	O	ILE A 43	15.249	0.058	2.690	1.00	21.26
	ATOM	267	N	PHE A 44	16.726	-1.332	3.674	1.00	21.01
	ATOM	268	CA	PHE A 44	16.010	-1.336	4.978	1.00	20.01
	ATOM	269	CB	PHE A 44	16.732	-2.199	6.044	1.00	19.41
	ATOM	270	CG	PHE A 44	17.852	-1.477	6.763	1.00	19.84
30	ATOM	271	CD1	PHE A 44	19.141	-1.478	6.254	1.00	18.51
	ATOM	272	CE1	PHE A 44	20.166	-0.785	6.899	1.00	18.40
	ATOM	273	CZ	PHE A 44	19.904	-0.073	8.068	1.00	19.46
	ATOM	274	CE2	PHE A 44	18.626	-0.064	8.581	1.00	19.23
	ATOM	275	CD2	PHE A 44	17.607	-0.756	7.931	1.00	18.50
35	ATOM	276	C	PHE A 44	15.836	0.106	5.492	1.00	19.94

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	ATOM	277	O	PHE A 44	14.796	0.446	6.068	1.00	19.11
	ATOM	278	N	LEU A 45	16.848	0.949	5.275	1.00	20.05
	ATOM	279	CA	LEU A 45	16.805	2.315	5.829	1.00	19.87
	ATOM	280	CB	LEU A 45	18.205	2.954	5.954	1.00	20.08
5	ATOM	281	CG	LEU A 45	18.248	4.282	6.740	1.00	19.74
	ATOM	282	CD1	LEU A 45	19.645	4.948	6.763	1.00	20.32
	ATOM	283	CD2	LEU A 45	17.753	4.075	8.149	1.00	20.08
	ATOM	284	C	LEU A 45	15.847	3.227	5.073	1.00	20.02
	ATOM	285	O	LEU A 45	15.178	4.053	5.691	1.00	20.23
10	ATOM	286	N	ARG A 46	15.792	3.066	3.750	1.00	20.72
	ATOM	287	CA	ARG A 46	14.822	3.752	2.893	1.00	21.13
	ATOM	288	CB	ARG A 46	14.965	3.291	1.437	1.00	21.95
	ATOM	289	CG	ARG A 46	13.987	3.971	0.460	1.00	24.16
	ATOM	290	CD	ARG A 46	13.879	3.195	-0.847	1.00	28.00
15	ATOM	291	NE	ARG A 46	13.278	1.883	-0.627	1.00	33.54
	ATOM	292	CZ	ARG A 46	13.514	0.808	-1.374	1.00	36.00
	ATOM	293	NH1	ARG A 46	14.348	0.876	-2.409	1.00	37.87
	ATOM	294	NH2	ARG A 46	12.917	-0.340	-1.079	1.00	36.69
	ATOM	295	C	ARG A 46	13.421	3.444	3.380	1.00	21.00
20	ATOM	296	O	ARG A 46	12.585	4.345	3.484	1.00	20.61
	ATOM	297	N	GLU A 47	13.166	2.167	3.666	1.00	20.38
	ATOM	298	CA	GLU A 47	11.848	1.762	4.161	1.00	20.88
	ATOM	299	CB	GLU A 47	11.733	0.236	4.239	1.00	21.04
	ATOM	300	CG	GLU A 47	11.760	-0.440	2.855	1.00	23.05
25	ATOM	301	CD	GLU A 47	10.692	0.099	1.915	1.00	27.38
	ATOM	302	OE1	GLU A 47	9.518	0.275	2.335	1.00	27.90
	ATOM	303	OE2	GLU A 47	11.032	0.357	0.753	1.00	29.10
	ATOM	304	C	GLU A 47	11.469	2.403	5.484	1.00	20.17
	ATOM	305	O	GLU A 47	10.345	2.874	5.632	1.00	20.85
30	ATOM	306	N	LEU A 48	12.401	2.426	6.436	1.00	20.16
	ATOM	307	CA	LEU A 48	12.181	3.094	7.726	1.00	19.77
	ATOM	308	CB	LEU A 48	13.364	2.853	8.665	1.00	19.93
	ATOM	309	CG	LEU A 48	13.494	1.478	9.325	1.00	20.77
	ATOM	310	CD1	LEU A 48	14.958	1.176	9.588	1.00	21.36
35	ATOM	311	CD2	LEU A 48	12.712	1.446	10.636	1.00	21.54

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	ATOM	312	C	LEU A 48	11.913	4.591	7.540	1.00	20.00
	ATOM	313	O	LEU A 48	10.939	5.125	8.058	1.00	18.59
	ATOM	314	N	ILE A 49	12.753	5.257	6.759	1.00	19.48
	ATOM	315	CA	ILE A 49	12.573	6.695	6.519	1.00	20.50
5	ATOM	316	CB	ILE A 49	13.805	7.298	5.788	1.00	19.99
	ATOM	317	CG1	ILE A 49	15.034	7.205	6.709	1.00	20.63
	ATOM	318	CD1	ILE A 49	16.379	7.523	6.035	1.00	20.79
	ATOM	319	CG2	ILE A 49	13.539	8.758	5.389	1.00	21.83
	ATOM	320	C	ILE A 49	11.255	6.995	5.805	1.00	20.54
10	ATOM	321	O	ILE A 49	10.560	7.970	6.139	1.00	20.83
	ATOM	322	N	SER A 50	10.893	6.135	4.854	1.00	20.02
	ATOM	323	CA	SER A 50	9.629	6.271	4.143	1.00	20.33
	ATOM	324	CB	SER A 50	9.541	5.271	2.985	0.65	20.03
	ATOM	325	OG	SER A 50	8.259	5.291	2.389	0.65	20.44
15	ATOM	326	C	SER A 50	8.435	6.127	5.094	1.00	20.02
	ATOM	327	O	SER A 50	7.462	6.861	4.967	1.00	19.48
	ATOM	328	N	ASN A 51	8.516	5.203	6.055	1.00	19.91
	ATOM	329	CA	ASN A 51	7.415	5.050	7.008	1.00	20.06
	ATOM	330	CB	ASN A 51	7.486	3.716	7.759	1.00	19.89
20	ATOM	331	CG	ASN A 51	7.096	2.522	6.878	1.00	21.39
	ATOM	332	OD1	ASN A 51	6.309	2.650	5.938	1.00	22.88
	ATOM	333	ND2	ASN A 51	7.643	1.353	7.195	1.00	21.62
	ATOM	334	C	ASN A 51	7.326	6.243	7.967	1.00	19.72
	ATOM	335	O	ASN A 51	6.230	6.656	8.340	1.00	19.53
25	ATOM	336	N	SER A 52	8.484	6.801	8.334	1.00	19.49
	ATOM	337	CA	SER A 52	8.538	8.022	9.158	1.00	19.90
	ATOM	338	CB	SER A 52	9.984	8.369	9.552	1.00	18.99
	ATOM	339	OG	SER A 52	10.509	7.454	10.502	1.00	16.95
	ATOM	340	C	SER A 52	7.911	9.199	8.414	1.00	20.71
30	ATOM	341	O	SER A 52	7.111	9.943	8.993	1.00	20.97
	ATOM	342	N	SER A 53	8.264	9.352	7.139	1.00	21.68
	ATOM	343	CA	SER A 53	7.752	10.453	6.290	1.00	23.05
	ATOM	344	CB	SER A 53	8.416	10.431	4.905	1.00	23.36
	ATOM	345	OG	SER A 53	7.889	11.455	4.071	1.00	26.63
35	ATOM	346	C	SER A 53	6.236	10.398	6.160	1.00	23.52

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	ATOM	347	O	SER A	53	5.554	11.431	6.221	1.00	23.18
	ATOM	348	N	ASP A	54	5.717	9.181	5.989	1.00	23.75
	ATOM	349	CA	ASP A	54	4.277	8.915	6.001	1.00	24.65
	ATOM	350	CB	ASP A	54	4.022	7.419	5.749	1.00	24.86
5	ATOM	351	CG	ASP A	54	2.541	7.076	5.659	1.00	28.59
	ATOM	352	OD1	ASP A	54	1.923	7.299	4.587	1.00	32.06
	ATOM	353	OD2	ASP A	54	1.995	6.559	6.657	1.00	31.92
	ATOM	354	C	ASP A	54	3.612	9.365	7.308	1.00	23.61
	ATOM	355	O	ASP A	54	2.544	9.984	7.278	1.00	23.65
10	ATOM	356	N	ALA A	55	4.250	9.061	8.438	1.00	22.93
	ATOM	357	CA	ALA A	55	3.733	9.417	9.765	1.00	22.71
	ATOM	358	CB	ALA A	55	4.506	8.701	10.857	1.00	22.25
	ATOM	359	C	ALA A	55	3.775	10.923	9.996	1.00	22.36
	ATOM	360	O	ALA A	55	2.890	11.484	10.637	1.00	21.86
15	ATOM	361	N	LEU A	56	4.820	11.557	9.467	1.00	22.48
	ATOM	362	CA	LEU A	56	4.998	13.012	9.546	1.00	22.61
	ATOM	363	CB	LEU A	56	6.449	13.383	9.212	1.00	21.67
	ATOM	364	CG	LEU A	56	7.458	12.981	10.300	1.00	21.77
	ATOM	365	CD1	LEU A	56	8.867	12.728	9.738	1.00	21.24
20	ATOM	366	CD2	LEU A	56	7.497	13.990	11.427	1.00	21.19
	ATOM	367	C	LEU A	56	3.999	13.760	8.667	1.00	23.20
	ATOM	368	O	LEU A	56	3.407	14.764	9.102	1.00	23.86
	ATOM	369	N	ASP A	57	3.786	13.262	7.448	1.00	24.09
	ATOM	370	CA	ASP A	57	2.704	13.753	6.569	1.00	25.05
25	ATOM	371	CB	ASP A	57	2.572	12.886	5.309	1.00	25.01
	ATOM	372	CG	ASP A	57	3.607	13.208	4.244	1.00	25.60
	ATOM	373	OD1	ASP A	57	4.349	14.201	4.377	1.00	25.91
	ATOM	374	OD2	ASP A	57	3.674	12.452	3.251	1.00	26.54
	ATOM	375	C	ASP A	57	1.352	13.773	7.306	1.00	25.58
30	ATOM	376	O	ASP A	57	0.650	14.786	7.294	1.00	25.62
	ATOM	377	N	LYS A	58	1.004	12.663	7.961	1.00	25.99
	ATOM	378	CA	LYS A	58	-0.286	12.545	8.657	1.00	26.71
	ATOM	379	CB	LYS A	58	-0.491	11.132	9.210	1.00	26.76
	ATOM	380	CG	LYS A	58	-0.647	10.072	8.115	1.00	27.54
35	ATOM	381	CD	LYS A	58	-1.048	8.717	8.692	1.00	28.53

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	ATOM	382	CE	LYS	A	58	-0.967	7.601	7.633	1.00	30.71
	ATOM	383	NZ	LYS	A	58	-1.586	7.999	6.327	1.00	33.81
	ATOM	384	C	LYS	A	58	-0.490	13.591	9.758	1.00	26.99
	ATOM	385	O	LYS	A	58	-1.531	14.235	9.797	1.00	27.26
5	ATOM	386	N	ILE	A	59	0.494	13.766	10.642	1.00	26.84
	ATOM	387	CA	ILE	A	59	0.380	14.799	11.671	1.00	27.47
	ATOM	388	CB	ILE	A	59	1.406	14.627	12.857	1.00	27.66
	ATOM	389	CG1	ILE	A	59	1.103	15.591	14.017	1.00	28.30
	ATOM	390	CD1	ILE	A	59	-0.209	15.312	14.770	1.00	28.67
10	ATOM	391	CG2	ILE	A	59	2.850	14.765	12.388	1.00	28.69
	ATOM	392	C	ILE	A	59	0.405	16.193	11.043	1.00	27.72
	ATOM	393	O	ILE	A	59	-0.389	17.055	11.422	1.00	27.31
	ATOM	394	N	ARG	A	60	1.277	16.398	10.059	1.00	27.90
	ATOM	395	CA	ARG	A	60	1.375	17.697	9.410	1.00	28.89
15	ATOM	396	CB	ARG	A	60	2.443	17.704	8.330	1.00	29.00
	ATOM	397	CG	ARG	A	60	2.573	19.056	7.673	1.00	31.18
	ATOM	398	CD	ARG	A	60	3.764	19.132	6.771	1.00	35.20
	ATOM	399	NE	ARG	A	60	3.617	18.269	5.608	1.00	38.26
	ATOM	400	CZ	ARG	A	60	4.110	18.548	4.406	1.00	41.08
20	ATOM	401	NH1	ARG	A	60	4.774	19.679	4.190	1.00	41.29
	ATOM	402	NH2	ARG	A	60	3.931	17.689	3.416	1.00	43.14
	ATOM	403	C	ARG	A	60	0.040	18.162	8.815	1.00	29.35
	ATOM	404	O	ARG	A	60	-0.458	19.234	9.157	1.00	29.04
	ATOM	405	N	TYR	A	61	-0.530	17.359	7.921	1.00	29.71
25	ATOM	406	CA	TYR	A	61	-1.743	17.785	7.219	1.00	31.01
	ATOM	407	CB	TYR	A	61	-2.011	16.917	5.987	1.00	31.00
	ATOM	408	CG	TYR	A	61	-1.013	17.171	4.893	1.00	31.56
	ATOM	409	CD1	TYR	A	61	-0.087	16.197	4.533	1.00	31.05
	ATOM	410	CE1	TYR	A	61	0.847	16.433	3.541	1.00	32.05
30	ATOM	411	CZ	TYR	A	61	0.870	17.659	2.901	1.00	32.05
	ATOM	412	OH	TYR	A	61	1.803	17.884	1.917	1.00	33.65
	ATOM	413	CE2	TYR	A	61	-0.031	18.654	3.246	1.00	32.48
	ATOM	414	CD2	TYR	A	61	-0.969	18.405	4.239	1.00	31.30
	ATOM	415	C	TYR	A	61	-2.954	17.857	8.135	1.00	31.63
35	ATOM	416	O	TYR	A	61	-3.784	18.766	8.000	1.00	31.82

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	ATOM	417	N	GLU A 62	-3.043	16.920	9.074	1.00	32.30
	ATOM	418	CA	GLU A 62	-4.122	16.932	10.058	1.00	33.28
	ATOM	419	CB	GLU A 62	-4.093	15.671	10.916	1.00	33.67
	ATOM	420	CG	GLU A 62	-4.828	14.499	10.287	1.00	36.61
5	ATOM	421	CD	GLU A 62	-4.758	13.253	11.141	1.00	39.56
	ATOM	422	OE1	GLU A 62	-4.762	13.384	12.390	1.00	40.68
	ATOM	423	OE2	GLU A 62	-4.692	12.144	10.558	1.00	40.81
	ATOM	424	C	GLU A 62	-4.084	18.159	10.958	1.00	33.31
	ATOM	425	O	GLU A 62	-5.130	18.668	11.360	1.00	33.26
10	ATOM	426	N	SER A 63	-2.882	18.640	11.271	1.00	33.33
	ATOM	427	CA	SER A 63	-2.746	19.817	12.129	1.00	33.38
	ATOM	428	CB	SER A 63	-1.336	19.905	12.725	1.00	32.96
	ATOM	429	OG	SER A 63	-0.368	20.182	11.723	1.00	33.21
	ATOM	430	C	SER A 63	-3.121	21.125	11.419	1.00	33.73
15	ATOM	431	O	SER A 63	-3.245	22.168	12.065	1.00	33.86
	ATOM	432	N	LEU A 64	-3.306	21.075	10.100	1.00	34.49
	ATOM	433	CA	LEU A 64	-3.643	22.276	9.330	1.00	35.10
	ATOM	434	CB	LEU A 64	-3.583	22.014	7.823	1.00	34.97
	ATOM	435	CG	LEU A 64	-2.211	21.829	7.159	1.00	35.14
20	ATOM	436	CD1	LEU A 64	-2.364	21.888	5.636	1.00	35.50
	ATOM	437	CD2	LEU A 64	-1.195	22.878	7.629	1.00	34.86
	ATOM	438	C	LEU A 64	-5.009	22.831	9.714	1.00	35.85
	ATOM	439	O	LEU A 64	-5.271	24.030	9.567	1.00	35.91
	ATOM	440	N	THR A 65	-5.875	21.954	10.208	1.00	36.59
25	ATOM	441	CA	THR A 65	-7.201	22.370	10.660	1.00	37.17
	ATOM	442	CB	THR A 65	-8.313	21.780	9.783	1.00	37.20
	ATOM	443	OG1	THR A 65	-7.937	20.465	9.372	1.00	37.35
	ATOM	444	CG2	THR A 65	-8.527	22.650	8.553	1.00	38.21
	ATOM	445	C	THR A 65	-7.440	22.042	12.130	1.00	37.42
30	ATOM	446	O	THR A 65	-8.480	22.396	12.688	1.00	37.53
	ATOM	447	N	ASP A 66	-6.479	21.356	12.748	1.00	37.42
	ATOM	448	CA	ASP A 66	-6.454	21.224	14.204	1.00	37.04
	ATOM	449	CB	ASP A 66	-7.024	19.882	14.673	1.00	37.04
	ATOM	450	CG	ASP A 66	-7.301	19.859	16.173	1.00	37.54
35	ATOM	451	OD1	ASP A 66	-7.012	20.866	16.856	1.00	37.62

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	ATOM	452	OD2 ASP A 66	-7.807	18.836	16.672	1.00	37.10
	ATOM	453	C ASP A 66	-5.039	21.433	14.742	1.00	37.02
	ATOM	454	O ASP A 66	-4.322	20.459	15.007	1.00	36.80
	ATOM	455	N PRO A 67	-4.649	22.707	14.940	1.00	36.74
5	ATOM	456	CA PRO A 67	-3.298	23.053	15.389	1.00	36.44
	ATOM	457	CB PRO A 67	-3.323	24.593	15.444	1.00	36.53
	ATOM	458	CG PRO A 67	-4.464	24.991	14.550	1.00	36.87
	ATOM	459	CD PRO A 67	-5.484	23.910	14.757	1.00	36.78
	ATOM	460	C PRO A 67	-2.946	22.467	16.758	1.00	36.00
10	ATOM	461	O PRO A 67	-1.763	22.298	17.064	1.00	35.87
	ATOM	462	N SER A 68	-3.963	22.143	17.557	1.00	35.52
	ATOM	463	CA SER A 68	-3.770	21.573	18.895	1.00	35.17
	ATOM	464	CB SER A 68	-5.106	21.495	19.639	1.00	35.42
	ATOM	465	OG SER A 68	-5.894	20.422	19.144	1.00	36.19
15	ATOM	466	C SER A 68	-3.131	20.181	18.869	1.00	34.65
	ATOM	467	O SER A 68	-2.661	19.689	19.894	1.00	34.54
	ATOM	468	N LYS A 69	-3.126	19.551	17.698	1.00	33.65
	ATOM	469	CA LYS A 69	-2.483	18.246	17.523	1.00	33.02
	ATOM	470	CB LYS A 69	-2.906	17.622	16.193	1.00	33.12
20	ATOM	471	CG LYS A 69	-4.363	17.188	16.186	1.00	33.72
	ATOM	472	CD LYS A 69	-4.763	16.553	14.875	1.00	36.01
	ATOM	473	CE LYS A 69	-6.029	15.717	15.060	1.00	36.03
	ATOM	474	NZ LYS A 69	-6.477	15.120	13.771	1.00	38.51
	ATOM	475	C LYS A 69	-0.956	18.352	17.618	1.00	32.39
25	ATOM	476	O LYS A 69	-0.269	17.354	17.841	1.00	31.86
	ATOM	477	N LEU A 70	-0.446	19.570	17.466	1.00	31.81
	ATOM	478	CA LEU A 70	0.988	19.842	17.620	1.00	31.53
	ATOM	479	CB LEU A 70	1.467	20.838	16.560	1.00	31.31
	ATOM	480	CG LEU A 70	1.407	20.414	15.091	1.00	31.65
30	ATOM	481	CD1 LEU A 70	1.858	21.567	14.193	1.00	31.92
	ATOM	482	CD2 LEU A 70	2.223	19.147	14.825	1.00	30.74
	ATOM	483	C LEU A 70	1.356	20.349	19.016	1.00	31.40
	ATOM	484	O LEU A 70	2.480	20.807	19.230	1.00	31.38
	ATOM	485	N ASP A 71	0.419	20.267	19.962	1.00	30.83
35	ATOM	486	CA ASP A 71	0.717	20.596	21.365	1.00	30.62

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	ATOM	487	CB	ASP	A	71	-0.550	20.611	22.224	1.00	30.74
	ATOM	488	CG	ASP	A	71	-1.493	21.744	21.858	1.00	30.65
	ATOM	489	OD1	ASP	A	71	-1.139	22.585	21.001	1.00	30.14
	ATOM	490	OD2	ASP	A	71	-2.608	21.778	22.416	1.00	31.86
5	ATOM	491	C	ASP	A	71	1.747	19.640	21.959	1.00	30.34
	ATOM	492	O	ASP	A	71	2.495	20.014	22.863	1.00	30.38
	ATOM	493	N	SER	A	72	1.789	18.416	21.430	1.00	29.75
	ATOM	494	CA	SER	A	72	2.792	17.421	21.804	1.00	29.44
	ATOM	495	CB	SER	A	72	2.240	16.010	21.571	1.00	29.36
10	ATOM	496	OG	SER	A	72	1.750	15.886	20.247	1.00	28.56
	ATOM	497	C	SER	A	72	4.124	17.572	21.055	1.00	29.27
	ATOM	498	O	SER	A	72	5.008	16.722	21.186	1.00	29.07
	ATOM	499	N	GLY	A	73	4.269	18.645	20.282	1.00	29.10
	ATOM	500	CA	GLY	A	73	5.515	18.916	19.555	1.00	29.28
15	ATOM	501	C	GLY	A	73	5.290	19.492	18.171	1.00	28.94
	ATOM	502	O	GLY	A	73	4.587	18.898	17.346	1.00	28.80
	ATOM	503	N	LYS	A	74	5.887	20.653	17.916	1.00	28.76
	ATOM	504	CA	LYS	A	74	5.742	21.325	16.631	1.00	29.02
	ATOM	505	CB	LYS	A	74	5.865	22.842	16.774	1.00	29.46
20	ATOM	506	CG	LYS	A	74	4.680	23.494	17.459	1.00	30.40
	ATOM	507	CD	LYS	A	74	4.766	25.000	17.318	1.00	32.30
	ATOM	508	CE	LYS	A	74	3.723	25.670	18.187	1.00	34.55
	ATOM	509	NZ	LYS	A	74	3.978	27.127	18.200	1.00	36.69
	ATOM	510	C	LYS	A	74	6.752	20.845	15.606	1.00	29.12
25	ATOM	511	O	LYS	A	74	6.450	20.820	14.411	1.00	29.19
	ATOM	512	N	GLU	A	75	7.950	20.485	16.070	1.00	28.88
	ATOM	513	CA	GLU	A	75	9.032	20.104	15.162	1.00	28.65
	ATOM	514	CB	GLU	A	75	10.383	20.070	15.885	1.00	29.01
	ATOM	515	CG	GLU	A	75	10.650	21.245	16.823	1.00	29.80
30	ATOM	516	CD	GLU	A	75	12.070	21.241	17.381	0.30	29.42
	ATOM	517	OE1	GLU	A	75	12.594	22.338	17.678	0.30	30.17
	ATOM	518	OE2	GLU	A	75	12.665	20.147	17.522	0.30	29.28
	ATOM	519	C	GLU	A	75	8.751	18.740	14.539	1.00	28.23
	ATOM	520	O	GLU	A	75	8.544	17.759	15.252	1.00	28.73
35	ATOM	521	N	LEU	A	76	8.759	18.697	13.210	1.00	27.00

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	ATOM	522	CA	LEU A 76	8.511	17.475	12.457	1.00	26.29
	ATOM	523	CB	LEU A 76	7.388	17.695	11.436	1.00	26.28
	ATOM	524	CG	LEU A 76	6.060	18.218	11.999	1.00	26.87
	ATOM	525	CD1	LEU A 76	5.052	18.392	10.886	1.00	28.84
5	ATOM	526	CD2	LEU A 76	5.513	17.289	13.073	1.00	26.21
	ATOM	527	C	LEU A 76	9.794	17.072	11.756	1.00	25.66
	ATOM	528	O	LEU A 76	10.199	17.694	10.774	1.00	25.18
	ATOM	529	N	HIS A 77	10.443	16.036	12.275	1.00	25.06
	ATOM	530	CA	HIS A 77	11.745	15.638	11.754	1.00	24.78
10	ATOM	531	CB	HIS A 77	12.832	16.607	12.249	1.00	25.48
	ATOM	532	CG	HIS A 77	13.052	16.573	13.728	1.00	28.21
	ATOM	533	ND1	HIS A 77	14.309	16.556	14.290	1.00	31.34
	ATOM	534	CE1	HIS A 77	14.201	16.520	15.607	1.00	31.69
	ATOM	535	NE2	HIS A 77	12.917	16.520	15.917	1.00	30.36
15	ATOM	536	CD2	HIS A 77	12.178	16.555	14.762	1.00	29.59
	ATOM	537	C	HIS A 77	12.078	14.198	12.123	1.00	23.80
	ATOM	538	O	HIS A 77	11.309	13.532	12.820	1.00	22.74
	ATOM	539	N	ILE A 78	13.230	13.742	11.635	1.00	22.86
	ATOM	540	CA	ILE A 78	13.733	12.389	11.845	1.00	22.29
20	ATOM	541	CB	ILE A 78	13.794	11.603	10.497	1.00	22.20
	ATOM	542	CG1	ILE A 78	12.415	11.559	9.827	1.00	22.05
	ATOM	543	CD1	ILE A 78	12.419	11.225	8.356	1.00	21.87
	ATOM	544	CG2	ILE A 78	14.357	10.179	10.707	1.00	22.34
	ATOM	545	C	ILE A 78	15.152	12.483	12.423	1.00	22.63
25	ATOM	546	O	ILE A 78	15.983	13.267	11.929	1.00	23.11
	ATOM	547	N	ASN A 79	15.430	11.701	13.460	1.00	22.30
	ATOM	548	CA	ASN A 79	16.803	11.543	13.972	1.00	22.08
	ATOM	549	CB	ASN A 79	16.868	11.845	15.477	1.00	22.51
	ATOM	550	CG	ASN A 79	16.504	13.294	15.828	1.00	23.25
30	ATOM	551	OD1	ASN A 79	16.079	13.574	16.955	1.00	24.43
	ATOM	552	ND2	ASN A 79	16.703	14.212	14.895	1.00	21.15
	ATOM	553	C	ASN A 79	17.342	10.133	13.732	1.00	21.73
	ATOM	554	O	ASN A 79	16.634	9.145	13.951	1.00	21.66
	ATOM	555	N	LEU A 80	18.597	10.032	13.298	1.00	20.56
35	ATOM	556	CA	LEU A 80	19.261	8.738	13.177	1.00	20.75

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	ATOM	557	CB	LEU	A	80	19.872	8.545	11.786	1.00	20.64
	ATOM	558	CG	LEU	A	80	18.971	8.701	10.571	1.00	21.55
	ATOM	559	CD1	LEU	A	80	19.774	8.519	9.286	1.00	23.34
	ATOM	560	CD2	LEU	A	80	17.816	7.697	10.654	1.00	22.17
5	ATOM	561	C	LEU	A	80	20.357	8.650	14.236	1.00	20.81
	ATOM	562	O	LEU	A	80	21.199	9.537	14.333	1.00	19.28
	ATOM	563	N	ILE	A	81	20.329	7.578	15.028	1.00	20.85
	ATOM	564	CA	ILE	A	81	21.248	7.423	16.141	1.00	22.18
	ATOM	565	CB	ILE	A	81	20.547	7.687	17.521	1.00	22.16
10	ATOM	566	CG1	ILE	A	81	19.627	8.912	17.439	1.00	23.90
	ATOM	567	CD1	ILE	A	81	18.722	9.129	18.645	1.00	24.17
	ATOM	568	CG2	ILE	A	81	21.600	7.827	18.650	1.00	22.39
	ATOM	569	C	ILE	A	81	21.927	6.049	16.158	1.00	22.21
	ATOM	570	O	ILE	A	81	21.372	5.099	16.695	1.00	21.56
15	ATOM	571	N	PRO	A	82	23.137	5.942	15.560	1.00	22.67
	ATOM	572	CA	PRO	A	82	23.955	4.736	15.677	1.00	23.52
	ATOM	573	CB	PRO	A	82	24.994	4.901	14.554	1.00	23.01
	ATOM	574	CG	PRO	A	82	25.116	6.359	14.367	1.00	23.77
	ATOM	575	CD	PRO	A	82	23.781	6.969	14.722	1.00	22.53
20	ATOM	576	C	PRO	A	82	24.649	4.656	17.041	1.00	24.29
	ATOM	577	O	PRO	A	82	25.108	5.679	17.574	1.00	24.68
	ATOM	578	N	ASN	A	83	24.699	3.454	17.602	1.00	24.84
	ATOM	579	CA	ASN	A	83	25.341	3.211	18.890	1.00	25.58
	ATOM	580	CB	ASN	A	83	24.300	3.065	20.017	1.00	25.89
25	ATOM	581	CG	ASN	A	83	24.936	2.823	21.402	1.00	27.07
	ATOM	582	OD1	ASN	A	83	26.031	2.269	21.520	1.00	27.97
	ATOM	583	ND2	ASN	A	83	24.225	3.227	22.454	1.00	28.91
	ATOM	584	C	ASN	A	83	26.193	1.961	18.743	1.00	25.58
	ATOM	585	O	ASN	A	83	25.681	0.838	18.685	1.00	25.09
30	ATOM	586	N	LYS	A	84	27.500	2.171	18.649	1.00	25.86
	ATOM	587	CA	LYS	A	84	28.432	1.081	18.381	1.00	26.94
	ATOM	588	CB	LYS	A	84	29.767	1.647	17.894	1.00	26.96
	ATOM	589	CG	LYS	A	84	29.673	2.308	16.531	1.00	27.27
	ATOM	590	CD	LYS	A	84	31.050	2.599	15.922	1.00	28.69
35	ATOM	591	CE	LYS	A	84	30.886	3.076	14.483	1.00	30.48

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	ATOM	592	NZ	LYS	A	84	32.019	3.925	14.041	1.00	31.97
	ATOM	593	C	LYS	A	84	28.628	0.177	19.603	1.00	27.93
	ATOM	594	O	LYS	A	84	29.004	-0.996	19.477	1.00	28.49
	ATOM	595	N	GLN	A	85	28.374	0.736	20.781	1.00	28.49
5	ATOM	596	CA	GLN	A	85	28.543	0.015	22.035	1.00	29.68
	ATOM	597	CB	GLN	A	85	28.568	1.008	23.194	1.00	29.87
	ATOM	598	CG	GLN	A	85	29.256	0.541	24.454	1.00	33.41
	ATOM	599	CD	GLN	A	85	29.146	1.568	25.557	1.00	35.69
	ATOM	600	OE1	GLN	A	85	28.240	1.504	26.384	1.00	39.32
10	ATOM	601	NE2	GLN	A	85	30.047	2.547	25.554	1.00	38.48
	ATOM	602	C	GLN	A	85	27.428	-1.027	22.189	1.00	29.30
	ATOM	603	O	GLN	A	85	27.700	-2.182	22.516	1.00	29.93
	ATOM	604	N	ASP	A	86	26.194	-0.619	21.895	1.00	29.35
	ATOM	605	CA	ASP	A	86	25.002	-1.468	22.013	1.00	29.45
15	ATOM	606	CB	ASP	A	86	23.769	-0.600	22.326	1.00	30.58
	ATOM	607	CG	ASP	A	86	23.882	0.154	23.652	1.00	34.01
	ATOM	608	OD1	ASP	A	86	24.735	-0.189	24.508	1.00	36.00
	ATOM	609	OD2	ASP	A	86	23.094	1.106	23.844	1.00	38.47
	ATOM	610	C	ASP	A	86	24.715	-2.237	20.721	1.00	28.37
20	ATOM	611	O	ASP	A	86	23.847	-3.101	20.695	1.00	27.83
	ATOM	612	N	ARG	A	87	25.438	-1.893	19.654	1.00	26.85
	ATOM	613	CA	ARG	A	87	25.193	-2.382	18.295	1.00	25.70
	ATOM	614	CB	ARG	A	87	25.600	-3.845	18.121	1.00	26.03
	ATOM	615	CG	ARG	A	87	25.994	-4.161	16.699	1.00	28.20
25	ATOM	616	CD	ARG	A	87	25.807	-5.617	16.379	1.00	30.24
	ATOM	617	NE	ARG	A	87	26.786	-6.464	17.042	1.00	31.75
	ATOM	618	CZ	ARG	A	87	26.652	-7.779	17.203	1.00	31.42
	ATOM	619	NH1	ARG	A	87	25.566	-8.418	16.761	1.00	28.59
	ATOM	620	NH2	ARG	A	87	27.613	-8.455	17.811	1.00	29.73
30	ATOM	621	C	ARG	A	87	23.760	-2.137	17.819	1.00	24.68
	ATOM	622	O	ARG	A	87	23.120	-3.029	17.239	1.00	24.43
	ATOM	623	N	THR	A	88	23.257	-0.932	18.075	1.00	22.75
	ATOM	624	CA	THR	A	88	21.910	-0.583	17.645	1.00	22.00
	ATOM	625	CB	THR	A	88	20.995	-0.261	18.848	1.00	21.75
35	ATOM	626	OG1	THR	A	88	21.561	0.812	19.599	1.00	20.93

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	ATOM	627	CG2 THR A 88	20.841	-1.465	19.743	1.00	21.79
	ATOM	628	C THR A 88	21.914	0.624	16.721	1.00	21.44
	ATOM	629	O THR A 88	22.728	1.545	16.887	1.00	21.31
	ATOM	630	N LEU A 89	20.989	0.626	15.767	1.00	20.95
5	ATOM	631	CA LEU A 89	20.695	1.828	15.000	1.00	20.36
	ATOM	632	CB LEU A 89	20.853	1.581	13.493	1.00	20.49
	ATOM	633	CG LEU A 89	20.491	2.744	12.549	0.65	19.36
	ATOM	634	CD1 LEU A 89	21.328	4.003	12.825	0.65	16.93
	ATOM	635	CD2 LEU A 89	20.605	2.309	11.074	0.65	19.33
10	ATOM	636	C LEU A 89	19.264	2.229	15.351	1.00	20.24
	ATOM	637	O LEU A 89	18.340	1.429	15.191	1.00	20.39
	ATOM	638	N THR A 90	19.101	3.446	15.860	1.00	20.08
	ATOM	639	CA THR A 90	17.788	3.950	16.276	1.00	20.49
	ATOM	640	CB THR A 90	17.840	4.493	17.730	1.00	20.31
15	ATOM	641	OG1 THR A 90	18.233	3.441	18.620	1.00	21.44
	ATOM	642	CG2 THR A 90	16.481	5.052	18.184	1.00	21.34
	ATOM	643	C THR A 90	17.329	5.027	15.298	1.00	20.47
	ATOM	644	O THR A 90	18.117	5.896	14.897	1.00	21.09
	ATOM	645	N ILE A 91	16.067	4.951	14.895	1.00	20.44
20	ATOM	646	CA ILE A 91	15.481	5.918	13.991	1.00	20.79
	ATOM	647	CB ILE A 91	14.977	5.266	12.675	1.00	20.67
	ATOM	648	CG1 ILE A 91	16.121	4.571	11.915	1.00	22.90
	ATOM	649	CD1 ILE A 91	16.434	3.155	12.394	1.00	25.38
	ATOM	650	CG2 ILE A 91	14.304	6.296	11.793	1.00	22.52
25	ATOM	651	C ILE A 91	14.293	6.501	14.737	1.00	20.57
	ATOM	652	O ILE A 91	13.376	5.767	15.100	1.00	20.69
	ATOM	653	N VAL A 92	14.312	7.808	14.963	1.00	20.77
	ATOM	654	CA VAL A 92	13.244	8.465	15.726	1.00	20.94
	ATOM	655	CB VAL A 92	13.769	9.141	17.036	1.00	21.35
30	ATOM	656	CG1 VAL A 92	12.601	9.575	17.931	1.00	22.59
	ATOM	657	CG2 VAL A 92	14.697	8.205	17.815	1.00	22.93
	ATOM	658	C VAL A 92	12.565	9.516	14.880	1.00	20.67
	ATOM	659	O VAL A 92	13.234	10.309	14.200	1.00	20.26
	ATOM	660	N ASP A 93	11.229	9.532	14.914	1.00	20.16
35	ATOM	661	CA ASP A 93	10.482	10.582	14.256	1.00	20.22

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	ATOM	662	CB	ASP	A	93	9.829	10.109	12.944	1.00	20.77
	ATOM	663	CG	ASP	A	93	8.688	9.125	13.163	1.00	22.11
	ATOM	664	OD1	ASP	A	93	7.621	9.537	13.700	1.00	21.32
	ATOM	665	OD2	ASP	A	93	8.854	7.948	12.757	1.00	19.83
5	ATOM	666	C	ASP	A	93	9.458	11.173	15.203	1.00	20.25
	ATOM	667	O	ASP	A	93	9.134	10.574	16.232	1.00	19.66
	ATOM	668	N	THR	A	94	8.998	12.364	14.849	1.00	21.03
	ATOM	669	CA	THR	A	94	7.933	13.043	15.583	1.00	21.19
	ATOM	670	CB	THR	A	94	8.369	14.467	15.962	1.00	21.14
10	ATOM	671	OG1	THR	A	94	8.746	15.165	14.776	1.00	21.29
	ATOM	672	CG2	THR	A	94	9.556	14.409	16.913	1.00	21.39
	ATOM	673	C	THR	A	94	6.647	13.066	14.760	1.00	21.81
	ATOM	674	O	THR	A	94	5.899	14.067	14.766	1.00	21.70
	ATOM	675	N	GLY	A	95	6.382	11.954	14.058	1.00	22.03
15	ATOM	676	CA	GLY	A	95	5.133	11.762	13.301	1.00	21.58
	ATOM	677	C	GLY	A	95	3.928	11.473	14.187	1.00	22.02
	ATOM	678	O	GLY	A	95	3.989	11.656	15.400	1.00	22.03
	ATOM	679	N	ILE	A	96	2.840	10.999	13.578	1.00	22.76
	ATOM	680	CA	ILE	A	96	1.543	10.828	14.270	1.00	22.72
20	ATOM	681	CB	ILE	A	96	0.360	10.675	13.245	1.00	23.06
	ATOM	682	CG1	ILE	A	96	-1.005	10.898	13.918	1.00	22.93
	ATOM	683	CD1	ILE	A	96	-2.093	11.377	12.971	1.00	23.52
	ATOM	684	CG2	ILE	A	96	0.423	9.301	12.522	1.00	20.87
	ATOM	685	C	ILE	A	96	1.562	9.698	15.313	1.00	23.31
25	ATOM	686	O	ILE	A	96	0.737	9.677	16.238	1.00	23.37
	ATOM	687	N	GLY	A	97	2.514	8.772	15.187	1.00	22.89
	ATOM	688	CA	GLY	A	97	2.618	7.671	16.131	1.00	22.98
	ATOM	689	C	GLY	A	97	1.533	6.634	15.898	1.00	23.18
	ATOM	690	O	GLY	A	97	0.770	6.715	14.917	1.00	23.86
30	ATOM	691	N	MET	A	98	1.455	5.667	16.801	1.00	23.76
	ATOM	692	CA	MET	A	98	0.503	4.568	16.675	1.00	24.94
	ATOM	693	CB	MET	A	98	1.208	3.314	16.133	1.00	24.36
	ATOM	694	CG	MET	A	98	1.611	3.400	14.671	1.00	24.10
	ATOM	695	SD	MET	A	98	2.664	2.017	14.144	1.00	26.24
35	ATOM	696	CE	MET	A	98	4.176	2.332	15.035	1.00	25.71

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	ATOM	697	C	MET A 98	-0.180	4.236	18.000	1.00	25.13
	ATOM	698	O	MET A 98	0.416	4.329	19.061	1.00	24.71
	ATOM	699	N	THR A 99	-1.439	3.824	17.908	1.00	26.05
	ATOM	700	CA	THR A 99	-2.163	3.315	19.057	1.00	27.31
5	ATOM	701	CB	THR A 99	-3.692	3.405	18.821	1.00	27.18
	ATOM	702	OG1	THR A 99	-4.045	2.610	17.683	1.00	29.32
	ATOM	703	CG2	THR A 99	-4.106	4.847	18.551	1.00	28.59
	ATOM	704	C	THR A 99	-1.743	1.863	19.308	1.00	27.41
	ATOM	705	O	THR A 99	-1.097	1.238	18.460	1.00	26.95
10	ATOM	706	N	LYS A 100	-2.090	1.338	20.480	1.00	27.58
	ATOM	707	CA	LYS A 100	-1.874	-0.072	20.792	1.00	27.79
	ATOM	708	CB	LYS A 100	-2.391	-0.387	22.202	1.00	28.15
	ATOM	709	CG	LYS A 100	-2.216	-1.825	22.628	1.00	29.66
	ATOM	710	CD	LYS A 100	-2.578	-1.998	24.084	1.00	32.73
15	ATOM	711	CE	LYS A 100	-3.354	-3.278	24.282	1.00	33.21
	ATOM	712	NZ	LYS A 100	-3.386	-3.649	25.709	1.00	34.56
	ATOM	713	C	LYS A 100	-2.526	-0.987	19.739	1.00	27.53
	ATOM	714	O	LYS A 100	-1.899	-1.945	19.279	1.00	27.56
	ATOM	715	N	ALA A 101	-3.760	-0.667	19.342	1.00	27.07
20	ATOM	716	CA	ALA A 101	-4.475	-1.426	18.315	1.00	27.02
	ATOM	717	CB	ALA A 101	-5.894	-0.917	18.144	1.00	27.25
	ATOM	718	C	ALA A 101	-3.729	-1.408	16.985	1.00	26.92
	ATOM	719	O	ALA A 101	-3.587	-2.450	16.350	1.00	26.64
	ATOM	720	N	ASP A 102	-3.236	-0.228	16.590	1.00	26.90
25	ATOM	721	CA	ASP A 102	-2.400	-0.068	15.387	1.00	26.87
	ATOM	722	CB	ASP A 102	-1.854	1.371	15.283	1.00	27.17
	ATOM	723	CG	ASP A 102	-2.914	2.393	14.924	1.00	28.56
	ATOM	724	OD1	ASP A 102	-3.934	2.024	14.307	1.00	27.83
	ATOM	725	OD2	ASP A 102	-2.720	3.589	15.256	1.00	29.01
30	ATOM	726	C	ASP A 102	-1.220	-1.044	15.369	1.00	26.26
	ATOM	727	O	ASP A 102	-0.955	-1.674	14.349	1.00	26.37
	ATOM	728	N	LEU A 103	-0.510	-1.159	16.489	1.00	25.93
	ATOM	729	CA	LEU A 103	0.625	-2.098	16.600	1.00	26.07
	ATOM	730	CB	LEU A 103	1.311	-1.965	17.965	1.00	25.56
35	ATOM	731	CG	LEU A 103	2.088	-0.683	18.281	1.00	24.85

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	ATOM	732	CD1 LEU A 103	2.452	-0.652	19.752	1.00	23.97
	ATOM	733	CD2 LEU A 103	3.358	-0.542	17.407	1.00	25.36
	ATOM	734	C LEU A 103	0.218	-3.556	16.393	1.00	26.81
	ATOM	735	O LEU A 103	0.864	-4.303	15.655	1.00	26.66
5	ATOM	736	N ILE A 104	-0.851	-3.957	17.071	1.00	26.77
	ATOM	737	CA ILE A 104	-1.330	-5.335	17.020	1.00	27.74
	ATOM	738	CB ILE A 104	-2.353	-5.589	18.162	1.00	27.36
	ATOM	739	CG1 ILE A 104	-1.662	-5.422	19.518	1.00	27.86
	ATOM	740	CD1 ILE A 104	-2.619	-5.280	20.685	1.00	27.10
10	ATOM	741	CG2 ILE A 104	-2.985	-6.981	18.044	1.00	28.77
	ATOM	742	C ILE A 104	-1.917	-5.658	15.645	1.00	27.80
	ATOM	743	O ILE A 104	-1.602	-6.699	15.051	1.00	28.38
	ATOM	744	N ASN A 105	-2.739	-4.749	15.129	1.00	28.42
	ATOM	745	CA ASN A 105	-3.454	-4.965	13.873	1.00	28.61
15	ATOM	746	CB ASN A 105	-4.617	-3.980	13.734	1.00	28.78
	ATOM	747	CG ASN A 105	-5.747	-4.267	14.690	1.00	28.96
	ATOM	748	OD1 ASN A 105	-5.931	-5.398	15.144	1.00	29.88
	ATOM	749	ND2 ASN A 105	-6.527	-3.239	14.992	1.00	30.10
	ATOM	750	C ASN A 105	-2.572	-4.833	12.650	1.00	28.73
20	ATOM	751	O ASN A 105	-2.719	-5.603	11.699	1.00	28.85
	ATOM	752	N ASN A 106	-1.666	-3.857	12.673	1.00	28.66
	ATOM	753	CA ASN A 106	-0.887	-3.497	11.485	1.00	28.83
	ATOM	754	CB ASN A 106	-0.930	-1.979	11.225	1.00	29.22
	ATOM	755	CG ASN A 106	-2.352	-1.427	11.128	1.00	31.86
25	ATOM	756	OD1 ASN A 106	-3.313	-2.145	10.801	1.00	34.05
	ATOM	757	ND2 ASN A 106	-2.491	-0.139	11.420	1.00	32.81
	ATOM	758	C ASN A 106	0.563	-3.974	11.494	1.00	28.15
	ATOM	759	O ASN A 106	1.245	-3.884	10.471	1.00	28.43
	ATOM	760	N LEU A 107	1.037	-4.468	12.636	1.00	27.31
30	ATOM	761	CA LEU A 107	2.402	-4.997	12.742	1.00	26.67
	ATOM	762	CB LEU A 107	3.277	-4.129	13.659	1.00	26.69
	ATOM	763	CG LEU A 107	3.870	-2.809	13.167	1.00	27.67
	ATOM	764	CD1 LEU A 107	4.863	-2.282	14.204	1.00	28.29
	ATOM	765	CD2 LEU A 107	4.553	-2.974	11.808	1.00	27.39
35	ATOM	766	C LEU A 107	2.452	-6.460	13.208	1.00	26.15

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	ATOM	767	O	LEU A 107	3.289	-6.838	14.039	1.00	25.83
	ATOM	768	N	GLY A 108	1.556	-7.283	12.685	1.00	25.42
	ATOM	769	CA	GLY A 108	1.789	-8.724	12.755	1.00	25.73
	ATOM	770	C	GLY A 108	0.626	-9.685	12.742	1.00	26.17
5	ATOM	771	O	GLY A 108	0.795	-10.832	12.323	1.00	25.66
	ATOM	772	N	THR A 109	-0.538	-9.262	13.238	1.00	26.59
	ATOM	773	CA	THR A 109	-1.676	-10.193	13.329	1.00	27.51
	ATOM	774	CB	THR A 109	-2.574	-9.930	14.570	1.00	27.25
	ATOM	775	OG1	THR A 109	-3.176	-8.639	14.456	1.00	27.98
10	ATOM	776	CG2	THR A 109	-1.768	-10.016	15.862	1.00	26.95
	ATOM	777	C	THR A 109	-2.547	-10.257	12.057	1.00	28.19
	ATOM	778	O	THR A 109	-3.326	-11.197	11.892	1.00	27.89
	ATOM	779	N	ILE A 110	-2.424	-9.269	11.168	1.00	28.94
	ATOM	780	CA	ILE A 110	-3.215	-9.268	9.928	1.00	30.35
15	ATOM	781	CB	ILE A 110	-4.276	-8.139	9.900	1.00	30.31
	ATOM	782	CG1	ILE A 110	-5.119	-8.144	11.175	1.00	30.70
	ATOM	783	CD1	ILE A 110	-6.021	-6.916	11.330	1.00	30.59
	ATOM	784	CG2	ILE A 110	-5.172	-8.281	8.656	1.00	30.87
	ATOM	785	C	ILE A 110	-2.353	-9.160	8.675	1.00	30.90
20	ATOM	786	O	ILE A 110	-1.571	-8.219	8.535	1.00	30.79
	ATOM	787	N	ALA A 111	-2.502	-10.122	7.762	1.00	31.94
	ATOM	788	CA	ALA A 111	-1.835	-10.049	6.466	1.00	33.31
	ATOM	789	CB	ALA A 111	-1.789	-11.421	5.797	1.00	33.20
	ATOM	790	C	ALA A 111	-2.562	-9.042	5.585	1.00	34.32
25	ATOM	791	O	ALA A 111	-3.691	-9.291	5.136	1.00	35.21
	ATOM	792	N	LYS A 112	-1.938	-7.888	5.367	1.00	35.17
	ATOM	793	CA	LYS A 112	-2.523	-6.882	4.485	1.00	36.27
	ATOM	794	CB	LYS A 112	-1.913	-5.505	4.744	1.00	36.60
	ATOM	795	CG	LYS A 112	-1.869	-5.079	6.217	1.00	37.64
30	ATOM	796	CD	LYS A 112	-3.258	-5.020	6.850	1.00	39.74
	ATOM	797	CE	LYS A 112	-3.194	-4.434	8.249	1.00	40.58
	ATOM	798	NZ	LYS A 112	-4.523	-4.533	8.916	1.00	43.18
	ATOM	799	C	LYS A 112	-2.299	-7.311	3.036	1.00	37.02
	ATOM	800	O	LYS A 112	-1.384	-8.096	2.754	1.00	37.08
35	ATOM	801	N	SER A 113	-3.141	-6.826	2.122	1.00	37.38

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	ATOM	802	CA	SER A 113	-2.965	-7.150	0.704	1.00	37.55
	ATOM	803	CB	SER A 113	-4.070	-6.540	-0.171	1.00	37.77
	ATOM	804	OG	SER A 113	-3.823	-5.173	-0.478	1.00	39.69
	ATOM	805	C	SER A 113	-1.590	-6.672	0.277	1.00	36.74
5	ATOM	806	O	SER A 113	-1.159	-5.582	0.653	1.00	37.49
	ATOM	807	N	GLY A 114	-0.902	-7.508	-0.489	1.00	36.34
	ATOM	808	CA	GLY A 114	0.514	-7.317	-0.774	1.00	34.72
	ATOM	809	C	GLY A 114	1.355	-8.406	-0.128	1.00	33.98
	ATOM	810	O	GLY A 114	2.342	-8.850	-0.701	1.00	33.11
10	ATOM	811	N	THR A 115	0.952	-8.855	1.061	1.00	33.54
	ATOM	812	CA	THR A 115	1.776	-9.792	1.831	1.00	33.09
	ATOM	813	CB	THR A 115	1.281	-9.942	3.288	1.00	33.21
	ATOM	814	OG1	THR A 115	1.221	-8.649	3.898	1.00	31.40
	ATOM	815	CG2	THR A 115	2.224	-10.827	4.097	1.00	32.33
15	ATOM	816	C	THR A 115	1.871	-11.152	1.143	1.00	33.59
	ATOM	817	O	THR A 115	2.968	-11.590	0.797	1.00	33.17
	ATOM	818	N	LYS A 116	0.722	-11.803	0.950	1.00	34.02
	ATOM	819	CA	LYS A 116	0.648	-13.075	0.222	1.00	35.15
	ATOM	820	CB	LYS A 116	-0.816	-13.478	0.004	1.00	35.02
20	ATOM	821	CG	LYS A 116	-1.020	-14.918	-0.490	1.00	35.94
	ATOM	822	CD	LYS A 116	-2.504	-15.257	-0.612	1.00	36.48
	ATOM	823	CE	LYS A 116	-2.730	-16.503	-1.471	1.00	38.17
	ATOM	824	NZ	LYS A 116	-4.176	-16.705	-1.796	1.00	39.19
	ATOM	825	C	LYS A 116	1.380	-12.988	-1.118	1.00	35.25
25	ATOM	826	O	LYS A 116	2.150	-13.880	-1.460	1.00	35.46
	ATOM	827	N	ALA A 117	1.143	-11.897	-1.853	1.00	35.63
	ATOM	828	CA	ALA A 117	1.743	-11.658	-3.172	1.00	36.00
	ATOM	829	CB	ALA A 117	1.109	-10.435	-3.835	1.00	35.78
	ATOM	830	C	ALA A 117	3.264	-11.522	-3.157	1.00	35.87
30	ATOM	831	O	ALA A 117	3.948	-12.137	-3.975	1.00	36.41
	ATOM	832	N	PHE A 118	3.794	-10.709	-2.248	1.00	35.70
	ATOM	833	CA	PHE A 118	5.242	-10.570	-2.137	1.00	35.78
	ATOM	834	CB	PHE A 118	5.632	-9.367	-1.272	1.00	34.98
	ATOM	835	CG	PHE A 118	7.091	-8.996	-1.374	1.00	34.15
35	ATOM	836	CD1	PHE A 118	7.638	-8.588	-2.592	1.00	33.19

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	ATOM	837	CE1 PHE A 118	8.982	-8.242	-2.692	1.00	33.20
	ATOM	838	CZ PHE A 118	9.798	-8.301	-1.563	1.00	33.24
	ATOM	839	CE2 PHE A 118	9.261	-8.700	-0.342	1.00	33.52
	ATOM	840	CD2 PHE A 118	7.916	-9.047	-0.255	1.00	32.91
5	ATOM	841	C PHE A 118	5.870	-11.855	-1.591	1.00	36.36
	ATOM	842	O PHE A 118	6.934	-12.267	-2.054	1.00	36.25
	ATOM	843	N MET A 119	5.200	-12.471	-0.613	1.00	37.16
	ATOM	844	CA MET A 119	5.628	-13.756	-0.042	1.00	38.61
	ATOM	845	CB MET A 119	4.601	-14.258	0.981	1.00	38.35
10	ATOM	846	CG MET A 119	5.031	-15.459	1.810	1.00	38.78
	ATOM	847	SD MET A 119	3.599	-16.262	2.569	1.00	40.01
	ATOM	848	CE MET A 119	2.866	-17.137	1.179	1.00	40.42
	ATOM	849	C MET A 119	5.825	-14.780	-1.158	1.00	39.05
	ATOM	850	O MET A 119	6.905	-15.362	-1.280	1.00	39.74
15	ATOM	851	N GLU A 120	4.788	-14.966	-1.979	1.00	39.56
	ATOM	852	CA GLU A 120	4.823	-15.872	-3.134	1.00	40.30
	ATOM	853	CB GLU A 120	3.448	-15.951	-3.814	1.00	40.28
	ATOM	854	CG GLU A 120	2.368	-16.635	-2.987	1.00	39.76
	ATOM	855	CD GLU A 120	0.973	-16.543	-3.613	1.00	40.01
20	ATOM	856	OE1 GLU A 120	0.115	-17.380	-3.256	1.00	39.72
	ATOM	857	OE2 GLU A 120	0.727	-15.641	-4.449	1.00	37.15
	ATOM	858	C GLU A 120	5.885	-15.491	-4.167	1.00	40.94
	ATOM	859	O GLU A 120	6.500	-16.370	-4.774	1.00	41.23
	ATOM	860	N ALA A 121	6.098	-14.192	-4.373	1.00	41.60
25	ATOM	861	CA ALA A 121	7.155	-13.734	-5.277	1.00	42.35
	ATOM	862	CB ALA A 121	7.086	-12.228	-5.488	1.00	42.01
	ATOM	863	C ALA A 121	8.536	-14.146	-4.753	1.00	43.23
	ATOM	864	O ALA A 121	9.377	-14.625	-5.522	1.00	43.24
	ATOM	865	N LEU A 122	8.755	-13.982	-3.446	1.00	43.79
30	ATOM	866	CA LEU A 122	10.032	-14.360	-2.827	1.00	44.75
	ATOM	867	CB LEU A 122	10.158	-13.813	-1.399	1.00	44.30
	ATOM	868	CG LEU A 122	10.381	-12.314	-1.151	1.00	43.98
	ATOM	869	CD1 LEU A 122	10.612	-12.085	0.332	1.00	42.82
	ATOM	870	CD2 LEU A 122	11.548	-11.748	-1.954	1.00	42.97
35	ATOM	871	C LEU A 122	10.250	-15.873	-2.835	1.00	45.33

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	ATOM	872	O	LEU A 122	11.379	-16.339	-3.022	1.00	45.40
	ATOM	873	N	GLN A 123	9.168	-16.626	-2.625	1.00	46.14
	ATOM	874	CA	GLN A 123	9.176	-18.091	-2.756	1.00	46.84
	ATOM	875	CB	GLN A 123	7.815	-18.676	-2.360	1.00	46.72
5	ATOM	876	CG	GLN A 123	7.547	-18.630	-0.866	1.00	47.04
	ATOM	877	CD	GLN A 123	6.130	-19.022	-0.471	1.00	46.97
	ATOM	878	OE1	GLN A 123	5.308	-19.396	-1.304	1.00	46.77
	ATOM	879	NE2	GLN A 123	5.843	-18.931	0.820	1.00	48.12
	ATOM	880	C	GLN A 123	9.549	-18.528	-4.176	1.00	47.32
10	ATOM	881	O	GLN A 123	9.943	-19.679	-4.409	1.00	47.70
	ATOM	882	N	ALA A 124	9.419	-17.599	-5.116	1.00	47.52
	ATOM	883	CA	ALA A 124	9.845	-17.817	-6.486	1.00	47.88
	ATOM	884	CB	ALA A 124	8.707	-17.500	-7.448	1.00	47.88
	ATOM	885	C	ALA A 124	11.069	-16.944	-6.766	1.00	48.05
15	ATOM	886	O	ALA A 124	11.110	-16.207	-7.752	1.00	48.51
	ATOM	887	N	GLY A 125	12.042	-17.014	-5.856	1.00	47.99
	ATOM	888	CA	GLY A 125	13.363	-16.385	-6.002	1.00	47.78
	ATOM	889	C	GLY A 125	13.445	-14.930	-6.434	1.00	47.50
	ATOM	890	O	GLY A 125	14.395	-14.544	-7.116	1.00	47.91
20	ATOM	891	N	ALA A 126	12.474	-14.111	-6.034	1.00	47.07
	ATOM	892	CA	ALA A 126	12.454	-12.705	-6.452	1.00	46.38
	ATOM	893	CB	ALA A 126	11.033	-12.149	-6.409	1.00	46.55
	ATOM	894	C	ALA A 126	13.408	-11.825	-5.635	1.00	46.02
	ATOM	895	O	ALA A 126	13.920	-12.246	-4.595	1.00	45.78
25	ATOM	896	N	ASP A 127	13.626	-10.608	-6.143	1.00	45.50
	ATOM	897	CA	ASP A 127	14.440	-9.550	-5.532	1.00	44.68
	ATOM	898	CB	ASP A 127	14.627	-8.434	-6.570	1.00	45.03
	ATOM	899	CG	ASP A 127	15.818	-7.542	-6.279	1.00	46.83
	ATOM	900	OD1	ASP A 127	16.714	-7.953	-5.506	1.00	50.02
30	ATOM	901	OD2	ASP A 127	15.867	-6.420	-6.832	1.00	48.32
	ATOM	902	C	ASP A 127	13.758	-8.983	-4.274	1.00	43.69
	ATOM	903	O	ASP A 127	12.591	-9.300	-4.017	1.00	43.62
	ATOM	904	N	ILE A 128	14.473	-8.142	-3.512	1.00	42.16
	ATOM	905	CA	ILE A 128	13.955	-7.564	-2.246	1.00	40.69
35	ATOM	906	CB	ILE A 128	14.885	-7.902	-1.013	1.00	40.44

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	ATOM	907	CG1 ILE A 128	14.129	-7.824	0.323	1.00	39.35
	ATOM	908	CD1 ILE A 128	13.230	-8.999	0.612	1.00	38.26
	ATOM	909	CG2 ILE A 128	16.112	-7.007	-0.969	1.00	39.58
	ATOM	910	C ILE A 128	13.662	-6.050	-2.284	1.00	40.21
5	ATOM	911	O ILE A 128	12.874	-5.557	-1.482	1.00	39.54
	ATOM	912	N SER A 129	14.288	-5.318	-3.210	1.00	39.68
	ATOM	913	CA SER A 129	14.132	-3.854	-3.283	1.00	39.11
	ATOM	914	CB SER A 129	15.001	-3.250	-4.394	1.00	39.45
	ATOM	915	OG SER A 129	14.936	-1.826	-4.369	1.00	41.04
10	ATOM	916	C SER A 129	12.681	-3.409	-3.479	1.00	38.02
	ATOM	917	O SER A 129	12.340	-2.261	-3.184	1.00	38.04
	ATOM	918	N MET A 130	11.850	-4.331	-3.960	1.00	36.49
	ATOM	919	CA MET A 130	10.439	-4.090	-4.271	1.00	35.47
	ATOM	920	CB MET A 130	9.980	-5.017	-5.415	1.00	36.44
15	ATOM	921	CG MET A 130	10.880	-5.011	-6.655	1.00	38.63
	ATOM	922	SD MET A 130	11.192	-3.355	-7.303	1.00	46.12
	ATOM	923	C MET A 130	9.513	-4.294	-3.073	1.00	33.61
	ATOM	924	O MET A 130	8.290	-4.195	-3.206	1.00	33.12
	ATOM	925	N ILE A 131	10.097	-4.585	-1.911	1.00	31.33
20	ATOM	926	CA ILE A 131	9.325	-4.848	-0.690	1.00	29.03
	ATOM	927	CB ILE A 131	10.266	-5.219	0.499	1.00	28.52
	ATOM	928	CG1 ILE A 131	9.455	-5.691	1.710	1.00	27.01
	ATOM	929	CD1 ILE A 131	10.218	-6.625	2.654	1.00	26.13
	ATOM	930	CG2 ILE A 131	11.205	-4.043	0.844	1.00	27.34
25	ATOM	931	C ILE A 131	8.358	-3.709	-0.299	1.00	28.42
	ATOM	932	O ILE A 131	7.223	-3.963	0.129	1.00	27.69
	ATOM	933	N GLY A 132	8.816	-2.467	-0.450	1.00	28.21
	ATOM	934	CA GLY A 132	8.028	-1.291	-0.062	1.00	27.85
	ATOM	935	C GLY A 132	6.749	-1.156	-0.872	1.00	28.02
30	ATOM	936	O GLY A 132	5.700	-0.790	-0.326	1.00	27.91
	ATOM	937	N GLN A 133	6.838	-1.485	-2.164	1.00	27.31
	ATOM	938	CA GLN A 133	5.694	-1.381	-3.083	1.00	28.17
	ATOM	939	CB GLN A 133	6.136	-1.543	-4.536	1.00	28.29
	ATOM	940	CG GLN A 133	7.261	-0.608	-4.953	1.00	32.37
35	ATOM	941	CD GLN A 133	6.858	0.846	-4.921	1.00	36.47

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	ATOM	942	OE1	GLN A 133	5.903	1.247	-5.581	1.00	39.54
	ATOM	943	NE2	GLN A 133	7.586	1.650	-4.151	1.00	39.31
	ATOM	944	C	GLN A 133	4.567	-2.370	-2.760	1.00	27.32
	ATOM	945	O	GLN A 133	3.407	-2.117	-3.099	1.00	26.63
5	ATOM	946	N	PHE A 134	4.908	-3.478	-2.099	1.00	26.88
	ATOM	947	CA	PHE A 134	3.907	-4.471	-1.673	1.00	26.52
	ATOM	948	CB	PHE A 134	4.488	-5.895	-1.743	1.00	26.94
	ATOM	949	CG	PHE A 134	4.676	-6.422	-3.156	1.00	26.91
	ATOM	950	CD1	PHE A 134	3.794	-7.360	-3.685	1.00	27.82
10	ATOM	951	CE1	PHE A 134	3.960	-7.865	-4.991	1.00	27.80
	ATOM	952	CZ	PHE A 134	5.015	-7.416	-5.776	1.00	28.00
	ATOM	953	CE2	PHE A 134	5.905	-6.472	-5.261	1.00	29.02
	ATOM	954	CD2	PHE A 134	5.724	-5.975	-3.951	1.00	27.69
	ATOM	955	C	PHE A 134	3.345	-4.182	-0.274	1.00	26.46
15	ATOM	956	O	PHE A 134	2.591	-4.985	0.287	1.00	26.76
	ATOM	957	N	GLY A 135	3.708	-3.033	0.290	1.00	25.96
	ATOM	958	CA	GLY A 135	3.181	-2.613	1.588	1.00	25.25
	ATOM	959	C	GLY A 135	3.718	-3.347	2.807	1.00	24.52
	ATOM	960	O	GLY A 135	3.123	-3.260	3.881	1.00	24.52
20	ATOM	961	N	VAL A 136	4.841	-4.060	2.644	1.00	23.52
	ATOM	962	CA	VAL A 136	5.485	-4.818	3.731	1.00	22.72
	ATOM	963	CB	VAL A 136	5.453	-6.347	3.475	1.00	22.79
	ATOM	964	CG1	VAL A 136	4.096	-6.924	3.866	1.00	23.64
	ATOM	965	CG2	VAL A 136	5.797	-6.670	2.012	1.00	22.92
25	ATOM	966	C	VAL A 136	6.931	-4.372	4.041	1.00	21.95
	ATOM	967	O	VAL A 136	7.699	-5.119	4.654	1.00	21.68
	ATOM	968	N	GLY A 137	7.262	-3.142	3.655	1.00	21.49
	ATOM	969	CA	GLY A 137	8.585	-2.538	3.890	1.00	20.62
	ATOM	970	C	GLY A 137	9.144	-2.619	5.306	1.00	20.35
30	ATOM	971	O	GLY A 137	10.353	-2.786	5.493	1.00	19.58
	ATOM	972	N	PHE A 138	8.277	-2.488	6.312	1.00	20.08
	ATOM	973	CA	PHE A 138	8.722	-2.611	7.702	1.00	20.05
	ATOM	974	CB	PHE A 138	7.538	-2.640	8.678	1.00	19.94
	ATOM	975	CG	PHE A 138	7.928	-3.050	10.072	1.00	20.86
35	ATOM	976	CD1	PHE A 138	8.630	-2.173	10.902	1.00	20.36

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	ATOM	977	CE1 PHE A 138	9.025	-2.562	12.180	1.00	21.52
	ATOM	978	CZ PHE A 138	8.704	-3.843	12.650	1.00	20.92
	ATOM	979	CE2 PHE A 138	8.016	-4.724	11.830	1.00	21.99
	ATOM	980	CD2 PHE A 138	7.632	-4.328	10.546	1.00	21.90
5	ATOM	981	C PHE A 138	9.590	-3.838	7.940	1.00	19.48
	ATOM	982	O PHE A 138	10.613	-3.758	8.633	1.00	19.46
	ATOM	983	N TYR A 139	9.191	-4.957	7.341	1.00	19.30
	ATOM	984	CA TYR A 139	9.835	-6.246	7.594	1.00	19.36
	ATOM	985	CB TYR A 139	8.930	-7.424	7.195	1.00	19.59
10	ATOM	986	CG TYR A 139	7.657	-7.454	8.024	1.00	20.49
	ATOM	987	CD1 TYR A 139	7.658	-7.923	9.350	1.00	21.23
	ATOM	988	CE1 TYR A 139	6.472	-7.930	10.110	1.00	20.24
	ATOM	989	CZ TYR A 139	5.307	-7.459	9.547	1.00	21.34
	ATOM	990	OH TYR A 139	4.121	-7.426	10.264	1.00	21.33
15	ATOM	991	CE2 TYR A 139	5.296	-6.981	8.257	1.00	21.16
	ATOM	992	CD2 TYR A 139	6.464	-6.985	7.501	1.00	20.92
	ATOM	993	C TYR A 139	11.239	-6.362	7.022	1.00	18.75
	ATOM	994	O TYR A 139	11.988	-7.221	7.466	1.00	18.40
	ATOM	995	N SER A 140	11.594	-5.461	6.098	1.00	18.62
20	ATOM	996	CA SER A 140	12.974	-5.325	5.604	1.00	18.45
	ATOM	997	CB SER A 140	13.087	-4.229	4.526	1.00	19.37
	ATOM	998	OG SER A 140	12.871	-2.926	5.056	1.00	18.95
	ATOM	999	C SER A 140	13.996	-5.089	6.720	1.00	18.23
	ATOM	1000	O SER A 140	15.184	-5.342	6.545	1.00	17.91
25	ATOM	1001	N ALA A 141	13.537	-4.615	7.880	1.00	17.90
	ATOM	1002	CA ALA A 141	14.426	-4.400	9.026	1.00	18.22
	ATOM	1003	CB ALA A 141	13.646	-3.905	10.209	1.00	17.84
	ATOM	1004	C ALA A 141	15.182	-5.688	9.383	1.00	18.22
	ATOM	1005	O ALA A 141	16.334	-5.653	9.811	1.00	18.42
30	ATOM	1006	N TYR A 142	14.531	-6.821	9.169	1.00	19.13
	ATOM	1007	CA TYR A 142	15.116	-8.127	9.490	1.00	19.67
	ATOM	1008	CB TYR A 142	14.008	-9.168	9.702	1.00	19.50
	ATOM	1009	CG TYR A 142	13.236	-8.848	10.965	1.00	20.26
	ATOM	1010	CD1 TYR A 142	13.716	-9.254	12.217	1.00	19.73
35	ATOM	1011	CE1 TYR A 142	13.021	-8.945	13.396	1.00	20.96

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	ATOM	1012	CZ	TYR A 142	11.843	-8.213	13.316	1.00	20.06
	ATOM	1013	OH	TYR A 142	11.156	-7.885	14.473	1.00	21.48
	ATOM	1014	CE2	TYR A 142	11.361	-7.781	12.094	1.00	19.63
	ATOM	1015	CD2	TYR A 142	12.059	-8.096	10.917	1.00	20.99
5	ATOM	1016	C	TYR A 142	16.177	-8.609	8.503	1.00	20.33
	ATOM	1017	O	TYR A 142	16.790	-9.660	8.716	1.00	20.68
	ATOM	1018	N	LEU A 143	16.403	-7.841	7.437	1.00	20.20
	ATOM	1019	CA	LEU A 143	17.606	-8.062	6.607	1.00	20.32
	ATOM	1020	CB	LEU A 143	17.568	-7.181	5.361	1.00	19.86
10	ATOM	1021	CG	LEU A 143	16.519	-7.437	4.278	1.00	20.48
	ATOM	1022	CD1	LEU A 143	16.392	-6.196	3.380	1.00	19.53
	ATOM	1023	CD2	LEU A 143	16.849	-8.704	3.470	1.00	20.54
	ATOM	1024	C	LEU A 143	18.900	-7.778	7.379	1.00	20.65
	ATOM	1025	O	LEU A 143	19.925	-8.421	7.140	1.00	21.28
15	ATOM	1026	N	VAL A 144	18.859	-6.788	8.276	1.00	20.36
	ATOM	1027	CA	VAL A 144	20.047	-6.339	8.999	1.00	20.16
	ATOM	1028	CB	VAL A 144	20.459	-4.857	8.647	1.00	20.04
	ATOM	1029	CG1	VAL A 144	20.615	-4.668	7.137	1.00	20.62
	ATOM	1030	CG2	VAL A 144	19.462	-3.836	9.223	1.00	20.07
20	ATOM	1031	C	VAL A 144	19.953	-6.503	10.521	1.00	20.00
	ATOM	1032	O	VAL A 144	20.969	-6.444	11.200	1.00	19.13
	ATOM	1033	N	ALA A 145	18.742	-6.715	11.049	1.00	20.65
	ATOM	1034	CA	ALA A 145	18.533	-6.783	12.507	1.00	20.36
	ATOM	1035	CB	ALA A 145	17.572	-5.685	12.970	1.00	21.12
25	ATOM	1036	C	ALA A 145	18.024	-8.144	12.973	1.00	20.33
	ATOM	1037	O	ALA A 145	17.199	-8.763	12.305	1.00	20.08
	ATOM	1038	N	GLU A 146	18.545	-8.587	14.118	1.00	20.96
	ATOM	1039	CA	GLU A 146	18.132	-9.822	14.772	1.00	22.03
	ATOM	1040	CB	GLU A 146	19.314	-10.453	15.546	1.00	21.93
30	ATOM	1041	CG	GLU A 146	19.932	-9.577	16.641	1.00	23.11
	ATOM	1042	CD	GLU A 146	21.259	-10.101	17.145	1.00	24.54
	ATOM	1043	OE1	GLU A 146	21.828	-11.008	16.504	1.00	28.10
	ATOM	1044	OE2	GLU A 146	21.733	-9.614	18.195	1.00	27.38
	ATOM	1045	C	GLU A 146	16.947	-9.535	15.690	1.00	22.13
35	ATOM	1046	O	GLU A 146	16.138	-10.421	15.959	1.00	22.96

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	ATOM	1047	N	LYS A 147	16.837	-8.286	16.145	1.00	22.04
	ATOM	1048	CA	LYS A 147	15.723	-7.882	16.996	1.00	22.28
	ATOM	1049	CB	LYS A 147	16.086	-7.999	18.483	1.00	22.08
	ATOM	1050	CG	LYS A 147	14.997	-7.482	19.462	1.00	24.93
5	ATOM	1051	CD	LYS A 147	15.250	-7.905	20.925	1.00	24.27
	ATOM	1052	CE	LYS A 147	16.582	-7.391	21.471	1.00	28.12
	ATOM	1053	NZ	LYS A 147	16.831	-7.769	22.907	1.00	28.87
	ATOM	1054	C	LYS A 147	15.328	-6.467	16.652	1.00	21.28
	ATOM	1055	O	LYS A 147	16.184	-5.615	16.390	1.00	21.03
10	ATOM	1056	N	VAL A 148	14.023	-6.226	16.626	1.00	20.65
	ATOM	1057	CA	VAL A 148	13.508	-4.904	16.341	1.00	19.68
	ATOM	1058	CB	VAL A 148	12.801	-4.865	14.964	1.00	19.80
	ATOM	1059	CG1	VAL A 148	12.173	-3.476	14.683	1.00	20.55
	ATOM	1060	CG2	VAL A 148	13.786	-5.273	13.829	1.00	18.59
15	ATOM	1061	C	VAL A 148	12.546	-4.531	17.468	1.00	20.06
	ATOM	1062	O	VAL A 148	11.665	-5.324	17.814	1.00	19.03
	ATOM	1063	N	THR A 149	12.752	-3.342	18.034	1.00	19.77
	ATOM	1064	CA	THR A 149	11.842	-2.758	19.033	1.00	20.67
	ATOM	1065	CB	THR A 149	12.591	-2.376	20.327	1.00	20.54
20	ATOM	1066	OG1	THR A 149	13.410	-3.472	20.757	1.00	22.01
	ATOM	1067	CG2	THR A 149	11.612	-1.997	21.449	1.00	21.10
	ATOM	1068	C	THR A 149	11.218	-1.516	18.410	1.00	20.92
	ATOM	1069	O	THR A 149	11.920	-0.692	17.781	1.00	20.77
	ATOM	1070	N	VAL A 150	9.900	-1.380	18.565	1.00	20.63
25	ATOM	1071	CA	VAL A 150	9.202	-0.199	18.093	1.00	20.24
	ATOM	1072	CB	VAL A 150	8.150	-0.523	16.999	1.00	20.68
	ATOM	1073	CG1	VAL A 150	7.311	0.717	16.660	1.00	19.79
	ATOM	1074	CG2	VAL A 150	8.818	-1.074	15.718	1.00	19.79
	ATOM	1075	C	VAL A 150	8.541	0.453	19.313	1.00	20.91
30	ATOM	1076	O	VAL A 150	7.727	-0.177	19.980	1.00	20.50
	ATOM	1077	N	ILE A 151	8.942	1.685	19.609	1.00	20.88
	ATOM	1078	CA	ILE A 151	8.351	2.476	20.693	1.00	21.91
	ATOM	1079	CB	ILE A 151	9.430	3.136	21.581	1.00	22.18
	ATOM	1080	CG1	ILE A 151	10.530	2.139	21.996	1.00	23.97
35	ATOM	1081	CD1	ILE A 151	10.154	1.111	23.023	1.00	27.31

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	ATOM	1082	CG2 ILE A 151	8.790	3.924	22.754	1.00	21.89
	ATOM	1083	C ILE A 151	7.531	3.556	20.022	1.00	21.91
	ATOM	1084	O ILE A 151	7.985	4.171	19.053	1.00	21.70
	ATOM	1085	N THR A 152	6.312	3.790	20.504	1.00	21.99
5	ATOM	1086	CA THR A 152	5.438	4.708	19.795	1.00	21.88
	ATOM	1087	CB THR A 152	4.685	4.015	18.638	1.00	21.74
	ATOM	1088	OG1 THR A 152	4.120	5.004	17.773	1.00	22.54
	ATOM	1089	CG2 THR A 152	3.571	3.092	19.146	1.00	21.50
	ATOM	1090	C THR A 152	4.484	5.454	20.728	1.00	22.51
10	ATOM	1091	O THR A 152	4.043	4.898	21.736	1.00	22.69
	ATOM	1092	N LYS A 153	4.204	6.704	20.369	1.00	22.65
	ATOM	1093	CA LYS A 153	3.314	7.581	21.140	1.00	22.89
	ATOM	1094	CB LYS A 153	4.138	8.470	22.070	1.00	22.56
	ATOM	1095	CG LYS A 153	3.330	9.504	22.882	1.00	22.98
15	ATOM	1096	CD LYS A 153	2.489	8.840	23.951	1.00	23.75
	ATOM	1097	CE LYS A 153	1.717	9.892	24.773	1.00	23.27
	ATOM	1098	NZ LYS A 153	0.584	10.447	23.979	1.00	24.90
	ATOM	1099	C LYS A 153	2.390	8.398	20.226	1.00	23.43
	ATOM	1100	O LYS A 153	2.850	9.201	19.409	1.00	23.16
20	ATOM	1101	N HIS A 154	1.079	8.177	20.372	1.00	23.89
	ATOM	1102	CA HIS A 154	0.052	8.874	19.599	1.00	24.81
	ATOM	1103	CB HIS A 154	-0.949	7.832	19.082	1.00	25.37
	ATOM	1104	CG HIS A 154	-1.925	8.340	18.064	1.00	25.81
	ATOM	1105	ND1 HIS A 154	-2.995	9.149	18.390	1.00	26.84
25	ATOM	1106	CE1 HIS A 154	-3.695	9.409	17.301	1.00	26.96
	ATOM	1107	NE2 HIS A 154	-3.136	8.774	16.286	1.00	28.23
	ATOM	1108	CD2 HIS A 154	-2.035	8.089	16.739	1.00	25.52
	ATOM	1109	C HIS A 154	-0.651	9.851	20.544	1.00	25.53
	ATOM	1110	O HIS A 154	-0.804	9.548	21.728	1.00	25.56
30	ATOM	1111	N ASN A 155	-1.076	11.004	20.031	1.00	26.81
	ATOM	1112	CA ASN A 155	-1.856	11.952	20.841	1.00	28.16
	ATOM	1113	CB ASN A 155	-2.359	13.128	19.997	1.00	28.01
	ATOM	1114	CG ASN A 155	-1.248	14.119	19.623	1.00	27.71
	ATOM	1115	OD1 ASN A 155	-0.197	14.182	20.265	1.00	27.79
35	ATOM	1116	ND2 ASN A 155	-1.488	14.895	18.575	1.00	27.52

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	ATOM	1117	C	ASN A 155	-3.030	11.227	21.505	1.00	29.47
	ATOM	1118	O	ASN A 155	-3.671	10.361	20.890	1.00	29.57
	ATOM	1119	N	ASP A 156	-3.271	11.556	22.773	1.00	31.26
	ATOM	1120	CA	ASP A 156	-4.408	11.033	23.547	1.00	32.80
5	ATOM	1121	CB	ASP A 156	-5.732	11.348	22.835	1.00	33.37
	ATOM	1122	CG	ASP A 156	-5.882	12.818	22.518	1.00	35.56
	ATOM	1123	OD1	ASP A 156	-5.932	13.638	23.463	1.00	37.98
	ATOM	1124	OD2	ASP A 156	-5.930	13.154	21.318	1.00	39.04
	ATOM	1125	C	ASP A 156	-4.345	9.548	23.921	1.00	33.18
10	ATOM	1126	O	ASP A 156	-5.336	8.993	24.403	1.00	33.57
	ATOM	1127	N	ASP A 157	-3.190	8.909	23.714	1.00	33.35
	ATOM	1128	CA	ASP A 157	-2.981	7.515	24.121	1.00	33.17
	ATOM	1129	CB	ASP A 157	-3.018	6.589	22.911	1.00	33.92
	ATOM	1130	CG	ASP A 157	-3.663	5.245	23.215	1.00	36.04
15	ATOM	1131	OD1	ASP A 157	-3.552	4.731	24.359	1.00	37.42
	ATOM	1132	OD2	ASP A 157	-4.300	4.700	22.289	1.00	39.60
	ATOM	1133	C	ASP A 157	-1.639	7.346	24.832	1.00	32.61
	ATOM	1134	O	ASP A 157	-0.799	8.244	24.788	1.00	32.89
	ATOM	1135	N	GLU A 158	-1.444	6.194	25.470	1.00	31.42
20	ATOM	1136	CA	GLU A 158	-0.211	5.892	26.190	1.00	31.10
	ATOM	1137	CB	GLU A 158	-0.433	4.754	27.190	1.00	31.03
	ATOM	1138	CG	GLU A 158	-1.091	5.158	28.514	1.00	32.62
	ATOM	1139	CD	GLU A 158	-1.026	4.034	29.540	1.00	33.07
	ATOM	1140	OE1	GLU A 158	-1.652	2.975	29.310	1.00	36.81
25	ATOM	1141	OE2	GLU A 158	-0.334	4.198	30.571	1.00	36.86
	ATOM	1142	C	GLU A 158	0.910	5.506	25.217	1.00	29.71
	ATOM	1143	O	GLU A 158	0.659	5.277	24.025	1.00	29.35
	ATOM	1144	N	GLN A 159	2.135	5.448	25.737	1.00	28.35
	ATOM	1145	CA	GLN A 159	3.301	4.993	24.977	1.00	27.26
30	ATOM	1146	CB	GLN A 159	4.559	5.685	25.499	1.00	27.30
	ATOM	1147	CG	GLN A 159	5.865	5.347	24.785	1.00	26.86
	ATOM	1148	CD	GLN A 159	6.953	6.363	25.108	1.00	27.06
	ATOM	1149	OE1	GLN A 159	6.743	7.578	24.985	1.00	27.83
	ATOM	1150	NE2	GLN A 159	8.111	5.878	25.523	1.00	26.13
35	ATOM	1151	C	GLN A 159	3.451	3.475	25.080	1.00	26.75

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	ATOM	1152	O	GLN A 159	3.442	2.911	26.177	1.00	26.29
	ATOM	1153	N	TYR A 160	3.611	2.822	23.930	1.00	25.74
	ATOM	1154	CA	TYR A 160	3.681	1.369	23.889	1.00	25.46
	ATOM	1155	CB	TYR A 160	2.478	0.794	23.132	1.00	26.41
5	ATOM	1156	CG	TYR A 160	1.151	1.147	23.761	1.00	28.09
	ATOM	1157	CD1	TYR A 160	0.700	0.491	24.910	1.00	29.91
	ATOM	1158	CE1	TYR A 160	-0.526	0.830	25.495	1.00	30.25
	ATOM	1159	CZ	TYR A 160	-1.301	1.823	24.923	1.00	30.07
	ATOM	1160	OH	TYR A 160	-2.514	2.163	25.486	1.00	30.87
10	ATOM	1161	CE2	TYR A 160	-0.874	2.484	23.786	1.00	30.83
	ATOM	1162	CD2	TYR A 160	0.349	2.140	23.209	1.00	29.27
	ATOM	1163	C	TYR A 160	4.971	0.927	23.218	1.00	24.52
	ATOM	1164	O	TYR A 160	5.556	1.688	22.436	1.00	23.95
	ATOM	1165	N	ALA A 161	5.386	-0.291	23.542	1.00	22.91
15	ATOM	1166	CA	ALA A 161	6.555	-0.938	22.948	1.00	22.19
	ATOM	1167	CB	ALA A 161	7.630	-1.147	24.003	1.00	21.83
	ATOM	1168	C	ALA A 161	6.159	-2.277	22.310	1.00	22.28
	ATOM	1169	O	ALA A 161	5.530	-3.125	22.962	1.00	22.45
	ATOM	1170	N	TRP A 162	6.511	-2.432	21.031	1.00	21.61
20	ATOM	1171	CA	TRP A 162	6.351	-3.664	20.258	1.00	21.16
	ATOM	1172	CB	TRP A 162	5.753	-3.302	18.893	1.00	21.81
	ATOM	1173	CG	TRP A 162	5.583	-4.395	17.846	1.00	21.71
	ATOM	1174	CD1	TRP A 162	4.399	-4.972	17.467	1.00	21.80
	ATOM	1175	NE1	TRP A 162	4.615	-5.888	16.457	1.00	21.69
25	ATOM	1176	CE2	TRP A 162	5.954	-5.912	16.148	1.00	21.70
	ATOM	1177	CD2	TRP A 162	6.601	-4.970	16.985	1.00	21.86
	ATOM	1178	CE3	TRP A 162	7.991	-4.791	16.855	1.00	19.94
	ATOM	1179	CZ3	TRP A 162	8.682	-5.565	15.899	1.00	21.79
	ATOM	1180	CH2	TRP A 162	8.004	-6.488	15.083	1.00	21.28
30	ATOM	1181	CZ2	TRP A 162	6.646	-6.675	15.188	1.00	21.68
	ATOM	1182	C	TRP A 162	7.766	-4.221	20.103	1.00	21.51
	ATOM	1183	O	TRP A 162	8.714	-3.459	19.940	1.00	20.18
	ATOM	1184	N	GLU A 163	7.931	-5.532	20.203	1.00	21.32
	ATOM	1185	CA	GLU A 163	9.263	-6.114	19.988	1.00	23.26
35	ATOM	1186	CB	GLU A 163	10.057	-6.142	21.306	1.00	23.19

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	ATOM	1187	CG	GLU A 163	11.519	-6.606	21.190	1.00	26.67
	ATOM	1188	CD	GLU A 163	12.300	-6.373	22.470	1.00	27.38
	ATOM	1189	OE1	GLU A 163	12.455	-7.338	23.261	1.00	32.73
	ATOM	1190	OE2	GLU A 163	12.746	-5.219	22.695	1.00	33.19
5	ATOM	1191	C	GLU A 163	9.163	-7.504	19.400	1.00	22.43
	ATOM	1192	O	GLU A 163	8.260	-8.273	19.749	1.00	21.10
	ATOM	1193	N	SER A 164	10.104	-7.837	18.515	1.00	22.00
	ATOM	1194	CA	SER A 164	10.178	-9.189	17.997	1.00	21.58
	ATOM	1195	CB	SER A 164	9.227	-9.394	16.807	1.00	21.81
10	ATOM	1196	OG	SER A 164	9.225	-10.742	16.367	1.00	20.81
	ATOM	1197	C	SER A 164	11.592	-9.544	17.592	1.00	22.11
	ATOM	1198	O	SER A 164	12.331	-8.723	17.028	1.00	21.02
	ATOM	1199	N	SER A 165	11.950	-10.784	17.881	1.00	22.35
	ATOM	1200	CA	SER A 165	13.168	-11.352	17.361	1.00	22.87
15	ATOM	1201	CB	SER A 165	13.974	-11.982	18.494	1.00	22.54
	ATOM	1202	OG	SER A 165	14.530	-10.967	19.303	1.00	21.84
	ATOM	1203	C	SER A 165	12.822	-12.367	16.284	1.00	23.82
	ATOM	1204	O	SER A 165	13.610	-13.275	16.003	1.00	24.14
	ATOM	1205	N	ALA A 166	11.655	-12.183	15.656	1.00	24.57
20	ATOM	1206	CA	ALA A 166	11.075	-13.162	14.739	1.00	25.84
	ATOM	1207	CB	ALA A 166	11.982	-13.390	13.511	1.00	26.24
	ATOM	1208	C	ALA A 166	10.780	-14.455	15.504	1.00	26.62
	ATOM	1209	O	ALA A 166	10.402	-14.398	16.671	1.00	27.98
	ATOM	1210	N	GLY A 167	10.947	-15.618	14.885	1.00	27.40
25	ATOM	1211	CA	GLY A 167	10.605	-16.869	15.583	1.00	26.68
	ATOM	1212	C	GLY A 167	9.106	-17.058	15.790	1.00	26.65
	ATOM	1213	O	GLY A 167	8.663	-17.925	16.580	1.00	26.70
	ATOM	1214	N	GLY A 168	8.321	-16.248	15.088	1.00	25.49
	ATOM	1215	CA	GLY A 168	6.889	-16.475	14.992	1.00	24.71
30	ATOM	1216	C	GLY A 168	6.026	-15.722	15.990	1.00	24.30
	ATOM	1217	O	GLY A 168	4.808	-15.880	15.974	1.00	24.09
	ATOM	1218	N	SER A 169	6.635	-14.914	16.856	1.00	23.57
	ATOM	1219	CA	SER A 169	5.848	-14.104	17.784	1.00	23.58
	ATOM	1220	CB	SER A 169	5.611	-14.840	19.112	1.00	24.02
35	ATOM	1221	OG	SER A 169	6.817	-15.050	19.820	1.00	26.82

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	ATOM	1222	C	SER A 169	6.408	-12.702	18.040	1.00	23.07
	ATOM	1223	O	SER A 169	7.569	-12.397	17.724	1.00	21.88
	ATOM	1224	N	PHE A 170	5.559	-11.845	18.603	1.00	22.22
	ATOM	1225	CA	PHE A 170	5.976	-10.519	19.029	1.00	22.28
5	ATOM	1226	CB	PHE A 170	5.721	-9.453	17.945	1.00	22.42
	ATOM	1227	CG	PHE A 170	4.252	-9.208	17.613	1.00	21.08
	ATOM	1228	CD1	PHE A 170	3.527	-8.209	18.269	1.00	21.63
	ATOM	1229	CE1	PHE A 170	2.185	-7.948	17.935	1.00	20.76
	ATOM	1230	CZ	PHE A 170	1.563	-8.677	16.935	1.00	20.46
10	ATOM	1231	CE2	PHE A 170	2.276	-9.684	16.260	1.00	21.47
	ATOM	1232	CD2	PHE A 170	3.622	-9.925	16.597	1.00	23.04
	ATOM	1233	C	PHE A 170	5.277	-10.170	20.336	1.00	22.89
	ATOM	1234	O	PHE A 170	4.312	-10.842	20.720	1.00	22.97
	ATOM	1235	N	THR A 171	5.788	-9.158	21.029	1.00	22.20
15	ATOM	1236	CA	THR A 171	5.149	-8.697	22.259	1.00	22.78
	ATOM	1237	CB	THR A 171	6.031	-8.878	23.511	1.00	22.78
	ATOM	1238	OG1	THR A 171	7.247	-8.126	23.379	1.00	23.59
	ATOM	1239	CG2	THR A 171	6.334	-10.362	23.744	1.00	23.11
	ATOM	1240	C	THR A 171	4.742	-7.254	22.169	1.00	23.07
20	ATOM	1241	O	THR A 171	5.348	-6.456	21.440	1.00	22.21
	ATOM	1242	N	VAL A 172	3.700	-6.925	22.923	1.00	23.23
	ATOM	1243	CA	VAL A 172	3.265	-5.562	23.076	1.00	23.73
	ATOM	1244	CB	VAL A 172	1.965	-5.263	22.298	1.00	23.94
	ATOM	1245	CG1	VAL A 172	1.521	-3.815	22.543	1.00	24.87
25	ATOM	1246	CG2	VAL A 172	2.154	-5.515	20.789	1.00	25.53
	ATOM	1247	C	VAL A 172	3.076	-5.285	24.567	1.00	24.12
	ATOM	1248	O	VAL A 172	2.498	-6.100	25.294	1.00	23.24
	ATOM	1249	N	ARG A 173	3.585	-4.144	25.011	1.00	24.81
	ATOM	1250	CA	ARG A 173	3.431	-3.726	26.407	1.00	26.09
30	ATOM	1251	CB	ARG A 173	4.590	-4.256	27.258	1.00	26.12
	ATOM	1252	CG	ARG A 173	5.962	-3.683	26.881	1.00	26.10
	ATOM	1253	CD	ARG A 173	7.078	-4.533	27.456	1.00	27.32
	ATOM	1254	NE	ARG A 173	7.317	-5.718	26.634	1.00	26.74
	ATOM	1255	CZ	ARG A 173	7.909	-6.828	27.062	1.00	29.58
35	ATOM	1256	NH1	ARG A 173	8.301	-6.933	28.325	1.00	31.07

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	ATOM	1257	NH2	ARG A 173	8.080	-7.850	26.233	1.00	29.33
	ATOM	1258	C	ARG A 173	3.361	-2.209	26.511	1.00	27.30
	ATOM	1259	O	ARG A 173	3.747	-1.489	25.588	1.00	27.01
	ATOM	1260	N	THR A 174	2.860	-1.724	27.643	1.00	28.55
5	ATOM	1261	CA	THR A 174	3.002	-0.317	27.983	1.00	30.04
	ATOM	1262	CB	THR A 174	2.105	0.047	29.179	1.00	29.97
	ATOM	1263	OG1	THR A 174	0.743	-0.149	28.791	1.00	30.00
	ATOM	1264	CG2	THR A 174	2.304	1.487	29.591	1.00	31.26
	ATOM	1265	C	THR A 174	4.476	-0.021	28.274	1.00	30.71
10	ATOM	1266	O	THR A 174	5.113	-0.721	29.054	1.00	31.22
	ATOM	1267	N	ASP A 175	5.018	0.995	27.613	1.00	32.10
	ATOM	1268	CA	ASP A 175	6.440	1.322	27.736	1.00	33.41
	ATOM	1269	CB	ASP A 175	6.917	2.116	26.511	1.00	33.59
	ATOM	1270	CG	ASP A 175	8.426	2.334	26.503	1.00	33.56
15	ATOM	1271	OD1	ASP A 175	9.153	1.534	27.117	1.00	34.94
	ATOM	1272	OD2	ASP A 175	8.886	3.314	25.894	1.00	34.04
	ATOM	1273	C	ASP A 175	6.727	2.091	29.033	1.00	34.54
	ATOM	1274	O	ASP A 175	6.132	3.135	29.287	1.00	34.58
	ATOM	1275	N	THR A 176	7.630	1.551	29.847	1.00	35.92
20	ATOM	1276	CA	THR A 176	8.038	2.181	31.113	1.00	37.54
	ATOM	1277	CB	THR A 176	8.481	1.137	32.161	1.00	37.49
	ATOM	1278	OG1	THR A 176	9.431	0.235	31.572	1.00	38.88
	ATOM	1279	CG2	THR A 176	7.286	0.357	32.683	1.00	37.91
	ATOM	1280	C	THR A 176	9.191	3.163	30.921	1.00	38.07
25	ATOM	1281	O	THR A 176	9.440	4.010	31.784	1.00	39.04
	ATOM	1282	N	GLY A 177	9.882	3.047	29.789	1.00	38.21
	ATOM	1283	CA	GLY A 177	11.073	3.842	29.503	1.00	38.23
	ATOM	1284	C	GLY A 177	10.820	5.300	29.177	1.00	37.92
	ATOM	1285	O	GLY A 177	9.739	5.831	29.426	1.00	37.86
30	ATOM	1286	N	GLU A 178	11.835	5.935	28.599	1.00	37.89
	ATOM	1287	CA	GLU A 178	11.836	7.375	28.327	1.00	37.84
	ATOM	1288	CB	GLU A 178	13.197	7.787	27.765	1.00	37.87
	ATOM	1289	CG	GLU A 178	14.319	7.727	28.818	1.00	39.11
	ATOM	1290	CD	GLU A 178	15.713	7.794	28.228	1.00	39.23
35	ATOM	1291	OE1	GLU A 178	16.667	7.386	28.932	1.00	42.61

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	ATOM	1292	OE2	GLU A 178	15.863	8.247	27.071	1.00	40.32
	ATOM	1293	C	GLU A 178	10.685	7.865	27.420	1.00	37.22
	ATOM	1294	O	GLU A 178	10.580	7.448	26.263	1.00	36.69
	ATOM	1295	N	PRO A 179	9.807	8.736	27.964	1.00	36.70
5	ATOM	1296	CA	PRO A 179	8.662	9.324	27.250	1.00	36.44
	ATOM	1297	CB	PRO A 179	8.016	10.227	28.310	1.00	36.39
	ATOM	1298	CG	PRO A 179	8.451	9.648	29.611	1.00	36.68
	ATOM	1299	CD	PRO A 179	9.850	9.181	29.368	1.00	36.61
	ATOM	1300	C	PRO A 179	9.071	10.154	26.034	1.00	36.31
10	ATOM	1301	O	PRO A 179	10.132	10.787	26.048	1.00	35.89
	ATOM	1302	N	MET A 180	8.210	10.170	25.012	1.00	36.06
	ATOM	1303	CA	MET A 180	8.528	10.769	23.706	1.00	36.38
	ATOM	1304	CB	MET A 180	8.256	9.767	22.582	1.00	36.19
	ATOM	1305	CG	MET A 180	8.957	8.429	22.699	1.00	37.85
15	ATOM	1306	SD	MET A 180	8.832	7.551	21.130	1.00	39.39
	ATOM	1307	CE	MET A 180	9.957	8.543	20.179	1.00	37.87
	ATOM	1308	C	MET A 180	7.771	12.050	23.357	1.00	35.26
	ATOM	1309	O	MET A 180	8.262	12.885	22.598	1.00	36.28
	ATOM	1310	N	GLY A 181	6.556	12.197	23.852	1.00	34.11
20	ATOM	1311	CA	GLY A 181	5.766	13.354	23.442	1.00	31.85
	ATOM	1312	C	GLY A 181	4.871	12.970	22.281	1.00	29.73
	ATOM	1313	O	GLY A 181	3.659	13.011	22.405	1.00	29.70
	ATOM	1314	N	ARG A 182	5.468	12.594	21.147	1.00	27.72
	ATOM	1315	CA	ARG A 182	4.698	12.092	19.994	1.00	25.61
25	ATOM	1316	CB	ARG A 182	3.805	13.181	19.377	1.00	25.96
	ATOM	1317	CG	ARG A 182	2.839	12.687	18.275	1.00	24.46
	ATOM	1318	CD	ARG A 182	2.309	13.830	17.397	1.00	24.59
	ATOM	1319	NE	ARG A 182	3.384	14.482	16.645	1.00	23.13
	ATOM	1320	CZ	ARG A 182	3.821	15.722	16.867	1.00	24.13
30	ATOM	1321	NH1	ARG A 182	3.253	16.489	17.799	1.00	22.04
	ATOM	1322	NH2	ARG A 182	4.816	16.209	16.135	1.00	22.51
	ATOM	1323	C	ARG A 182	5.648	11.554	18.930	1.00	25.12
	ATOM	1324	O	ARG A 182	6.637	12.206	18.572	1.00	24.50
	ATOM	1325	N	GLY A 183	5.333	10.367	18.432	1.00	23.71
35	ATOM	1326	CA	GLY A 183	6.085	9.791	17.324	1.00	22.73

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	ATOM	1327	C	GLY A 183	6.437	8.339	17.540	1.00	22.20
	ATOM	1328	O	GLY A 183	5.833	7.647	18.365	1.00	21.94
	ATOM	1329	N	THR A 184	7.432	7.888	16.790	1.00	21.40
	ATOM	1330	CA	THR A 184	7.798	6.487	16.764	1.00	21.48
5	ATOM	1331	CB	THR A 184	7.204	5.784	15.528	1.00	21.32
	ATOM	1332	OG1	THR A 184	5.780	5.781	15.639	1.00	22.32
	ATOM	1333	CG2	THR A 184	7.696	4.330	15.409	1.00	21.09
	ATOM	1334	C	THR A 184	9.302	6.399	16.729	1.00	21.39
	ATOM	1335	O	THR A 184	9.962	7.139	15.986	1.00	21.06
10	ATOM	1336	N	LYS A 185	9.824	5.510	17.551	1.00	21.05
	ATOM	1337	CA	LYS A 185	11.244	5.221	17.597	1.00	21.36
	ATOM	1338	CB	LYS A 185	11.786	5.591	18.974	1.00	21.59
	ATOM	1339	CG	LYS A 185	13.052	4.876	19.407	1.00	23.90
	ATOM	1340	CD	LYS A 185	13.688	5.575	20.597	1.00	28.13
15	ATOM	1341	CE	LYS A 185	12.961	5.276	21.906	1.00	30.15
	ATOM	1342	NZ	LYS A 185	13.502	6.103	23.031	1.00	31.53
	ATOM	1343	C	LYS A 185	11.442	3.742	17.293	1.00	21.03
	ATOM	1344	O	LYS A 185	10.835	2.874	17.938	1.00	20.58
	ATOM	1345	N	VAL A 186	12.292	3.457	16.309	1.00	20.60
20	ATOM	1346	CA	VAL A 186	12.577	2.088	15.938	1.00	20.73
	ATOM	1347	CB	VAL A 186	12.314	1.833	14.431	1.00	20.94
	ATOM	1348	CG1	VAL A 186	12.602	0.373	14.063	1.00	19.60
	ATOM	1349	CG2	VAL A 186	10.868	2.175	14.072	1.00	20.34
	ATOM	1350	C	VAL A 186	14.039	1.788	16.290	1.00	21.09
25	ATOM	1351	O	VAL A 186	14.945	2.508	15.865	1.00	20.83
	ATOM	1352	N	ILE A 187	14.241	0.744	17.088	1.00	21.09
	ATOM	1353	CA	ILE A 187	15.557	0.344	17.556	1.00	21.45
	ATOM	1354	CB	ILE A 187	15.605	0.190	19.099	1.00	21.79
	ATOM	1355	CG1	ILE A 187	15.025	1.440	19.779	1.00	21.43
30	ATOM	1356	CD1	ILE A 187	14.873	1.326	21.269	1.00	23.22
	ATOM	1357	CG2	ILE A 187	17.047	-0.079	19.563	1.00	20.34
	ATOM	1358	C	ILE A 187	15.940	-0.971	16.885	1.00	20.90
	ATOM	1359	O	ILE A 187	15.334	-2.004	17.144	1.00	20.99
	ATOM	1360	N	LEU A 188	16.942	-0.918	16.009	1.00	20.64
35	ATOM	1361	CA	LEU A 188	17.397	-2.107	15.292	1.00	20.54

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	ATOM	1362	CB	LEU A 188	17.751	-1.786	13.844	1.00	20.84
	ATOM	1363	CG	LEU A 188	16.710	-1.201	12.885	1.00	22.68
	ATOM	1364	CD1	LEU A 188	17.313	-1.134	11.494	1.00	24.88
	ATOM	1365	CD2	LEU A 188	15.488	-2.049	12.839	1.00	21.50
5	ATOM	1366	C	LEU A 188	18.624	-2.680	15.970	1.00	20.84
	ATOM	1367	O	LEU A 188	19.681	-2.032	16.006	1.00	20.10
	ATOM	1368	N	HIS A 189	18.483	-3.895	16.491	1.00	20.11
	ATOM	1369	CA	HIS A 189	19.594	-4.605	17.109	1.00	20.75
	ATOM	1370	CB	HIS A 189	19.096	-5.568	18.200	1.00	20.75
10	ATOM	1371	CG	HIS A 189	18.526	-4.867	19.396	1.00	22.67
	ATOM	1372	ND1	HIS A 189	19.272	-4.595	20.523	1.00	26.02
	ATOM	1373	CE1	HIS A 189	18.520	-3.945	21.398	1.00	27.17
	ATOM	1374	NE2	HIS A 189	17.313	-3.794	20.882	1.00	25.16
	ATOM	1375	CD2	HIS A 189	17.288	-4.368	19.633	1.00	24.29
15	ATOM	1376	C	HIS A 189	20.253	-5.363	15.984	1.00	20.12
	ATOM	1377	O	HIS A 189	19.733	-6.380	15.522	1.00	19.92
	ATOM	1378	N	LEU A 190	21.386	-4.845	15.520	1.00	20.17
	ATOM	1379	CA	LEU A 190	21.973	-5.344	14.284	1.00	20.34
	ATOM	1380	CB	LEU A 190	22.954	-4.323	13.691	1.00	20.08
20	ATOM	1381	CG	LEU A 190	22.403	-2.943	13.307	1.00	18.77
	ATOM	1382	CD1	LEU A 190	23.542	-2.076	12.782	1.00	20.00
	ATOM	1383	CD2	LEU A 190	21.292	-3.027	12.279	1.00	19.23
	ATOM	1384	C	LEU A 190	22.671	-6.688	14.445	1.00	21.13
	ATOM	1385	O	LEU A 190	23.307	-6.969	15.473	1.00	20.41
25	ATOM	1386	N	LYS A 191	22.563	-7.500	13.404	1.00	22.12
	ATOM	1387	CA	LYS A 191	23.300	-8.761	13.332	1.00	23.62
	ATOM	1388	CB	LYS A 191	22.841	-9.555	12.120	1.00	23.35
	ATOM	1389	CG	LYS A 191	21.480	-10.178	12.300	1.00	25.86
	ATOM	1390	CD	LYS A 191	21.100	-11.054	11.123	1.00	29.59
30	ATOM	1391	CE	LYS A 191	20.396	-10.269	10.035	1.00	30.04
	ATOM	1392	NZ	LYS A 191	19.218	-11.057	9.532	1.00	33.86
	ATOM	1393	C	LYS A 191	24.794	-8.490	13.256	1.00	24.31
	ATOM	1394	O	LYS A 191	25.202	-7.439	12.764	1.00	24.27
	ATOM	1395	N	GLU A 192	25.603	-9.450	13.720	1.00	25.16
35	ATOM	1396	CA	GLU A 192	27.062	-9.261	13.854	1.00	26.83

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	ATOM	1397	CB	GLU A 192	27.756	-10.530	14.390	1.00	27.09
	ATOM	1398	CG	GLU A 192	27.481	-11.827	13.596	1.00	30.76
	ATOM	1399	CD	GLU A 192	28.594	-12.218	12.606	1.00	35.82
	ATOM	1400	OE1	GLU A 192	28.394	-13.202	11.858	1.00	37.71
5	ATOM	1401	OE2	GLU A 192	29.663	-11.559	12.570	1.00	38.39
	ATOM	1402	C	GLU A 192	27.765	-8.785	12.583	1.00	26.86
	ATOM	1403	O	GLU A 192	28.730	-8.006	12.662	1.00	26.87
	ATOM	1404	N	ASP A 193	27.290	-9.255	11.430	1.00	26.82
	ATOM	1405	CA	ASP A 193	27.937	-8.944	10.147	1.00	27.33
10	ATOM	1406	CB	ASP A 193	27.933	-10.166	9.216	1.00	27.66
	ATOM	1407	CG	ASP A 193	26.533	-10.612	8.806	1.00	29.50
	ATOM	1408	OD1	ASP A 193	25.527	-10.237	9.455	1.00	32.14
	ATOM	1409	OD2	ASP A 193	26.438	-11.383	7.831	1.00	32.39
	ATOM	1410	C	ASP A 193	27.360	-7.719	9.435	1.00	27.08
15	ATOM	1411	O	ASP A 193	27.722	-7.438	8.284	1.00	27.46
	ATOM	1412	N	GLN A 194	26.477	-6.990	10.117	1.00	26.40
	ATOM	1413	CA	GLN A 194	25.808	-5.833	9.517	1.00	25.61
	ATOM	1414	CB	GLN A 194	24.286	-6.083	9.457	1.00	25.68
	ATOM	1415	CG	GLN A 194	23.864	-7.351	8.669	1.00	25.78
20	ATOM	1416	CD	GLN A 194	24.180	-7.274	7.171	1.00	27.37
	ATOM	1417	OE1	GLN A 194	24.117	-6.210	6.573	1.00	28.42
	ATOM	1418	NE2	GLN A 194	24.541	-8.411	6.574	1.00	26.88
	ATOM	1419	C	GLN A 194	26.152	-4.504	10.217	1.00	25.18
	ATOM	1420	O	GLN A 194	25.435	-3.505	10.079	1.00	24.28
25	ATOM	1421	N	THR A 195	27.275	-4.483	10.938	1.00	24.30
	ATOM	1422	CA	THR A 195	27.654	-3.313	11.732	1.00	24.44
	ATOM	1423	CB	THR A 195	28.765	-3.627	12.779	1.00	24.42
	ATOM	1424	OG1	THR A 195	29.991	-3.922	12.101	1.00	26.34
	ATOM	1425	CG2	THR A 195	28.377	-4.803	13.682	1.00	25.28
30	ATOM	1426	C	THR A 195	28.075	-2.101	10.890	1.00	23.97
	ATOM	1427	O	THR A 195	28.295	-1.012	11.432	1.00	23.90
	ATOM	1428	N	GLU A 196	28.192	-2.288	9.575	1.00	24.29
	ATOM	1429	CA	GLU A 196	28.522	-1.171	8.675	1.00	24.46
	ATOM	1430	CB	GLU A 196	28.672	-1.634	7.225	1.00	24.42
35	ATOM	1431	CG	GLU A 196	27.380	-1.980	6.519	1.00	24.75

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	ATOM	1432	CD	GLU A 196	27.595	-2.739	5.222	1.00	25.98
	ATOM	1433	OE1	GLU A 196	28.182	-3.848	5.269	1.00	27.84
	ATOM	1434	OE2	GLU A 196	27.163	-2.226	4.162	1.00	25.27
	ATOM	1435	C	GLU A 196	27.480	-0.067	8.784	1.00	23.83
5	ATOM	1436	O	GLU A 196	27.795	1.097	8.595	1.00	24.20
	ATOM	1437	N	TYR A 197	26.247	-0.431	9.137	1.00	23.57
	ATOM	1438	CA	TYR A 197	25.162	0.554	9.248	1.00	23.48
	ATOM	1439	CB	TYR A 197	23.805	-0.130	9.022	1.00	23.65
	ATOM	1440	CG	TYR A 197	23.773	-0.826	7.683	1.00	23.65
10	ATOM	1441	CD1	TYR A 197	23.791	-0.081	6.497	1.00	22.45
	ATOM	1442	CE1	TYR A 197	23.782	-0.698	5.269	1.00	23.06
	ATOM	1443	CZ	TYR A 197	23.791	-2.076	5.196	1.00	23.74
	ATOM	1444	OH	TYR A 197	23.785	-2.663	3.963	1.00	25.68
	ATOM	1445	CE2	TYR A 197	23.787	-2.851	6.353	1.00	24.21
15	ATOM	1446	CD2	TYR A 197	23.789	-2.220	7.592	1.00	21.58
	ATOM	1447	C	TYR A 197	25.196	1.410	10.522	1.00	23.36
	ATOM	1448	O	TYR A 197	24.267	2.162	10.803	1.00	23.62
	ATOM	1449	N	LEU A 198	26.282	1.302	11.277	1.00	23.17
	ATOM	1450	CA	LEU A 198	26.533	2.187	12.415	1.00	23.36
20	ATOM	1451	CB	LEU A 198	26.978	1.388	13.635	1.00	23.58
	ATOM	1452	CG	LEU A 198	26.010	0.288	14.060	1.00	23.78
	ATOM	1453	CD1	LEU A 198	26.669	-0.550	15.133	1.00	25.09
	ATOM	1454	CD2	LEU A 198	24.712	0.922	14.552	1.00	25.44
	ATOM	1455	C	LEU A 198	27.607	3.195	12.065	1.00	24.07
25	ATOM	1456	O	LEU A 198	27.947	4.065	12.881	1.00	23.81
	ATOM	1457	N	GLU A 199	28.141	3.070	10.854	1.00	24.99
	ATOM	1458	CA	GLU A 199	29.244	3.917	10.420	1.00	26.08
	ATOM	1459	CB	GLU A 199	30.204	3.140	9.515	1.00	26.14
	ATOM	1460	CG	GLU A 199	30.847	1.950	10.250	0.65	26.62
30	ATOM	1461	CD	GLU A 199	31.762	1.114	9.386	0.65	27.46
	ATOM	1462	OE1	GLU A 199	32.101	1.546	8.261	0.65	29.11
	ATOM	1463	OE2	GLU A 199	32.151	0.016	9.844	0.65	30.34
	ATOM	1464	C	GLU A 199	28.722	5.186	9.764	1.00	26.23
	ATOM	1465	O	GLU A 199	27.840	5.139	8.902	1.00	26.37
35	ATOM	1466	N	GLU A 200	29.257	6.319	10.212	1.00	26.27

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	ATOM	1467	CA	GLU A 200	28.847	7.636	9.738	1.00	27.10
	ATOM	1468	CB	GLU A 200	29.774	8.696	10.341	1.00	27.24
	ATOM	1469	CG	GLU A 200	29.614	10.079	9.771	1.00	29.21
	ATOM	1470	CD	GLU A 200	30.563	11.087	10.388	1.00	30.12
5	ATOM	1471	OE1	GLU A 200	30.315	12.296	10.214	1.00	32.69
	ATOM	1472	OE2	GLU A 200	31.553	10.677	11.040	1.00	34.90
	ATOM	1473	C	GLU A 200	28.829	7.725	8.204	1.00	26.21
	ATOM	1474	O	GLU A 200	27.835	8.143	7.613	1.00	25.10
	ATOM	1475	N	ARG A 201	29.930	7.321	7.566	1.00	26.20
10	ATOM	1476	CA	ARG A 201	30.039	7.397	6.107	1.00	26.49
	ATOM	1477	CB	ARG A 201	31.431	6.964	5.628	1.00	26.49
	ATOM	1478	CG	ARG A 201	31.624	7.063	4.102	1.00	28.45
	ATOM	1479	CD	ARG A 201	33.068	6.754	3.712	1.00	29.22
	ATOM	1480	NE	ARG A 201	33.960	7.811	4.180	1.00	35.23
15	ATOM	1481	CZ	ARG A 201	35.188	7.610	4.641	1.00	37.40
	ATOM	1482	NH1	ARG A 201	35.913	8.642	5.055	1.00	38.73
	ATOM	1483	NH2	ARG A 201	35.689	6.381	4.701	1.00	40.32
	ATOM	1484	C	ARG A 201	28.964	6.593	5.379	1.00	25.17
	ATOM	1485	O	ARG A 201	28.338	7.099	4.452	1.00	25.30
20	ATOM	1486	N	ARG A 202	28.776	5.340	5.801	1.00	24.12
	ATOM	1487	CA	ARG A 202	27.848	4.404	5.166	1.00	23.35
	ATOM	1488	CB	ARG A 202	27.992	3.009	5.796	1.00	23.14
	ATOM	1489	CG	ARG A 202	27.094	1.932	5.180	1.00	24.85
	ATOM	1490	CD	ARG A 202	27.604	1.461	3.811	1.00	26.40
25	ATOM	1491	NE	ARG A 202	26.832	0.317	3.323	1.00	27.92
	ATOM	1492	CZ	ARG A 202	26.163	0.275	2.173	1.00	27.95
	ATOM	1493	NH1	ARG A 202	26.183	1.307	1.331	1.00	29.78
	ATOM	1494	NH2	ARG A 202	25.482	-0.818	1.850	1.00	27.29
	ATOM	1495	C	ARG A 202	26.402	4.867	5.286	1.00	22.42
30	ATOM	1496	O	ARG A 202	25.629	4.758	4.335	1.00	22.07
	ATOM	1497	N	ILE A 203	26.053	5.370	6.467	1.00	21.98
	ATOM	1498	CA	ILE A 203	24.722	5.927	6.713	1.00	21.64
	ATOM	1499	CB	ILE A 203	24.545	6.336	8.199	1.00	22.12
	ATOM	1500	CG1	ILE A 203	24.537	5.089	9.097	0.50	19.77
35	ATOM	1501	CD1	ILE A 203	24.749	5.393	10.576	0.50	20.87

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	ATOM	1502	CG2	ILE A 203	23.247	7.133	8.409	0.50	20.26
	ATOM	1503	C	ILE A 203	24.471	7.099	5.758	1.00	22.44
	ATOM	1504	O	ILE A 203	23.479	7.112	5.046	1.00	21.94
	ATOM	1505	N	LYS A 204	25.412	8.040	5.701	1.00	23.01
5	ATOM	1506	CA	LYS A 204	25.296	9.198	4.804	1.00	24.23
	ATOM	1507	CB	LYS A 204	26.464	10.175	4.990	1.00	23.57
	ATOM	1508	CG	LYS A 204	26.417	10.941	6.319	1.00	25.23
	ATOM	1509	CD	LYS A 204	27.354	12.133	6.360	1.00	25.76
	ATOM	1510	CE	LYS A 204	28.792	11.739	6.515	1.00	29.79
10	ATOM	1511	NZ	LYS A 204	29.681	12.932	6.670	1.00	30.11
	ATOM	1512	C	LYS A 204	25.171	8.779	3.342	1.00	24.07
	ATOM	1513	O	LYS A 204	24.373	9.345	2.599	1.00	24.63
	ATOM	1514	N	GLU A 205	25.950	7.777	2.944	1.00	24.70
	ATOM	1515	CA	GLU A 205	25.904	7.230	1.586	1.00	24.97
15	ATOM	1516	CB	GLU A 205	26.871	6.052	1.449	1.00	24.94
	ATOM	1517	CG	GLU A 205	26.807	5.377	0.079	1.00	26.00
	ATOM	1518	CD	GLU A 205	27.813	4.273	-0.077	1.00	29.37
	ATOM	1519	OE1	GLU A 205	27.972	3.457	0.859	1.00	29.92
	ATOM	1520	OE2	GLU A 205	28.441	4.211	-1.149	1.00	32.07
20	ATOM	1521	C	GLU A 205	24.507	6.777	1.189	1.00	25.01
	ATOM	1522	O	GLU A 205	23.994	7.165	0.138	1.00	24.39
	ATOM	1523	N	ILE A 206	23.895	5.957	2.044	1.00	24.99
	ATOM	1524	CA	ILE A 206	22.611	5.346	1.714	1.00	25.10
	ATOM	1525	CB	ILE A 206	22.366	4.010	2.493	1.00	25.11
25	ATOM	1526	CG1	ILE A 206	22.219	4.241	3.999	1.00	24.96
	ATOM	1527	CD1	ILE A 206	21.941	2.935	4.821	1.00	25.19
	ATOM	1528	CG2	ILE A 206	23.478	3.018	2.184	1.00	24.86
	ATOM	1529	C	ILE A 206	21.433	6.315	1.822	1.00	25.14
	ATOM	1530	O	ILE A 206	20.484	6.216	1.046	1.00	24.77
30	ATOM	1531	N	VAL A 207	21.508	7.264	2.748	1.00	25.22
	ATOM	1532	CA	VAL A 207	20.500	8.331	2.823	1.00	25.85
	ATOM	1533	CB	VAL A 207	20.664	9.211	4.092	1.00	26.05
	ATOM	1534	CG1	VAL A 207	19.704	10.400	4.072	1.00	25.12
	ATOM	1535	CG2	VAL A 207	20.436	8.353	5.365	1.00	25.18
35	ATOM	1536	C	VAL A 207	20.537	9.170	1.544	1.00	26.67

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	ATOM	1537	O	VAL A 207	19.505	9.411	0.927	1.00	26.92
	ATOM	1538	N	LYS A 208	21.738	9.569	1.132	1.00	26.92
	ATOM	1539	CA	LYS A 208	21.933	10.327	-0.104	1.00	27.99
	ATOM	1540	CB	LYS A 208	23.411	10.704	-0.265	1.00	27.59
5	ATOM	1541	CG	LYS A 208	23.673	11.743	-1.366	1.00	28.46
	ATOM	1542	C	LYS A 208	21.451	9.568	-1.341	1.00	28.65
	ATOM	1543	O	LYS A 208	20.800	10.138	-2.214	1.00	28.78
	ATOM	1544	N	LYS A 209	21.776	8.281	-1.407	1.00	29.67
	ATOM	1545	CA	LYS A 209	21.453	7.456	-2.561	1.00	31.15
10	ATOM	1546	CB	LYS A 209	22.301	6.172	-2.534	1.00	31.00
	ATOM	1547	CG	LYS A 209	22.238	5.342	-3.810	1.00	32.58
	ATOM	1548	CD	LYS A 209	23.325	4.265	-3.832	1.00	32.43
	ATOM	1549	C	LYS A 209	19.958	7.126	-2.649	1.00	31.64
	ATOM	1550	O	LYS A 209	19.351	7.237	-3.721	1.00	31.61
15	ATOM	1551	N	HIS A 210	19.363	6.746	-1.520	1.00	32.17
	ATOM	1552	CA	HIS A 210	18.026	6.162	-1.526	1.00	33.19
	ATOM	1553	CB	HIS A 210	18.060	4.786	-0.867	1.00	33.52
	ATOM	1554	CG	HIS A 210	18.988	3.825	-1.532	1.00	35.65
	ATOM	1555	ND1	HIS A 210	18.640	3.120	-2.665	1.00	37.98
20	ATOM	1556	CE1	HIS A 210	19.648	2.345	-3.022	1.00	39.10
	ATOM	1557	NE2	HIS A 210	20.638	2.529	-2.166	1.00	39.37
	ATOM	1558	CD2	HIS A 210	20.250	3.450	-1.225	1.00	36.81
	ATOM	1559	C	HIS A 210	16.926	6.983	-0.863	1.00	33.27
	ATOM	1560	O	HIS A 210	15.747	6.639	-1.002	1.00	33.15
25	ATOM	1561	N	SER A 211	17.299	8.038	-0.141	1.00	33.60
	ATOM	1562	CA	SER A 211	16.331	8.849	0.610	1.00	34.27
	ATOM	1563	CB	SER A 211	16.390	8.488	2.097	1.00	33.95
	ATOM	1564	OG	SER A 211	16.034	7.133	2.305	1.00	30.19
	ATOM	1565	C	SER A 211	16.528	10.361	0.401	1.00	35.80
30	ATOM	1566	O	SER A 211	16.617	11.139	1.353	1.00	35.79
	ATOM	1567	N	GLN A 212	16.569	10.765	-0.861	1.00	37.49
	ATOM	1568	CA	GLN A 212	16.916	12.142	-1.236	1.00	39.49
	ATOM	1569	CB	GLN A 212	17.720	12.178	-2.555	1.00	39.58
	ATOM	1570	CG	GLN A 212	17.768	10.869	-3.378	1.00	41.89
35	ATOM	1571	CD	GLN A 212	16.411	10.209	-3.597	1.00	44.61

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	ATOM	1572	OE1	GLN A 212	15.400	10.881	-3.799	1.00	46.54
	ATOM	1573	NE2	GLN A 212	16.388	8.882	-3.553	1.00	46.02
	ATOM	1574	C	GLN A 212	15.748	13.144	-1.283	1.00	39.83
	ATOM	1575	O	GLN A 212	15.984	14.350	-1.409	1.00	40.82
5	ATOM	1576	N	PHE A 213	14.505	12.668	-1.180	1.00	40.12
	ATOM	1577	CA	PHE A 213	13.342	13.575	-1.158	1.00	40.49
	ATOM	1578	CB	PHE A 213	12.650	13.623	-2.532	1.00	41.41
	ATOM	1579	CG	PHE A 213	13.557	14.056	-3.661	1.00	42.33
	ATOM	1580	CD1	PHE A 213	13.937	15.388	-3.798	1.00	43.79
10	ATOM	1581	CE1	PHE A 213	14.776	15.790	-4.845	1.00	44.58
	ATOM	1582	CZ	PHE A 213	15.238	14.843	-5.770	1.00	44.30
	ATOM	1583	CE2	PHE A 213	14.861	13.508	-5.638	1.00	44.11
	ATOM	1584	CD2	PHE A 213	14.024	13.126	-4.589	1.00	43.99
	ATOM	1585	C	PHE A 213	12.336	13.269	-0.034	1.00	39.98
15	ATOM	1586	O	PHE A 213	11.181	12.912	-0.286	1.00	40.31
	ATOM	1587	N	ILE A 214	12.785	13.445	1.205	1.00	38.90
	ATOM	1588	CA	ILE A 214	12.009	13.087	2.399	1.00	37.81
	ATOM	1589	CB	ILE A 214	12.949	12.929	3.627	1.00	37.79
	ATOM	1590	CG1	ILE A 214	13.972	11.818	3.379	1.00	37.71
20	ATOM	1591	CD1	ILE A 214	15.197	11.883	4.291	1.00	38.56
	ATOM	1592	CG2	ILE A 214	12.153	12.663	4.904	1.00	37.64
	ATOM	1593	C	ILE A 214	10.883	14.084	2.723	1.00	36.93
	ATOM	1594	O	ILE A 214	9.777	13.687	3.121	1.00	37.39
	ATOM	1595	N	GLY A 215	11.174	15.372	2.580	1.00	35.69
25	ATOM	1596	CA	GLY A 215	10.204	16.424	2.896	1.00	34.20
	ATOM	1597	C	GLY A 215	10.256	16.882	4.338	1.00	33.08
	ATOM	1598	O	GLY A 215	9.488	17.761	4.751	1.00	33.03
	ATOM	1599	N	TYR A 216	11.163	16.278	5.104	1.00	31.65
	ATOM	1600	CA	TYR A 216	11.392	16.612	6.504	1.00	30.16
30	ATOM	1601	CB	TYR A 216	10.636	15.635	7.422	1.00	29.85
	ATOM	1602	CG	TYR A 216	9.157	15.678	7.129	1.00	29.33
	ATOM	1603	CD1	TYR A 216	8.347	16.658	7.702	1.00	29.55
	ATOM	1604	CE1	TYR A 216	6.990	16.734	7.406	1.00	29.29
	ATOM	1605	CZ	TYR A 216	6.437	15.845	6.505	1.00	29.73
35	ATOM	1606	OH	TYR A 216	5.097	15.934	6.203	1.00	29.11

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	ATOM	1607	CE2 TYR A 216	7.224	14.868	5.901	1.00	29.77
	ATOM	1608	CD2 TYR A 216	8.581	14.794	6.210	1.00	29.07
	ATOM	1609	C TYR A 216	12.879	16.568	6.771	1.00	29.68
	ATOM	1610	O TYR A 216	13.585	15.760	6.159	1.00	29.40
5	ATOM	1611	N PRO A 217	13.370	17.449	7.665	1.00	29.29
	ATOM	1612	CA PRO A 217	14.780	17.411	8.054	1.00	28.65
	ATOM	1613	CB PRO A 217	14.921	18.577	9.036	1.00	28.79
	ATOM	1614	CG PRO A 217	13.553	18.906	9.469	1.00	29.74
	ATOM	1615	CD PRO A 217	12.642	18.541	8.336	1.00	29.24
10	ATOM	1616	C PRO A 217	15.172	16.109	8.731	1.00	28.19
	ATOM	1617	O PRO A 217	14.411	15.557	9.526	1.00	28.22
	ATOM	1618	N ILE A 218	16.354	15.621	8.391	1.00	27.72
	ATOM	1619	CA ILE A 218	16.918	14.436	9.022	1.00	27.03
	ATOM	1620	CB ILE A 218	16.966	13.229	8.030	1.00	27.16
15	ATOM	1621	CG1 ILE A 218	17.497	11.965	8.709	1.00	28.19
	ATOM	1622	CD1 ILE A 218	17.074	10.686	8.002	1.00	28.84
	ATOM	1623	CG2 ILE A 218	17.765	13.567	6.750	1.00	28.60
	ATOM	1624	C ILE A 218	18.281	14.791	9.633	1.00	26.38
	ATOM	1625	O ILE A 218	19.088	15.500	9.011	1.00	25.79
20	ATOM	1626	N THR A 219	18.502	14.349	10.869	1.00	25.45
	ATOM	1627	CA THR A 219	19.763	14.618	11.568	1.00	25.37
	ATOM	1628	CB THR A 219	19.588	15.588	12.768	1.00	25.49
	ATOM	1629	OG1 THR A 219	18.872	16.755	12.341	1.00	25.84
	ATOM	1630	CG2 THR A 219	20.950	16.022	13.325	1.00	26.78
25	ATOM	1631	C THR A 219	20.425	13.325	12.006	1.00	24.60
	ATOM	1632	O THR A 219	19.793	12.465	12.642	1.00	23.87
	ATOM	1633	N LEU A 220	21.690	13.176	11.620	1.00	24.14
	ATOM	1634	CA LEU A 220	22.524	12.067	12.070	1.00	24.37
	ATOM	1635	CB LEU A 220	23.460	11.609	10.950	1.00	23.79
30	ATOM	1636	CG LEU A 220	24.407	10.448	11.264	1.00	24.59
	ATOM	1637	CD1 LEU A 220	23.640	9.175	11.619	1.00	22.49
	ATOM	1638	CD2 LEU A 220	25.335	10.193	10.075	1.00	24.32
	ATOM	1639	C LEU A 220	23.352	12.441	13.296	1.00	25.04
	ATOM	1640	O LEU A 220	24.133	13.397	13.254	1.00	25.13
35	ATOM	1641	N PHE A 221	23.199	11.679	14.378	1.00	25.33

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	ATOM	1642	CA	PHE A 221	23.991	11.912	15.593	1.00	26.39
	ATOM	1643	CB	PHE A 221	23.098	11.872	16.841	1.00	26.73
	ATOM	1644	CG	PHE A 221	22.067	12.972	16.868	1.00	26.79
	ATOM	1645	CD1	PHE A 221	22.363	14.207	17.449	1.00	27.08
5	ATOM	1646	CE1	PHE A 221	21.429	15.237	17.451	1.00	27.41
	ATOM	1647	CZ	PHE A 221	20.180	15.046	16.868	1.00	27.57
	ATOM	1648	CE2	PHE A 221	19.878	13.829	16.265	1.00	27.21
	ATOM	1649	CD2	PHE A 221	20.824	12.797	16.262	1.00	26.61
	ATOM	1650	C	PHE A 221	25.169	10.947	15.706	1.00	27.07
10	ATOM	1651	O	PHE A 221	24.982	9.727	15.780	1.00	27.17
	ATOM	1652	N	VAL A 222	26.377	11.505	15.708	1.00	27.39
	ATOM	1653	CA	VAL A 222	27.604	10.717	15.698	1.00	28.83
	ATOM	1654	CB	VAL A 222	28.552	11.138	14.537	1.00	28.79
	ATOM	1655	CG1	VAL A 222	29.842	10.276	14.524	1.00	29.42
15	ATOM	1656	CG2	VAL A 222	27.843	11.022	13.195	1.00	28.86
	ATOM	1657	C	VAL A 222	28.317	10.859	17.039	1.00	29.39
	ATOM	1658	O	VAL A 222	28.619	11.971	17.483	1.00	29.44
	ATOM	1659	N	GLU A 223	28.588	9.724	17.672	1.00	30.40
	ATOM	1660	CA	GLU A 223	29.257	9.703	18.962	1.00	31.98
20	ATOM	1661	CB	GLU A 223	29.136	8.308	19.584	1.00	32.02
	ATOM	1662	CG	GLU A 223	29.727	8.149	20.986	1.00	32.42
	ATOM	1663	CD	GLU A 223	28.986	8.934	22.067	1.00	31.70
	ATOM	1664	OE1	GLU A 223	29.652	9.308	23.047	1.00	33.87
25	ATOM	1665	OE2	GLU A 223	27.762	9.171	21.953	1.00	29.95
	ATOM	1666	C	GLU A 223	30.717	10.111	18.809	1.00	33.12
	ATOM	1667	O	GLU A 223	31.416	9.597	17.940	1.00	32.76
	ATOM	1668	N	LYS A 224	31.149	11.058	19.642	1.00	34.64
	ATOM	1669	CA	LYS A 224	32.569	11.423	19.803	1.00	36.26
30	ATOM	1670	CB	LYS A 224	33.224	10.548	20.887	1.00	36.62
	ATOM	1671	CG	LYS A 224	32.576	10.694	22.276	1.00	36.59
	ATOM	1672	CD	LYS A 224	33.078	9.656	23.268	1.00	36.92
	ATOM	1673	CE	LYS A 224	32.684	10.013	24.716	1.00	38.25
	ATOM	1674	NZ	LYS A 224	33.534	11.096	25.309	1.00	39.28
35	ATOM	1675	C	LYS A 224	33.376	11.362	18.503	1.00	36.99

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	ATOM	1676	O	LYS A 224	34.523	10.881	18.478	1.00	38.18
	ATOM	1677	S22	LIG A 501	0.703	6.258	10.649	1.00	26.70
	ATOM	1678	C9	LIG A 501	2.090	5.962	11.511	1.00	24.71
	ATOM	1679	N8	LIG A 501	3.160	5.369	10.977	1.00	25.32
5	ATOM	1680	C12	LIG A 501	3.284	4.965	9.569	1.00	30.06
	ATOM	1681	C13	LIG A 501	3.056	3.504	9.296	1.00	31.24
	ATOM	1682	C14	LIG A 501	3.587	2.989	8.104	1.00	32.67
	ATOM	1683	C15	LIG A 501	3.443	1.649	7.731	1.00	33.61
	ATOM	1684	C16	LIG A 501	2.737	0.850	8.610	1.00	32.84
10	ATOM	1685	O19	LIG A 501	2.431	-0.480	8.529	1.00	33.08
	ATOM	1686	C20	LIG A 501	1.663	-0.826	9.693	1.00	33.58
	ATOM	1687	O21	LIG A 501	1.554	0.383	10.495	1.00	33.58
	ATOM	1688	C17	LIG A 501	2.181	1.390	9.843	1.00	32.68
	ATOM	1689	C18	LIG A 501	2.336	2.719	10.198	1.00	31.77
15	ATOM	1690	C7	LIG A 501	4.071	5.267	11.942	1.00	21.78
	ATOM	1691	N11	LIG A 501	3.602	5.780	13.085	1.00	23.22
	ATOM	1692	N10	LIG A 501	2.375	6.199	12.807	1.00	24.05
	ATOM	1693	C3	LIG A 501	5.432	4.667	11.805	1.00	21.14
	ATOM	1694	C4	LIG A 501	6.674	5.477	11.811	1.00	19.92
20	ATOM	1695	O27	LIG A 501	6.590	6.820	12.022	1.00	19.49
	ATOM	1696	C5	LIG A 501	7.908	4.856	11.596	1.00	19.48
	ATOM	1697	C6	LIG A 501	7.971	3.478	11.365	1.00	19.59
	ATOM	1698	O23	LIG A 501	9.178	2.868	11.167	1.00	19.42
	ATOM	1699	C1	LIG A 501	6.721	2.651	11.356	1.00	19.70
25	ATOM	1700	C2	LIG A 501	5.498	3.296	11.570	1.00	19.89
	ATOM	1701	C24	LIG A 501	6.822	1.170	11.137	1.00	18.90
	ATOM	1702	C25	LIG A 501	5.553	0.480	10.630	1.00	19.98
	ATOM	1703	C26	LIG A 501	7.210	0.573	12.481	1.00	18.30
	ATOM	1704	O	HOH W 1	28.632	-4.835	7.916	1.00	27.13
30	ATOM	1705	O	HOH W 2	5.293	8.388	14.153	1.00	19.00
	ATOM	1706	O	HOH W 3	13.173	6.820	2.275	1.00	21.88
	ATOM	1707	O	HOH W 4	-0.545	-6.873	10.634	1.00	26.43
	ATOM	1708	O	HOH W 5	11.033	5.985	13.496	1.00	20.85
	ATOM	1709	O	HOH W 6	7.099	-5.364	23.832	1.00	21.75
35	ATOM	1710	O	HOH W 7	18.096	5.252	2.598	1.00	31.44

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	ATOM	1711	O	HOH W	8	13.515	-1.506	7.491	1.00	27.40
	ATOM	1712	O	HOH W	9	8.466	-14.305	12.913	1.00	25.66
	ATOM	1713	O	HOH W	10	23.607	-5.930	1.589	1.00	30.72
	ATOM	1714	O	HOH W	11	20.946	3.483	18.798	1.00	24.42
5	ATOM	1715	O	HOH W	12	24.625	-5.281	4.109	1.00	26.39
	ATOM	1716	O	HOH W	13	32.367	6.465	8.913	1.00	27.50
	ATOM	1717	O	HOH W	14	1.399	12.336	22.131	1.00	25.58
	ATOM	1718	O	HOH W	15	23.511	11.739	3.468	1.00	23.38
	ATOM	1719	O	HOH W	16	29.064	-2.555	16.958	1.00	29.89
10	ATOM	1720	O	HOH W	17	18.287	2.850	1.991	1.00	23.97
	ATOM	1721	O	HOH W	18	-0.685	11.813	17.209	1.00	27.19
	ATOM	1722	O	HOH W	19	0.138	5.601	21.586	1.00	24.33
	ATOM	1723	O	HOH W	20	19.907	-10.369	-4.072	1.00	34.69
	ATOM	1724	O	HOH W	21	3.952	-3.323	7.012	1.00	42.26
15	ATOM	1725	O	HOH W	22	9.043	-16.241	11.113	1.00	24.70
	ATOM	1726	O	HOH W	23	16.151	-13.158	15.168	1.00	31.60
	ATOM	1727	O	HOH W	24	24.175	-11.771	14.834	1.00	28.79
	ATOM	1728	O	HOH W	26	-3.329	13.007	16.401	1.00	22.45
	ATOM	1729	O	HOH W	27	-0.441	1.451	11.806	1.00	33.06
20	ATOM	1730	O	HOH W	28	11.177	4.493	11.004	1.00	21.58
	ATOM	1731	O	HOH W	29	25.227	8.288	17.757	1.00	29.54
	ATOM	1732	O	HOH W	30	10.287	-12.953	18.908	1.00	27.89
	ATOM	1733	O	HOH W	31	0.897	-7.271	6.277	1.00	33.57
	ATOM	1734	O	HOH W	32	-6.605	2.748	17.228	1.00	33.66
25	ATOM	1735	O	HOH W	33	0.852	9.562	4.949	1.00	43.02
	ATOM	1736	O	HOH W	35	5.753	-0.814	2.482	1.00	32.67
	ATOM	1737	O	HOH W	36	-2.295	-17.323	10.475	1.00	30.98
	ATOM	1738	O	HOH W	37	3.956	-19.462	8.919	1.00	31.72
	ATOM	1739	O	HOH W	38	9.539	0.867	9.131	1.00	24.28
30	ATOM	1740	O	HOH W	39	9.382	11.280	18.869	1.00	29.99
	ATOM	1741	O	HOH W	40	15.127	14.517	1.620	1.00	52.10
	ATOM	1742	O	HOH W	41	-4.936	-11.879	7.926	1.00	33.94
	ATOM	1743	O	HOH W	42	29.758	-6.171	10.914	1.00	43.96
	ATOM	1744	O	HOH W	43	21.616	4.671	21.425	1.00	32.46
35	ATOM	1745	O	HOH W	45	1.987	-6.303	8.905	1.00	32.23

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	ATOM	1746	O	HOH	W	46	-5.836	-8.237	14.774	1.00	42.33
	ATOM	1747	O	HOH	W	47	28.055	-3.377	1.592	1.00	35.58
	ATOM	1748	O	HOH	W	48	-5.650	1.080	20.826	1.00	34.49
	ATOM	1749	O	HOH	W	49	20.605	-13.567	16.474	1.00	34.82
5	ATOM	1750	O	HOH	W	50	20.079	-17.689	-0.219	1.00	29.99
	ATOM	1751	O	HOH	W	52	11.454	-1.186	9.234	1.00	23.56
	ATOM	1752	O	HOH	W	53	5.006	9.609	26.124	1.00	31.87
	ATOM	1753	O	HOH	W	54	-0.134	24.327	17.144	1.00	29.63
	ATOM	1754	O	HOH	W	55	6.602	15.659	19.311	1.00	37.32
10	ATOM	1755	O	HOH	W	56	-5.057	-6.828	28.721	1.00	50.59
	ATOM	1756	O	HOH	W	58	16.275	16.189	12.428	1.00	31.49
	ATOM	1757	O	HOH	W	59	2.310	-3.197	33.395	1.00	33.83
	ATOM	1758	O	HOH	W	61	3.855	-12.242	-6.573	1.00	39.44
	ATOM	1759	O	HOH	W	62	28.121	6.942	16.590	1.00	37.00
15	ATOM	1760	O	HOH	W	63	9.310	-9.340	22.417	1.00	39.30
	ATOM	1761	O	HOH	W	64	-3.973	7.467	20.448	1.00	54.78
	ATOM	1762	O	HOH	W	65	11.748	-16.207	10.958	1.00	35.98
	ATOM	1763	O	HOH	W	66	18.701	-11.956	4.296	1.00	36.37
	ATOM	1764	O	HOH	W	67	28.447	6.570	13.797	1.00	34.47
20	ATOM	1765	O	HOH	W	68	28.379	-8.278	5.740	1.00	36.04
	ATOM	1766	O	HOH	W	69	-1.771	13.869	23.782	1.00	33.43
	ATOM	1767	O	HOH	W	70	-3.086	-13.658	13.283	1.00	45.28
	ATOM	1768	O	HOH	W	72	13.902	-17.777	10.689	1.00	46.78
	ATOM	1769	O	HOH	W	73	24.887	8.479	20.388	1.00	27.32
25	ATOM	1770	O	HOH	W	74	-4.126	2.368	22.415	1.00	37.26
	ATOM	1771	O	HOH	W	75	18.174	-8.288	-3.343	1.00	39.53
	ATOM	1772	O	HOH	W	77	1.906	-3.528	29.615	1.00	31.37
	ATOM	1773	O	HOH	W	78	30.428	4.381	2.253	1.00	31.14
	ATOM	1774	O	HOH	W	79	8.083	17.452	17.921	1.00	37.74
30	ATOM	1775	O	HOH	W	80	23.175	-2.787	0.534	1.00	32.79
	ATOM	1776	O	HOH	W	81	10.010	-4.238	24.649	1.00	39.68
	ATOM	1777	O	HOH	W	82	-1.580	-18.286	18.273	1.00	37.51
	ATOM	1778	O	HOH	W	83	28.629	4.662	18.973	1.00	37.60
	ATOM	1779	O	HOH	W	84	-3.966	-15.838	11.912	1.00	36.36
35	ATOM	1780	O	HOH	W	85	-5.571	-0.044	14.196	1.00	39.92

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	ATOM	1781	O	HOH W 86	2.701	6.802	28.219	1.00	33.37
	ATOM	1782	O	HOH W 87	4.054	22.591	20.709	1.00	36.51
	ATOM	1783	O	HOH W 89	10.564	3.353	0.239	1.00	39.34
	ATOM	1784	O	HOH W 90	17.392	3.900	21.177	1.00	33.71
5	ATOM	1785	O	HOH W 91	8.886	21.290	11.834	1.00	29.45
	ATOM	1786	O	HOH W 92	-1.873	21.216	25.302	1.00	57.39
	ATOM	1787	O	HOH W 93	20.431	1.294	22.313	1.00	39.11
	ATOM	1788	O	HOH W 94	0.395	-18.800	-7.247	1.00	56.50
	ATOM	1789	O	HOH W 95	24.269	-12.973	10.438	1.00	39.24
10	ATOM	1790	O	HOH W 96	22.249	-5.099	19.977	1.00	32.06
	ATOM	1791	O	HOH W 97	6.727	22.511	20.150	1.00	40.10
	ATOM	1792	O	HOH W 98	2.279	10.244	3.022	1.00	37.67
	ATOM	1793	O	HOH W 99	-1.251	-10.009	-1.419	1.00	30.76
	ATOM	1794	O	HOH W 101	17.181	-11.067	11.339	1.00	34.01
15	ATOM	1795	O	HOH W 102	29.663	3.774	21.254	1.00	43.76
	ATOM	1796	O	HOH W 103	29.196	-5.298	17.621	1.00	44.15
	ATOM	1797	O	HOH W 104	5.091	7.786	28.473	1.00	37.08
	ATOM	1798	O	HOH W 106	9.797	-1.018	-2.978	1.00	53.59
	ATOM	1799	O	HOH W 107	3.392	-17.181	13.840	1.00	39.37
20	ATOM	1800	O	HOH W 108	27.213	-5.898	4.004	1.00	37.23
	ATOM	1801	O	HOH W 109	-2.075	-13.855	15.641	1.00	30.68
	ATOM	1802	O	HOH W 110	28.368	-13.607	16.364	1.00	66.41
	ATOM	1803	O	HOH W 111	15.678	11.849	19.117	1.00	32.96
	ATOM	1804	O	HOH W 113	5.638	-1.459	6.258	1.00	38.93
25	ATOM	1805	O	HOH W 114	31.539	2.519	3.888	1.00	35.63
	ATOM	1806	O	HOH W 115	5.760	10.633	2.737	1.00	36.92
	ATOM	1807	O	HOH W 116	24.376	-10.176	18.657	1.00	31.15
	ATOM	1808	O	HOH W 117	25.144	2.318	25.081	1.00	42.18
	ATOM	1809	O	HOH W 118	-6.269	7.743	19.632	1.00	35.61
30	ATOM	1810	O	HOH W 119	-0.722	-17.223	13.736	1.00	37.87
	ATOM	1811	O	HOH W 120	30.581	-0.124	13.098	1.00	30.69
	ATOM	1812	O	HOH W 121	8.038	1.100	3.904	1.00	36.82
	ATOM	1813	O	HOH W 122	35.258	12.568	16.291	1.00	55.49
	ATOM	1814	O	HOH W 124	5.192	-2.464	31.053	1.00	49.06
35	ATOM	1815	O	HOH W 125	0.014	-4.885	26.218	1.00	42.21

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	ATOM	1816	O	HOH W 126	6.606	-13.631	25.003	1.00	38.41
	ATOM	1817	O	HOH W 127	8.003	-13.734	22.774	1.00	45.68
	ATOM	1818	O	HOH W 128	-1.605	-14.636	19.174	1.00	40.49
	ATOM	1819	O	HOH W 129	11.428	16.397	19.562	1.00	52.41
5	ATOM	1820	O	HOH W 130	30.717	-1.349	15.435	1.00	29.72
	ATOM	1821	O	HOH W 131	-6.353	-4.780	18.264	1.00	48.81
	ATOM	1822	O	HOH W 132	31.720	10.900	6.890	1.00	42.74
	ATOM	1823	O	HOH W 133	21.804	13.566	2.479	1.00	35.25
	ATOM	1824	O	HOH W 134	17.979	4.901	-5.372	1.00	46.39
10	ATOM	1825	O	HOH W 135	-2.104	-10.435	1.248	1.00	34.38
	ATOM	1826	O	HOH W 136	6.670	3.448	2.750	1.00	41.00
	ATOM	1827	O	HOH W 137	3.800	4.243	4.489	1.00	46.31
	ATOM	1828	O	HOH W 138	-2.570	6.606	13.251	1.00	51.92
	ATOM	1829	O	HOH W 139	5.002	0.458	4.596	1.00	43.17
15	ATOM	1830	O	HOH W 140	1.493	-0.360	4.867	1.00	47.17
	ATOM	1831	O	HOH W 141	0.841	0.842	1.974	1.00	40.10
	ATOM	1832	O	HOH W 142	11.338	5.555	-0.800	1.00	55.45
	ATOM	1833	O	HOH W 143	14.883	5.969	-3.651	1.00	43.49
	ATOM	1834	O	HOH W 144	15.623	3.552	-3.956	1.00	48.33
20	ATOM	1835	O	HOH W 145	-0.346	3.916	0.863	1.00	44.74
	ATOM	1836	O	HOH W 146	-6.838	-0.890	22.055	1.00	42.49
	ATOM	1837	O	HOH W 147	-5.500	-3.094	21.306	1.00	35.44
	ATOM	1838	O	HOH W 148	-5.138	-6.252	23.720	1.00	44.34
	ATOM	1839	O	HOH W 149	2.990	13.801	24.910	1.00	35.58
25	ATOM	1840	O	HOH W 150	11.760	-3.968	42.092	1.00	50.02
	ATOM	1841	O	HOH W 151	11.845	11.900	28.107	1.00	40.30
	ATOM	1842	O	HOH W 152	12.936	10.826	29.989	1.00	35.98
	ATOM	1843	O	HOH W 153	10.548	13.577	29.455	1.00	49.16
	ATOM	1844	O	HOH W 154	12.434	8.763	31.573	1.00	39.73
30	ATOM	1845	O	HOH W 155	14.902	9.666	25.441	1.00	46.88
	ATOM	1846	O	HOH W 156	13.708	3.983	27.418	1.00	44.44
	ATOM	1847	O	HOH W 157	22.291	-6.886	18.125	1.00	44.80
	ATOM	1848	O	HOH W 158	18.405	-13.148	12.748	1.00	45.34
	ATOM	1849	O	HOH W 159	19.908	-13.597	8.758	1.00	43.46
35	ATOM	1850	O	HOH W 160	25.140	-9.317	3.826	1.00	30.14

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	ATOM	1851	O	HOH W 161	24.285	-8.799	1.293	1.00	41.36
	ATOM	1852	O	HOH W 162	0.157	-2.649	31.376	1.00	46.39
	ATOM	1853	O	HOH W 163	13.156	-16.477	13.339	1.00	94.75
	ATOM	1854	O	HOH W 164	8.516	-11.899	20.944	1.00	38.91
5	ATOM	1855	O	HOH W 165	12.795	-11.012	21.269	1.00	32.36
	ATOM	1856	O	HOH W 166	-5.669	-12.148	10.443	1.00	49.54
	ATOM	1857	O	HOH W 167	-4.040	-11.381	2.272	1.00	42.06
	ATOM	1858	O	HOH W 168	-0.517	-15.840	24.771	1.00	49.65
	ATOM	1859	O	HOH W 169	19.659	-17.851	8.990	1.00	51.32
10	ATOM	1860	O	HOH W 170	25.384	7.705	-2.161	1.00	39.22
	ATOM	1861	O	HOH W 171	27.242	5.706	-3.207	1.00	39.97
	ATOM	1862	O	HOH W 172	6.618	-3.190	-7.590	1.00	39.71
	ATOM	1863	O	HOH W 173	7.969	-6.150	-8.098	1.00	38.71
	ATOM	1864	O	HOH W 174	11.880	-14.554	-9.251	1.00	52.24
15	ATOM	1865	O	HOH W 175	17.124	-5.263	-4.764	1.00	49.56
	ATOM	1866	O	HOH W 176	31.345	6.267	12.321	1.00	31.49
	ATOM	1867	O	HOH W 177	-1.556	16.843	21.863	1.00	47.14

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What is claimed:

1. A composition of matter, comprising:
a compound that binds to the N-terminal ADP/ATP binding site of Hsp90,
wherein the compound interacts with the amino acid residue Lys58 of Hsp90, and
5 wherein the compound inhibits Hsp90 activity upon binding to the N-terminal
ADP/ATP binding site of Hsp90,
provided that the compounds are not the compounds of formulas (I) – (XXXIX) or
tautomers, pharmaceutically acceptable salts, solvates, clathrates or prodrugs thereof.
- 10 2. The composition of matter of claim 1, wherein the compound interacts with the
amino acid residue Lys58 of Hsp90 to alter the three-dimensional orientation of the amino
acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid
residue Lys58 of Hsp90 in the absence of the compound.
- 15 3. The composition of matter of claim 1, wherein the compound forms a hydrogen
bond with the amine group of the side chain of Lys58.
4. The composition of matter of claim 1, wherein the compound further interacts with
the amino acid residue Gly97 of Hsp90.
- 20 5. The composition of matter of claim 1, wherein the compound further interacts with
the amino acid residue Thr184 of Hsp90.
6. The composition of matter of claim 1, wherein the compound further interacts with
25 the amino acid residues Gly97 and Thr184 of Hsp90.
7. The composition of matter of claim 6, wherein the compound further interacts with
the amino acid residue Asp93 of Hsp90.
- 30 8. The composition of matter of claim 7, wherein the compound further interacts with
the amino acid residue Asn51 of Hsp90.
9. The composition of matter of claim 8, wherein the compound further interacts with
the amino acid residue Ser52 of Hsp90.

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10. The composition of matter of claim 9, wherein the compound further interacts with the amino acid residues Phe138, Leu107, and Val150 of Hsp90.
11. The composition of matter of any one of claims 1-10, wherein the recited amino acid residue has a three-dimensional orientation substantially corresponding to the atomic coordinates represented in Table 3 or the recited amino acid residues have a three-dimensional orientation substantially corresponding to the atomic coordinates represented in Table 3:
12. A composition of matter, comprising:
an inhibitor and Hsp90,
wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 3.
13. A composition of matter, comprising:
a compound that binds to the N-terminal ADP/ATP binding site of Hsp90,
wherein the compound interacts with the amino acid residue Gly97 of Hsp90, and
wherein the compound inhibits Hsp90 activity upon binding to the N-terminal ADP/ATP binding site of Hsp90,
provided that the compounds are not the compounds of formulas (I) – (XXXIX) or tautomers, pharmaceutically acceptable salts, solvates, clathrates or prodrugs thereof.
14. The composition of matter of claim 13, wherein the compound interacts with the amino acid residue Gly97 of Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 in the absence of the compound.
15. The composition of matter of claim 13, wherein the compound forms a hydrogen bond with the carbonyl group of Gly97.
16. The composition of matter of claim 13, wherein the compound further interacts with the amino acid residue Thr184 of Hsp90.

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17. The composition of matter of claim 16, wherein the compound further interacts with the amino acid residue Asp93 of Hsp90.
18. The composition of matter of claim 17, wherein the compound further interacts with the amino acid residue Asn51 of Hsp90.
19. The composition of matter of claim 18, wherein the compound further interacts with the amino acid residue Ser52 of Hsp90.
20. The composition of matter of claim 19, wherein the compound further interacts with the amino acid residues Phe138, Leu107, and Val150 of Hsp90.
21. The composition of matter of claim 13, wherein the recited amino acid residue has a three-dimensional orientation substantially corresponding to the atomic coordinates represented in Table 4 or Table 5 or the recited amino acid residues have a three-dimensional orientation substantially corresponding to the atomic coordinates represented in Table 4 or Table 5.
22. A composition of matter, comprising:
an inhibitor and Hsp90,
wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 4.
23. A composition of matter, comprising:
an inhibitor and Hsp90,
wherein, when the inhibitor is bound to Hsp90, the composition has a three-dimensional orientation substantially corresponding to atomic coordinates represented in Table 5.
24. A method of inhibiting Hsp90 activity, comprising:
exposing a compound to Hsp90, wherein the compound interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 in the absence of the compound,

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provided that the compounds are not the compounds of formulas (I) – (XXXIX) or tautomers, pharmaceutically acceptable salts, solvates, clathrates or prodrugs thereof.

25. The method of claim 24, wherein the compound interacts with Hsp90 to arrange the amino acid residue Lys58 of Hsp90 into a three-dimensional orientation substantially corresponding to the atomic coordinates represented in Table 3:

26. A method of identifying an inhibitor for Hsp90, comprising:
obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90;
determining a three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90 by computing atomic coordinates from X-ray diffraction data of the co-crystal; and
designing a compound capable of binding to the N-terminal ADP/ATP binding site of Hsp90 based on a three-dimensional shape complementarity or estimated interaction energy of the N-terminal ADP/ATP binding site of Hsp90.

27. A method of identifying an inhibitor for Hsp90, comprising:
obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Lys58 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90;
using the X-ray diffraction data to generate an electron density map consistent with the three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90; and
developing compounds for an inhibitor of Hsp90 based on the electron density map.

28. A method of inhibiting Hsp90 activity, comprising:
exposing a compound to Hsp90, wherein the compound interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to

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the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 in the absence of the compound,

provided that the compounds are not the compounds of formulas (I) – (XXXIX) or tautomers, pharmaceutically acceptable salts, solvates, clathrates or prodrugs thereof.

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29. The method of claim 28, wherein the compound interacts with Hsp90 to arrange the amino acid residue Gly97 of Hsp90 into a three-dimensional orientation substantially corresponding to the atomic coordinates represented in Table 4 or Table 5.

10

30. A method of identifying an inhibitor for Hsp90, comprising:

obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to the three-dimensional orientation of the amino acid residue

15

Gly97 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90;

determining a three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90 by computing atomic coordinates from X-ray diffraction data of the co-crystal; and

20

designing a compound capable of binding to the N-terminal ADP/ATP binding site of Hsp90 based on a three-dimensional shape complementarity or estimated interaction energy of the N-terminal ADP/ATP binding site of Hsp90.

25

31. A method of identifying an inhibitor for Hsp90, comprising:

obtaining X-ray diffraction data from a co-crystal comprising Hsp90 and an inhibitor bound to the N-terminal ADP/ATP binding site of Hsp90, wherein the inhibitor interacts with Hsp90 to alter the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 relative to the three-dimensional orientation of the amino acid residue Gly97 of Hsp90 when the inhibitor is not bound to the N-terminal ADP/ATP binding site of Hsp90;

30

using the X-ray diffraction data to generate an electron density map consistent with the three-dimensional orientation of the N-terminal ADP/ATP binding site of Hsp90; and developing compounds for an inhibitor of Hsp90 based on the electron density map.

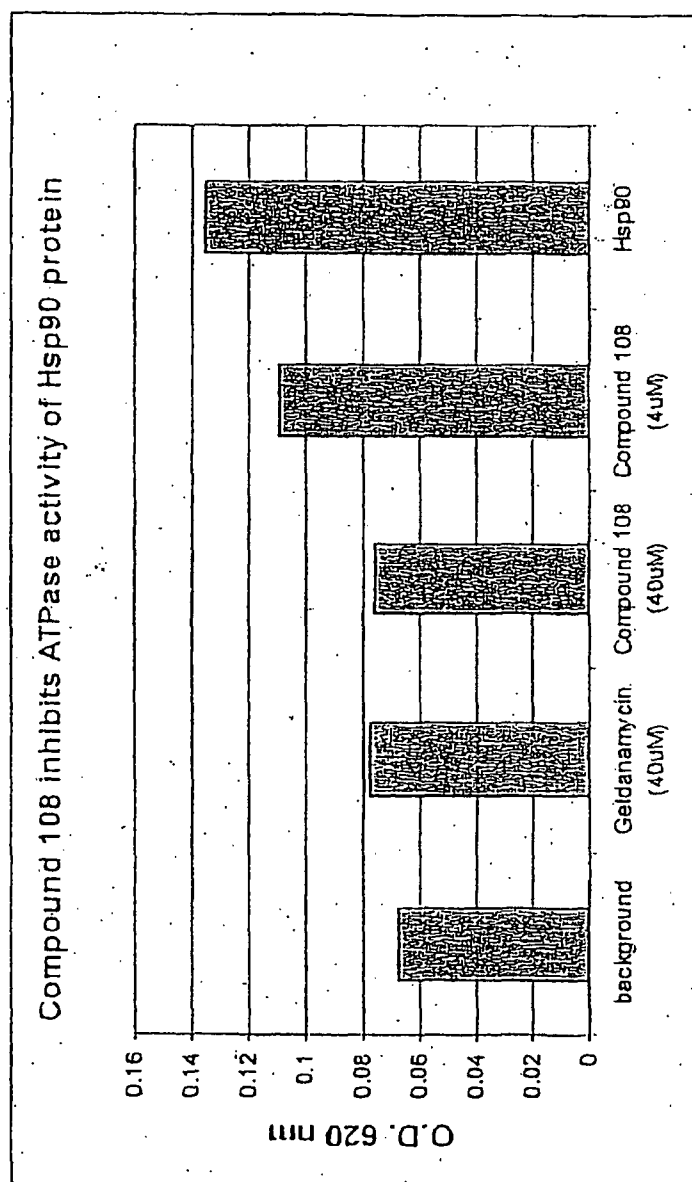


FIG. 1

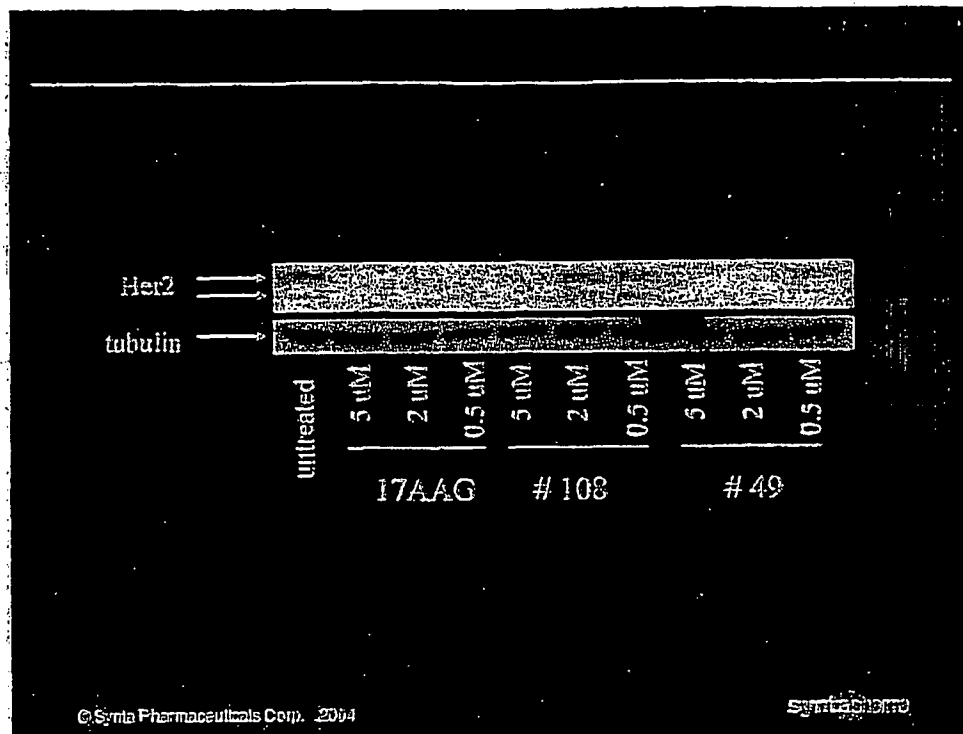


FIG. 2

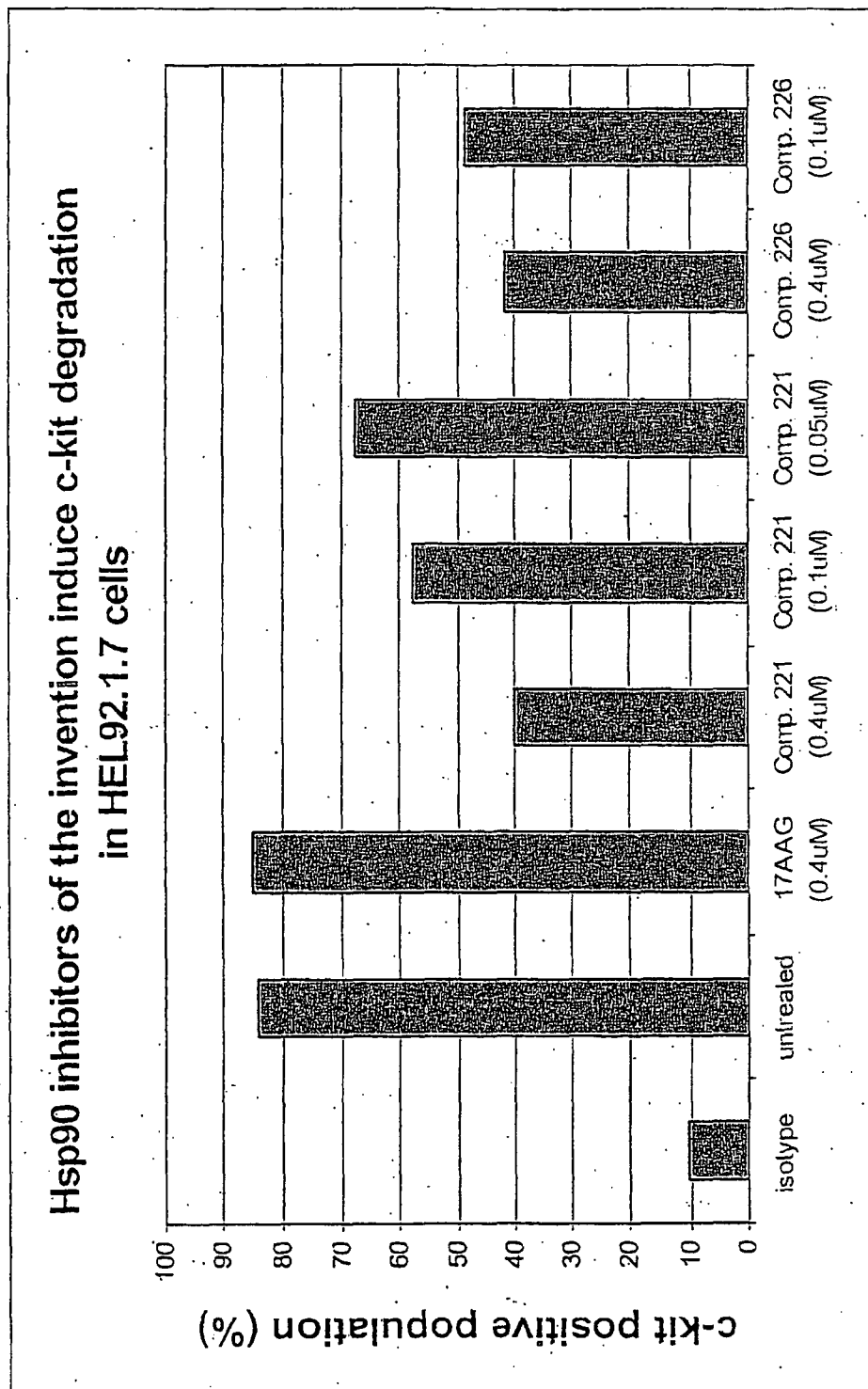


Fig. 3

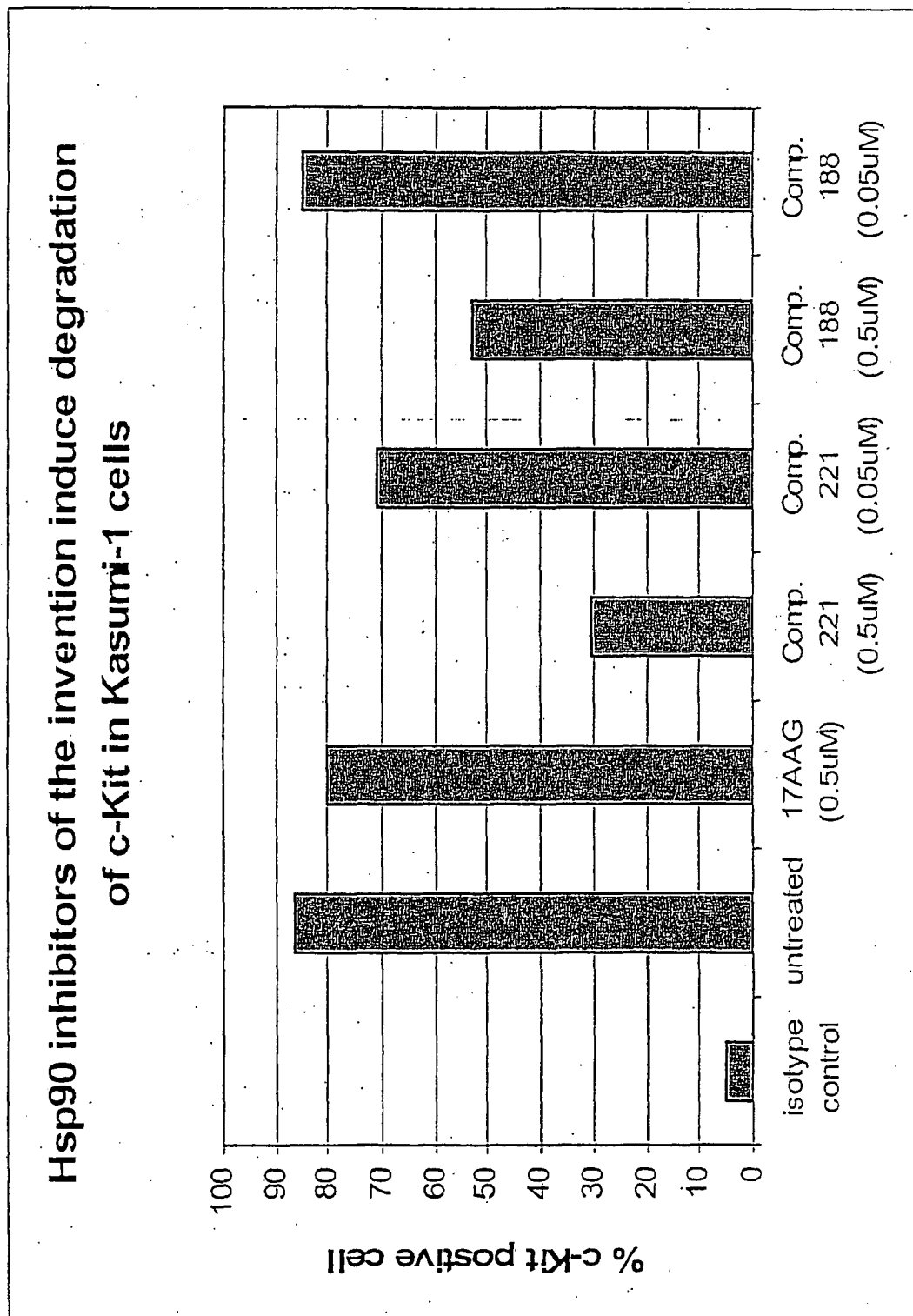


Fig. 4

Hsp90 inhibitors induce degradation of c-Kit in Kasumi-1 cells

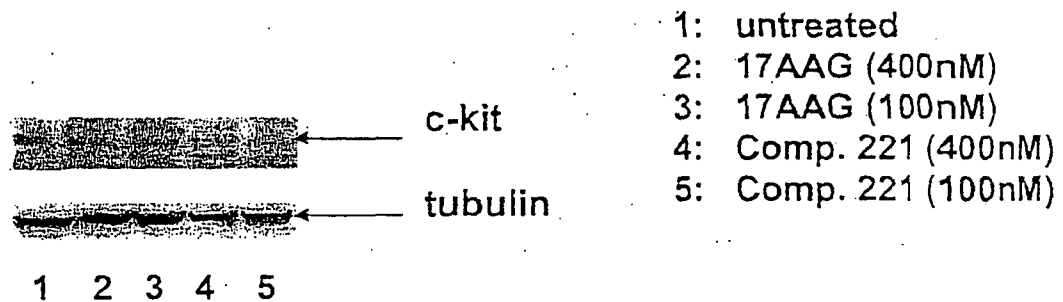


Fig. 5

C-Met Degradation induced by Hsp90 inhibitors in NCI-H1193 cells

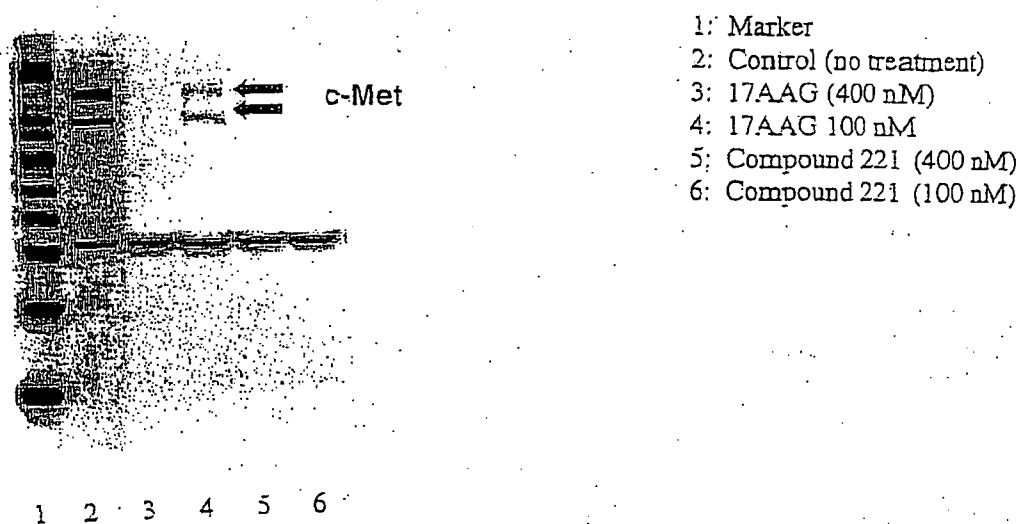


Fig. 6

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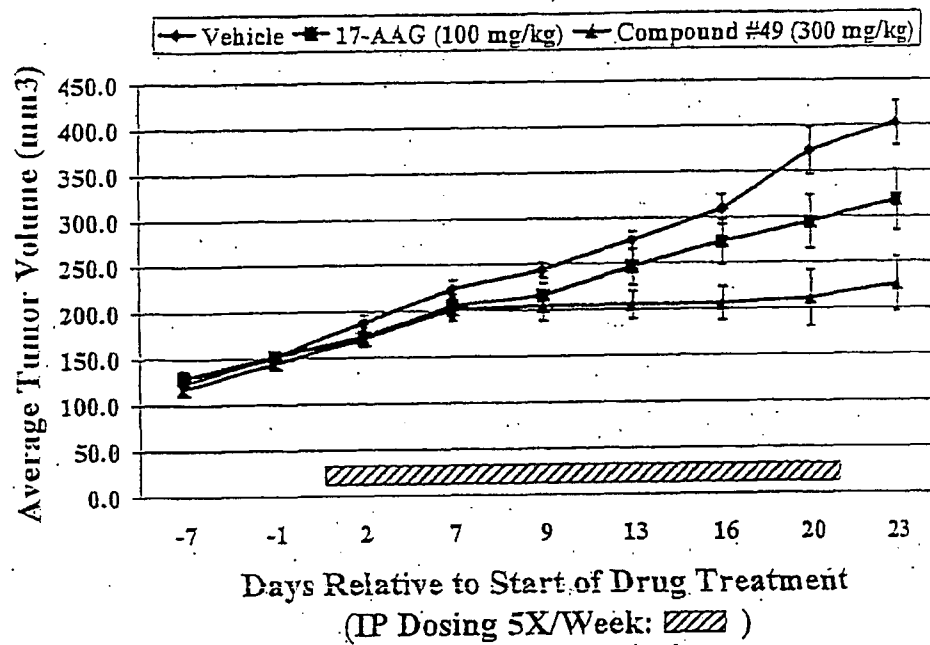


Fig. 7

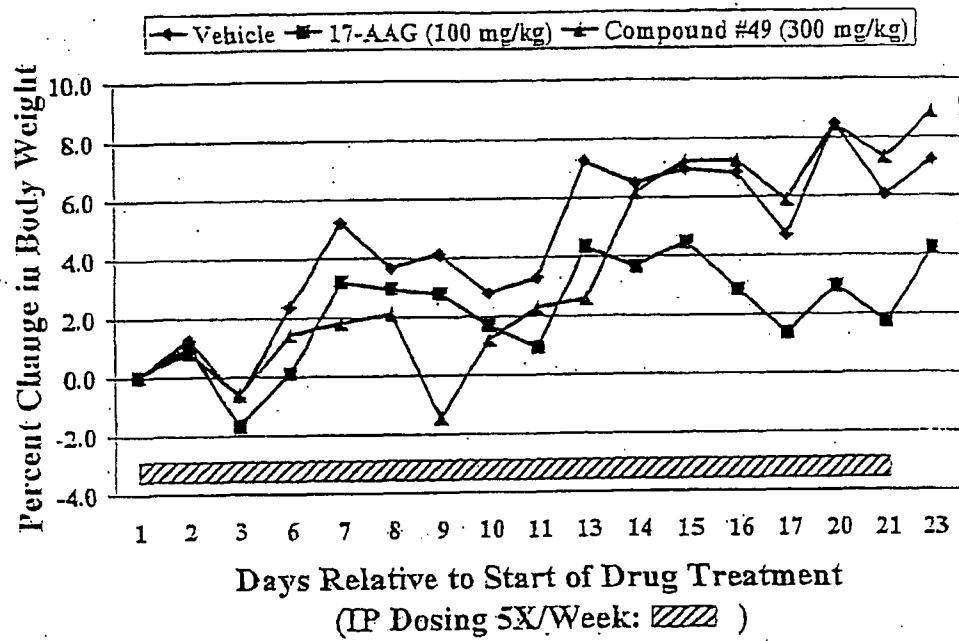


Fig. 8

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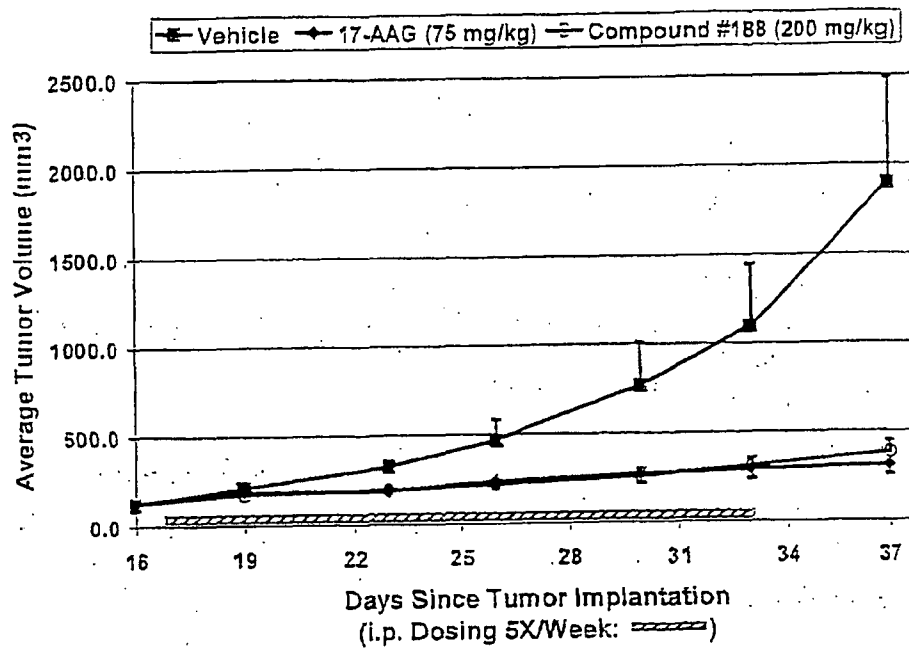


Fig. 9

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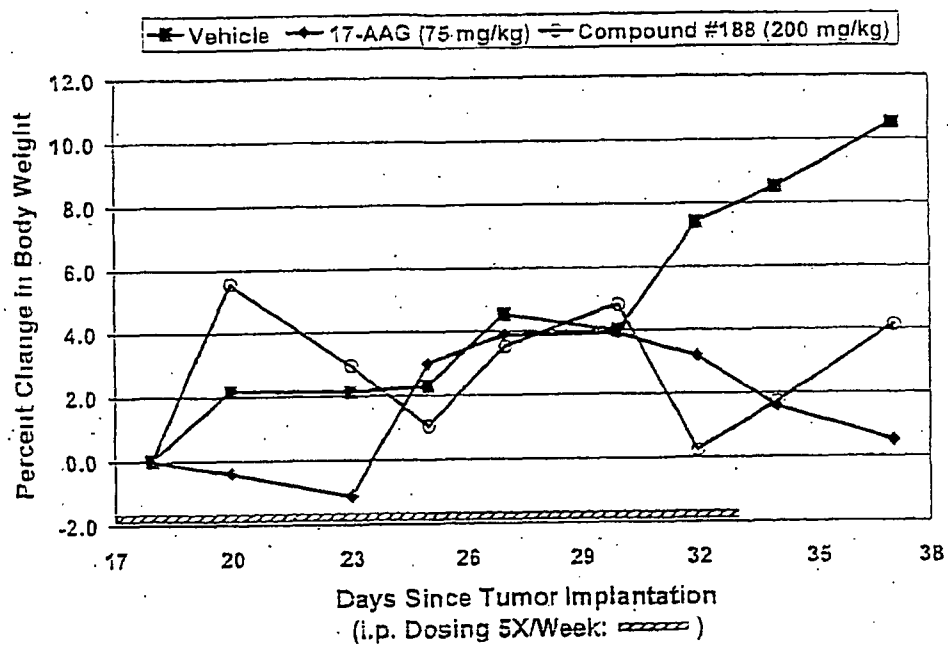
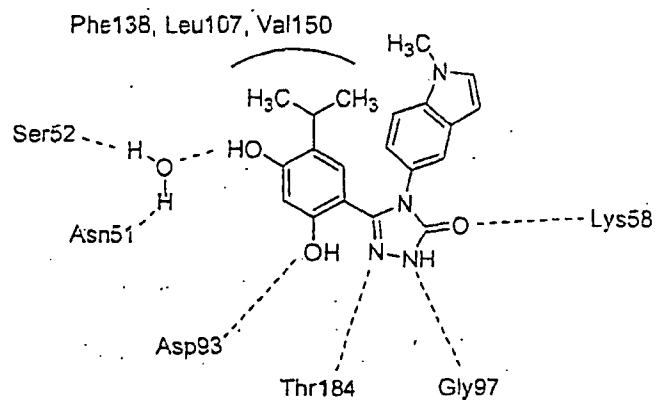
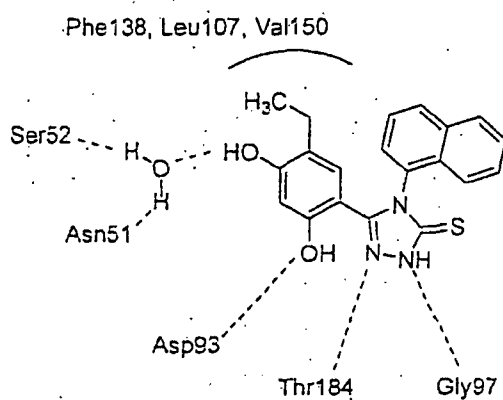


Fig. 10

a.)



b.)



c.)

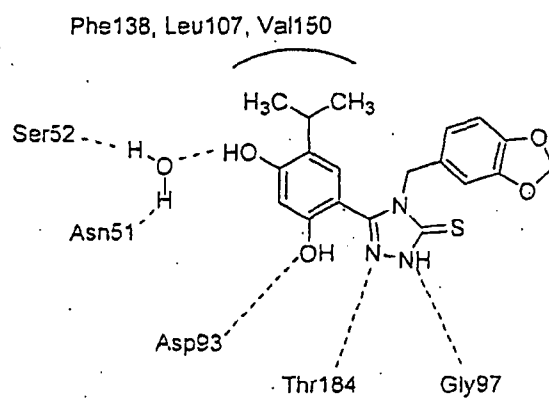


Fig. 11