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(54) Title: METHODS AND COMPOSITIONS FOR TREATING AND/OR PREVENTING A DISEASE OR DISORDER ASSOCIATED WITH ABNORMAL LEVEL AND/OR ACTIVITY OF THE IFP35 FAMILY OF PROTEINS

(57) Abstract: The present invention provides methods and compositions for treating and/or preventing a disease or disorder associated with abnormally high level of the IFP35 family of proteins, including IFP35 and NMI, methods and compositions for diagnosis, prognosis or treatment monitoring of a disease or disorder associated with abnormally high level of the IFP35 family of proteins, including IFP35 and NMI, and methods and compositions for identifying a modulator of the IFP35 family of proteins, including IFP35 and NMI.



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**METHODS AND COMPOSITIONS FOR TREATING AND/OR PREVENTING A  
DISEASE OR DISORDER ASSOCIATED WITH ABNORMAL LEVEL AND/OR  
ACTIVITY OF THE IFP35 FAMILY OF PROTEINS**

**Cross-Reference To Related Applications**

- 5       **[0001]**     The present application claims priority to Chinese patent application No. 201410418773.1, filed August 22, 2014, the disclosure of which is incorporated by reference in its entirety for all purposes.

**Technical Field**

- 10       **[0002]**     In some aspects, the present disclosure relates to methods and compositions for treating and/or preventing a disease or disorder associated with abnormally level and/or activity of the IFP35 family of proteins, including IFP35 and NMI; methods and compositions for diagnosis, prognosis or treatment monitoring of a disease or disorder associated with abnormally level and/or activity of the IFP35 family of proteins; and methods and compositions for identifying a modulator of the IFP35 family of  
15       proteins.

**Background Art**

- 20       **[0003]**     Endogenous danger signals are “damage-associated molecular patterns” (DAMPs) that are released from necrotic or stressed cells which trigger the inflammatory response. For instance, cells produce endogenous DAMPs for immune regulation after infection or injury. *See* Gallucci et al., *Current Opinion in Immunology* 13, 114-119 (2001); Matzinger, *Science* 296, 301-305 (2002); and Hirsiger et al., *Mediators of Inflammation*, 315941 (2012). The known DAMPs include not only small molecules such as uric acid, cholesterol and ATP (*see* Gombault et al., *Frontiers in Immunology* 3, 414 (2012); Heil et al., *Frontiers in Plant Science* 5, 578 (2014); and Shi, *Journal of Clinical Investigation* 120, 1809-1811 (2010)), but also proteins such as high-mobility group box protein 1 (HMGB1) (*see* Tsung et al., *Journal of Internal Medicine* 276, 425-443 (2014); and Wang et al., *Science* 285, 248-251 (1999)), heat shock proteins (HSPs) (*see* Tamura et al., *Immunotherapy* 4, 841-852 (2012)), interleukin-1 $\alpha$  (IL-1 $\alpha$ ) (*see*

Dinarello, Annual Review of Immunology 27, 519-550 (2009)), interleukin-33 (IL-33) (see Liew et al., Nature Reviews Immunology 10, 103-110 (2010)), myeloid-related protein-8 (Mrp8) and myeloid-related protein-14 (Mrp14) (see Vogl et al., Nature Medicine 13, 1042-1049 (2007); and Austermann et al., Cell Reports 9, 2112-2123 (2014)). DAMPs may play important roles in pathogen elimination and damage repair. However, uncontrolled activation of inflammation by DAMPs will lead to persistent over-expression of toxic cytokines, which are major risk factors for sepsis shock and systemic inflammatory response syndrome. See Srikrishna et al., Neoplasia 11, 615-628 (2009); and Piccinini et al., Mediators of Inflammation, doi:10.1155/2010/672395 (2010).

10       **[0004]**   Thousands of cytokines are involved in the immune response. Being selectively activated or restrained, they constitute a complicate but precisely under-controlled network to perform antiviral or immune regulation functions. See Dinarello, Chest 118, 503-508 (2000). In addition, they are considered to be broadly involved in other cellular activities, for instance, suppressing tumor growth, promoting catabiosis, and inducing apoptosis. See Crusz et al., Nature Reviews Clinical Oncology, doi:10.1038/nrclinonc.2015.105 (2015); Chen et al., Drug Design, Development and Therapy 9, 2941-2946 (2015); Villeda et al., Nature 477, 90-94 (2011); and Eckhardt et al., Cell Death Disease 5, e1562 (2014). However, the functional mechanisms of these proteins are largely unclear.

## 20       **SUMMARY**

**[0005]**   In one aspect, disclosed herein is a method for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity of IFP35 (Interferon-induced Protein 35kD) and/or NMI (N-Myc-interacting protein) in a subject. In some embodiments, the method comprises administering, to a subject in need of such treatment and/or prevention, an effective amount of an agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in the subject.

**[0006]**   In any of the preceding embodiments, the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI can be associated with excessive immune response. In any of the preceding embodiments, the disease or disorder can be associated with cytokine storm. In any of the preceding embodiments,

the disease or disorder can be selected from the group consisting of inflammation, infection, organ damage, sepsis, and autoimmune disease. In any of the preceding embodiments, the method can be for treating a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI. In any of the preceding  
5    embodiments, the method can be for preventing a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

**[0007]** In any of the preceding embodiments, the agent can comprise a molecule, such as a small molecule or a polypeptide, that inhibits or reduces the expression and/or activity of IFP35 and/or NMI. In any of the preceding embodiments, the agent can  
10    comprise an antibody or antigen binding fragment thereof that inhibits or reduces the expression and/or activity of IFP35 and/or NMI. In any of the preceding embodiments, the agent can comprise a polynucleotide, such as an siRNA, shRNA, or miRNA, that targets the gene encoding IFP35 and/or NMI. In any of the preceding embodiments, the agent can comprise an antisense polynucleotide, such as an antisense RNA, that targets  
15    the gene encoding IFP35 and/or NMI. In any of the preceding embodiments, the agent can comprise a molecule that inhibits or reduces the oligomerization of IFP35 and/or NMI. In any of the preceding embodiments, the agent can comprise a molecule that inhibits or reduces the expression and/or activity of an interferon, thereby inhibiting or reducing the expression and/or activity of IFP35 and/or NMI. In any of the preceding  
20    embodiments, the agent can comprise a molecule that inhibits or reduces the secretion of IFP35 and/or NMI. In any of the preceding embodiments, the agent can comprise a molecule that inhibits or reduces the interaction between IFP35 and/or NMI and a cellular receptor of IFP35 and/or NMI. In any of the preceding embodiments, the agent can comprise a molecule that inhibits or reduces the interaction between IFP35 and/or  
25    NMI and a IFP35 and/or NMI cell surface receptor.

**[0008]** In any of the preceding embodiments, the prevention or reduction of the production and/or the activity of IFP35 and/or NMI can result in the inhibition or reduction of the expression and/or activity of an inflammatory factor, and/or inhibiting or reduction of NF- $\kappa$ B signaling. In one aspect, the inflammatory factor comprises IL-1 $\beta$ ,  
30    TNF- $\alpha$ , iNOS, and/or CD86, and the NF- $\kappa$ B signaling is mediate by a TLR such as TLR4.

**[0009]** In any of the preceding embodiments, the agent can comprise an antibody or antigen binding fragment that specifically binds to IFP35 and/or an antibody or antigen binding fragment that specifically binds to NMI. In one aspect, the antibody or antigen binding fragment specifically binds one or more NIDs (NMI/IFP35 domains).

5       **[0010]** In any of the preceding embodiments, the method can further comprise administering a pharmaceutically acceptable carrier or excipient. In any of the preceding embodiments, the agent can be administered via an oral, nasal, inhalational, parental, intravenous, intraperitoneal, subcutaneous, intramuscular, intradermal, topical, or rectal route. In any of the preceding embodiments, the agent can be administered at an amount  
10       that reduces production and/or an activity of IFP35 and/or NMI in the subject to a level that is substantially identical to a production and/or an activity level of IFP35 and/or NMI in a comparable subject that does not have a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

15       **[0011]** In any of the preceding embodiments, the subject can be a mammal. In some embodiments, the mammal is a human or a non-human mammal.

20       **[0012]** In another aspect, disclosed herein is a pharmaceutical composition for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject. In some aspects, the pharmaceutical composition comprises an effective amount of an agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in a subject and a pharmaceutically acceptable carrier or excipient. In any of the preceding embodiments, the pharmaceutical composition can further comprise an effective amount of a drug for the treatment and/or prevention of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in the subject.

25       **[0013]** In yet another aspect, disclosed herein is use of an effective amount of an agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in a subject for the manufacture of a medicament for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in the subject. In some aspects, the disease or disorder associated with abnormally high

level and/or activity of IFP35 and/or NMI is inflammation, infection, sepsis, organ damage, and autoimmune disease.

**[0014]** In still another aspect, disclosed herein is an antibody or antigen binding fragment thereof that specifically binds to IFP35 and/or NMI. In some aspects, the antibody or antigen binding fragment specifically binds to an epitope within SEQ ID NO: 2, SEQ ID NO: 4, SEQ ID NO: 6, or SEQ ID NO: 8. In some embodiments, the antibody or antigen binding fragment specifically binds to an epitope within amino acids 81-170, 177-268, or 136-216 of SEQ ID NO: 2. In other embodiments, the antibody or antigen binding fragment specifically binds to an epitope within amino acids 81-168, 175-266, or 134-214 of SEQ ID NO: 4. In still other embodiments, the antibody or antigen binding fragment specifically binds to an epitope within amino acids 104-193, 202-293, or 151-250 of SEQ ID NO: 6. In other embodiments, the antibody or antigen binding fragment specifically binds to an epitope within amino acids 103-192, 201-292, or 151-240 of SEQ ID NO: 8.

**[0015]** In another aspect, disclosed herein is an antibody or antigen binding fragment thereof that specifically binds to IFP35 and/or NMI, and the antibody or antigen binding fragment thereof comprises a heavy chain variable region comprising a complementarity determining region (CDR) consisting of the amino acid sequences of a CDR in the heavy chain variable region sequence set forth in SEQ ID NO: 9 and/or a light chain variable region comprising a CDR consisting of the amino acid sequence of a CDR in the light chain variable region sequence set forth in SEQ ID NO:10. In one embodiment, the antibody or antigen binding fragment thereof comprises a heavy chain variable region set forth in SEQ ID NO: 9 and a light chain variable region set forth in SEQ ID NO:10.

**[0016]** In any of the preceding embodiments, the antibody can be a monoclonal antibody, a polyclonal antibody, or a bi-specific antibody. In any of the preceding embodiments, the antigen binding fragment can be an Fab, F(ab')<sub>2</sub>, Fv or scFv fragment. In any of the preceding embodiments, the antibody or antigen binding fragment can further comprise a human heavy chain constant region and a human light chain constant region.

[0017] In any of the preceding embodiments, the antibody or antigen binding fragment can be a fully human antibody or antigen binding fragment or a humanized antibody or antigen binding fragment. In any of the preceding embodiments, the antibody or antigen binding fragment can be recombinantly produced.

5 [0018] In one aspect, disclosed herein is a method for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity and/or activity of IFP35 and/or NMI in a subject. The method can comprise administering, to a subject in need of such treatment and/or prevention, an effective amount of the antibody or antigen binding fragment according to any of the preceding embodiments. In any of the  
10 preceding embodiments, the disease or disorder can be associated with excessive immune response. In any of the preceding embodiments, the disease or disorder can be associated with cytokine storm. In any of the preceding embodiments, the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI can be selected from the group consisting of inflammation, infection, organ damage, sepsis, and  
15 autoimmune disease. In any of the preceding embodiments, the prevention or reduction of the production and/or the activity of IFP35 and/or NMI can result in the inhibition or reduction of the expression and/or activity of an inflammatory factor, and/or inhibiting or reduction of NF- $\kappa$ B signaling. In one aspect, the inflammatory factor comprises IL-1 $\beta$ , TNF- $\alpha$ , iNOS, and/or CD86, and the NF- $\kappa$ B signaling is mediate by a TLR such as TLR4.

20 [0019] In one aspect, disclosed herein is an isolated polynucleotide encoding an antibody or antigen binding fragment thereof that specifically binds to IFP35 and/or NMI. In some embodiments, the antibody or antigen binding fragment thereof comprises a heavy chain variable region comprising a complementarity determining region (CDR) consisting of the amino acid sequence of a CDR in the heavy chain variable region  
25 sequence set forth in SEQ ID NO: 9 and/or a light chain variable region comprising a CDR consisting of the amino acid sequences of a CDR in the light chain variable region sequence set forth in SEQ ID NO: 10. In some aspects, the antibody or antigen binding fragment thereof comprises a heavy chain variable region set forth in SEQ ID NO: 9 and a light chain variable region set forth in SEQ ID NO:10.

30 [0020] In one aspect, also disclosed herein is an isolated vector comprising the polynucleotide according to any of the preceding embodiments. In another aspect, also

disclosed herein is an isolated host cell comprising the vector according to any of the preceding embodiments.

[0021] In another aspect, disclosed herein is a host cell which is selected from the group consisting of the following: (a) a host cell transformed with an expression vector comprising a polynucleotide comprising a sequence encoding a heavy chain variable region of an antibody or antigen binding fragment thereof and a polynucleotide comprising a sequence encoding a light chain variable region of an antibody or antigen binding fragment thereof; and (b) a host cell transformed with an expression vector comprising a polynucleotide comprising a sequence encoding a heavy chain variable region of an antibody or antigen binding fragment thereof and an expression vector comprising a polynucleotide comprising a sequence encoding a light chain variable region of an antibody or antigen binding fragment thereof. In some embodiments, the antibody or fragment comprises a heavy chain variable region comprising a complementarity determining region (CDR) consisting of the amino acid sequences of a CDR in the heavy chain variable region sequence set forth in SEQ ID NO: 9 and/or a light chain variable region comprising a CDR consisting of the amino acid sequences of a CDR in the light chain variable region sequence set forth in SEQ ID NO: 10. In any of the preceding embodiments, the host cell can be a eukaryotic cell such as a CHO cell.

[0022] In another aspect, disclosed herein is a method of making an anti-IFP35 antibody or antigen binding fragment thereof and/or an anti-NMI antibody or antigen binding fragment thereof. In some aspects, the method comprises: a) culturing the host cell of any one of preceding embodiments under conditions suitable for expression of the polynucleotide encoding the antibody or antigen binding fragment; and b) isolating the antibody or antigen binding fragment. In one aspect, also disclosed herein is an antibody or antigen binding fragment produced by the method according to any of the preceding embodiments.

[0023] In some embodiments, disclosed herein is an isolated polypeptide comprising, consisting essentially of, or consisting of: (1) the sequence set forth in amino acids 81-170, 177-268, or 136-216 of SEQ ID NO: 2; or (2) the sequence set forth in amino acids 81-168, 175-266, or 134-214 of SEQ ID NO: 4; or (3) the sequence set forth

in amino acids 104-193, 202-293 or 151-250 of SEQ ID NO: 6; or (4) the sequence set forth in amino acids 103-192, 201-292, or 151-240 of SEQ ID NO: 8.

**[0024]** In some embodiments, disclosed herein is an isolated polypeptide comprising, consisting essentially of, or consisting of the sequence set forth in amino acids 81-170, 177-268, or 136-216 of SEQ ID NO: 2, wherein one or more of the amino acid residues at positions 145, 147, 150, 151, 172, 173, 175, 177, 182, 188, 192, 212, 199, 201, 207, 208, 210, 214, and 216 of SEQ ID NO: 2 (Ser145, Arg147, Glu150, Glu151, Asp172, Val173, Glu175, Leu177, Met182, Asp188, Gln192, Arg212, Gln199, Thr201, Gln207, Gln208, Pro210, Ser214, and Tyr216) are mutated and/or modified. In some aspects, according to structure-based sequence alignment, the left NID domain outside of the determined IFP35 NID-H domain structure has similar structure to NID-H. Ser234, Leu236, Arg110, Arg 108, Arg233, Leu 82, Glu268, Thr271, Val273, Glu92, Asp87, Asp245, and Gly246 of SEQ ID NO: 2 are the amino acid residues in the left NID domain that correspond to the surface residues in the determined NID domain structure of IFP35. In any of the preceding embodiments, the mutation(s) can substantially reduce or eliminate binding of the polypeptide to a IFP35 receptor or an inhibitory antibody specific for IFP35.

**[0025]** In some embodiments, disclosed herein is an isolated polypeptide comprising, consisting essentially of, or consisting of the sequence set forth in amino acids 81-168, 175-266, or 134-214 of SEQ ID NO: 4, wherein one or more of the amino acid residues at positions 143, 145, 148, 149, 170, 172, 173, 175, 180, 186, 190, 210, 197, 199, 204, 205, 206, 208, 212, and 214 of SEQ ID NO: 4 (Ser143, Arg145, Glu148, Glu149, Glu170, Arg172, Glu173, Leu175, Met180, Glu186, Gln190, Arg210, Gln197, Arg199, Arg204, Gln205, Gln206, Leu208, Ser212, and Tyr214) are mutated and/or modified. In any of the preceding embodiments, the mutation(s) can substantially reduce or eliminate binding of the polypeptide to a IFP35 receptor or an inhibitory antibody specific for IFP35.

**[0026]** In some embodiments, disclosed herein is an isolated polypeptide comprising, consisting essentially of, or consisting of the sequence set forth in amino acids 104-193, 202-293, or 151-250 of SEQ ID NO: 6, wherein one or more of the amino acid residues at positions 107, 112, 117, 159, 172, 173, 192, 197, 215, 256, 267, and 292

of SEQ ID NO: 6 (Leu107, Lys112, Gln117, Lys159, Glu172, Glu173, Glu192, Asp197, Asp215, Lys256, Asp267, and Glu292) are mutated and/or modified. In any of the preceding embodiments, the mutation(s) can substantially reduce or eliminate binding of the polypeptide to a NMI receptor or an inhibitory antibody specific for NMI.

5           **[0027]** In some embodiments, disclosed herein is an isolated polypeptide comprising, consisting essentially of, or consisting of the sequence set forth in amino acids 103-192, 201-292, or 151-240 of SEQ ID NO: 8, wherein one or more of the amino acid residues at positions 106, 111, 116, 158, 171, 172, 191, 196, 214, 255, 266, and 291 of SEQ ID NO: 8 (Leu106, Lys111, Gln116, Lys158, Glu171, Asp172, Asp191, Asp196, 10 Asp214, Arg255, Asp266, and Asp291) are mutated and/or modified. In any of the preceding embodiments, the mutation(s) can substantially reduce or eliminate binding of the polypeptide to a NMI receptor or an inhibitory antibody specific for NMI.

**[0028]** In one aspect, disclosed herein is a pharmaceutical composition comprising the polypeptide of any one of the preceding embodiments. In some 15 embodiments, the pharmaceutical composition comprises a pharmaceutically acceptable carrier or excipient.

**[0029]** In one aspect, disclosed herein is a method for stimulating an immune response in a subject, and the method comprises administering, to a subject in need of such stimulation, an effective amount of the polypeptide or the pharmaceutical 20 composition of any one of the preceding embodiments. In one aspect, the subject has a proliferation disorder, a neoplasm, a tumor or a cancer. In another aspect, the proliferation disorder is selected from the group consisting of sarcoma, epidermoid cancer, fibrosarcoma, cervical cancer, gastric carcinoma, skin cancer, leukemia, lymphoma, lung cancer, non- small cell lung cancer, colon cancer, CNS cancer, 25 melanoma, ovarian cancer, renal cancer, prostate cancer, breast cancer, liver cancer, head and neck cancers, pancreatic cancer, bladder cancer and esophageal cancer. In any of the preceding embodiments, the stimulation of the immune response can comprise stimulation of the expression and/or activity of an inflammatory factor, the recruitment of immune cells such as neutrophils, and/or NF- $\kappa$ B signaling. In some aspects, the 30 inflammatory factor comprises IL-1 $\beta$ , TNF- $\alpha$ , iNOS, and/or CD86, and the NF- $\kappa$ B signaling is mediated by a TLR such as TLR4. In any one of the preceding embodiments,

the stimulation of NF- $\kappa$ B signaling can comprise an increase in phosphorylated I $\kappa$ B $\alpha$  and/or a reduction in total I $\kappa$ B $\alpha$ .

- 5       **[0030]** In some aspects, provided herein are compositions and methods for activating, boosting, augmenting, and/or potentiating immune response in a subject. The present compositions and methods can be used to treat and/or prevent any suitable disease or disorder associated with abnormally low level of a IFP35 family protein such as IFP35 and/or NMI in a subject. For example, the disease or disorder associated with abnormally low level of IFP35 and/or NMI in a subject can be a proliferation disorder, a neoplasm, a tumor or a cancer. Exemplary proliferation disorders include sarcoma, epidermoid cancer, fibrosarcoma, cervical cancer, gastric carcinoma, skin cancer, leukemia, lymphoma, lung cancer, *e.g.*, non-small cell lung cancer (NSCLC), colon cancer, CNS cancer, melanoma, ovarian cancer, renal cancer, prostate cancer, breast cancer, liver cancer, head and neck cancers, pancreatic cancer, bladder cancer and esophageal cancer.
- 10       **[0031]** In another aspect, disclosed herein is an isolated polynucleotide encoding a polypeptide comprising the polypeptide of any one of the preceding embodiments. In yet another aspect, disclosed herein is an isolated vector comprising the polynucleotide of any one of the preceding embodiments. In still another aspect, disclosed herein is an isolated host cell comprising the vector of any one of the preceding embodiments. In some aspects, the host cell is a eukaryotic cell such as a CHO cell. In some aspects, disclosed herein is a method of making an isolated polynucleotide, and the method comprises: a) culturing the host cell under conditions suitable for expression of the polynucleotide encoding a polypeptide comprising the polypeptide of any of the preceding embodiments; and b) isolating the polypeptide.
- 20       **[0032]** In some aspects, disclosed herein is a method of diagnosis, prognosis or treatment monitoring of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject. In some aspects, the method comprises assessing the level and/or an activity of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI. In one embodiment, the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is associated with
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- 30

excessive immune response. In another embodiment, the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is associated with cytokine storm. In any of the preceding embodiments, the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI can be selected from the group consisting of inflammation, infection, organ damage, sepsis, and autoimmune disease.

**[0033]** In any of the preceding embodiments, the method can be used for diagnosis of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject, and wherein a level and/or an activity of IFP35 and/or NMI in a subject that is at least 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, 100%, 150%, 200%, 300%, 400%, or 500% higher than a level and/or an activity of IFP35 and/or NMI in a comparable subject that does not have a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI, e.g., inflammation, infection, organ damage, sepsis, and autoimmune disease, indicates that the subject has the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

**[0034]** In any of the preceding embodiments, the method can further comprise assessing the level of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI. In any of the preceding embodiments, the method can comprise assessing an activity of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI. In any of the preceding embodiments, the level and/or an activity of IFP35 and/or NMI can be assessed at the DNA, RNA and/or protein level. In one aspect, the level of IFP35 and/or NMI is assessed at the DNA and/or RNA level using a polynucleotide that is complementary to at least 10 consecutive nucleotides in the IFP35 and/or NMI DNA or RNA. In another aspect, the level of IFP35 and/or NMI is assessed at the protein level using an antibody that specifically binds to IFP35 and/or NMI.

**[0035]** Also disclosed herein, in one aspect, is a kit of diagnosis, prognosis or treatment monitoring of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject. In some aspects, the kit comprises a

means for assessing the level and/or an activity of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

**[0036]** Also disclosed herein, in one aspect, is a method of companion  
5 diagnostics of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject. In some aspects, the method comprises determining the genetic status of IFP35 and/or NMI gene in a subject being treated for the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI. In one aspect, the genetic status of IFP35 and/or NMI gene in a subject is determined using  
10 a polynucleotide that is complementary to at least 10 consecutive nucleotides in the IFP35 and/or NMI DNA or RNA.

**[0037]** Also disclosed herein, in one aspect, is a kit of companion diagnostics of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject. In one aspect, the kit comprises a means for determining the genetic  
15 status of IFP35 and/or NMI gene in a subject being treated for the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

**[0038]** In one aspect, disclosed herein is a method for identifying a modulator of IFP35 and/or NMI. In some aspects, the method comprises: a) contacting IFP35 and/or NMI with a test substance and assessing an activity of IFP35 and/or NMI that has been  
20 contacted by the test substance; b) assessing an activity of the IFP35 and/or NMI that has not been contacted by the test substance; and c) comparing the activities of IFP35 and/or NMI assessed in steps a) and b), and identifying the test substance as a modulator of IFP35 and/or NMI when the activities of IFP35 and/or NMI assessed in steps a) and b) are different. In one aspect, the test substances are small molecules, a polypeptide library  
25 comprising mutants and/or fragments of IFP35 and/or NMI, antibodies that specifically bind IFP35 and/or NMI, a polynucleotide, such as an siRNA, shRNA, miRNA, or antisense RNAs. In any of the preceding embodiments, the method can be used to identify an inhibitor of an activity of IFP35 and/or NMI. In any of the preceding embodiments, the method can be used to identify a drug for treating and/or preventing a  
30 disease or disorder associated with abnormal level and/or activity of IFP35 and/or NMI in a subject. In some aspects, the disease or disorder associated with abnormal level

and/or activity of IFP35 and/or NMI is a proliferation disorder, a neoplasm, a tumor or a cancer. In some embodiments, the disease or disorder, such as a proliferation disorder, a neoplasm, a tumor or a cancer, is associated with abnormally low level and/or activity of a IFP35 family protein such as IFP35 or NMI.

- 5           **[0039]** In some aspects, also disclosed herein is a drug candidate identified by a method of any one of the preceding embodiments.

### **Brief Description of the Drawings**

- [0040]** **Fig. 1** shows a crystal structure of NID-H (heterozygous NID). **a.** Truncations and putative domains of IFP35 are shown and the boundaries between  
10 domains are noted in the sequence. **b.** The structure of the IFP35 dimer (closed conformational dimer, c-dimer) with secondary structure elements noted. **c.** Residues involved in the intra-molecule interactions are labeled and shown in sticks. For clarity, only half of the interactions are shown. **d.** The ring structure of the octamer, in which monomers are shown. **e.** Dimer with domain-swapping conformation (open  
15 conformational dimer, o-dimer) is highlighted with secondary structure elements noted on the upper panel. A NID-H molecule from c-dimer is superimposed on the o-dimer as shown in the lower panel.

- [0041]** **Fig. 2** shows the two stable aggregation states, dimer and octamer, of NID-H. **a.** Size-exclusion chromatography analysis of NID-H using Superdex-200  
20 (16/60 or 10/30) column (GE). The UV absorptions at 280 nm are shown in blue. The elution volumes of two peaks are 75ml and 90ml, suggesting dimer and octamer formation. **b.** O-dimer and c-dimer superimposed on the octamer. Four o-dimers interact with one another through  $\alpha 1$ - $\alpha 1$  interactions, and form a ring like octamer structure. **c.** Structure comparison between NID-H and RNA recognition motif (RRM). The R.M.S.D.  
25 between them is about 1.3 Å.

**[0042]** **Fig. 3** shows that the open conformational dimer (o-dimer) of NID-H is responsible for immune response stimulation. **a.** Octameric NID-H up-regulates the transcription of TNF- $\alpha$  and IL-1 $\beta$  in RAW 264.7 cells. The cellular mRNA of TNF- $\alpha$  and IL-1 $\beta$  were detected by RT-PCR using GAPDH as internal control. **b.** Dimeric

stated mutation on  $\alpha 1$ , K156E/K163E/R165E, partially up-regulates the transcription of TNF- $\alpha$  and IL-1 $\beta$ . **c.** IFP35 without the L-zip domain ( $\Delta$  N) stimulated immune response more effectively than NID-H octamer. **d.** Similar with LPS,  $\Delta$  N could effectively stimulate the TNF- $\alpha$  release of RAW264.7 cells. TNF- $\alpha$  levels in cell culture were  
 5 determined by ELISA after 4 h of incubation.

**[0043]** **Fig. 4** shows that human source NMI protein up-regulates the transcription of TNF- $\alpha$  and IL-1 $\beta$  in THP1 cells. PBS buffer was used as negative control (NC). Results came from an average of three independently replicates. Error bars indicate the standard deviation among them.

10 **[0044]** **Fig. 5** shows IFP35 possesses characteristics of endogenous DAMPs. **a.** IFP35 released by RAW264.7 cells stimulated by LPS. RAW 264.7 macrophages were pretreated with 100ng/mL LPS. Cell lysate and supernatants at 0, 1, 2, 3, 5, 9 hours were analyzed by western blot of IFP35, HMGB1 and  $\beta$ -Actin. **b.** IFP35 is accumulated in the serum of LPS induced septic mice. Serum concentrations of IFP35 in mice were  
 15 determined by ELISA 3h and 6h after injection of LPS. **c.** IFP35 is accumulated in the serum of septic patients. This data was obtained from the serum of 12 patients and 8 normal individuals. **d.** Survival rate of the septic mice administrated with IgG and IFP35 monoclonal antibodies (Anti-NID-H) was presented. Mice received LPS injection (i.p.) followed by treatment with anti-IFP35 antibody or IgG. Animal survival rate was  
 20 assessed in  $n = 15$  mice/group. **e.** Anti-NID-H neutralization attenuated the release of early inflammatory cytokines such as IL-6, TNF- $\alpha$  and IL-1 $\beta$ , detected using ELISA. **f.** Survival of wild-type ( $n=12$ ) and *IFP35*<sup>-/-</sup> mice ( $n=12$ ) treated with LPS and D-gal. **g.** The release of early inflammatory cytokines in the serum of IFP35 knock-out mice is reduced. Serum concentrations of IL-6, TNF- $\alpha$  and IL-1 $\beta$  in *IFP35*<sup>-/-</sup> and wild-type mice  
 25 as determined by ELISA 1h and 3h after injection of LPS and D-gal.

**[0045]** **Fig. 6** shows IFP35 family members are released as endogenous DAMPs. **a.** IFP35 released by RAW cells stimulated by 10 ng/ml INF- $\gamma$ . **b.** NMI released by RAW cells stimulated by Salmonella (SR). **c** and **d.** The aggregation state of IFP35 (panel c) and NMI (panel d) were detected. After stimulating the RAW cells with SR, the  
 30 cell culture were collected and the released IFP35 family members were detected the by

gel filtration (Superdex-200 (16/60 or 10/30) column, GE) and western blot. The elution volume of IFP 35 is about 90ml, as shown in panel c, suggesting a 35kD monomer. NMI showed multiple aggregation states detected by gel filtration. The elution volume of its major conformation is about 76-82ml, indicating that released NMI existed as dimer in solution. **e.** NMI is accumulated in the serum of LPS induced septic mice, as determined by ELISA 3h and 6h after injection of LPS. **f.** NMI is accumulated in the serum of septic patients. Serum was obtained from 8 healthy people and 12 septic patients. Serum concentrations of NMI were determined by ELISA. **g.** NMI knock-out mice is resistant to LPS challenge. The survival rate of wide type (WT) (n=14) and *Nmi*<sup>-/-</sup> mice (KO) (n=14) administrated with LPS was presented. **h.** The release of inflammatory cytokines such as IL-6, TNF- $\alpha$  and IL-1 $\beta$  in the serum of *Nmi*<sup>-/-</sup> mice is reduced. The results got from WT and KO mice are shown in gray and black, respectively. All the results were confirmed by multiple independently analyzed biological replicates.

**[0046]** **Fig. 7** shows IFP35 stimulates the cytokines storm based on TLR4/MD2/CD14 complex. **a.** Octameric NID-H induced NF- $\kappa$ B promoter activity in a HEK293 cell line transfected with TLR4, CD14, MD2 and NF- $\kappa$ B promoter luciferase plasmid. 24 hours after transfection, cells were stimulated with 10 $\mu$ g/ml Octameric NID-H or 100 ng/ml LPS for 4 h (in the presence or absence of 25 mg/ml polymyxin B) and assayed for luciferase activity. The luciferase activity triggered by LPS can be blocked by polymyxin B, an effective antibiotic for Gram-negative infections. **b.** Purified IFP35 ( $\Delta$ N), a N-terminal truncation of IFP35 and LPS induce NF- $\kappa$ B and AP-1 but not IRF3 promoter activity. The genes of TLR4, MD2 and CD14 and NF- $\kappa$ B promoter (or AP-1, IRF3) with luciferase activity were transiently transfected into HEK293 cells. IFP35 was used at 1  $\mu$ g/ml, while 100 ng/ml LPS were administrated as positive control.

**[0047]** **Fig. 8** shows the structure model of tandem NID domains in IFP35. **a** and **b.** Secondary structure elements and sequence alignment of A and A' as well as B and B' are shown in panel a. The identical residues are labeled with "\*", while residues with similar features are labeled with ":" or ".". Residues in the hydrophobic core of NID-H structure are shown in panel b which is highlighted in squares in panel a. **c.** The double-barrel structure of tandem NIDs. Part B' is shown in green and Part A' is shown in cyan. The NID-H structure is shown in purple.

- [0048] Fig. 9 shows sequence alignment of IFP35 and NMI generated by ClustalW. The identical residues are labeled with “\*”, while residues with similar features are labeled with “:” or “.”. The secondary structure elements of NMI are predicted by PsiPred. The  $\alpha$ -helices and  $\beta$ -strands are shown in red and yellow, respectively. The two NID domains parallel to those in IFP35 are labeled and highlighted in squares.
- [0049] Fig. 10 illustrates the process of IFP35 protein purification.
- [0050] Fig. 11 shows the different oligomer states of IFP35.
- [0051] Fig. 12 shows the IFP35-NID crystal.
- 10 [0052] Fig. 13 shows the structure of the dimeric IFP35-NID.
- [0053] Fig. 14 shows the structure of the octameric IFP35-NID.
- [0054] Fig. 15 shows the structure of dimer with domain-swapping conformation.
- [0055] Fig. 16 shows the residues of some areas.
- [0056] Fig. 17 shows the purification of the recombinant NMI.
- 15 [0057] Fig. 18 reveals the expression level of IFP35 when stimulated by salmonella.
- [0058] Fig. 19 shows that the abundance of IFP35 changed with time as measured by immunofluorescence.
- [0059] Fig. 20 shows the abundance of IFP35 secreted to the medium at different periods when cells are infected by the virus.
- 20 [0060] Fig. 21 shows a model of mouse peritonitis.
- [0061] Fig. 22 shows the contribution of the IFP35 with different oligomer states during the process of stimulating inflammation.
- [0062] Fig. 23 shows the result of Flow cytometry analysis, which illustrates octameric IFP35-nid can recruit large amount of neutrophil granulocytes.
- 25 [0063] Fig. 24 shows exogenous octameric IFP35-NID can stimulate NF- $\kappa$ B pathway in macrophages.

[0064] Fig. 25 illustrates that IFP35 can stimulate inflammation through myd88 signal pathway.

[0065] Fig. 26 shows the levels of IL-1 $\beta$  and TNF among WT, TLR9-/- and TLR4-/- mouse as induced by IFP35.

5 [0066] Fig. 27A shows the amount of IFP35 in the serum of septic mice. Fig. 27B shows the survival rate of the septic mice was increased when administrated with IFP35 monoclonal antibodies.

[0067] Fig. 28 shows that the block of IFP35 attenuated the release of induced IL-6 by LPS in mice.

10 [0068] Fig. 29 shows the abundance of NMI in cell lysate and supernatant of Thp1 cells stimulated by salmonella.

[0069] Fig. 30 demonstrates that mouse source NMI protein can up-regulate the transcription of TNF $\alpha$  and IL-1 $\beta$  in Thp1 cells.

[0070] Fig. 31 shows the detection of the aggregation state of NMI.

15 [0071] Fig. 32 shows a secondary structure prediction of human IFP35.

[0072] Fig. 33 shows the crystal structure coordinates of the NID-H dimer.

[0073] Fig. 34 shows the crystal structure coordinates of the NID-H octamer.

## **Detailed Description of the Invention**

### **A. GENERAL TECHNIQUES**

20 [0074] The practice of the present invention will employ, unless otherwise indicated, conventional techniques of molecular biology (including recombinant techniques), microbiology, cell biology, biochemistry, immunology, and pharmacology, which are within the skill of the art. Such techniques are explained fully in the literature, such as, Molecular Cloning: A Laboratory Manual, 2<sup>nd</sup> ed. (Sambrook et al., 1989);  
 25 Oligonucleotide Synthesis (M. J. Gait, ed., 1984); Animal Cell Culture (R. I. Freshney, ed., 1987); Methods in Enzymology (Academic Press, Inc.); Current Protocols in Molecular Biology (F. M. Ausubel et al., eds., 1987, and periodic updates); PCR: The

Polymerase Chain Reaction (Mullis et al., eds., 1994); and Remington, The Science and Practice of Pharmacy, 20<sup>th</sup> ed., (Lippincott, Williams & Wilkins 2003).

#### Definitions

**[0075]** Unless defined otherwise, all technical and scientific terms used herein have the same meaning as is commonly understood by one of ordinary skill in the art to which this invention belongs. All patents, patent applications (published or unpublished), and other publications referred to herein are incorporated by reference in their entireties. If a definition set forth in this section is contrary to or otherwise inconsistent with a definition set forth in the patents, applications, published applications and other publications that are herein incorporated by reference, the definition set forth in this section prevails over the definition that is incorporated herein by reference.

**[0076]** As used herein, “a” or “an” means “at least one” or “one or more.”

**[0077]** The terms “polypeptide,” “oligopeptide,” “peptide,” and “protein” are used interchangeably herein to refer to polymers of amino acids of any length, *e.g.*, at least 5, 6, 7, 8, 9, 10, 20, 30, 40, 50, 100, 200, 300, 400, 500, 1,000 or more amino acids. The polymer may be linear or branched, it may comprise modified amino acids, and it may be interrupted by non-amino acids. The terms also encompass an amino acid polymer that has been modified naturally or by intervention; for example, disulfide bond formation, glycosylation, lipidation, acetylation, phosphorylation, or any other manipulation or modification, such as conjugation with a labeling component. Also included within the definition are, for example, polypeptides containing one or more analogs of an amino acid (including, for example, unnatural amino acids, etc.), as well as other modifications known in the art.

**[0078]** As used herein, the terms “variant” is used in reference to polypeptides that have some degree of amino acid sequence identity to a parent polypeptide sequence. A variant is similar to a parent sequence, but has at least one substitution, deletion or insertion in their amino acid sequence that makes them different in sequence from a parent polypeptide. Additionally, a variant may retain the functional characteristics of the parent polypeptide, *e.g.*, maintaining a biological activity that is at least 50%, 60%, 70%, 80%, 90%, 95%, 98%, or 99% of that of the parent polypeptide.

[0079] An “antibody” is an immunoglobulin molecule capable of specific binding to a target, such as a carbohydrate, polynucleotide, lipid, polypeptide, etc., through at least one antigen recognition site, located in the variable region of the immunoglobulin molecule, and can be an immunoglobulin of any class, *e.g.*, IgG, IgM, IgA, IgD and IgE. IgY, which is the major antibody type in avian species such as chicken, is also included within the definition. As used herein, the term encompasses not only intact polyclonal or monoclonal antibodies, but also fragments thereof (such as Fab, Fab’, F(ab’)<sub>2</sub>, Fv), single chain (ScFv), mutants thereof, naturally occurring variants, fusion proteins comprising an antibody portion with an antigen recognition site of the required specificity, humanized antibodies, chimeric antibodies, and any other modified configuration of the immunoglobulin molecule that comprises an antigen recognition site of the required specificity.

[0080] As used herein, the term “antigen” refers to a target molecule that is specifically bound by an antibody through its antigen recognition site. The antigen may be monovalent or polyvalent, *i.e.*, it may have one or more epitopes recognized by one or more antibodies. Examples of kinds of antigens that can be recognized by antibodies include polypeptides, oligosaccharides, glycoproteins, polynucleotides, lipids, etc.

[0081] As used herein, the term “epitope” refers to a portion of an antigen, *e.g.*, a peptide sequence of at least about 3 to 5, preferably about 5 to 10 or 15, and not more than about 1,000 amino acids (or any integer there between), which define a sequence that by itself or as part of a larger sequence, binds to an antibody generated in response to such sequence. There is no critical upper limit to the length of the fragment, which may, for example, comprise nearly the full-length of the antigen sequence, or even a fusion protein comprising two or more epitopes from the target antigen. An epitope for use in the subject invention is not limited to a peptide having the exact sequence of the portion of the parent protein from which it is derived, but also encompasses sequences identical to the native sequence, as well as modifications to the native sequence, such as deletions, additions and substitutions (conservative in nature).

[0082] As used herein, the term “specifically binds” refers to the binding specificity of a specific binding pair. Recognition by an antibody of a particular target in the presence of other potential targets is one characteristic of such binding. Specific

binding involves two different molecules wherein one of the molecules specifically binds with the second molecule through chemical or physical means. The two molecules are related in the sense that their binding with each other is such that they are capable of distinguishing their binding partner from other assay constituents having similar characteristics. The members of the binding component pair are referred to as ligand and receptor (anti-ligand), specific binding pair (SBP) member and SBP partner, and the like. A molecule may also be an SBP member for an aggregation of molecules; for example an antibody raised against an immune complex of a second antibody and its corresponding antigen may be considered to be an SBP member for the immune complex.

10       **[0083]** As used herein, a “tag” or an “epitope tag” refers to a sequence of amino acids, typically added to the N- and/or C- terminus of a polypeptide. The inclusion of tags fused to a polypeptide can facilitate polypeptide purification and/or detection. Typically a tag or tag polypeptide refers to polypeptide that has enough residues to provide an epitope recognized by an antibody or can serve for detection or purification, yet is short enough such that it does not interfere with activity of chimeric polypeptide to which it is linked. The tag polypeptide typically is sufficiently unique so an antibody that specifically binds thereto does not substantially cross-react with epitopes in the polypeptide to which it is linked. Suitable tag polypeptides generally have at least 5 or 6 amino acid residues and usually between about 8-50 amino acid residues, typically between 9-30 residues. The tags can be linked to one or more chimeric polypeptides in a multimer and permit detection of the multimer or its recovery from a sample or mixture. Such tags are well known and can be readily synthesized and designed. Exemplary tag polypeptides include those used for affinity purification and include His tags, the influenza hemagglutinin (HA) tag polypeptide and its antibody 12CA5; the c-myc tag and the 8F9, 3C7, 6E10, G4, B7 and 9E10 antibodies thereto; and the Herpes Simplex virus glycoprotein D (gD) tag and its antibody. *See, e.g.,* Field et al. (1988) *Mol. Cell. Biol.* 8:2159-2165; Evan et al. (1985) *Mol. Cell. Biol.* 5:3610-3616; Paborsky et al. (1990) *Protein Engineering* 3:547-553.

30       **[0084]** “Polynucleotide,” or “nucleic acid,” as used interchangeably herein, refer to polymers of nucleotides of any length, and include DNA and RNA. The nucleotides can be deoxyribonucleotides, ribonucleotides, modified nucleotides or bases, and/or their

analog, or any substrate that can be incorporated into a polymer by DNA or RNA polymerase. A polynucleotide may comprise modified nucleotides, such as methylated nucleotides and their analogs. If present, modification to the nucleotide structure may be imparted before or after assembly of the polymer. The sequence of nucleotides may be interrupted by non-nucleotide components. A polynucleotide may be further modified after polymerization, such as by conjugation with a labeling component. Other types of modifications include, for example, "caps", substitution of one or more of the naturally occurring nucleotides with an analog, internucleotide modifications such as, for example, those with uncharged linkages (*e.g.*, methyl phosphonates, phosphotriesters, phosphoamidates, cabamates, etc.) and with charged linkages (*e.g.*, phosphorothioates, phosphorodithioates, etc.), those containing pendant moieties, such as, for example, proteins (*e.g.*, nucleases, toxins, antibodies, signal peptides, ply-L-lysine, etc.), those with intercalators (*e.g.*, acridine, psoralen, etc.), those containing chelators (*e.g.*, metals, radioactive metals, boron, oxidative metals, etc.), those containing alkylators, those with modified linkages (*e.g.*, alpha anomeric nucleic acids, etc.), as well as unmodified forms of the polynucleotide(s). Further, any of the hydroxyl groups ordinarily present in the sugars may be replaced, for example, by phosphonate groups, phosphate groups, protected by standard protecting groups, or activated to prepare additional linkages to additional nucleotides, or may be conjugated to solid supports. The 5' and 3' terminal OH can be phosphorylated or substituted with amines or organic capping groups moieties of from 1 to 20 carbon atoms. Other hydroxyls may also be derivatized to standard protecting groups. Polynucleotides can also contain analogous forms of ribose or deoxyribose sugars that are generally known in the art, including, for example, 2'-O-methyl-2'-O-allyl, 2'-fluoro- or 2'-azido-ribose, carbocyclic sugar analogs,  $\alpha$ -anomeric sugars, epimeric sugars such as arabinose, xyloses or lyxoses, pyranose sugars, furanose sugars, sedoheptuloses, acyclic analogs and abasic nucleoside analogs such as methyl riboside. One or more phosphodiester linkages may be replaced by alternative linking groups. These alternative linking groups include, but are not limited to, embodiments wherein phosphate is replaced by P(O)S("thioate"), P(S)S("dithioate"), "(O)NR<sub>2</sub> ("amidate"), P(O)R, P(O)OR', CO or CH<sub>2</sub> ("formacetal"), in which each R or R' is independently H or substituted or unsubstituted alkyl (1-20 C) optionally containing an

ether (--O--) linkage, aryl, alkenyl, cycloalkyl, cycloalkenyl or araldyl. Not all linkages in a polynucleotide need be identical. The preceding description applies to all polynucleotides referred to herein, including RNA and DNA.

[0085] “Oligonucleotide,” as used herein, generally refers to short, generally  
5 single stranded, generally synthetic polynucleotides that are generally, but not necessarily, less than about 200 nucleotides in length. The terms “oligonucleotide” and “polynucleotide” are not mutually exclusive. The description above for polynucleotides is equally and fully applicable to oligonucleotides.

[0086] As used herein, the term “homologue” is used to refer to a nucleic acid  
10 which differs from a naturally occurring nucleic acid (e.g., the “prototype” or “wild-type” nucleic acid) by minor modifications to the naturally occurring nucleic acid, but which maintains the basic nucleotide structure of the naturally occurring form. Such changes include, but are not limited to: changes in one or a few nucleotides, including deletions (e.g., a truncated version of the nucleic acid) insertions and/or substitutions. A  
15 homologue can have enhanced, decreased, or substantially similar properties as compared to the naturally occurring nucleic acid. A homologue can be complementary or matched to the naturally occurring nucleic acid. Homologues can be produced using techniques known in the art for the production of nucleic acids including, but not limited to, recombinant DNA techniques, chemical synthesis, etc.

[0087] As used herein, “substantially complementary or substantially matched”  
20 means that two nucleic acid sequences have at least 90% sequence identity. Preferably, the two nucleic acid sequences have at least 95%, 96%, 97%, 98%, 99% or 100% of sequence identity. Alternatively, “substantially complementary or substantially matched” means that two nucleic acid sequences can hybridize under high stringency  
25 condition(s).

[0088] In general, the stability of a hybrid is a function of the ion concentration and temperature. Typically, a hybridization reaction is performed under conditions of lower stringency, followed by washes of varying, but higher, stringency. Moderately stringent hybridization refers to conditions that permit a nucleic acid molecule such as a  
30 probe to bind a complementary nucleic acid molecule. The hybridized nucleic acid

molecules generally have at least 60% identity, including for example at least any of 70%, 75%, 80%, 85%, 90%, or 95% identity. Moderately stringent conditions are conditions equivalent to hybridization in 50% formamide, 5x Denhardt's solution, 5x SSPE, 0.2% SDS at 42°C, followed by washing in 0.2x SSPE, 0.2% SDS, at 42°C. High stringency conditions can be provided, for example, by hybridization in 50% formamide, 5x Denhardt's solution, 5x SSPE, 0.2% SDS at 42°C, followed by washing in 0.1x SSPE, and 0.1% SDS at 65°C. Low stringency hybridization refers to conditions equivalent to hybridization in 10% formamide, 5x Denhardt's solution, 6x SSPE, 0.2% SDS at 22°C, followed by washing in 1x SSPE, 0.2% SDS, at 37°C. Denhardt's solution contains 1% Ficoll, 1% polyvinylpyrrolidone, and 1% bovine serum albumin (BSA). 20x SSPE (sodium chloride, sodium phosphate, ethylene diamide tetraacetic acid (EDTA)) contains 3M sodium chloride, 0.2M sodium phosphate, and 0.025 M (EDTA). Other suitable moderate stringency and high stringency hybridization buffers and conditions are well known to those of skill in the art.

**[0089]** As used herein, the term “RNA interference” or “RNAi” refers generally to a process in which a double-stranded RNA molecule or a short hairpin RNA molecule reducing or inhibiting the expression of a nucleic acid sequence with which the double-stranded or short hairpin RNA molecule shares substantial or total homology. The term “short interfering RNA” or “siRNA” or “RNAi agent” refers to an RNA (or RNA analog) sequence comprising between about 10-50 nucleotides (or nucleotide analogs) that elicits RNA interference. *See* Kreutzer et al., WO 00/44895; Zernicka-Goetz et al., WO 01/36646; Fire, WO 99/32619; Mello & Fire, WO 01/29058. As used herein, siRNA molecules include RNA molecules encompassing chemically modified nucleotides and non-nucleotides. The term “ddRNAi agent” refers to a DNA-directed RNAi agent that is transcribed from an exogenous vector. The terms “short hairpin RNA” or “shRNA” refer to an RNA structure having a duplex region and a loop region. In certain embodiments, ddRNAi agents are expressed initially as shRNAs.

**[0090]** As used herein, “vector (or plasmid)” refers to discrete elements that are used to introduce heterologous DNA into cells for either expression or replication thereof. Selection and use of such vehicles are well known within the skill of the artisan. An expression vector includes vectors capable of expressing DNA's that are operatively

linked with regulatory sequences, such as promoter regions, that are capable of effecting expression of such DNA fragments. Thus, an expression vector refers to a recombinant DNA or RNA construct, such as a plasmid, a phage, recombinant virus or other vector that, upon introduction into an appropriate host cell, results in expression of the cloned  
5 DNA. Appropriate expression vectors are well known to those of skill in the art and include those that are replicable in eukaryotic cells and/or prokaryotic cells and those that remain episomal or those which integrate into the host cell genome.

[0091] As used herein, “a promoter region or promoter element” refers to a segment of DNA or RNA that controls transcription of the DNA or RNA to which it is  
10 operatively linked. The promoter region includes specific sequences that are sufficient for RNA polymerase recognition, binding and transcription initiation. This portion of the promoter region is referred to as the promoter. In addition, the promoter region includes sequences that modulate this recognition, binding and transcription initiation activity of RNA polymerase. These sequences may be cis acting or may be responsive to trans  
15 acting factors. Promoters, depending upon the nature of the regulation, may be constitutive or regulated. Exemplary promoters contemplated for use in prokaryotes include the bacteriophage T7 and T3 promoters, and the like.

[0092] As used herein, “operatively linked or operationally associated” refers to the functional relationship of DNA with regulatory and effector sequences of nucleotides,  
20 such as promoters, enhancers, transcriptional and translational stop sites, and other signal sequences. For example, operative linkage of DNA to a promoter refers to the physical and functional relationship between the DNA and the promoter such that the transcription of such DNA is initiated from the promoter by an RNA polymerase that specifically recognizes, binds to and transcribes the DNA. In order to optimize expression and/or *in*  
25 *vitro* transcription, it may be necessary to remove, add or alter 5' untranslated portions of the clones to eliminate extra, potential inappropriate alternative translation initiation (i.e., start) codons or other sequences that may interfere with or reduce expression, either at the level of transcription or translation. Alternatively, consensus sites can be inserted immediately 5' of the start codon and may enhance expression. *See, e.g., Kozak (1991) J.*  
30 *Biol. Chem.* 266:19867-19870. The desirability of (or need for) such modification may be empirically determined.

[0093] “Treating” or “treatment” or “alleviation” refers to therapeutic treatment wherein the object is to slow down (lessen) if not cure the targeted pathologic condition or disorder or prevent recurrence of the condition. A subject is successfully “treated” if, after receiving a therapeutic amount of a therapeutic agent or treatment, the subject  
5 shows observable and/or measurable reduction in or absence of one or more signs and symptoms of the particular disease. Reduction of the signs or symptoms of a disease may also be felt by the patient. A patient is also considered treated if the patient experiences stable disease. In some embodiments, treatment with a therapeutic agent is effective to result in the patients being disease-free 3 months after treatment, preferably 6  
10 months, more preferably one year, even more preferably 2 or more years post treatment. These parameters for assessing successful treatment and improvement in the disease are readily measurable by routine procedures familiar to a physician of appropriate skill in the art. In some embodiments, “treatment” means any manner in which the symptoms of a condition, disorder or disease are ameliorated or otherwise beneficially altered.  
15 Treatment also encompasses any pharmaceutical use of the compositions herein. In some embodiments, “amelioration” of the symptoms of a particular disorder by administration of a particular pharmaceutical composition refers to any lessening, whether permanent or temporary, lasting or transient that can be attributed to or associated with administration of the composition.

20 [0094] The term “prediction” or “prognosis” is used herein to refer to the likelihood that a patient will respond either favorably or unfavorably to a drug or set of drugs, or the likely outcome of a disease. In one embodiment, the prediction relates to the extent of those responses or outcomes. In one embodiment, the prediction relates to whether and/or the probability that a patient will survive or improve following treatment,  
25 for example treatment with a particular therapeutic agent, and for a certain period of time without disease recurrence. The predictive methods of the invention can be used clinically to make treatment decisions by choosing the most appropriate treatment modalities for any particular patient. The predictive methods of the present invention are valuable tools in predicting if a patient is likely to respond favorably to a treatment  
30 regimen, such as a given therapeutic regimen, including for example, administration of a given therapeutic agent or combination, surgical intervention, steroid treatment, etc.

[0095] As used herein the language “pharmaceutically acceptable carrier” is intended to include any and all solvents, dispersion media, coatings, isotonic and absorption delaying agents, and the like, compatible with pharmaceutical administration. The use of such media and agents for pharmaceutically active substances is well known in the art. *See, e.g.,* Remington, The Science and Practice of Pharmacy, 20<sup>th</sup> ed., (Lippincott, Williams & Wilkins 2003). Except insofar as any conventional media or agent is incompatible with the active compound, such use in the compositions is contemplated.

[0096] A “pharmaceutically acceptable salt” is intended to mean a salt of a free acid or base of a compound represented herein that is non-toxic, biologically tolerable, or otherwise biologically suitable for administration to the subject. *See, generally,* Berge, et al., *J. Pharm. Sci.*, 1977, 66, 1-19. Preferred pharmaceutically acceptable salts are those that are pharmacologically effective and suitable for contact with the tissues of subjects without undue toxicity, irritation, or allergic response. A compound described herein may possess a sufficiently acidic group, a sufficiently basic group, both types of functional groups, or more than one of each type, and accordingly react with a number of inorganic or organic bases, and inorganic and organic acids, to form a pharmaceutically acceptable salt.

[0097] Examples of pharmaceutically acceptable salts include sulfates, pyrosulfates, bisulfates, sulfites, bisulfites, phosphates, monohydrogen-phosphates, dihydrogenphosphates, metaphosphates, pyrophosphates, chlorides, bromides, iodides, acetates, propionates, decanoates, caprylates, acrylates, formates, isobutyrate, caproates, heptanoates, propiolates, oxalates, malonates, succinates, suberates, sebacates, fumarates, maleates, butyne-1,4-dioates, hexyne-1,6-dioates, benzoates, chlorobenzoates, methylbenzoates, dinitrobenzoates, hydroxybenzoates, methoxybenzoates, phthalates, sulfonates, methylsulfonates, propylsulfonates, besylates, xylenesulfonates, naphthalene-1-sulfonates, naphthalene-2-sulfonates, phenylacetates, phenylpropionates, phenylbutyrates, citrates, lactates,  $\gamma$ -hydroxybutyrates, glycolates, tartrates, and mandelates.

[0098] As used herein, the term “therapeutically effective amount” or “effective amount” refers to an amount of a therapeutic agent that when administered alone or in

combination with an additional therapeutic agent to a cell, tissue, or subject is effective to prevent or ameliorate a disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject. A therapeutically effective dose further refers to that amount of the therapeutic agent sufficient to result in amelioration of symptoms, *e.g.*,  
5 treatment, healing, prevention or amelioration of the relevant medical condition, or an increase in rate of treatment, healing, prevention or amelioration of such conditions. When applied to an individual active ingredient administered alone, a therapeutically effective dose refers to that ingredient alone. When applied to a combination, a therapeutically effective dose refers to combined amounts of the active ingredients that  
10 result in the therapeutic effect, whether administered in combination, serially or simultaneously. In some embodiment, “an effective amount of a compound for treating a particular disease” is an amount that is sufficient to ameliorate, or in some manner reduce the symptoms associated with the disease. Such amount may be administered as a single dosage or may be administered according to a regimen, whereby it is effective. The  
15 amount may cure the disease but, typically, is administered in order to ameliorate the symptoms of the disease. Repeated administration may be required to achieve the desired amelioration of symptoms.

[0099] The term “combination” refers to either a fixed combination in one dosage unit form, or a kit of parts for the combined administration where a compound and a  
20 combination partner (*e.g.*, another drug as explained below, also referred to as “therapeutic agent” or “co-agent”) may be administered independently at the same time or separately within time intervals, especially where these time intervals allow that the combination partners show a cooperative, *e.g.*, synergistic effect. The terms “co-administration” or “combined administration” or the like as utilized herein are meant to  
25 encompass administration of the selected combination partner to a single subject in need thereof (*e.g.*, a patient), and are intended to include treatment regimens in which the agents are not necessarily administered by the same route of administration or at the same time. The term “pharmaceutical combination” as used herein means a product that results from the mixing or combining of more than one active ingredient and includes  
30 both fixed and non-fixed combinations of the active ingredients. The term “fixed combination” means that the active ingredients, *e.g.*, a compound and a combination

partner, are both administered to a patient simultaneously in the form of a single entity or dosage. The term “non-fixed combination” means that the active ingredients, *e.g.*, a compound and a combination partner, are both administered to a patient as separate entities either simultaneously, concurrently or sequentially with no specific time limits, 5 wherein such administration provides therapeutically effective levels of the two compounds in the body of the patient. The latter also applies to cocktail therapy, *e.g.*, the administration of three or more active ingredients.

[00100] As used herein, “biological sample” refers to any sample obtained from a living or viral source or other source of macromolecules and biomolecules, and includes 10 any cell type or tissue of a subject from which nucleic acid or protein or other macromolecule can be obtained. The biological sample can be a sample obtained directly from a biological source or a sample that is processed. For example, isolated nucleic acids that are amplified constitute a biological sample. Biological samples include, but are not limited to, body fluids, such as blood, plasma, serum, cerebrospinal 15 fluid, synovial fluid, urine and sweat, tissue and organ samples from animals and plants and processed samples derived therefrom.

[00101] The terms “level” or “levels” are used to refer to the presence and/or amount of a target, *e.g.*, a protein or polynucleotide, and can be determined qualitatively or quantitatively. A “qualitative” change in the target, protein or polynucleotide level 20 refers to the appearance or disappearance of a target, protein or polynucleotide that is not detectable or is present in samples obtained from normal controls. A “quantitative” change in the levels of one or more targets, proteins or polynucleotides refers to a measurable increase or decrease in the target, protein or polynucleotide levels when compared to a healthy control.

25 [00102] A “healthy control” or “normal control” is a biological sample taken from an individual who does not suffer from a disease or disorder associated with abnormally high level of IFP35 and/or NMI. A “negative control” is a sample that lacks any of the specific analyte the assay is designed to detect and thus provides a reference baseline for the assay.

[00103] As used herein, “mammal” refers to any of the mammalian class of species. Frequently, the term “mammal,” as used herein, refers to humans, human subjects or human patients. “Mammal” also refers to any of the non-human mammalian class of species, *e.g.*, experimental, companion or economic non-human mammals.

5 Exemplary non-human mammals include mice, rats, rabbits, cats, dogs, pigs, cattle, sheep, goats, horses, monkeys, Gorillas and chimpanzees.

[00104] As used herein, “production by recombinant means” refers to production methods that use recombinant nucleic acid methods that rely on well-known methods of molecular biology for expressing proteins encoded by cloned nucleic acids.

10 [00105] As used herein, the term “subject” is not limited to a specific species or sample type. For example, the term “subject” may refer to a patient, and frequently a human patient. However, this term is not limited to humans and thus encompasses a variety of non-human animal or mammalian species.

[00106] As used herein, a “prodrug” is a compound that, upon *in vivo*  
15 administration, is metabolized or otherwise converted to the biologically, pharmaceutically or therapeutically active form of the compound. To produce a prodrug, the pharmaceutically active compound is modified such that the active compound will be regenerated by metabolic processes. The prodrug may be designed to alter the metabolic stability or the transport characteristics of a drug, to mask side effects or toxicity, to  
20 improve the flavor of a drug or to alter other characteristics or properties of a drug. By virtue of knowledge of pharmacodynamic processes and drug metabolism *in vivo*, those of skill in this art, once a pharmaceutically active compound is known, can design prodrugs of the compound (*see, e.g.*, Nogrady (1985) Medicinal Chemistry A Biochemical Approach, Oxford University Press, New York, pages 388-392).

25 [00107] As used herein, “test substance (or candidate compound)” refers to a chemically defined compound (*e.g.*, organic molecules, inorganic molecules, organic/inorganic molecules, proteins, peptides, nucleic acids, oligonucleotides, lipids, polysaccharides, saccharides, or hybrids among these molecules such as glycoproteins, etc.) or mixtures of compounds (*e.g.*, a library of test compounds, natural extracts or

culture supernatants, etc.) whose effect on IFP35 and/or NMI is determined by the disclosed and/or claimed methods herein.

5       **[00108]** As used herein, high-throughput screening (HTS) refers to processes that test a large number of samples, such as samples of diverse chemical structures against disease targets to identify “hits” (*see, e.g.,* Broach, *et al.*, High throughput screening for drug discovery, *Nature*, 384:14-16 (1996); Janzen, *et al.*, High throughput screening as a discovery tool in the pharmaceutical industry, *Lab Robotics Automation*: 8261-265 (1996); Fernandes, P.B., Letter from the society president, *J. Biomol. Screening*, 2:1 (1997); Burbaum, *et al.*, New technologies for high-throughput screening, *Curr. Opin. Chem. Biol.*, 1:72-78 (1997)). HTS operations are highly automated and computerized to handle sample preparation, assay procedures and the subsequent processing of large volumes of data.

**[00109]** It is understood that aspects and embodiments of the invention described herein include “consisting” and/or “consisting essentially of” aspects and embodiments.

15       **[00110]** Throughout this disclosure, various aspects of this invention are presented in a range format. It should be understood that the description in range format is merely for convenience and brevity and should not be construed as an inflexible limitation on the scope of the invention. Accordingly, the description of a range should be considered to have specifically disclosed all the possible sub-ranges as well as individual numerical values within that range. For example, description of a range such as from 1 to 6 should be considered to have specifically disclosed sub-ranges such as from 1 to 3, from 1 to 4, from 1 to 5, from 2 to 4, from 2 to 6, from 3 to 6 etc., as well as individual numbers within that range, for example, 1, 2, 3, 4, 5, and 6. This applies regardless of the breadth of the range.

25       **[00111]** Other objects, advantages and features of the present invention will become apparent from the following specification taken in conjunction with the accompanying drawings.

### C、METHODS FOR TREATING AND/OR PREVENTING A DISEASE OR DISORDER ASSOCIATED WITH ABNORMALLY HIGH LEVEL AND/OR ACTIVITY OF THE IFP35 FAMILY OF PROTEINS

[00112] The IFP35 family proteins, including IFP35 and NMI, can be rapidly up-regulated by type I or type II interferon in numerous immune cells. Yang et al., PLoS One 7, e50932 (2012); Das et al., Journal of Virology 88, 3103-3113 (2014); Zhu et al., Cell 96, 121-130 (1999); and Lebrun et al., Journal of Interferon & Cytokine Research 18, 767-771 (1998). The functions of IFP35 family members are not clear. IFP35 family members are predicted to consist of a Leucine-zipper (L-zip) domain in their N-termini, followed by two tandem structural and functional unknown NMI/IFP35 domains (NIDs). In the early report, people found IFP35 and NMI located in the cytoplasm using immunofluorescence microscopy. Lebrun et al., Journal of Interferon & Cytokine Research 18, 767-771 (1998). They could assemble into high molecular mass complex (HMMC) mediated by their NID domains and further into functional unknown speckle-like aggregations. Zhou et al., JBC 275, 21364-21371 (2000); and Chen et al., JBC 275, 36278-84 (2000). It was known that IFP35 could recognize specific viral nucleic acids from bovine foamy virus, and inhibit the virus transcription. Tan et al., Journal of Virology 82, 4275-4283 (2008). However, recent results suggested that it could support vesicular stomatitis virus replication, by specifically interacted with RIG-1 (retinoic acid-inducible gene I) and negatively regulated the host innate immune response. Das et al., Journal of Virology 88, 3103-3113 (2014). Investigations of NMI mainly focused on its inhibitory effects on the proliferation and metastasis of cancer cells, by regulating multiple signaling pathways. Li et al., Mol Biol Cell 23, 4635-4646 (2012); Fillmore et al., International Journal of Cancer 125, 556-64 (2009); and Li et al., JBC 277, 20965-73 (2002). To further explore the potential functions and mechanisms of IFP35 family members, the inventors determined the X-ray crystallography structure of the NID domain in IFP35. It was found that IFP35 and NMI could serve as DAMPs for immune modulation. Some DAMP proteins were reported to be recognized by specific cell-surface receptor, TLR4, with the help of MD2 and other associated proteins. See Yang et al., PNAS 107, 11942-11947 (2010); Nagai et al., Nature Immunology 3, 667-672 (2002); and Zanoni et al., Cell 147, 868-880 (2011). A complex signal cascade can be triggered to activate the transcription factor NF- $\kappa$ B, resulting in cytokines release and enhanced host

inflammatory response. *See* Meylan et al., *Nature Immunology* 5, 503-507 (2004); Moynagh, *Trends in Immunology* 26, 469-476 (2005); and Lu et al., *Cytokine* 42, 145-151 (2008).

[00113] In some aspects, disclosed herein is a use of a truncated IFP35 protein (e.g., octamer of the truncated protein) or a truncated NMI protein in preparation of an agent for regulating the inflammatory response. In some aspects, disclosed herein is a use of a truncated IFP35 protein (e.g., octamer of the truncated protein) or a truncated NMI protein in preparation of antineoplastic products. In some aspects, by using a IFP35 antibody or NMI antibody to neutralize IFP35 or NMI in cells or the humoral fluids, it can effectively regulate IFP35 or NMI protein overexpression-induced excessive inflammatory response, inhibit inflammatory effect, avoid the generation of body and tissue damage by inflammation and dramatically improve the survival rate of a subject, such as a subject with a bacterial or viral infection or autoimmune disease. In some embodiments, the subject is with a viral infection (such as influenza virus, SARS, MERS, HBV, HCV), bacterial infection (such as *Mycobacterium tuberculosis*), fungal infection, and/or infection caused by other pathogens. In some aspects, the infections provoke expression of a IFP35 family protein, such as IFP35 and/or NMI expression. Overexpression of IFP35 and/or NMI in the infected patients may lead to severe damage of their organs and bodies. Abnormally high level of IFP35 may lead to tissue or organ damage because of provoking of cytokine storm.

[00114] Thus, the present compositions and/or methods can be used to treat, ameliorate, and/or prevent a number of infectious diseases, infection states, inflammation, autoimmune disease, graft-versus-host disease, or conditions associated with over-activation of the immune system in a subject. Pathogenic viruses include, but are not limited to, Retroviridae (e.g., human immunodeficiency viruses, such as HIV-1 (also referred to as HTLV-III, LAV or HTLV-III/LAV, or HIV-III); and other isolates, such as HIV-LP; Picornaviridae (e.g., polio viruses, hepatitis A virus; enteroviruses, human coxsackie viruses, rhinoviruses, echoviruses); Calciviridae (e.g., strains that cause gastroenteritis); Togaviridae (e.g., equine encephalitis viruses, rubella viruses); Flaviridae (e.g., dengue viruses, encephalitis viruses, yellow fever viruses); Coronaviridae (e.g., coronaviruses); Rhabdoviridae (e.g., vesicular stomatitis viruses,

rabies viruses); *Filoviridae* (e.g., ebola viruses); *Paramyxoviridae* (e.g., parainfluenza viruses, mumps virus, measles virus, respiratory syncytial virus); *Orthomyxoviridae* (e.g., influenza viruses); *Bunyaviridae* (e.g., Hantaan viruses, bunya viruses, phleboviruses and Nairo viruses); *Arena viridae* (hemorrhagic fever viruses); *Reoviridae* (e.g., reoviruses, orbiviruses and rotaviruses); *Bimaviridae*; *Hepadnaviridae* (Hepatitis B virus); *Parvoviridae* (parvoviruses); *Papovaviridae* (papilloma viruses, polyoma viruses); *Adenoviridae* (most adenoviruses); *Herpesviridae* (herpes simplex virus (HSV) 1 and 2, varicella zoster virus, cytomegalovirus (CMV), herpes viruses); *Poxviridae* (variola viruses, vaccinia viruses, pox viruses); and *Iridoviridae* (e.g., African swine fever virus); Hepatitis C virus; and unclassified viruses (e.g., the agent of delta hepatitis (thought to be a defective satellite of hepatitis B virus); Norwalk and related viruses, and astroviruses).

**[00115]** Pathogenic bacteria include, but are not limited to, *Helicobacter pylori*, *Borrelia burgdorferi*, *Legionella pneumophila*, *Mycobacteria* sps (e.g. *M. tuberculosis*, *M. avium*, *M. intracellulare*, *M. kansasii*, *M. goodii*), *Staphylococcus aureus*, *Neisseria gonorrhoeae*, *Neisseria meningitidis*, *Listeria monocytogenes*, *Streptococcus pyogenes* (Group A *Streptococcus*), *Streptococcus agalactiae* (Group B *Streptococcus*), *Streptococcus* (viridans group), *Streptococcus faecalis*, *Streptococcus bovis*, *Streptococcus* (anaerobic sps.), *Streptococcus pneumoniae*, pathogenic *Campylobacter* sp., *Enterococcus* sp., *Haemophilus influenzae*, *Bacillus anthracis*, *Corynebacterium diphtheriae*, *Corynebacterium* sp., *Erysipelothrix rhusiopathiae*, *Clostridium perfringens*, *Clostridium tetani*, *Enterobacter aerogenes*, *Klebsiella pneumoniae*, *Pasteurella multocida*, *Bacteroides* sp., *Fusobacterium nucleatum*, pathogenic strains of *Escherichia coli*, *Streptobacillus moniliformis*, *Treponema pallidum*, *Treponema pertenue*, *Leptospira*, and *Actinomyces israelii*.

**[00116]** Infectious fungi include, but are not limited to, *Cryptococcus neoformans*, *Histoplasma capsulatum*, *Coccidioides immitis*, *Blastomyces dermatitidis*, *Chlamydia trachomatis*, *Candida albicans*.

**[00117]** Infectious protozoa include, but are not limited to, *Plasmodium* spp., e.g., *Plasmodium falciparum*; Trypanosomes, e.g., *Trypanosoma cruzi*; and *Toxoplasma gondii*.

[00118] Allergens include, but are not limited to, pollens, insect venoms, animal dander dust, fungal spores and drugs (e.g. penicillin). Examples of natural, animal and plant allergens include proteins specific to the following genera: Canine (*Canis familiaris*); *Dermatophagoides* (e.g. *Dermatophagoides farinae*); *Felis* (*Felis domesticus*); *Ambrosia* (*Ambrosia artemisiifolia*; *Lolium* (e.g. *Lolium perenne* or *Lolium multiflorum*); *Cryptomeria* (*Cryptomeria japonica*); *Alternaria* (*Alternaria alternata*); Alder; *Alnus* (*Alnus gultinosa*); *Betula* (*Betula verrucosa*); *Quercus* (*Quercus alba*); *Olea* (*Olea europa*); *Artemisia* (*Artemisia vulgaris*); *Plantago* (e.g. *Plantago lanceolata*); *Parietaria* (e.g. *Parietaria officinalis* or *Parietaria judaica*); *Blattella* (e.g. *Blattella germanica*); *Apis* (e.g. *Apis multiflorum*); *Cupressus* (e.g. *Cupressus sempervirens*, *Cupressus arizonica* and *Cupressus macrocarpa*); *Juniperus* (e.g. *Juniperus sabinoides*, *Juniperus virginiana*, *Juniperus communis* and *Juniperus ashei*); *Thuya* (e.g. *Thuya orientalis*); *Chamaecyparis* (e.g. *Chamaecyparis obtusa*); *Periplaneta* (e.g. *Periplaneta americana*); *Agropyron* (e.g. *Agropyron repens*); *Secale* (e.g. *Secale cereale*); *Triticum* (e.g. *Triticum aestivum*); *Dactylis* (e.g. *Dactylis glomerata*); *Festuca* (e.g. *Festuca elatior*); *Poa* (e.g. *Poa pratensis* or *Poa compressa*); *Avena* (e.g. *Avena sativa*); *Holcus* (e.g. *Holcus lanatus*); *Anthoxanthum* (e.g. *Anthoxanthum odoratum*); *Arrhenatherum* (e.g. *Arrhenatherum elatius*); *Agrostis* (e.g. *Agrostis alba*); *Phleum* (e.g. *Phleum pratense*); *Phalaris* (e.g. *Phalaris arundinacea*); *Paspalum* (e.g. *Paspalum notatum*); *Sorghum* (e.g. *Sorghum halepensis*); and *Bromus* (e.g. *Bromus inermis*). Use of epitopes from the above allergens in the present methods for antibody detection and analysis is also envisaged.

[00119] In some aspects, the present compositions and/or methods can also be used for relieving disease-induced or associated suppression of a subject's immune system, such as cancer-induced or associated suppression of the subject's immune system. For example, by administering a IFP35 family protein or analog or derivative therefore, the subject's immune response can be activated and/or augmented in order to overcome the disease-causing vector's ability to evade an immune reaction. This therapeutic approach is applicable to disease states whereby immune system suppression has been demonstrated, such as bacterial infections, parasitic infections including malaria and

typanosomiasis, viral infections, peptic ulcers and gastric cancer due to *H. Pylori* infection together with prevention of pregnancy.

[00120] In some aspects, provided herein are the amino acid residues that are involved in binding with a IFP35 receptor or an antagonist antibody against IFP35. In one aspect, the domain-swapping dimer form an arc intersecting surface area, and the dimer provides some residues such as Ser145, Asp172, Val173, Leu177, Arg212, Gln199, Gln207, Gln208, Pro210, Ser214, Thr201, and Tyr216 to form a large exposed surface as shown in **Fig. 16A**. Among the residues, residues Glu150, Glu175, Leu177, Gln207, and Gln208 are in a more prominent position (**Fig. 16A**). Consequently, they are more likely to bind the receptor or antibody.

[00121] In some aspects, other residues on the inner surface of the ring structure formed by the IFP5-NID octamer participate in the interaction with other proteins. These residues can include Ser145, Arg147, Glu150, Glu151, Val173, Gly206, Gln207, and Gln208. In some aspects, Arg147, Gln207, Gln208, Glu150, and Glu151 provide extended side chains that protrude from the inner surface of octamer ring structure (**Fig. 16B**).

[00122] Based on the structure of the dimer or the octamer, there are some relatively large amino acid residues near the top of the amino terminus and the carboxyl terminus of the  $\beta$  sheet barrel-like structure of the single monomer or domain-swapping monomer; these relatively large amino acid residues extend outwards. These residues can include Arg187, Glu188, Gln192, Gln196, Arg212, and Tyr216, and they are close in distance. Furthermore, some amino acid residues may participate in binding to other proteins, antibodies, or small molecules (**Fig. 16C**).

[00123] These residues above are located on the surface of the structure. In some embodiments, these residues participate in binding with the receptor or the antibody and are the key position for drug inhibition.

[00124] In some aspects, the present inventors have expressed, purified, and crystalized IFP35 and NMI, and have also determined the structure of one fragment of IFP35. The fragment of IFP35 can induce inflammatory response and further IFP35 and NMI can be secreted out from the cell to stimulate intense inflammatory response. It can

be effective to control the excessive inflammatory response caused by the excessive secretory expression of IFP35 or NMI through neutralization of IFP 35 or NMI in cell solution or body fluids using a IFP35 antibody or a NMI antibody. In some aspects, the present disclosure avoids the damage of the body and the tissue and raises the survival rates of the subjects. The results indicate that a disease or condition associated with the excessive expression of IFP35 and NMI, such as bacterial infections, virus invasions, autoimmune diseases, tumor, and other infections, may be controlled by the reduction of the concentration of IFP35 and/or NMI. Meanwhile, diseases caused by the defect or deficiency of the expression and/or procession (such as secretion) of IFP35 and/or NMI may be improved through the addition of the proteins.

**[00125]** Below is a sequence alignment of human IFP35 (hIFP), mouse IFP35 (mIFP), human NMI (hNMI) and mouse NMI (mNMI), using CLUSTAL 2.1 multiple sequence alignment.

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15 hNMI      MEADKDDTQQILKEHSPD-EFIKDEQNKGLIDEITKKNIQLKKEIQKLETELQEATKEFQ 59
   mNMI      MDADKDNIKQACDERSAEMDDMRGEQSMGLVHEIMSENKELDEEIKKLEAELQSDAREFQ 60
   hIFP      -----MSAPLDAALHALQEEQARLKMRLWDLQQLRKELGDSPK 38
   mIFP      -----MSVTIQTVLYSLQEEQARLKMRLQELQQLKRERTGSPG 38
      :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :
20 hNMI      IKEDIPETKMKFLSVETPENDSQLSNISCSFQVSSKVPYEQKQALITFEKEEVAQN 119
   mNMI      IKENVPEKKLKLTSVESPKDGCDFSNSSCSFQVSSQILYELQEGQALITFEKEEVAQN 120
   hIFP      DKVPFVSPKIPLVFRGHTQQDPEVPKSLVS---NLRHCPPLLAGSALITFDDPKVAEQVL 95
   mIFP      AKIPFSVPEVPLVFQGGTKQGRQVPKFVVS---NLKVCCPLPEGSALVTFEDPKVVDRL 95
      *  ..  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :
25 hNMI      SMSKHHVQIKDVNLEVTAKPVPVLSGVRQVY--VEVSKMKINVTEIPD--TLREDQMRD 175
   mNMI      SMGNHVVQMEGTPVKVSAHPVPLNTGVRQVH--VDISKMKINVTGIPD--ELSEEQTRD 176
   hIFP      QQKEHTINMEECRLRVQVQPLELPMVTTIQVMMSSQLSGRRVLVTGFPASLRLSEELLD 155
   mIFP      QQKEHRVNLEDCLRVQVQPLELPMVTNIQV--SSQPDNHRVLVSGFPAGLRLSEELLD 153
      .  :  *  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :
30 hNMI      KLELSFSKSRNGGGEVDRVDYDRQSSAVITFVEIGVADKILKKKEYPLYINQTC 235
   mNMI      KLELSFCKSRNGGGEVESVDYDRKSRSAVITFVETGVVDKILKKKTYPLYMNQKCHSV 236
   hIFP      KLEIFFGKTRNGGGEVDVDR--ELLPGSVMLGFARDGVAQRQCIGQFTVPLGGQVPLRV 213
   mIFP      KLEIFFGKAKNGGGEVDVETR--EMLQGTVMLGFADEEVAQHLCQIGQFRVPLDRQQV 211
      ***  *  *  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :
35 hNMI      SPYTEIHLKKYQIFSGTSKRTVLLTGMIEGIQMDDEEIVEDLINIHFQRAKNGGGEVDVVK 295
   mNMI      SPCIERCLEKYQVFSAVSKKTVLLTGLEGIPVDEETGEDLLNIHFQKNNNGGGEVEVVK 296
   hIFP      SPYVNGEIQKAEIRSQPVPRSVLVLNIPDI-LDGPVLHDVLEIHFQKPTRGGGEVEALT 272
   mIFP      SPYVSGEIQKAEIKFQQAPHSVLVTNIPDV-MDAQELHDILEIHFQKPTRGGGEVEALT 270
      **  .  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :  :
40 hNMI      S-LGQPHIAYFEE----- 307
   mNMI      S-LDQSFAAYFKEEARETI 314
   hIFP      VPQGQQLAVFTSESG--- 288
   mIFP      VPSGQQLAIFTSESS--- 286
      .  *  *  *  .

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**[00126]** In some embodiments, provided herein is a method of using a IFP35 family protein in provoking an immune response. In another embodiment, provided herein is a method of inhibiting and/or reducing a IFP35 family protein, such as IFP35 and NMI, in order to inhibit cytokine storm, such as by infection of bacteria, viruses or

organ damaging induced by abnormal high level of IFP35/NMI by food or drug. The organ may include lung, kidney, liver or others organs.

5       **[00127]** In some embodiments, provided herein is an antagonist compound for a IFP35 family protein, such as an antibody or a small molecule compound, for treating or preventing a disease or condition associated with or caused by abnormal levels of the IFP35 family protein.

10       **[00128]** In other embodiments, provided herein is a method for applying the crystal structure method for further designing and/or selecting an antibody or compound. In one aspect, the structure is used to see how drugs or antibody binds to the target protein, and then the antibody or compound can be further modified. From the target protein/antibody co-crystal structure, epitope of the target protein can also be identified.

15       **[00129]** Embodiment 1: Application of truncated IFP35 protein in preparing reagents/products to provoke immune response and inflammation or in preparing anti-tumor products, wherein said truncated IFP35 is human IFP35 or mouse IFP35, wherein said truncated human IFP35 is as 1) or 2) below:

**[00130]** 1)       protein with residues as in SEQ ID NO: 2, from residues 136-216;

**[00131]** 2)       said protein sequence as in 1), wherein 1-10 additional residues are added to the sequence's amino or/and carboxyl terminus, and the sequence homology is at least about 90% to the sequence of 1);

20       **[00132]** wherein said truncated mouse IFP35 is as 3) or 4) below:

**[00133]** 3)       protein with residues as in SEQ ID NO: 4, from residues 134-216;

**[00134]** 4)       said protein sequence as in 3), wherein 1-10 additional residues are added to the sequence's amino or/and carboxyl terminus, and the sequence homology is at least about 90% to the sequence of 3).

25       **[00135]** Embodiment 2:       A method of Embodiment 1, wherein the truncated human IFP35 protein as shown in SEQ ID NO: 2, from residues 124-220.

**[00136]** Embodiment 3:       A method in preparing products to provoke immune response/inflammation by IFP35 protein or in preparing products to against tumor/cancer, wherein said sequence of IFP35 protein is shown as in SEQ ID NO: 2 or SEQ ID NO: 4.

[00137] Embodiment 4: A method in preparing products to provoke immune response/inflammation by IFP35 mutant proteins or in preparing products to against tumor/cancer, wherein said IFP35 mutant protein has at least one mutation and/or modification of a residue involved in binding a IFP35 receptor or an inhibitory antibody, which mutation and/or modification leads to reduced or no binding of IFP35 to the IFP35 receptor or inhibitory antibody, wherein said residue involved in receptor binding/antibody binding is Ser145, Asp172, Val 173, Leu 177, Arg212, Gln199, Gln207, Gln 208, Pro210, Ser214, Thr201, Tyr216, Glu150, Glu175, Gln208, Arg147, Glu151, or Gly206, or any combination thereof. According to the structure comparison results, corresponding position residues that are in sequences from other sources of IFP35 and NMI are within the present disclosure. According to the structure comparison results, IFP35 and NMI both have two NID domains, these two NID domains are homologs to each other, therefore, corresponding NID region residues of IFP35 and NMI outside the structure determined IFP35 NID domain are within the present disclosure.

[00138] Embodiment 5: The method according to any of Embodiments 1-4, wherein the method induces immune response/inflammation to increase expression of inflammation factors, recruitments of neutrophils or stimulate NF- $\kappa$ B pathway, wherein said inflammation factors include: IL-1 $\beta$ , TNF- $\alpha$ , iNOS, or CD86, and wherein said stimulating NF- $\kappa$ B pathway is to increase I $\kappa$ B $\alpha$  to reduce the total I $\kappa$ B $\alpha$  amount.

[00139] Embodiment 6: A method to inhibit diseases by abnormal high amount of IFP35 induced over immune response or application of product that inhibit IFP35 protein to inhibit inflammation factor expression/reaction.

[00140] Embodiment 7: The method of Embodiment 6, wherein said inhibitory product or reagent is a IFP35 antibody that inhibits IFP35 protein activity, and/or wherein the antibody is monoclonal or polyclonal, and/or wherein said disease is sepsis, and/or wherein said inflammation factors include: IL-1 $\beta$ , TNF- $\alpha$ , iNOS, or CD86.

[00141] Embodiment 8: Use of a truncated NMI protein in preparing reagents/products to provoke immune response and inflammation or in preparing anti-tumor products, wherein said truncated NMI is truncated human NMI or mouse NMI, wherein said truncated human NMI protein has a sequence set forth in SEQ ID NO: 8,

from residues 155-240, and said truncated mouse NMI protein has a sequence set forth in SEQ ID NO: 6, from residues 151-250.

5       **[00142]** Embodiment 9:       A method in preparing products to provoke immune response/inflammation by NMI protein or in preparing products to against tumor/cancer, wherein said NMI protein is human or mouse NMI protein, said sequence of human NMI is set forth in SEQ ID NO: 8, or said sequence of mouse IFP35 is set forth in SEQ ID NO: 6.

10       **[00143]** Embodiment 10:       A method in preparing products to provoke immune response/inflammation by NMI mutant proteins or in preparing products to against tumor/cancer, wherein said NMI mutant protein is that involved residues are mutated, leading to no binding of NMI to NMI receptor or inhibitory antibody.

15       **[00144]** Embodiment 11:       The method according to any of Embodiments 8-11, wherein said provoking the immune response/inflammation stimulates inflammation factors expression and/or stimulates NF- $\kappa$ B pathway signaling, wherein said inflammation factors include: IL-1 $\beta$ , TNF- $\alpha$ , iNOS, or CD86, and wherein said stimulating NF- $\kappa$ B pathway is to increase I $\kappa$ B $\alpha$  to reduce the total I $\kappa$ B $\alpha$  amount.

20       **[00145]** Embodiment 12:       A method of preparing a product that inhibits NMI protein activity to treat diseases induced by abnormal high expression of NMI or a product that inhibits NMI to inhibit inflammation factors expression.

25       **[00146]** Embodiment 13:       The method according to Embodiment 12, wherein said product is a NMI antibody, optionally wherein said antibody is a monoclonal or polyclonal antibody, optionally wherein said disease is sepsis, optionally wherein said inflammation factors include: IL-1 $\beta$ , TNF- $\alpha$ , iNOS, or CD86.

**[00147]** Embodiment 14:       A method to over-express and crystallize truncated IFP35 protein, comprising:

**[00148]** 1)       Using bacteria cells to express the truncated protein as said in Embodiment 1;

**[00149]** 2)       Purifying said truncated IFP35 protein;

**[00150]** 3)       Crystalizing the purified truncated protein.

[00151] Embodiment 15: The method according to Embodiment 14, further comprising: cloning the truncated IFP35 NID fragment genes to a vector (e.g., pGEX-6p-1 vector) in order to express a N terminal GST-tagged fusion protein (GST-IFP35-NID), then transforming this plasmid vector to an *E.coli* cell, after IPTG induction, then  
5 collecting bacteria for purification, wherein said purification step comprises: an affinity chromatography (glutathione column) step, removing of GST fusion tag by enzyme, and/or an ion exchange column step, and/or a gel filtration column step.

[00152] Embodiment 16: A method to crystalize NMI protein or its truncations, comprising:

10 [00153] 1) Expressing the NMI truncation proteins described as in Embodiment 8 in eukaryotic cells;

[00154] 2) Purifying these truncated proteins;

[00155] 3) Crystallizing these proteins.

[00156] Embodiment 17: The method according to Embodiment 14, further  
15 comprising: cloning the truncated NMI NID fragment genes to a vector (e.g., pGEX-6p-1 vector) in order to express a N terminal GST-tagged fusion protein (GST-NMI-NID), then transforming this plasmid vector to an *E.coli* cell, after IPTG induction, then collecting bacteria for purification, wherein said purification step comprises: an affinity chromatography (glutathione column) step, removing of GST fusion tag by enzyme,  
20 and/or an ion exchange column step, and/or a gel filtration column step.

[00157] Embodiment 18: A method of designing or modifying a IFP35 family protein, such as IFP35 and NMI, in order to treat tumor, immune deficient diseases, etc., by targeting the IFP35 family protein to treat the disease.

[00158] Embodiment 19: A structure having a root mean square deviation  
25 (RMSD) in its core region less than about 1.5 anstrom to the IFP35-NID structure disclosed herein, according to the atom coordinates of the IFP35-NID crystal structure disclosed herein.

[00159] Embodiment 20. An atomic level structure having a root mean square deviation (RMSD) less than 1.5 Å to the core region of IFP35-NID domain (includes residues 136-216).

[00160] Embodiment 21. A IFP35 antibody, 1D7, produced against human IFP35 in mouse, and deposited in China General Microbiological Culture Collection Center (CGMCC) under CGMCC 9573.

[00161] Embodiment 22. A IFP35 truncation protein having a human or mouse origin, wherein said human IFP35 truncation is:

[00162] 1) A protein with sequence as shown in SEQ ID NO: 4, from residues 134-216; or

[00163] 2) A protein with sequences same to 1) but with additional 1-10 residues at its amino or carboxyl terminus, wherein the homology of the protein to the protein in 1) is at least about 90%.

[00164] Embodiment 23. A IFP35 family protein having a mutation at a residue involved in binding of the IFP35 family protein to a receptor or a neutralizing antibody, wherein the mutation disrupts or reduces binding to the receptor or neutralizing antibody, wherein the residue is: Ser145, Asp172, Val 173, Leu 177, Arg212, Gln199, Gln207, Gln 208, Pro210, Ser214, Thr201, Tyr216, Glu150, Glu175, Gln208, Arg147, Glu151, or/and Gly206 of human IFP set forth in SEQ ID NO: 2, or a residue in the IFP35 family protein that corresponds to the listed residue of SEQ ID NO: 2.

[00165] Embodiment 25. A NMI truncation protein from residues 155-240 (for human NMI set forth in SEQ ID NO: 8) and from residues 151-250 (for mouse NMI set forth in SEQ ID NO: 6).

#### **D、PHARMACEUTICAL COMPOSITIONS FOR TREATING AND/OR PREVENTING A DISEASE OR DISORDER ASSOCIATED WITH ABNORMALLY HIGH LEVEL AND/OR ACTIVITY OF IFP35 AND/OR NMI**

[00166] In another aspect, the present disclosure provides for a pharmaceutical composition for treating and/or preventing a disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject, which pharmaceutical

composition comprises an effective amount of an agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in a subject and a pharmaceutically acceptable carrier or excipient.

5       **[00167]** The present pharmaceutical compositions can be used to treat and/or prevent any suitable disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject.

10       **[00168]** In some embodiments, the present pharmaceutical compositions can be used to treat a disease or disorder associated with abnormally high level of IFP35 and/or NMI. In other embodiments, the present pharmaceutical compositions can be used to prevent a disease or disorder associated with abnormally high level of IFP35 and/or NMI.

15       **[00169]** Any suitable agents can be used in the present pharmaceutical compositions to treat and/or prevent any suitable disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject. For example, a suitable agent can be used to reduce copy number of IFP35 and/or NMI gene, to block or reduce replication of IFP35 and/or NMI gene, to block or reduce transcription of IFP35 and/or NMI gene, to block or reduce translation of IFP35 and/or NMI mRNA, and/or to inhibit one, some or all activities of IFP35 and/or NMI. In some embodiments, the agent comprises a polynucleotide (such as an siRNA, shRNA, or miRNA) targeting the gene encoding IFP35 and/or NMI. The siRNA can target any suitable portion of the IFP35 and/or NMI gene. For example, the siRNA can target a portion of the IFP35 and/or NMI gene that encodes one or more NIDs. In other embodiments, the agent comprises an antisense RNA targeting the gene encoding IFP35 and/or NMI. The antisense RNA can target any suitable portion of the IFP35 and/or NMI gene.

25       **[00170]** In still other embodiments, the agent inhibits or modifies a nuclear factor that controls IFP35 and/or NMI transcription. Any suitable agent that inhibits or modifies a nuclear factor that controls IFP35 and/or NMI transcription can be used in the present methods.

30       **[00171]** In yet other embodiments, the agent comprises an antibody that specifically binds to IFP35 and/or NMI. The antibody can specifically bind to any suitable portion of the IFP35 and/or NMI. For example, the antibody can specifically

bind to one or more NIDs of IFP35 and/or NMI. In another example, the antibody can specifically bind to a portion of IFP35 and/or NMI that interacts with the cellular IFP35 and/or NMI receptors.

**[00172]** In some aspects, disclosed herein is an antibody or antigen binding  
 5 fragment thereof that specifically binds to IFP35 and/or NMI, and the antibody or antigen binding fragment thereof comprises a heavy chain variable region comprising a complementarity determining region (CDR) consisting of the amino acid sequences of a CDR in the heavy chain variable region sequence set forth in SEQ ID NO: 9 and/or a  
 10 light chain variable region comprising a CDR consisting of the amino acid sequence of a CDR in the light chain variable region sequence set forth in SEQ ID NO:10. In one embodiment, the antibody or antigen binding fragment thereof comprises a heavy chain variable region set forth in SEQ ID NO: 9 and a light chain variable region set forth in SEQ ID NO:10. Conservative substitution(s) may be introduced into the CDRs and/or framework regions (FRs) of an antibody disclosed herein.

15 **[00173]** VQLVESGPELK KPGETVKISCKASGYTFTNYGM  
 NWVKQAPGKGLKWMGWINTYTGEPTFADDFKGRFAFSL  
 ETSASTAYLQINNLKNEDTATYFCARYGYSWAMDYWGQ  
 GTSVTVSSAST (SEQ ID NO: 9).

**[00174]** DIVMTQSPAIM SASPGEKVTMTCSASSSVSYMH  
 20 WYQQKSGTSPKRWIYDTSKLASGVPARFSGSGSGTSSSLT  
 ISSMEAEDAATYYCQQWSSNPPIITFGAGTKLEIK (SEQ  
 ID NO: 10).

**[00175]** In one aspect, disclosed herein is an isolated polynucleotide encoding an antibody or antigen binding fragment thereof that specifically binds to IFP35 and/or NMI.  
 25 In some embodiments, the antibody or antigen binding fragment thereof comprises a heavy chain variable region comprising a complementarity determining region (CDR) consisting of the amino acid sequence of a CDR in the heavy chain variable region sequence set forth in SEQ ID NO: 9 and/or a light chain variable region comprising a CDR consisting of the amino acid sequences of a CDR in the light chain variable region  
 30 sequence set forth in SEQ ID NO: 10. In some aspects, the antibody or antigen binding

fragment thereof comprises a heavy chain variable region set forth in SEQ ID NO: 9 and a light chain variable region set forth in SEQ ID NO:10. In other embodiments, the isolated polynucleotide comprises the nucleic acid sequence set forth in SEQ ID NO: 11 and/or SEQ ID NO: 12.

5       **[00176]** TGGTCGACGCTGAGGAGACGGTGACTGAGGTTCTTGACCCCA  
 GTAGTCCATAGCCCAAGAGTACCCGTATCTTGACAGAAATATGTAGCCGTG  
 TCCTCATTCTTGAGGTTGTTGATCTGCAAATAGGCAGTGCTGGCAGAGGTTTC  
 CAAAGAGAAGGCAAACCGTCCCTTGAAGTCATCAGCAAATGTTGGCTCTCCA  
 GTGTAGGTGTTTATCCAGCCCATCCACTTTAAACCCTTTCCTGGAGCCTGCTT  
 10   CACCCAGTTCATTCCATAGTTTGTGAAGGTATACCCAGAAGCCTTGCAGGAG  
 ATCTTGACTGTCTCTCCTGACTCCTTAAGCTGCACCT       (SEQ ID NO: 11).

**[00177]** GACATTGTGATGACCCAGTCTCCAGCAATCATGTCTGCATCTCC  
 AGGGGAGAAGGTCACCATGACCTGCAGTGCCAGCTCAAGTGTAAGTTACATG  
 CACTGGTACCAGCAGAAGTCAGGCACCTCCCCCAAAGATGGATTTATGACA  
 15   CATCCAAACTGGCTTCTGGAGTCCCTGCTCGCTTCAGTGGCAGTGGGTCTGGG  
 ACCTCTTACTCTCTCACAATCAGCAGCATGGAGGCTGAAGATGCTGCCACTT  
 ATTACTGCCAGCAGTGGAGTAGTAACCCACCCATCACGTTCGGTGCTGGCAC  
 CAAGCTGGAAATCAAA       (SEQ ID NO: 12).

**[00178]** The terms “complementarity determining region,” and “CDR,” are known  
 20   in the art to refer to non-contiguous sequences of amino acids within antibody variable  
 regions, which confer antigen specificity and binding affinity. In general, there are three  
 (3) CDRs in each heavy chain variable region (CDR-H1, CDR-H2, CDR-H3) and three  
 (3) CDRs in each light chain variable region (CDR-L1, CDR-L2, CDR-L3).

**[00179]** The precise amino acid sequence boundaries of a given CDR can be  
 25   readily determined using any of a number of well-known schemes, including those  
 described by Kabat *et al.* (1991), “Sequences of Proteins of Immunological Interest,” 5th  
 Ed. Public Health Service, National Institutes of Health, Bethesda, MD (“Kabat”  
 numbering scheme), Al-Lazikani *et al.*, (1997) JMB 273,927-948 (“Chothia” numbering  
 scheme), MacCallum *et al.*, J. Mol. Biol. 262:732-745 (1996), “Antibody-antigen  
 30   interactions: Contact analysis and binding site topography,” *J. Mol. Biol.* 262, 732-745.”

(Contact” numbering scheme), Lefranc MP *et al.*, “IMGT unique numbering for immunoglobulin and T cell receptor variable domains and Ig superfamily V-like domains,” *Dev Comp Immunol*, 2003 Jan;27(1):55-77 (“IMGT” numbering scheme), and Honegger A and Plückthun A, “Yet another numbering scheme for immunoglobulin variable domains: an automatic modeling and analysis tool,” *J Mol Biol*, 2001 Jun 8;309(3):657-70, (AHO numbering scheme).

[00180] The boundaries of a given CDR may vary depending on the scheme used for identification. For example, the Kabat scheme is based structural alignments, while the Chothia scheme is based on structural information. Numbering for both the Kabat and Chothia schemes is based upon the most common antibody region sequence lengths, with insertions accommodated by insertion letters, for example, “30a,” and deletions appearing in some antibodies. The two schemes place certain insertions and deletions (“indels”) at different positions, resulting in differential numbering. The Contact scheme is based on analysis of complex crystal structures and is similar in many respects to the Chothia numbering scheme.

[00181] Thus, unless otherwise specified, the terms “CDR” and “complementary determining region” of a given antibody or region thereof, such as a variable region, as well as individual CDRs (*e.g.*, “CDR-H1, CDR-H2) of the antibody or region thereof, should be understood to encompass the complementary determining region as defined by any of the known schemes described herein above.

[00182] As used herein, the term “conservative substitution” refers to substitutions of amino acids and/or amino acid sequences that are known to those of skill in this art and may be made generally without altering the biological activity of the resulting molecule. Those of skill in this art recognize that, in general, single amino acid substitutions in non-essential regions of a polypeptide do not substantially alter biological activity (see, *e.g.*, Watson, *et al.*, MOLECULAR BIOLOGY OF THE GENE, The Benjamin/Cummings Pub. Co., p. 224 (4th Edition 1987)). For example, such changes include substituting any of isoleucine (I), valine (V), and leucine (L) for any other of these hydrophobic amino acids; aspartic acid (D) for glutamic acid (E) and vice versa; glutamine (Q) for asparagine (N) and vice versa; and serine (S) for threonine (T) and vice versa. Other substitutions can also be considered conservative, depending on the

environment of the particular amino acid and its role in the three-dimensional structure of the protein. For example, glycine (G) and alanine (A) can frequently be interchangeable, as can alanine (A) and valine (V). Methionine (M), which is relatively hydrophobic, can frequently be interchanged with leucine and isoleucine, and sometimes with valine.

- 5 Lysine (K) and arginine (R) are frequently interchangeable in locations in which the significant feature of the amino acid residue is its charge and the differing pK's of these two amino acid residues are not significant. Still other changes can be considered "conservative" in particular environments (see, pages 13-15 "Biochemistry" 2nd ED. Lubert Stryer ed (Stanford University); Henikoff *et al.*, PNAS 1992 Vol 89 10915-10919; 10 Lei *et al.*, J Biol Chem 1995 May 19; 270(20):11882-6). Other substitutions are also permissible and may be determined empirically or in accord with known conservative substitutions.

- [00183] In yet other embodiments, the agent can comprise a variant form of IFP35 and/or NMI. Any suitable variant form of IFP35 and/or NMI can be used in the present 15 methods. For example, the variant form of IFP35 and/or NMI can be a mutant IFP35 and/or NMI and/or a fragment of IFP35 and/or NMI.

- [00184] The pharmaceutical compositions can be administered via any suitable route. For example, the pharmaceutical compositions can be administered via an oral, nasal, inhalational, parental, intravenous, intraperitoneal, subcutaneous, intramuscular, 20 intradermal, topical, or rectal route.

- [00185] In some embodiments, the present pharmaceutical compositions can further comprise another suitable therapeutic or preventive substance or treatment. For example, the pharmaceutical compositions can further comprise an effective amount of a drug for the treatment and/or prevention of a proliferation disorder, a neoplasm, a tumor 25 or a cancer in the subject.

[00186] The present pharmaceutical compositions can be used at any suitable amount or dosage. For example, the present pharmaceutical compositions can be administered at an amount that reduces production and/or an activity of IFP35 and/or NMI in the subject to a level that is substantially identical to a production and/or an

activity level of IFP35 and/or NMI in a comparable subject that does not have a disease or disorder associated with abnormally high level of IFP35 and/or NMI.

[00187] The present pharmaceutical compositions can be used to treat and/or prevent a disease or disorder in any suitable subject. For example, the subject can be a mammal. In some embodiments, the mammal is a human. In other embodiments, the subject is a non-human animal or non-human mammal, *e.g.*, experimental, companion or economic non-human animal or non-human mammal.

10 **E、USE OF AN EFFECTIVE AMOUNT OF AN AGENT THAT PREVENTS OR REDUCES PRODUCTION AND/OR AN ACTIVITY OF IFP35 AND/OR NMI IN A SUBJECT FOR THE MANUFACTURE OF A MEDICAMENT**

[00188] In still another aspect, the present disclosure provides for a use of an effective amount of an agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in a subject for the manufacture of a medicament for treating and/or preventing a disease or disorder associated with abnormally high level of IFP35 and/or NMI in said subject.

[00189] An agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in a subject can be used for the manufacture of a medicament for treating and/or preventing any suitable disease or disorder associated with abnormally high level of IFP35 and/or NMI in said subject.

[00190] In some embodiments, agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in a subject can be used for the manufacture of a medicament for treating any suitable disease or disorder associated with abnormally high level of IFP35 and/or NMI in said subject. In other embodiments, agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in a subject can be used for the manufacture of a medicament for preventing any suitable disease or disorder associated with abnormally high level of IFP35 and/or NMI in said subject.

[00191] Any suitable agents can be used for the manufacture of a medicament for treating any suitable disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject. For example, a suitable agent can be used to reduce copy number of IFP35 and/or NMI gene, to block or reduce replication of IFP35 and/or NMI

gene, to block or reduce transcription of IFP35 and/or NMI gene, to block or reduce translation of IFP35 and/or NMI mRNA, and/or to inhibit one, some or all activities of IFP35 and/or NMI. In some embodiments, the agent comprises an siRNA targeting the gene encoding IFP35 and/or NMI. The siRNA can target any suitable portion of the  
5 IFP35 and/or NMI gene. For example, the siRNA can target a portion of the IFP35 and/or NMI gene that encodes one or more NID domains.

[00192] In other embodiments, the agent comprises an antisense RNA targeting the gene encoding IFP35 and/or NMI. The antisense RNA can target any suitable portion of the IFP35 and/or NMI gene. For example, the antisense RNA can target a portion of  
10 the IFP35 and/or NMI gene that encodes one or more NID domains.

[00193] In still other embodiments, the agent inhibits or modifies a nuclear factor that controls IFP35 and/or NMI transcription. Any suitable agent that inhibits or modifies a nuclear factor that controls IFP35 and/or NMI transcription can be used for the manufacture of a medicament for treating and/or preventing a disease or disorder  
15 associated with abnormally high level of IFP35 and/or NMI in a subject.

[00194] In yet other embodiments, the agent comprises an antibody that specifically binds to IFP35 and/or NMI. The antibody can specifically bind to any suitable portion of the IFP35 and/or NMI. For example, the antibody can specifically bind to one or more NID domains of IFP35 and/or NMI. In another example, the  
20 antibody can specifically bind to a portion of a NID domain of IFP35 and/or NMI.

[00195] In yet other embodiments, the agent can comprise a variant form of IFP35 and/or NMI. Any suitable variant form of IFP35 and/or NMI can be used in the present methods. For example, the variant form of IFP35 and/or NMI can be a mutant IFP35 and/or NMI and/or a fragment of IFP35 and/or NMI, *e.g.*, a fragment comprising one or  
25 more NID domains of IFP35 and/or NMI, or a fragment comprising a portion of a NID domain of IFP35 and/or NMI. The agent can also comprise fusion proteins between a variant form of IFP35 and/or NMI and a heterologous protein (such as an Fc portion).

[00196] The medicament can be manufactured for administration via any suitable route. For example, the medicament can be administered via an oral, nasal, inhalational,

parental, intravenous, intraperitoneal, subcutaneous, intramuscular, intradermal, topical, or rectal route.

[00197] In some embodiments, the present medicaments can further comprise another suitable therapeutic or preventive substance or treatment. For example, the medicaments can further comprise an effective amount of a drug for the treatment and/or prevention of a proliferation disorder, a neoplasm, a tumor or a cancer in the subject.

[00198] The present medicaments can be used at any suitable amount or dosage. For example, the present medicaments can be administered at an amount that reduces production and/or an activity of IFP35 and/or NMI in the subject to a level that is substantially identical to a production and/or an activity level of IFP35 and/or NMI in a comparable subject that does not have a disease or disorder associated with abnormally high level of IFP35 and/or NMI.

[00199] The present medicaments can be used to treat and/or prevent a disease or disorder in any suitable subject. For example, the subject can be a mammal. In some embodiments, the mammal is a human. In other embodiments, the subject is a non-human animal or non-human mammal, *e.g.*, experimental, companion or economic non-human animal or non-human mammal.

[00200] Any suitable formulation of the compounds described herein can be prepared. *See, generally, Remington's Pharmaceutical Sciences*, (2000) Hoover, J. E. editor, 20th edition, Lippincott Williams and Wilkins Publishing Company, Easton, Pa., pages 780-857. A formulation is selected to be suitable for an appropriate route of administration. Some routes of administration are oral, parenteral, by inhalation, topical, rectal, nasal, buccal, vaginal, via an implanted reservoir, or other drug administration methods. In cases where compounds are sufficiently basic or acidic to form stable nontoxic acid or base salts, administration of the compounds as salts may be appropriate. Examples of pharmaceutically acceptable salts are organic acid addition salts formed with acids that form a physiological acceptable anion, for example, tosylate, methanesulfonate, acetate, citrate, malonate, tartarate, succinate, benzoate, ascorbate,  $\alpha$ -ketoglutarate, and  $\alpha$ -glycerophosphate. Suitable inorganic salts may also be formed, including hydrochloride, sulfate, nitrate, bicarbonate, and carbonate salts.

Pharmaceutically acceptable salts are obtained using standard procedures well known in the art, for example, by a sufficiently basic compound such as an amine with a suitable acid, affording a physiologically acceptable anion. Alkali metal (*e.g.*, sodium, potassium or lithium) or alkaline earth metal (*e.g.*, calcium) salts of carboxylic acids also are made.

5           **[00201]** Where contemplated compounds are administered in a pharmacological composition, it is contemplated that the compounds can be formulated in admixture with a pharmaceutically acceptable excipient and/or carrier. For example, contemplated compounds can be administered orally as neutral compounds or as pharmaceutically acceptable salts, or intravenously in a physiological saline solution. Conventional buffers  
10 such as phosphates, bicarbonates or citrates can be used for this purpose. Of course, one of ordinary skill in the art may modify the formulations within the teachings of the specification to provide numerous formulations for a particular route of administration. In particular, contemplated compounds may be modified to render them more soluble in water or other vehicle, which for example, may be easily accomplished with minor  
15 modifications (salt formulation, esterification, etc.) that are well within the ordinary skill in the art. It is also well within the ordinary skill of the art to modify the route of administration and dosage regimen of a particular compound in order to manage the pharmacokinetics of the present compounds for maximum beneficial effect in a patient.

**[00202]** The agents as described herein can be or can be made generally soluble in  
20 organic solvents such as chloroform, dichloromethane, ethyl acetate, ethanol, methanol, isopropanol, acetonitrile, glycerol, *N,N*-dimethylformamide, *N,N*-dimethylacetamide, dimethylsulfoxide, etc. In one embodiment, the present invention provides formulations prepared by mixing an agent with a pharmaceutically acceptable carrier. In one aspect, the formulation may be prepared using a method comprising: a) dissolving a described  
25 agent in a water-soluble organic solvent, a non-ionic solvent, a water-soluble lipid, a cyclodextrin, a vitamin such as tocopherol, a fatty acid, a fatty acid ester, a phospholipid, or a combination thereof, to provide a solution; and b) adding saline or a buffer containing 1-10% carbohydrate solution. In one example, the carbohydrate comprises dextrose. The pharmaceutical compositions obtained using the present methods are  
30 stable and useful for animal and clinical applications.

[00203] Illustrative examples of water soluble organic solvents for use in the present methods and compositions include and are not limited to polyethylene glycol (PEG), alcohols, acetonitrile, *N*-methyl-2-pyrrolidone, *N,N*-dimethylformamide, *N,N*-dimethylacetamide, dimethyl sulfoxide, or a combination thereof. Examples of alcohols  
5 include but are not limited to methanol, ethanol, isopropanol, glycerol, or propylene glycol.

[00204] Illustrative examples of water soluble non-ionic surfactants for use in the present methods and compositions include and are not limited to CREMOPHOR<sup>®</sup> EL, polyethylene glycol modified CREMOPHOR<sup>®</sup> (polyoxyethyleneglyceroltriricinoleat 35),  
10 hydrogenated CREMOPHOR<sup>®</sup> RH40, hydrogenated CREMOPHOR<sup>®</sup> RH60, PEG-succinate, polysorbate 20, polysorbate 80, SOLUTOL<sup>®</sup> HS (polyethylene glycol 660 12-hydroxystearate), sorbitan monooleate, poloxamer, LABRAFIL<sup>®</sup> (ethoxylated persic oil), LABRASOL<sup>®</sup> (capryl-caproyl macrogol-8-glyceride), GELUCIRE<sup>®</sup> (glycerol ester), SOFTIGEN<sup>®</sup> (PEG 6 caprylic glyceride), glycerin, glycol-polysorbate, or a combination  
15 thereof.

[00205] Illustrative examples of water soluble lipids for use in the present methods and compositions include but are not limited to vegetable oils, triglycerides, plant oils, or a combination thereof. Examples of lipid oils include but are not limited to castor oil, polyoxyl castor oil, corn oil, olive oil, cottonseed oil, peanut oil, peppermint oil,  
20 safflower oil, sesame oil, soybean oil, hydrogenated vegetable oil, hydrogenated soybean oil, a triglyceride of coconut oil, palm seed oil, and hydrogenated forms thereof, or a combination thereof.

[00206] Illustrative examples of fatty acids and fatty acid esters for use in the present methods and compositions include but are not limited to oleic acid, monoglycerides, diglycerides, a mono- or di-fatty acid ester of PEG, or a combination  
25 thereof.

[00207] Illustrative examples of cyclodextrins for use in the present methods and compositions include but are not limited to alpha-cyclodextrin, beta-cyclodextrin, hydroxypropyl-beta-cyclodextrin, or sulfobutyl ether-beta-cyclodextrin.

[00208] Illustrative examples of phospholipids for use in the present methods cyclodextrin include but are not limited to soy phosphatidylcholine, or distearoyl phosphatidylglycerol, and hydrogenated forms thereof, or a combination thereof.

[00209] One of ordinary skill in the art may modify the formulations within the teachings of the specification to provide numerous formulations for a particular route of administration. In particular, the compounds may be modified to render them more soluble in water or other vehicle. It is also well within the ordinary skill of the art to modify the route of administration and dosage regimen of a particular compound in order to manage the pharmacokinetics of the present compounds for maximum beneficial effect in a patient.

## **F. METHOD OF DIAGNOSIS, PROGNOSIS OR TREATMENT MONITORING**

[00210] In yet another aspect, the present disclosure provides for a method of diagnosis, prognosis or treatment monitoring of a disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject, which method comprises assessing the level and/or an activity of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level of IFP35 and/or NMI.

[00211] The present methods can be used for diagnosis, prognosis or treatment monitoring of any suitable disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject.

[00212] In some embodiments, the present methods are used for diagnosis of a disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject, and wherein a level and/or an activity of IFP35 and/or NMI in a subject that is at least 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, 100%, 150%, 200%, 300%, 400%, or 500% higher than a level and/or an activity of IFP35 and/or NMI in a comparable subject that does not have a disease or disorder associated with abnormally high level of IFP35 and/or NMI, *e.g.*, a proliferation disorder, a neoplasm, a tumor or a cancer, indicates that the subject has the disease or disorder associated with abnormally high level of IFP35 and/or NMI.

[00213] In some embodiments, the present methods are used for treatment monitoring of a disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject to adjust further treatment of the subject, *e.g.*, to increase or decrease the dosage, or to extend, shorten or stop the treatment.

5 [00214] In some embodiments, the present methods comprise assessing the level of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level of IFP35 and/or NMI. In other embodiments, the present methods comprise assessing an activity of IFP35 and/or NMI in a subject  
10 level of IFP35 and/or NMI. Any suitable IFP35 and/or NMI activity can be assessed, *e.g.*, binding to a cellular receptor or an antibody. In still other embodiments, the present methods comprise assessing the level and an activity of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level of IFP35 and/or NMI.

15 [00215] The level and/or an activity of IFP35 and/or NMI can be assessed at any suitable level. For example, the level and/or an activity of IFP35 and/or NMI can be assessed at the DNA, RNA and/or protein level. The level of IFP35 and/or NMI DNA and/or RNA can be assessed using any suitable means or methods. For example, the level of IFP35 and/or NMI DNA and/or RNA can be assessed using a polynucleotide that  
20 is complementary to at least 10, 15, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1,000 or more consecutive nucleotides in the IFP35 and/or NMI DNA or RNA. The level of IFP35 and/or NMI protein can be assessed using any suitable means or methods. For example, the level of IFP35 and/or NMI protein can be assessed using an antibody that specifically binds to IFP35 and/or NMI. Any suitable antibody  
25 can be used. For example, the antibody can specifically bind to a portion of a NID domain, or one or more NID domains of IFP35 and/or NMI. In still another example, the antibody is a polyclonal antibody.

[00216] In yet another aspect, the present disclosure provides for a kit of diagnosis, prognosis or treatment monitoring of a disease or disorder associated with abnormally  
30 high level of IFP35 and/or NMI in a subject, which kit comprises means for assessing the

level and/or an activity of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level of IFP35 and/or NMI.

[00217] Any suitable means can be used in the present kits. For example, the means can be used in assessing an activity of IFP35 and/or NMI. In another example, the means can be a polynucleotide that is complementary to at least 10, 15, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1,000 or more consecutive nucleotides in the IFP35 and/or NMI DNA or RNA for assessing the level of IFP35 and/or NMI DNA and/or RNA. In still another example, the means can be an antibody that specifically binds to IFP35 and/or NMI for assessing the level of IFP35 and/or NMI protein. The suitable means can be contained in any suitable single or multiple containers, *e.g.*, test tubes, microtiter plates, etc. The suitable means can also be immobilized on any suitable single or multiple surfaces, *e.g.*, beads, chips or microfluidic devices, etc.

[00218] In yet another aspect, the present disclosure provides for a method of companion diagnostics of a disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject, which method comprises determining the genetic status of IFP35 and/or NMI gene in a subject being treated for the disease or disorder associated with abnormally high level of IFP35 and/or NMI.

[00219] The genetic status of IFP35 and/or NMI gene in a subject can be assessed using any suitable methods or means. For example, the genetic status of IFP35 and/or NMI gene in a subject can be determined using a polynucleotide that is complementary to at least 10, 15, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1,000 consecutive nucleotides in the IFP35 and/or NMI DNA or RNA.

[00220] In yet another aspect, the present disclosure provides for a kit of companion diagnostics of a disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject, which kit comprises means for determining the genetic status of IFP35 and/or NMI gene in a subject being treated for the disease or disorder associated with abnormally high level of IFP35 and/or NMI.

[00221] Any suitable means can be used in the present kits. For example, the present kits can comprise a polynucleotide that is complementary to at least 10, 15, 20,

30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1,000 consecutive nucleotides in the IFP35 and/or NMI DNA or RNA for determining the genetic status of IFP35 and/or NMI gene in a subject. The suitable means can be contained in any suitable single or multiple containers, e.g., test tubes, microtiter plates, etc. The suitable means  
5 can also be immobilized on any suitable single or multiple surfaces, e.g., beads, chips or microfluidic devices, etc.

**[00222]** The present methods can be conducted in any suitable manner. For example, the present methods can be conducted manually. In another example, the present methods can be conducted in a semi-automatic or an automatic fashion. The  
10 present methods can be conducted at any suitable location. For example, the present methods can be conducted at a hospital, a clinic, a doctor's office, a clinical lab, a pharmacy, an office or a home. The present methods can be conducted at by any suitable personnel. For example, the present methods can be conducted by a physician, a nurse, a lab technician, a caregiver or a patient.

15 **[00223]** The present kits can comprises additional suitable components, e.g., means for obtaining a sample from a subject, assay standard, identifier of the test subject and/or test instructions, etc. The present kits can be standalone kits or can be part of an assay system, e.g., automated assay systems.

## 20 **G、METHODS FOR IDENTIFYING A MODULATOR OF IFP35 AND/OR NMI**

**[00224]** In yet another aspect, the present disclosure provides for a method for identifying a modulator of IFP35 and/or NMI, which method comprises: a) contacting IFP35 and/or NMI with a test substance and assessing an activity of IFP35 and/or NMI that has been contacted by said test substance; b) assessing an activity of said IFP35  
25 and/or NMI that has not been contacted by said test substance; and c) comparing said activities of IFP35 and/or NMI assessed in steps a) and b), and identifying said test substance as a modulator of IFP35 and/or NMI when said activities of IFP35 and/or NMI assessed in steps a) and b) are different.

**[00225]** Any suitable test substances can be used in the present methods. For  
30 example, the test substances can be small molecules, a polypeptide library comprising

mutants and/or fragments of IFP35 and/or NMI, antibodies that specifically bind IFP35 and/or NMI, siRNAs or antisense RNAs.

**[00226]** In some embodiments, the present methods can be used to identify an inhibitor of an activity of IFP35 and/or NMI.

5 **[00227]** In some embodiments, the present methods can be used to identify a drug for treating and/or preventing a disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject. The present methods can be used to identify a drug for treating and/or preventing any suitable disease or disorder associated with abnormally high level of IFP35 and/or NMI in a subject. For example, the disease or disorder  
10 associated with abnormally high level of IFP35 and/or NMI in a subject can be a proliferation disorder, a neoplasm, a tumor or a cancer.

**[00228]** The present methods can be conducted using any suitable assay format. Preferably, the present methods can be conducted using a high-throughput assay format.

**[00229]** In some embodiments, the present disclosure provides for a modulator of  
15 IFP35 and/or NMI or a drug candidate that is identified by present methods.

## H、EXAMPLES

### Example 1: IFP35 family members as early endogenous DAMPs

#### Abstract

**[00230]** In this example, the structures of a hybrid NID domain (NID-H) of IFP35  
20 were determined. NID-H could fold into an open or a closed conformation. NID-H in the open conformation showed high virulence to mice by inducing cytokine cascade in macrophages, characterized by the up-regulation of the expression of some early inflammation factors. Furthermore, IFP35 and NMI were released into the cell culture media of monocytes or macrophages, 1 hour after stimulated by LPS or IFN- $\gamma$ . The  
25 accumulation of IFP35 and NMI were also detected in the serum of LPS shocked mice and septic patients. A neutralizing antibody to IFP35 NID-H attenuated the LPS induced inflammatory response, and effectively improved the survival rate of septic mice. Besides, IFP35 or NMI knock-out mice were resistant to LPS challenge. Compared to HMGB-1, a known late DAMP, the IFP35 family members could serve as endogenous

ligands of TLR4, leading to the activation of the transcription factor NF- $\kappa$ B. Therefore, in some aspects, IFP35 family members with one or more NID domains, including IFP35 and NMI, could serve as early endogenous DAMPs. In some aspects, use of IFP35 and/or NMI or binding partners in the diagnosis and/or treatment of infection and injury is provided.

## Results

### 1. The structures of NID revealed its open and closed conformations.

[00231] According to sequence analysis, IFP35 has an L-zip domain at its N-terminus containing the first 80 amino acids, following by two tandem NID domains covering the 81-170 and 177-268 amino acids, respectively (**Fig. 1a**). Truncated protein constructs were constructed according to secondary structure prediction. A truncated IFP35 protein containing the 124<sup>th</sup> to the 220<sup>th</sup> amino acids expressed well in *E. coli*. Since this truncated IFP35 protein spreads across the two predicted NID domains, it was termed NID-H (heterozygous NID) (**Fig. 1a**). During the purification process, NID-H was found to exist in at least two stable aggregation states, dimer and octamer (**Fig. 2a**).

[00232] Well-diffracted NID-H crystals with both dimeric and octameric states were obtained. The crystal of dimeric NID-H with seleno-L-methionine derivation diffracted at 2.2 Å. The structure was determined by single-wavelength anomalous diffraction (SAD) method (Table 1). The SAD method is disclosed in Chayen & Saridakis, Nature methods 5, 147-153 (2008). The NID-H folds into barrel-like structure, formed by five  $\beta$ -strands and two  $\alpha$ -helices which connect with each other in the order of  $\beta$ 1- $\alpha$ 1- $\beta$ 2- $\beta$ 3- $\alpha$ 2- $\beta$ 4- $\beta$ 5 (**Fig. 1b**). Several pairs of residues on helix  $\alpha$ 1 and the following loop (L1) connecting  $\alpha$ 1 and  $\beta$ 2 play important roles for dimer formation. Based on the structure, at least five pairs of interactions could be observed (**Fig. 1c**), including: the hydrophobic interaction between the side chains of Ile159 from each monomer; the electronic interactions between Lys163 and Glu158, as well as Asp155 and Lys156; the interaction between the side chain of Asp170 and the amino group on the backbone of Thr164; the interaction between the side chain of Arg165 and carbonyl group on the backbone of Val171.

[00233] Table 1. Data collection and refinement statistics

|                                          | <b>Dimer (Se-Met)</b>             | <b>Octamer (Native)</b> |
|------------------------------------------|-----------------------------------|-------------------------|
| <b>Data Collection</b>                   |                                   |                         |
| Beamline                                 | BL17U1                            | BL17U1                  |
| Wavelength (Å)                           | 0.9798                            | 0.9792                  |
| Resolution range (Å)                     | 40.0-2.3 (2.34-2.30) <sup>a</sup> | 50.0-2.5 (2.54-2.50)    |
| Space group                              | H3                                | P2 <sub>1</sub>         |
| <b>Cell dimensions</b>                   |                                   |                         |
| a, b, c (Å)                              | 170.3, 170.3, 53.0                | 44.4, 125.3, 77.2       |
| $\alpha$ , $\beta$ , $\gamma$ (°)        | 90.0, 90.0, 120.0                 | 90.0, 90.3, 90.0        |
| Total reflections                        | 25,256 (1,263)                    | 29,326 (1,447)          |
| Unique reflections                       | 1,148                             | 6,110                   |
| Completeness (%)                         | 99.9 (100.0)                      | 97.8 (99.9)             |
| Mean I/ $\sigma$                         | 74.2 (21.3)                       | 21.1 (5.4)              |
| Multiplicity                             | 22.0 (22.5)                       | 4.8 (5.4)               |
| R <sub>sys</sub> (%)                     | 12.5 (69.9)                       | 10.8 (57.9)             |
| <b>Refinement</b>                        |                                   |                         |
| Resolution range (Å)                     | 32.38-2.30                        | 36.71-2.50              |
| R <sub>work</sub> /R <sub>free</sub> (%) | 18.1/22.9                         | 20.6/25.3               |
| Rmsd bond length (Å)                     | 0.002                             | 0.003                   |
| Rmsd bond angles (°)                     | 0.619                             | 0.639                   |
| <b>Ramachandran plot</b>                 |                                   |                         |
| Most favored (%)                         | 98.2                              | 97.6                    |

|                                     |      |      |
|-------------------------------------|------|------|
| Additional allowed (%)              | 1.8  | 2.4  |
| Disallowed (%)                      | 0.0  | 0.0  |
| Average B factor ( $\text{\AA}^2$ ) | 29.0 | 55.0 |

<sup>a</sup> Values in parentheses are for the highest resolution shell.

[00234] Subsequently, the octameric structure of NID-H was determined at 2.8 Å resolution by molecular replacement (MR) method (**Fig. 1d**, **Table 1**). A domain-swapping conformation between two monomers can be observed in the octameric structure. The specific manner is that  $\beta 1$ - $\alpha 1$ - $\beta 2$  from one monomer interact with  $\beta 3$ - $\alpha 2$ - $\beta 4$ - $\beta 5$  from another monomer and fold into a barrel-like structure (**Fig. 1d**). In this way, two monomers piled up head-to-end and interact tightly in the dimer. For clarity, this domain-swapping dimer was named the open conformational dimer (o-dimer). The dimer without domain-swapping is called the closed conformational dimer (c-dimer). Four o-dimers further interact with each other through  $\alpha 1$ - $\alpha 1$  interactions, as described in c-dimer, and form a ring like structure (**Fig. 2b**). The monomer in o-dimer is quite similar to that in the c-dimer (**Fig. 1e**). The root mean square deviation (RMSD) between them is only about 0.7 Å. The major difference is that the  $\beta$ -turn (T1) in c-dimer connecting  $\beta 2$  and  $\beta 3$  is straightened in the o-dimer, in which it forms a loop (L2) and connects the two barrel-like structures. The crystal structure coordinates of the dimer structure and the octamer structure are provided in **Fig. 33** and **Fig. 34**, respectively.

[00235] Using Dali server, a powerful structure comparison tool, known structures in PDB were compared to the barrel-like structure of NID-H. The NID-H structure was found to be very similar to that of RNA recognition motif (RRM) (**Fig. 2c**). The RRM are widely used to identify RNAs of different sequences and structures. However, there is no obvious RNA binding site in the structure of NID-H indicated by its surface charge distribution. EMSA experiment using NID-H and RNAs with different sequences were also performed, and no interaction between NID-H and the tested RNA sequences was found (data not shown).

2. The open conformation of IFP35 NID-H stimulated immune response.

[00236] NID-H domain was used as antigen to stimulate polyclonal antibodies production in mice for IFP35 detection. The NID-H octamer caused a 100% mortality rate for all four mice used. Besides, all the mice died with swelled belly and obviously increased ascites. This phenomenon indicated that the NID-H octamer might have cellular toxicity. Because IFP35 typically is specifically expressed in immune cells, such as monocytes, macrophages, dendritic cells and lymphocytes, the NID-H octamer could stimulate inflammatory response.

[00237] The transcription level of pro-inflammatory factors, such as TNF- $\alpha$  and IL-1 $\beta$ , were up-regulated in the presence of NID-H octamer in murine macrophage-like RAW264.7 cells (**Fig. 3a**). This result was similar to lipopolysaccharide (LPS) induced inflammatory cytokines production. By comparison, the NID-H dimer (c-dimer) did not have this effect. Based on these results, NID-H in its octameric structure tends to induce cytokine storm related to TNF- $\alpha$  and IL-1 $\beta$ .

[00238] Since the c-dimer itself could not induce inflammation, the o-dimer in the NID-H octamer could serve as the active conformation. To verify whether the octameric skeleton is necessary for its cellular toxicity, a mutant with three point mutations, K156E/K163E/R165E, on the  $\alpha 1$  helix as shown in **Fig. 1c**, was constructed. These mutations were supposed to partially destroy the c-dimer formation, which leads to the de-polymerization of the octamer. Therefore, some independent o-dimer should be produced. The results showed that the mutated and/or modified dimer could partially up-regulate the transcription of TNF- $\alpha$  and IL-1 $\beta$  (**Fig. 3b**), which could be ascribed to the formation of independent o-dimers. The results showed that o-dimer is the active state of NID-H to induce cytokine storm.

[00239] Since NID-H can activate the innate immune response, IFP35 full length protein was expressed. However, IFP35 had low yield in eukaryotic cells and formed inclusion body in *E. coil.*, probably due to the hydrophobic L-zip domain at its N terminus. A truncated IFP35 with 34 amino acids deletion at its N terminal ( $\Delta N$ ) was constructed and expressed using prokaryotic expression system. Soluble  $\Delta N$  protein was obtained, and the  $\Delta N$  protein stimulated the transcription of TNF- $\alpha$  and IL-1 $\beta$  more effectively than NID-H octamer (**Fig. 3c**). Compared to the effective dose of NID-H (about 10-50 $\mu$ g/ml), the effective dose of  $\Delta N$  was about 1 $\mu$ g/ml, which was comparable

to that of HMGB-1 or Mrps. Besides,  $\Delta N$  has a strong effects to stimulate the release of inflammation cytokines such as TNF- $\alpha$  at low dose. Detected by ELISA, 100-200 pg/ml TNF- $\alpha$  could be released into culture by RAW 264.7 cells, stimulated by  $\Delta N$  or LPS at 1  $\mu$ g/ml. (**Fig. 3d**). Moreover, when RAW264.7 cells were stimulated using recombinant mNMI protein, similar inflammation response was also detected (**Fig. 4**). Based on these results, IFP35 family members can serve as endogenous DAMP proteins.

**[00240]** A secondary structure prediction of human IFP35 is shown in **Fig. 32**. According to the prediction, in some aspects, removal of the first 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, or 78 residues in human IFP35 would produce similar results as  $\Delta N$  used in this example.

3. IFP35 family members possess the typical characteristics of endogenous DAMP.

**[00241]** DAMPs, including HSPs, HMGB-1, Mrp8 and Mrp14, are secreted by cells and are then recognized by the pattern recognition receptors (PRRs) on the cell surface. Kawai *et al.*, Immunity 34, 637-650 (2011); Wu & Chen, Annual Review of Immunology 32, 461-488 (2014); and Zhong *et al.*, Frontiers in Immunology 4, 333 (2013). IFP35 and NMI were reported to localize in cytoplasm after being up-regulated by IFN- $\gamma$ . However, in this example, within 3 hour after stimulated by IFN- $\gamma$ , or within 1 hour after stimulated by LPS or Salmonella, IFP35 and NMI were secreted and detected in the culture supernatant of RAW 264.7 cells (**Fig. 5a, Fig. 6a, Fig. 6b and Figs. 18-21**). In the following several hours, IFP35 and NMI accumulated in the culture in a time-dependent manner as revealed by immunoblot result. In contrast, early and late mediators of endotoxemia, TNF- $\alpha$  and HMGB-1, were released at several minutes and at 6-8 hours, respectively. Wang *et al.*, Science 285, 248-251 (1999); and Tracey *et al.*, Science 234, 470-474 (1986). IFP35 was reported to bind NMI in cells, forming HMMC and further into speckle-like aggregations. Chen *et al.*, JBC 275, 36278-84 (2000). Secreted IFP35 and NMI in the culture of RAW264.7 cells stimulated by Salmonella SR-11 were analyzed using gel filtration and western blot. The results showed that secreted IFP35 existed as monomer and NMI existed as dimer in solution (**Fig. 6c and Fig. 6d**). Similar to HMGB-1 and Mrps, there is no obvious transmembrane signal peptide in the

sequences of the IFP35 family members. Therefore, the IFP35 family of proteins can serve as early DAMPs.

[00242] DAMPs were reported to be closely related to the infection and injury. Hirsiger et al., *Mediators of Inflammation*, 315941 (2012); and Bianchi, *Journal of Leukocyte Biology* 81, 1-5 (2007). The concentrations of known DAMPs, such as HMGB-1 and Mrps, are significantly increased in the serum of septic patients. Wang et al., *Science* 285, 248-251 (1999); Austermann et al., *Cell Reports* 9, 2112-2123 (2014); and Sunden-Cullberg et al., *Critical Care Medicine* 33, 564-573 (2005). In order to determine if IFP35 and NMI were released in serum during infection, mice were challenged using LPS and detected them in the serum of septic mice. IFP35 and NMI were secreted within 3 hours after LPS exposure. Compared with the control group, the serum IFP35 and NMI in LPS administrated mice increased sharply with a dose dependent manner, up to about 120ng/ml within 6 hours (**Fig. 5b** and **Fig. 6e**). In addition, serum of the patients with sepsis was analyzed and the concentrations of IFP35 in almost all of the 12 samples were elevated. Although great deviations existed among these cases, probably caused by different pathogens and physical conditions, the serum IFP35 could be quantified at 1-10ng/ml, while the protein was barely detectable in the serum of normal individuals (**Fig. 5c** and **Fig. 6f**). These results demonstrated that IFP35 is released into serum during infection.

[00243] Different from HMGB-1, IFP35 family members could be released within the first hour after LPS stimulation. Administration of antibodies to NID-H (anti-NID-H) before lethal dose ( $LD_{100}$ ) of LPS exposure could provide effective protection to mice. Compared with the 0% survival rate in control, more than 60% of the anti-NID-H treated mice survived in 7 days after LPS exposure (**Fig. 5d**). Because the toxic effects of LPS are partly mediated by inflammatory cytokines such as TNF- $\alpha$ , IL-1 $\beta$  and IL-6, the concentrations of these cytokines in serum after the administration of LPS and anti-IFP35 monoclonal antibody were examined. Consistent with this phenomenon, administration of anti-NID-H could decrease the release of some toxic inflammatory factors in the serum of septic mice such as TNF- $\alpha$ , IL-1 $\beta$  and IL-6, by about 20%-50% (**Fig. 5e**). IFP35 and NMI knock-out mice were produced using CRISPPR-Cas9 technology. Ran et al., *Nature Protocols* 8, 2281-2308 (2013). The reaction to bacterial LPS in

conjunction with galactosamine (D-gal) is a well-characterized model of endotoxic shock in mice that is mediated by inflammatory cytokines. Vogl et al., Nature Medicine 13, 1042-1049 (2007); and Galanos et al., PNAS 76, 5939-5943 (1979). After intraperitoneal injection of LPS and D-gal, wild-type animals showed symptoms of acute illness and died within 5–8 h. In contrast, *IFP35*<sup>-/-</sup> mice were less severely affected and survived significantly longer (**Fig. 5f**). Resistant of *IFP35*<sup>-/-</sup> and *NMI*<sup>-/-</sup> mice to LPS – induced lethal toxicity was also observed when mice were injected with a large amount of LPS without D-gal. Compared with the normal mice whose lethality is almost 100% under administration of lethal dose of LPS, the lethality of NMI knock-out mice are improved (**Fig. 6g**). During LPS exposure, the concentrations of known pro-inflammatory factors were greatly decreased in the serum of these knock-out mice (**Fig. 5g** and **Fig. 6h**). Therefore, all these results demonstrated that IFP35 could serve as DAMP and cause strong inflammatory response.

4. IFP35 stimulates the cytokines storm potentially based on the TLR4 pathway.

[00244] Based on previous reports, HMGB-1 and Mrps induce immune response through triggering the activation of NF-κB by TLR4 signal pathway. Vogl et al., Nature Medicine 13, 1042-1049 (2007); Yang et al., PNAS 107, 11942-11947 (2010); and Yu et al., Shock 26, 174-179 (2006). Accordingly, several key players in this pathway were detected and their effects in immune response induced by IFP35 family members were analyzed. First of all, the activation of NF-κB promoter by NID-H was detected using luciferase assay. HEK293 cells were transiently transfected with plasmids such as TLR4, CD14, MD2 and luciferase following NF-κB promoter. 24 hours after transfection, cells were incubated with 10μg/ml purified octameric NID-H protein. The luciferase activity is dependent on the transcription level of luciferase gene by transcriptional factor, phosphorylated NF-κB, hence it was used to represent the activation of NF-κB. The luciferase activity triggered by NID-H was not strong but obvious (**Fig. 7a**). The activity of LPS can be blocked by polymyxin B, an effective antibiotic for Gram-negative infections. However, the activity of NID-H was not affected. Since IFP35(ΔN), a N-terminal truncation of IFP35, has high efficiency to trigger the inflammation response, its abilities to active transcription factors were also detected. The results showed that purified ΔN induced strong NF-κB and AP-1 promoter activities. In contrast, it has no

effects to IRF3 promoter (**Fig. 7b**). These results suggest that IFP35 active NF- $\kappa$ B and AP-1 but not IRF-3, probably through Myd88 dependent pathway and the mechanism of IFP35 family members should be parallel to the known DAMPs. After stimulation by interferon, IFP35 family members can be released as danger signal, then lead to cytokine storm through TLR4-MyD88-NF- $\kappa$ B/AP-1 signaling pathway.

## Discussion

[00245] In this example, the structure of the NID domain, the characteristic domain of IFP35 family members, was determined. It is found that the open conformation of NID-H could activate the innate immune response. The results indicate that the IFP35 family members can act as early DAMPs and activate transcriptional factor NF- $\kappa$ B through the TLR4 pathway and lead to cytokine storm. However, the structures and functions of IFP35 family members still need be discussed and illustrated.

### 1. The structures of the tandem NID domains

[00246] There are two tandem NID domains in both IFP35 and NMI. The structure of NID-H crosses two predicted NID domains in IFP35. It could be divided into two fragments,  $\beta$ 1- $\alpha$ 1- $\beta$ 2 (termed as “A part”) and  $\beta$ 3- $\alpha$ 2- $\beta$ 4- $\beta$ 5 (termed as “B part”), covering 131-179 and 180-228 amino acids in the sequence, respectively. Based on the secondary structure prediction results, the fragment covering 80-130 contains  $\beta$ - $\alpha$ - $\beta$  secondary structure elements, and it was termed “B’ part”, compared to B part. Similarly, an “A’ part” covering 229-276 contains  $\beta$ - $\alpha$ - $\beta$  secondary structure elements. By sequence alignment, parts A’ and B’ are comparable with parts A and B (**Fig. 8a**). Residues involved in the hydrophobic core of NID-H structure were found out as shown in **Fig. 8b**. These residues are almost completely conserved in these two groups, A with A’ and B with B’ (**Fig. 8a**). Therefore, members in the same group can replace with each other. According to previous domain predication, A and B’ belong to the first NID domain, while A’ and B belong to the second. According to the structure of NID-H, the structure of the two tandem NID domains in IFP35 could fold into a double-barrel structure (**Fig. 8c**).

[00247] In this model, the NID-H region, consisting of part A and part B, exist as the open conformation. The skeletons of the tandem NIDs model and NID-H o-dimer

structure are similar. Nevertheless, there are many differences between them. For example, the surface residues in A' and B' are not exactly same with those in A and B. Besides, it is reasonable that the relative position of these two NIDs should be flexible, which might be adjusted during receptor reorganization. In contrast, the o-dimer  
 5 conformation of the NID-H is stable because it is fixed in ring structure of the octamer. Based on these, it is understandable that the NID-H octamer only has about 5-10% activity compared with  $\Delta N$ . A long loop (LL) is supposed to be existed in the putative NID domain. It connects the two parts of the NID domain, which fold into a  $\beta$ - $\alpha$ - $\beta$ - $\beta$ -LL- $\beta$ - $\alpha$ - $\beta$  structure. In IFP35, these two long loops cover 115-130 and 220-228 amino acids,  
 10 respectively. The features of these amino acids indicate that these two loops are flexible. Therefore, these two loops might take part in the HMMC formation in cells or receptor recognition on the out membrane. The structure and functional mechanism of NMI, the homologous protein of IFP35 could also be inferred from the structure of IFP35 (**Fig. 9**).

## 2. The recognition between IFP35 and TLR4

15 **[00248]** To verify the recognition between IFP35 and TLR4, an in vitro binding assay was used to pull down IFP35 by TLR4, TLR4/MD2 and TLR4/MD2/CD14 complex. The bait was fused with 6\*His and immobilized on Ni-NTA beads. The treated beads were used to pull down full-length or truncated IFP35 proteins, including purified NID-H octamer,  $\Delta N$ , and released IFP35 in RAW cell culture. The results showed that  
 20 only the release IFP35 could be captured by TLR4/MD2 complex in the presence of CD14 (Data not shown). Therefore, TLR4, MD2 and CD14 can work coordinately during IFP35 recognition.

## 3. The differences between IFP35 family members and known DAMPs

25 **[00249]** Although the IFP35 family members can stimulate NF- $\kappa$ B through TLR4 pathway, similar to the known late DAMPs, in fact, they are expected to have more differences. As early DAMPs, IFP35 and NMI are released in the first hour after cells are stimulated by pathogens, compared to the 6-8 hours for HMGB-1. Playing crucial role in the early state of immune response, IFP35 family members may crosstalk with known other early inflammatory factors such as TNF- $\alpha$ , IL-1 $\beta$ . From the results herein, the  
 30 antibody of NID-H are effective to down regulate the expression of these inflammatory

cytokines, so it could provide more efficient protection for LPS challenged mice. Besides, their concentrations in patients' serum are far from that of HMGB-1, but comparable to other cytokines, they are more likely to work as signal molecules rather than effectors.

[00250] On one hand, IFP35 tends to aggregate because it contains a hydrophobic L-zip domain, on the other hand, it is easy to degrade due to the flexibility of two NID domains. Therefore, IFP35 protein could not fold well in many expression systems. The released IFP35 by immune cells are limited and glycosylated. A NID-H fragment which folds into an active octameric conformation has a high yield in *E. coil*. Since the active conformation is stabilized and the binding surface is exposed in the octamer structure, the NID-H octamer will be very powerful for monoclonal antibody screening. A monoclonal antibody of NID-H neutralized IFP35 and provided protection for septic mice. Besides, soluble  $\Delta$ N could also be used to prepare monoclonal antibody. Even though further evidences are still needed, their applications in fighting against infections and injuries could be expected.

[00251] These data demonstrated a type of early DAMP, IFP35 family members. They are released when the immune cells are stimulated by pathogen or interferon, and further enhance the immune response through TLR4 Signal pathway. The structure of NID-H shed light on the mechanism of these new DAMPs. The results herein provide a way in diagnosis and treatment for infection and injury related diseases.

## 20 Methods

[00252] **Plasmid Construction.** The cDNA of Homo sapiens IFP35 and *Mus musculus* NMI were amplified from reverse-transcribed cDNA from THP1 and RAW264.7 cells (accession No.: NP\_005524.2 and NP\_001135421.1). Standard methods for primer design, PCR amplification, digestion and recovery were used. The DNA sequences corresponding to amino acids 124-240 and 35-289 of human IPF35 protein (NID-H and  $\Delta$ N) were inserted into pGEX-6p-1 vector (Invitrogen) using the BamH I and Xho I sites with an N-terminal GST tag. And the DNA sequences of mouse NMI protein was inserted into RSFDuet vector (Novagen) using the BamH I and Xho I sites. All the plasmids were verified by DNA sequencing.

**[00253] IFP35 (NID-H and  $\Delta$ N) purification.** The plasmids were transformed into *Escherichia coli* BL21 (DE3) expression strain (for native protein expression) and *Escherichia coli* B834 (DE3) expression strain (for Selenomethionine derivative (Se-Met) expression). Cells for native or Se-Met protein expression were cultured in the presence  
5 of 0.1 g/L Ampicillin in Lenox Broth medium or in SelenoMet Medium Base (Molecular Dimensions Limited) at 37 °C until the OD<sub>600</sub> reached 0.8-1.0 and were then induced with 0.5 mM isopropyl- $\beta$ -D-thiogalactopyranoside (IPTG) at 37 °C for 5 hours.

**[00254]** Cells containing over-expressed native or Se-Met IFP35 (residues 124-220) were harvested and resuspended in cold 1x PBS buffer (137 mM NaCl, 2.7 mM KCl,  
10 10 mM Na<sub>2</sub>HPO<sub>4</sub>, 1.8 mM KH<sub>2</sub>PO<sub>4</sub>, pH 7.4), and lysed by passing the cell suspension two times through an EmulsiFlex-C5 homogenizer (Avestin) at 5,000 psi and 15,000 psi, respectively. Cell lysate was centrifuged at 30,700 g/4 °C/40 min and the supernatant was incubated with Glutathione Sepharose 4B resin (GE Healthcare) at a ratio of 100 ml supernatant per ml resin at 4 °C for 30 - 60 min. After incubation, the GST resin was  
15 washed with 1x PBS buffer and equilibrated with a buffer of 150 mM NaCl, 20 mM Tris-HCl, pH 8.0. The recombinant protein was eluted with 20 mM GSH and the GST tag was cleaved overnight at 4 °C by PreScission Protease (PPase). After cleavage, the recombinant protein was further purified through a HiTrap Q HP (GE Healthcare) column and eluted with a linear gradient of 150 to 1,000 mM NaCl. A HiLoad 16/60  
20 Superdex 200 (GE Healthcare) column (prep grade) equilibrated with 150 mM NaCl, 20 mM Tris-HCl, pH 8.0 was used as the last purification step. Protein content of each fraction from elution peaks was analyzed by SDS-PAGE. Two peaks with target protein were pooled separately, concentrated, flash-frozen in liquid nitrogen, and stored at -80 °C until further use.

**[00255] NMI, GFP-NID-H and GFP-NMI purification.** The plasmids were transformed into *E. coli* strain BL21 (DE3). Cells were cultured in LB medium at 37°C with 100 mg/L ampicillin. When the OD<sub>600</sub> reached 0.8–1.0, the culture was induced by addition of isopropyl-thio-D-galactosidase (IPTG) (Sigma) to a final concentration of 0.5mM for 20 h at 16°C. Cells were harvested by centrifugation at 5000rpm for 10 min.  
30 Pellets were resuspended in Tris buffer (20 mM Tris at pH 8.0, 150mM NaCl) and lysed by sonication. The lysate was separated by centrifugation at 16,000 rpm for 30 min, and

the recovered supernatant was applied to a Ni-NTA affinity column (Qiagen), followed by intensive washing with washing buffer (20 mM Tris at pH 8.0, 150 mM NaCl, 50 mM imidazole). Recombinant protein was eluted from the Ni-NTA affinity column using elution buffer (20 mM Tris at pH 8.0, 150 mM NaCl, 500 mM imidazole) and further  
5 purified by gel filtration with a Superdex200 column (GE Healthcare) using Tris buffer as described above on an FPLC protein purification system.

[00256] The purity and integrity of all recombinant proteins were verified by Coomassie blue staining after SDS-PAGE, with a purity predominantly >90%. The LPS content in all proteins preparations is undetectable or <10 pg/mg protein as measured by  
10 Limulus assay.

[00257] **Crystallization and Data Collection** Both the native and Se-Met IFP35 fragments exhibited two oligomeric states on the Superdex 200 column: octamer and dimer. Both forms of protein were used for crystallization screening. Ultimately, the native IFP35 (residues 124-220) was crystallized in its octameric form by the hanging  
15 drop method with a drop consisting of 1  $\mu$ L 6 mg/mL protein and 1  $\mu$ L well solution (0.2 M  $(\text{NH}_4)_2\text{SO}_4$ , 0.1 M Bis-Tris-HCl, 20 % [w/v] PEG3350, pH 5.4) at 16 °C for 14 days. Crystals of Se-Met IFP35 (residues 124-220) were grown in its dimeric form by the hanging drop method from a solution consisting of 1  $\mu$ L 10 mg/mL protein and 1  $\mu$ L well solution (0.2 M  $(\text{NH}_4)_2\text{SO}_4$ , 0.1 M Bis-Tris-HCl, 22 % [w/v] PEG3350, 0.1 M K Na  
20 Tartrate, pH 5.5) at 16 °C for 50 days.

[00258] Crystals were flash-frozen in liquid nitrogen until data collection. For Se-Met crystals, an additional 20 % [v/v] Glycerol was used as a cryo-protectant. The X-ray diffraction data of native and Se-Met proteins were collected on beamline BL17U at Shanghai Synchrotron Radiation Facility (SSRF) at wavelengths of 0.9798 Å and 0.9792  
25 Å, respectively. The collected data were integrated and scaled using HKL-2000 (Otwinowski, Methods in Enzymology 276, 307-326 (1997)), Selenium-labeled positions in Se-Met protein were determined using SHELXD from the CCP4 suite (Schneider et al., Acta Crystallographica, Section D, Biological Crystallography 58, 1772-1779 (2002); and Winn et al., Acta Crystallographica, Section D, Biological Crystallography 67, 235-  
30 242 (2011)) and six selenium sites were found.

**[00259] Structure Determination and Refinement.** The structure of IFP35 (residues 124-220) in dimeric form was determined using SAD in the Phenix suite. Adams et al., *Acta Crystallographica, Section D, Biological Crystallography* 66, 213-221 (2010). AutoSol was used to obtain the initial phase. The missing region in the model was rebuilt with AutoBuild or Coot. Emsley et al., *Acta Crystallographica, Section D, Biological Crystallography* 66, 486-501 (2010). The model was further refined with phenix.refine in iterative cycles until R values converged. Six molecules were found in one asymmetric unit with a Matthews coefficient value calculated to  $2.39 \text{ \AA}^3 \text{ Da}^{-1}$  and the solvent content was 48.6 %. Matthews, *J Mol Biol* 33, 491-497 (1968).

**[00260]** Structure of the octameric form was solved by molecular replacement using Phaser-MR (Adams et al., *Acta Crystallographica, Section D, Biological Crystallography* 66, 213-221 (2010)) and the dimeric structure as a search model. The model was rebuilt with Coot (Emsley et al., *Acta Crystallographica, Section D, Biological Crystallography* 66, 486-501 (2010)) and refined with phenix.refine. Adams et al., *Acta Crystallographica, Section D, Biological Crystallography* 66, 213-221 (2010). At the final step, TLS refinement was introduced and the TLS groups were suggested by the TLSMD server. Painter et al., *Acta Crystallographica, Section D, Biological Crystallography* 62, 439-450 (2006). Eight molecules were found in the asymmetric unit. The calculated Matthews coefficient and solvent content were  $2.61 \text{ \AA}^3 \text{ Da}^{-1}$  and 52.8 %, respectively. Matthews, *J Mol Biol* 33, 491-497 (1968). Inter-molecular interactions were analyzed by PISA. Krissinel et al., *J Mol Biol* 372, 774-797 (2007). All crystal structure-related figures were prepared with PyMOL ([www.pymol.org](http://www.pymol.org)).

**[00261] Antibodies and reagents.** Anti-IFP35 antibody was obtained from Abnova (D01P). Anti-HMGB1 antibody was obtained from Abcam (ab79823). Anti- $\beta$ -Actin antibody was obtained from Sigma-Aldrich (A5441). Anti-CD11b (M1/70) and Gr-1 (RB6-8C5) antibody was obtained from BD Biosciences. Anti-I $\kappa$ Ba antibody and pI $\kappa$ Ba antibody were obtained from Abcam. IFN $\gamma$ , trichloroacetic acid (TCA), Lipopolysaccharide (LPS) from *E.coli* 055:5 and D-galactosamine (D-gal) were purchased from Sigma-Aldrich. MCSF was purchased from Peprotech.

**[00262] Cells and cell culture conditions.** RAW 264.7 macrophages (from ATCC) were cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with

10% fetal bovine serum at 37°C. B6/C57 mice-derived *wt*, *Tlr3*<sup>-/-</sup>, *Tlr4*<sup>-/-</sup>, *Tlr7*<sup>-/-</sup>, *Tlr9*<sup>-/-</sup>, *Myd88*<sup>-/-</sup> BMDM cells were cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum and 20 ng/ml MCSF at 37°C. THP1 cells were cultured in RPMI 1640 medium supplemented with 10% fetal bovine serum at 37°C. RAW 264.7 macrophages, BMDM and THP1 cells were seeded in 6-well plates at a density of  $2 \times 10^6$  cells/well and grown overnight. Then the cells were stimulated with LPS (100 ng/mL), varying concentrations of Salmonella SR-11, IFN- $\gamma$ , purified recombinant proteins IFP35-NID or NMI for different times as indicated in the figure legends.

10        **[00263] RNA isolation and q-PCR.** The total RNA was extracted from RAW 264.7, THP1 and BMDM cells using Trizol reagent (Invitrogen) according to the manufacturer's instructions. The first strand of cDNA was synthesized from 1  $\mu$ g of total RNA using random primers and MMLV reverse transcriptase (Invitrogen). Real-time RT-PCR was performed using the SYBR Green PCR kit (Bio-Rad) and Real-time  
15        quantitative polymerase chain reaction analyses were performed using the CFX96 Real-Time PCR System (Bio-Rad). Each measurement was set up in duplicates, and three independent experiments were performed. The primer sequences were as follows:

**[00264]** mouse (m) GAPDH: sense, CAGAACATCATCCCTGCATC; antisense, TACTTGGCAGGTTTCTCCAG;

20        **[00265]** mTNF $\alpha$ : sense, CCAGTGTGGGAAGCTGTCTT; antisense, AAGCAAAAGAGGAGGCAACA;

**[00266]** mIL-1 $\beta$ : sense, AAGGAGAACCAAGCAACGACAAAA; antisense, TGGGGAACTCTGCAGACTCAAAC.

**[00267] Western blot.** RAW 264.7 macrophages and THP1 cells were pretreated  
25        with 100ng/mL LPS or Salmonella SR-11 for 1h, 2h, 3h, 5h and 9h. Then the cells were washed twice with cold PBS, scraped, and collected in lysis buffer (20mM Tris, pH 7.4, 150mM NaCl, 5mM EDTA, 0.5%NP-40, 10%glycerol, protease inhibitor cocktail(Roche)). The whole cell lysates were incubated at 4°C for 45min, followed by centrifugation (12 000  $g \times 15$  min, 4°C). Secretory protein in the cell culture supernatant  
30        was collected by trichloroacetic acid (TCA)/acetone precipitation. The cell culture

supernatant was added 0.11 volumes of ice-cold 100% TCA and placed on ice for 2h, followed by centrifuge at 20,000g for 30 min. Then carefully remove the supernatant, add 500  $\mu$ L of acetone, centrifuge at 20,000g for 10 min, carefully remove the supernatant and dry the protein pellet in a vacuum evaporator. Protein samples were separated by SDS-PAGE, transferred to a PVDF membrane, and probed with specific antibodies against IFP35, HMGB1, and NMI.

[00268] BMDM cells were treated with purified recombinant proteins IFP35-NID or NMI for 5min, 15min, 30min, 60min. Then the cells were washed twice with cold PBS, scraped, and collected in lysis buffer. The whole cell lysates were incubated at 4°C for 45min, followed by centrifugation. Protein samples were prepared for western blot. IkBa, pIkBa,  $\beta$ -Actin were detected by WB.

[00269] **LPS-induced shock model.** LPS from E. coli 055:B5 and D-gal were diluted in pyrogen-free saline. A combination of LPS (50  $\mu$ g per kg body weight) and D-gal (1.0 g per kg body weight) was injected intraperitoneally in *IFP35*<sup>-/-</sup>, *NMI*<sup>-/-</sup> and wild-type mice. Resistant of *IFP35*<sup>-/-</sup> and *NMI*<sup>-/-</sup> mice to LPS induced lethal toxicity were also observed when mice were injected with a large amount of LPS (50 mg per kg body weight) without D-gal. Observe and record the mortality of mice for 1 week.

[00270] **IFP35 monoclonal antibody protects LPS shocked mice.** In the survival experiment, IFP35 mAb and IgG1 (10 $\mu$ g per mouse) were injected intraperitoneally in B6/C57 mice 4h before the injection of LPS (50 mg per kg body weight). Additional doses (10 $\mu$ g per mouse) were administered at 2h after LPS injection. Delayed doses (10  $\mu$ g per mouse) was administrated every 24 hours for 4 times. Observe and record the mortality of mice for week.

[00271] **Determination of cytokine concentrations.** IFP35 and NMI in human and mouse serum were measured with ELISA kits (CUSABIO).Release of cytokines (IL-1 $\beta$ , IL-6, and TNF $\alpha$ ) in the culture supernatants or in mouse serum were measured by ELISA Kit (Biolegend, Thermo Fisher).

[00272] **Generation of IFP35<sup>-/-</sup> mice.** Genomic engineering of *IFP35* was achieved with the CRISPR/Cas9 system as described.

[00273] **Flow cytometry.** Recombinant protein IFP35 NID-H, NMI or PBS were injected intraperitoneally in B6/C57 mice for 24 h, respectively. The mouse ascites was incubated with antibody to CD11b and Gr-1, followed by FITC-conjugated secondary antibody. Cells were analyzed on a FACSCalibur machine (BD Biosciences) to detect the  
5 peritoneal neutrophils and data were analyzed using CellQuestPro software.

[00274] B6/C57 mice-derived *wt* or *Tlr4*<sup>-/-</sup> cells were incubated with GFP-NID-H and GFP-NMI in PBS buffer (containing 2% FBS) for 1h. Cells were analyzed on a FACSCalibur machine (BD Biosciences) and data were analyzed using CellQuestPro software.

10 [00275] Citation of the publications or documents herein is not intended as an admission that any of the foregoing is pertinent prior art, nor does it constitute any admission as to the contents or date of these publications or documents.

#### **Example 2: Use of IFP35 Family Proteins**

[00276] IFP35 and NMI can be rapidly up-regulated by interferon (IFN). The  
15 protein level of IFP35 in cells is low without the induction of IFN. IFP35 and NMI can be induced by type I or type II interferon (IFN $\alpha/\beta/\gamma$ ) in numerous immune cells. The amount of IFP35 protein and mRNA level increased dramatically after stimulation of IFN  $\gamma$  for 6h and reached the maximum level at 24h, revealed a 25-fold increase compared with non-treatment. Most cells can express NMI, and similarity with IFP35,  
20 the expression of NMI increased 2-20 fold after IFN treatment.

[00277] Homo sapiens IFP35 is located in the 17q21, with a NCBI Accession No. NP\_005524.2. The cDNA sequence encodes a 288-amino acid protein with a deduced molecular mass of 31.8 KDa. A natural mutant with methionine at position 128 mutated and/or modified to valine (M128V) exists. Homo sapiens NMI is located on  
25 chromosome 2, with a NCBI Accession No. AAC12949.1, including 307 amino acids.

[00278] IFP35 and NMI are homologous protein. According to the structure prediction, they both include two tandem N-Myc binding protein/IFP35 domain (Nmi/IFP35 domains, NIDs). According to sequence analysis, IFP35 has an L-zip domain at its N-terminus containing the first 80 amino acids, following by two tandem  
30 NID domains covering the 81-170 and 177-268 amino acids, respectively.

[00279] IFP35 and NMI are co-located in the cytoplasm in different cell types by immunofluorescence microscopy techniques. NMI and IFP35 proteins can form a high molecular mass complex (HMMC) of 300-400 kDa through NID domain as determined by native gel electrophoresis and gel filtration which suppress the IFP35 degradation by proteasome. IFP35 and NMI can form speckle-like aggregations after stimulation of IFN $\gamma$  called NMI/IFP35 speckles (NIS). In IFN $\gamma$ -treated apoptotic cells, the NIS dissociates, but the high molecular mass complex does not dissociate.

[00280] It is reported that IFP35 can regard as antiviral protein and inhibit the Bovine Foamy Virus replication. The second NID domain of IFP35 can bind the long terminal repeat sequences of early regulatory protein BTas (Bovine transactivator protein) of Bovine Foamy Virus, thus inhibiting the transcription activity to suppress the virus infecting cells. In addition, high throughput screening showed that IFP35 protein could interact with CLEC4G (C-type lectin domain family member 4 G) in the Ras-MAPK/PI3K pathway.

[00281] NMI can participate in the JAK-STAT pathway induced by IFN. NMI interacts with all STATs except Stat2, and enhances the association of mutual activation factor CBP/p300, thus enhances STATs-mediated transcription level of downstream genes.

[00282] The mRNA level of NMI in malignant breast cancer cell lines decreased 25-45 fold compared to the normal breast cells and the protein level of NMI was also significantly lower than the normal breast cells. Continuous telomerase activity is considered as one of the prerequisite for cancer, and NMI can bind breast cancer susceptibility protein BRCA1 (breast cancer type 1 susceptibility protein) and c-Myc to form a ternary complexes and down-regulate the promoter activity of anthropogenic telomerase reverse transcriptase gene (human telomerase reverse transcriptase gene, hTERT). *hTERT* promoter activity was decreased by about 75% when co-transfected the Flag-Nmi and HA-BRCA1 into cells. In addition, when detected the protein Dkk1 (Dickkopf-1) in the Wnt/ $\beta$ -catenin pathway, the data suggest that overexpression NMI inhibits the Wnt/ $\beta$ -catenin signaling via up-regulation of Dkk1 and retards tumor growth.

[00283] NMI can up-regulate the negative feedback regulating factors SMAD7 in the TGF/SMAD  $\beta$  signaling pathway to inhibit TGF/SMAD  $\beta$  signaling pathways and reduce the aggressiveness and mobility of the breast cancer cells. IFP35 and NMI are associated with inflammatory signals.

5 [00284] Fig. 10 illustrates the process of IFP35 protein purification. (A) SDS-PAGE analysis of IFP35-NID. The left lane: molecule marker. Lane 1: GST-tagged IFP35-NID after purification of affinity chromatography. Lane 2: the mixture of proteins after digestion by PPase. Lane 3: the IFP35-NID eluted from the GST resin column. Lane 4: IFP35-NID purified after size-exclusion chromatography. (B) Size-exclusion  
10 chromatography analysis (superdex-200(16/60)). The elution volume of the peak suggesting the aggregation state of the protein is close to dimer

[00285] Fig. 11 shows the different oligomer states of IFP35. (A) Anion exchange column analysis. (B) Size-exclusion chromatography analysis. The elution volumes of two peaks suggesting different oligomer formation. (C) SDS-PAGE analysis for the  
15 whole process of purification. Lane 1: GST-tagged IFP35. Lane 2: IFP35 eluted from the GST column. Lane 3: IFP35 after digestion by PPase. Lane 4: sample binding to anion exchange column. Lane 5: sample that did not bind to anion exchange column. Lane 6: protein eluted from size-exclusion chromatography superdex-200 (the elution volume of the peak was 72-74ml). Lane 7: protein eluted from size-exclusion  
20 chromatography superdex-200 (the elution volume of the peak was 90-92ml).

[00286] Fig. 12 shows the IFP35-NID crystal. (A) Native octamer crystal. The protein was crystalized in reservoir solution with 0.2 M ammonium sulfate, 0.1M Bis-tris, 25% [w/v] PEG3350, pH5.5, in which the drop was set up at 1 $\mu$ l protein and 1 $\mu$ l reservoir solution. The crystal was grown for 14 days at the temperature of 289k. (B)  
25 Native octamer crystal. The native IFP35-NID (residues 124-220) was crystallized in its octameric form by the hanging drop method with a drop containing 1  $\mu$ L protein and 1  $\mu$ L well solution (0.2 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 0.1 M Bis-Tris-HCl, 20 % [w/v] PEG3350, pH 5.4), with 30% [w/v] d-glucose as an additive, at 16 °C for 1-14 days. (C) Crystals of Se-Met IFP35-NID (residues 124-220) were grown in its dimeric form, with the hanging drop  
30 method from a solution consisting of 1  $\mu$ L protein and 1  $\mu$ L well solution (0.2 M (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 0.1 M Bis-Tris-HCl, 22 % [w/v] PEG3350, pH 5.4) at 16 °C for 7 days.

Scale bar = 100  $\mu\text{m}$ . (D) Crystals of Se-Met IFP35 (residues 124-220) were grown in its dimeric form, with the hanging drop method from a solution consisting of 1  $\mu\text{L}$  protein and 1  $\mu\text{L}$  well solution (0.2 M  $(\text{NH}_4)_2\text{SO}_4$ , 0.1 M Bis-Tris-HCl, 22 % [w/v] PEG3350, pH 5.5) at 16  $^\circ\text{C}$  for 30 days. Scale bar = 200  $\mu\text{m}$ . The crystals are identified with  
 5 arrows.

[00287] **Fig. 13** shows the structure of the dimeric IFP35-NID. (A) and (B) are the whole structure from different views. (C) and (D) indicate residues (shown in sticks) involved in the intra-molecule interaction from different views. H1 indicates  $\alpha$ -helix mainly involved in dimer formation. A single molecule is shown in red or blue.\

10 [00288] **Fig. 14** shows the structure of the octameric IFP35-NID. Monomers are shown in different colors. The octamer were formed with four domain-swapping dimers in the manner similar to the interaction that form the dimer. The amino terminal and carboxyl terminal of molecule A are indicated with A-N and A-C.

[00289] **Fig. 15** shows the structure of dimer with domain-swapping conformation.  
 15 The domain-swapping model of octamer. A-dimer and B-dimer are extracted from the octamer. Red and blue indicate one molecule respectively. Two molecules can bind to each other. The dimers finally form a ring structure of octamer through interaction between the side H1  $\alpha$ -helix of one dimer and the H1 $\alpha$ -helix of its neighbor dimer.

[00290] **Fig. 16** shows the residues of some areas. (A) Residues on the arc  
 20 intersecting surface area (atoms on side chain are labelled and shown in sticks, atoms on the main chain are not labelled). (B) Residues on the inner surface of the octamer ring structure (atoms on side chain are labelled and shown in sticks, atoms on the main chain are not labelled). (C) Residues on the head of a monomer within a dimer (from two molecules, atoms on side chain are labelled and shown in sticks, atoms on the main chain are not labelled). The whole structure are shown in ribbons, different colors indicate  
 25 different molecules.

[00291] **Fig. 17** shows the purification of the recombinant NMI. (A) The SDS-PAGE of the mouse NMI-NID fragment. (B) The size exclusion chromatography results of NMI-NID. (C) The SDS-PAGE of the full length mouse NMI with 6\*His tag. (D)

The size exclusion chromatography result of full length mouse NMI with 6\* His tag at its N terminal.

**[00292] Fig. 18** reveals the expression level of IFP35 and HMGB1 (as a control) when stimulated by salmonella.

5 **[00293] Fig. 19** shows that the abundance of IFP35 changed with time as measured by immunofluorescence when stimulated by salmonella.

**[00294] Fig. 20** shows the abundance of IFP35 secreted to the medium at different periods when cells are infected by the virus. (A) The abundance of secreted IFP35 at different times measured by western blot while the cells are infected by A59 and MHV68  
10 with different MOI. (B) The abundance of secreted HMGB1 at different times measured by western blot while the cells are infected by A59 and MHV68 with different MOI.

**[00295] Fig. 21** shows a model of mouse peritonitis. (A) In the model of peritonitis induced by mouse Standard strains of salmonella typhimurium SR-11, IFP35 was released to the medium when injected live SR-11 to the model. (B) IFP35 are  
15 released to the medium in case of that inflammasome is stimulated by LPS and ATP.

**[00296] Fig. 22** shows the contribution of the IFP35 with different oligomer states during the process of stimulating inflammation. Expression level of some inflammation factors are measured as indicated in the figure.

**[00297] Fig. 23** shows the result of Flow cytometry analysis, which illustrates  
20 octameric IFP35-nid can recruit large amount of neutrophil granulocytes.

**[00298] Fig. 24** shows exogenous octameric IFP35-NID can stimulate NF-κB pathway in macrophages.

**[00299] Fig. 25** illustrates that IFP35 can stimulate inflammation through myd88 signal pathway.

25 **[00300] Fig. 26** shows the levels of IL-1β and TNF among WT, *Tlr9*<sup>-/-</sup> and *Tlr4*<sup>-/-</sup> mouse as induced by IFP35.

**[00301] Fig. 27A** shows the amount of IFP35 in the serum of septic mice. **Fig. 27B** shows the survival rate of the septic mice was increased when administrated with IFP35 monoclonal antibodies.

[00302] Fig. 28 shows that the block of IFP35 attenuated the release of induced IL-6 by LPS in mice.

[00303] Fig. 29 shows the abundance of NMI in cell lysate and supernatant of Thp1 cells stimulated by salmonella.

5 [00304] Fig. 30 demonstrates that mouse source NMI protein can up-regulate the transcription of TNF $\alpha$  and IL-1 $\beta$  in Thp1 cells.

[00305] Fig. 31 shows the SDS-PAGE detection of the aggregation state of NMI by running size exclusion chromatography. The digits labeled on each protein lanes indicate elution volume. Since there is a sustained NMI elution profile, the result  
10 suggested that NMI may exist as different oligomers in mouse serum.

[00306] Fig. 32 shows a secondary structure prediction of human IFP35 (performed by PSIPred (<http://bioinf.cs.ucl.ac.uk/psipred/>)).

[00307] The experimental methods used in the following protocols are all conventional methods unless otherwise specified. All the materials and reagents used in  
15 the following protocols can be commercially obtained unless otherwise specified. The results of IFP35-NID1 and IFP35-NID2 in the following protocols have no significant differences.

[00308] The expression, purification, and crystallization of IFP35 and NMI.

[00309] 1. Plasmid Construction

20 [00310] The cDNA of Homo sapiens IFP35 and Mus musculus NMI were amplified from reverse-transcribed cDNA from THP1 and RAW264.7 cells (Accession No.: NP\_005524.2 and NP\_001135421.1). The sequence of IFP35 was verified to be the wild variant of M128V by DNA sequencing.

[00311] SEQ ID NO: 1 is the cDNA sequence of Homo sapiens IFP35. SEQ ID  
25 NO: 2 is the amino acid sequence of Homo sapiens IFP35. In one aspect, a NID of IFP35 is encoded by nucleic acid 372 to 660 of SEQ ID NO: 1 (from the 5' end), which encodes amino acid residues 124 to 220 of SEQ ID NO: 2 (from the N-terminus). In one aspect, a NID of IFP35 is encoded by nucleic acid 408 to 648 of SEQ ID NO: 1 (from the

5' end), which encodes amino acid residues 136 to 216 of SEQ ID NO: 2 (from the N-terminus).

**[00312]** SEQ ID NO: 3 is the cDNA sequence of *Mus musculus* IFP35. SEQ ID NO: 4 is the amino acid sequence of *Mus musculus* IFP35.

5 **[00313]** SEQ ID NO: 5 is the cDNA sequence of *Mus musculus* NMI. SEQ ID NO: 6 is the amino acid sequence of *Mus musculus* NMI. NMI-NID is encoded by nucleic acid 453 to 750 of SEQ ID NO: 5 (from the 5' end), which encodes amino acid residues 151 to 250 of SEQ ID NO: 6 (from the N-terminus).

10 **[00314]** SEQ ID NO: 7 is the cDNA sequence of *Homo sapiens* NMI. SEQ ID NO: 8 is the amino acid sequence of *Homo sapiens* NMI. NMI-NID is encoded by nucleic acid 465 to 720 of SEQ ID NO: 7 (from the 5' end), which encodes amino acid residues 155 to 240 of SEQ ID NO: 8 (from the N-terminus).

**[00315]** The PCR primers used in this protocol are synthesized by Beijing Synthesis, Sangon Biological Engineering (Shanghai) Co., LTD. The superstar high-fidelity DNA polymerases used were purchased from GenStar Biosolutions Co., Ltd. The restriction endonucleases were bought from Takara biotechnology (Dalian) Co., LTD. The agarose was purchased from Biowest (US). The quick gel extraction kit was purchased from Beijing Transgen Biotechnology Co., LTD. The *E. coli* expression vector pGEX-6p-1 is from GE Healthcare Incorporation. The DH5 $\alpha$ , BL21 (DE3) chemically competent cells and B834 defect competent cells are purchased from Invitrogen Company. DNA sequencing was performed by Beijing Liuhe Genomics Technology Co., LTD.

## **[00316]** 2. Protein Expression and Purification

25 **[00317]** Tryptone and yeast extracts used to cultivate *E. coli* are purchased from Thermo Fisher Oxoid (UK). High pressure homogenization cell cracker EmulsiFlex-C5 used for cell crash is purchased from Avestin (Canada). Prescission protease (Ppase) is purified from a *E. coli* strain. GST affinity column (Glutathione Sepharose 4B), anion exchange column (HiTrap\_Q\_HP\_5 ml), size-exclusion chromatography column (HiLoad\_16/60\_Superdex200\_prep grad and Superdex 200 10/300 GL, 24 ml), protein purification system(ÄKTApurifier) are purchased from GE healthcare life sciences. The

30

NanoDrop 2000 spectrophotometer used for concentration detection is purchased from Thermo (US).

**[00318]** Other biochemical Reagents used are purchased from Sigma Aldrich Company or Beijing Chemical Reagent Company.

5           **[00319]** 3.       Crystallization and Data Collection

**[00320]** Crystallization screening kits and Se-Met are purchased from Hampton Research Incorporation. Buffers including Tris-base, Bis-Tris, and polymer PEG3350 are purchased from Sigma-Aldrich (US). Home Source X-ray diffractometer is purchased from Rigaku Incorporation (Japan).

10           **[00321]** IFP35 Expression, Purification, and Crystallization

**[00322]** For purification, many tags such as 6×HIS, GST, or MBP can be chosen. Take GST-tagged protein as an example, the DNA sequences corresponding to amino acids 1-288, 128-216 and 136-216 of Homo sapiens IPF35 protein were inserted into pGEX-6p-1 vector (Invitrogen) using the BamH I and Xho I sites with an N-terminal  
15   GST tag. All the plasmids were verified by DNA sequencing. The recombinant protein obtained in this way can be cleaved by PreScission Protease (PPase). The recombinant plasmids of full-length IFP35 and other fragments are constructed in the similar way.

**[00323]** pGEX-6p-1 vector has GST tag and PPase cleavage site in front of the multiple cloning site.

20           **[00324]** (1).     Plasmid Construction

**[00325]** Take the cDNA sequence of IFP35 as the template, pairs of primers for PCR amplification were used to get full length IFP35 protein-coding gene, IFP35 NID1 encoding gene, IFP35 NID2 encoding gene respectively, which were digested by BamH1 and EcoRI restriction endonucleases and then ligated to the vector pGEX-6p-1 cleaved  
25   by the same restriction enzymes. Following the ligation reaction, the ligated plasmid DNA was transformed into competent cells such as *E. coli* DH5α (Invitrogen) using heat-shock method. The bacteria were spread thin on the plate with consistent antibiotic resistance (100 µg/ml ampicillin) and plates were incubated at 37°C overnight. The next day, several colonies were picked into 2ml LB medium and cultivated at 37°C for 10h for

plasmid extraction to confirm the presence of the recombinant plasmid by DNA sequencing. Once it has been established that the insert is in the proper orientation and the correct junctions are present, the plasmids are used for protein expression.

[00326] By DNA sequencing, Plasmid 1 is the GST-IFP35 recombinant plasmid containing SEQ ID NO: 1 inserted into pGEX-6p-1 using the BamH I and Xho I sites. Plasmid 2 is the GST-IFP35-NID1 recombinant plasmid containing DNA sequence 372-660 from the 5' end of SEQ ID NO: 1, which is inserted into pGEX-6p-1 using the BamH I and Xho I sites and was added with a termination codon. Plasmid 3 is the GST-IFP35-NID2 recombinant plasmid containing DNA sequence 408-648 from the 5' end of SEQ ID NO: 1, which is inserted into pGEX-6p-1 using the BamH I and Xho I sites and was added with a termination codon.

[00327] The primers for amplification of full-length IFP35:

Upstream primers: 5' GG TAGATCTATGTCAGCCCCACTGGATG3'

Downstream primers: 5' GGT GAATTCCTAGCCTGACTCAGAGGTGAAGACT3'

[00328] The primers for amplification of IFP35-NID1 (amino acids 124-220 of SEQ ID NO: 2):

Upstream primers: 5' GGTGGATCCCCAGGTGATGATGTCCAGCCA3'

Downstream primers: 5' GGTGAATTCTTACTCCCCGTTACATACGGAGAGAC3'

The primers for amplification of IFP35-NID2 (amino acids 136-216 of SEQ ID NO: 2):

Upstream primers: 5' GGTGAATTCAGGGTGTGTTGGTCACTGGATTTCCT3'

Downstream primers: 5' GGTGAATTCTTACTCCCCGTTACATACGGAGAGAC3'

[00328] (2). Protein Expression

[00329] *E. coli* BL21 (DE3) cells were transformed with the recombinant plasmids and grown on LB agar plates containing 100 µg/ml ampicillin. Following overnight incubation at 37 °C, single colonies were transferred into 100ml LB broth containing 100 µg/ml ampicillin and grown overnight at 37 °C with shaking (200 rev min<sup>-1</sup>). The cells were diluted 1/400 in flasks containing 1L LB broth supplemented with 100µg ml<sup>-1</sup> ampicillin and cultivated at 37 °C with continuous shaking (200 rev min<sup>-1</sup>) until an OD<sub>600nm</sub> of 0.6 was reached. The cells were subsequently treated with 1 mM IPTG to induce the expression of recombinant proteins. After 5 h of incubation with continuous

shaking (200 rev min<sup>-1</sup>) at 37°C, the cells were harvested by centrifugation at 4000 rev min<sup>-1</sup> for 30 min at 4 °C.

[00330] Cells containing over-expressed proteins were harvested and resuspended 10/1 in cold 1x PBS buffer (137 mM NaCl, 2.7 mM KCl, 10 mM Na<sub>2</sub>HPO<sub>4</sub>, 1.8 mM KH<sub>2</sub>PO<sub>4</sub>, pH 7.4), and lysed by passing the cell suspension two times through an EmulsiFlex-C5 homogenizer (Avestin) at 5,000 psi and 15,000 psi, respectively. Cell lysate was centrifuged at 30,700 g/4 °C/40 min and collect the supernatant.

[00331] (3). Protein Purification

[00332] 1) Affinity Chromatography

10 [00333] After centrifugation, the supernatant was incubated with Glutathione Sepharose 4B resin (GE Healthcare) at a ratio of 100 ml supernatant per ml resin at 4 °C for 30 - 60 min. After incubation, the GST resin was added to the gravity column for the separation of the resin from the solution mixture, then the column was washed about 10 resin volumes with 1× PBS buffer to bind the GST-tagged proteins on the resin.

15 [00334] Next, the GST resin was equilibrated with a buffer of 150 mM NaCl, 20 mM Tris-HCl, pH 8.0. The recombinant protein was cleaved overnight at 4 °C by PreScission Protease (PPase) and then eluted with 2 column volumes buffer containing 15 mM GSH, 150 mM NaCl, 20 mM Tris-HCl, pH 8.0. at the speed of 1mL/min for 30min. After cleavage and elution, IFP35, IFP35 NID1, and IFP35 NID2 (all the elution  
20 volumes are about 50ml) were obtained.

[00335] 2) Anion-exchange Chromatography

[00336] Proteins digested by protease PPase enzyme were injected into anion exchange column (HiTrap\_Q\_HP\_5 ml, GE Healthcare company), which is fixed to the FPLC purifier (GE Healthcare) and was balanced with 20mM Tris - HCl (PH8.0), 50 mM NaCl before injection. With the elution buffer (20mM Tris HCl (PH8.0), 1 M NaCl) to carry on the gradient elution at the flow rate of 1 ml/min and the elution volume 100ml, samples of the corresponding protein were collected according to the 280 nm and 260nm ultraviolet absorption.

[00337] 3) Size-exclusion Chromatography

[00338] A HiLoad 16/60 Superdex 200 (GE Healthcare) column (prep grade) equilibrated with 150 mM NaCl, 20 mM Tris-HCl, 5% gly, pH 8.0 was used as the next purification step after anion-exchange chromatography. The column was fixed to the FPLC purifier (GE Healthcare) as the same and the flow rate was 1ml/min eluted for  
5 120min. The full-length human IFP35 protein and IFP35-NID were collected at elution volume of about 45 ml and 90-92ml respectively. Finally, the purified IFP35 (elution volume of 45 ml), IFP35 NID1 (elution volume is 90-92 ml), and IFP35 NID2 (elution volume is 90-92 ml) were obtained.

[00339] Size-exclusion chromatography of IFP35-NID1 and IFP35-NID2 are  
10 shown in **Fig. 10**. The elution volumes of IFP35-NID1 and IFP35-NID2 samples are 90-92ml corresponding to the molecular weight 17-43KD. Results of centrifugal analysis and crystal structure indicated that the IFP35-NID1 and IFP35-NID2 were dimers.

[00340] During the purification of IFP35-NID1 and IFP35-NID2, two different oligomer states of the proteins corresponding to the elution volumes of 72ml and 90-  
15 92ml can be obtained (**Fig. 11**). When the proteins were eluted down from the resin column before the digestion of PPase, two peaks, one at volume 72ml and the other at volume 90-92ml, were observed. The peak at volume 72ml corresponded to molecular weight of 70kd - 100kd, and the peak at volume 90-92ml corresponded to the dimer. The peaks of elution volumes of IFP35-NID1 and IFP35-NID2 suggested dimer and octamer.

20 [00341] The SDS-PAGE analysis of IFP35-NID1 and IFP35-NID2 had no significant differences.

#### [00342] 4) Se-Met IFP35-NID Purification

[00343] The purification of Se-Met IFP35-NID was similar to native IFP35-NID. The difference is the application of Escherichia coli B834 (DE3) expression strain (for  
25 Selenomethionine derivative (Se-Met) expression) and the M9 medium with additive Se-Met. Methionine of proteins expressed by b834 with M9 medium was replaced with Se-Met. Crystal obtained in this method can be used to determine crystal phase and further for structure determination.

#### [00344] (4). Protein Crystalization

**[00345]** 1) Crystallization

**[00346]** Both the native and Se-Met IFP35-nid1 and IFP35-nid2 fragments exhibited two oligomeric states on the Superdex 200 column: octamer and dimer. Both forms of protein were used for crystallization screening performed using multiple  
5 conditions from the commercially available kits (Hampton Research). The purified proteins are centrifuged at 14000rpm/10min/4 °C to remove precipitation and bubble. Crystallization trials were carried out by the sitting-drop vapor-diffusion method, mixing 1 µl of the protein sample with an equal volume of screening solution on the Siliconized slides and equilibrated over 200µl of the latter in the reservoir. The crystals are grown  
10 at 16 °C. Crystals of IFP35-NID1 are shown in **Fig. 12**.

**[00347]** 2) Structure Determination and Refinement

**[00348]** In the crystal structure of dimeric IFP35-NID1 or IFP35-NID2 (**Fig. 13**), there are six molecules within each asymmetric unit, and the structure of the six IFP35-NID1 or IFP35-NID2 molecules are the same. Electron density chart can clearly show  
15 that residues of amino acids 136 to 216 in IFP35, but the crystal structure can not clearly completely display the residues (124-135) at the amino terminus and the residues (216-220) at the carboxyl terminus. This phenomenon illustrated that the core of the IFP35 - NID domain structure is mainly composed of amino acids 136-216, the increase or decrease of individual residues at the carboxyl terminal and amino terminal is not  
20 important to the overall structure. Hence, these residues are dispensable in crystal structure analysis and crystallization experiments. In IFP35-NID structure, five antiparallel beta piece (named B1-B5 according to the sequence order respectively) made up the barrel structure, which surrounded an alpha helix (H1) to form a complete barrel structure (**Fig. 13A** and **Fig. 13B**).

25 **[00349]** IFP35-NID2 formed dimer on the interface where alpha helix (H1) located through hydrogen bonds and hydrophobic interaction, van der Waals force and so on (**Fig. 13C** and **Fig. 13D**). The size of the interaction surface calculated by PISA (Protein Interface, Surface and Assemblies) is about 586.5 Å square. Residues mainly participated in dimer formation included Glu150, Glu151, Asp155, Lys158, Ile159,  
30 Arg165 and Asp172 on the alpha helix (H1).

[00350] Eight NID-1 or 2 molecules interacted with each other and formed a ring like structure. The monomer in octamer is quite similar to the monomer in the dimer that the monomer folds into barrel-like structure formed by five  $\beta$ -strands and two  $\alpha$ -helices. Several pairs of residues on helix  $\alpha 1$  in octameric structure play important roles for  
5 interaction between molecules and to mediate dimer formation, which are the same as the dimeric structure. As for the difference, the antiparallel  $\beta 2$  and  $\beta 3$  (177Lue-216Tyr) in dimer is straightened in octamer and inserted into the structure of the adjacent molecule being part of the neighbor NID domain. In this way, two monomers piled up a dimer and formed a domain-swapping conformation between two monomers, which makes it  
10 different from the dimer.

[00351] For clarity, this domain-swapping dimer was named open conformational dimer (o-dimer). By comparison, the above mentioned dimer without domain-swapping is called closed conformational dimer (c-dimer). The o-dimer folded in the same way as c-dimer, so the structure of the swapping NID domain is similar to that of the monomer  
15 in c-dimer (**Fig. 15**). When the adjacent o-dimer interact using the same H1 $\alpha$  helix used in c-dimer, the four o-dimer formed the four-angle star structure (**Fig. 14**). The eight monomer was marked A to G started from N-terminal in the clockwise orientation and the whole structure could be divided into four pairs of o-dimer A/B, C/D, E/F and G/H respectively, among which the structural details of A/B and E/F or C/D and G/H are  
20 similar and structural differences of the loop distinguished A/B and E/F from C/D and G/H. For the four domain-swapping dimers (o-dimer) formed the four-angle star, the diameter of the inner hole is 35 Å and The outer diameter is 80 Å. The octamer formed a new arc intersecting surface through cross-over of two swapping molecules, which is absent from c-dimer. The octameric ring structure was absent from c-dimer. The  
25 structural differences may be the basis for the functional differences between different oligomer states.

[00352] Based on the octameric structure, some residues are observed to be involved in structure formation, and others are observed to be mainly exposed on the surface of the whole structure and are supposed to be interacted with other proteins.  
30 These external residues mainly distributed in three areas as follows:

[00353] The domain-swapping dimer form an arc intersecting surface area on which the dimer provide some residues such as Ser145, Asp172, Val173, Leu177, Arg212, Gln199, Gln207, Gln208, Pro210, Ser214, Thr201, and Tyr216 to form a large exposed surface(**Fig. 16A**). Among them, residues Glu150, Glu175, Leu177, Gln207, and Gln208 are in a more prominent position (**Fig. 16A**).

[00354] Other residues on the inner surface of the ring structure formed by the octameric IFP5-NID can participate in the interaction with other proteins. These residues include Ser145, Arg147, Glu150, Glu151, Val173, Gly206, Gln207, and Gln208. In some aspects, Arg147, Gln207, Gln208, Glu150, and Glu151 provide extended side chains that protrude from the inner surface of octamer ring structure (**Fig. 16B**).

[00355] Based on the structure of the dimer or the octamer, there are some relatively large amino acid residues near the top of the amino terminus and the carboxyl terminus of the  $\beta$  sheet barrel-like structure of the single monomer or domain-swapping monomer; these relatively large amino acid residues extend outwards. These residues can include Arg187, Glu188, Gln192, Gln196, Arg212, and Tyr216, and they are close in distance. Furthermore, some amino acid residues may participate in binding to other proteins, antibodies, or small molecules (**Fig. 16C**).

### [00356] 3) Data Collection and Structure Determination

[00357] The prepared crystal was tested on Rigaku-007 X-ray diffractometer and the diffraction data were collected on beamline BL17U at Shanghai Synchrotron Radiation Facility (SSRF). X-ray diffraction data were calculated with existing common structure determination or analysis software or package including data analysis software such as HKL2000 and Mosflm, Image processing software coot and pymol, Heavy atoms solve software shelx, and Structure refinement software Phenix and CCP4. Mainly used methods here are Single wavelength anomalous scattering and molecular displacement.

[00358] The X-ray diffraction data of Se-Met proteins were collected on beamline BL17U at Shanghai Synchrotron Radiation Facility (SSRF) at wavelengths of 0.979 Å. 720 images were collected with Rotation range 1° per image and were integrated and scaled using HKL-2000. After calculation, the resolution ratio was 2.3 Å and the space group was H3. Selenium-labeled positions elenium-labeled positions in Se-Met protein

were determined using SAD OF SHELXD and six selenium sites were found. AutoSol was used to obtain the initial phase. The model was rebuilt with AutoBuild and was further refined with coot and phenix.refine.

5       **[00359]** The 2.5Å X-ray diffraction data of native octameric crystal was obtained at Shanghai Synchrotron Radiation Facility as the same. Structure of the octameric form was solved by molecular replacement using Phaser-MR in Phenix and the dimeric structure as a search model, and was further refined with coot and phenix.refine.

10       **[00360]** All the results above indicated that the full-length IFP35 or the NID fragments predicted could not express or were expressed as high polymer, making it difficult to get proteins with uniform states. However, the second half of the first NID domain and the first half of the second NID domain (residues 124-220 or 134-216, which are named IFP35-NID1 and IFP35-NID2, respectively, which are collectively referred to as IFP35-NID because of the similar purification results) were expressed and purified well. Using methods above, a large amount of high purity soluble IFP35-NID can be  
15       obtained, especially when they were fused to GST. GST fused protein is referred to as GST-IFP35-NID.

**[00361]** During purification, there were two stable aggregation states of IFP35-NID and well-diffracted crystals with both states can be obtained.

**[00362]** Expression and purification of NMI

20       **[00363]** Take the cDNA sequence of NMI as the template, pairs of primers for PCR amplification were used to get full length human NMI protein-coding genes (1-924 from 5' end of SEQ ID NO: 7), human NMI-NID (residues corresponding to amino acid residues 155-240) encoding gene (465-720 from 5' end of SEQ ID NO: 7), mus musculus NMI encoding gene (1-945 from 5' end of SEQ ID NO: 5), mus musculus NMI-NID  
25       (residues corresponding to amino acid residues 151-250) encoding gene (453-750 from 5' end of SEQ ID NO: 5), respectively, which were digested by BamH1 and XhoI restriction endonucleases and then ligated to the vector pGEX-6p-1 cleaved by the same restriction enzymes. In this way, the recombinant plasmids that express GST-human-NMI, GST-human-NMI-NID, GST-mouse-NMI, and GST-mouse-NMI-NID, with added  
30       termination codon at the 3' terminus, were obtained.

**[00364]** Primers for amplification of full-length human NMI:

Upstream primer: 5' GGT GGATCC ATGGAAGCTGATAAAGATGAC 3'

Downstream primer: 5' GGT CTCGAG CTATTCTTCAAAGTATGCTATGTG3'

**[00365]** Primers for amplification of human NMI (155-240):

5 Upstream primer: 5' GGT GGATCC TCTAAAATGAAAATCAATGTTAC 3'

Downstream primer: 5' GGT CTCGAG TTATTCTGTGTATGGAGAAACAG 3

**[00366]** Primers for amplification of full-length mouse NMI:

Upstream primer: 5' CGCGGATCCATGGATGCTGATAAAGACAAC 3'

Downstream primer: 5' CCGCTCGAGTCATATGGTTTCTCTGGCCTC3'

10 **[00367]** Primers for amplification of mouse NMI (151-250):

Upstream primer: 5' CGCGGATCCGTTTCATGTGGACATTTCTAAAATG 3'

Downstream primer: 5' CCGCTCGAGTCAAACACCTGGTACTTTTCTAAG3'

**[00368]** The mouse and human full length or fragments of NMI were expressed using E. coli prokaryotic expression system. Reagents and expression methods used are  
15 basically the same as IFP35 protein expression.

**[00369]** The protocol for NMI expression was essentially the same with IFP35.

The protocol of NMI purification was essentially the same with IFP35. The purification was divided into 4 steps: GST gravity column affinity chromatography, cleavage of GST with PPase, anion exchange chromatography, and gel filtration chromatography.

20 **[00370]** 1) GST affinity chromatography

**[00371]** After centrifugation, the supernatant was incubated with Glutathione Sepharose 4B resin (GE Healthcare) at a ratio of 100 ml supernatant per ml resin at 4 °C for 1 - 2 h. After incubation, the GST resin was added to the gravity column for the separation of the resin from the solution mixture. Then the column was washed with 1×  
25 PBS buffer until there were no miscellaneous proteins on the resin.

**[00372]** The GST tagged NMI was eluted the elution buffer containing 10 mM GSH and then cleaved by PPase for 8h at 4°C. After cleavage and elution, mouse NMI and mouse NMI-NID were obtained (the elution volumes were about 30ml respectively).

Proteins were eluted with buffer contained 10 mM GSH, 150 mM NaCl, 20 mM Tris-HCl, pH 8.0. at the speed of 1mL/min for 30min.

**[00373]** 2) Size-exclusion chromatography

**[00374]** Proteins digested by PPase were further purified by Size-exclusion chromatography (HiLoad\_16/60\_ Superdex200\_prep grad and Superdex 200 10/300 GL, 24 ml). The column was balanced with 150 mM NaCl, 20 mM Tris-HCl, 5% gly, pH 8.0, and the flow rate was 1ml/min eluted for 120min. The full-length mus musculus NMI protein and NMI-NID were collected at elution volume of about 30 ml and 120 ml respectively. Finally, the purified NMI (elution volume of 30ml), NMI NID (elution volume of 120 ml) were obtained.

**[00375]** The full-length and fragments of mus musculus NMI can be expressed in *E. coli* and purified, but no different oligomer states similar to IFP35-NID were observed in NMI-NID. The full-length NMI and fragments of NMI exhibited polymerized states.

**[00376]** Human NMI and NMI-NID were purified in the same way as mus musculus NMI related proteins.

**[00377]** This example shows that there are two oligomer states of IFP35-NID: dimer and octamer. The two NID domains in IFP35 are probably not two independent domains but two swapping-interacting domains. The two aggregation states of the IFP35-NID indicated that IFP35 may have two different oligomer states in cells which most likely are in accordance with the functions. NMI had similar function with IFP35, and their structures may be similar. However, NMI did not have different oligomer states when compared to IFP35. NMI secreted out from cells was homogenous polymer states. Based on estimation by the weight, the secreted NMI was possibly a dimer or a tetramer.

**[00378]** In the subsequent function experiments, it was found that only octameric IFP35-NID can induce the same inflammation induced by NMI, suggesting that the octameric IFP35-NID possessed same structural features with the full-length IFP35. Therefore, finding amino acids on the octameric surface which are involved in the binding of IFP35 to receptors and blocking the binding may block IFP35 from functioning normally. Similarly, inhibitory antibodies for IFP35 and/or NMI can be

developed to target the amino acid residues that participate in the interaction of IFP35 with its cellular receptors.

### Example 3 Analysis of IFP35 Immune Function

**[00379]** IFP35 causes excessive immune response

5       **[00380]** Homo sapiens IFP35-NID1, IFP35-NID2, or IFP35-NID-H domain (dimer or octamer) can be used as antigen to stimulate mice immune response. Four mice were used for each protein, each mouse immune for four times, 0.2mg protein per body was injected intraperitoneally in mice. Then mice strengthen immune once every 14 days after the first time of immune, a total of four times.

10       **[00381]** In the immune process, using Homo sapiens IFP35-NID dimer to immune mice can get corresponding antibody as expected and NID-H octamer caused swelled belly when immune to the third time and almost all the mice died with swelled belly when immune to the fourth time. The NID-H octamer could stimulate inflammatory response. RAW 264.7 macrophages (from ATCC) were cultured in high-glucose  
15 Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum at 37°C.

**[00382]** IFP35-NID1 and IFP35-NID2 had no significant difference.

**[00383]** IFP35 immunological function in vivo

**[00384]** BMDM cell culture: Kill the mice through breaking the mice neck, take  
20 the two hind legs of mice, soak the legs in 70% alcohol for 1min, and try to eliminate the muscles of the back bone, flush the marrow cavity with PBS. Then centrifuge at 400g for 100 min and carefully remove the supernatant. Erythrocyte cells were collected in cell lysis buffer and then add 10 ml PBS to neutralize the cell lysis buffer. The BMDM cells cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10%  
25 fetal bovine serum, 1% penicillin-streptomycin, 1% L-glutamine and 20 ng/ml MCSF at 37°C.

**[00385]** RAW 264.7 macrophages (from ATCC) were cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum at 37°C.

[00386] 1. Infection by **salmonella** in macrophages264.7 and BMDM causes IFP release

[00387] Cells were washed three times with preheat PBS. Raw 264.7 and BMDM cells were digested by pancreatic enzyme and counted by the hemocytometer to confirm the number of the cells in every hole. 1 ml of preheating DMEM was added to the cell culture dishes. Salmonella SR-11 were centrifuged at 12000RPM for 10 min and washed twice with PBS. Salmonella were suspended and counted by the hemocytometer. The Raw264.7 cells were added the Salmonella according to the multiplex of infection (1:100 or 1:10), while BMDM cells according to the multiplex of infection (1:10 or 1:2). Cell culture dishes were centrifuged at 1500RPM for 10 min at room temperature which is benefit for bacteria to adsorb on the cells. When Raw264.7 cells were infected with Salmonella for 1 hour and BMDM were infected with Salmonella for 0.5 hours, the salmonella in the cell culture were removed and 100 µg/ml Amikacin DMEM was added in the medium. When Raw 264.7 cells were infected with Salmonella for 3 hour and BMDM cells were infected with Salmonella for 1 hour, 10 µg/ml Amikacin DMEM was added in the medium. Secretory protein in the cell culture supernatant was collected after Raw 264, 7 and BMDM cells were infected with Salmonella for 1, 3, 5, 9 h or 0.5, 1, 2, 4h, respectively.

[00388] Concentrate the cell culture supernatant and extract the whole cell lysates after cells were infected with Salmonella: Concentrate the cell culture supernatant: (1)The cell culture supernatant was added 0.1 volumes of ice-cold 100% TCA and placed on ice for 2h. (2) Centrifuge at12,000 g for 30 min at 4°C. (3) Carefully remove the supernatant, wash the sediment twice with cold acetone. (4)Centrifuge at 12,000g for 10 min at 4°C. (5) The sediment was heated at 95°C for 5 minutes in the 30ul 1 x SDS-PAGE loading buffer.

[00389] Extract the whole cell lysates after cells were infected with Salmonella: (1) Collect the cells: Remove the cell culture supernatant, wash the cells twice with PBS, add 1ml PBS to the cell culture dishes, scrape the cells with cell scratcher, transfer the cell suspension to 1.5 ml tube with pipet, centrifuge at 1500RPM for 5 min and remove the supernatant. Cell sedimentation is used to extract total protein. (2)Cell lysis: Take appropriate amount of RIPA lysis buffer, add PMSF to the lysis buffer with a final

concentration of 1 mm, proteinase inhibitors cocktail (Roche). Add 150ul RIPA lysis buffer to each hole in the cell culture dishes and split the cells for 15 min on ice.

(3) Collect the cell lysis buffer: centrifuge at 12000RPM for 5 min at 4°C after cells were splitted completely and transfer the supernatant to a new tube. (4) Boil the sampe: The  
5 cell lysis buffer was heated at 95°C for 5 minutes in the 150ul 2 x SDS-PAGE loading buffer.

[00390] As shown in **Fig. 18**, there is no or little IFP35 in the in the cell culture supernatant. However, within 1 hour after stimulated by Salmonella, released IFP35 could be detected in the culture supernatant of RAW 264.7 cells. In the following several  
10 hours, they cumulated in the culture in time-dependent manner. In contrast, the release time of IFP35 is earlier than the known danger signals HMGB-1. And the protein level of IFP35 in cells decrease (**Fig. 18A**). Same results were obtained when BMDM and PBDM cells were used (**Fig. 18B** and **Fig. 18C**).

[00391] To better observe the change of intracellular IFP35 protein content after  
15 infected with salmonella, immunofluorescence method was used to detect the IFP35 protein. As shown in **Fig. 19**, IFP35 was stained by red and DAPI was stained by blue. The two different schemes of infection, which is the ratio of the cells number to MOI is 1:2 or 1:10 respectively, were used to observe the change of IFP35 protein content from 0 to 3 hours. It was found that the intracellular IFP35 protein content gradually reduced  
20 as the extension of time, and the IFP35 reduced faster in the higher MOI infected cells. It further proved that the infection induced IFP35 accumulation was not occurring inside the cells, but largely secreted to the outside of the cells. This result is in agreement with the previous research that the change of the intracellular IFP protein content.

## [00392] 2. The release of IFP35 in the virus infection

25 [00393] Experimental method: The Raw264.7 cells were added the virus according to the multiplex of infection. Collect the cell culture supernatant in time-dependent manner. Centrifuge at 200g for 30 min at 4°C. Collect the supernatant by trichloroacetic acid (TCA), western blot.

[00394] Whether DNA virus (MHV68), or RNA viruses (A59) infect the  
30 Raw264.7 in vitro, IFP35 release as early as 8 hours after infection when the multiplex of

infection(MOI) is 0.2. Under the same conditions, HMGB1 is not release .Increase the multiplex of infection to 5, HMGB1 release obviously after infection for 24h. Similar with bacterial infected cells in vitro, IFP35 release earlier than HMGB1, illustrated that IFP35 is a very important danger signal molecules.

### 5 [00395] 3. The model of mice peritonitis

[00396] Fig. 21A shows that in the standard strains of salmonella SR-11 caused mice peritonitis model, IFP35 could be released. Injecting with Live salmonella (Live SR-11) caused mice peritonitis, IFP35 could be released to the mice ascites. While injecting with symbiotic *E. coli* (*E. coli* Stable3) and heat death of salmonella (HK SR-11, 10 heat killed SR-11) does not cause inflammation and IFP35 could not be detected. The result illustrated that IFP35 has correlation with the inflammatory response.

[00397] The establishment of the standard strains of salmonella SR-11 caused mice peritonitis model. Wash the mice ascites with 8ml PBS after inject bacteria for 2 h, 4 h, 8 h, extract 4ml ascites wash buffer. Trichloroacetic acid (TCA) precipitation and 15 detect the IFP35 by western blot. (1) C57 / B6 mice, male, 8 to 10 weeks, weight about 20 g, ban water and food for 4 hours. (2) Each mice inject  $2 \times 10^5$  bacteria. (3) Wash the mice ascites with 8ml PBS after inject bacteria for 2 h, 4 h, 8 h, extract 4ml ascites wash buffer. (4)Centrifuge at 200g for 10 min at 4°C, collect the cell culture, Trichloroacetic acid (TCA) precipitation. (5) Detect the IFP35 by western blot.

20 [00398] As shown in Fig. 21B, when LPS, ATP activate inflammasome, IFP35 could be released. Experimental Method: (1) Raw264.7 cells were stimulated by LPS (1 µg/ml) for 4 h; (2) Cells were continue stimulated by ATP (5 mM) for 10, 30, 60 min; (3) Centrifuge at 200g for 10 min at 4°C, collect the cell culture, Trichloroacetic acid (TCA) precipitation; (4) Detect the IFP35 by western blot.

### 25 [00399] IFP35 in inflammatory response

[00400] 1. IFP35 induces the **production** of inflammatory cytokines

[00401] Experiment procedure: Wipe out the endotoxin of IFP35 dimer and octamer in the example 1, add them to the BMDM cell culture medium (final

concentration of 5, 25, 50  $\mu\text{g/ml}$ ), stimulate for 4 hours and detect the known pro-inflammatory factors, TNF- $\alpha$  and IL-1 $\beta$  using Q-PCR, GAPDH as internal.

**[00402]** Q-PCR amplification primers:

**[00403]** IL-1 $\beta$ :

5 Sense: 5'AAGGAGAACCAAGCAACGACAAAA 3'

Antisense: 5'TGGGGAACTCTGCAGACTCAAAC 3'

**[00404]** TNF- $\alpha$ :

Sense: 5'CCAGTGTGGGAAGCTGTCTT 3'

Antisense: 5'AAGCAAAAGAGGAGGCAACA 3'

10 **[00405]** GAPDH:

Sense: 5'AGGTCGGTGTGAACGGATTTG 3'

Antisense: 5'TGTAGACCATGTAGTTGAGGTCA3'

**[00406]** As shown in **Fig. 22**, the known pro-inflammatory factors, TNF- $\alpha$ , IL-1 $\beta$ , iNOS and CD86 can be up-regulated in the presence of NID-H octamer in BMDM cells,  
15 but the NID-H dimer did not have this effect. The result demonstrated that different aggregation states of IFP35-NID have different effect.

**[00407]** IFP35 NID1 and IFP35 NID2 use the same method and the results have no significant difference.

**[00408]** **2. IFP35 leads to excessive inflammatory response**

20 **[00409]** IFP35-NID dimer and octamer were injected into mouse peritoneal. 8 hours later, IFP35-NID octamer caused an acute inflammatory response, manifested by neutrophil accumulation. This effect should be the reason why the mice abdominal distension and death in the early inflammatory response. The result demonstrated that IFP35-NID octamer not only induce the macrophage to produce inflammation factor in  
25 vitro, but also have the ability to regulate inflammatory responses in mice.

**[00410]** **3. IFP35 activates the NF- $\kappa$ B pathway in macrophages**

[00411] The activation of NF- $\kappa$ B by IFP35-NID octamer was observed. NF- $\kappa$ B pathway is an important pathway of macrophage activation. Detection method: Add endotoxin free protein of IFP35-NID dimer and octamer to the Raw264.7 cells, stimulate for 15, 30, and 60min. The cells were collected in the RIPA (Proteinase inhibitor cocktail, Roche) buffer for 30min on ice. Centrifuge at 12,000rpm for 10 min at 4°C. Collect the supernatant and heat at 95°C for 10 minutes in the SDS-PAGE loading buffer. Save the sample at -70 degrees. Western blot was used to detect the phosphorylation of suppressor I $\kappa$ B $\alpha$  in the NF- $\kappa$ B signaling pathway. Phospho-I $\kappa$ B $\alpha$  and I $\kappa$ B $\alpha$  antibody were from CST. Results as shown in **Fig. 24**, after adding the prokaryotic expressed different polymeric state of endotoxin free protein, expression of the octamer of IFP35-NID recombined protein increased the phosphorylation of I $\kappa$ B $\alpha$ , but reduced the total I $\kappa$ B $\alpha$  protein level. It suggested the octamer of IFP35-NID recombined protein could activate NF- $\kappa$ B signaling pathway. Taken together, these results indicated that the octamer may induce macrophage activation to produce a large number of inflammatory cytokines by activating NF- $\kappa$ B signaling pathway, but not the dimer.

[00412] The cell surface receptor of IFP35

[00413] Since IFP35 induced inflammatory response by secreted to extracellular or in body fluids, the example aims to identify the cell surface receptor that mediated IFP35 activity, and then to detect the biological function of TLR-Myd88 pathway in this process.

[00414] BMDM cell culture: Kill the mice through breaking the mice neck, take the two hind legs of mice, soak the legs in 70% alcohol for 1min, and try to eliminate the muscles of the back bone, flush the marrow cavity with PBS. Then centrifuge at 400g for 100 min and carefully remove the supernatant. Erythrocyte cells were collected in cell lysis buffer and then add 10 ml PBS to neutralize the cell lysis buffer. The BMDM cells cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum, 1% penicillin-streptomycin, 1% L-glutamine and 20 ng/ml MCSF at 37°C.

[00415] IFP35 or NMI stimulation: Add IFP35-NID dimer, octamer or NMI (5, 25, or 50 $\mu$ g/mL) to stimulate the BMDM cells for 4h, IL-1 $\beta$ , and TNF- $\alpha$  were detected by Q-PCR.

[00416] Extract the cell total RNA: The total RNA was extracted from BMDM cells using the RNA extract Kit from KangWei Company(Cat No. CW 0597). The total RNA was extracted from RAW 264.7 cells using Trizol reagent (Invitrogen).

[00417] Reverse transcription: The first strand of cDNA was synthesized from 1 $\mu$ g of total RNA using PrimeScript™ II 1st Strand cDNA Synthesis Kit (Cat.No.6210A).Real-time RT-PCR was performed using the SYBR® Premix Ex Taq™ (Tli RNaseH Plus) and ROX plus Q-PCR kit (Cat.NO.RR42LR). As shown in **Fig. 25**, treating Myd88 knock-out BMDM cells using IFP35-NID protein, the activity of NID-H were sharply reduced in these cells, IL-1 $\beta$  (**Fig. 25A**) and TNF- $\alpha$ (**Fig. 25B**) could not be induced by IFP35-NID. IFP35 likely binds to the TLR receptor in the cell surface to active NF- $\kappa$ B through Myd88 dependent pathway and produce inflammation factors.

[00418] TLR-4 and TLR-9 are the two main cell surface receptor proteins which can induce the inflammation response. As shown in **Fig. 26**, TLR4 mediate the increase of IL-1 $\beta$  (**Fig. 26A**) and TNF- $\alpha$  (**Fig. 26B**) through the IFP35-NID. Compared the NID-H octamer could up-regulated the TNF- $\alpha$  and IL-1 $\beta$  in WT, TLR9 -/- and TLR4 -/- mice BMDM cells, IFP35 family proteins can also be identified by TLR4, directly or indirectly.

**[00419] IFP35 monoclonal antibody in treating the diseases caused by excessive inflammatory response such as sepsis**

[00420] Because IFP35-NID can activate macrophages and induce inflammation response, IFP35 may play a role in sepsis in which IFP35 can exacerbate cytokine storm in sepsis and lead to the death of mice.

**[00421] 1. The expression of IFP35 in sepsis mice**

[00422] The establishment of LPS-induced shock model: (1) the B6 / C57 mice were banned water and food for 1 night; (2) LPS (5 mg and 10mg per kg body weight) was injected intraperitoneally in mice the next day morning; (3) Take the blood using the

capillary 3 hours after injection; (4) Remove the mice eye and take blood 6 hours after injection.

[00423] Detect the concentration of IFP35 in the LPS-induced shock model using ELISA. (1)Antibodies are coated: purified monoclonal antibody of IFP35 1D7 diluted  
5 with PBS to 2 mg/ml, 100  $\mu$ l per hole in enzyme label plate, 4  $^{\circ}$ C, over night; (2)Wash: wash three times with PBST (0.05% Tween-20); (3)Block: PBST (0.05% Tween-20) containing 2%BSA place on shaking table to fade, room temperature, 1h; (4)Add diluted standard and samples, 100 $\mu$ l per hole, 4  $^{\circ}$ C, over night; (5)Wash: wash three times with PBST (0.05% Tween-20), wash twice with ddH<sub>2</sub>O. (6) Color:Add 100 $\mu$ l TMB to each  
10 well, avoid light, place on shaking table for 10-20min. (7) Stop the reaction: Add 50 $\mu$ l 2M H<sub>2</sub>SO<sub>4</sub> to each well; (8)Enzyme label plate, 450nm scan OD.

[00424] Quantitative detecting the IFP35 concentration in blood of sepsis mice model shows high concentration of IFP35 in the blood of LPS-induced sepsis mice, which reaches nanogram level (about 8ng). But the level of HMGB1 is pg600-800  
15 according to the previous paper. And it depends on the time or dose of LPS injection (for 3 hours and 6 hours, LPS dose of 5 mg and 10 milligrams per kilogram of body weight).

[00425] 2. Increased survival rate of septic mice by injecting IFP35 monoclonal antibodies

[00426] IFP35 monoclonal antibody 1D7 was injected into mice. As shown in **Fig.**  
20 **27**, IFP35 monoclonal antibody could increase the survival rate of septic mice. The results demonstrated that IFP35 monoclonal antibody 1D7 could protect the mice from death effectively in bacteremic model. The medial death time of mice that accepted the treatment of 1D7 (n=10) was 107 hours, while it was 50 hours of the control.

[00427] 3. For detecting the expression of inflammation factor IL-6 in mice after  
25 IFP35 monoclonal antibody injection, the specific method was as follows: IL-6 ELISA kit was from BD Biosciences, the detailed operating information see the specification of the product.

[00428] Results as shown in **Fig. 28**, for the mice with severe sepsis, the IL-6 protein was highly expressed in body fluids of mice by injecting IFP35 antibody (1D7) but not in non-injected.

[00429] IFP35 and anti-tumor treatment

5        [00430] The protein level of NMI is reduced in some tumors. Since IFP35 and NMI highlighted a variety of functions in biological progressions, such as promoting inflammatory response of biological organisms, activating immune system, and promoting the release of inflammatory cytokines, the injection of purified IFP35 or NMI into blood may activate and/or enhance anti-tumor treatments. Therefore, IFP35 or NMI  
10      protein might be a promising anti-cancer drug.

#### Example 4      NMI immune function analysis

[00431] NMI cause excessive immune response

[00432] Full length NMI and NMI-NID used as antigen to stimulate mice immune response. Four mice were used for each protein, each mouse immune for four times,  
15      0.2mg protein per body was injected intraperitoneally in mice. Then mice strengthen immune once every 14 days after the first time of immune, a total of four times.

[00433] In the immune process, using Mouse NMI-NID to immune mice can cause swelled belly when immune to the third time and almost all the mice died with swelled belly when immune to the fourth time. So it is difficult to get antibodies in mice. Thus,  
20      the NID-H octamer may stimulate inflammatory response.

[00434] NMI immunological function research in vivo

[00435] 1. NMI is secreted to the extracellular space when cells are infected by bacteria

[00436] The NMI and IFP35 are homologous protein. IFP35 and NMI can  
25      assemble into high molecular mass complex (HMMC). In this example, NMI was detected.

[00437] BMDM cell culture: Kill the mice through breaking the mice neck, take the two hind legs of mice, soak the legs in 70% alcohol for 1min, and try to eliminate the muscles of the back bone, flush the marrow cavity with PBS. Then centrifuge at 400g for

100 min and carefully remove the supernatant. Erythrocyte cells were collected in cell lysis buffer and then add 10 ml PBS to neutralize the cell lysis buffer. The BMDM cells cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum, 1% penicillin-streptomycin, 1% L-glutamine and 20 ng/ml MCSF at  
5 37°C.

[00438] RAW 264.7 macrophages (from ATCC) were cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum at 37°C.

[00439] 2. Infection by **salmonella** in THP1 cells and detection of the protein level  
10 of NMI in the cell lysate and supernatant.

[00440] Experimental method: Collect the THP1 cells in the 15ml tube, centrifuge at 500g for 5 min, remove the supernatant, wash the cells with preheat PBS, centrifuge at 500g for 5 min, remove the supernatant. Suspend the cells with DMEM and count the cells by the hemocytometer. Add  $3 \times 10^5$  cells in every hole. Add 1 ml of preheating  
15 DMEM to the cell culture dishes. Salmonella SR – 11 were centrifuged at 12000RPM for 10 min and washed twice with PBS. Salmonella were suspended and counted by the hemocytometer. The THP1 cells were added the Salmonella according to the multiplex of infection (1:100 or 1:10). Cell culture dishes were centrifuged at 1500RPM for 10 min at room temperature which is benefit for bacteria to adsorb on the cells. When THP1  
20 cells were infected with Salmonella for 1 hour, remove the salmonella in the cell culture and add 100 µg/ml Amikacin DMEM in the medium. When THP1 cells were infected with Salmonella for 3 hour, add 10 µg/ml Amikacin DMEM in the medium. Secretory protein in the cell culture supernatant was collected after THP1 cells were infected with Salmonella for 1, 3, 5, and 9h.

25 [00441] Concentrate the cell culture supernatant and extract the whole cell lysates after cells were infected with Salmonella: Concentrate the cell culture supernatant: The cell culture supernatant was added 0.1 volumes of ice-cold 100% TCA and placed on ice for 2h. Centrifuge at 12,000g for 30 min at 4°C. Carefully remove the supernatant, wash the sediment twice with cold acetone. (4)Centrifuge at 12,000g for 10 min at 4°C. (5)

The sediment was heated at 95°C for 5 minutes in the 30ul 1 x SDS-PAGE loading buffer.

[00442] Extract the whole cell lysates after cells were infected with Salmonella: (1) Collect the cells: Collect the THP1 cells in the 15ml tube, centrifuge at 500g for 5 min, 5 remove the supernatant, wash the cells with preheat PBS, centrifuge at 500g for 5 min, remove the supernatant. Cell sedimentation is used to extract total protein. (2) Cell lysis: Take appropriate amount of RIPA lysis buffer, add PMSF to the lysis buffer with a final concentration of 1 mm, proteinase inhibitors cocktail (Roche). Add 150ul RIPA lysis buffer to each hole in the cell culture dishes and split the cells for 15 min on ice. 10 (3) Collect the cell lysis buffer: centrifuge at 12000RPM for 5 min at 4°C after cells were split completely and transfer the supernatant to a new tube. (4) Boil the sample: The cell lysis buffer was heated at 95°C for 5 minutes in the 150ul 2 x SDS-PAGE loading buffer.

[00443] THP1 cell culture: THP1 cells were cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum at 37°C.

15 [00444] As shown in **Fig. 29**, there is no or little NMI in the in the cell culture supernatant. However, within 1 hour after stimulated by Salmonella, released NMI could be detected in the culture supernatant of THP1 cells. Meanwhile, the NMI in the cells does not change much. The result demonstrated that NMI could be secreted into the extracellular when infected by the bacteria.

20 [00445] NMI in inflammatory response

[00446] Add the mouse full length NMI to the THP1 cell culture medium (final concentration of 5, 25, 50 µg/ml), stimulate for 4 hours and detect the known pro-inflammatory factors, TNF-α and IL-1β.

25 [00447] Raw264.7 cell culture: Cells were cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum at 37°C.

[00448] Extract the cell total RNA: The total RNA was extracted from BMDM cells using the RNA extract Kit from KangWei Company (Cat No. CW 0597). The total RNA was extracted from RAW 264.7 cells using Trizol reagent (Invitrogen).

[00449] Reverse transcription: The first strand of cDNA was synthesized from 1 $\mu$ g of total RNA using PrimeScript™ II 1st Strand cDNA Synthesis Kit (Cat.No.6210A).Real-time RT-PCR was performed using the SYBR® Premix Ex Taq™ (Tli RNaseH Plus) and ROX plus Q-PCR kit (Cat.NO.RR42LR).

5        [00450] As shown in **Fig. 30**, add control, LPS, NMI protein (5 $\mu$ g/mL, 25 $\mu$ g/mL or 50 $\mu$ g/mL), the known pro-inflammatory factors, TNF- $\alpha$  and IL-1 $\beta$  can be up-regulated in the presence of NMI in THP1 cells. The result demonstrated that NMI also could induce other inflammatory factors similar with IFP35.

10       [00451] NMI-NID1 and full length NMI were tested using the same method and the results are not significantly different.

[00452] **NMI protein aggregation state**

15       [00453] The aggregation state of NMI that secreted by cells after stimulated by bacteria were tested. NMI can be secreted into cell culture medium when salmonella infected the THP1 cells. As shown in **Fig. 31**, 10 ml cell culture medium which contains the secreted NMI concentrate to 2ml using Millipore concentration tube. The samples separated by chromatographic separation using Superdex S-200 molecular sieve column. And then, the eluted samples were tested by western and the elution peak position of NMI was tested by NMI antibody. The numbers in the figure is the volume of the elution buffer. It shows that the top of NMI elution peak primary at 78ml, the corresponding  
20       molecular weight is from 70KDa to 140KDa.

[00454] **The cell surface receptor of NMI**

[00455] Since NMI can be secreted out of the cell and into body fluid to induce inflammation response, this example aims to identify the cell surface receptor of NMI and then to detect the biological function of TLR-Myd88 pathway in this process.

25       [00456] BMDM cell culture: Kill the mice through breaking the mice neck, take the two hind legs of mice, soak the legs in 70% alcohol for 1min, and try to eliminate the muscles of the back bone, flush the marrow cavity with PBS. Then centrifuge at 400g for 100 min and carefully remove the supernatant. Erythrocyte cells were collected in cell lysis buffer and then add 10 ml PBS to neutralize the cell lysis buffer. The BMDM cells

cultured in high-glucose Dulbecco's modified Eagle's medium supplemented with 10% fetal bovine serum, 1% penicillin-streptomycin, 1% L-glutamine and 20 ng/ml MCSF at 37°C.

[00457] Extract the cell total RNA: The total RNA was extracted from BMDM  
5 cells using the RNA extract Kit from KangWei Company (Cat No. CW 0597). The total RNA was extracted from RAW 264.7 cells using Trizol reagent (Invitrogen).

[00458] Reverse transcription: The first strand of cDNA was synthesized from 1µg of total RNA using PrimeScript™ II 1st Strand cDNA Synthesis Kit (Cat.No.6210A).Real-time RT-PCR was performed using the SYBR® Premix Ex Taq™  
10 (Tli RNaseH Plus) and ROX plus Q-PCR kit (Cat.NO.RR42LR).

**[00459] NMI monoclonal antibody in treating the diseases caused by excessive inflammatory response such as sepsis**

[00460] Because of the high similarity of NMI structure and function with IFP35, and the cooperation of these two proteins, inhibition of NMI may have the same effect  
15 with IFP35 to inhibit the NMI-induced overactive immune response. Therefore, the NMI inhibitor is expected to treat septicemia, virus infection-induced NMI over-expression, and autoimmune diseases and so on, like IFP35 inhibitors.

**[00461] The expression of NMI in sepsis mice**

[00462] The establishment of LPS-induced shock model: (1) the B6 / C57 mice  
20 were banned water and food for 1 night; (2) LPS (5 mg and 10mg per kg body weight) was injected intraperitoneally in mice the next day morning; (3) Take the blood using the capillary 3 hours after injection; (4) Remove the mice eye and take blood 6 hours after injection.

[00463] Detect the concentration of NMI in the LPS-induced shock model using  
25 ELISA. Quantitative detecting the NMI concentration in blood of sepsis mice model, it shows high concentration of NMI in the blood of LPS-induced sepsis mice, that reaches nanogram level. But the level of HMGB1 is pg600-800 according to the previous paper. And it depends on the time or dose of LPS injection (for 3 hours and 6 hours, LPS dose

of 5 mg and 10 milligrams per kilogram of body weight). NMI monoclonal antibody can increase the survival rate of septic mice.

**[00464]** Overreaction for immune response

5 **[00465]** The different length of purified proteins that expressed by exogenous prokaryotic system, were injected into mice abdominal cavity, 100mg protein per mouse, after eliminating the endotoxin. The recruitment of some immune cells by IFP35 and NMI in mice abdominal cavity, such as neutrophils, was detected by flow cytometry.

**[00466]** NMI in cancer treatment

10 **[00467]** Based on the present disclosure of IFP and NMI, drugs can be developed to treat sepsis, inflammation storm, autoimmune diseases and other diseases, which are associated with abnormally high levels of IFP35 and/or NMI expression, secretion, and/or activity. In some aspects, provided herein are (1) small compounds or peptides to inhibit IFP35 and NMI release; (2) antibodies to IFP35 and/or NMI to suppress the generation and function of IFP35 and NMI; (3) a small molecule to interference the  
15 formation of IFP35 or NMI polymer in vivo; (4) agents that inhibit the secretion of interferon to reduce the generation of IFP35; (5) agents that inhibit the interaction between IFP35 and NMI with their cell surface receptors to suppress IFP35 and/or NMI function; (6) agents that inhibit the interaction of IFP35 and NMI with their receptors to suppress their function. Likewise, under the condition of low immunity or immune  
20 suppression, such as in tumor tissues, the function of immune response could enhance by supply IFP35 or NMI to the organism or a part of it.

**[00468]** The techniques to achieve this purpose may: (1) directly inject IFP35 or NMI protein or their targeted derivative into the organism; (2) directly offer a derived peptide or small molecule by IFP35 or NMI or their targeted derivative. In addition, in  
25 terms of diagnosis of sepsis and inflammatory response, ELISA kits can be developed. Because it is only a fragment of IFP35 that expressed and crystallized in vitro, the full length of IFP35 may not have to form polymers to perform the function to induct cytokine storm. In mice, using the neutralizing monoclonal antibody of IFP35 could inhibit cytokine storm. This result suggests that IFP35 is a factor which causes cytokine  
30 storm no matter what polymeric state it exists. Therefore, IFP35 might be a primary

reason that causes cytokine storm, which makes it become a target for inhibition of cytokine storm. Thus, the proper use of IFP35 monoclonal antibody or other inhibitory molecules of IFP35 could be helpful to inhibit cytokine storm. Because of the high similarity of NMI structure and function with IFP35, and the cooperation of these two proteins that both secrete to the outside of the cells, and the functions like induce the generation of cell inflammation factors, it indicate that NMI may have the same or similarity function with IFP35. Therefore, the inhibition of NMI could also inhibit the inflammation, and also be able to protect animals from overreacted inflammation response. Therefore, in some aspects, death or injury induced by overproduction of NMI or NMI mediated excessive inflammatory response can be avoided. Due to the less expression of NMI in some tumors, supplement of NMI provides an anti-tumor function. The similarity of NMI with IFP35 shows the two aspects of function, one is to enhance the immunity of organism to inhibit cancer or avoid infection, second is that they could become the target of tumor treatment to curb excessive immune function by inhibiting their activity, and then to prevent and treat the organism damage by inflammatory outbreak. Taken together, these results indicate the crucial function to induce inflammation response by IFP35 and NMI expression, and further demonstrate their significant value in medical science.

#### **Example 5    Generation of IFP35 antibody**

**[00469]** To clone the sequences of the variable regions in the antibody, 7 pairs PCR primer were designed for the light chains variable region (VL), according to the 6 families of light chain. Primers P1-P7 are 7 upstream primers starting from FWR1 region, and P8 is the downstream primer ended at the end of FWR4 region. According to the 4 families of heavy chains variable regions, 5 pairs of heavy chain VH primers were designed for PCR amplification. Primers P9-P12 are the upstream primers, starting from FWR1 region; Primer 13 is the downstream primer ended at the end of FWR4.

**[00470]** The sequences of these primers are listed below:

|    |                         |
|----|-------------------------|
| P1 | GACATTGTGATGWCACAGTCTCC |
| P2 | GATRTTKTGATGACYCARRCTCC |
| P3 | GACATTGTGCTGACCCAATCTCC |
| P4 | GACATTGTGCTGACACAGTCTCC |
| P5 | SAAAWTGTKCTCACCCAGTCTCC |
| P6 | GAYATYMGATGACMCAGWC     |

P7 GAYATTGTGATGACMCAGWCT  
 P8 (VL-R) TTTBAKYTCCAGCTTGGTSCC  
 P9 AGGTGCAGCTKMAGGAGTCAGG  
 P10 AGGTYCAGCTKCARSARTCT  
 5 P11 AGGTCCARCTGCAGCAGYCT  
 P12 AGGTGMAGCTKGWGGARTCTGG  
 P13 (VH-R) TGGTCGACGCTGAGGAGACGGT

[00471] IFP35 antibody hybridoma cells were cultured and collected, using Trizol reagents (Life Technologies Inc.) to extract total RNA. Then using the extracted RNA as  
 10 template to synthesize cDNA by using cDNA synthesis reagent kit from Life Technologies Inc. The PCR fragment products of light chain variable regions and heavy chain regions were recovered from the agarose gel and then cloned to T-vector (GE Healthcare). These constructs were transformed to E.coli DH5 $\alpha$  competent cells and single clones were selected and sequenced.

15 [00472] Sequencing comparison results of our heavy and light chains comparing with sequences in NCBI BLAST shows that our sequences harbor similar feature of mouse IgG.

[00473] GACATTGTGATGACCCAGTCTCCAGCAATCATGTCTGCATCTCC  
 AGGGGAGAAGGTCACCATGACCTGCAGTGCCAGCTCAAGTGTAAGTTACATG  
 20 CACTGGTACCAGCAGAAGTCAGGCACCTCCCCCAAAGATGGATTTATGACA  
 CATCCAAACTGGCTTCTGGAGTCCCTGCTCGCTTCAGTGGCAGTGGGTCTGGG  
 ACCTCTTACTCTCTCACAATCAGCAGCATGGAGGCTGAAGATGCTGCCACTT  
 ATTACTGCCAGCAGTGGAGTAGTAACCCACCCATCACGTTTCGGTGCTGGCAC  
 CAAGCTGGAAATCAAA (SEQ ID NO: 12)

25 Mus musculus isolate AIDKO-glmnB-1 immunoglobulin kappa light chain variable region gene, partial sequence  
 Sequence ID: [gi|EE543882.1](#) Length: 444 Number of Matches: 1

| Range 1: 31 to 329 GenBank Graphics |                                                                   |              |           | ▼ Next Match ▲ Previous Match |
|-------------------------------------|-------------------------------------------------------------------|--------------|-----------|-------------------------------|
| Score                               | Expect                                                            | Identities   | Gaps      | Strand                        |
| 347 bits(296)                       | 3e-152                                                            | 298/299(99%) | 0/299(0%) | Plus/Plus                     |
| Query 18                            | CAGACTCCACAAATCATGTCTGCATCTCCAGGGGAGAAGGTCACCATGACCTGCATGTC       | 75           |           |                               |
| Subject 31                          | CAGCTCCACGCAATCAATGTCTGCATCTCCAGGGGAGAAGGTCACCATGACCTGCATGTC      | 80           |           |                               |
| Query 76                            | AGTCAAGTGTAAATTACATGCTACTGTTACTGCAAAAGTCAAGTCACTTCTTCAAAAG        | 135          |           |                               |
| Subject 91                          | AGTCAAGTGTAAATTACATGCTACTGTTACTGCAAAAGTCAAGTCACTTCTTCAAAAG        | 130          |           |                               |
| Query 136                           | TGACTTTATGACATCCAACTGCTTCTGGAGTCCCTGCTCGCTTCAGTGGCAGTGGGTCTGGG    | 195          |           |                               |
| Subject 151                         | TGACTTTATGACATCCAACTGCTTCTGGAGTCCCTGCTCGCTTCAGTGGCAGTGGGTCTGGG    | 210          |           |                               |
| Query 196                           | TCTGAGCTCTTACTCTCTCACAATCAGCAGCATGGAGGCTGAAGATGCTGCCACTT          | 255          |           |                               |
| Subject 211                         | TCTGAGCTCTTACTCTCTCACAATCAGCAGCATGGAGGCTGAAGATGCTGCCACTT          | 270          |           |                               |
| Query 256                           | TACTGCTGACATGAGTAGTAACCCACCCATCACGTTTCGGTGCTGGCACCAAGCTGGAAATCAAA | 314          |           |                               |
| Subject 271                         | TACTGCTGACATGAGTAGTAACCCACCCATCACGTTTCGGTGCTGGCACCAAGCTGGAAATCAAA | 329          |           |                               |

[00474] TGGTCGACGCTGAGGAGACGGTGACTGAGGTTTCCTTGACCCCA  
 GTAGTCCATAGCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG  
 TCCTCATTCTTGAGGTTGTTGATCTGCAAATAGGCAGTGCTGGCAGAGGTTTC  
 5 CAAAGAGAAGGCAAACCGTCCCTTGAAGTCATCAGCAAATGTTGGCTCTCCA  
 GTGTAGGTGTTTATCCAGCCCATCCACTTTAAACCCCTTTCCTGGAGCCTGCTT  
 CACCCAGTTCATTCCATAGTTTGTGAAGGTATACCCAGAAGCCTTGCAGGAG  
 ATCTTGACTGTCTCTCCTGACTCCTTAAGCTGCACCT (SEQ ID NO: 11)

Mus musculus clone nat26H immunoglobulin heavy chain variable region mRNA, partial cds  
 Sequence ID: [gi541044655.1](#) Length: 331 Number of Matches: 1

| Range 1: 8 to 331 |                                                                                              | GenBank      | Graphics  | ▼ Next Match ▲ Previous Match |  |
|-------------------|----------------------------------------------------------------------------------------------|--------------|-----------|-------------------------------|--|
| Score             | Expect                                                                                       | Identities   | Gaps      | Strand                        |  |
| 518 bits(280)     | 3e-143                                                                                       | 313/328(95%) | 5/328(1%) | Plus/Minus                    |  |
| Query 10          | CTGAGGAGACGGTGACTGAGGTTTCCTTGACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG                     | 68           |           |                               |  |
| Subject 331       | CTGAGGAGACGGTGACTGAGGTTTCCTTGACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG                     | 276          |           |                               |  |
| Query 68          | TATCTTGCACAGAAATATGTAGCCGTGCTCTTATCTTGAGGTTTCCTTGACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG | 128          |           |                               |  |
| Subject 275       | TATCTTGCACAGAAATATGTAGCCGTGCTCTTATCTTGAGGTTTCCTTGACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG | 218          |           |                               |  |
| Query 128         | GCAGTCTGCTGAGGTTTCCTTGACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG                            | 188          |           |                               |  |
| Subject 215       | GCAGTCTGCTGAGGTTTCCTTGACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG                            | 158          |           |                               |  |
| Query 188         | GTTGCTCTCTGAGGTTTCCTTGACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG                            | 248          |           |                               |  |
| Subject 155       | GTTGCTCTCTGAGGTTTCCTTGACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG                            | 95           |           |                               |  |
| Query 248         | TGCTTACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG                                             | 308          |           |                               |  |
| Subject 95        | TGCTTACCCCAAGAGTACCCGTATCTTGCACAGAAATATGTAGCCGTG                                             | 35           |           |                               |  |
| Query 308         | TTGACTGTCTCTCCTGACTCCTTAAGCTGCACCT                                                           | 336          |           |                               |  |
| Subject 35        | TTGACTGTCTCTCCTGACTCCTTAAGCTGCACCT                                                           | 8            |           |                               |  |

10 [00475] Translated light chain protein sequence and heavy chain protein sequence  
 based on the DNA sequences:

[00476] Light Chain: DIVMTQSPAIMASAPGEKVTMTCSASS  
 SVSYMHWYQQKSGTSPKRWIYDTSKLASGVPARFSGSGS  
 GTSYSLTISSMEAEDAATYYCQQWSSNPPIITFGAGTKLEI  
 15 K (SEQ ID NO: 10);

[00477] Heavy Chain: VQLVESGPGLKKPGETVKISCKASGY  
 TFTNYGMNWVKQAPGKGLKWMGWINTYTGEPTFADDFK

GRFAFSLETSASTAYLQINNLIK NEDTATYFCARYGYSWA  
MDYWGQGTSVTVSSAST (SEQ ID NO: 9).

## Claims

1. A method for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity of IFP35 (Interferon-induced Protein 35kD) and/or NMI (N-Myc-interacting protein) in a subject, which method comprises  
5 administering, to a subject in need of such treatment and/or prevention, an effective amount of an agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in said subject.
2. The method of claim 1, wherein the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is associated with excessive  
10 immune response.
3. The method of claim 1 or 2, wherein the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is associated with cytokine storm.
4. The method of any one of claims 1-3, wherein the disease or disorder  
15 associated with abnormally high level and/or activity of IFP35 and/or NMI is selected from the group consisting of inflammation, infection, sepsis, and autoimmune disease.
5. The method of any one of claims 1-4, which is for treating a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.
6. The method of any one of claims 1-4, which is for preventing a disease or  
20 disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.
7. The method of any one of claims 1-6, wherein the agent comprises a molecule, such as a small molecule or a polypeptide, that inhibits or reduces the expression and/or activity of IFP35 and/or NMI.

8. The method of any one of claims 1-7, wherein the agent comprises an antibody or antigen binding fragment thereof that inhibits or reduces the expression and/or activity of IFP35 and/or NMI.

9. The method of any one of claims 1-8, wherein the agent comprises a  
5 polynucleotide (such as an siRNA, shRNA, or miRNA) targeting the gene encoding IFP35 and/or NMI.

10. The method of any one of claims 1-9, wherein the agent comprises an antisense RNA targeting the gene encoding IFP35 and/or NMI.

11. The method of any one of claims 1-10, wherein the agent comprises a  
10 molecule that inhibits or reduces the oligomerization of IFP35 and/or NMI.

12. The method of any one of claims 1-11, wherein the agent comprises a molecule that inhibits or reduces the expression and/or activity of an interferon, thereby inhibiting or reducing the expression and/or activity of IFP35 and/or NMI.

13. The method of any one of claims 1-12, wherein the agent comprises a  
15 molecule that inhibits or reduces the secretion of IFP35 and/or NMI.

14. The method of any one of claims 1-13, wherein the agent comprises a molecule that inhibits or reduces the interaction between IFP35 and/or NMI and a cellular receptor of IFP35 and/or NMI.

15. The method of any one of claims 1-14, wherein the agent comprises a  
20 molecule that inhibits or reduces the interaction between IFP35 and/or NMI and a IFP35 and/or NMI cell surface receptor.

16. The method of any one of claims 1-15, wherein the prevention or reduction of the production and/or the activity of IFP35 and/or NMI results in the

inhibition or reduction of the expression and/or activity of an inflammatory factor, and/or inhibiting or reduction of NF- $\kappa$ B signaling.

17. The method of claim 16, wherein the inflammatory factor comprises IL-1 $\beta$ , TNF- $\alpha$ , iNOS, and/or CD86, and the NF- $\kappa$ B signaling is mediate by a TLR such as  
5 TLR4.

18. The method of any one of claims 1-17, wherein the agent comprises an antibody or antigen binding fragment that specifically binds to IFP35 and/or an antibody or antigen binding fragment that specifically binds to NMI.

19. The method of claim 18, wherein the antibody or antigen binding  
10 fragment specifically binds one or more NIDs (NMI/IFP35 domains).

20. The method of any one of claims 1-19, further comprising administering a pharmaceutically acceptable carrier or excipient.

21. The method of any one of claims 1-19, wherein the agent is administered via an oral, nasal, inhalational, parental, intravenous, intraperitoneal, subcutaneous,  
15 intramuscular, intradermal, topical, or rectal route.

22. The method of any one of claims 1-21, wherein the agent is administered at an amount that reduces production and/or an activity of IFP35 and/or NMI in the subject to a level that is substantially identical to a production and/or an activity level of IFP35 and/or NMI in a comparable subject that does not have a disease or disorder  
20 associated with abnormally high level and/or activity of IFP35 and/or NMI.

23. The method of any one of claims 1-22, wherein the subject is a mammal.

24. The method of claim 23, wherein the mammal is a human or a non-human mammal.

25. A pharmaceutical composition for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject, which pharmaceutical composition comprises an effective amount of an agent that prevents or reduces production and/or an activity of IFP35 and/or NMI in a subject  
5 and a pharmaceutically acceptable carrier or excipient.

26. The pharmaceutical composition of claim 25, further comprising an effective amount of a drug for the treatment and/or prevention of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in the subject.

27. Use of an effective amount of an agent that prevents or reduces production  
10 and/or an activity of IFP35 and/or NMI in a subject for the manufacture of a medicament for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in said subject.

28. The use of claim 27, wherein the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is inflammation, infection,  
15 sepsis, organ damage, and autoimmune disease.

29. An antibody or antigen binding fragment thereof that specifically binds to IFP35 and/or NMI, wherein the antibody or antigen binding fragment specifically binds to an epitope within SEQ ID NO: 2, SEQ ID NO: 4, SEQ ID NO: 6, or SEQ ID NO: 8.

30. The antibody or antigen binding fragment of claim 29, wherein the  
20 antibody or antigen binding fragment specifically binds to an epitope within amino acids 81-170, 177-268, or 136-216 of SEQ ID NO: 2.

31. The antibody or antigen binding fragment of claim 29, wherein the antibody or antigen binding fragment specifically binds to an epitope within amino acids 81-168, 175-266, or 134-214 of SEQ ID NO: 4.

32. The antibody or antigen binding fragment of claim 29, wherein the antibody or antigen binding fragment specifically binds to an epitope within amino acids 104-193, 202-293, or 151-250 of SEQ ID NO: 6.

33. The antibody or antigen binding fragment of claim 29, wherein the  
5 antibody or antigen binding fragment specifically binds to an epitope within amino acids 103-192, 201-292, or 151-240 of SEQ ID NO: 8.

34. An antibody or antigen binding fragment thereof that specifically binds to IFP35 and/or NMI, wherein the antibody or antigen binding fragment thereof comprises a heavy chain variable region comprising a complementarity determining region (CDR)  
10 consisting of the amino acid sequences of a CDR in the heavy chain variable region sequence set forth in SEQ ID NO: 9 and/or a light chain variable region comprising a CDR consisting of the amino acid sequence of a CDR in the light chain variable region sequence set forth in SEQ ID NO:10.

35. The antibody or antigen binding fragment of claim 34, wherein the  
15 antibody or antigen binding fragment thereof comprises a heavy chain variable region set forth in SEQ ID NO: 9 and a light chain variable region set forth in SEQ ID NO:10.

36. The antibody or antigen binding fragment of any one of claims 29-35, wherein the fragment is an Fab, F(ab $\square$ )<sub>2</sub>, Fv or scFv fragment, and wherein the antibody is a monoclonal antibody, a polyclonal antibody, or a bi-specific antibody.

20 37. The antibody or antigen binding fragment of any one of claims 29-36, further comprising a human heavy chain constant region and a human light chain constant region.

38. The antibody or antigen binding fragment of any one of claims 29-37, wherein the antibody is a fully human antibody or a humanized antibody.

39. The antibody or antigen binding fragment of any one of claims 29-38, wherein the antibody is recombinantly produced.

40. A method for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity and/or activity of IFP35 (Interferon-induced Protein 35kD) and/or NMI (N-Myc-interacting protein) in a subject, which method  
5 comprises administering, to a subject in need of such treatment and/or prevention, an effective amount of the antibody or antigen binding fragment thereof of any one of claims 29-39 in said subject.

41. The method of claim 40, wherein the disease or disorder associated with  
10 abnormally high level and/or activity of IFP35 and/or NMI is associated with excessive immune response.

42. The method of claim 40 or 41, wherein the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is associated with cytokine storm.

43. The method of any one of claims 40-42, wherein the disease or disorder  
15 associated with abnormally high level and/or activity of IFP35 and/or NMI is selected from the group consisting of inflammation, infection, sepsis, and autoimmune disease.

44. The method of any one of claims 40-43, wherein the prevention or reduction of the production and/or the activity of IFP35 and/or NMI results in the  
20 inhibition or reduction of the expression and/or activity of an inflammatory factor, and/or inhibiting or reduction of NF- $\kappa$ B signaling.

45. The method of claim 44, wherein the inflammatory factor comprises IL-1 $\beta$ , TNF- $\alpha$ , iNOS, and/or CD86, and the NF- $\kappa$ B signaling is mediate by a TLR such as TLR4.

46. An isolated polynucleotide encoding an antibody or antigen binding fragment thereof that specifically binds to IFP35 and/or NMI, wherein the antibody or antigen binding fragment thereof comprises a heavy chain variable region comprising a complementarity determining region (CDR) consisting of the amino acid sequence of a CDR in the heavy chain variable region sequence set forth in SEQ ID NO: 9 and/or a light chain variable region comprising a CDR consisting of the amino acid sequences of a CDR in the light chain variable region sequence set forth in SEQ ID NO:10.

47. The polynucleotide of claim 46, wherein the antibody or antigen binding fragment thereof comprises a heavy chain variable region set forth in SEQ ID NO: 9 and a light chain variable region set forth in SEQ ID NO:10.

48. An isolated vector comprising the polynucleotide of claim 46 or 47.

49. An isolated host cell comprising the vector of claim 48.

50. A host cell which is selected from the group consisting of the following:

(a) a host cell transformed with an expression vector comprising a polynucleotide comprising a sequence encoding a heavy chain variable region of an antibody or antigen binding fragment thereof and a polynucleotide comprising a sequence encoding a light chain variable region of an antibody or antigen binding fragment thereof; and

(b) a host cell transformed with an expression vector comprising a polynucleotide comprising a sequence encoding a heavy chain variable region of an antibody or antigen binding fragment thereof and an expression vector comprising a polynucleotide comprising a sequence encoding a light chain variable region of an antibody or antigen binding fragment thereof,

wherein the antibody or fragment comprises a heavy chain variable region comprising a complementarity determining region (CDR) consisting of the amino acid sequences of a CDR in the heavy chain variable region sequence set forth in SEQ ID NO: 9 and/or a light chain variable region comprising a CDR consisting of the amino acid sequences of a CDR in the light chain variable region sequence set forth in SEQ ID NO:10.

51. The host cell of claim 49 or claim 50, wherein the host cell is a eukaryotic cell such as a CHO cell.

52. A method of making an anti-IFP35 antibody or antigen binding fragment thereof and/or an anti-NMI antibody or antigen binding fragment thereof, wherein the  
5 method comprises:

- a) culturing the host cell of any one of claims 49-51 under conditions suitable for expression of the polynucleotide encoding the antibody or antigen binding fragment; and
- b) isolating the antibody or antigen binding fragment.

10 53. The antibody or antigen binding fragment produced by the method of claim 52.

54. An isolated polypeptide comprising, consisting essentially of, or consisting of:

- (1) the sequence set forth in amino acids 81-170, 177-268, or 136-216 of SEQ  
15 ID NO: 2; or
- (2) the sequence set forth in amino acids 81-168, 175-266, or 134-214 of SEQ ID NO: 4; or
- (3) the sequence set forth in amino acids 104-193, 202-293 or 151-250 of SEQ ID NO: 6; or
- 20 (4) the sequence set forth in amino acids 103-192, 201-292, or 151-240 of SEQ ID NO: 8.

55. An isolated polypeptide comprising, consisting essentially of, or consisting of the sequence set forth in amino acids 81-170, 177-268, or 136-216 of SEQ ID NO: 2, wherein one or more of the amino acid residues at positions 145, 147, 150, 151,  
25 172, 173, 175, 177, 182, 188, 192, 212, 199, 201, 207, 208, 210, 214, and 216 of SEQ ID NO: 2 (Ser145, Arg147, Glu150, Glu151, Asp172, Val173, Glu175, Leu177, Met182, Asp188, Gln192, Arg212, Gln199, Thr201, Gln207, Gln208, Pro210, Ser214, and Tyr216) are mutated and/or modified.

56. The isolated polypeptide of claim 55, wherein the mutation(s) substantially reduce(s) or eliminate(s) binding of the polypeptide to a IFP35 receptor or an inhibitory antibody specific for IFP35.

57. An isolated polypeptide comprising, consisting essentially of, or  
5 consisting of the sequence set forth in amino acids 81-168, 175-266, or 134-214 of SEQ ID NO: 4, wherein one or more of the amino acid residues at positions 143, 145, 148, 149, 170, 172, 173, 175, 180, 186, 190, 210, 197, 199, 204, 205, 206, 208, 212, and 214 of SEQ ID NO: 4 (Ser143, Arg145, Glu148, Glu149, Glu170, Arg172, Glu173, Leu175, Met180, Glu186, Gln190, Arg210, Gln197, Arg199, Arg204, Gln205, Gln206, Leu208,  
10 Ser212, and Tyr214) are mutated and/or modified.

58. The isolated polypeptide of claim 57, wherein the mutation(s) substantially reduce(s) or eliminate(s) binding of the polypeptide to a IFP35 receptor or an inhibitory antibody specific for IFP35.

59. An isolated polypeptide comprising, consisting essentially of, or  
15 consisting of the sequence set forth in amino acids 104-193, 202-293, or 151-250 of SEQ ID NO: 6, wherein one or more of the amino acid residues at positions 107, 112, 117, 159, 172, 173, 192, 197, 215, 256, 267, and 292 of SEQ ID NO: 6 (Leu107, Lys112, Gln117, Lys159, Glu172, Glu173, Glu192, Asp197, Asp215, Lys256, Asp267, and Glu292) are mutated and/or modified.

20 60. The isolated polypeptide of claim 59, wherein the mutation(s) substantially reduce(s) or eliminate(s) binding of the polypeptide to a NMI receptor or an inhibitory antibody specific for NMI.

61. An isolated polypeptide comprising, consisting essentially of, or  
25 consisting of the sequence set forth in amino acids 103-192, 201-292, or 151-240 of SEQ ID NO: 8, wherein one or more of the amino acid residues at positions 106, 111, 116, 158, 171, 172, 191, 196, 214, 255, 266, and 291 of SEQ ID NO: 8 (Leu106, Lys111, Gln116,

Lys158, Glu171, Asp172, Asp191, Asp196, Asp214, Arg255, Asp266, and Asp291) are mutated and/or modified.

62. The isolated polypeptide of claim 61, wherein the mutation(s) substantially reduce(s) or eliminate(s) binding of the polypeptide to a NMI receptor or an inhibitory antibody specific for NMI.

63. A pharmaceutical composition comprising the polypeptide of any one of claims 54-62 and optionally a pharmaceutically acceptable carrier or excipient.

64. A method for stimulating an immune response in a subject, which method comprises administering, to a subject in need of such stimulation, an effective amount of the polypeptide of any one of claims 54-62 or the pharmaceutical composition of claim 63 in said subject.

65. The method of claim 64, wherein the subject has a proliferation disorder, a neoplasm, a tumor or a cancer.

66. The method of claim 65, wherein the proliferation disorder is selected from the group consisting of sarcoma, epidermoid cancer, fibrosarcoma, cervical cancer, gastric carcinoma, skin cancer, leukemia, lymphoma, lung cancer, non-small cell lung cancer, colon cancer, CNS cancer, melanoma, ovarian cancer, renal cancer, prostate cancer, breast cancer, liver cancer, head and neck cancers, pancreatic cancer, bladder cancer and esophageal cancer.

67. The method of any one of claims 64-66, wherein the stimulation of the immune response comprises stimulation of the expression and/or activity of an inflammatory factor, the recruitment of immune cells such as neutrophils, and/or NF- $\kappa$ B signaling.

68. The method of claim 67, wherein the inflammatory factor comprises IL-1 $\beta$ , TNF- $\alpha$ , iNOS, and/or CD86, and the NF- $\kappa$ B signaling is mediated by a TLR such as TLR4.

69. The method of claim 67 or 68, wherein the stimulation of NF- $\kappa$ B  
5 signaling comprises an increase in phosphorylated I $\kappa$ B $\alpha$  and/or a reduction in total I $\kappa$ B $\alpha$ .

70. An isolated polynucleotide encoding a polypeptide comprising the polypeptide of any one of claims 54-62.

71. An isolated vector comprising the polynucleotide of claim 70.

72. An isolated host cell comprising the vector of claim 71, wherein the host  
10 cell is optionally a eukaryotic cell such as a CHO cell.

73. A method of making an isolated polynucleotide, wherein the method comprises:

a) culturing the host cell of claim 72 under conditions suitable for expression of the polynucleotide encoding a polypeptide comprising the polypeptide of any one of  
15 claims 54-62; and

b) isolating the polypeptide.

74. A method of diagnosis, prognosis or treatment monitoring of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject, which method comprises assessing the level and/or an activity of IFP35 and/or  
20 NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

75. The method of claim 74, wherein the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is associated with excessive immune response.

76. The method of claim 74 or 75, wherein the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is associated with cytokine storm.

77. The method of any one of claims 74-76, wherein the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is selected from the group consisting of inflammation, infection, sepsis, and autoimmune disease.

78. The method of any one of claims 74-77, which is used for diagnosis of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject, and wherein a level and/or an activity of IFP35 and/or NMI in a subject that is at least 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, 100%, 150%, 200%, 300%, 400%, or 500% higher than a level and/or an activity of IFP35 and/or NMI in a comparable subject that does not have a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI, e.g., inflammation, infection, sepsis, and autoimmune disease, indicates that the subject has the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

79. The method of any one of claims 74-78, which comprises assessing the level of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

80. The method of any one of claims 74-78, which comprises assessing an activity of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

81. The method of any one of claims 74-80, wherein the level and/or an activity of IFP35 and/or NMI is assessed at the DNA, RNA and/or protein level.

82. The method of claim 81, wherein the level of IFP35 and/or NMI is assessed at the DNA and/or RNA level using a polynucleotide that is complementary to at least 10 consecutive nucleotides in the IFP35 and/or NMI DNA or RNA.

83. The method of claim 81, wherein the level of IFP35 and/or NMI is assessed at the protein level using an antibody that specifically binds to IFP35 and/or NMI.

84. A kit of diagnosis, prognosis or treatment monitoring of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject, which kit comprises a means for assessing the level and/or an activity of IFP35 and/or NMI in a subject suspected of or being treated for a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

85. A method of companion diagnostics of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject, which method comprises determining the genetic status of IFP35 and/or NMI gene in a subject being treated for the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

86. The method of claim 85, wherein the genetic status of IFP35 and/or NMI gene in a subject is determined using a polynucleotide that is complementary to at least 10 consecutive nucleotides in the IFP35 and/or NMI DNA or RNA.

87. A kit of companion diagnostics of a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject, which kit comprises a means for determining the genetic status of IFP35 and/or NMI gene in a subject being treated for the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI.

88. A method for identifying a modulator of IFP35 and/or NMI, which method comprises:

- a) contacting IFP35 and/or NMI with a test substance and assessing an activity of IFP35 and/or NMI that has been contacted by said test substance;
- b) assessing an activity of said IFP35 and/or NMI that has not been contacted by said test substance; and

c) comparing said activities of IFP35 and/or NMI assessed in steps a) and b), and identifying said test substance as a modulator of IFP35 and/or NMI when said activities of IFP35 and/or NMI assessed in steps a) and b) are different.

89. The method of claim 88, wherein the test substances are small molecules,  
5 a polypeptide library comprising mutants and/or fragments of IFP35 and/or NMI, antibodies that specifically bind IFP35 and/or NMI, siRNAs or antisense RNAs.

90. The method of claim 88 or 89, which is used to identify an inhibitor of an activity of IFP35 and/or NMI.

91. The method of any one of claims 88-90, which is used to identify a drug  
10 for treating and/or preventing a disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI in a subject.

92. The method of claim 91, wherein the disease or disorder associated with abnormally high level and/or activity of IFP35 and/or NMI is a proliferation disorder, a neoplasm, a tumor or a cancer.

15 93. A drug candidate identified by any one of claims 88-92.

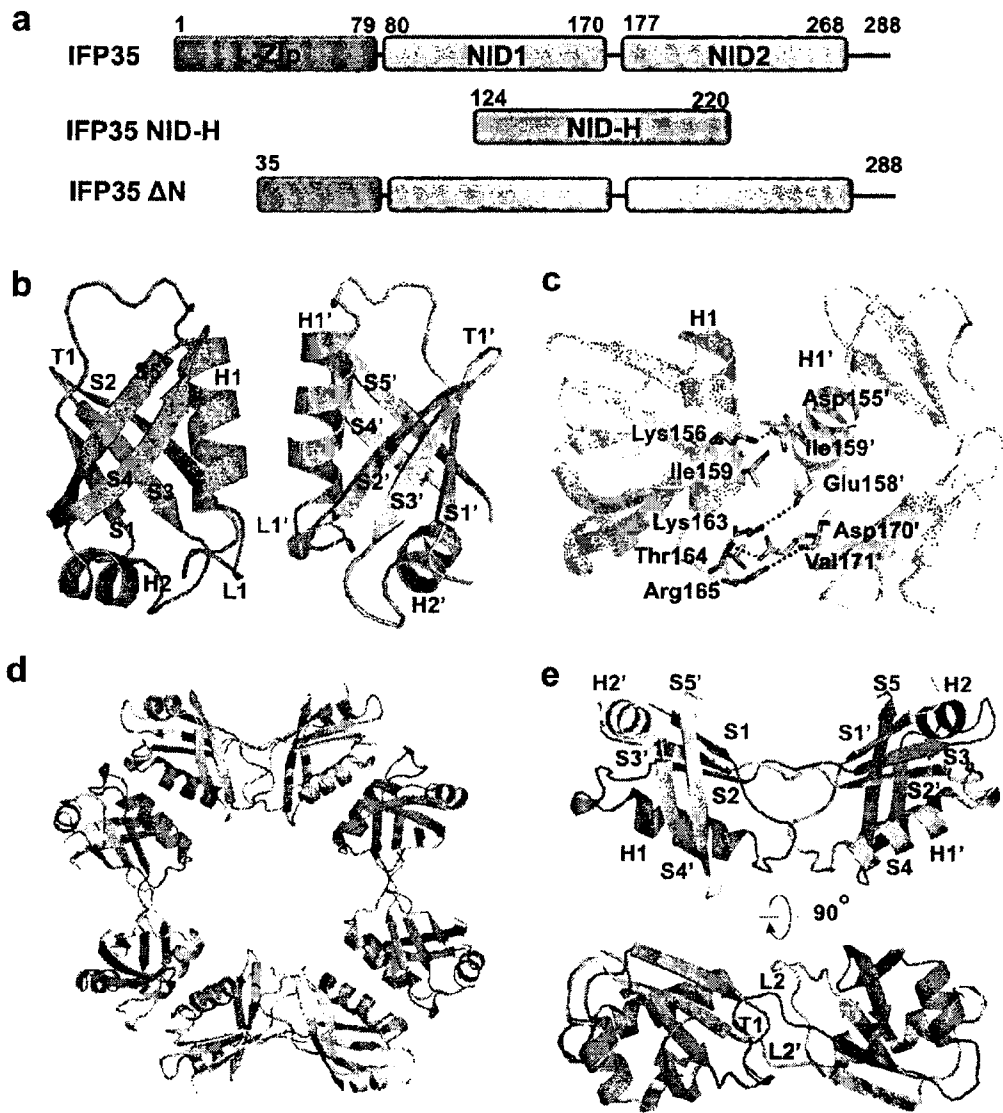


FIGURE 1

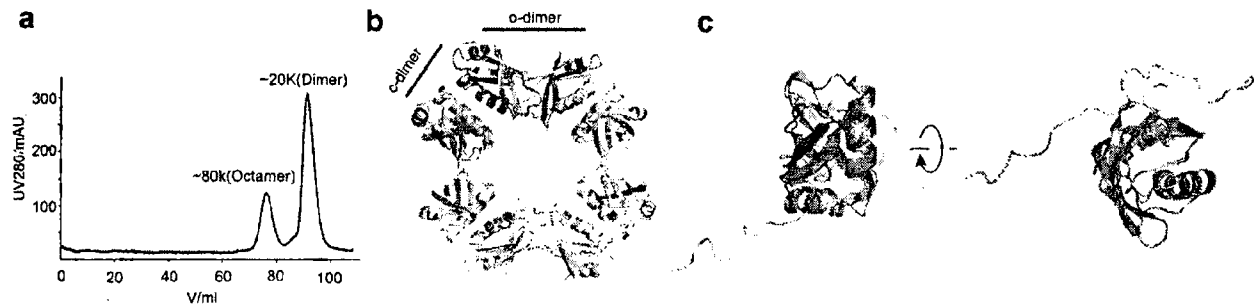


FIGURE 2

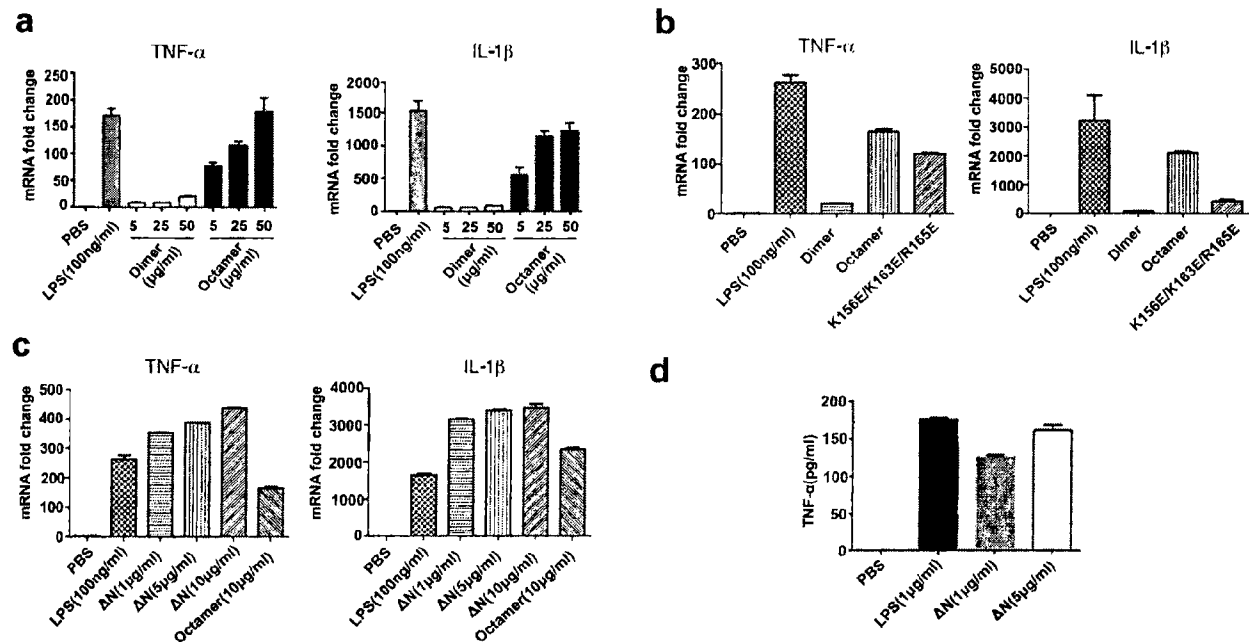


FIGURE 3

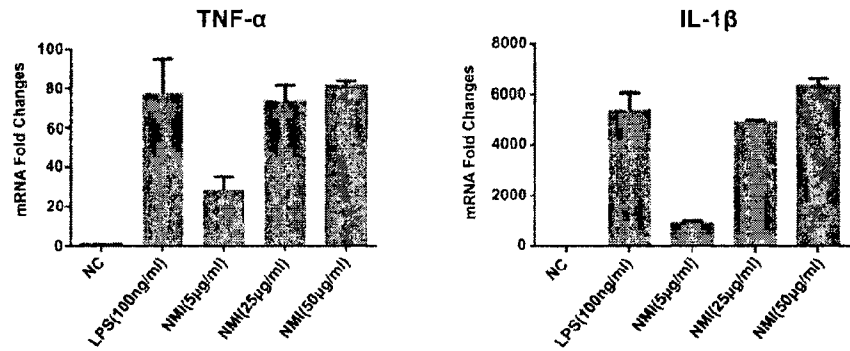


FIGURE 4

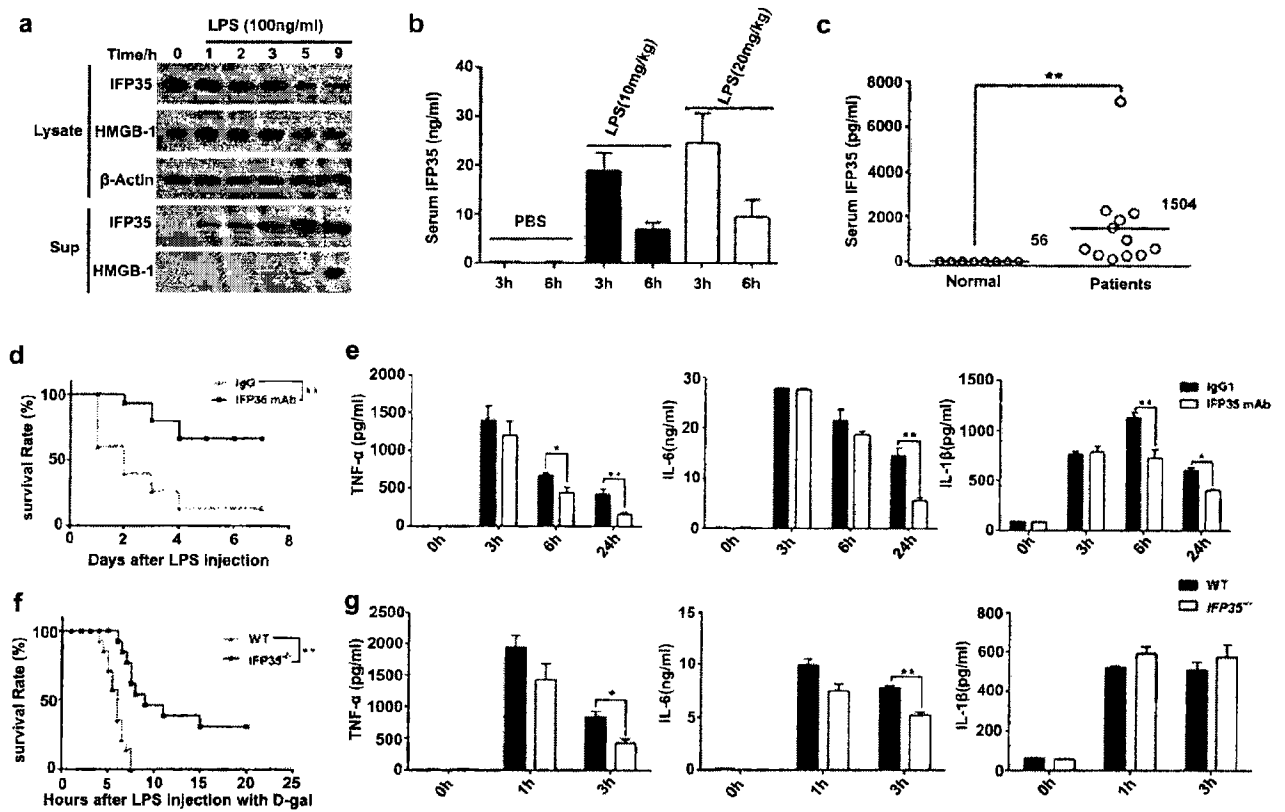


FIGURE 5

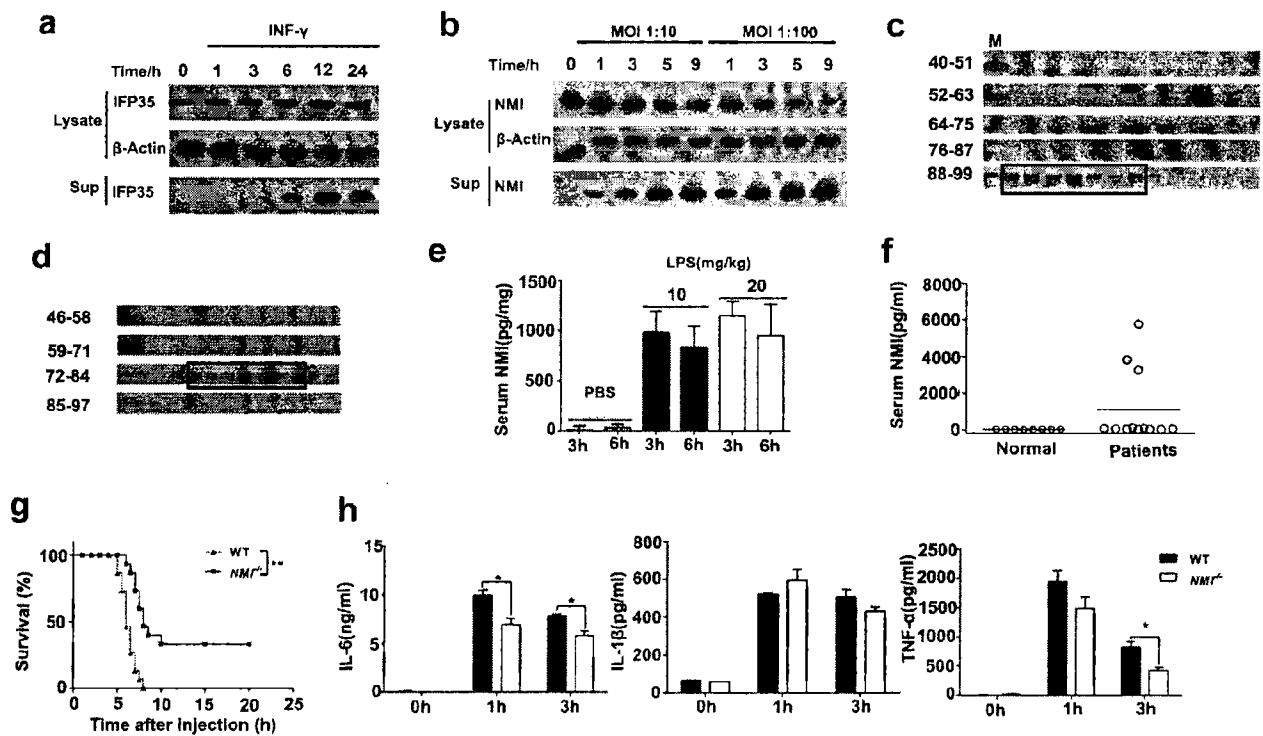


FIGURE 6

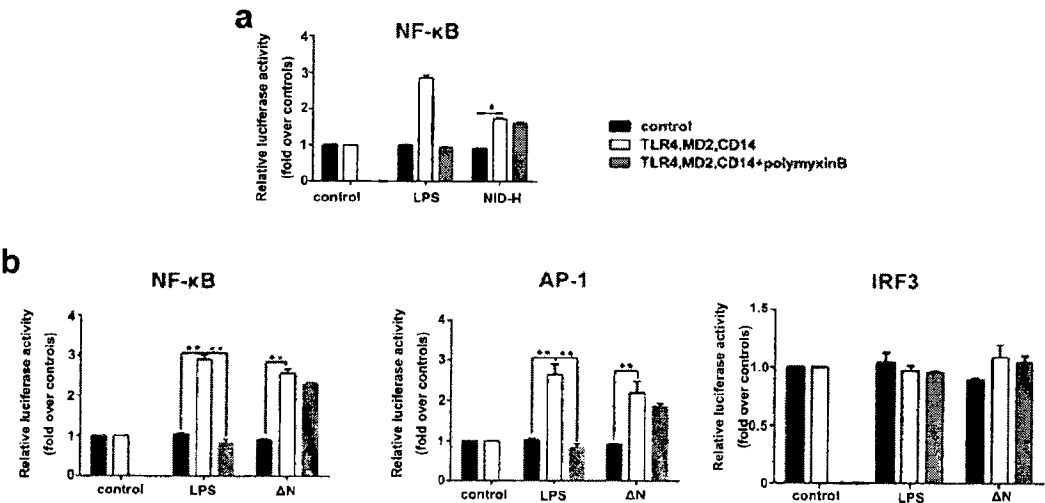


FIGURE 7

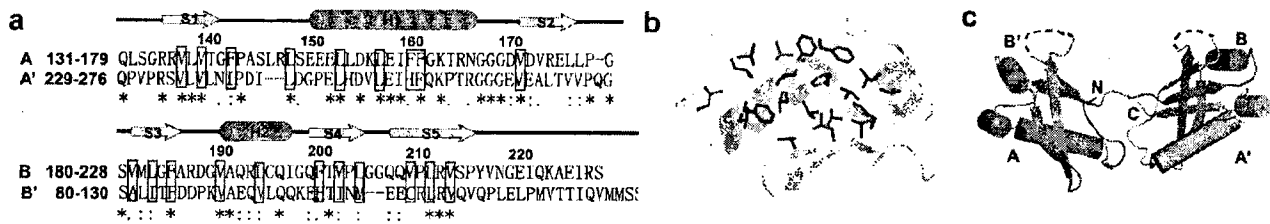


FIGURE 8

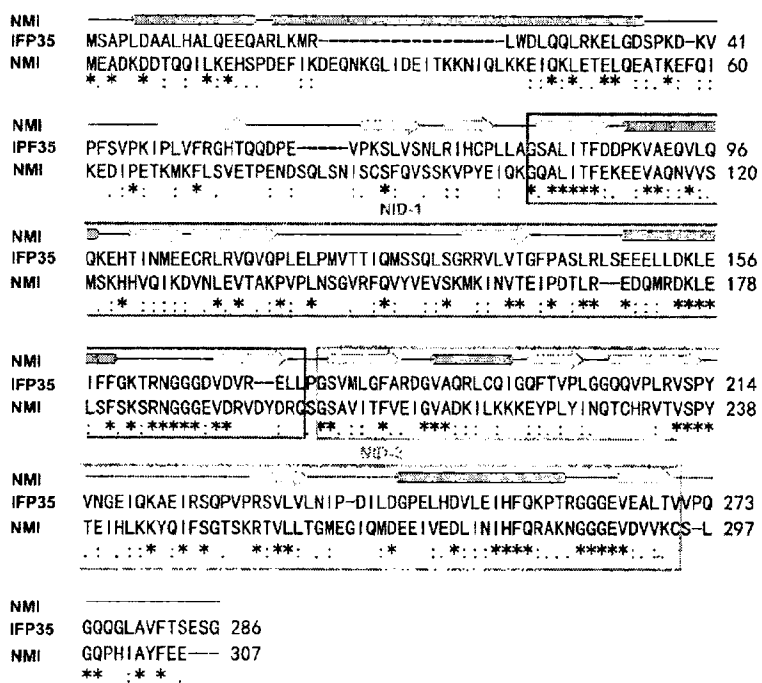


FIGURE 9

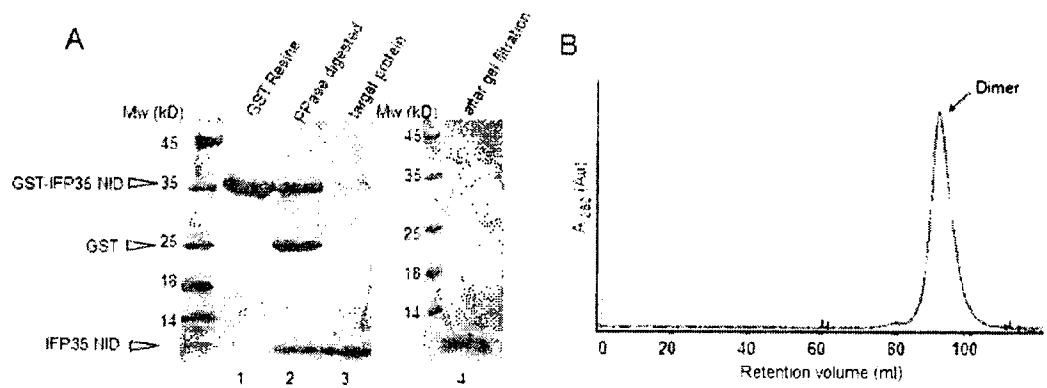


FIGURE 10

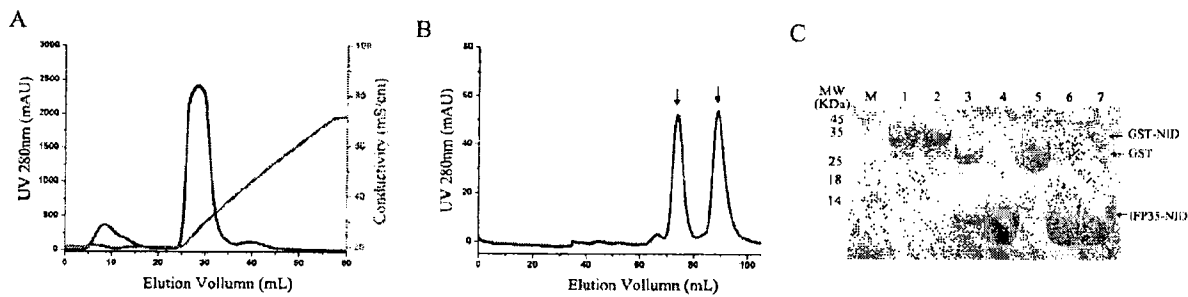


FIGURE 11

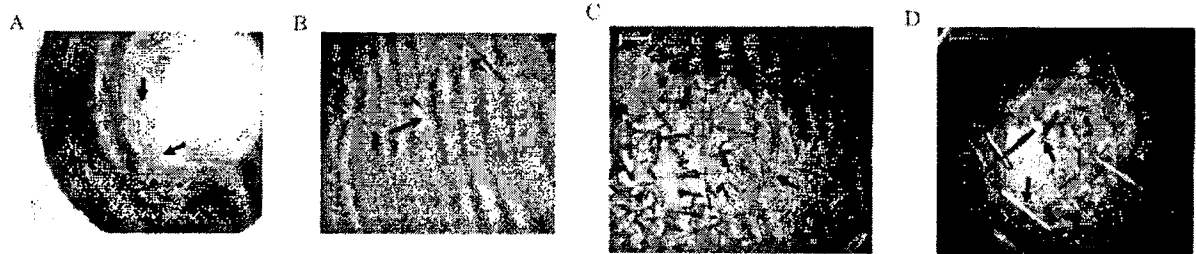


FIGURE 12



FIGURE 13

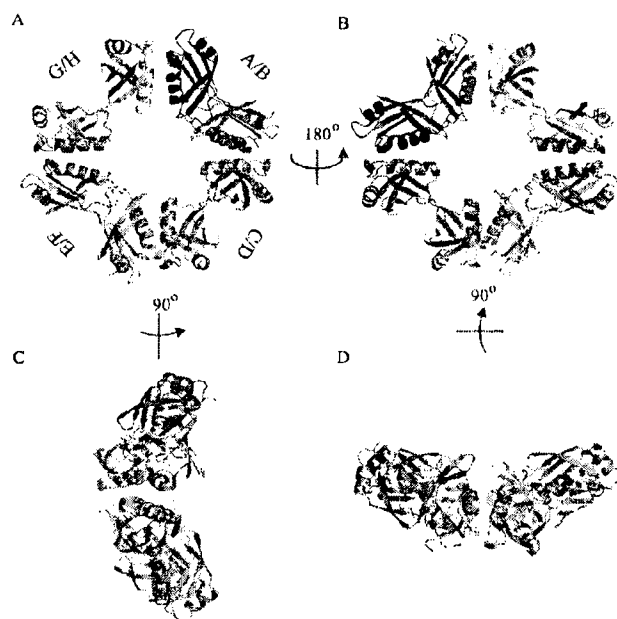


FIGURE 14

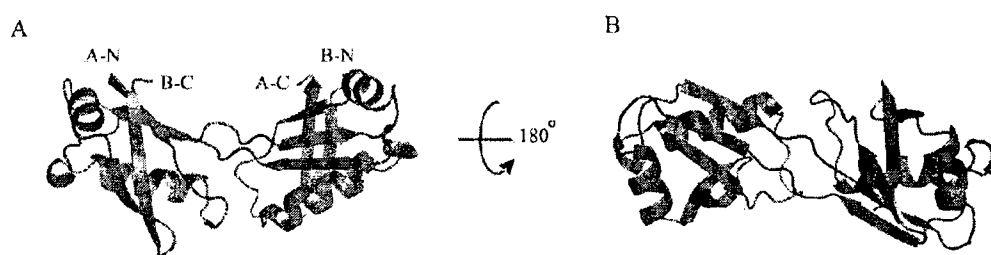


FIGURE 15



FIGURE 16

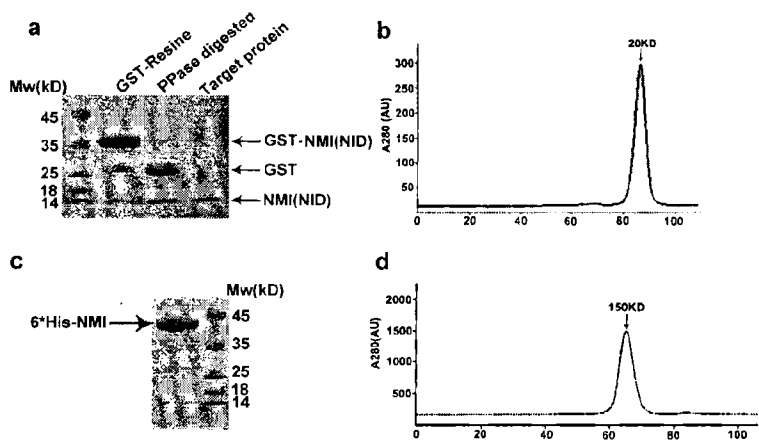


FIGURE 17

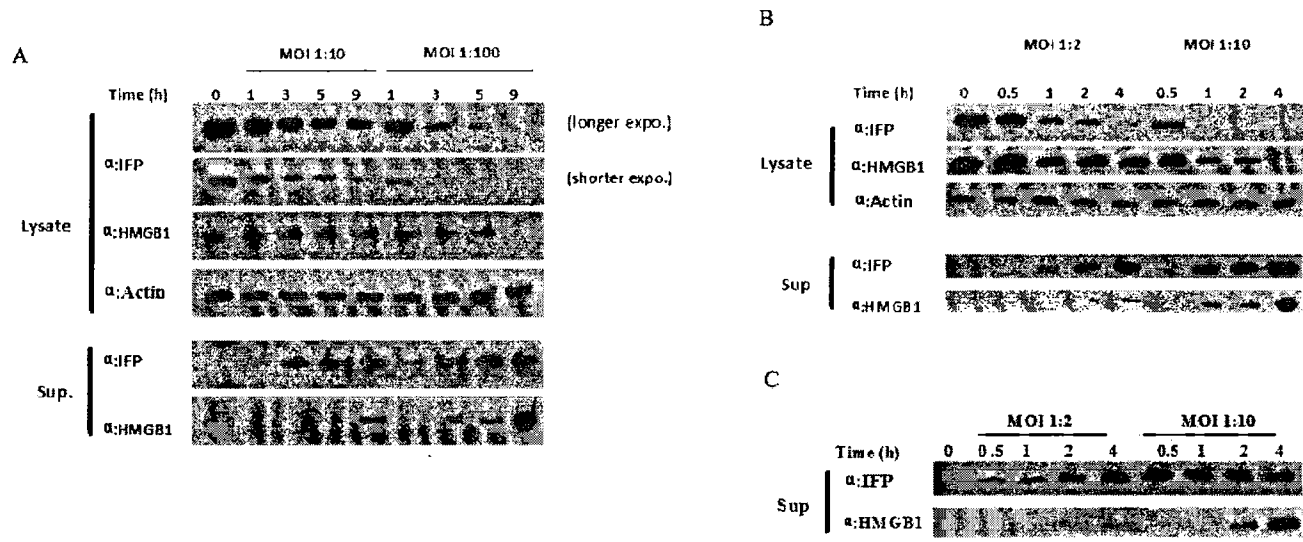


FIGURE 18

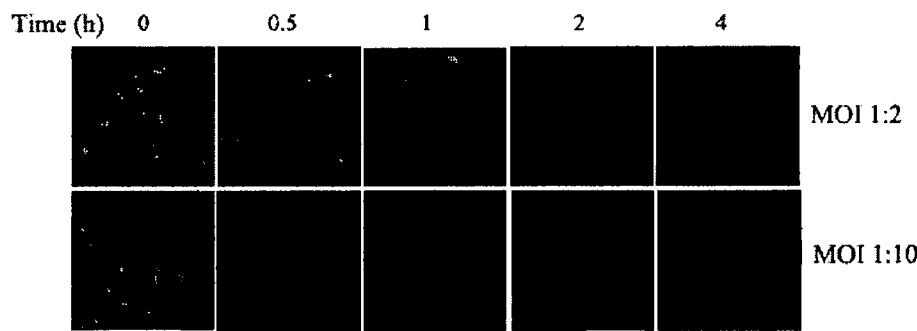


FIGURE 19

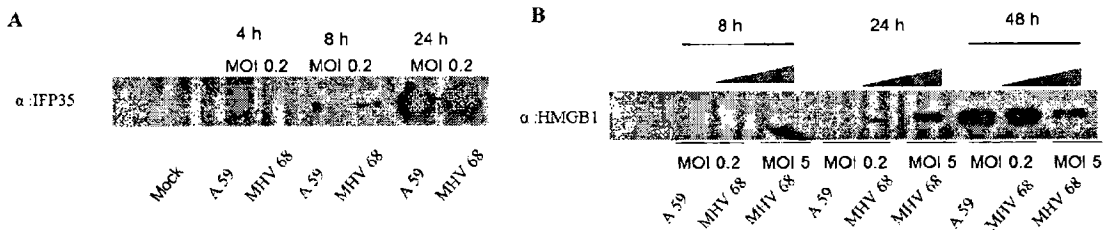


FIGURE 20

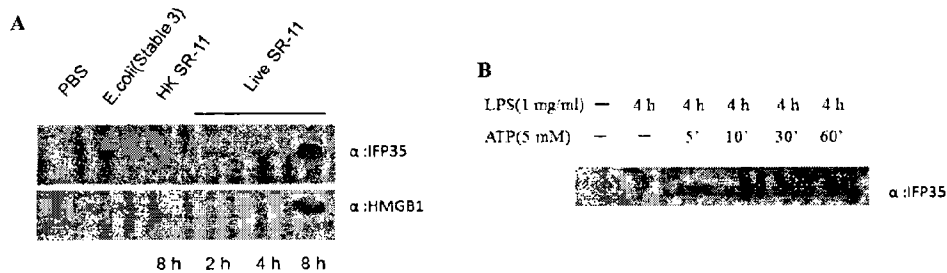


FIGURE 21

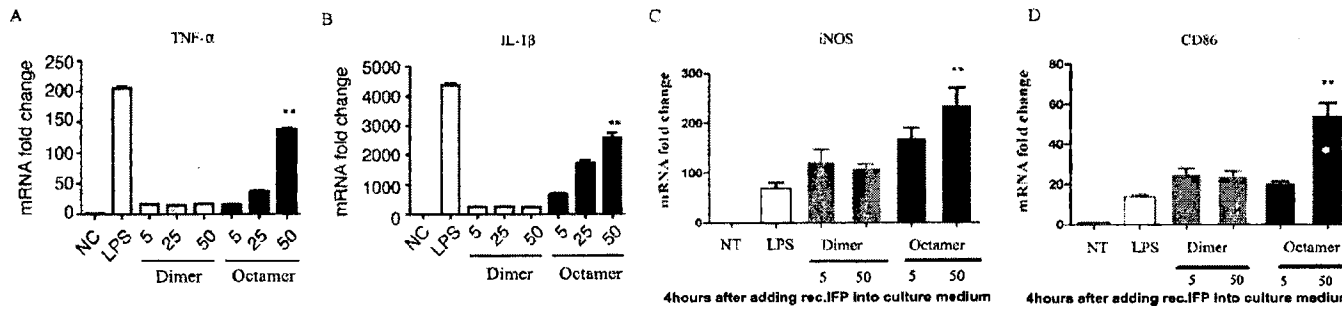


FIGURE 22

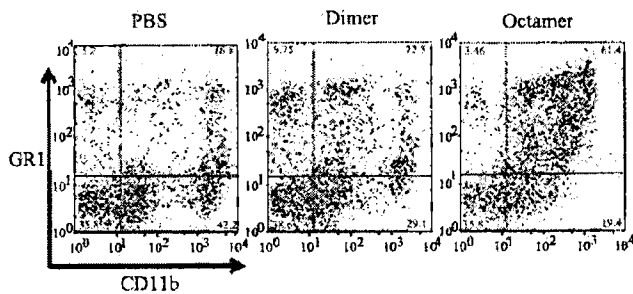


FIGURE 23

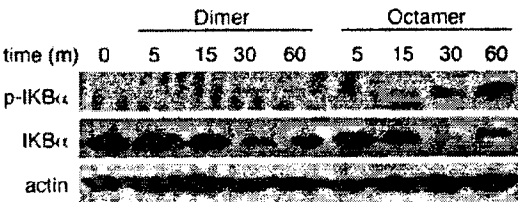


FIGURE 24

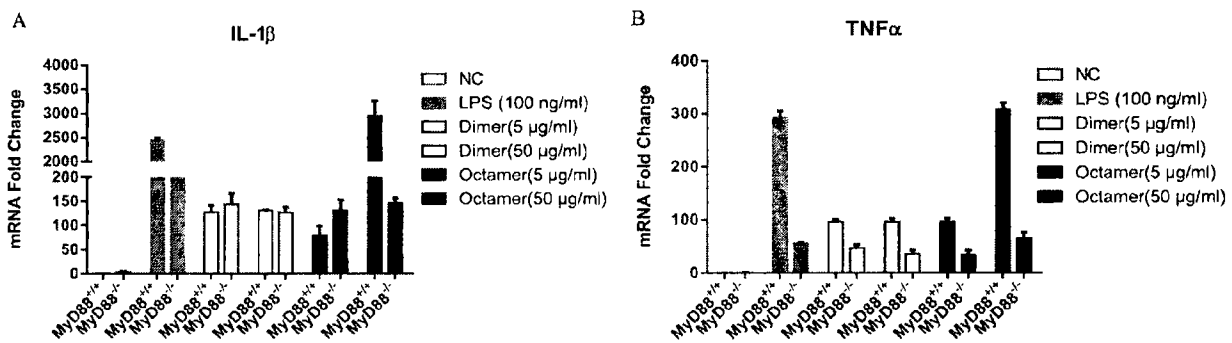


FIGURE 25

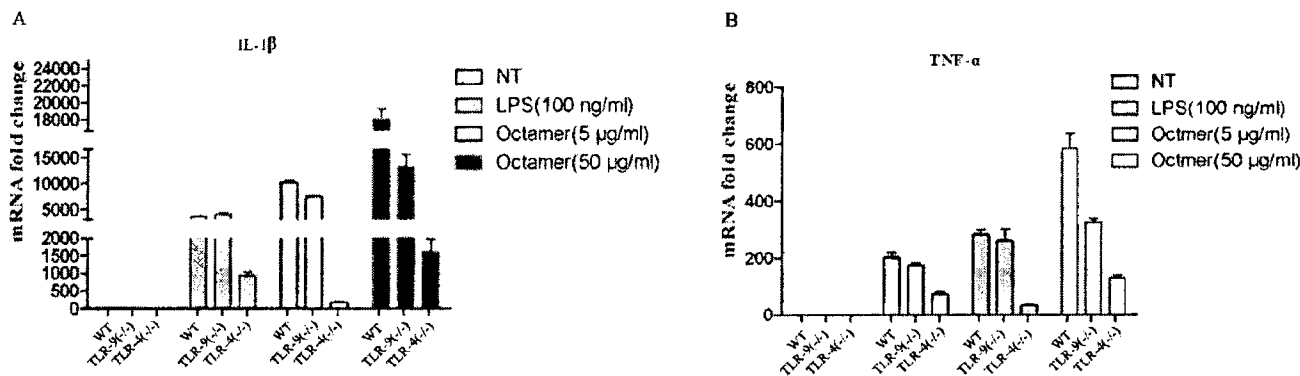


FIGURE 26

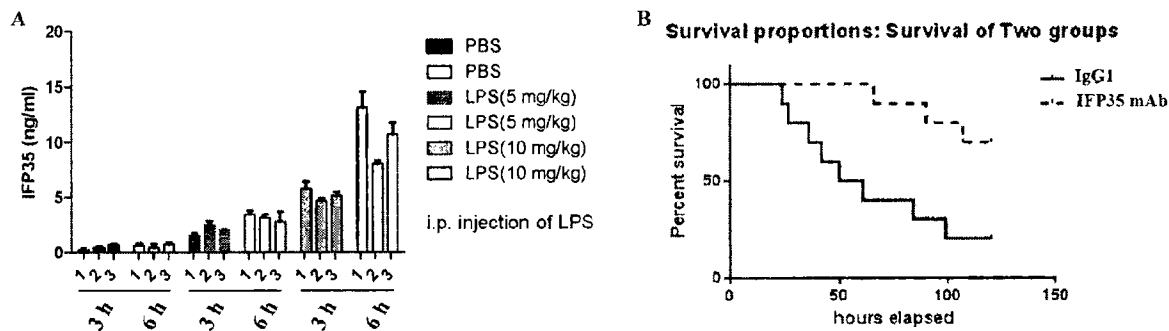


FIGURE 27

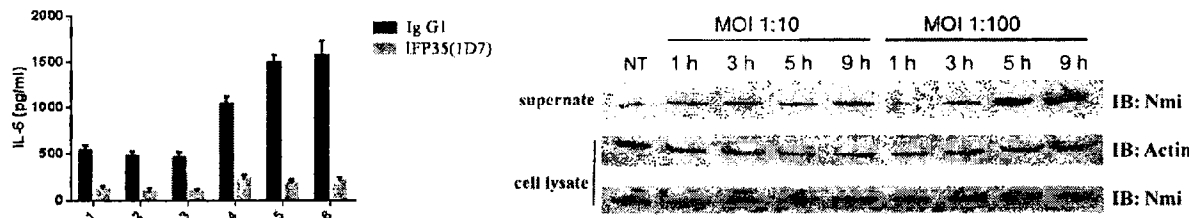


FIGURE 28

FIGURE 29

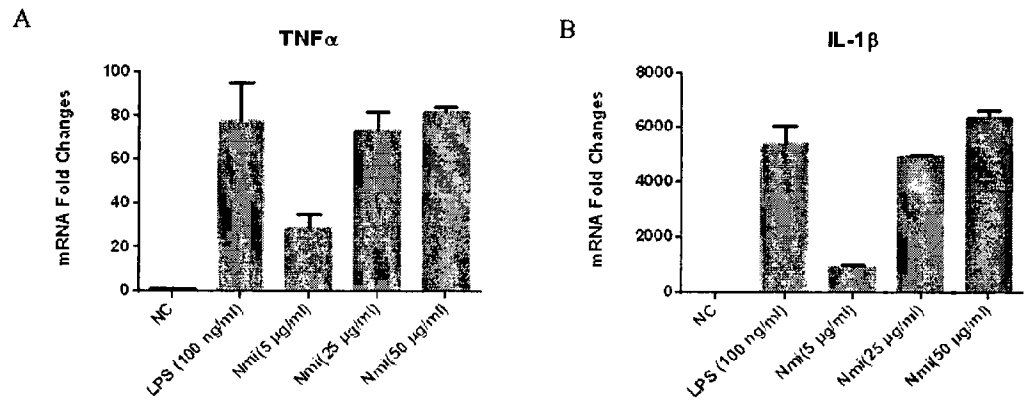


FIGURE 30

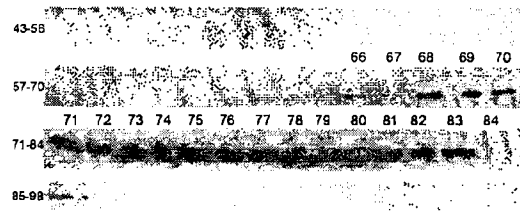


FIGURE 31

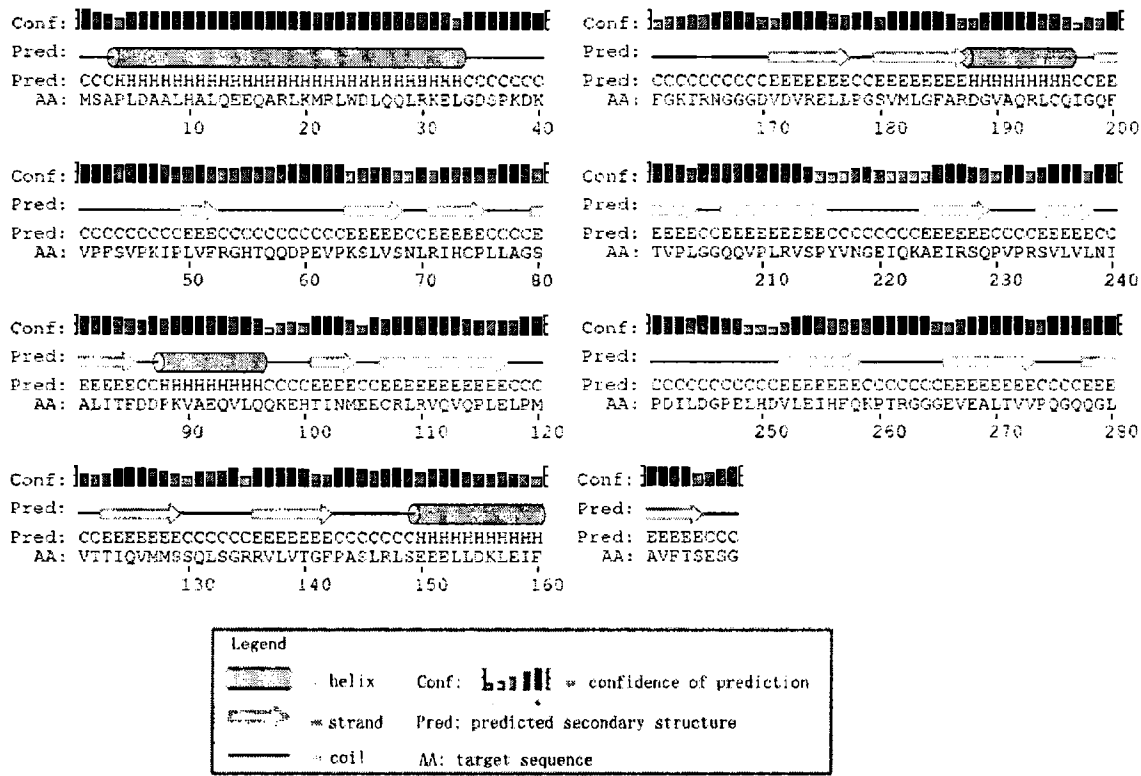


FIGURE 32

```

REMARK Date 2012-08-15 Time 17:29:02 CST +0800 (1345022942.94 s)
REMARK PHENIX refinement
REMARK ***** INPUT FILES AND LABELS *****
REMARK Reflections:
REMARK file name : R3.mtz
REMARK labels : ['I-obs(-), SIGI-obs(+), I-obs(-), SIGI-obs(-)']
REMARK K-free flags:
REMARK file name : R3.mtz
REMARK label : R-free-flags(+), R-free-flags(-)
REMARK test_flag_value: 1
REMARK Model file name(s):
REMARK /home/lab/hh1ang/shenjia/se/refine/4.pdb
REMARK ***** REFINEMENT SUMMARY: QUICK FACTS *****
REMARK Start: r_work = 0.1979 r_free = 0.2206 bonds = 0.027 angles = 1.212
REMARK Final: r_work = 0.1891 r_free = 0.2164 bonds = 0.014 angles = 1.073
REMARK ***** REFINEMENT STATISTICS STEP BY STEP *****
REMARK leading digit, like 1., means number of macro-cycles
REMARK 0 : statistics at the very beginning when nothing is done yet
REMARK 1 : bulk solvent correction and/or (anisotropic) scaling
REMARK 2 : refinement of coordinates
REMARK 3 : refinement of ADPs (Atomic Displacement Parameters)
REMARK 4 : ordered solvent update (add / remove)
REMARK 5 : refinement of occupancies
REMARK ***** R-factors, x-ray target values and norm of gradient of x-ray target *****
REMARK stage r-work r-free xray_target-u xray_target-t
REMARK 0 : 0.1982 0.2227 2.584130e+00 2.690833e+00
REMARK 1_bss: 0.1979 0.2206 2.579446e+00 2.674047e+00
REMARK 1_xyz: 0.1972 0.2271 2.563918e+00 2.691198e+00
REMARK 1_adp: 0.1929 0.2265 2.561187e+00 2.689500e+00
REMARK 2_bss: 0.1905 0.2238 2.556120e+00 2.680442e+00
REMARK 2_xyz: 0.1893 0.2203 2.545982e+00 2.666609e+00
REMARK 2_adp: 0.1885 0.2212 2.545223e+00 2.670100e+00
REMARK 3_bss: 0.1884 0.2201 2.544938e+00 2.691160e+00
REMARK 3_xyz: 0.1873 0.2191 2.538317e+00 2.661769e+00
REMARK 3_adp: 0.1867 0.2190 2.535566e+00 2.662260e+00
REMARK 3_bss: 0.1891 0.2164 2.543833e+00 2.649104e+00
REMARK ***** Overall statistics *****
REMARK stage k_sol b_sol b11 b22 b33 b12 b13 b23
REMARK 0 : 0.394 42.713 0.493 0.493 -0.981 -0.000 0.000 -0.000
REMARK 1_bss: 0.394 42.716 0.510 0.510 -1.019 -0.000 -0.000 0.000
REMARK 1_xyz: 0.394 42.716 0.510 0.510 -1.019 -0.000 -0.000 0.000
REMARK 1_adp: 0.394 42.716 0.510 0.510 -1.019 -0.000 -0.000 0.000
REMARK 2_bss: 0.394 42.969 0.530 0.530 -1.060 -0.000 -0.000 0.000
REMARK 2_xyz: 0.394 42.969 0.530 0.530 -1.060 -0.000 -0.000 0.000
REMARK 2_adp: 0.394 42.969 0.530 0.530 -1.060 -0.000 -0.000 0.000
REMARK 3_bss: 0.394 43.491 0.547 0.547 -1.095 -0.000 -0.000 0.000
REMARK 3_xyz: 0.394 43.491 0.547 0.547 -1.095 -0.000 -0.000 0.000
REMARK 3_adp: 0.394 43.491 0.547 0.547 -1.095 -0.000 -0.000 0.000
REMARK 3_bss: 0.395 44.043 0.645 0.645 -1.289 -0.000 -0.000 0.000
REMARK ***** Deviation of refined model from start model *****
REMARK stage max min max min max min max min
REMARK 0 : 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
REMARK 1_bss: 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
REMARK 1_xyz: 7.613 0.002 0.075 0.075 0.000 0.000 0.000 0.000
REMARK 1_adp: 7.613 0.002 0.075 0.075 0.000 0.000 0.000 0.000
REMARK 2_bss: 7.613 0.002 0.065 0.065 0.000 0.000 0.000 0.000
REMARK 2_xyz: 7.613 0.002 0.065 0.065 0.000 0.000 0.000 0.000
REMARK 2_adp: 7.613 0.002 0.065 0.065 0.000 0.000 0.000 0.000
REMARK 3_bss: 7.613 0.002 0.065 0.065 0.000 0.000 0.000 0.000
REMARK 3_xyz: 7.920 0.001 0.068 0.068 0.000 0.000 0.000 0.000
REMARK 3_adp: 7.920 0.001 0.068 0.068 0.000 0.000 0.000 0.000
REMARK 3_bss: 7.920 0.001 0.068 0.068 0.000 0.000 0.000 0.000
REMARK ***** stage number of ordered solvent *****
REMARK 0 : 157
REMARK ***** dimer-PDB-coordinates.txt *****
REMARK 1_bss: 157
REMARK 1_xyz: 157
REMARK 1_adp: 157
REMARK 2_bss: 243
REMARK 2_xyz: 243
REMARK 2_adp: 243
REMARK 3_bss: 243
REMARK 3_xyz: 263
REMARK 3_adp: 263
REMARK 3_bss: 247
REMARK ***** MODEL CONTENT *****
REMARK ELEMENT ATOM RECORD COUNT OCCUPANCY SUM
REMARK C 2430 2430.00
REMARK S 12 12.00
REMARK O 941 941.00
REMARK N 693 693.00
REMARK TOTAL 4076 4076.00
REMARK r_free_flags.md5.hexdigest 2a5644da3038c7a7af52eb7881d6dc1
REMARK IF THIS FILE IS FOR PDB DEPOSITION: REMOVE ALL FROM THIS LINE UP.
REMARK ***** REFINEMENT *****
REMARK PROGRAM : PHENIX (phenix.refine: 1.6.4.466)
REMARK AUTHORS : Adams, Afonine, Chen, Davis, Echols, Gopal,
REMARK Gross-Kunstleve, Hoare, Hung, Immerminger, Isenger, McCoy,
REMARK McKee, Moras, Paj, Read, Richardson, Richardson, Romo-
REMARK Sacchettini, Sauter, Smith, Stojanovic, Terwilliger, Zwart
REMARK ***** REFINEMENT TARGET : ML *****
REMARK ***** DATA USED IN REFINEMENT *****
REMARK RESOLUTION RANGE HIGH (ANGSTROMS) : 2.304
REMARK RESOLUTION RANGE LOW (ANGSTROMS) : 32.176
REMARK MIN(FOBS/SIGMA_FOBS) : 0.16
REMARK COMPLETENESS FOR RANGE (%) : 98.16
REMARK NUMBER OF REFLECTIONS : 49665
REMARK ***** FIT TO DATA USED IN REFINEMENT *****
REMARK R VALUE (WORKING + TEST SET) : 0.1891
REMARK R VALUE (WORKING SET) : 0.1891
REMARK FREE R VALUE : 0.2164
REMARK FREE R VALUE TEST SET SIZE (%) : 7.89
REMARK FREE R VALUE TEST SET COUNT : 3920
REMARK ***** FIT TO DATA USED IN REFINEMENT (IN BINS) *****
REMARK BIN RESOLUTION RANGE COMPLET. NWORK NFREE RWORK RFREE
REMARK 1 32.3789 - 6.9743 1.00 1663 148 0.1970 0.1931
REMARK 2 6.9743 - 5.5448 1.00 1648 144 0.2219 0.2490
REMARK 3 5.5448 - 4.8465 1.00 1666 146 0.1613 0.1740
REMARK 4 4.8465 - 4.4046 1.00 1678 142 0.1399 0.1474
REMARK 5 4.4046 - 4.0895 1.00 1653 146 0.1480 0.1679
REMARK 6 4.0895 - 3.8488 0.99 1642 143 0.1596 0.1643
REMARK 7 3.8488 - 3.6563 0.99 1666 138 0.1722 0.2083
REMARK 8 3.6563 - 3.4974 0.91 1518 132 0.2078 0.2077
REMARK 9 3.4974 - 3.3429 1.00 1630 140 0.1836 0.2170
REMARK 10 3.3429 - 3.2469 1.00 1664 141 0.1867 0.2252
REMARK 11 3.2469 - 3.1455 1.00 1669 143 0.1970 0.1891
REMARK 12 3.1455 - 3.0557 1.00 1667 144 0.1921 0.2309
REMARK 13 3.0557 - 2.9753 1.00 1680 135 0.1939 0.2142
REMARK 14 2.9753 - 2.9027 0.99 1649 143 0.1975 0.2096
REMARK 15 2.9027 - 2.8368 0.99 1656 145 0.2119 0.2850
REMARK ***** dimer-PDB-coordinates.txt *****
REMARK 3_bss: 23.129 0.8495 0.0182 35.896
REMARK 3_xyz: 22.872 0.8462 0.0182 35.386
REMARK 3_adp: 22.859 0.8462 0.0181 35.384
REMARK 3_bss: 22.550 0.8495 0.0185 34.758
REMARK ***** Maximal deviations *****
REMARK stage angl bond chir dihe plan repu lgradl
REMARK 0 : 22.479 0.354 0.222 70.433 0.055 1.121 3.3787e-01
REMARK 1_bss: 22.479 0.354 0.222 70.433 0.055 1.121 3.3787e-01
REMARK 1_xyz: 13.927 0.192 0.239 76.938 0.040 1.659 1.2796e-01
REMARK 1_adp: 13.927 0.192 0.239 76.938 0.040 1.659 1.2796e-01
REMARK 2_bss: 13.927 0.192 0.239 76.938 0.040 1.659 1.2796e-01
REMARK 2_xyz: 6.154 0.122 0.237 75.781 0.016 1.935 5.0119e-02
REMARK 2_adp: 6.154 0.122 0.237 75.781 0.016 1.935 5.0119e-02
REMARK 3_bss: 5.848 0.120 0.233 78.234 0.016 2.013 5.7365e-02
REMARK 3_xyz: 5.848 0.120 0.233 78.234 0.016 2.013 5.7365e-02
REMARK 3_adp: 5.848 0.120 0.233 78.234 0.016 2.013 5.7365e-02
REMARK 3_bss: 5.848 0.120 0.233 78.234 0.016 2.013 5.7365e-02
REMARK ***** Overall statistics *****
REMARK stage b_max b_min b_ave b_max b_min b_ave b_max b_min b_ave
REMARK 0 : 98.48 3.56 29.52 98.48 3.56 29.43 47.16 15.33 31.69
REMARK 1_bss: 98.48 3.56 29.52 98.48 3.56 29.44 47.16 15.33 31.69
REMARK 1_xyz: 98.48 3.56 29.52 98.48 3.56 29.44 47.16 15.33 31.69
REMARK 1_adp: 98.48 3.56 29.52 98.48 3.56 29.44 47.16 15.33 31.69
REMARK 2_bss: 99.17 2.99 29.32 99.17 2.99 29.23 49.06 14.87 31.56
REMARK 2_xyz: 99.17 2.99 29.32 99.17 2.99 29.23 49.06 14.87 31.56
REMARK 2_adp: 99.17 2.99 29.32 99.17 2.99 29.23 49.06 14.87 31.56
REMARK 3_bss: 96.71 2.77 29.84 96.71 2.77 29.38 67.41 12.79 36.59
REMARK 3_xyz: 96.71 2.77 29.84 96.71 2.77 29.38 67.41 12.79 36.59
REMARK 3_adp: 97.27 2.77 29.84 97.27 2.77 29.38 67.41 12.79 36.59
REMARK 3_bss: 97.82 2.39 30.09 97.82 2.39 29.72 36.36 15.72 35.74
REMARK ***** Deviation of refined model from start model *****
REMARK stage max min max min max min max min
REMARK 0 : 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
REMARK 1_bss: 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
REMARK 1_xyz: 7.613 0.002 0.075 0.075 0.000 0.000 0.000 0.000
REMARK 1_adp: 7.613 0.002 0.075 0.075 0.000 0.000 0.000 0.000
REMARK 2_bss: 7.613 0.002 0.065 0.065 0.000 0.000 0.000 0.000
REMARK 2_xyz: 7.613 0.002 0.065 0.065 0.000 0.000 0.000 0.000
REMARK 2_adp: 7.613 0.002 0.065 0.065 0.000 0.000 0.000 0.000
REMARK 3_bss: 7.613 0.002 0.065 0.065 0.000 0.000 0.000 0.000
REMARK 3_xyz: 7.920 0.001 0.068 0.068 0.000 0.000 0.000 0.000
REMARK 3_adp: 7.920 0.001 0.068 0.068 0.000 0.000 0.000 0.000
REMARK 3_bss: 7.920 0.001 0.068 0.068 0.000 0.000 0.000 0.000
REMARK ***** stage number of ordered solvent *****
REMARK 0 : 157
REMARK ***** dimer-PDB-coordinates.txt *****
REMARK 3 16 2.8368 - 2.7764 1.00 1411 0.2062 0.2758
REMARK 3 17 2.7764 - 2.7209 0.99 1722 0.1896 0.2290
REMARK 3 18 2.7209 - 2.6896 0.99 1603 0.2300 0.2766
REMARK 3 19 2.6896 - 2.6202 0.99 1629 0.2270 0.2767
REMARK 3 20 2.6202 - 2.5775 0.99 1604 0.2306 0.2773
REMARK 3 21 2.5775 - 2.5360 0.98 1613 0.2319 0.2975
REMARK 3 22 2.5360 - 2.4870 0.98 1645 0.2156 0.2776
REMARK 3 23 2.4870 - 2.4603 0.99 1700 0.2364 0.2532
REMARK 3 24 2.4603 - 2.4256 0.98 1563 0.236 0.2518
REMARK 3 25 2.4256 - 2.3929 0.98 1665 0.2340 0.2545
REMARK 3 26 2.3929 - 2.3618 0.96 1412 0.1864 0.2417
REMARK 3 27 2.3618 - 2.3323 0.97 1631 0.2172 0.2335
REMARK 3 28 2.3323 - 2.3042 0.92 1335 0.2353 0.2762
REMARK ***** R FACTOR FORMULA *****
REMARK R = SUM(|F_OBS| - SCALE * |F_MODEL|) / SUM(|F_OBS|)
REMARK ***** TOTAL MODEL STRUCTURE FACTOR (F_MODEL) *****
REMARK F_MODEL = F_BULK * EXP((F_CALC_ATOMS + F_BULK) / F_CALC_ATOMS)
REMARK F_CALC_ATOMS = ATOMIC MODEL STRUCTURE FACTORS
REMARK F_BULK = EXP((H(1) - AC(1) - C(1) - AC(1) - H(1)
REMARK A = ORTHOGONALIZATION MATRIX, H = MILLER INDEX
REMARK C = TRANSCIPSE, (-1) = TRANSPOSE
REMARK ***** STRUCTURE FACTORS CALCULATION ALGORITHM : FFT *****
REMARK ***** DEVIATIONS FROM IDEAL VALUES *****
REMARK DOND : 0.014 0.120 4000
REMARK ANGLE : 1.073 5.848 5240
REMARK CHIRALITY : 0.006 0.243 566
REMARK PLANARITY : 0.003 0.016 659
REMARK DIHEDRAL : 15.18 78.234 1462
REMARK MIN NONBONDED DISTANCE : 1.906
REMARK ***** ATOMIC DISPLACEMENT PARAMETERS *****
REMARK WILSON 3 : None
REMARK RMS(B_ISO_OR_EQUIVALENT_BONDED) : 6.84
REMARK ATOMS : NUMBER OF ATOMS
REMARK ISO : ANISO

```

|                           |          |                        |                              |          |          |        |      |       |           |                           |        |        |      |       |  |  |  |  |  |
|---------------------------|----------|------------------------|------------------------------|----------|----------|--------|------|-------|-----------|---------------------------|--------|--------|------|-------|--|--|--|--|--|
| dimer-PDB-coordinates.txt |          |                        |                              |          |          |        |      |       |           | dimer-PDB-coordinates.txt |        |        |      |       |  |  |  |  |  |
| REMARK                    | 3        | ALL                    | :                            | 4076     | 0        | ATOM   | 25   | CA    | ARG A 135 | -5.233                    | 21.857 | 30.748 | 1.00 | 29.86 |  |  |  |  |  |
| REMARK                    | 3        | ALL (NO H)             | :                            | 4076     | 0        | ATOM   | 26   | C8    | ARG A 135 | -4.425                    | 20.636 | 31.164 | 1.00 | 22.95 |  |  |  |  |  |
| REMARK                    | 3        | SOLVENT                | :                            | 247      | 0        | ATOM   | 27   | CG    | ARG A 135 | -5.182                    | 19.335 | 31.024 | 1.00 | 29.84 |  |  |  |  |  |
| REMARK                    | 3        | NON-SOLVENT            | :                            | 3829     | 0        | ATOM   | 28   | CD    | ARG A 135 | -4.852                    | 18.403 | 32.139 | 1.00 | 35.49 |  |  |  |  |  |
| REMARK                    | 3        | HYDROGENS              | :                            | 0        | 0        | ATOM   | 29   | NE    | ARG A 135 | -4.376                    | 17.124 | 31.648 | 1.00 | 49.93 |  |  |  |  |  |
| REMARK                    | 3        |                        |                              |          |          | ATOM   | 30   | CZ    | ARG A 135 | -3.099                    | 16.831 | 31.451 | 1.00 | 62.45 |  |  |  |  |  |
| REMARK                    | 3        | NCS DETAILS            |                              |          |          | ATOM   | 31   | NH1   | ARG A 135 | -2.162                    | 17.733 | 31.693 | 1.00 | 40.97 |  |  |  |  |  |
| REMARK                    | 3        | NUMBER OF NCS GROUPS : | 1                            |          |          | ATOM   | 32   | NH2   | ARG A 135 | -2.781                    | 15.626 | 31.014 | 1.00 | 81.20 |  |  |  |  |  |
| REMARK                    | 3        | NCS GROUP :            | 1                            |          |          | ATOM   | 33   | C     | ARG A 135 | -4.440                    | 23.124 | 31.059 | 1.00 | 22.78 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 34   | O     | ARG A 135 | -3.885                    | 23.258 | 32.145 | 1.00 | 23.74 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain B and (resseq 10:92) |          |          | ATOM   | 35   | N     | ARG A 136 | -4.382                    | 24.037 | 30.099 | 1.00 | 15.08 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 36   | CA    | ARG A 136 | -3.534                    | 25.205 | 30.212 | 1.00 | 22.37 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.054                      |          |          | ATOM   | 37   | CB    | ARG A 136 | -2.509                    | 25.241 | 29.071 | 1.00 | 23.59 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 2                            |          |          | ATOM   | 38   | CG    | ARG A 136 | -1.659                    | 24.001 | 29.009 | 1.00 | 30.35 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 39   | CD    | ARG A 136 | -0.513                    | 24.070 | 27.925 | 1.00 | 26.43 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain C and (resseq 10:92) |          |          | ATOM   | 40   | NE    | ARG A 136 | 0.167                     | 22.936 | 27.918 | 1.00 | 58.81 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 41   | 72    | ARG A 136 | 1.172                     | 22.584 | 27.084 | 1.00 | 40.33 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.039                      |          |          | ATOM   | 42   | NH1   | ARG A 136 | 1.345                     | 23.451 | 26.174 | 1.00 | 30.48 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 3                            |          |          | ATOM   | 43   | NH2   | ARG A 136 | 1.802                     | 21.423 | 27.164 | 1.00 | 32.12 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 44   | C     | ARG A 136 | -4.318                    | 26.496 | 30.210 | 1.00 | 15.47 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain D and (resseq 10:92) |          |          | ATOM   | 45   | O     | ARG A 136 | -5.335                    | 26.611 | 29.549 | 1.00 | 21.97 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 46   | N     | VAL A 137 | -3.810                    | 27.474 | 30.943 | 1.00 | 18.32 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.057                      |          |          | ATOM   | 47   | CA    | VAL A 137 | -4.391                    | 28.802 | 30.993 | 1.00 | 18.35 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 4                            |          |          | ATOM   | 48   | CB    | VAL A 137 | -5.204                    | 29.036 | 32.298 | 1.00 | 19.36 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 49   | CG1   | VAL A 137 | -6.296                    | 28.011 | 32.423 | 1.00 | 18.04 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain E and (resseq 10:92) |          |          | ATOM   | 50   | CG2   | VAL A 137 | -4.301                    | 28.581 | 33.520 | 1.00 | 13.98 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 51   | C     | VAL A 137 | -3.297                    | 29.849 | 30.909 | 1.00 | 18.17 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.046                      |          |          | ATOM   | 52   | O     | VAL A 137 | -2.115                    | 29.558 | 31.138 | 1.00 | 16.31 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 5                            |          |          | ATOM   | 53   | N     | LEU A 138 | -3.714                    | 31.063 | 30.557 | 1.00 | 18.51 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 54   | CA    | LEU A 138 | -2.863                    | 32.232 | 30.561 | 1.00 | 19.92 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain F and (resseq 10:92) |          |          | ATOM   | 55   | C     | LEU A 138 | -2.958                    | 32.798 | 29.233 | 1.00 | 20.37 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 56   | CG    | LEU A 138 | -2.007                    | 32.445 | 28.027 | 1.00 | 16.83 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.045                      |          |          | ATOM   | 57   | CD1   | LEU A 138 | -2.167                    | 33.507 | 26.946 | 1.00 | 36.14 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 6                            |          |          | ATOM   | 58   | CD2   | LEU A 138 | -0.600                    | 33.034 | 28.422 | 1.00 | 27.90 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 59   | C     | LEU A 138 | -3.319                    | 33.146 | 31.688 | 1.00 | 20.35 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain G and (resseq 10:92) |          |          | ATOM   | 60   | O     | LEU A 138 | -4.517                    | 33.388 | 31.870 | 1.00 | 11.67 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 61   | N     | VAL A 139 | -1.346                    | 33.663 | 32.428 | 1.00 | 15.28 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.045                      |          |          | ATOM   | 62   | CA    | VAL A 139 | -2.393                    | 34.596 | 32.731 | 1.00 | 25.57 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 7                            |          |          | ATOM   | 63   | CB    | VAL A 139 | -1.947                    | 34.123 | 34.829 | 1.00 | 19.42 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 64   | CG1   | VAL A 139 | -2.307                    | 35.081 | 35.958 | 1.00 | 13.63 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain H and (resseq 10:92) |          |          | ATOM   | 65   | CG2   | VAL A 139 | -2.376                    | 32.690 | 35.154 | 1.00 | 16.03 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 66   | C     | VAL A 139 | -1.999                    | 35.936 | 33.114 | 1.00 | 23.00 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.057                      |          |          | ATOM   | 67   | N     | VAL A 139 | -0.820                    | 36.020 | 32.731 | 1.00 | 20.66 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 8                            |          |          | ATOM   | 68   | N     | THR A 140 | -2.818                    | 36.982 | 33.207 | 1.00 | 17.88 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 69   | CA    | THR A 140 | -2.394                    | 38.312 | 32.771 | 1.00 | 27.24 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain I and (resseq 10:92) |          |          | ATOM   | 70   | CB    | THR A 140 | -2.980                    | 38.686 | 31.384 | 1.00 | 21.11 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 71   | CG1   | THR A 140 | -4.406                    | 38.580 | 31.438 | 1.00 | 22.20 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.046                      |          |          | ATOM   | 72   | CG2   | THR A 140 | -2.449                    | 37.744 | 30.306 | 1.00 | 25.26 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 9                            |          |          | ATOM   | 73   | C     | THR A 140 | -2.851                    | 38.358 | 33.768 | 1.00 | 15.47 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 74   | O     | THR A 140 | -3.738                    | 39.093 | 34.593 | 1.00 | 21.56 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain J and (resseq 10:92) |          |          | ATOM   | 75   | N     | GLY A 141 | -2.240                    | 40.539 | 33.659 | 1.00 | 26.14 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 76   | CA    | GLY A 141 | -2.636                    | 41.675 | 34.507 | 1.00 | 24.91 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.045                      |          |          | ATOM   | 77   | C     | GLY A 141 | -1.579                    | 42.216 | 35.456 | 1.00 | 21.73 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 10                           |          |          | ATOM   | 78   | O     | GLY A 141 | -1.669                    | 43.400 | 36.314 | 1.00 | 31.66 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 79   | N     | PHE A 142 | -0.747                    | 43.951 | 35.905 | 1.00 | 16.83 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain K and (resseq 10:92) |          |          | ATOM   | 80   | CA    | PHE A 142 | 0.728                     | 42.181 | 36.190 | 1.00 | 21.74 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 81   | CB    | PHE A 142 | 1.956                     | 41.295 | 35.974 | 1.00 | 22.57 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.045                      |          |          | ATOM   | 82   | CG    | PHE A 142 | 1.641                     | 39.940 | 35.959 | 1.00 | 28.82 |  |  |  |  |  |
| REMARK                    | 3        | NCS OPERATOR :         | 11                           |          |          | ATOM   | 83   | CD1   | PHE A 142 | 1.506                     | 39.140 | 37.155 | 1.00 | 23.23 |  |  |  |  |  |
| REMARK                    | 3        | REFERENCE SELECTION:   | chain A and (resseq 10:92)   |          |          | ATOM   | 84   | CD2   | PHE A 142 | 1.196                     | 37.799 | 37.137 | 1.00 | 23.64 |  |  |  |  |  |
| REMARK                    | 3        | SELECTION              | : chain L and (resseq 10:92) |          |          | ATOM   | 85   | C     | PHE A 142 | 0.007                     | 37.142 | 35.963 | 1.00 | 20.40 |  |  |  |  |  |
| REMARK                    | 3        | ATOM PAIRS NUMBER :    | 635                          |          |          | ATOM   | 86   | CE    | PHE A 142 | 1.133                     | 37.828 | 34.772 | 1.00 | 26.73 |  |  |  |  |  |
| REMARK                    | 3        | RMSD                   | : 0.045                      |          |          | ATOM   | 87   | CD2   | PHE A 142 | 1.446                     | 39.175 | 34.779 | 1.00 | 26.48 |  |  |  |  |  |
| CRYST1                    | 170.285  | 170.285                | 52.980                       | 90.00    | 90.00    | 120.00 | H 3  |       |           |                           |        |        |      |       |  |  |  |  |  |
| SCALE1                    | 0.005873 | 0.003390               | 0.000000                     | 0.000000 | 0.000000 |        |      |       |           |                           |        |        |      |       |  |  |  |  |  |
| SCALE2                    | 0.000000 | 0.006781               | 0.000000                     | 0.000000 | 0.000000 |        |      |       |           |                           |        |        |      |       |  |  |  |  |  |
| SCALE3                    | 0.000000 | 0.000000               | 0.018875                     | 0.000000 | 0.000000 |        |      |       |           |                           |        |        |      |       |  |  |  |  |  |
| ATOM                      | 1        | O                      | ALA A 131                    | -2.052   | 14.406   | 26.595 | 1.00 | 56.29 |           |                           |        |        |      |       |  |  |  |  |  |
| ATOM                      | 2        | N                      | ALA A 131                    | -3.626   | 13.169   | 30.963 | 1.00 | 42.82 |           |                           |        |        |      |       |  |  |  |  |  |
| ATOM                      | 3        | CA                     | ALA A 131                    | -2.768   | 15.333   | 28.931 | 1.00 | 61.54 |           |                           |        |        |      |       |  |  |  |  |  |
| ATOM                      | 4        | C                      | ALA A 131                    | -3.525   | 14.297   | 27.832 | 1.00 | 58.93 |           |                           |        |        |      |       |  |  |  |  |  |
|                           |          |                        |                              |          |          |        |      |       |           |                           |        |        |      |       |  |  |  |  |  |

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|---------------------------|-----|-----|-----------|
| ATOM                      | 214 | OE1 | GLU A 158 |
| ATOM                      | 215 | OE2 | GLU A 158 |
| ATOM                      | 216 | C   | GLU A 158 |
| ATOM                      | 217 | O   | GLU A 158 |
| ATOM                      | 218 | ILE | A 159     |
| ATOM                      | 219 | ILE | A 159     |
| ATOM                      | 220 | CB  | ILE A 159 |
| ATOM                      | 221 | CG1 | ILE A 159 |
| ATOM                      | 222 | CG2 | ILE A 159 |
| ATOM                      | 223 | CG2 | ILE A 159 |
| ATOM                      | 224 | C   | ILE A 159 |
| ATOM                      | 225 | O   | ILE A 159 |
| ATOM                      | 226 | N   | PHE A 160 |
| ATOM                      | 227 | CA  | PHE A 160 |
| ATOM                      | 228 | CB  | PHE A 160 |
| ATOM                      | 229 | CG  | PHE A 160 |
| ATOM                      | 230 | CD1 | PHE A 160 |
| ATOM                      | 231 | CE1 | PHE A 160 |
| ATOM                      | 232 | CZ  | PHE A 160 |
| ATOM                      | 233 | CE2 | PHE A 160 |
| ATOM                      | 234 | CD2 | PHE A 160 |
| ATOM                      | 235 | C   | PHE A 160 |
| ATOM                      | 236 | O   | PHE A 160 |
| ATOM                      | 237 | N   | PHE A 161 |
| ATOM                      | 238 | CA  | PHE A 161 |
| ATOM                      | 239 | CB  | PHE A 161 |
| ATOM                      | 240 | CG  | PHE A 161 |
| ATOM                      | 241 | CD1 | PHE A 161 |
| ATOM                      | 242 | CE1 | PHE A 161 |
| ATOM                      | 243 | CZ  | PHE A 161 |
| ATOM                      | 244 | CE2 | PHE A 161 |
| ATOM                      | 245 | CD2 | PHE A 161 |
| ATOM                      | 246 | C   | PHE A 161 |
| ATOM                      | 247 | O   | PHE A 161 |
| ATOM                      | 248 | N   | GLY A 162 |
| ATOM                      | 249 | CA  | GLY A 162 |
| ATOM                      | 250 | C   | GLY A 162 |
| ATOM                      | 251 | O   | GLY A 162 |
| ATOM                      | 252 | N   | LYS A 163 |
| ATOM                      | 253 | CA  | LYS A 163 |
| ATOM                      | 254 | CB  | LYS A 163 |
| ATOM                      | 255 | CG  | LYS A 163 |
| ATOM                      | 256 | CD  | LYS A 163 |
| ATOM                      | 257 | CE  | LYS A 163 |
| ATOM                      | 258 | CF  | LYS A 163 |
| ATOM                      | 259 | C   | LYS A 163 |
| ATOM                      | 260 | O   | LYS A 163 |
| ATOM                      | 261 | N   | THR A 164 |
| ATOM                      | 262 | CA  | THR A 164 |
| ATOM                      | 263 | CB  | THR A 164 |
| ATOM                      | 264 | CG  | THR A 164 |
| ATOM                      | 265 | CD  | THR A 164 |
| ATOM                      | 266 | C   | THR A 164 |
| ATOM                      | 267 | O   | THR A 164 |
| ATOM                      | 268 | N   | ARG A 165 |
| ATOM                      | 269 | CA  | ARG A 165 |
| ATOM                      | 270 | CB  | ARG A 165 |
| ATOM                      | 271 | CG  | ARG A 165 |
| ATOM                      | 272 | CD  | ARG A 165 |
| ATOM                      | 273 | CE  | ARG A 165 |
| ATOM                      | 274 | CZ  | ARG A 165 |
| ATOM                      | 275 | NH1 | ARG A 165 |
| ATOM                      | 276 | NH2 | ARG A 165 |

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|---------------------------|-----|-----|-----------|
| ATOM                      | 340 | N   | GLU A 175 |
| ATOM                      | 341 | CA  | GLU A 175 |
| ATOM                      | 342 | CB  | GLU A 175 |
| ATOM                      | 343 | CG  | GLU A 175 |
| ATOM                      | 344 | CD  | GLU A 175 |
| ATOM                      | 345 | OE1 | GLU A 175 |
| ATOM                      | 346 | OE2 | GLU A 175 |
| ATOM                      | 347 | C   | GLU A 175 |
| ATOM                      | 348 | O   | GLU A 175 |
| ATOM                      | 349 | N   | LEU A 176 |
| ATOM                      | 350 | CA  | LEU A 176 |
| ATOM                      | 351 | CB  | LEU A 176 |
| ATOM                      | 352 | CG  | LEU A 176 |
| ATOM                      | 353 | CD1 | LEU A 176 |
| ATOM                      | 354 | CD2 | LEU A 176 |
| ATOM                      | 355 | C   | LEU A 176 |
| ATOM                      | 356 | O   | LEU A 176 |
| ATOM                      | 357 | N   | LEU A 177 |
| ATOM                      | 358 | CA  | LEU A 177 |
| ATOM                      | 359 | CB  | LEU A 177 |
| ATOM                      | 360 | CG  | LEU A 177 |
| ATOM                      | 361 | CD1 | LEU A 177 |
| ATOM                      | 362 | CD2 | LEU A 177 |
| ATOM                      | 363 | C   | LEU A 177 |
| ATOM                      | 364 | O   | LEU A 177 |
| ATOM                      | 365 | N   | PRO A 178 |
| ATOM                      | 366 | CA  | PRO A 178 |
| ATOM                      | 367 | CB  | PRO A 178 |
| ATOM                      | 368 | CG  | PRO A 178 |
| ATOM                      | 369 | CD  | PRO A 178 |
| ATOM                      | 370 | C   | PRO A 178 |
| ATOM                      | 371 | O   | PRO A 178 |
| ATOM                      | 372 | N   | GLY A 179 |
| ATOM                      | 373 | CA  | GLY A 179 |
| ATOM                      | 374 | C   | GLY A 179 |
| ATOM                      | 375 | O   | GLY A 179 |
| ATOM                      | 376 | N   | SER A 180 |
| ATOM                      | 377 | CA  | SER A 180 |
| ATOM                      | 378 | CB  | SER A 180 |
| ATOM                      | 379 | CG  | SER A 180 |
| ATOM                      | 380 | C   | SER A 180 |
| ATOM                      | 381 | O   | SER A 180 |
| ATOM                      | 382 | N   | VAL A 181 |
| ATOM                      | 383 | CA  | VAL A 181 |
| ATOM                      | 384 | CB  | VAL A 181 |
| ATOM                      | 385 | CG1 | VAL A 181 |
| ATOM                      | 386 | CG2 | VAL A 181 |
| ATOM                      | 387 | C   | VAL A 181 |
| ATOM                      | 388 | O   | VAL A 181 |
| ATOM                      | 389 | N   | MET A 182 |
| ATOM                      | 390 | CA  | MET A 182 |
| ATOM                      | 391 | CB  | MET A 182 |
| ATOM                      | 392 | CG  | MET A 182 |
| ATOM                      | 393 | CD  | MET A 182 |
| ATOM                      | 394 | CE  | MET A 182 |
| ATOM                      | 395 | C   | MET A 182 |
| ATOM                      | 396 | O   | MET A 182 |
| ATOM                      | 397 | N   | LEU A 183 |
| ATOM                      | 398 | CA  | LEU A 183 |
| ATOM                      | 399 | CB  | LEU A 183 |
| ATOM                      | 400 | CG  | LEU A 183 |
| ATOM                      | 401 | CD1 | LEU A 183 |
| ATOM                      | 402 | CD2 | LEU A 183 |

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|---------------------------|------|-----|-----------|
| O                         | ATOM | 277 | C         |
| O                         | ATOM | 278 | O         |
| O                         | ATOM | 279 | N         |
| O                         | ATOM | 280 | CA        |
| O                         | ATOM | 281 | CB        |
| O                         | ATOM | 282 | CG        |
| O                         | ATOM | 283 | CD1       |
| O                         | ATOM | 284 | CD2       |
| O                         | ATOM | 285 | C         |
| O                         | ATOM | 286 | O         |
| O                         | ATOM | 287 | N         |
| O                         | ATOM | 288 | CA        |
| O                         | ATOM | 289 | CB        |
| O                         | ATOM | 290 | CG        |
| O                         | ATOM | 291 | CD        |
| O                         | ATOM | 292 | CE        |
| O                         | ATOM | 293 | C         |
| O                         | ATOM | 294 | O         |
| O                         | ATOM | 295 | N         |
| O                         | ATOM | 296 | CA        |
| O                         | ATOM | 297 | CB        |
| O                         | ATOM | 298 | CG        |
| O                         | ATOM | 299 | CD        |
| O                         | ATOM | 300 | CE        |
| O                         | ATOM | 301 | C         |
| O                         | ATOM | 302 | O         |
| O                         | ATOM | 303 | N         |
| O                         | ATOM | 304 | CA        |
| O                         | ATOM | 305 | CB        |
| O                         | ATOM | 306 | CG        |
| O                         | ATOM | 307 | CD        |
| O                         | ATOM | 308 | CE        |
| O                         | ATOM | 309 | C         |
| O                         | ATOM | 310 | VAL A 171 |
| O                         | ATOM | 311 | CG2       |
| O                         | ATOM | 312 | C         |
| O                         | ATOM | 313 | O         |
| O                         | ATOM | 314 | N         |
| O                         | ATOM | 315 | CA        |
| O                         | ATOM | 316 | CB        |
| O                         | ATOM | 317 | CG        |
| O                         | ATOM | 318 | CD1       |
| O                         | ATOM | 319 | CD2       |
| O                         | ATOM | 320 | C         |
| O                         | ATOM | 321 | O         |
| O                         | ATOM | 322 | N         |
| O                         | ATOM | 323 | CA        |
| O                         | ATOM | 324 | CB        |
| O                         | ATOM | 325 | CG        |
| O                         | ATOM | 326 | CD        |
| O                         | ATOM | 327 | C         |
| O                         | ATOM | 328 | O         |
| O                         | ATOM | 329 | N         |
| O                         | ATOM | 330 | CA        |
| O                         | ATOM | 331 | CB        |
| O                         | ATOM | 332 | CG        |
| O                         | ATOM | 333 | CD        |
| O                         | ATOM | 334 | CE        |
| O                         | ATOM | 335 | C         |
| O                         | ATOM | 336 | O         |
| O                         | ATOM | 337 | NH2       |
| O                         | ATOM | 338 | C         |
| O                         | ATOM | 339 | O         |

| dimer-PDB-coordinates.txt |      |     |    |
|---------------------------|------|-----|----|
| O                         | ATOM | 403 | C  |
| O                         | ATOM | 404 | O  |
| O                         | ATOM | 405 | N  |
| O                         | ATOM | 406 | CA |
| O                         | ATOM | 407 | CB |
| O                         | ATOM | 408 | CG |
| O                         | ATOM | 409 | CD |
| O                         | ATOM | 410 | CE |
| O                         | ATOM | 411 | C  |
| O                         | ATOM | 412 | O  |
| O                         | ATOM | 413 | N  |
| O                         | ATOM | 414 | CA |
| O                         | ATOM | 415 | CB |
| O                         | ATOM | 416 | CG |
| O                         | ATOM | 417 | CD |
| O                         | ATOM | 418 | CE |
| O                         | ATOM | 419 | C  |
| O                         | ATOM | 420 | O  |
| O                         | ATOM | 421 | N  |
| O                         | ATOM | 422 | CA |
| O                         | ATOM | 423 | CB |
| O                         | ATOM | 424 | CG |
| O                         | ATOM | 425 | CD |
| O                         | ATOM | 426 | CE |
| O                         | ATOM | 427 | C  |
| O                         | ATOM | 428 | O  |
| O                         | ATOM | 429 | N  |
| O                         | ATOM | 430 | CA |
| O                         | ATOM | 431 | CB |
| O                         | ATOM | 432 | CG |
| O                         | ATOM | 433 | CD |
| O                         | ATOM | 434 | CE |
| O                         | ATOM | 435 | C  |
| O                         | ATOM | 436 | O  |
| O                         | ATOM | 437 | N  |
| O                         | ATOM | 438 | CA |
| O                         | ATOM | 439 | CB |
| O                         | ATOM | 440 | CG |
| O                         | ATOM | 441 | CD |
| O                         | ATOM | 442 | CE |
| O                         | ATOM | 443 | C  |
| O                         | ATOM | 444 | O  |
| O                         | ATOM | 445 | N  |
| O                         | ATOM | 446 | CA |
| O                         | ATOM | 447 | CB |
| O                         | ATOM | 448 | CG |
| O                         | ATOM | 449 | CD |
| O                         | ATOM | 450 | CE |
| O                         | ATOM | 451 | C  |
| O                         | ATOM | 452 | O  |
| O                         | ATOM | 453 | N  |
| O                         | ATOM | 454 | CA |
| O                         | ATOM | 455 | CB |
| O                         | ATOM | 456 | CG |
| O                         | ATOM | 457 | CD |
| O                         | ATOM | 458 | CE |
| O                         | ATOM | 459 | C  |
| O                         | ATOM | 460 | O  |
| O                         | ATOM | 461 | N  |
| O                         | ATOM | 462 | CA |
| O                         | ATOM | 463 | CB |
| O                         | ATOM | 464 | CG |
| O                         | ATOM | 465 | CD |

| dimer-PDB-coordinates.txt |     |     |           |                                  |
|---------------------------|-----|-----|-----------|----------------------------------|
| ATOM                      | 466 | NE2 | GLN A 192 | -10.517 23.112 29.759 1.00 43.33 |
| ATOM                      | 467 | C   | GLN A 192 | -11.584 25.951 34.040 1.00 32.42 |
| ATOM                      | 468 | O   | GLN A 192 | -13.157 27.009 33.881 1.00 25.76 |
| ATOM                      | 469 | N   | ARG A 193 | -12.462 25.365 35.223 1.00 22.13 |
| ATOM                      | 470 | CA  | ARG A 193 | -12.985 26.029 36.411 1.00 24.31 |
| ATOM                      | 471 | CB  | ARG A 193 | -12.719 25.124 37.637 1.00 22.62 |
| ATOM                      | 472 | CG  | ARG A 193 | -13.223 25.819 38.913 1.00 25.92 |
| ATOM                      | 473 | CD  | ARG A 193 | -12.500 25.315 40.151 1.00 32.86 |
| ATOM                      | 474 | NE  | ARG A 193 | -12.790 23.945 40.533 1.00 32.67 |
| ATOM                      | 475 | CZ  | ARG A 193 | -12.879 23.022 40.803 1.00 40.87 |
| ATOM                      | 476 | NH1 | ARG A 193 | -10.597 23.318 40.748 1.00 35.20 |
| ATOM                      | 477 | NH2 | ARG A 193 | -12.260 21.800 41.425 1.00 32.13 |
| ATOM                      | 478 | C   | ARG A 193 | -12.350 27.417 38.586 1.00 20.89 |
| ATOM                      | 479 | O   | ARG A 193 | -13.052 28.420 36.777 1.00 20.09 |
| ATOM                      | 480 | N   | LEU A 194 | -11.021 27.482 36.525 1.00 18.75 |
| ATOM                      | 481 | CA  | LEU A 194 | -10.330 25.755 36.749 1.00 18.43 |
| ATOM                      | 482 | CB  | LEU A 194 | -8.807 25.575 36.742 1.00 16.00  |
| ATOM                      | 483 | CG  | LEU A 194 | -6.208 21.924 37.508 1.00 21.55  |
| ATOM                      | 484 | CD  | LEU A 194 | -6.726 27.576 37.701 1.00 15.82  |
| ATOM                      | 485 | CE  | LEU A 194 | -8.449 25.521 39.205 1.00 19.51  |
| ATOM                      | 486 | C   | LEU A 194 | -10.733 29.771 35.655 1.00 22.95 |
| ATOM                      | 487 | O   | LEU A 194 | -10.690 30.967 35.850 1.00 20.00 |
| ATOM                      | 488 | N   | PRO A 195 | -10.414 33.125 36.185 1.00 21.72 |
| ATOM                      | 489 | CA  | PRO A 195 | -11.358 30.133 38.369 1.00 24.28 |
| ATOM                      | 490 | CB  | PRO A 195 | -11.196 29.377 39.039 1.00 28.70 |
| ATOM                      | 491 | CG  | PRO A 195 | -11.610 30.301 39.554 1.00 58.72 |
| ATOM                      | 492 | C   | PRO A 195 | -12.791 30.653 38.584 1.00 22.41 |
| ATOM                      | 493 | CD  | PRO A 195 | -13.075 31.110 39.343 1.00 19.38 |
| ATOM                      | 494 | CE  | PRO A 195 | -13.679 29.802 39.898 1.00 19.67 |
| ATOM                      | 495 | CA  | GLN A 196 | -15.030 30.221 34.440 1.00 27.66 |
| ATOM                      | 496 | CB  | GLN A 196 | -15.662 29.040 34.926 1.00 26.25 |
| ATOM                      | 497 | CG  | GLN A 196 | -16.426 28.148 33.623 1.00 51.12 |
| ATOM                      | 498 | C   | GLN A 196 | -16.749 26.735 34.301 1.00 63.53 |
| ATOM                      | 499 | CD  | GLN A 196 | -16.861 26.375 35.501 1.00 50.35 |
| ATOM                      | 500 | NE2 | GLN A 196 | -16.892 25.813 35.354 1.00 47.43 |
| ATOM                      | 501 | C   | GLN A 196 | -14.993 31.306 35.507 1.00 27.39 |
| ATOM                      | 502 | O   | GLN A 196 | -15.694 32.306 35.356 1.00 24.15 |
| ATOM                      | 503 | N   | ILE A 197 | -14.190 31.115 36.554 1.00 29.11 |
| ATOM                      | 504 | CA  | ILE A 197 | -14.069 31.157 37.589 1.00 23.11 |
| ATOM                      | 505 | CB  | ILE A 197 | -13.183 31.710 38.757 1.00 22.35 |
| ATOM                      | 506 | CG  | ILE A 197 | -13.625 30.514 39.476 1.00 19.67 |
| ATOM                      | 507 | CD  | ILE A 197 | -12.839 29.774 40.407 1.00 24.55 |
| ATOM                      | 508 | CE  | ILE A 197 | -12.949 32.881 39.722 1.00 19.50 |
| ATOM                      | 509 | C   | ILE A 197 | -13.516 33.443 36.973 1.00 26.10 |
| ATOM                      | 510 | NE  | ILE A 197 | -14.031 34.531 37.223 1.00 23.02 |
| ATOM                      | 511 | N   | GLY A 198 | -12.451 31.122 36.185 1.00 21.72 |
| ATOM                      | 512 | CA  | GLY A 198 | -11.980 34.400 35.350 1.00 19.99 |
| ATOM                      | 513 | C   | GLY A 198 | -11.152 35.488 36.009 1.00 24.60 |
| ATOM                      | 514 | O   | GLY A 198 | -10.071 35.816 35.533 1.00 24.65 |
| ATOM                      | 515 | N   | GLN A 199 | -11.660 36.071 37.088 1.00 22.31 |
| ATOM                      | 516 | CA  | GLN A 199 | -10.918 37.123 37.777 1.00 28.60 |
| ATOM                      | 517 | CB  | GLN A 199 | -11.761 38.187 37.866 1.00 28.27 |
| ATOM                      | 518 | CG  | GLN A 199 | -11.989 39.052 36.520 1.00 46.50 |
| ATOM                      | 519 | CD  | GLN A 199 | -12.540 40.450 36.658 1.00 71.20 |
| ATOM                      | 520 | CE  | GLN A 199 | -11.814 41.383 37.013 1.00 73.18 |
| ATOM                      | 521 | NE2 | GLN A 199 | -13.835 40.606 36.394 1.00 61.94 |
| ATOM                      | 522 | C   | GLN A 199 | -10.566 36.703 38.221 1.00 23.76 |
| ATOM                      | 523 | O   | GLN A 199 | -11.468 36.014 39.889 1.00 27.81 |
| ATOM                      | 524 | N   | PHE A 200 | -9.257 37.119 39.557 1.00 18.81  |
| ATOM                      | 525 | CA  | PHE A 200 | -6.755 36.734 40.857 1.00 16.65  |
| ATOM                      | 526 | CB  | PHE A 200 | -7.816 35.531 40.723 1.00 19.81  |
| ATOM                      | 527 | CG  | PHE A 200 | -8.438 34.339 40.058 1.00 19.49  |
| ATOM                      | 528 | CD  | PHE A 200 | -8.927 33.281 40.818 1.00 15.69  |

| dimer-PDB-coordinates.txt |     |     |           |                                  |
|---------------------------|-----|-----|-----------|----------------------------------|
| ATOM                      | 592 | CG  | VAL A 209 | -2.093 41.922 41.412 1.00 23.13  |
| ATOM                      | 593 | CD  | VAL A 209 | -2.055 42.270 39.931 1.00 24.29  |
| ATOM                      | 594 | CE  | VAL A 209 | -0.799 42.539 42.095 1.00 16.99  |
| ATOM                      | 595 | C   | VAL A 209 | -4.489 42.667 41.482 1.00 19.82  |
| ATOM                      | 596 | O   | VAL A 209 | -4.658 40.465 41.638 1.00 22.08  |
| ATOM                      | 597 | N   | PRO A 210 | -5.320 42.416 40.769 1.00 23.67  |
| ATOM                      | 598 | CA  | PRO A 210 | -4.409 42.400 40.903 1.00 24.00  |
| ATOM                      | 599 | CB  | PRO A 210 | -7.354 42.947 39.700 1.00 20.14  |
| ATOM                      | 600 | CG  | PRO A 210 | -6.448 44.155 39.672 1.00 23.58  |
| ATOM                      | 601 | CD  | PRO A 210 | -5.324 43.884 40.650 1.00 17.97  |
| ATOM                      | 602 | CE  | PRO A 210 | -5.861 44.260 38.796 1.00 22.62  |
| ATOM                      | 603 | C   | PRO A 210 | -5.322 43.854 40.654 1.00 22.62  |
| ATOM                      | 604 | N   | LEU A 211 | -5.987 39.846 36.586 1.00 20.01  |
| ATOM                      | 605 | CA  | LEU A 211 | -5.451 39.086 37.471 1.00 21.86  |
| ATOM                      | 606 | CB  | LEU A 211 | -4.455 38.037 37.954 1.00 13.26  |
| ATOM                      | 607 | CG  | LEU A 211 | -3.167 38.506 38.654 1.00 18.62  |
| ATOM                      | 608 | C   | LEU A 211 | -2.337 37.309 39.107 1.00 15.91  |
| ATOM                      | 609 | CD  | LEU A 211 | -2.314 38.392 37.763 1.00 19.14  |
| ATOM                      | 610 | CE  | LEU A 211 | -6.581 38.391 36.712 1.00 25.45  |
| ATOM                      | 611 | O   | LEU A 211 | -7.644 36.089 37.273 1.00 20.26  |
| ATOM                      | 612 | N   | ARG A 212 | -6.336 36.144 35.428 1.00 21.36  |
| ATOM                      | 613 | CA  | ARG A 212 | -7.285 37.448 34.587 1.00 21.56  |
| ATOM                      | 614 | CB  | ARG A 212 | -7.549 38.219 33.501 1.00 29.44  |
| ATOM                      | 615 | CG  | ARG A 212 | -8.262 39.349 33.305 1.00 29.40  |
| ATOM                      | 616 | CD  | ARG A 212 | -9.737 39.366 33.234 1.00 68.47  |
| ATOM                      | 617 | CE  | ARG A 212 | -10.467 40.628 33.233 1.00 65.17 |
| ATOM                      | 618 | C   | ARG A 212 | -11.792 40.705 33.230 1.00 72.06 |
| ATOM                      | 619 | NH1 | ARG A 212 | -12.516 39.591 33.228 1.00 66.62 |
| ATOM                      | 620 | NH2 | ARG A 212 | -12.392 41.889 32.236 1.00 70.06 |
| ATOM                      | 621 | C   | ARG A 212 | -6.695 36.112 34.399 1.00 26.61  |
| ATOM                      | 622 | O   | ARG A 212 | -5.493 36.008 33.915 1.00 16.12  |
| ATOM                      | 623 | N   | VAL A 213 | -7.555 35.101 34.177 1.00 21.30  |
| ATOM                      | 624 | CA  | VAL A 213 | -7.208 33.794 33.668 1.00 22.30  |
| ATOM                      | 625 | CB  | VAL A 213 | -7.504 32.701 34.705 1.00 20.15  |
| ATOM                      | 626 | CG  | VAL A 213 | -7.396 31.335 35.050 1.00 17.48  |
| ATOM                      | 627 | CD  | VAL A 213 | -6.536 32.817 35.850 1.00 18.71  |
| ATOM                      | 628 | C   | VAL A 213 | -6.019 33.540 32.403 1.00 26.82  |
| ATOM                      | 629 | O   | VAL A 213 | -9.238 33.683 32.403 1.00 26.34  |
| ATOM                      | 630 | N   | SER A 214 | -7.338 33.173 31.327 1.00 20.92  |
| ATOM                      | 631 | CA  | SER A 214 | -7.987 32.925 30.037 1.00 30.35  |
| ATOM                      | 632 | CB  | SER A 214 | -7.611 34.016 29.037 1.00 27.75  |
| ATOM                      | 633 | CG  | SER A 214 | -7.813 35.301 29.583 1.00 45.62  |
| ATOM                      | 634 | C   | SER A 214 | -7.506 32.592 29.493 1.00 26.23  |
| ATOM                      | 635 | O   | SER A 214 | -6.469 31.105 29.919 1.00 22.15  |
| ATOM                      | 636 | N   | PRO A 215 | -8.244 31.006 28.540 1.00 31.13  |
| ATOM                      | 637 | CA  | PRO A 215 | -7.791 29.739 27.430 1.00 39.78  |
| ATOM                      | 638 | CB  | PRO A 215 | -8.942 29.347 27.022 1.00 39.78  |
| ATOM                      | 639 | CG  | PRO A 215 | -10.101 30.203 27.430 1.00 43.19 |
| ATOM                      | 640 | CD  | PRO A 215 | -9.506 31.469 27.945 1.00 35.86  |
| ATOM                      | 641 | C   | PRO A 215 | -6.512 29.947 27.147 1.00 29.53  |
| ATOM                      | 642 | O   | PRO A 215 | -6.286 31.041 26.837 1.00 33.72  |
| ATOM                      | 643 | N   | TYR A 216 | -5.677 28.920 27.041 1.00 29.46  |
| ATOM                      | 644 | CA  | TYR A 216 | -4.455 29.020 26.256 1.00 38.33  |
| ATOM                      | 645 | CB  | TYR A 216 | -3.351 28.171 26.878 1.00 39.21  |
| ATOM                      | 646 | CG  | TYR A 216 | -2.014 26.322 26.199 1.00 44.95  |
| ATOM                      | 647 | CD  | TYR A 216 | -1.466 29.580 25.865 1.00 51.11  |
| ATOM                      | 648 | CE  | TYR A 216 | -0.240 29.732 25.264 1.00 51.64  |
| ATOM                      | 649 | CZ  | TYR A 216 | -0.459 28.647 24.959 1.00 59.06  |
| ATOM                      | 650 | OH  | TYR A 216 | -1.684 26.773 24.348 1.00 61.10  |
| ATOM                      | 651 | CH2 | TYR A 216 | -0.963 27.353 25.165 1.00 56.66  |
| ATOM                      | 652 | CD2 | TYR A 216 | -1.295 27.213 25.781 1.00 46.46  |
| ATOM                      | 653 | C   | TYR A 216 | -4.697 28.559 24.820 1.00 38.96  |
| ATOM                      | 654 | O   | TYR A 216 | -5.226 27.483 24.597 1.00 42.30  |

| dimer-PDB-coordinates.txt |     |     |           |                                 |
|---------------------------|-----|-----|-----------|---------------------------------|
| N                         | 529 | CE2 | PHE A 200 | -9.510 32.173 40.205 1.00 17.08 |
| O                         | 530 | CE  | PHE A 200 | -9.602 31.123 38.818 1.00 14.67 |
| N                         | 531 | CE1 | PHE A 200 | -9.120 33.177 38.060 1.00 17.45 |
| C                         | 532 | CD1 | PHE A 200 | -8.540 34.275 36.674 1.00 16.76 |
| C                         | 533 | C   | PHE A 200 | -7.948 37.887 41.437 1.00 22.12 |
| C                         | 534 | O   | PHE A 200 | -7.379 38.654 40.706 1.00 24.64 |
| C                         | 535 | N   | THR A 201 | -7.944 38.002 42.753 1.00 20.04 |
| N                         | 536 | CA  | THR A 201 | -7.068 38.953 43.399 1.00 20.47 |
| C                         | 537 | CB  | THR A 201 | -7.824 39.803 44.436 1.00 22.49 |
| N                         | 538 | CG1 | THR A 201 | -8.860 40.526 43.763 1.00 20.50 |
| N                         | 539 | CG2 | THR A 201 | -8.891 40.804 45.087 1.00 23.11 |
| N                         | 540 | O   | THR A 201 | -8.567 38.160 44.055 1.00 17.05 |
| O                         | 541 | O   | THR A 201 | -8.221 37.317 44.905 1.00 24.00 |
| N                         | 542 | N   | VAL A 202 | -4.732 38.420 43.647 1.00 21.35 |
| C                         | 543 | CA  | VAL A 202 | -3.603 37.617 44.088 1.00 18.60 |
| C                         | 544 | CB  | VAL A 202 | -2.877 36.903 42.892 1.00 20.63 |
| C                         | 545 | CG1 | VAL A 202 | -1.841 35.987 43.342 1.00 16.00 |
| C                         | 546 | CG2 | VAL A 202 | -1.409 36.131 42.453 1.00 14.83 |
| C                         | 547 | C   | VAL A 202 | -2.153 38.472 44.756 1.00 20.80 |
| C                         | 548 | O   | VAL A 202 | -2.101 39.460 44.238 1.00 21.47 |
| O                         | 549 | N   | PRO A 203 | -2.168 38.079 45.014 1.00 22.76 |
| N                         | 550 | CA  | PRO A 203 | -1.582 36.771 46.722 1.00 25.70 |
| C                         | 551 | CB  | PRO A 203 | -1.661 35.068 45.103 1.00 25.89 |
| C                         | 552 | CG  | PRO A 203 | -2.372 37.360 46.212 1.00 24.66 |
| S                         | 553 | CD  | PRO A 203 | -2.730 36.972 46.806 1.00 18.98 |
| C                         | 554 | C   | PRO A 203 | -0.265 38.564 46.022 1.00 24.40 |
| O                         | 555 | O   | PRO A 203 | -0.714 37.436 45.886 1.00 31.01 |
| C                         | 556 | N   | LEU A 204 | -2.058 37.589 45.410 1.00 23.90 |
| C                         | 557 | CA  | LEU A 204 | -2.193 39.602 44.922 1.00 29.64 |
| C                         | 558 | CB  | LEU A 204 | -2.037 39.706 43.393 1.00 22.17 |
| C                         | 559 | CG  | LEU A 204 | -1.232 38.583 42.748 1.00 20.57 |
| C                         | 560 | CD1 | LEU A 204 | -1.008 38.877 41.303 1.00 21.61 |
| O                         | 561 | CD2 | LEU A 204 | -1.371 37.269 42.935 1.00 25.87 |
| C                         | 562 | C   | LEU A 204 | -1.050 38.759 45.410 1.00 21.47 |
| N                         | 563 | O   | LEU A 204 | -2.764 44.934 45.114 1.00 31.62 |
| C                         | 564 | N   | GLY A 205 | -4.391 40.455 46.177 1.00 37.30 |
| C                         | 565 | CA  | GLY A 205 | -5.028 44.473 46.608 1.00 30.28 |
| N                         | 566 | C   | GLY A 205 | -4.409 42.705 47.252 1.00 41.43 |
| C                         | 567 | O   | GLY A 205 | -4.643 42.841 45.310 1.00 21.44 |
| C                         | 568 | N   | GLY A 206 | -3.578 42.490 48.266 1.00 28.63 |
| C                         | 569 | CA  | GLY A 206 | -2.961 43.398 48.962 1.00 20.68 |
| C                         | 570 | C   | GLY A 206 | -1.697 44.141 48.309 1.00 24.80 |
| C                         | 571 | O   | GLY A 206 | -0.877 44.780 45.373 1.00 23.63 |
| C                         | 572 | N   | GLN A 207 | -2.534 42.850 47.013 1.00 19.58 |
| O                         | 573 | CA  | GLN A 207 | -0.353 44.366 46.304 1.00 20.37 |
| C                         | 574 | CB  | GLN A 207 | -0.724 44.839 44.838 1.00 18.51 |
| C                         | 575 | CG  | GLN A 207 | -1.711 45.832 44.886 1.00 16.32 |
| C                         | 576 | CD  | GLN A 207 | -2.716 46.377 44.386 1.00 21.66 |
| C                         | 577 | OE1 | GLN A 207 | -2.190 46.838 44.386 1.00 20.66 |
| N                         | 578 | NE2 | GLN A 207 | -3.271 46.295 42.987 1.00 21.44 |
| C                         | 579 | C   | GLN A 207 | -0.709 43.265 46.259 1.00 25.03 |
| O                         | 580 | O   | GLN A 207 | -0.402 43.066 46.397 1.00 22.56 |
| C                         | 581 | N   | GLN A 208 | -3.631 42.568 45.410 1.00 21.47 |
| C                         | 582 | CA  | GLN A 208 | -3.036 42.688 46.847 1.00 24.09 |
| C                         | 583 | CB  | GLN A 208 | -4.194 42.589 46.808 1.00 21.15 |
| C                         | 584 | CG  | GLN A 208 | -3.778 43.327 45.163 1.00 39.39 |
| N                         | 585 | CD  | GLN A 208 | -3.615 42.179 49.089 1.00 45.64 |
| C                         | 586 | OE1 | GLN A 208 | -4.621 42.719 45.410 1.00 54.47 |
| N                         | 587 | NE2 | GLN A 208 | -3.360 42.476 50.359 1.00 21.47 |
| C                         | 588 | C   | GLN A 208 | -3.555 42.959 44.462 1.00 18.80 |
| C                         | 589 | O   | GLN A 208 | -4.279 42.981 44.249 1.00 19.93 |
| N                         | 590 | N   | VAL A 209 | -3.202 42.084 43.593 1.00 21.38 |
| C                         | 591 | CA  | VAL A 209 | -3.202 42.084 43.593 1.00 21.38 |

| dimer-PDB-coordinates.txt |     |     |           |                                 |
|---------------------------|-----|-----|-----------|---------------------------------|
| ATOM                      | 718 | CD1 | PHE B 142 | 14.725 23.416 55.057 1.00 24.22 |
| ATOM                      | 719 | CE1 | PHE B 142 | 13.362 23.283 55.028 1.00 23.95 |
| ATOM                      | 720 | CZ  | PHE B 142 | 12.666 23.132 56.190 1.00 27.45 |
| ATOM                      | 721 | CE2 | PHE B 142 | 13.327 23.124 57.396 1.00 27.98 |
| ATOM                      | 722 | CD2 | PHE B 142 | 14.695 23.253 57.425 1.00 29.81 |
| ATOM                      | 723 | C   | PHE B 142 | 15.123 22.243 56.284 1.00 36.83 |
| ATOM                      | 724 | O   | PHE B 142 | 19.566 22.490 57.425 1.00 30.31 |
| ATOM                      | 725 | N   | PRO B 143 | 18.906 22.327 55.214 1.00 31.38 |
| ATOM                      | 726 | CA  | PRO B 143 | 21.351 22.524 55.346 1.00 31.95 |
| ATOM                      | 727 | CB  | PRO B 143 | 21.886 22.049 53.985 1.00 25.87 |
| ATOM                      | 728 | CG  | PRO B 143 | 20.756 22.365 53.031 1.00 29.07 |
| ATOM                      | 729 | CD  | PRO B 143 | 19.498 22.060 53.818 1.00 24.25 |
| ATOM                      | 730 | C   | PRO B 143 | 21.713 22.999 55.374 1.00 32.26 |
| ATOM                      | 731 | O   | PRO B 143 | 21.034 24.854 55.066 1.00 31.43 |
| ATOM                      | 732 | N   | ALA B 144 | 22.794 24.238 56.309 1.00 31.47 |
| ATOM                      | 733 | CA  | ALA B 144 | 23.259 25.592 56.589 1.00 32.22 |
| ATOM                      | 734 | CB  | ALA B 144 | 24.473 25.542 57.520 1.00 30.92 |
| ATOM                      | 735 | C   | ALA B 144 | 23.599 26.364 55.315 1.00 31.34 |
| ATOM                      | 736 | O   | ALA B 144 | 25.607 27.589 55.311 1.00 38.94 |
| ATOM                      | 737 | N   | SER B 145 | 23.866 25.649 54.237 1.00 29.70 |
| ATOM                      | 738 | CA  | SER B 145 | 24.313 26.281 52.993 1.00 25.41 |
| ATOM                      | 739 | CB  | SER B 145 | 24.985 25.241 52.106 1.00 29.27 |
| ATOM                      | 740 | OG  | SER B 145 | 24.056 24.226 51.757 1.00 31.88 |
| ATOM                      | 741 | C   | SER B 145 | 25.173 26.941 52.198 1.00 34.19 |
| ATOM                      | 742 | O   | SER B 145 | 23.418 27.635 51.109 1.00 39.77 |
| ATOM                      | 743 | N   | LEU B 146 | 21.927 26.706 52.604 1.00 34.04 |
| ATOM                      | 744 | CA  | LEU B 146 | 20.783 27.286 52.891 1.00 32.84 |
| ATOM                      | 745 | CB  | LEU B 146 | 19.468 26.852 52.531 1.00 30.73 |
| ATOM                      | 746 | CG  | LEU B 146 | 18.761 25.651 51.929 1.00 37.14 |
| ATOM                      | 747 | CD  | LEU B 146 | 17.350 25.158 52.492 1.00 39.37 |
| ATOM                      | 748 | CE  | LEU B 146 | 18.741 25.768 50.416 1.00 29.19 |
| ATOM                      | 749 | C   | LEU B 146 | 20.838 28.616 51.849 1.00 35.57 |
| ATOM                      | 750 | O   | LEU B 146 | 21.023 29.468 52.878 1.00 41.65 |
| ATOM                      | 751 | N   | ARG B 147 | 20.647 29.376 50.658 1.00 42.01 |
| ATOM                      | 752 | CA  | ARG B 147 | 20.765 30.818 50.439 1.00 52.36 |
| ATOM                      | 753 | CB  | ARG B 147 | 21.437 31.085 49.083 1.00 62.60 |
| ATOM                      | 754 | CG  | ARG B 147 | 22.823 30.489 48.935 1.00 73.15 |
| ATOM                      | 755 | CD  | ARG B 147 | 23.835 31.202 49.805 1.00 75.47 |
| ATOM                      | 756 | CE  | ARG B 147 | 25.195 30.960 49.337 1.00 88.18 |
| ATOM                      | 757 | C   | ARG B 147 | 26.172 31.859 49.401 1.00 93.64 |
| ATOM                      | 758 | OG1 | ARG B 147 | 25.931 31.060 49.913 1.00 88.39 |
| ATOM                      | 759 | NH2 | ARG B 147 | 27.365 31.558 48.951 1.00 76.60 |
| ATOM                      | 760 | C   | ARG B 147 | 19.410 31.528 50.442 1.00 1.11  |
| ATOM                      | 761 | O   | ARG B 147 | 19.345 32.760 50.419 1.00 56.19 |
| ATOM                      | 762 | N   | LEU B 148 | 18.337 30.746 50.449 1.00 41.27 |
| ATOM                      | 763 | CA  | LEU B 148 | 16.982 31.275 50.370 1.00 35.67 |
| ATOM                      | 764 | CB  | LEU B 148 | 15.981 30.116 50.329 1.00 30.58 |
| ATOM                      | 765 | CG  | LEU B 148 | 16.237 29.079 49.227 1.00 39.77 |
| ATOM                      | 766 | CD  | LEU B 148 | 15.250 27.914 49.307 1.00 26.88 |
| ATOM                      | 767 | CE  | LEU B 148 | 16.179 29.733 47.843 1.00 36.56 |
| ATOM                      | 768 | C   | LEU B 148 | 16.641 32.194 51.535 1.00 28.82 |
| ATOM                      | 769 | O   | LEU B 148 | 17.009 31.922 52.687 1.00 34.89 |
| ATOM                      | 770 | N   | SER B 149 | 15.940 33.284 51.231 1.00 24.60 |
| ATOM                      | 771 | CA  | SER B 149 | 15.187 34.060 52.272 1.00 30.90 |
| ATOM                      | 772 | CB  | SER B 149 | 14.606 35.293 51.665 1.00 33.00 |
| ATOM                      | 773 | CG  | SER B 149 | 13.436 34.883 50.975 1.00 32.66 |
| ATOM                      | 774 | C   | SER B 149 | 14.206 33.234 52.947 1.00 32.06 |
| ATOM                      | 775 | O   | SER B 149 | 13.815 32.183 52.438 1.00 31.51 |
| ATOM                      | 776 | N   | GLU B 150 | 13.702 32.701 54.079 1.00 29.61 |
| ATOM                      | 777 | CA  | GLU B 150 | 12.685 34.504 54.804 1.00 37.11 |
| ATOM                      | 778 | CB  | GLU B 150 | 12.381 33.617 56.142 1.00 37.86 |
| ATOM                      | 779 | CG  | GLU B 150 | 13.525 33.504 57.148 1.00 43.79 |
| ATOM                      | 780 | C   | GLU B 150 | 13.272 34.292 58.439 1.00 63.81 |

| dimer-PDB-coordinates.txt |     |     |           |                                 |
|---------------------------|-----|-----|-----------|---------------------------------|
| ATOM                      | 844 | N   | GLU B 158 | 5.778 25.277 50.515 1.00 17.94  |
| ATOM                      | 845 | CA  | GLU B 158 | 4.332 25.260 50.342 1.00 20.95  |
| ATOM                      | 846 | CB  | GLU B 158 | 3.192 26.641 50.556 1.00 25.54  |
| ATOM                      | 847 | CG  | GLU B 158 | 2.229 26.677 50.306 1.00 30.15  |
| ATOM                      | 848 | CD  | GLU B 158 | 1.560 27.907 50.881 1.00 35.54  |
| ATOM                      | 849 | CE  | GLU B 158 | 0.205 27.938 50.905 1.00 34.42  |
| ATOM                      | 850 | OE1 | GLU B 158 | 2.866 28.898 51.329 1.00 36.12  |
| ATOM                      | 851 | C   | GLU B 158 | 3.999 24.721 49.956 1.00 28.78  |
| ATOM                      | 852 | O   | GLU B 158 | 3.006 24.031 48.766 1.00 31.05  |
| ATOM                      | 853 | N   | ILE B 159 | 4.857 25.020 47.985 1.00 25.70  |
| ATOM                      | 854 | CA  | ILE B 159 | 4.681 24.496 46.650 1.00 29.15  |
| ATOM                      | 855 | CB  | ILE B 159 | 5.652 25.124 45.651 1.00 29.08  |
| ATOM                      | 856 | CG1 | ILE B 159 | 5.213 26.549 45.324 1.00 38.61  |
| ATOM                      | 857 | CG2 | ILE B 159 | 6.069 27.194 44.295 1.00 50.53  |
| ATOM                      | 858 | C   | ILE B 159 | 5.647 24.310 44.163 1.00 31.05  |
| ATOM                      | 859 | O   | ILE B 159 | 4.864 22.951 46.617 1.00 33.21  |
| ATOM                      | 860 | O   | ILE B 159 | 4.062 22.261 46.012 1.00 34.65  |
| ATOM                      | 861 | N   | PHE B 160 | 5.912 22.488 47.264 1.00 25.05  |
| ATOM                      | 862 | CA  | PHE B 160 | 6.098 22.041 47.310 1.00 16.59  |
| ATOM                      | 863 | CB  | PHE B 160 | 7.470 20.688 47.879 1.00 19.74  |
| ATOM                      | 864 | CG  | PHE B 160 | 7.784 19.231 47.810 1.00 19.49  |
| ATOM                      | 865 | CD1 | PHE B 160 | 7.427 18.354 48.847 1.00 17.24  |
| ATOM                      | 866 | CE1 | PHE B 160 | 7.694 17.014 48.776 1.00 19.01  |
| ATOM                      | 867 | CZ  | PHE B 160 | 8.336 16.485 47.663 1.00 19.85  |
| ATOM                      | 868 | CD2 | PHE B 160 | 8.702 17.337 46.621 1.00 21.16  |
| ATOM                      | 869 | CE2 | PHE B 160 | 8.410 18.701 46.694 1.00 18.31  |
| ATOM                      | 870 | C   | PHE B 160 | 5.000 20.259 48.084 1.00 20.37  |
| ATOM                      | 871 | O   | PHE B 160 | 4.376 19.361 47.360 1.00 18.51  |
| ATOM                      | 872 | N   | PHE B 161 | 4.766 20.716 49.324 1.00 17.62  |
| ATOM                      | 873 | CA  | PHE B 161 | 3.843 20.014 50.210 1.00 19.99  |
| ATOM                      | 874 | CB  | PHE B 161 | 4.227 20.221 51.682 1.00 17.60  |
| ATOM                      | 875 | CG  | PHE B 161 | 5.501 19.514 52.070 1.00 15.31  |
| ATOM                      | 876 | CD1 | PHE B 161 | 5.542 18.137 52.173 1.00 13.38  |
| ATOM                      | 877 | CE1 | PHE B 161 | 6.724 17.486 52.511 1.00 16.96  |
| ATOM                      | 878 | CZ  | PHE B 161 | 7.878 18.216 52.752 1.00 12.93  |
| ATOM                      | 879 | CE2 | PHE B 161 | 7.841 19.593 52.635 1.00 18.02  |
| ATOM                      | 880 | CD2 | PHE B 161 | 6.659 20.227 52.299 1.00 11.96  |
| ATOM                      | 881 | C   | PHE B 161 | 2.380 20.370 49.962 1.00 22.22  |
| ATOM                      | 882 | O   | PHE B 161 | 1.481 19.724 50.530 1.00 15.92  |
| ATOM                      | 883 | N   | GLY B 162 | 2.150 21.391 49.133 1.00 15.86  |
| ATOM                      | 884 | CA  | GLY B 162 | 0.804 21.740 48.729 1.00 16.20  |
| ATOM                      | 885 | C   | GLY B 162 | 0.257 20.806 47.668 1.00 19.14  |
| ATOM                      | 886 | O   | GLY B 162 | -0.933 20.639 47.368 1.00 23.18 |
| ATOM                      | 887 | N   | LYS B 163 | 1.117 19.969 47.103 1.00 15.79  |
| ATOM                      | 888 | CA  | LYS B 163 | 0.709 19.109 45.986 1.00 18.68  |
| ATOM                      | 889 | CB  | LYS B 163 | 1.875 18.891 45.034 1.00 19.35  |
| ATOM                      | 890 | CG  | LYS B 163 | 2.128 20.071 44.125 1.00 21.19  |
| ATOM                      | 891 | CD  | LYS B 163 | 3.408 19.902 43.350 1.00 35.62  |
| ATOM                      | 892 | CE  | LYS B 163 | 3.529 20.985 42.284 1.00 39.17  |
| ATOM                      | 893 | NZ  | LYS B 163 | 3.202 22.333 42.832 1.00 37.77  |
| ATOM                      | 894 | C   | LYS B 163 | 0.150 17.764 46.416 1.00 23.00  |
| ATOM                      | 895 | O   | LYS B 163 | 0.790 17.010 47.164 1.00 22.62  |
| ATOM                      | 896 | N   | THR B 164 | 1.047 17.371 45.931 1.00 22.58  |
| ATOM                      | 897 | CA  | THR B 164 | -1.630 16.445 46.074 1.00 26.83 |
| ATOM                      | 898 | CB  | THR B 164 | -2.937 16.038 45.254 1.00 32.04 |
| ATOM                      | 899 | OG1 | THR B 164 | -3.936 16.863 45.864 1.00 36.94 |
| ATOM                      | 900 | CG2 | THR B 164 | -3.431 14.616 45.219 1.00 36.14 |
| ATOM                      | 901 | C   | THR B 164 | -0.680 15.049 45.648 1.00 20.71 |
| ATOM                      | 902 | O   | THR B 164 | -0.525 14.045 46.339 1.00 27.83 |
| ATOM                      | 903 | N   | ARG B 165 | -0.532 15.232 44.326 1.00 23.67 |
| ATOM                      | 904 | CA  | ARG B 165 | 0.931 14.176 44.020 1.00 24.22  |
| ATOM                      | 905 | CB  | ARG B 165 | 1.274 14.438 42.579 1.00 31.17  |
| ATOM                      | 906 | CG  | ARG B 165 | 2.322 15.622 42.389 1.00 40.32  |

| dimer-PDB-coordinates.txt |      |     |     |                                           |
|---------------------------|------|-----|-----|-------------------------------------------|
| C                         | ATOM | 781 | OE1 | GLU B 150 12.299 35.091 58.502 1.00 58.04 |
| C                         | ATOM | 782 | OE2 | GLU B 150 14.056 34.106 59.395 1.00 60.21 |
| C                         | ATOM | 783 | C   | GLU B 150 11.411 32.792 53.974 1.00 30.83 |
| C                         | ATOM | 784 | O   | GLU B 150 10.817 31.708 53.915 1.00 28.18 |
| C                         | ATOM | 785 | N   | GLU B 151 11.011 33.880 53.327 1.00 25.86 |
| C                         | ATOM | 786 | CA  | GLU B 151 9.851 33.868 52.464 1.00 24.76  |
| C                         | ATOM | 787 | CB  | GLU B 151 9.537 35.272 51.933 1.00 33.58  |
| C                         | ATOM | 788 | CG  | GLU B 151 8.266 35.316 51.062 1.00 49.98  |
| C                         | ATOM | 789 | CD  | GLU B 151 7.399 36.536 51.331 1.00 67.27  |
| C                         | ATOM | 790 | OE1 | GLU B 151 7.941 37.555 51.808 1.00 72.81  |
| C                         | ATOM | 791 | OE2 | GLU B 151 6.173 36.473 51.031 1.00 60.56  |
| C                         | ATOM | 792 | C   | GLU B 151 10.400 37.468 51.107 1.00 24.93 |
| C                         | ATOM | 793 | O   | GLU B 151 9.054 32.138 51.001 1.00 27.40  |
| C                         | ATOM | 794 | N   | GLU B 152 11.173 32.835 50.675 1.00 20.29 |
| C                         | ATOM | 795 | CA  | GLU B 152 11.406 31.913 49.560 1.00 22.98 |
| C                         | ATOM | 796 | CB  | GLU B 152 12.763 32.159 48.897 1.00 29.87 |
| C                         | ATOM | 797 | CG  | GLU B 152 12.922 34.290 48.193 1.00 44.86 |
| C                         | ATOM | 798 | CD  | GLU B 152 14.307 33.660 47.589 1.00 59.41 |
| C                         | ATOM | 799 | OE1 | GLU B 152 15.302 33.716 48.358 1.00 41.78 |
| C                         | ATOM | 800 | OE2 | GLU B 152 14.397 33.716 46.342 1.00 61.65 |
| C                         | ATOM | 801 | C   | GLU B 152 11.357 30.467 50.031 1.00 24.11 |
| C                         | ATOM | 802 | O   | GLU B 152 10.807 29.599 49.354 1.00 24.87 |
| C                         | ATOM | 803 | N   | LEU B 153 11.945 30.107 50.144 1.00 25.51 |
| C                         | ATOM | 804 | CA  | LEU B 153 11.933 28.674 51.739 1.00 19.38 |
| C                         | ATOM | 805 | CB  | LEU B 153 12.742 28.841 53.060 1.00 20.63 |
| C                         | ATOM | 806 | CG  | LEU B 153 12.697 27.491 53.785 1.00 23.83 |
| C                         | ATOM | 807 | CD  | LEU B 153 11.292 26.403 52.913 1.00 22.86 |
| C                         | ATOM | 808 | CE  | LEU B 153 13.416 27.359 51.114 1.00 30.98 |
| C                         | ATOM | 809 | C   | LEU B 153 10.503 28.409 52.019 1.00 19.19 |
| C                         | ATOM | 810 | N   | LEU B 153 10.139 27.262 51.710 1.00 19.57 |
| C                         | ATOM | 811 | O   | LEU B 154 9.701 29.307 52.594 1.00 19.12  |
| C                         | ATOM | 812 | CA  | LEU B 154 8.302 29.007 52.875 1.00 21.28  |
| C                         | ATOM | 813 | N   | LEU B 154 7.647 30.125 52.693 1.00 18.44  |
| C                         | ATOM | 814 | CB  | LEU B 154 8.103 30.193 52.188 1.00 21.98  |
| C                         | ATOM | 815 | CD  | LEU B 154 7.573 31.443 55.840 1.00 32.24  |
| C                         | ATOM | 816 | CE  | LEU B 154 7.695 28.946 55.920 1.00 18.29  |
| C                         | ATOM | 817 | C   | LEU B 154 7.337 26.757 51.586 1.00 20.86  |
| C                         | ATOM | 818 | O   | LEU B 154 6.814 27.779 51.479 1.00 20.61  |
| C                         | ATOM | 819 | N   | LEU B 155 7.723 29.620 50.594 1.00 18.30  |
| C                         | ATOM | 820 | CA  | ASP B 155 7.090 29.419 49.394 1.00 21.94  |
| C                         | ATOM | 821 | CB  | ASP B 155 7.417 30.568 48.333 1.00 23.52  |
| C                         | ATOM | 822 | CG  | ASP B 155 6.664 31.844 48.676 1.00 30.68  |
| C                         | ATOM | 823 | OD1 | ASP B 155 5.709 31.785 49.492 1.00 29.49  |
| C                         | ATOM | 824 | OD2 | ASP B 155 5.016 3                         |

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|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 970  | CZ  | ARG | B | 174 | 4.506  | 31.252 | 52.603 | 1.00 | 29.51 |
| ATOM | 971  | NH1 | ARG | B | 174 | 4.415  | 30.334 | 51.637 | 1.00 | 17.66 |
| ATOM | 972  | NH2 | ARG | B | 174 | 5.040  | 32.437 | 52.343 | 1.00 | 24.13 |
| ATOM | 973  | C   | ARG | B | 174 | 3.858  | 29.046 | 58.700 | 1.00 | 21.50 |
| ATOM | 974  | O   | ARG | B | 174 | 3.713  | 30.264 | 58.632 | 1.00 | 21.16 |
| ATOM | 975  | N   | GLU | B | 175 | 4.731  | 28.463 | 59.526 | 1.00 | 21.43 |
| ATOM | 976  | CA  | GLU | B | 175 | 5.478  | 29.225 | 60.322 | 1.00 | 24.46 |
| ATOM | 977  | CB  | GLU | B | 175 | 4.875  | 29.008 | 61.646 | 1.00 | 25.15 |
| ATOM | 978  | CG  | GLU | B | 175 | 3.609  | 29.763 | 62.191 | 1.00 | 25.56 |
| ATOM | 979  | CD  | GLU | B | 175 | 3.259  | 29.762 | 63.680 | 1.00 | 48.07 |
| ATOM | 980  | OE1 | GLU | B | 175 | 3.835  | 28.932 | 64.426 | 1.00 | 49.32 |
| ATOM | 981  | OE2 | GLU | B | 175 | 2.443  | 30.600 | 64.102 | 1.00 | 37.40 |
| ATOM | 982  | C   | GLU | B | 175 | 6.923  | 28.791 | 60.606 | 1.00 | 22.09 |
| ATOM | 983  | O   | GLU | B | 175 | 7.237  | 27.606 | 60.473 | 1.00 | 22.56 |
| ATOM | 984  | N   | LEU | B | 176 | 7.802  | 29.748 | 60.871 | 1.00 | 20.50 |
| ATOM | 985  | CA  | LEU | B | 176 | 9.199  | 29.437 | 61.160 | 1.00 | 26.04 |
| ATOM | 986  | CB  | LEU | B | 176 | 10.097 | 30.590 | 60.724 | 1.00 | 16.94 |
| ATOM | 987  | CG  | LEU | B | 176 | 9.964  | 30.871 | 59.228 | 1.00 | 28.39 |
| ATOM | 988  | CH  | LEU | B | 176 | 10.502 | 32.251 | 58.941 | 1.00 | 37.73 |
| ATOM | 989  | CD  | LEU | B | 176 | 10.660 | 29.799 | 58.400 | 1.00 | 25.96 |
| ATOM | 990  | C   | LEU | B | 176 | 9.373  | 29.176 | 62.657 | 1.00 | 34.23 |
| ATOM | 991  | O   | LEU | B | 176 | 9.121  | 30.063 | 63.482 | 1.00 | 26.05 |
| ATOM | 992  | N   | LEU | B | 177 | 9.769  | 27.352 | 63.001 | 1.00 | 30.92 |
| ATOM | 993  | CA  | LEU | B | 177 | 10.137 | 27.618 | 64.374 | 1.00 | 24.18 |
| ATOM | 994  | CB  | LEU | B | 177 | 9.405  | 26.368 | 64.831 | 1.00 | 22.26 |
| ATOM | 995  | CG  | LEU | B | 177 | 7.979  | 26.325 | 65.353 | 1.00 | 35.13 |
| ATOM | 996  | CD  | LEU | B | 177 | 7.201  | 27.519 | 64.537 | 1.00 | 42.51 |
| ATOM | 997  | CE  | LEU | B | 177 | 7.271  | 25.180 | 65.363 | 1.00 | 33.12 |
| ATOM | 998  | C   | LEU | B | 177 | 11.644 | 27.380 | 64.431 | 1.00 | 30.87 |
| ATOM | 999  | O   | LEU | B | 177 | 12.115 | 27.285 | 63.389 | 1.00 | 33.71 |
| ATOM | 1000 | N   | PRO | B | 178 | 12.195 | 27.482 | 65.645 | 1.00 | 41.48 |
| ATOM | 1001 | CA  | PRO | B | 178 | 13.638 | 27.042 | 65.759 | 1.00 | 35.28 |
| ATOM | 1002 | CB  | PRO | B | 178 | 13.836 | 26.868 | 67.267 | 1.00 | 48.50 |
| ATOM | 1003 | CG  | PRO | B | 178 | 12.727 | 27.703 | 67.879 | 1.00 | 41.65 |
| ATOM | 1004 | CD  | PRO | B | 178 | 11.354 | 27.478 | 66.960 | 1.00 | 39.29 |
| ATOM | 1005 | C   | PRO | B | 178 | 14.088 | 25.797 | 64.886 | 1.00 | 31.64 |
| ATOM | 1006 | O   | PRO | B | 178 | 14.594 | 24.564 | 65.315 | 1.00 | 37.07 |
| ATOM | 1007 | N   | GLY | B | 179 | 14.867 | 25.444 | 65.943 | 1.00 | 38.13 |
| ATOM | 1008 | CA  | GLY | B | 179 | 15.394 | 24.944 | 63.104 | 1.00 | 35.03 |
| ATOM | 1009 | C   | GLY | B | 179 | 14.347 | 24.135 | 62.355 | 1.00 | 43.71 |
| ATOM | 1010 | O   | GLY | B | 179 | 14.630 | 23.035 | 61.879 | 1.00 | 40.20 |
| ATOM | 1011 | N   | SER | B | 180 | 12.136 | 24.658 | 62.227 | 1.00 | 37.93 |
| ATOM | 1012 | CA  | SER | B | 180 | 12.429 | 24.899 | 61.503 | 1.00 | 34.80 |
| ATOM | 1013 | CB  | SER | B | 180 | 11.491 | 22.846 | 62.423 | 1.00 | 31.67 |
| ATOM | 1014 | CG  | SER | B | 180 | 10.547 | 23.447 | 63.262 | 1.00 | 40.85 |
| ATOM | 1015 | C   | SER | B | 180 | 11.037 | 24.743 | 60.877 | 1.00 | 32.77 |
| ATOM | 1016 | O   | SER | B | 180 | 10.901 | 25.933 | 61.172 | 1.00 | 28.65 |
| ATOM | 1017 | N   | VAL | B | 181 | 10.136 | 24.126 | 60.624 | 1.00 | 37.93 |
| ATOM | 1018 | CA  | VAL | B | 181 | 9.904  | 24.823 | 59.489 | 1.00 | 21.66 |
| ATOM | 1019 | CB  | VAL | B | 181 | 9.140  | 24.982 | 57.953 | 1.00 | 19.58 |
| ATOM | 1020 | CG  | VAL | B | 181 | 7.771  | 25.392 | 57.403 | 1.00 | 15.52 |
| ATOM | 1021 | CD  | VAL | B | 181 | 10.194 | 25.997 | 57.564 | 1.00 | 20.24 |
| ATOM | 1022 | C   | VAL | B | 181 | 7.833  | 24.080 | 59.869 | 1.00 | 18.67 |
| ATOM | 1023 | O   | VAL | B | 181 | 7.751  | 22.882 | 59.696 | 1.00 | 24.08 |
| ATOM | 1024 | N   | MET | B | 182 | 6.853  | 24.787 | 60.406 | 1.00 | 18.43 |
| ATOM | 1025 | CA  | MET | B | 182 | 5.601  | 24.147 | 60.763 | 1.00 | 17.08 |
| ATOM | 1026 | CB  | MET | B | 182 | 5.132  | 24.673 | 62.111 | 1.00 | 23.02 |
| ATOM | 1027 | CG  | MET | B | 182 | 4.145  | 23.801 | 62.833 | 1.00 | 32.06 |
| ATOM | 1028 | CD  | MET | B | 182 | 2.846  | 24.734 | 65.207 | 1.00 | 61.02 |
| ATOM | 1029 | C   | MET | B | 182 | 1.885  | 24.127 | 65.448 | 1.00 | 59.16 |
| ATOM | 1030 | O   | MET | B | 182 | 4.569  | 24.441 | 59.683 | 1.00 | 13.65 |
| ATOM | 1031 | O   | MET | B | 182 | 4.409  | 25.593 | 59.247 | 1.00 | 14.49 |
| ATOM | 1032 | N   | LEU | B | 183 | 3.851  | 27.396 | 59.240 | 1.00 | 16.18 |

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|      |      |     |     |   |     |         |        |        |      |       |
|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 1095 | CA  | GLN | B | 192 | 11.006  | 11.758 | 58.631 | 1.00 | 26.50 |
| ATOM | 1097 | CB  | GLN | B | 192 | -2.215  | 11.102 | 59.147 | 1.00 | 27.98 |
| ATOM | 1098 | CG  | GLN | B | 192 | -2.712  | 11.477 | 60.541 | 1.00 | 35.42 |
| ATOM | 1099 | CD  | GLN | B | 192 | -3.181  | 12.925 | 60.637 | 1.00 | 42.46 |
| ATOM | 1100 | OE1 | GLN | B | 192 | -3.721  | 13.490 | 59.641 | 1.00 | 35.69 |
| ATOM | 1101 | OE2 | GLN | B | 192 | -3.971  | 13.932 | 61.801 | 1.00 | 40.40 |
| ATOM | 1102 | C   | GLN | B | 192 | -0.362  | 11.159 | 57.525 | 1.00 | 27.92 |
| ATOM | 1103 | O   | GLN | B | 192 | -0.595  | 10.411 | 57.687 | 1.00 | 32.64 |
| ATOM | 1104 | N   | ARG | B | 193 | -0.892  | 11.384 | 56.334 | 1.00 | 22.76 |
| ATOM | 1105 | CA  | ARG | B | 193 | -0.279  | 10.831 | 55.135 | 1.00 | 26.32 |
| ATOM | 1106 | CB  | ARG | B | 193 | -1.092  | 11.226 | 53.904 | 1.00 | 23.50 |
| ATOM | 1107 | CG  | ARG | B | 193 | -1.583  | 10.584 | 52.665 | 1.00 | 20.42 |
| ATOM | 1108 | CD  | ARG | B | 193 | -0.902  | 11.187 | 53.449 | 1.00 | 30.42 |
| ATOM | 1109 | CE  | ARG | B | 193 | -2.307  | 11.399 | 51.077 | 1.00 | 36.39 |
| ATOM | 1110 | CZ  | ARG | B | 193 | -3.038  | 12.475 | 50.793 | 1.00 | 49.94 |
| ATOM | 1111 | NH1 | ARG | B | 193 | -2.512  | 13.692 | 50.866 | 1.00 | 41.60 |
| ATOM | 1112 | NH2 | ARG | B | 193 | -4.308  | 12.338 | 50.439 | 1.00 | 54.88 |
| ATOM | 1113 | C   | ARG | B | 193 | -1.182  | 10.475 | 52.212 | 1.00 | 32.12 |
| ATOM | 1114 | O   | ARG | B | 193 | -2.077  | 10.450 | 54.738 | 1.00 | 29.48 |
| ATOM | 1115 | N   | LEU | B | 194 | -1.431  | 12.575 | 55.084 | 1.00 | 23.39 |
| ATOM | 1116 | CA  | LEU | B | 194 | -2.796  | 13.077 | 54.906 | 1.00 | 21.96 |
| ATOM | 1117 | CB  | LEU | B | 194 | -2.845  | 14.609 | 54.978 | 1.00 | 20.11 |
| ATOM | 1118 | CG  | LEU | B | 194 | -2.188  | 15.356 | 53.878 | 1.00 | 25.30 |
| ATOM | 1119 | CD  | LEU | B | 194 | -1.206  | 16.858 | 54.075 | 1.00 | 29.45 |
| ATOM | 1120 | CE  | LEU | B | 194 | -2.915  | 15.600 | 52.532 | 1.00 | 21.82 |
| ATOM | 1121 | C   | LEU | B | 194 | -3.707  | 12.470 | 55.964 | 1.00 | 24.47 |
| ATOM | 1122 | O   | LEU | B | 194 | -4.863  | 12.125 | 55.689 | 1.00 | 25.86 |
| ATOM | 1123 | N   | CYS | B | 195 | -3.178  | 12.343 | 57.177 | 1.00 | 23.27 |
| ATOM | 1124 | CA  | CYS | B | 195 | -3.946  | 11.789 | 58.281 | 1.00 | 20.45 |
| ATOM | 1125 | CB  | CYS | B | 195 | -3.196  | 12.036 | 59.615 | 1.00 | 37.13 |
| ATOM | 1126 | CG  | CYS | B | 195 | -4.084  | 11.481 | 61.104 | 1.00 | 65.27 |
| ATOM | 1127 | C   | CYS | B | 195 | -4.274  | 10.296 | 58.045 | 1.00 | 25.73 |
| ATOM | 1128 | O   | CYS | B | 195 | -5.381  | 9.895  | 58.318 | 1.00 | 33.59 |
| ATOM | 1129 | N   | GLN | B | 196 | -3.316  | 9.559  | 57.491 | 1.00 | 30.12 |
| ATOM | 1130 | CA  | GLN | B | 196 | -3.541  | 9.178  | 57.109 | 1.00 | 33.19 |
| ATOM | 1131 | CB  | GLN | B | 196 | -2.259  | 7.528  | 56.571 | 1.00 | 30.35 |
| ATOM | 1132 | CG  | GLN | B | 196 | -1.285  | 7.080  | 57.654 | 1.00 | 52.05 |
| ATOM | 1133 | CD  | GLN | B | 196 | -0.152  | 6.976  | 57.145 | 1.00 | 71.23 |
| ATOM | 1134 | OE1 | GLN | B | 196 | -0.357  | 6.329  | 55.931 | 1.00 | 66.64 |
| ATOM | 1135 | OE2 | GLN | B | 196 | -1.110  | 6.953  | 58.074 | 1.00 | 54.96 |
| ATOM | 1136 | C   | GLN | B | 196 | -4.645  | 8.071  | 56.078 | 1.00 | 21.74 |
| ATOM | 1137 | O   | GLN | B | 196 | -5.529  | 7.235  | 56.208 | 1.00 | 30.39 |
| ATOM | 1138 | N   | ILE | B | 197 | -4.599  | 8.925  | 55.047 | 1.00 | 35.77 |
| ATOM | 1139 | CA  | ILE | B | 197 | -5.677  | 6.939  | 54.047 | 1.00 | 24.09 |
| ATOM | 1140 | CB  | ILE | B | 197 | -5.383  | 9.896  | 52.866 | 1.00 | 26.99 |
| ATOM | 1141 | CG  | ILE | B | 197 | -4.163  | 9.393  | 52.100 | 1.00 | 22.34 |
| ATOM | 1142 | CD  | ILE | B | 197 | -3.539  | 10.449 | 51.210 | 1.00 | 22.35 |
| ATOM | 1143 | CE  | ILE | B | 197 | -6.801  | 10.013 | 51.967 | 1.00 | 22.35 |
| ATOM | 1144 | C   | ILE | B | 197 | -7.007  | 9.293  | 54.710 | 1.00 | 31.18 |
| ATOM | 1145 | O   | ILE | B | 197 | -8.016  | 8.627  | 54.479 | 1.00 | 28.61 |
| ATOM | 1146 | N   | GLY | B | 198 | -7.003  | 10.358 | 55.533 | 1.00 | 28.58 |
| ATOM | 1147 | CA  | GLY | B | 198 | -8.133  | 9.624  | 54.624 | 1.00 | 24.35 |
| ATOM | 1148 | CB  | GLY | B | 198 | -9.200  | 11.327 | 55.767 | 1.00 | 25.74 |
| ATOM | 1149 | CG  | GLY | B | 198 | -9.786  | 12.333 | 56.305 | 1.00 | 33.35 |
| ATOM | 1150 | C   | GLY | B | 198 | -9.834  | 10.799 | 54.662 | 1.00 | 21.81 |
| ATOM | 1151 | O   | GLY | B | 198 | -11.027 | 11.373 | 54.055 | 1.00 | 30.05 |
| ATOM | 1152 | N   | GLN | B | 199 | -12.150 | 10.345 | 54.903 | 1.00 | 32.32 |
| ATOM | 1153 | CA  | GLN | B | 199 | -12.784 | 10.065 | 55.347 | 1.00 | 49.75 |
| ATOM | 1154 | CB  | GLN | B | 199 | -14.099 | 9.312  | 55.236 | 1.00 | 74.04 |
| ATOM | 1155 | CG  | GLN | B | 199 | -15.132 | 9.301  | 54.693 | 1.00 | 71.19 |
| ATOM | 1156 | CD  | GLN | B | 199 | -14.064 | 8.902  | 55.457 | 1.00 | 67.30 |
| ATOM | 1157 | CE  | GLN | B | 199 | -10.736 | 11.857 | 55.658 | 1.00 | 24.62 |
| ATOM | 1158 | O   | GLN | B | 199 | -9.990  | 11.270 | 51.914 | 1.00 | 26.63 |

dimer-PDB-coordinates.txt

|      |      |    |     |   |     |       |        |        |      |       |
|------|------|----|-----|---|-----|-------|--------|--------|------|-------|
| ATOM | 1033 | CA | LEU | B | 183 | 2.641 | 23.556 | 58.222 | 1.00 | 21.13 |
| ATOM | 1034 | CB | LEU | B | 183 | 3.214 | 22.822 | 56.923 | 1.00 | 15.3  |

| dimer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |      | dimer-PDB-coordinates.txt |   |      |      |     |     |     |        |        |        |        |       |       |   |
|---------------------------|------|-----|-----|---|-----|--------|--------|--------|------|---------------------------|---|------|------|-----|-----|-----|--------|--------|--------|--------|-------|-------|---|
| A                         | T    | A   | T   | A | T   | A      | T      | A      | T    | A                         | T | A    | T    | A   | T   | A   | T      | A      | T      |        |       |       |   |
| AT01                      | 1348 | O   | GLY | C | 141 | 39.604 | 20.152 | 43.929 | 1.00 | 33.41                     | 0 | AT01 | 1411 | N   | GLU | C   | 150    | 27.111 | 28.413 | 42.054 | 1.00  | 27.97 | N |
| AT01                      | 1349 | N   | PHE | C | 142 | 37.761 | 20.784 | 45.021 | 1.00 | 21.24                     | 0 | AT01 | 1412 | C   | GLU | C   | 150    | 26.840 | 26.963 | 42.802 | 1.00  | 31.00 | C |
| AT01                      | 1350 | C   | PHE | C | 142 | 37.549 | 21.931 | 44.130 | 1.00 | 27.00                     | 0 | AT01 | 1413 | C   | GLU | C   | 150    | 26.183 | 27.311 | 44.139 | 1.00  | 38.78 | C |
| AT01                      | 1351 | CB  | PHE | C | 142 | 36.149 | 22.503 | 44.327 | 1.00 | 26.17                     | 0 | AT01 | 1414 | CG  | GLU | C   | 150    | 27.147 | 27.967 | 45.136 | 1.00  | 40.19 | C |
| AT01                      | 1352 | CB  | PHE | C | 142 | 35.075 | 22.455 | 44.324 | 1.00 | 26.16                     | 0 | AT01 | 1415 | CG  | GLU | C   | 150    | 26.464 | 28.246 | 46.418 | 1.00  | 56.91 | C |
| AT01                      | 1353 | CD1 | PHE | C | 142 | 34.555 | 20.982 | 43.136 | 1.00 | 26.16                     | 0 | AT01 | 1416 | OE1 | GLU | C   | 150    | 25.213 | 27.405 | 45.018 | 1.00  | 55.18 | C |
| AT01                      | 1354 | CE1 | PHE | C | 142 | 33.579 | 20.005 | 43.127 | 1.00 | 25.25                     | 0 | AT01 | 1417 | OE2 | GLU | C   | 150    | 27.194 | 28.801 | 47.361 | 1.00  | 68.50 | C |
| AT01                      | 1355 | CE2 | PHE | C | 142 | 33.123 | 19.478 | 44.326 | 1.00 | 28.91                     | 0 | AT01 | 1418 | C   | GLU | C   | 150    | 35.970 | 26.010 | 43.954 | 1.00  | 31.20 | C |
| AT01                      | 1356 | CE3 | PHE | C | 142 | 33.647 | 19.938 | 45.118 | 1.00 | 27.10                     | 0 | AT01 | 1419 | O   | GLU | C   | 150    | 26.227 | 24.802 | 42.155 | 1.00  | 29.37 | C |
| AT01                      | 1357 | CE4 | PHE | C | 142 | 34.616 | 20.921 | 45.114 | 1.00 | 27.44                     | 0 | AT01 | 1420 | N   | GLU | C   | 151    | 24.934 | 26.863 | 41.137 | 1.00  | 29.56 | N |
| AT01                      | 1358 | C   | PHE | C | 142 | 38.603 | 23.025 | 45.140 | 1.00 | 31.49                     | 0 | AT01 | 1421 | C   | GLU | C   | 151    | 24.067 | 25.777 | 40.971 | 1.00  | 30.17 | C |
| AT01                      | 1359 | O   | PHE | C | 142 | 38.857 | 23.436 | 45.465 | 1.00 | 31.49                     | 0 | AT01 | 1422 | C   | GLU | C   | 151    | 24.067 | 25.777 | 40.971 | 1.00  | 30.17 | C |
| AT01                      | 1360 | N   | PRO | C | 143 | 39.223 | 23.494 | 43.469 | 1.00 | 31.07                     | 0 | AT01 | 1423 | CG  | GLU | C   | 151    | 21.916 | 23.824 | 39.126 | 1.00  | 49.38 | C |
| AT01                      | 1361 | C   | PRO | C | 143 | 40.436 | 24.585 | 43.443 | 1.00 | 30.30                     | 0 | AT01 | 1424 | CG  | GLU | C   | 151    | 20.463 | 26.213 | 39.394 | 1.00  | 71.47 | C |
| AT01                      | 1362 | C   | PRO | C | 143 | 40.902 | 24.535 | 43.443 | 1.00 | 30.30                     | 0 | AT01 | 1425 | OE1 | GLU | C   | 151    | 20.260 | 27.349 | 39.861 | 1.00  | 71.71 | C |
| AT01                      | 1363 | CG  | PRO | C | 143 | 39.864 | 24.020 | 41.062 | 1.00 | 24.81                     | 0 | AT01 | 1426 | OE2 | GLU | C   | 151    | 19.561 | 25.375 | 39.151 | 1.00  | 55.12 | C |
| AT01                      | 1364 | CD  | PRO | C | 143 | 39.070 | 23.010 | 41.665 | 1.00 | 21.21                     | 0 | AT01 | 1427 | CG  | GLU | C   | 151    | 24.067 | 25.777 | 39.126 | 1.00  | 30.17 | C |
| AT01                      | 1365 | C   | PRO | C | 143 | 39.525 | 25.948 | 43.534 | 1.00 | 29.62                     | 0 | AT01 | 1428 | O   | GLU | C   | 151    | 24.530 | 22.944 | 39.023 | 1.00  | 26.74 | O |
| AT01                      | 1366 | CG  | PRO | C | 143 | 38.430 | 26.191 | 43.010 | 1.00 | 29.25                     | 0 | AT01 | 1429 | N   | GLU | C   | 152    | 25.734 | 25.815 | 38.691 | 1.00  | 24.20 | N |
| AT01                      | 1367 | O   | PRO | C | 143 | 40.207 | 26.483 | 44.257 | 1.00 | 30.67                     | 0 | AT01 | 1430 | C   | GLU | C   | 152    | 26.506 | 25.238 | 37.691 | 1.00  | 27.41 | C |
| AT01                      | 1368 | C   | ALA | C | 144 | 39.688 | 28.179 | 44.525 | 1.00 | 33.67                     | 0 | AT01 | 1431 | C   | GLU | C   | 152    | 27.813 | 26.431 | 37.939 | 1.00  | 39.40 | C |
| AT01                      | 1369 | CG  | ALA | C | 144 | 40.616 | 28.929 | 45.457 | 1.00 | 32.86                     | 0 | AT01 | 1432 | CG  | GLU | C   | 152    | 26.676 | 27.409 | 36.220 | 1.00  | 52.66 | C |
| AT01                      | 1370 | C   | ALA | C | 144 | 39.449 | 28.970 | 45.138 | 1.00 | 31.70                     | 0 | AT01 | 1433 | CG  | GLU | C   | 152    | 27.647 | 28.399 | 35.746 | 1.00  | 60.95 | C |
| AT01                      | 1371 | O   | ALA | C | 144 | 38.665 | 29.916 | 45.108 | 1.00 | 30.02                     | 0 | AT01 | 1434 | OE1 | GLU | C   | 152    | 25.377 | 27.109 | 36.263 | 1.00  | 41.29 | C |
| AT01                      | 1372 | C   | ALA | C | 144 | 39.215 | 28.535 | 45.165 | 1.00 | 30.40                     | 0 | AT01 | 1435 | OE2 | GLU | C   | 152    | 27.637 | 25.431 | 34.297 | 1.00  | 57.90 | C |
| AT01                      | 1373 | C   | SER | C | 145 | 40.042 | 29.277 | 46.033 | 1.00 | 24.50                     | 0 | AT01 | 1436 | GLU | C   | 152 | 26.136 | 27.394 | 34.436 | 1.00   | 59.06 | C     |   |
| AT01                      | 1374 | CG  | SER | C | 145 | 41.240 | 26.912 | 46.033 | 1.00 | 29.29                     | 0 | AT01 | 1437 | O   | GLU | C   | 152    | 27.456 | 23.055 | 37.442 | 1.00  | 21.17 | O |
| AT01                      | 1375 | OG  | SER | C | 145 | 41.201 | 27.529 | 39.716 | 1.00 | 31.72                     | 0 | AT01 | 1438 | N   | LEU | C   | 153    | 27.886 | 24.272 | 39.255 | 1.00  | 22.30 | N |
| AT01                      | 1376 | C   | SER | C | 145 | 38.761 | 29.014 | 40.099 | 1.00 | 29.30                     | 0 | AT01 | 1439 | C   | LEU | C   | 153    | 25.867 | 23.271 | 39.823 | 1.00  | 24.22 | C |
| AT01                      | 1377 | O   | SER | C | 145 | 38.524 | 29.679 | 39.995 | 1.00 | 30.40                     | 0 | AT01 | 1440 | C   | LEU | C   | 153    | 29.510 | 23.791 | 41.111 | 1.00  | 21.60 | C |
| AT01                      | 1378 | N   | LEU | C | 146 | 37.959 | 28.045 | 40.514 | 1.00 | 28.85                     | 0 | AT01 | 1441 | C   | LEU | C   | 153    | 29.510 | 23.791 | 41.111 | 1.00  | 21.60 | C |
| AT01                      | 1379 | C   | LEU | C | 146 | 36.682 | 27.767 | 39.836 | 1.00 | 30.42                     | 0 | AT01 | 1442 | CD1 | LEU | C   | 153    | 31.321 | 22.267 | 40.983 | 1.00  | 21.57 | C |
| AT01                      | 1380 | CB  | LEU | C | 146 | 35.961 | 26.610 | 40.511 | 1.00 | 33.56                     | 0 | AT01 | 1443 | CD2 | LEU | C   | 153    | 30.852 | 23.306 | 43.173 | 1.00  | 22.65 | C |
| AT01                      | 1381 | CG  | LEU | C | 146 | 36.172 | 25.223 | 39.927 | 1.00 | 35.76                     | 0 | AT01 | 1444 | C   | LEU | C   | 153    | 29.050 | 22.016 | 40.108 | 1.00  | 21.32 | C |
| AT01                      | 1382 | CD  | LEU | C | 146 | 35.140 | 24.280 | 40.515 | 1.00 | 30.49                     | 0 | AT01 | 1445 | O   | LEU | C   | 153    | 28.462 | 20.896 | 39.780 | 1.00  | 22.60 | O |
| AT01                      | 1383 | CD2 | LEU | C | 146 | 35.067 | 25.255 | 39.646 | 1.00 | 36.75                     | 0 | AT01 | 1446 | N   | LEU | C   | 154    | 29.882 | 22.040 | 40.709 | 1.00  | 20.70 | N |
| AT01                      | 1384 | C   | LEU | C | 146 | 35.727 | 28.976 | 39.767 | 1.00 | 36.87                     | 0 | AT01 | 1447 | C   | LEU | C   | 154    | 26.011 | 21.083 | 41.037 | 1.00  | 21.31 | C |
| AT01                      | 1385 | O   | LEU | C | 146 | 35.459 | 29.620 | 40.808 | 1.00 | 34.73                     | 0 | AT01 | 1448 | C   | LEU | C   | 154    | 24.795 | 21.593 | 41.939 | 1.00  | 47.72 | C |
| AT01                      | 1386 | N   | ARG | C | 147 | 35.129 | 29.254 | 36.596 | 1.00 | 42.42                     | 0 | AT01 | 1449 | CG  | LEU | C   | 154    | 25.117 | 21.932 | 43.286 | 1.00  | 27.28 | C |
| AT01                      | 1387 | C   | ARG | C | 147 | 34.372 | 30.439 | 38.362 | 1.00 | 33.54                     | 0 | AT01 | 1450 | CD1 | LEU | C   | 154    | 23.920 | 22.572 | 43.987 | 1.00  | 22.50 | C |
| AT01                      | 1388 | CB  | ARG | C | 147 | 34.710 | 31.058 | 37.004 | 1.00 | 37.02                     | 0 | AT01 | 1451 | CD2 | LEU | C   | 154    | 23.920 | 22.572 | 43.987 | 1.00  | 22.50 | C |
| AT01                      | 1389 | CG  | ARG | C | 147 | 36.161 | 31.489 | 36.823 | 1.00 | 70.19                     | 0 | AT01 | 1452 | O   | LEU | C   | 154    | 25.567 | 20.375 | 39.744 | 1.00  | 22.10 | O |
| AT01                      | 1390 | CD  | ARG | C | 147 | 36.468 | 32.695 | 37.681 | 1.00 | 76.21                     | 0 | AT01 | 1453 | C   | LEU | C   | 154    | 35.564 | 19.149 | 39.682 | 1.00  | 19.01 | C |
| AT01                      | 1391 | NE  | ARG | C | 147 | 37.681 | 33.384 | 37.202 | 1.00 | 85.10                     | 0 | AT01 | 1454 | N   | ASP | C   | 155    | 25.180 | 20.142 | 38.726 | 1.00  | 16.57 | N |
| AT01                      | 1392 | CZ  | ARG | C | 147 | 37.843 | 34.703 | 37.231 | 1.00 | 89.68                     | 0 | AT01 | 1455 | C   | ASP | C   | 155    | 24.799 | 20.546 | 37.556 | 1.00  | 21.43 | C |
| AT01                      | 1393 | NH1 | ARG | C | 147 | 35.683 | 35.476 | 36.720 | 1.00 | 84.49                     | 0 | AT01 | 1456 | CG  | ASP | C   | 155    | 27.302 | 21.611 | 36.470 | 1.00  | 20.40 | C |
| AT01                      | 1394 | NH2 | ARG | C | 147 | 39.961 | 35.249 | 36.720 | 1.00 | 81.29                     | 0 | AT01 | 1457 | CG  | ASP | C   | 155    | 22.906 | 22.131 | 36.813 | 1.00  | 34.02 | C |
| AT01                      | 1395 | C   | ARG | C | 147 | 32.881 | 30.110 | 38.388 | 1.00 | 55.51                     | 0 | AT01 | 1458 | OD1 | ASP | C   | 155    | 22.209 | 21.487 | 37.646 | 1.00  | 35.30 | C |
| AT01                      | 1396 | O   | ARG | C | 147 | 32.035 | 31.006 | 38.358 | 1.00 | 55.73                     | 0 | AT01 | 1459 | OD2 | ASP | C   | 155    | 22.497 | 23.185 | 36.231 | 1.00  | 38.57 | C |
| AT01                      | 1397 | N   | LEU | C | 148 | 32.567 | 28.821 | 38.428 | 1.00 | 42.44                     | 0 | AT01 | 1460 | C   | ASP | C   | 155    | 25.919 | 19.729 | 36.831 | 1.00  | 21.61 | C |
| AT01                      | 1398 | C   | LEU | C | 148 | 31.193 | 28.356 | 38.346 | 1.00 | 35.63                     | 0 | AT01 | 1461 | O   | ASP | C   | 155    | 25.659 | 18.694 | 36.605 | 1.00  | 20.58 | O |
| AT01                      | 1399 | CB  | LEU | C | 148 | 29.630 | 27.377 | 38.111 | 1.00 | 30.93                     | 0 | AT01 | 1462 | C   | LYS | C   | 156    | 26.721 | 19.783 | 36.784 | 1.00  | 21.04 | C |
| AT01                      | 1400 | CG  | LEU | C | 148 | 32.032 | 26.174 | 37.244 | 1.00 | 36.17                     | 0 | AT01 | 1463 | C   | LYS | C   | 156    | 28.259 | 19.558 | 36.187 | 1.00  | 22.61 | C |
| AT01                      | 1401 | CD1 | LEU | C | 148 | 32.006 | 24.664 | 37.401 | 1.00 | 26.97                     | 0 | AT01 | 1464 | C   | LYS | C   | 156    | 29.523 | 20.411 | 36.152 | 1.00  | 24.52 | C |
| AT01                      | 1402 | CD2 | LEU | C | 148 | 31.570 | 26.579 | 35.835 | 1.00 | 32.22                     | 0 | AT01 | 1465 | CG  | LYS | C   | 156    | 29.523 | 20.411 | 35.808 | 1.00  | 32.74 | C |
| AT01                      | 1403 | O   | LEU | C | 148 | 30.327 | 28.669 | 35.863 | 1.00 | 34.66                     | 0 | AT01 | 1466 | CG  | LYS | C   | 156    | 29.523 | 20.411 | 35.808 | 1.00  | 32.74 | C |
| AT01                      | 1404 | O   | LEU | C | 148 | 30.761 | 28.561 | 35.863 | 1.00 | 34.67                     | 0 | AT01 | 1467 | CE  | LYS | C   | 156    | 29.523 | 20.411 | 35.808 | 1.00  | 32.74 | C |
| AT01                      | 1405 | N   | SER | C | 149 | 29.054 | 29.221 | 39.182 | 1.00 | 23.02                     | 0 | AT01 | 1468 | NZ  | LYS | C   | 156    | 29.007 | 22.987 | 31.954 | 1.00  | 39.04 | N |
| AT01                      | 1406 | C   | SER | C | 149 | 28.087 | 29.445 | 40.224 | 1.00 | 28.77                     | 0 | AT01 | 1469 | C   | LYS | C   | 156    | 28.559 | 18.272 | 36.952 | 1.00  | 25.81 | C |
| AT01                      | 1407 | CB  | SER | C | 149 | 26.773 | 29.936 | 39.620 | 1.00 | 29.57                     | 0 | AT01 | 1470 | O   | LYS | C   | 156    | 28.860 | 17.237 | 36.942 | 1.00  | 27.44 | O |
| AT01                      | 1408 | CG  | SER | C | 149 |        |        |        |      |                           |   |      |      |     |     |     |        |        |        |        |       |       |   |

dimer-PDB-coordinates.txt

|      |      |     |     |   |     |        |        |        |      |       |  |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|--|
| ATOM | 1474 | CG  | LEU | C | 157 | 30.171 | 18.325 | 40.906 | 1.00 | 23.36 |  |
| ATOM | 1475 | CD1 | LEU | C | 157 | 30.122 | 18.922 | 32.142 | 1.00 | 21.16 |  |
| ATOM | 1476 | CD2 | LEU | C | 157 | 30.140 | 17.522 | 40.640 | 1.00 | 21.66 |  |
| ATOM | 1477 | C   | LEU | C | 157 | 27.695 | 16.103 | 38.891 | 1.00 | 15.41 |  |
| ATOM | 1478 | O   | LEU | C | 157 | 27.884 | 14.909 | 38.799 | 1.00 | 17.36 |  |
| ATOM | 1479 | N   | GLU | C | 158 | 26.540 | 16.543 | 38.818 | 1.00 | 19.09 |  |
| ATOM | 1480 | CE2 | GLU | C | 158 | 25.349 | 15.616 | 38.622 | 1.00 | 24.23 |  |
| ATOM | 1481 | CB  | GLU | C | 158 | 25.959 | 16.201 | 38.814 | 1.00 | 20.14 |  |
| ATOM | 1482 | CG  | GLU | C | 158 | 22.841 | 15.354 | 38.613 | 1.00 | 27.53 |  |
| ATOM | 1483 | CD  | GLU | C | 158 | 22.517 | 15.883 | 39.144 | 1.00 | 36.52 |  |
| ATOM | 1484 | OE1 | GLU | C | 158 | 20.526 | 15.129 | 39.133 | 1.00 | 33.06 |  |
| ATOM | 1485 | OE2 | GLU | C | 158 | 21.449 | 17.050 | 39.621 | 1.00 | 36.36 |  |
| ATOM | 1486 | C   | GLU | C | 158 | 23.413 | 14.952 | 37.247 | 1.00 | 27.62 |  |
| ATOM | 1487 | O   | GLU | C | 158 | 25.537 | 13.802 | 37.092 | 1.00 | 31.70 |  |
| ATOM | 1488 | N   | ILE | C | 159 | 25.880 | 15.706 | 36.252 | 1.00 | 18.51 |  |
| ATOM | 1489 | CA  | ILE | C | 159 | 26.060 | 15.126 | 34.933 | 1.00 | 25.75 |  |
| ATOM | 1490 | CB  | ILE | C | 159 | 26.390 | 16.189 | 33.871 | 1.00 | 29.81 |  |
| ATOM | 1491 | CG1 | ILE | C | 159 | 25.147 | 17.093 | 33.552 | 1.00 | 35.53 |  |
| ATOM | 1492 | CG2 | ILE | C | 159 | 25.407 | 16.118 | 32.547 | 1.00 | 30.52 |  |
| ATOM | 1493 | CG2 | ILE | C | 159 | 26.893 | 15.445 | 32.607 | 1.00 | 28.01 |  |
| ATOM | 1494 | C   | ILE | C | 159 | 27.172 | 14.075 | 34.968 | 1.00 | 29.03 |  |
| ATOM | 1495 | O   | ILE | C | 159 | 26.985 | 12.961 | 34.492 | 1.00 | 36.37 |  |
| ATOM | 1496 | N   | PHE | C | 160 | 28.326 | 14.418 | 35.533 | 1.00 | 24.61 |  |
| ATOM | 1497 | CA  | PHE | C | 160 | 29.423 | 13.459 | 35.587 | 1.00 | 17.12 |  |
| ATOM | 1498 | CB  | PHE | C | 160 | 30.582 | 12.013 | 36.135 | 1.00 | 14.41 |  |
| ATOM | 1499 | CG  | PHE | C | 160 | 31.883 | 11.209 | 36.075 | 1.00 | 20.23 |  |
| ATOM | 1500 | CD1 | PHE | C | 160 | 32.158 | 12.342 | 37.124 | 1.00 | 15.04 |  |
| ATOM | 1501 | CD1 | PHE | C | 160 | 32.734 | 11.487 | 37.065 | 1.00 | 17.01 |  |
| ATOM | 1502 | CD2 | PHE | C | 160 | 34.058 | 11.486 | 35.948 | 1.00 | 19.54 |  |
| ATOM | 1503 | CD2 | PHE | C | 160 | 33.802 | 12.357 | 34.907 | 1.00 | 16.33 |  |
| ATOM | 1504 | CD2 | PHE | C | 160 | 32.712 | 12.013 | 34.958 | 1.00 | 14.28 |  |
| ATOM | 1505 | C   | PHE | C | 160 | 29.075 | 17.188 | 36.392 | 1.00 | 20.46 |  |
| ATOM | 1506 | O   | PHE | C | 160 | 29.211 | 13.068 | 35.899 | 1.00 | 16.09 |  |
| ATOM | 1507 | N   | PHE | C | 161 | 28.628 | 11.378 | 37.628 | 1.00 | 13.73 |  |
| ATOM | 1508 | CA  | PHE | C | 161 | 28.383 | 11.269 | 36.545 | 1.00 | 20.23 |  |
| ATOM | 1509 | CB  | PHE | C | 161 | 28.551 | 11.715 | 40.003 | 1.00 | 15.80 |  |
| ATOM | 1510 | CG  | PHE | C | 161 | 29.972 | 11.019 | 40.363 | 1.00 | 14.28 |  |
| ATOM | 1511 | CD1 | PHE | C | 161 | 30.903 | 10.991 | 40.466 | 1.00 | 12.48 |  |
| ATOM | 1512 | CD1 | PHE | C | 161 | 32.237 | 11.262 | 40.791 | 1.00 | 15.39 |  |
| ATOM | 1513 | CD2 | PHE | C | 161 | 32.644 | 12.579 | 40.983 | 1.00 | 14.31 |  |
| ATOM | 1514 | CD2 | PHE | C | 161 | 31.712 | 13.614 | 40.979 | 1.00 | 16.35 |  |
| ATOM | 1515 | CD2 | PHE | C | 161 | 31.388 | 13.320 | 40.566 | 1.00 | 10.43 |  |
| ATOM | 1516 | C   | PHE | C | 161 | 27.046 | 10.578 | 38.337 | 1.00 | 17.17 |  |
| ATOM | 1517 | O   | PHE | C | 161 | 26.809 | 9.520  | 35.907 | 1.00 | 16.21 |  |
| ATOM | 1518 | N   | GLY | C | 162 | 26.190 | 11.168 | 37.507 | 1.00 | 13.89 |  |
| ATOM | 1519 | CA  | GLY | C | 162 | 24.960 | 10.512 | 37.111 | 1.00 | 14.99 |  |
| ATOM | 1520 | CB  | GLY | C | 162 | 25.171 | 9.455  | 35.037 | 1.00 | 16.48 |  |
| ATOM | 1521 | O   | GLY | C | 162 | 24.260 | 8.711  | 35.715 | 1.00 | 17.45 |  |
| ATOM | 1522 | N   | LYS | C | 163 | 26.372 | 9.383  | 35.484 | 1.00 | 15.61 |  |
| ATOM | 1523 | CA  | LYS | C | 163 | 26.606 | 8.469  | 34.363 | 1.00 | 19.34 |  |
| ATOM | 1524 | CB  | LYS | C | 163 | 27.621 | 9.045  | 33.381 | 1.00 | 19.27 |  |
| ATOM | 1525 | CG  | LYS | C | 163 | 27.064 | 10.138 | 32.500 | 1.00 | 26.94 |  |
| ATOM | 1526 | CD  | LYS | C | 163 | 26.151 | 10.762 | 33.644 | 1.00 | 37.10 |  |
| ATOM | 1527 | CE  | LYS | C | 163 | 27.544 | 10.772 | 30.590 | 1.00 | 31.26 |  |
| ATOM | 1528 | NZ  | LYS | C | 163 | 26.427 | 12.482 | 31.143 | 1.00 | 36.93 |  |
| ATOM | 1529 | C   | LYS | C | 163 | 27.059 | 7.078  | 34.786 | 1.00 | 21.26 |  |
| ATOM | 1530 | O   | LYS | C | 163 | 26.019 | 6.914  | 35.531 | 1.00 | 17.22 |  |
| ATOM | 1531 | N   | THR | C | 164 | 26.357 | 6.076  | 34.286 | 1.00 | 19.36 |  |
| ATOM | 1532 | CA  | THR | C | 164 | 26.736 | 4.696  | 34.498 | 1.00 | 27.57 |  |
| ATOM | 1533 | CB  | THR | C | 164 | 25.793 | 3.745  | 33.743 | 1.00 | 21.28 |  |
| ATOM | 1534 | CG1 | THR | C | 164 | 24.505 | 3.757  | 34.366 | 1.00 | 35.94 |  |
| ATOM | 1535 | CG2 | THR | C | 164 | 26.323 | 2.339  | 32.732 | 1.00 | 14.19 |  |
| ATOM | 1536 | C   | THR | C | 164 | 26.202 | 4.483  | 34.059 | 1.00 | 24.12 |  |

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|      |      |     |     |   |     |        |        |        |      |       |  |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|--|
| ATOM | 1600 | CA  | ARG | C | 174 | 22.561 | 14.045 | 48.057 | 1.00 | 20.10 |  |
| ATOM | 1601 | CB  | ARG | C | 174 | 22.747 | 17.426 | 44.566 | 1.00 | 16.53 |  |
| ATOM | 1602 | CG  | ARG | C | 174 | 21.814 | 15.507 | 44.017 | 1.00 | 26.85 |  |
| ATOM | 1603 | CD  | ARG | C | 174 | 21.809 | 18.576 | 42.468 | 1.00 | 21.00 |  |
| ATOM | 1604 | NE  | ARG | C | 174 | 21.470 | 19.927 | 42.012 | 1.00 | 27.78 |  |
| ATOM | 1605 | C   | ARG | C | 174 | 20.720 | 17.711 | 43.783 | 1.00 | 27.16 |  |
| ATOM | 1606 | NH1 | ARG | C | 174 | 27.135 | 19.504 | 39.816 | 1.00 | 20.86 |  |
| ATOM | 1607 | NH2 | ARG | C | 174 | 21.332 | 21.635 | 40.489 | 1.00 | 23.76 |  |
| ATOM | 1608 | C   | ARG | C | 174 | 22.604 | 15.360 | 46.920 | 1.00 | 19.64 |  |
| ATOM | 1609 | O   | ARG | C | 174 | 21.689 | 15.187 | 46.904 | 1.00 | 20.98 |  |
| ATOM | 1610 | N   | GLU | C | 175 | 23.680 | 16.377 | 47.731 | 1.00 | 21.91 |  |
| ATOM | 1611 | CA  | GLU | C | 175 | 23.762 | 15.574 | 46.707 | 1.00 | 28.63 |  |
| ATOM | 1612 | CB  | GLU | C | 175 | 23.440 | 15.091 | 50.121 | 1.00 | 23.46 |  |
| ATOM | 1613 | CG  | GLU | C | 175 | 21.964 | 18.826 | 50.299 | 1.00 | 34.78 |  |
| ATOM | 1614 | CD  | GLU | C | 175 | 21.718 | 18.531 | 51.878 | 1.00 | 44.30 |  |
| ATOM | 1615 | OE1 | GLU | C | 175 | 22.686 | 18.383 | 51.623 | 1.00 | 46.92 |  |
| ATOM | 1616 | OE2 | GLU | C | 175 | 20.934 | 18.737 | 52.286 | 1.00 | 37.15 |  |
| ATOM | 1617 | C   | GLU | C | 175 | 25.144 | 16.068 | 48.572 | 1.00 | 21.97 |  |
| ATOM | 1618 | O   | GLU | C | 175 | 26.137 | 19.456 | 48.575 | 1.00 | 19.41 |  |
| ATOM | 1619 | N   | LEU | C | 176 | 25.201 | 21.467 | 49.018 | 1.00 | 21.61 |  |
| ATOM | 1620 | CA  | LEU | C | 176 | 26.466 | 22.145 | 49.274 | 1.00 | 26.42 |  |
| ATOM | 1621 | CB  | LEU | C | 176 | 26.407 | 23.597 | 48.810 | 1.00 | 17.94 |  |
| ATOM | 1622 | CG  | LEU | C | 176 | 26.107 | 23.683 | 47.315 | 1.00 | 27.61 |  |
| ATOM | 1623 | CD1 | LEU | C | 176 | 25.586 | 25.067 | 46.950 | 1.00 | 16.86 |  |
| ATOM | 1624 | CD2 | LEU | C | 176 | 27.366 | 23.351 | 46.534 | 1.00 | 26.17 |  |
| ATOM | 1625 | C   | LEU | C | 176 | 26.761 | 22.080 | 50.753 | 1.00 | 32.12 |  |
| ATOM | 1626 | O   | LEU | C | 176 | 25.984 | 22.572 | 51.564 | 1.00 | 28.66 |  |
| ATOM | 1627 | N   | LEU | C | 177 | 27.868 | 21.433 | 51.109 | 1.00 | 32.12 |  |
| ATOM | 1628 | CA  | LEU | C | 177 | 28.370 | 21.429 | 52.181 | 1.00 | 24.16 |  |
| ATOM | 1629 | CB  | LEU | C | 177 | 28.622 | 20.001 | 52.957 | 1.00 | 21.99 |  |
| ATOM | 1630 | CG  | LEU | C | 177 | 27.440 | 19.718 | 53.513 | 1.00 | 16.18 |  |
| ATOM | 1631 | CD1 | LEU | C | 177 | 26.196 | 19.454 | 53.705 | 1.00 | 42.88 |  |
| ATOM | 1632 | CD2 | LEU | C | 177 | 27.763 | 17.751 | 53.712 | 1.00 | 35.08 |  |
| ATOM | 1633 | C   | LEU | C | 177 | 29.668 | 22.211 | 51.510 | 1.00 | 29.86 |  |
| ATOM | 1634 | O   | LEU | C | 177 | 30.235 | 22.524 | 51.453 | 1.00 | 29.28 |  |
| ATOM | 1635 | N   | PRO | C | 178 | 30.160 | 22.532 | 51.720 | 1.00 | 43.78 |  |
| ATOM | 1636 | CA  | PRO | C | 178 | 31.412 | 23.293 | 53.624 | 1.00 | 40.09 |  |
| ATOM | 1637 | CB  | PRO | C | 178 | 31.670 | 23.321 | 55.329 | 1.00 | 45.81 |  |
| ATOM | 1638 | CG  | PRO | C | 178 | 30.294 | 23.127 | 55.937 | 1.00 | 42.11 |  |
| ATOM | 1639 | CD  | PRO | C | 178 | 29.561 | 22.771 | 55.041 | 1.00 | 40.73 |  |
| ATOM | 1640 | C   | PRO | C | 178 | 32.561 | 22.607 | 53.071 | 1.00 | 31.16 |  |
| ATOM | 1641 | O   | PRO | C | 178 | 32.976 | 21.506 | 53.423 | 1.00 | 28.26 |  |
| ATOM | 1642 | N   | GLY | C | 179 | 33.036 | 23.257 | 52.013 | 1.00 | 36.53 |  |
| ATOM | 1643 | CA  | GLY | C | 179 | 34.111 | 22.725 | 51.189 | 1.00 | 36.32 |  |
| ATOM | 1644 | CB  | GLY | C | 179 | 33.825 | 21.497 | 50.471 | 1.00 | 40.47 |  |
| ATOM | 1645 | O   | GLY | C | 179 | 34.744 | 20.740 | 50.010 | 1.00 | 38.32 |  |
| ATOM | 1646 | N   | SER | C | 180 | 32.561 | 21.045 | 50.329 | 1.00 | 31.20 |  |
| ATOM | 1647 | CA  | SER | C | 180 | 32.281 | 19.800 | 49.638 | 1.00 | 28.67 |  |
| ATOM | 1648 | CB  | SER | C | 180 | 32.480 | 18.620 | 50.582 | 1.00 | 27.98 |  |
| ATOM | 1649 | CG  | SER | C | 180 | 31.389 | 18.487 | 51.442 | 1.00 | 40.80 |  |
| ATOM | 1650 | CD  | SER | C | 180 | 30.884 | 19.739 | 49.024 | 1.00 | 31.53 |  |
| ATOM | 1651 | O   | SER | C | 180 | 30.001 | 20.555 | 49.310 | 1.00 | 23.73 |  |
| ATOM | 1652 | N   | VAL | C | 181 | 30.684 | 18.746 | 48.160 | 1.00 | 22.83 |  |
| ATOM | 1653 | CA  | VAL | C | 181 | 29.349 | 18.522 | 47.635 | 1.00 | 21.12 |  |
| ATOM | 1654 | CB  | VAL | C | 181 | 29.297 | 18.635 | 46.125 | 1.00 | 18.23 |  |
| ATOM | 1655 | CG1 | VAL | C | 181 | 27.972 | 18.162 | 45.895 | 1.00 | 17.12 |  |
| ATOM | 1656 | CG2 | VAL | C | 181 | 29.476 | 20.078 | 45.695 | 1.00 | 18.93 |  |
| ATOM | 1657 | C   | VAL | C | 181 | 28.868 | 17.153 | 45.063 | 1.00 | 20.98 |  |
| ATOM | 1658 | O   | VAL | C | 181 | 29.571 | 16.282 | 47.916 | 1.00 |       |  |

| dimer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |            |
|---------------------------|------|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM                      | 1726 | CA  | ALA | C | 191 | 27.755 | 5.098  | 46.309 | 1.00 19.18 |
| ATOM                      | 1727 | CB  | ALA | C | 191 | 27.027 | 5.471  | 47.600 | 1.00 18.69 |
| ATOM                      | 1728 | CD  | ALA | C | 191 | 26.993 | 4.255  | 46.595 | 1.00 23.10 |
| ATOM                      | 1729 | O   | ALA | C | 191 | 30.111 | 4.768  | 46.572 | 1.00 26.17 |
| ATOM                      | 1730 | N   | GLN | C | 192 | 28.804 | 2.962  | 46.842 | 1.00 20.53 |
| ATOM                      | 1731 | CA  | GLN | C | 192 | 29.946 | 2.111  | 47.176 | 1.00 25.59 |
| ATOM                      | 1732 | CB  | GLN | C | 192 | 29.505 | 0.716  | 47.642 | 1.00 26.25 |
| ATOM                      | 1733 | CD  | GLN | C | 192 | 28.911 | 0.709  | 49.038 | 1.00 37.72 |
| ATOM                      | 1734 | OE1 | GLN | C | 192 | 27.619 | 1.323  | 49.141 | 1.00 47.20 |
| ATOM                      | 1735 | OE2 | GLN | C | 192 | 26.816 | 1.600  | 48.185 | 1.00 40.55 |
| ATOM                      | 1736 | NE2 | GLN | C | 192 | 27.417 | 2.142  | 50.308 | 1.00 47.68 |
| ATOM                      | 1737 | C   | GLN | C | 192 | 30.898 | 1.980  | 46.011 | 1.00 26.69 |
| ATOM                      | 1738 | O   | GLN | C | 192 | 32.118 | 2.011  | 46.180 | 1.00 27.73 |
| ATOM                      | 1739 | N   | ARG | C | 193 | 30.841 | 1.416  | 44.821 | 1.00 24.34 |
| ATOM                      | 1740 | CA  | ARG | C | 193 | 31.176 | 1.745  | 43.434 | 1.00 27.43 |
| ATOM                      | 1741 | CB  | ARG | C | 193 | 30.317 | 1.506  | 42.398 | 1.00 20.89 |
| ATOM                      | 1742 | CG  | ARG | C | 193 | 31.142 | 1.299  | 41.149 | 1.00 25.19 |
| ATOM                      | 1743 | CD  | ARG | C | 193 | 30.319 | 1.747  | 39.957 | 1.00 38.68 |
| ATOM                      | 1744 | OE1 | ARG | C | 193 | 28.337 | 0.840  | 39.571 | 1.00 47.74 |
| ATOM                      | 1745 | OE2 | ARG | C | 193 | 27.990 | 1.213  | 39.314 | 1.00 47.37 |
| ATOM                      | 1746 | NH1 | ARG | C | 193 | 27.609 | 2.457  | 39.455 | 1.00 34.93 |
| ATOM                      | 1747 | NH2 | ARG | C | 193 | 27.079 | 0.321  | 38.930 | 1.00 61.47 |
| ATOM                      | 1748 | C   | ARG | C | 193 | 32.013 | 3.026  | 43.453 | 1.00 18.59 |
| ATOM                      | 1749 | O   | ARG | C | 193 | 33.220 | 2.969  | 43.215 | 1.00 20.52 |
| ATOM                      | 1750 | N   | LEU | C | 194 | 31.165 | 1.181  | 42.561 | 1.00 24.13 |
| ATOM                      | 1751 | CA  | LEU | C | 194 | 32.071 | 1.446  | 43.348 | 1.00 19.28 |
| ATOM                      | 1752 | CB  | LEU | C | 194 | 31.115 | 0.639  | 43.392 | 1.00 13.72 |
| ATOM                      | 1753 | CG  | LEU | C | 194 | 30.140 | 0.783  | 42.228 | 1.00 22.89 |
| ATOM                      | 1754 | CD  | LEU | C | 194 | 29.183 | 7.920  | 42.455 | 1.00 14.01 |
| ATOM                      | 1755 | OE1 | LEU | C | 194 | 30.888 | 0.857  | 40.920 | 1.00 19.69 |
| ATOM                      | 1756 | OE2 | LEU | C | 194 | 28.151 | 1.487  | 40.920 | 1.00 19.69 |
| ATOM                      | 1757 | O   | LEU | C | 194 | 34.235 | 0.114  | 44.331 | 1.00 21.76 |
| ATOM                      | 1758 | N   | CYS | C | 195 | 32.843 | 1.193  | 45.624 | 1.00 23.04 |
| ATOM                      | 1759 | CA  | CYS | C | 195 | 33.798 | 1.243  | 46.720 | 1.00 25.54 |
| ATOM                      | 1760 | CB  | CYS | C | 195 | 33.072 | 1.934  | 46.045 | 1.00 32.89 |
| ATOM                      | 1761 | CG  | CYS | C | 195 | 34.068 | 1.112  | 49.631 | 1.00 66.52 |
| ATOM                      | 1762 | C   | CYS | C | 195 | 34.999 | 4.304  | 46.476 | 1.00 23.99 |
| ATOM                      | 1763 | O   | CYS | C | 195 | 36.152 | 4.672  | 46.746 | 1.00 20.72 |
| ATOM                      | 1764 | N   | CYS | C | 196 | 34.736 | 3.115  | 45.934 | 1.00 23.91 |
| ATOM                      | 1765 | CA  | GLN | C | 196 | 35.804 | 2.187  | 45.574 | 1.00 29.44 |
| ATOM                      | 1766 | CB  | GLN | C | 196 | 35.037 | 0.851  | 45.073 | 1.00 26.84 |
| ATOM                      | 1767 | CG  | GLN | C | 196 | 34.780 | -0.081 | 46.182 | 1.00 32.78 |
| ATOM                      | 1768 | CD  | GLN | C | 196 | 33.777 | -1.119 | 45.698 | 1.00 70.18 |
| ATOM                      | 1769 | OE1 | GLN | C | 196 | 33.621 | -1.330 | 44.487 | 1.00 66.66 |
| ATOM                      | 1770 | OE2 | GLN | C | 196 | 33.042 | -1.768 | 46.642 | 1.00 58.45 |
| ATOM                      | 1771 | O   | GLN | C | 196 | 36.715 | 2.796  | 44.517 | 1.00 26.60 |
| ATOM                      | 1772 | O   | GLN | C | 196 | 37.738 | 2.681  | 46.608 | 1.00 24.73 |
| ATOM                      | 1773 | N   | ILE | C | 197 | 36.132 | 3.439  | 43.511 | 1.00 29.67 |
| ATOM                      | 1774 | CA  | ILE | C | 197 | 36.941 | 4.106  | 42.484 | 1.00 23.22 |
| ATOM                      | 1775 | CB  | ILE | C | 197 | 36.078 | 4.627  | 41.317 | 1.00 25.75 |
| ATOM                      | 1776 | CG1 | ILE | C | 197 | 35.420 | 3.448  | 40.576 | 1.00 21.59 |
| ATOM                      | 1777 | CG2 | ILE | C | 197 | 35.866 | 3.845  | 39.617 | 1.00 21.36 |
| ATOM                      | 1778 | CD1 | ILE | C | 197 | 36.928 | 1.444  | 40.346 | 1.00 19.84 |
| ATOM                      | 1779 | C   | ILE | C | 197 | 37.735 | 5.251  | 43.116 | 1.00 26.47 |
| ATOM                      | 1780 | O   | ILE | C | 197 | 38.937 | 5.410  | 42.876 | 1.00 27.85 |
| ATOM                      | 1781 | N   | GLY | C | 198 | 37.051 | 6.051  | 43.926 | 1.00 26.82 |
| ATOM                      | 1782 | CA  | GLY | C | 198 | 37.710 | 7.025  | 44.777 | 1.00 21.79 |
| ATOM                      | 1783 | CB  | GLY | C | 198 | 37.482 | 6.140  | 44.420 | 1.00 21.79 |
| ATOM                      | 1784 | O   | GLY | C | 198 | 37.885 | 9.385  | 44.615 | 1.00 26.39 |
| ATOM                      | 1785 | N   | GLN | C | 199 | 36.925 | 6.191  | 43.022 | 1.00 21.42 |
| ATOM                      | 1786 | CA  | GLN | C | 199 | 39.467 | 9.377  | 42.369 | 1.00 28.04 |
| ATOM                      | 1787 | CB  | GLN | C | 199 | 40.997 | 9.315  | 42.305 | 1.00 28.73 |
| ATOM                      | 1788 | CG  | GLN | C | 199 | 42.672 | 9.495  | 43.642 | 1.00 47.78 |

| dimer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |            |
|---------------------------|------|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM                      | 1852 | CA  | GLN | C | 208 | 39.967 | 12.133 | 34.432 | 1.00 22.64 |
| ATOM                      | 1853 | CB  | GLN | C | 208 | 40.726 | 18.264 | 33.454 | 1.00 20.63 |
| ATOM                      | 1854 | CG  | GLN | C | 208 | 40.930 | 18.869 | 32.107 | 1.00 34.94 |
| ATOM                      | 1855 | CD  | GLN | C | 208 | 39.827 | 18.427 | 31.176 | 1.00 46.05 |
| ATOM                      | 1856 | OE1 | GLN | C | 208 | 40.688 | 17.747 | 31.536 | 1.00 33.77 |
| ATOM                      | 1857 | OE2 | GLN | C | 208 | 39.947 | 18.803 | 29.987 | 1.00 32.77 |
| ATOM                      | 1858 | C   | GLN | C | 208 | 40.477 | 18.834 | 35.820 | 1.00 18.64 |
| ATOM                      | 1859 | O   | GLN | C | 208 | 41.692 | 18.763 | 36.051 | 1.00 19.60 |
| ATOM                      | 1860 | N   | VAL | C | 209 | 39.547 | 18.554 | 36.742 | 1.00 20.59 |
| ATOM                      | 1861 | CA  | VAL | C | 209 | 39.853 | 18.698 | 35.152 | 1.00 20.08 |
| ATOM                      | 1862 | CB  | VAL | C | 209 | 38.781 | 19.536 | 36.089 | 1.00 21.36 |
| ATOM                      | 1863 | CG1 | VAL | C | 209 | 39.103 | 15.648 | 40.374 | 1.00 21.93 |
| ATOM                      | 1864 | CG2 | VAL | C | 209 | 38.662 | 20.906 | 35.244 | 1.00 16.64 |
| ATOM                      | 1865 | C   | VAL | C | 209 | 39.683 | 17.316 | 36.780 | 1.00 17.13 |
| ATOM                      | 1866 | O   | VAL | C | 209 | 38.936 | 16.548 | 38.637 | 1.00 22.14 |
| ATOM                      | 1867 | N   | PRO | C | 210 | 40.972 | 16.991 | 39.482 | 1.00 24.15 |
| ATOM                      | 1868 | CA  | PRO | C | 210 | 42.004 | 16.232 | 40.332 | 1.00 25.77 |
| ATOM                      | 1869 | CB  | PRO | C | 210 | 42.493 | 15.534 | 40.521 | 1.00 22.20 |
| ATOM                      | 1870 | CG  | PRO | C | 210 | 43.048 | 16.946 | 40.565 | 1.00 24.22 |
| ATOM                      | 1871 | CD  | PRO | C | 210 | 42.219 | 17.766 | 39.610 | 1.00 21.44 |
| ATOM                      | 1872 | O   | PRO | C | 210 | 40.196 | 15.847 | 41.533 | 1.00 23.68 |
| ATOM                      | 1873 | O   | PRO | C | 210 | 40.509 | 16.662 | 42.386 | 1.00 20.77 |
| ATOM                      | 1874 | N   | LEU | C | 211 | 39.150 | 15.046 | 42.552 | 1.00 20.74 |
| ATOM                      | 1875 | CA  | LEU | C | 211 | 36.232 | 15.096 | 42.762 | 1.00 20.14 |
| ATOM                      | 1876 | CB  | LEU | C | 211 | 36.817 | 15.361 | 42.249 | 1.00 15.36 |
| ATOM                      | 1877 | CG  | LEU | C | 211 | 36.520 | 16.709 | 41.591 | 1.00 18.83 |
| ATOM                      | 1878 | CD1 | LEU | C | 211 | 35.063 | 16.781 | 41.126 | 1.00 18.12 |
| ATOM                      | 1879 | CD2 | LEU | C | 211 | 36.820 | 17.844 | 42.552 | 1.00 21.01 |
| ATOM                      | 1880 | C   | LEU | C | 211 | 36.243 | 13.751 | 41.499 | 1.00 25.72 |
| ATOM                      | 1881 | O   | LEU | C | 211 | 38.534 | 12.658 | 42.903 | 1.00 20.11 |
| ATOM                      | 1882 | N   | ARG | C | 212 | 37.927 | 13.612 | 44.790 | 1.00 19.56 |
| ATOM                      | 1883 | CA  | ARG | C | 212 | 37.815 | 12.624 | 45.621 | 1.00 23.24 |
| ATOM                      | 1884 | CB  | ARG | C | 212 | 38.619 | 12.793 | 46.917 | 1.00 22.06 |
| ATOM                      | 1885 | CG  | ARG | C | 212 | 40.110 | 12.981 | 46.746 | 1.00 47.45 |
| ATOM                      | 1886 | CD  | ARG | C | 212 | 40.741 | 11.527 | 46.977 | 1.00 67.53 |
| ATOM                      | 1887 | NE  | ARG | C | 212 | 42.199 | 11.583 | 46.965 | 1.00 68.16 |
| ATOM                      | 1888 | CZ  | ARG | C | 212 | 42.572 | 10.305 | 46.943 | 1.00 72.13 |
| ATOM                      | 1889 | NH1 | ARG | C | 212 | 42.420 | 9.295  | 46.936 | 1.00 64.80 |
| ATOM                      | 1890 | NH2 | ARG | C | 212 | 44.292 | 10.634 | 46.932 | 1.00 72.16 |
| ATOM                      | 1891 | C   | ARG | C | 212 | 36.366 | 12.980 | 46.004 | 1.00 21.24 |
| ATOM                      | 1892 | O   | ARG | C | 212 | 35.633 | 13.333 | 46.322 | 1.00 18.99 |
| ATOM                      | 1893 | N   | VAL | C | 213 | 35.974 | 11.125 | 45.997 | 1.00 22.35 |
| ATOM                      | 1894 | CA  | VAL | C | 213 | 34.681 | 10.725 | 46.508 | 1.00 23.15 |
| ATOM                      | 1895 | CB  | VAL | C | 213 | 33.904 | 9.900  | 45.467 | 1.00 23.76 |
| ATOM                      | 1896 | CG1 | VAL | C | 213 | 32.706 | 9.218  | 46.112 | 1.00 23.77 |
| ATOM                      | 1897 | CG2 | VAL | C | 213 | 33.471 | 10.796 | 44.297 | 1.00 17.93 |
| ATOM                      | 1898 | C   | VAL | C | 213 | 34.896 | 9.884  | 47.755 | 1.00 29.66 |
| ATOM                      | 1899 | O   | VAL | C | 213 | 35.660 | 8.921  | 47.720 | 1.00 25.10 |
| ATOM                      | 1900 | N   | SER | C | 214 | 34.222 | 10.250 | 48.846 | 1.00 22.13 |
| ATOM                      | 1901 | CA  | SER | C | 214 | 34.315 | 9.517  | 50.130 | 1.00 29.67 |
| ATOM                      | 1902 | CB  | SER | C | 214 | 35.086 | 10.437 | 51.149 | 1.00 29.31 |
| ATOM                      | 1903 | CG  | SER | C | 214 | 36.268 | 10.973 | 50.626 | 1.00 42.12 |
| ATOM                      | 1904 | C   | SER | C | 214 | 32.973 | 9.247  | 50.678 | 1.00 27.09 |
| ATOM                      | 1905 | O   | SER | C | 214 | 32.003 | 9.868  | 50.271 | 1.00 21.94 |
| ATOM                      | 1906 | N   | PRO | C | 215 | 32.881 | 8.289  | 51.621 | 1.00 35.90 |
| ATOM                      | 1907 | CA  | PRO | C | 215 | 31.565 | 7.984  | 52.192 | 1.00 37.18 |
| ATOM                      | 1908 | CB  | PRO | C | 215 | 31.846 | 6.796  | 53.109 | 1.00 37.23 |
| ATOM                      | 1909 | CG  | PRO | C | 215 | 33.181 | 6.267  | 52.676 | 1.00 44.29 |
| ATOM                      | 1910 | CD  | PRO | C | 215 | 33.942 | 7.459  | 52.292 | 1.00 36.29 |
| ATOM                      | 1911 | O   | PRO | C | 215 | 31.061 | 9.175  | 53.014 | 1.00 30.86 |
| ATOM                      | 1912 | O   | PRO | C | 215 | 31.865 | 9.942  | 53.530 | 1.00 36.88 |
| ATOM                      | 1913 | N   | TYR | C | 216 | 29.250 | 10.122 | 53.122 | 1.00 29.34 |
| ATOM                      | 1914 | CA  | TYR | C | 216 | 29.173 | 10.413 | 53.934 | 1.00 42.29 |

| dimer-PDB-coordinates.txt |      |    |     |   |     |        |       |        |            |
|---------------------------|------|----|-----|---|-----|--------|-------|--------|------------|
| ATOM                      | 1789 | CD | GLN | C | 199 | 43.154 | 9.775 | 43.495 | 1.00 71.34 |

| dimer-PDB-coordinates.txt |      |     |     |       |        |        |        |      |       | dimer-PDB-coordinates.txt |      |     |     |       |        |        |        |      |       |      |      |      |     |       |        |        |        |      |       |   |
|---------------------------|------|-----|-----|-------|--------|--------|--------|------|-------|---------------------------|------|-----|-----|-------|--------|--------|--------|------|-------|------|------|------|-----|-------|--------|--------|--------|------|-------|---|
| ATOM                      | 1978 | C   | THR | D 140 | 10.613 | 20.965 | 23.956 | 1.00 | 27.14 | ATOM                      | 2041 | CA  | SER | D 149 | 22.790 | 30.056 | 28.024 | 1.00 | 27.68 | ATOM | 2041 | CA   | SER | D 149 | 22.790 | 30.056 | 28.024 | 1.00 | 27.68 | C |
| ATOM                      | 1979 | N   | THR | D 140 | 10.139 | 20.213 | 27.800 | 1.00 | 23.60 | ATOM                      | 2042 | CB  | SER | D 149 | 24.176 | 30.133 | 28.651 | 1.00 | 33.14 | ATOM | 2042 | CB   | SER | D 149 | 24.176 | 30.133 | 28.651 | 1.00 | 33.14 | C |
| ATOM                      | 1980 | N   | GLY | D 141 | 10.287 | 22.278 | 24.859 | 1.00 | 31.00 | ATOM                      | 2043 | OG  | SER | D 149 | 24.457 | 28.930 | 29.345 | 1.00 | 30.41 | ATOM | 2043 | OG   | SER | D 149 | 24.457 | 28.930 | 29.345 | 1.00 | 30.41 | C |
| ATOM                      | 1981 | CA  | GLY | D 141 | 9.250  | 22.891 | 22.880 | 1.00 | 24.14 | ATOM                      | 2044 | C   | SER | D 149 | 22.672 | 28.697 | 27.347 | 1.00 | 16.81 | ATOM | 2044 | C    | SER | D 149 | 22.672 | 28.697 | 27.347 | 1.00 | 16.81 | C |
| ATOM                      | 1982 | C   | GLY | D 141 | 9.711  | 24.902 | 23.471 | 1.00 | 25.31 | ATOM                      | 2045 | O   | SER | D 149 | 22.010 | 27.731 | 27.856 | 1.00 | 35.28 | ATOM | 2045 | O    | SER | D 149 | 22.010 | 27.731 | 27.856 | 1.00 | 35.28 | C |
| ATOM                      | 1983 | O   | GLY | D 141 | 8.945  | 24.482 | 24.407 | 1.00 | 33.85 | ATOM                      | 2046 | N   | GLU | D 150 | 23.940 | 26.331 | 26.216 | 1.00 | 30.41 | ATOM | 2046 | N    | GLU | D 150 | 23.940 | 26.331 | 26.216 | 1.00 | 30.41 | C |
| ATOM                      | 1984 | N   | PHE | D 142 | 10.944 | 24.304 | 23.393 | 1.00 | 23.42 | ATOM                      | 2047 | CA  | GLU | D 150 | 23.240 | 27.281 | 25.474 | 1.00 | 38.12 | ATOM | 2047 | CA   | GLU | D 150 | 23.240 | 27.281 | 25.474 | 1.00 | 38.12 | C |
| ATOM                      | 1985 | CA  | PHE | D 142 | 11.483 | 25.546 | 24.260 | 1.00 | 24.86 | ATOM                      | 2048 | CB  | GLU | D 150 | 23.949 | 27.399 | 24.124 | 1.00 | 37.63 | ATOM | 2048 | CB   | GLU | D 150 | 23.949 | 27.399 | 24.124 | 1.00 | 37.63 | C |
| ATOM                      | 1986 | CB  | PHE | D 142 | 12.984 | 25.675 | 24.048 | 1.00 | 27.10 | ATOM                      | 2049 | CG  | GLU | D 150 | 23.227 | 28.313 | 23.125 | 1.00 | 45.10 | ATOM | 2049 | CG   | GLU | D 150 | 23.227 | 28.313 | 23.125 | 1.00 | 45.10 | C |
| ATOM                      | 1987 | CD  | PHE | D 142 | 14.696 | 24.362 | 24.035 | 1.00 | 21.74 | ATOM                      | 2050 | C   | GLU | D 150 | 24.012 | 28.339 | 21.621 | 1.00 | 62.99 | ATOM | 2050 | C    | GLU | D 150 | 24.012 | 28.339 | 21.621 | 1.00 | 62.99 | C |
| ATOM                      | 1988 | CE1 | PHE | D 142 | 14.057 | 23.785 | 23.250 | 1.00 | 20.67 | ATOM                      | 2051 | OE2 | GLU | D 150 | 25.212 | 27.113 | 21.719 | 1.00 | 59.96 | ATOM | 2051 | OE2  | GLU | D 150 | 25.212 | 27.113 | 21.719 | 1.00 | 59.96 | C |
| ATOM                      | 1989 | CE2 | PHE | D 142 | 14.756 | 22.558 | 23.267 | 1.00 | 28.26 | ATOM                      | 2052 | OE2 | GLU | D 150 | 23.419 | 29.079 | 20.861 | 1.00 | 65.38 | ATOM | 2052 | OE2  | GLU | D 150 | 23.419 | 29.079 | 20.861 | 1.00 | 65.38 | C |
| ATOM                      | 1990 | CZ  | PHE | D 142 | 15.006 | 21.900 | 24.081 | 1.00 | 24.97 | ATOM                      | 2053 | C   | GLU | D 150 | 23.797 | 26.120 | 26.294 | 1.00 | 29.11 | ATOM | 2053 | C    | GLU | D 150 | 23.797 | 26.120 | 26.294 | 1.00 | 29.11 | C |
| ATOM                      | 1991 | CE2 | PHE | D 142 | 14.610 | 22.467 | 22.872 | 1.00 | 26.87 | ATOM                      | 2054 | O   | GLU | D 150 | 23.211 | 23.036 | 26.347 | 1.00 | 27.79 | ATOM | 2054 | O    | GLU | D 150 | 23.211 | 23.036 | 26.347 | 1.00 | 27.79 | C |
| ATOM                      | 1992 | CD2 | PHE | D 142 | 13.958 | 23.692 | 22.663 | 1.00 | 26.24 | ATOM                      | 2055 | N   | GLU | D 151 | 24.920 | 26.368 | 26.947 | 1.00 | 25.88 | ATOM | 2055 | N    | GLU | D 151 | 24.920 | 26.368 | 26.947 | 1.00 | 25.88 | C |
| ATOM                      | 1993 | C   | PHE | D 142 | 10.804 | 26.896 | 24.037 | 1.00 | 30.49 | ATOM                      | 2056 | CA  | GLU | D 151 | 15.545 | 23.460 | 27.777 | 1.00 | 33.27 | ATOM | 2056 | CA   | GLU | D 151 | 15.545 | 23.460 | 27.777 | 1.00 | 33.27 | C |
| ATOM                      | 1994 | O   | PHE | D 142 | 10.654 | 27.332 | 22.903 | 1.00 | 33.65 | ATOM                      | 2057 | CB  | GLU | D 151 | 15.902 | 25.842 | 24.297 | 1.00 | 32.46 | ATOM | 2057 | CB   | GLU | D 151 | 15.902 | 25.842 | 24.297 | 1.00 | 32.46 | C |
| ATOM                      | 1995 | N   | PRO | D 143 | 10.385 | 27.558 | 25.123 | 1.00 | 26.85 | ATOM                      | 2058 | CG  | GLU | D 151 | 27.634 | 24.808 | 29.137 | 1.00 | 48.81 | ATOM | 2058 | CG   | GLU | D 151 | 27.634 | 24.808 | 29.137 | 1.00 | 48.81 | C |
| ATOM                      | 1996 | CA  | PRO | D 143 | 9.763  | 26.861 | 25.017 | 1.00 | 30.32 | ATOM                      | 2059 | CD  | GLU | D 151 | 29.140 | 24.755 | 28.880 | 1.00 | 67.19 | ATOM | 2059 | CD   | GLU | D 151 | 29.140 | 24.755 | 28.880 | 1.00 | 67.19 | C |
| ATOM                      | 1997 | CB  | PRO | D 143 | 9.106  | 29.071 | 26.393 | 1.00 | 24.73 | ATOM                      | 2060 | OE1 | GLU | D 151 | 29.703 | 25.757 | 28.381 | 1.00 | 75.31 | ATOM | 2060 | OE1  | GLU | D 151 | 29.703 | 25.757 | 28.381 | 1.00 | 75.31 | C |
| ATOM                      | 1998 | CG  | PRO | D 143 | 9.687  | 28.604 | 27.324 | 1.00 | 14.61 | ATOM                      | 2061 | OE2 | GLU | D 151 | 29.763 | 23.703 | 25.149 | 1.00 | 62.80 | ATOM | 2061 | OE2  | GLU | D 151 | 29.763 | 23.703 | 25.149 | 1.00 | 62.80 | C |
| ATOM                      | 1999 | CD  | PRO | D 143 | 10.435 | 27.080 | 26.518 | 1.00 | 23.65 | ATOM                      | 2062 | C   | GLU | D 151 | 24.649 | 24.939 | 28.844 | 1.00 | 30.70 | ATOM | 2062 | C    | GLU | D 151 | 24.649 | 24.939 | 28.844 | 1.00 | 30.70 | C |
| ATOM                      | 2000 | C   | PRO | D 143 | 10.806 | 29.978 | 24.792 | 1.00 | 29.73 | ATOM                      | 2063 | O   | GLU | D 151 | 24.547 | 23.752 | 29.248 | 1.00 | 24.97 | ATOM | 2063 | O    | GLU | D 151 | 24.547 | 23.752 | 29.248 | 1.00 | 24.97 | C |
| ATOM                      | 2001 | O   | PRO | D 143 | 11.930 | 28.894 | 25.302 | 1.00 | 31.42 | ATOM                      | 2064 | N   | GLU | D 152 | 24.003 | 25.904 | 29.593 | 1.00 | 20.79 | ATOM | 2064 | N    | GLU | D 152 | 24.003 | 25.904 | 29.593 | 1.00 | 20.79 | C |
| ATOM                      | 2002 | N   | ALA | D 144 | 10.420 | 31.015 | 24.056 | 1.00 | 31.09 | ATOM                      | 2065 | CA  | GLU | D 152 | 23.098 | 25.592 | 30.694 | 1.00 | 25.16 | ATOM | 2065 | CA   | GLU | D 152 | 23.098 | 25.592 | 30.694 | 1.00 | 25.16 | C |
| ATOM                      | 2003 | CA  | ALA | D 144 | 11.303 | 32.151 | 23.779 | 1.00 | 11.60 | ATOM                      | 2066 | CB  | GLU | D 152 | 22.549 | 26.862 | 31.349 | 1.00 | 28.41 | ATOM | 2066 | CB   | GLU | D 152 | 22.549 | 26.862 | 31.349 | 1.00 | 28.41 | C |
| ATOM                      | 2004 | CB  | ALA | D 144 | 10.592 | 33.145 | 23.860 | 1.00 | 33.89 | ATOM                      | 2067 | CG  | GLU | D 152 | 23.511 | 27.712 | 31.064 | 1.00 | 50.34 | ATOM | 2067 | CG   | GLU | D 152 | 23.511 | 27.712 | 31.064 | 1.00 | 50.34 | C |
| ATOM                      | 2005 | C   | ALA | D 144 | 11.760 | 32.852 | 25.054 | 1.00 | 31.89 | ATOM                      | 2068 | C   | GLU | D 152 | 22.961 | 28.945 | 32.709 | 1.00 | 59.82 | ATOM | 2068 | C    | GLU | D 152 | 22.961 | 28.945 | 32.709 | 1.00 | 59.82 | C |
| ATOM                      | 2006 | O   | ALA | D 144 | 12.806 | 33.513 | 25.050 | 1.00 | 34.17 | ATOM                      | 2069 | OE1 | GLU | D 152 | 22.434 | 29.820 | 31.972 | 1.00 | 43.97 | ATOM | 2069 | OE1  | GLU | D 152 | 22.434 | 29.820 | 31.972 | 1.00 | 43.97 | C |
| ATOM                      | 2007 | N   | SER | D 145 | 11.031 | 32.703 | 26.138 | 1.00 | 29.95 | ATOM                      | 2070 | OE2 | GLU | D 152 | 22.949 | 29.024 | 33.953 | 1.00 | 60.35 | ATOM | 2070 | OE2  | GLU | D 152 | 22.949 | 29.024 | 33.953 | 1.00 | 60.35 | C |
| ATOM                      | 2008 | CA  | SER | D 145 | 11.332 | 33.397 | 27.378 | 1.00 | 22.97 | ATOM                      | 2071 | C   | GLU | D 152 | 21.936 | 24.758 | 30.213 | 1.00 | 23.33 | ATOM | 2071 | C    | GLU | D 152 | 21.936 | 24.758 | 30.213 | 1.00 | 23.33 | C |
| ATOM                      | 2009 | CB  | SER | D 145 | 10.098 | 33.368 | 28.278 | 1.00 | 30.25 | ATOM                      | 2072 | O   | GLU | D 152 | 21.525 | 23.805 | 30.881 | 1.00 | 22.61 | ATOM | 2072 | O    | GLU | D 152 | 21.525 | 23.805 | 30.881 | 1.00 | 22.61 | C |
| ATOM                      | 2010 | OG  | SER | D 145 | 9.754  | 32.023 | 28.610 | 1.00 | 30.24 | ATOM                      | 2073 | N   | LEU | D 153 | 23.168 | 25.128 | 29.065 | 1.00 | 17.99 | ATOM | 2073 | N    | LEU | D 153 | 23.168 | 25.128 | 29.065 | 1.00 | 17.99 | C |
| ATOM                      | 2011 | C   | SER | D 145 | 12.508 | 32.794 | 28.151 | 1.00 | 14.73 | ATOM                      | 2074 | CA  | LEU | D 153 | 20.245 | 24.391 | 28.500 | 1.00 | 17.74 | ATOM | 2074 | CA   | LEU | D 153 | 20.245 | 24.391 | 28.500 | 1.00 | 17.74 | C |
| ATOM                      | 2012 | O   | SER | D 145 | 12.964 | 33.388 | 29.135 | 1.00 | 26.69 | ATOM                      | 2075 | CB  | LEU | D 153 | 19.773 | 25.053 | 27.200 | 1.00 | 21.75 | ATOM | 2075 | CB   | LEU | D 153 | 19.773 | 25.053 | 27.200 | 1.00 | 21.75 | C |
| ATOM                      | 2013 | N   | LEU | D 146 | 12.950 | 31.613 | 27.740 | 1.00 | 30.81 | ATOM                      | 2076 | CG  | LEU | D 153 | 18.636 | 24.313 | 26.482 | 1.00 | 25.67 | ATOM | 2076 | CG   | LEU | D 153 | 18.636 | 24.313 | 26.482 | 1.00 | 25.67 | C |
| ATOM                      | 2014 | CA  | LEU | D 146 | 12.094 | 32.094 | 28.443 | 1.00 | 30.50 | ATOM                      | 2077 | CD1 | LEU | D 153 | 17.423 | 24.220 | 27.380 | 1.00 | 20.18 | ATOM | 2077 | CD1  | LEU | D 153 | 17.423 | 24.220 | 27.380 | 1.00 | 20.18 | C |
| ATOM                      | 2015 | CB  | LEU | D 146 | 14.443 | 29.618 | 27.792 | 1.00 | 31.72 | ATOM                      | 2078 | CD2 | LEU | D 153 | 18.281 | 24.973 | 25.160 | 1.00 | 23.15 | ATOM | 2078 | CD2  | LEU | D 153 | 18.281 | 24.973 | 25.160 | 1.00 | 23.15 | C |
| ATOM                      | 2016 | CG  | LEU | D 146 | 13.838 | 28.354 | 28.383 | 1.00 | 36.61 | ATOM                      | 2079 | C   | LEU | D 153 | 20.635 | 22.946 | 28.237 | 1.00 | 19.84 | ATOM | 2079 | C    | LEU | D 153 | 20.635 | 22.946 | 28.237 | 1.00 | 19.84 | C |
| ATOM                      | 2017 | CD1 | LEU | D 146 | 14.567 | 27.153 | 27.821 | 1.00 | 28.33 | ATOM                      | 2080 | O   | LEU | D 153 | 19.887 | 22.014 | 28.572 | 1.00 | 20.25 | ATOM | 2080 | O    | LEU | D 153 | 19.887 | 22.014 | 28.572 | 1.00 | 20.25 | C |
| ATOM                      | 2018 | CD2 | LEU | D 146 | 13.926 | 28.385 | 29.906 | 1.00 | 30.84 | ATOM                      | 2081 | N   | LEU | D 154 | 21.814 | 22.767 | 27.639 | 1.00 | 20.91 | ATOM | 2081 | N    | LEU | D 154 | 21.814 | 22.767 | 27.639 | 1.00 | 20.91 | C |
| ATOM                      | 2019 | C   | LEU | D 146 | 14.355 | 31.851 | 28.603 | 1.00 | 35.32 | ATOM                      | 2082 | CA  | LEU | D 154 | 22.326 | 21.493 | 27.344 | 1.00 | 22.31 | ATOM | 2082 | CA   | LEU | D 154 | 22.326 | 21.493 | 27.344 | 1.00 | 22.31 | C |
| ATOM                      | 2020 | O   | LEU | D 146 | 15.802 | 31.360 | 27.483 | 1.00 | 40.45 | ATOM                      | 2083 | CB  | LEU | D 154 | 23.618 | 21.938 | 26.624 | 1.00 | 25.59 | ATOM | 2083 | CB   | LEU | D 154 | 23.618 | 21.938 | 26.624 | 1.00 | 25.59 | C |
| ATOM                      | 2021 | N   | ARG | D 147 | 15.938 | 31.950 | 29.689 | 1.00 | 40.42 | ATOM                      | 2084 | CG  | LEU | D 154 | 23.409 | 22.938 | 25.062 | 1.00 | 18.18 | ATOM | 2084 | CG</ |     |       |        |        |        |      |       |   |

| dimer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |      | dimer-PDB-coordinates.txt |      |      |     |     |   |     |        |        |        |      |       |     |
|---------------------------|------|-----|-----|---|-----|--------|--------|--------|------|---------------------------|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|-----|
| ATOM                      | 2230 | CG1 | VAL | D | 173 | 25.248 | 13.759 | 19.585 | 1.00 | 21.61                     | ATOM | 2293 | O   | VAL | D | 181 | 17.411 | 17.679 | 20.498 | 1.00 | 23.16 | O   |
| ATOM                      | 2231 | CG2 | VAL | D | 173 | 26.908 | 11.920 | 19.900 | 1.00 | 21.26                     | ATOM | 2294 | N   | MET | D | 182 | 19.493 | 17.973 | 19.498 | 1.00 | 19.33 | N   |
| ATOM                      | 2232 | C   | VAL | D | 173 | 25.011 | 14.222 | 22.293 | 1.00 | 12.70                     | ATOM | 2295 | CA  | MET | D | 182 | 19.637 | 16.575 | 19.427 | 1.00 | 19.20 | CA  |
| ATOM                      | 2233 | O   | VAL | D | 173 | 22.928 | 13.905 | 22.706 | 1.00 | 13.25                     | ATOM | 2296 | CB  | MET | D | 182 | 20.384 | 16.484 | 18.985 | 1.00 | 20.97 | CB  |
| ATOM                      | 2234 | N   | ARG | D | 174 | 25.172 | 15.491 | 21.172 | 1.00 | 16.99                     | ATOM | 2297 | CG  | MET | D | 182 | 20.170 | 15.219 | 17.342 | 1.00 | 14.66 | CG  |
| ATOM                      | 2235 | CA  | ARG | D | 174 | 24.399 | 16.564 | 21.352 | 1.00 | 19.60                     | ATOM | 2298 | SD  | MET | D | 182 | 21.769 | 14.492 | 16.987 | 1.00 | 16.32 | SD  |
| ATOM                      | 2236 | CB  | ARG | D | 174 | 24.317 | 16.988 | 23.835 | 1.00 | 19.46                     | ATOM | 2299 | CE  | MET | D | 182 | 21.921 | 13.703 | 18.520 | 1.00 | 2.39  | CE  |
| ATOM                      | 2237 | CG  | ARG | D | 174 | 25.561 | 17.700 | 24.361 | 1.00 | 22.05                     | ATOM | 2300 | C   | MET | D | 182 | 20.464 | 16.865 | 20.527 | 1.00 | 17.95 | C   |
| ATOM                      | 2238 | CD  | ARG | D | 174 | 25.570 | 17.611 | 25.801 | 1.00 | 18.71                     | ATOM | 2301 | O   | MET | D | 182 | 21.519 | 16.343 | 20.957 | 1.00 | 15.67 | O   |
| ATOM                      | 2239 | NE  | ARG | D | 174 | 26.322 | 18.983 | 26.349 | 1.00 | 24.12                     | ATOM | 2302 | N   | LEU | D | 183 | 19.941 | 14.733 | 20.988 | 1.00 | 21.84 | N   |
| ATOM                      | 2240 | CZ  | ARG | D | 174 | 26.318 | 19.461 | 27.596 | 1.00 | 28.06                     | ATOM | 2303 | CA  | LEU | D | 183 | 20.680 | 13.932 | 21.955 | 1.00 | 16.83 | CA  |
| ATOM                      | 2241 | NH1 | ARG | D | 174 | 25.612 | 18.670 | 28.547 | 1.00 | 19.96                     | ATOM | 2304 | CB  | LEU | D | 183 | 19.899 | 13.618 | 23.270 | 1.00 | 15.05 | CB  |
| ATOM                      | 2242 | NH2 | ARG | D | 174 | 27.004 | 20.555 | 27.896 | 1.00 | 22.19                     | ATOM | 2305 | CG  | LEU | D | 183 | 19.584 | 15.130 | 24.000 | 1.00 | 12.45 | CG  |
| ATOM                      | 2243 | C   | ARG | D | 174 | 24.713 | 17.758 | 21.459 | 1.00 | 19.40                     | ATOM | 2306 | CD1 | LEU | D | 183 | 18.745 | 14.837 | 25.221 | 1.00 | 15.59 | CD1 |
| ATOM                      | 2244 | O   | ARG | D | 174 | 25.809 | 18.300 | 21.494 | 1.00 | 22.78                     | ATOM | 2307 | CD2 | LEU | D | 183 | 20.843 | 15.877 | 24.386 | 1.00 | 11.58 | CD2 |
| ATOM                      | 2245 | N   | GLU | D | 175 | 23.745 | 18.337 | 20.649 | 1.00 | 20.19                     | ATOM | 2308 | C   | LEU | D | 183 | 20.910 | 12.550 | 21.373 | 1.00 | 18.74 | C   |
| ATOM                      | 2246 | CA  | GLU | D | 175 | 23.577 | 19.237 | 19.675 | 1.00 | 24.43                     | ATOM | 2309 | O   | LEU | D | 183 | 20.026 | 11.995 | 20.729 | 1.00 | 16.90 | O   |
| ATOM                      | 2247 | CB  | GLU | D | 175 | 24.147 | 18.649 | 18.276 | 1.00 | 27.21                     | ATOM | 2310 | N   | GLY | D | 184 | 22.101 | 12.006 | 21.579 | 1.00 | 21.36 | N   |
| ATOM                      | 2248 | CG  | GLU | D | 175 | 25.459 | 17.987 | 17.980 | 1.00 | 34.20                     | ATOM | 2311 | CA  | GLY | D | 184 | 22.390 | 10.628 | 21.204 | 1.00 | 17.26 | CA  |
| ATOM                      | 2249 | CD  | GLU | D | 175 | 25.630 | 17.717 | 16.487 | 1.00 | 40.61                     | ATOM | 2312 | C   | GLY | D | 184 | 22.786 | 9.844  | 22.439 | 1.00 | 15.60 | C   |
| ATOM                      | 2250 | OE1 | GLU | D | 175 | 24.627 | 17.733 | 15.743 | 1.00 | 48.70                     | ATOM | 2313 | O   | GLY | D | 184 | 22.620 | 40.297 | 23.255 | 1.00 | 20.13 | O   |
| ATOM                      | 2251 | OE2 | GLU | D | 175 | 26.772 | 17.501 | 18.055 | 1.00 | 11.35                     | ATOM | 2314 | N   | PHE | D | 185 | 22.178 | 8.672  | 22.609 | 1.00 | 16.24 | N   |
| ATOM                      | 2252 | C   | GLU | D | 175 | 22.815 | 20.217 | 19.602 | 1.00 | 21.47                     | ATOM | 2315 | CA  | PHE | D | 185 | 22.427 | 7.862  | 23.797 | 1.00 | 18.49 | CA  |
| ATOM                      | 2253 | O   | GLU | D | 175 | 21.649 | 19.819 | 19.704 | 1.00 | 20.68                     | ATOM | 2316 | CB  | PHE | D | 185 | 21.105 | 7.308  | 24.332 | 1.00 | 19.41 | CB  |
| ATOM                      | 2254 | N   | LEU | D | 176 | 23.135 | 21.490 | 19.384 | 1.00 | 21.14                     | ATOM | 2317 | CG  | PHE | D | 185 | 22.136 | 6.392  | 24.708 | 1.00 | 12.95 | CG  |
| ATOM                      | 2255 | CA  | LEU | D | 176 | 22.127 | 22.890 | 19.087 | 1.00 | 22.34                     | ATOM | 2318 | CD1 | PHE | D | 185 | 20.151 | 6.830  | 25.982 | 1.00 | 15.71 | CD1 |
| ATOM                      | 2256 | CB  | LEU | D | 176 | 22.623 | 23.853 | 19.519 | 1.00 | 17.07                     | ATOM | 2319 | CD2 | PHE | D | 185 | 19.297 | 9.959  | 26.324 | 1.00 | 18.58 | CD2 |
| ATOM                      | 2257 | CG  | LEU | D | 176 | 22.945 | 23.890 | 24.013 | 1.00 | 27.39                     | ATOM | 2320 | CZ  | PHE | D | 185 | 18.429 | 30.476 | 25.382 | 1.00 | 17.63 | CZ  |
| ATOM                      | 2258 | CD1 | LEU | D | 176 | 23.811 | 25.090 | 21.341 | 1.00 | 35.49                     | ATOM | 2321 | CE2 | PHE | D | 185 | 18.409 | 9.952  | 24.099 | 1.00 | 18.61 | CE2 |
| ATOM                      | 2259 | CD2 | LEU | D | 176 | 21.671 | 23.910 | 22.837 | 1.00 | 24.05                     | ATOM | 2322 | CD3 | PHE | D | 185 | 19.271 | 8.929  | 23.763 | 1.00 | 16.19 | CD3 |
| ATOM                      | 2260 | C   | LEU | D | 176 | 21.809 | 22.494 | 17.592 | 1.00 | 30.45                     | ATOM | 2323 | CD4 | PHE | D | 185 | 22.464 | 6.768  | 23.576 | 1.00 | 23.49 | CD4 |
| ATOM                      | 2261 | O   | LEU | D | 176 | 17.682 | 21.176 | 18.623 | 1.00 | 19.18                     | ATOM | 2324 | O   | PHE | D | 185 | 23.638 | 6.261  | 22.486 | 1.00 | 15.36 | O   |
| ATOM                      | 2262 | N   | LEU | D | 177 | 20.544 | 27.178 | 17.281 | 1.00 | 28.02                     | ATOM | 2325 | N   | ALA | D | 186 | 24.177 | 6.442  | 24.646 | 1.00 | 29.17 | N   |
| ATOM                      | 2263 | CA  | LEU | D | 177 | 20.084 | 22.315 | 15.878 | 1.00 | 31.86                     | ATOM | 2326 | CA  | ALA | D | 186 | 25.220 | 5.429  | 24.602 | 1.00 | 30.50 | CA  |
| ATOM                      | 2264 | CB  | LEU | D | 177 | 19.431 | 21.022 | 15.404 | 1.00 | 27.04                     | ATOM | 2327 | CB  | ALA | D | 186 | 25.972 | 5.384  | 25.936 | 1.00 | 24.38 | CB  |
| ATOM                      | 2265 | CG  | LEU | D | 177 | 20.332 | 19.914 | 14.861 | 1.00 | 35.05                     | ATOM | 2328 | O   | ALA | D | 186 | 24.633 | 4.671  | 24.274 | 1.00 | 26.07 | O   |
| ATOM                      | 2266 | CD1 | LEU | D | 177 | 11.548 | 19.786 | 15.671 | 1.00 | 31.20                     | ATOM | 2329 | C   | ALA | D | 186 | 23.215 | 3.111  | 25.712 | 1.00 | 28.61 | C   |
| ATOM                      | 2267 | CD2 | LEU | D | 177 | 14.865 | 18.665 | 18.363 | 1.00 | 36.20                     | ATOM | 2330 | N   | ARG | D | 187 | 23.470 | 3.769  | 24.829 | 1.00 | 29.77 | N   |
| ATOM                      | 2268 | C   | LEU | D | 177 | 19.068 | 23.450 | 15.838 | 1.00 | 31.77                     | ATOM | 2331 | CA  | ARG | D | 187 | 23.946 | 2.417  | 24.739 | 1.00 | 31.96 | CA  |
| ATOM                      | 2269 | O   | LEU | D | 177 | 15.644 | 23.966 | 16.695 | 1.00 | 29.67                     | ATOM | 2332 | CB  | ARG | D | 187 | 22.746 | 1.826  | 26.139 | 1.00 | 31.09 | CB  |
| ATOM                      | 2270 | N   | PRO | D | 178 | 18.667 | 23.857 | 14.623 | 1.00 | 43.26                     | ATOM | 2333 | CG  | ARG | D | 187 | 24.069 | 1.450  | 26.325 | 1.00 | 55.38 | CG  |
| ATOM                      | 2271 | CA  | PRO | D | 178 | 17.701 | 24.961 | 14.518 | 1.00 | 40.02                     | ATOM | 2334 | CD  | ARG | D | 187 | 23.084 | 0.181  | 27.512 | 1.00 | 32.49 | CD  |
| ATOM                      | 2272 | O   | PRO | D | 178 | 17.440 | 25.052 | 14.010 | 1.00 | 45.05                     | ATOM | 2335 | CE  | ARG | D | 187 | 23.997 | 0.344  | 28.959 | 1.00 | 31.60 | CE  |
| ATOM                      | 2273 | CG  | PRO | D | 178 | 18.713 | 24.525 | 12.380 | 1.00 | 49.82                     | ATOM | 2336 | NZ  | ARG | D | 187 | 25.000 | 0.770  | 29.723 | 1.00 | 36.15 | NZ  |
| ATOM                      | 2274 | CD  | PRO | D | 178 | 19.157 | 23.411 | 11.303 | 1.00 | 38.70                     | ATOM | 2337 | NH1 | ARG | D | 187 | 26.180 | 1.056  | 29.172 | 1.00 | 33.19 | NH1 |
| ATOM                      | 2275 | C   | PRO | D | 178 | 16.411 | 24.663 | 15.284 | 1.00 | 32.94                     | ATOM | 2338 | NH2 | ARG | D | 187 | 24.830 | 0.896  | 31.040 | 1.00 | 66.40 | NH2 |
| ATOM                      | 2276 | O   | PRO | D | 178 | 15.684 | 23.723 | 14.944 | 1.00 | 33.48                     | ATOM | 2339 | C   | ARG | D | 187 | 21.678 | 2.283  | 29.902 | 1.00 | 35.19 | C   |
| ATOM                      | 2277 | N   | GLY | D | 179 | 16.156 | 25.442 | 16.393 | 1.00 | 33.78                     | ATOM | 2340 | CA  | ARG | D | 187 | 20.838 | 3.188  | 29.856 | 1.00 | 32.95 | CA  |
| ATOM                      | 2278 | CB  | GLY | D | 179 | 14.975 | 25.247 | 15.479 | 1.00 | 17.00                     | ATOM | 2341 | N   | ASP | D | 188 | 21.536 | 1.125  | 23.259 | 1.00 | 41.41 | N   |
| ATOM                      | 2279 | C   | GLY | D | 179 | 14.862 | 23.902 | 17.871 | 1.00 | 44.04                     | ATOM | 2342 | CA  | ASP | D | 188 | 20.421 | 0.810  | 27.397 | 1.00 | 35.02 | CA  |
| ATOM                      | 2280 | O   | GLY | D | 179 | 13.767 | 23.503 | 18.273 | 1.00 | 39.78                     | ATOM | 2343 | CB  | ASP | D | 188 | 20.646 | -0.541 | 21.712 | 1.00 | 42.22 | CB  |
| ATOM                      | 2281 | N   | SER | D | 180 | 15.973 | 23.193 | 18.049 | 1.00 | 33.86                     | ATOM | 2344 | CG  | ASP | D | 188 | 21.795 | -0.509 | 20.718 | 1.00 | 35.81 | CG  |
| ATOM                      | 2282 | CA  | SER | D | 180 | 15.864 | 21.922 | 18.754 | 1.00 | 28.31                     | ATOM | 2345 | CD1 | ASP | D | 188 | 21.886 | 0.467  | 19.940 | 1.00 | 50.46 | CD1 |
| ATOM                      | 2283 | CD2 | SER | D | 180 | 15.340 | 20.837 | 18.829 | 1.00 | 28.00                     | ATOM | 2346 | CD2 | ASP | D | 188 | 21.604 | -1.462 | 20.718 | 1.00 | 36.62 | CD2 |
| ATOM                      | 2284 | OG  | SER | D | 180 | 16.347 | 20.890 | 16.922 | 1.00 | 19.18                     | ATOM | 2347 | C   | ASP | D | 188 | 19.130 | 0.745  | 23.197 | 1.00 | 32.16 | C   |
| ATOM                      | 2285 | C   | SER | D | 180 | 17.199 | 21.459 | 13.354 | 1.00 | 31.00                     | ATOM | 2348 | O   | ASP | D | 188 | 19.124 | 0.286  | 24.339 | 1.00 | 31.16 | O   |
| ATOM                      | 2286 | O   | SER | D | 180 | 18.268 | 21.993 | 19.050 | 1.00 | 24.66                     | ATOM | 2349 | N   | GLY | D | 189 | 18.046 | 1.200  | 22.579 | 1.00 | 26.72 | N   |
| ATOM                      | 2287 | N   | VAL | D | 181 | 17.116 | 20.453 | 20.214 | 1.00 | 25.76                     | ATOM | 2350 | CA  | GLY | D | 189 | 16.727 | 1.113  | 23.161 | 1.00 | 26.83 | CA  |
| ATOM                      | 2288 | CA  | VAL | D | 181 | 18.333 | 19.862 | 20.737 | 1.00 | 22.14                     | ATOM | 2351 | C   | GLY | D | 189 | 16.268 | 2.358  | 23.504 | 1.00 | 29.89 | C   |
| ATOM                      | 2289 | CB  | VAL | D | 181 | 18.435 | 19.985 | 22.254 | 1.00 | 17.00                     | ATOM | 2352 | O   | GLY | D | 189 | 17.058 | 1.880  | 24.323 | 1.00 | 28.41 | O   |
| ATOM                      | 2290 | CG1 | VAL | D | 181 | 19.399 | 19.076 | 21.795 | 1.00 | 16.47                     | ATOM | 2353 | N   | VAL | D | 190 | 17.215 | 3.158  | 24.395 | 1.00 | 19.67 | N   |
| ATOM                      | 2291 | CG2 | VAL | D | 181 | 18.691 | 21.424 | 21.648 | 1.00 | 22.23                     | ATOM | 2354 | CA  | VAL | D | 190 | 16.892 | 4.332  | 25.193 | 1.00 | 21.67 | CA  |
| ATOM                      | 2292 | C   | VAL | D | 181 | 18.371 | 18.404 | 20.322 | 1.00 |                           |      |      |     |     |   |     |        |        |        |      |       |     |

|                           |      |     |     |   |     |        |        |        |            |                           |      |      |     |     |   |     |        |        |        |            |   |      |      |     |     |   |     |        |        |        |            |   |
|---------------------------|------|-----|-----|---|-----|--------|--------|--------|------------|---------------------------|------|------|-----|-----|---|-----|--------|--------|--------|------------|---|------|------|-----|-----|---|-----|--------|--------|--------|------------|---|
| dimer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |            | dimer-PDB-coordinates.txt |      |      |     |     |   |     |        |        |        |            |   |      |      |     |     |   |     |        |        |        |            |   |
| ATOM                      | 2482 | OE1 | GLN | D | 207 | 8.933  | 29.600 | 30.790 | 1.00 24.98 | O                         | ATOM | 2545 | CD  | PRO | D | 215 | 10.684 | 10.545 | 16.335 | 1.00 36.48 | C | ATOM | 2545 | CD  | PRO | D | 215 | 10.684 | 10.545 | 16.335 | 1.00 36.48 | C |
| ATOM                      | 2483 | NE2 | GLN | D | 207 | 10.932 | 30.604 | 31.002 | 1.00 21.40 | N                         | ATOM | 2546 | C   | PRO | D | 215 | 13.925 | 11.846 | 15.526 | 1.00 34.99 | C | ATOM | 2546 | C   | PRO | D | 215 | 13.925 | 11.846 | 15.526 | 1.00 34.99 | C |
| ATOM                      | 2484 | C   | GLN | D | 207 | 9.887  | 25.714 | 31.311 | 1.00 26.12 | C                         | ATOM | 2547 | O   | PRO | D | 215 | 13.357 | 12.812 | 15.009 | 1.00 33.30 | C | ATOM | 2547 | O   | PRO | D | 215 | 13.357 | 12.812 | 15.009 | 1.00 33.30 | C |
| ATOM                      | 2485 | O   | GLN | D | 207 | 10.942 | 25.060 | 34.396 | 1.00 17.95 | C                         | ATOM | 2548 | N   | TYR | D | 216 | 15.230 | 11.120 | 15.403 | 1.00 32.28 | C | ATOM | 2548 | N   | TYR | D | 216 | 15.230 | 11.120 | 15.403 | 1.00 32.28 | C |
| ATOM                      | 2486 | N   | GLN | D | 208 | 8.678  | 25.163 | 34.176 | 1.00 21.84 | N                         | ATOM | 2549 | CA  | TYR | D | 216 | 16.077 | 11.982 | 14.582 | 1.00 41.66 | C | ATOM | 2549 | CA  | TYR | D | 216 | 16.077 | 11.982 | 14.582 | 1.00 41.66 | C |
| ATOM                      | 2487 | CA  | GLN | D | 208 | 8.495  | 23.732 | 33.983 | 1.00 22.60 | C                         | ATOM | 2550 | CB  | TYR | D | 216 | 17.484 | 12.080 | 15.177 | 1.00 40.16 | C | ATOM | 2550 | CB  | TYR | D | 216 | 17.484 | 12.080 | 15.177 | 1.00 40.16 | C |
| ATOM                      | 2488 | CB  | GLN | D | 208 | 7.504  | 23.167 | 34.975 | 1.00 23.33 | C                         | ATOM | 2551 | CG  | TYR | D | 216 | 18.363 | 13.066 | 14.469 | 1.00 47.15 | C | ATOM | 2551 | CG  | TYR | D | 216 | 18.363 | 13.066 | 14.469 | 1.00 47.15 | C |
| ATOM                      | 2489 | CG  | GLN | D | 208 | 7.550  | 23.811 | 36.317 | 1.00 18.38 | C                         | ATOM | 2552 | CD1 | TYR | D | 216 | 17.968 | 12.147 | 15.740 | 1.00 39.99 | C | ATOM | 2552 | CD1 | TYR | D | 216 | 17.968 | 12.147 | 15.740 | 1.00 39.99 | C |
| ATOM                      | 2490 | CD  | GLN | D | 208 | 8.423  | 23.063 | 37.258 | 1.00 46.79 | C                         | ATOM | 2553 | CE1 | TYR | D | 216 | 18.788 | 15.282 | 13.593 | 1.00 53.72 | C | ATOM | 2553 | CE1 | TYR | D | 216 | 18.788 | 15.282 | 13.593 | 1.00 53.72 | C |
| ATOM                      | 2491 | OE1 | GLN | D | 208 | 9.091  | 22.106 | 36.863 | 1.00 60.57 | C                         | ATOM | 2554 | C2  | TYR | D | 216 | 20.047 | 14.889 | 13.177 | 1.00 60.12 | C | ATOM | 2554 | C2  | TYR | D | 216 | 20.047 | 14.889 | 13.177 | 1.00 60.12 | C |
| ATOM                      | 2492 | NE2 | GLN | D | 208 | 8.430  | 23.478 | 38.517 | 1.00 46.74 | C                         | ATOM | 2555 | CE2 | TYR | D | 216 | 20.867 | 15.791 | 12.530 | 1.00 58.77 | C | ATOM | 2555 | CE2 | TYR | D | 216 | 20.867 | 15.791 | 12.530 | 1.00 58.77 | C |
| ATOM                      | 2493 | C   | GLN | D | 208 | 7.919  | 23.584 | 32.601 | 1.00 18.56 | N                         | ATOM | 2556 | CH  | TYR | D | 216 | 20.466 | 13.597 | 13.338 | 1.00 55.92 | C | ATOM | 2556 | CH  | TYR | D | 216 | 20.466 | 13.597 | 13.338 | 1.00 55.92 | C |
| ATOM                      | 2494 | O   | GLN | D | 208 | 6.760  | 23.906 | 32.367 | 1.00 21.12 | C                         | ATOM | 2557 | CD2 | TYR | D | 216 | 19.654 | 12.444 | 14.904 | 1.00 41.14 | C | ATOM | 2557 | CD2 | TYR | D | 216 | 19.654 | 12.444 | 14.904 | 1.00 41.14 | C |
| ATOM                      | 2495 | N   | VAL | D | 209 | 8.729  | 23.075 | 31.686 | 1.00 21.66 | N                         | ATOM | 2558 | O   | TYR | D | 216 | 16.167 | 14.553 | 13.159 | 1.00 30.36 | C | ATOM | 2558 | O   | TYR | D | 216 | 16.167 | 14.553 | 13.159 | 1.00 30.36 | C |
| ATOM                      | 2496 | CA  | VAL | D | 209 | 8.421  | 23.196 | 30.268 | 1.00 16.03 | C                         | ATOM | 2559 | C   | TYR | D | 216 | 16.533 | 10.303 | 12.956 | 1.00 40.04 | C | ATOM | 2559 | C   | TYR | D | 216 | 16.533 | 10.303 | 12.956 | 1.00 40.04 | C |
| ATOM                      | 2497 | CB  | VAL | D | 209 | 9.672  | 23.703 | 29.522 | 1.00 23.36 | C                         | ATOM | 2560 | O   | GLY | E | 124 | 55.117 | 12.055 | 38.367 | 1.00 38.64 | C | ATOM | 2560 | O   | GLY | E | 124 | 55.117 | 12.055 | 38.367 | 1.00 38.64 | C |
| ATOM                      | 2498 | CG1 | VAL | D | 209 | 9.363  | 23.923 | 28.045 | 1.00 23.23 | C                         | ATOM | 2561 | N   | GLY | E | 134 | 55.272 | 11.936 | 41.391 | 1.00 44.25 | C | ATOM | 2561 | N   | GLY | E | 134 | 55.272 | 11.936 | 41.391 | 1.00 44.25 | C |
| ATOM                      | 2499 | CG2 | VAL | D | 209 | 10.179 | 24.977 | 30.171 | 1.00 15.63 | C                         | ATOM | 2562 | C   | GLY | E | 134 | 54.468 | 11.923 | 40.648 | 1.00 42.19 | C | ATOM | 2562 | C   | GLY | E | 134 | 54.468 | 11.923 | 40.648 | 1.00 42.19 | C |
| ATOM                      | 2500 | C   | VAL | D | 209 | 8.002  | 21.877 | 29.659 | 1.00 19.19 | C                         | ATOM | 2563 | CA  | ARG | E | 135 | 52.202 | 12.943 | 39.177 | 1.00 38.48 | C | ATOM | 2563 | CA  | ARG | E | 135 | 52.202 | 12.943 | 39.177 | 1.00 38.48 | C |
| ATOM                      | 2501 | O   | VAL | D | 209 | 8.692  | 20.689 | 29.792 | 1.00 24.39 | C                         | ATOM | 2564 | N   | ARG | E | 135 | 52.944 | 12.956 | 38.821 | 1.00 26.82 | C | ATOM | 2564 | N   | ARG | E | 135 | 52.944 | 12.956 | 38.821 | 1.00 26.82 | C |
| ATOM                      | 2502 | N   | PRO | D | 210 | 6.854  | 21.873 | 28.983 | 1.00 23.97 | N                         | ATOM | 2565 | CA  | ARG | E | 135 | 52.578 | 12.583 | 37.430 | 1.00 31.79 | C | ATOM | 2565 | CA  | ARG | E | 135 | 52.578 | 12.583 | 37.430 | 1.00 31.79 | C |
| ATOM                      | 2503 | CA  | PRO | D | 210 | 6.433  | 20.663 | 28.261 | 1.00 24.19 | C                         | ATOM | 2566 | C8  | ARG | E | 135 | 51.407 | 11.687 | 37.031 | 1.00 25.83 | C | ATOM | 2566 | C8  | ARG | E | 135 | 51.407 | 11.687 | 37.031 | 1.00 25.83 | C |
| ATOM                      | 2504 | CB  | PRO | D | 210 | 4.959  | 20.931 | 27.969 | 1.00 22.38 | C                         | ATOM | 2567 | CG  | ARG | E | 135 | 51.727 | 10.212 | 37.110 | 1.00 28.30 | C | ATOM | 2567 | CG  | ARG | E | 135 | 51.727 | 10.212 | 37.110 | 1.00 28.30 | C |
| ATOM                      | 2505 | CG  | PRO | D | 210 | 4.855  | 22.445 | 27.889 | 1.00 24.55 | C                         | ATOM | 2568 | C1  | ARG | E | 135 | 51.080 | 9.901  | 36.884 | 1.00 27.05 | C | ATOM | 2568 | C1  | ARG | E | 135 | 51.080 | 9.901  | 36.884 | 1.00 27.05 | C |
| ATOM                      | 2506 | CD  | PRO | D | 210 | 5.906  | 22.997 | 28.827 | 1.00 20.96 | C                         | ATOM | 2569 | NE  | ARG | E | 135 | 50.243 | 8.367  | 36.481 | 1.00 52.74 | C | ATOM | 2569 | NE  | ARG | E | 135 | 50.243 | 8.367  | 36.481 | 1.00 52.74 | C |
| ATOM                      | 2507 | C   | PRO | D | 210 | 7.235  | 20.517 | 28.656 | 1.00 25.51 | C                         | ATOM | 2570 | C2  | ARG | E | 135 | 48.944 | 8.483  | 36.727 | 1.00 66.06 | C | ATOM | 2570 | C2  | ARG | E | 135 | 48.944 | 8.483  | 36.727 | 1.00 66.06 | C |
| ATOM                      | 2508 | O   | PRO | D | 210 | 7.195  | 21.389 | 26.099 | 1.00 25.65 | C                         | ATOM | 2571 | NH1 | ARG | E | 135 | 48.322 | 9.635  | 36.511 | 1.00 52.96 | C | ATOM | 2571 | NH1 | ARG | E | 135 | 48.322 | 9.635  | 36.511 | 1.00 52.96 | C |
| ATOM                      | 2509 | N   | LEU | D | 211 | 7.985  | 19.423 | 26.839 | 1.00 21.47 | N                         | ATOM | 2572 | NH2 | ARG | E | 135 | 48.259 | 7.443  | 37.183 | 1.00 53.17 | C | ATOM | 2572 | NH2 | ARG | E | 135 | 48.259 | 7.443  | 37.183 | 1.00 53.17 | C |
| ATOM                      | 2510 | CA  | LEU | D | 211 | 8.873  | 19.203 | 25.714 | 1.00 21.26 | C                         | ATOM | 2573 | O   | ARG | E | 135 | 52.221 | 14.036 | 37.164 | 1.00 22.67 | C | ATOM | 2573 | O   | ARG | E | 135 | 52.221 | 14.036 | 37.164 | 1.00 22.67 | C |
| ATOM                      | 2511 | CB  | LEU | D | 211 | 10.321 | 19.067 | 26.182 | 1.00 16.16 | C                         | ATOM | 2574 | C   | ARG | E | 135 | 52.700 | 13.387 | 36.130 | 1.00 31.57 | C | ATOM | 2574 | C   | ARG | E | 135 | 52.700 | 13.387 | 36.130 | 1.00 31.57 | C |
| ATOM                      | 2512 | CG  | LEU | D | 211 | 10.996 | 20.267 | 26.842 | 1.00 20.07 | C                         | ATOM | 2575 | N   | ARG | E | 136 | 52.499 | 14.900 | 38.131 | 1.00 19.70 | C | ATOM | 2575 | N   | ARG | E | 136 | 52.499 | 14.900 | 38.131 | 1.00 19.70 | C |
| ATOM                      | 2513 | CD1 | LEU | D | 211 | 12.411 | 19.910 | 27.275 | 1.00 20.71 | C                         | ATOM | 2576 | CA  | ARG | E | 136 | 52.032 | 16.279 | 38.066 | 1.00 20.85 | C | ATOM | 2576 | CA  | ARG | E | 136 | 52.032 | 16.279 | 38.066 | 1.00 20.85 | C |
| ATOM                      | 2514 | CD2 | LEU | D | 211 | 11.023 | 21.462 | 25.895 | 1.00 20.79 | C                         | ATOM | 2577 | CB  | ARG | E | 136 | 52.108 | 16.582 | 39.242 | 1.00 21.79 | C | ATOM | 2577 | CB  | ARG | E | 136 | 52.108 | 16.582 | 39.242 | 1.00 21.79 | C |
| ATOM                      | 2515 | C   | LEU | D | 211 | 8.468  | 17.329 | 25.010 | 1.00 23.75 | C                         | ATOM | 2578 | CG  | ARG | E | 136 | 49.904 | 15.668 | 39.500 | 1.00 26.96 | C | ATOM | 2578 | CG  | ARG | E | 136 | 49.904 | 15.668 | 39.500 | 1.00 26.96 | C |
| ATOM                      | 2516 | O   | LEU | D | 211 | 7.893  | 17.015 | 25.626 | 1.00 20.94 | C                         | ATOM | 2579 | CD  | ARG | E | 136 | 46.846 | 14.854 | 39.413 | 1.00 23.14 | C | ATOM | 2579 | CD  | ARG | E | 136 | 46.846 | 14.854 | 39.413 | 1.00 23.14 | C |
| ATOM                      | 2517 | N   | ARG | D | 212 | 8.779  | 17.876 | 23.718 | 1.00 23.29 | N                         | ATOM | 2580 | NE  | ARG | E | 136 | 47.802 | 15.184 | 40.416 | 1.00 37.89 | C | ATOM | 2580 | NE  | ARG | E | 136 | 47.802 | 15.184 | 40.416 | 1.00 37.89 | C |
| ATOM</                    |      |     |     |   |     |        |        |        |            |                           |      |      |     |     |   |     |        |        |        |            |   |      |      |     |     |   |     |        |        |        |            |   |

| dimer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |      | dimer-PDB-coordinates.txt |   |      |      |     |     |   |     |        |        |        |      |       |   |
|---------------------------|------|-----|-----|---|-----|--------|--------|--------|------|---------------------------|---|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM                      | 2234 | CB  | LYS | E | 156 | 47.893 | 27.648 | 24.417 | 1.00 | 25.06                     | C | ATOM | 2797 | CE  | LYS | E | 163 | 51.865 | 19.649 | 16.728 | 1.00 | 41.43 | C |
| ATOM                      | 2235 | CG  | LYS | E | 156 | 46.892 | 28.593 | 23.783 | 1.00 | 34.17                     | C | ATOM | 2798 | NZ  | LYS | E | 163 | 50.488 | 19.545 | 15.289 | 1.00 | 40.28 | C |
| ATOM                      | 2236 | CD  | LYS | E | 156 | 46.802 | 28.408 | 22.299 | 1.00 | 36.36                     | C | ATOM | 2799 | C   | LYS | E | 163 | 54.438 | 15.769 | 22.900 | 1.00 | 23.09 | C |
| ATOM                      | 2237 | CE  | LYS | E | 156 | 45.981 | 29.333 | 21.688 | 1.00 | 38.93                     | C | ATOM | 2800 | O   | LYS | E | 163 | 55.292 | 16.236 | 23.652 | 1.00 | 21.98 | C |
| ATOM                      | 2238 | NZ  | LYS | E | 156 | 45.792 | 29.307 | 20.233 | 1.00 | 36.42                     | N | ATOM | 2801 | N   | THR | E | 164 | 54.521 | 14.557 | 21.375 | 1.00 | 23.46 | C |
| ATOM                      | 2239 | C   | LYS | E | 156 | 48.536 | 25.388 | 25.182 | 1.00 | 26.96                     | C | ATOM | 2802 | CA  | THR | E | 164 | 55.709 | 13.735 | 22.539 | 1.00 | 28.84 | C |
| ATOM                      | 2240 | O   | LYS | E | 156 | 49.435 | 24.779 | 24.561 | 1.00 | 26.94                     | C | ATOM | 2803 | CB  | THR | E | 164 | 55.379 | 12.418 | 21.743 | 1.00 | 38.36 | C |
| ATOM                      | 2241 | N   | LEU | E | 157 | 48.442 | 25.368 | 26.518 | 1.00 | 18.82                     | N | ATOM | 2804 | CG1 | THR | E | 164 | 54.530 | 11.590 | 22.356 | 1.00 | 39.97 | C |
| ATOM                      | 2242 | CA  | LEU | E | 157 | 49.413 | 24.636 | 27.302 | 1.00 | 17.61                     | C | ATOM | 2805 | CG2 | THR | E | 164 | 56.906 | 11.664 | 21.730 | 1.00 | 38.37 | C |
| ATOM                      | 2243 | CB  | LEU | E | 157 | 49.309 | 24.978 | 26.788 | 1.00 | 16.25                     | C | ATOM | 2806 | C   | THR | E | 164 | 56.968 | 14.491 | 22.103 | 1.00 | 19.16 | C |
| ATOM                      | 2244 | CG  | LEU | E | 157 | 49.745 | 26.406 | 29.133 | 1.00 | 24.16                     | C | ATOM | 2807 | O   | THR | E | 164 | 58.000 | 14.453 | 22.796 | 1.00 | 24.06 | C |
| ATOM                      | 2245 | CD1 | LEU | E | 157 | 49.394 | 26.733 | 30.573 | 1.00 | 20.38                     | C | ATOM | 2808 | N   | ARG | E | 165 | 56.891 | 15.201 | 20.984 | 1.00 | 25.73 | C |
| ATOM                      | 2246 | CD2 | LEU | E | 157 | 51.249 | 26.591 | 28.877 | 1.00 | 17.59                     | C | ATOM | 2809 | CA  | ARG | E | 165 | 58.081 | 15.881 | 20.478 | 1.00 | 23.18 | C |
| ATOM                      | 2247 | C   | LEU | E | 157 | 49.747 | 23.138 | 27.069 | 1.00 | 17.52                     | C | ATOM | 2810 | CB  | ARG | E | 165 | 57.887 | 16.366 | 19.038 | 1.00 | 32.12 | C |
| ATOM                      | 2248 | O   | LEU | E | 157 | 50.227 | 22.466 | 26.961 | 1.00 | 17.10                     | O | ATOM | 2811 | CG  | ARG | E | 165 | 56.911 | 17.517 | 18.856 | 1.00 | 36.70 | C |
| ATOM                      | 2249 | N   | LEU | E | 158 | 48.005 | 22.686 | 16.979 | 1.00 | 17.54                     | N | ATOM | 2812 | CD  | ARG | E | 165 | 57.050 | 18.075 | 17.444 | 1.00 | 47.43 | C |
| ATOM                      | 2250 | CA  | GLU | E | 158 | 47.746 | 21.271 | 26.795 | 1.00 | 23.60                     | C | ATOM | 2813 | NE  | ARG | E | 165 | 55.800 | 18.602 | 16.906 | 1.00 | 56.64 | C |
| ATOM                      | 2251 | CB  | GLU | E | 158 | 46.266 | 20.936 | 27.065 | 1.00 | 20.75                     | C | ATOM | 2814 | CZ  | ARG | E | 165 | 55.444 | 19.882 | 16.961 | 1.00 | 73.51 | C |
| ATOM                      | 2252 | CG  | GLU | E | 158 | 45.963 | 19.475 | 26.750 | 1.00 | 25.90                     | C | ATOM | 2815 | NH1 | ARG | E | 165 | 56.240 | 20.778 | 17.344 | 1.00 | 64.88 | C |
| ATOM                      | 2253 | CD  | GLU | E | 158 | 44.625 | 19.038 | 27.324 | 1.00 | 38.04                     | C | ATOM | 2816 | NH2 | ARG | E | 165 | 54.248 | 20.269 | 16.434 | 1.00 | 64.07 | C |
| ATOM                      | 2254 | CE1 | GLU | E | 158 | 45.436 | 17.824 | 27.304 | 1.00 | 36.15                     | C | ATOM | 2817 | C   | ARG | E | 165 | 58.396 | 17.010 | 21.275 | 1.00 | 26.02 | C |
| ATOM                      | 2255 | CE2 | GLU | E | 158 | 43.850 | 19.907 | 27.799 | 1.00 | 35.76                     | C | ATOM | 2818 | O   | ARG | E | 165 | 59.731 | 17.444 | 21.216 | 1.00 | 30.09 | C |
| ATOM                      | 2256 | C   | GLU | E | 158 | 48.213 | 20.818 | 25.422 | 1.00 | 25.61                     | C | ATOM | 2819 | N   | ASN | E | 166 | 57.772 | 17.494 | 22.301 | 1.00 | 22.30 | C |
| ATOM                      | 2257 | O   | GLU | E | 158 | 48.694 | 19.701 | 25.270 | 1.00 | 29.14                     | O | ATOM | 2820 | CA  | ASN | E | 166 | 58.227 | 16.304 | 23.250 | 1.00 | 19.17 | C |
| ATOM                      | 2258 | N   | ILE | E | 159 | 48.076 | 21.693 | 24.428 | 1.00 | 23.65                     | N | ATOM | 2821 | CB  | ASN | E | 166 | 57.131 | 19.541 | 23.115 | 1.00 | 19.95 | C |
| ATOM                      | 2259 | CA  | ILE | E | 159 | 48.573 | 21.391 | 23.099 | 1.00 | 25.90                     | C | ATOM | 2822 | CG  | ASN | E | 166 | 56.847 | 20.443 | 22.333 | 1.00 | 22.10 | C |
| ATOM                      | 2260 | CB  | ILE | E | 159 | 48.126 | 22.435 | 22.059 | 1.00 | 26.57                     | C | ATOM | 2823 | CD1 | ASN | E | 166 | 57.800 | 20.736 | 21.522 | 1.00 | 28.34 | C |
| ATOM                      | 2261 | CG1 | ILE | E | 159 | 46.646 | 22.256 | 21.733 | 1.00 | 35.24                     | C | ATOM | 2824 | ND2 | ASN | E | 166 | 51.650 | 20.892 | 22.172 | 1.00 | 19.75 | C |
| ATOM                      | 2262 | CD1 | ILE | E | 159 | 46.156 | 23.239 | 20.726 | 1.00 | 28.86                     | C | ATOM | 2825 | C   | ASN | E | 166 | 58.634 | 17.875 | 24.574 | 1.00 | 23.62 | C |
| ATOM                      | 2263 | CG2 | ILE | E | 159 | 48.307 | 22.291 | 20.771 | 1.00 | 27.79                     | C | ATOM | 2826 | O   | ASN | E | 166 | 58.957 | 18.578 | 25.520 | 1.00 | 26.09 | C |
| ATOM                      | 2264 | C   | ILE | E | 159 | 50.989 | 22.082 | 23.111 | 1.00 | 30.23                     | C | ATOM | 2827 | N   | VAL | E | 167 | 58.603 | 16.544 | 24.636 | 1.00 | 22.98 | C |
| ATOM                      | 2265 | O   | ILE | E | 159 | 50.853 | 20.688 | 22.968 | 1.00 | 36.41                     | C | ATOM | 2828 | CA  | GLY | E | 167 | 56.910 | 15.825 | 25.485 | 1.00 | 26.37 | C |
| ATOM                      | 2266 | N   | PHE | E | 160 | 50.780 | 22.250 | 23.724 | 1.00 | 25.32                     | N | ATOM | 2829 | C   | GLY | E | 167 | 57.724 | 15.499 | 26.666 | 1.00 | 22.29 | C |
| ATOM                      | 2267 | CA  | PHE | E | 160 | 52.236 | 22.209 | 23.743 | 1.00 | 17.58                     | C | ATOM | 2830 | O   | GLY | E | 167 | 57.817 | 14.926 | 27.745 | 1.00 | 24.38 | C |
| ATOM                      | 2268 | CB  | PHE | E | 160 | 52.817 | 23.506 | 24.290 | 1.00 | 15.64                     | C | ATOM | 2831 | N   | GLY | E | 168 | 56.560 | 15.858 | 26.148 | 1.00 | 20.75 | C |
| ATOM                      | 2269 | CG  | PHE | E | 160 | 54.107 | 23.567 | 24.214 | 1.00 | 20.74                     | C | ATOM | 2832 | CA  | GLY | E | 168 | 55.336 | 15.716 | 26.903 | 1.00 | 17.79 | C |
| ATOM                      | 2270 | CD  | PHE | E | 160 | 52.084 | 23.074 | 24.314 | 1.00 | 18.72                     | C | ATOM | 2833 | C   | GLY | E | 168 | 54.390 | 14.424 | 26.328 | 1.00 | 20.86 | C |
| ATOM                      | 2271 | CE1 | PHE | E | 160 | 56.470 | 23.109 | 25.183 | 1.00 | 16.65                     | C | ATOM | 2834 | O   | GLY | E | 168 | 55.191 | 13.399 | 26.338 | 1.00 | 21.99 | C |
| ATOM                      | 2272 | CE2 | PHE | E | 160 | 57.095 | 23.670 | 24.074 | 1.00 | 19.15                     | C | ATOM | 2835 | N   | GLY | E | 169 | 53.265 | 14.473 | 26.749 | 1.00 | 17.67 | C |
| ATOM                      | 2273 | CE3 | PHE | E | 160 | 56.324 | 24.172 | 23.020 | 1.00 | 17.82                     | C | ATOM | 2836 | CA  | GLY | E | 169 | 52.432 | 13.290 | 26.574 | 1.00 | 16.77 | C |
| ATOM                      | 2274 | CD2 | PHE | E | 160 | 54.943 | 24.117 | 23.093 | 1.00 | 18.84                     | C | ATOM | 2837 | C   | GLY | E | 169 | 50.996 | 13.615 | 26.939 | 1.00 | 21.90 | C |
| ATOM                      | 2275 | C   | PHE | E | 160 | 52.773 | 21.012 | 24.430 | 1.00 | 21.46                     | C | ATOM | 2838 | CG1 | ASP | E | 170 | 50.694 | 24.731 | 27.333 | 1.00 | 19.60 | C |
| ATOM                      | 2276 | O   | PHE | E | 160 | 53.587 | 20.240 | 24.659 | 1.00 | 15.68                     | O | ATOM | 2839 | N   | ASP | E | 170 | 50.105 | 12.644 | 26.807 | 1.00 | 16.56 | C |
| ATOM                      | 2277 | N   | PHE | E | 161 | 52.321 | 20.881 | 25.789 | 1.00 | 16.36                     | N | ATOM | 2840 | CA  | ASP | E | 170 | 48.682 | 12.875 | 27.668 | 1.00 | 20.04 | C |
| ATOM                      | 2278 | CA  | PHE | E | 161 | 52.656 | 19.850 | 26.679 | 1.00 | 19.39                     | C | ATOM | 2841 | CB  | ASP | E | 170 | 47.880 | 11.568 | 27.013 | 1.00 | 20.22 | C |
| ATOM                      | 2279 | CB  | PHE | E | 161 | 52.723 | 20.286 | 28.150 | 1.00 | 16.61                     | C | ATOM | 2842 | CG  | ASP | E | 170 | 47.625 | 11.080 | 25.590 | 1.00 | 32.45 | C |
| ATOM                      | 2280 | CG  | PHE | E | 161 | 53.847 | 21.410 | 28.525 | 1.00 | 14.79                     | C | ATOM | 2843 | CD1 | ASP | E | 170 | 48.192 | 11.663 | 24.623 | 1.00 | 29.44 | C |
| ATOM                      | 2281 | CD1 | PHE | E | 161 | 54.994 | 21.216 | 28.623 | 1.00 | 13.64                     | C | ATOM | 2844 | ND2 | ASP | E | 170 | 48.856 | 10.093 | 25.445 | 1.00 | 26.37 | C |
| ATOM                      | 2282 | CE1 | PHE | E | 161 | 55.840 | 22.263 | 28.836 | 1.00 | 17.53                     | C | ATOM | 2845 | C   | ASP | E | 170 | 48.486 | 13.527 | 28.427 | 1.00 | 21.20 | C |
| ATOM                      | 2283 | CE2 | PHE | E | 161 | 55.311 | 23.544 | 29.158 | 1.00 | 15.94                     | C | ATOM | 2846 | O   | ASP | E | 170 | 48.979 | 13.044 | 29.461 | 1.00 | 18.40 | C |
| ATOM                      | 2284 | CE3 | PHE | E | 161 | 55.932 | 23.739 | 29.044 | 1.00 | 16.94                     | C | ATOM | 2847 | N   | VAL | E | 171 | 47.766 | 14.638 | 28.411 | 1.00 | 20.34 | C |
| ATOM                      | 2285 | CD2 | PHE | E | 161 | 53.102 | 22.672 | 26.734 | 1.00 | 8.49                      | C | ATOM | 2848 | CA  | VAL | E | 171 | 47.392 | 15.347 | 29.625 | 1.00 | 19.02 | C |
| ATOM                      | 2286 | C   | PHE | E | 161 | 52.258 | 18.446 | 26.438 | 1.00 | 21.50                     | C | ATOM | 2849 | CB  | VAL | E | 171 | 47.757 | 16.946 | 29.354 | 1.00 | 20.05 | C |
| ATOM                      | 2287 | O   | PHE | E | 161 | 52.736 | 17.802 | 27.030 | 1.00 | 9.01                      | O | ATOM | 2850 | CG1 | VAL | E | 171 | 46.622 | 17.543 | 30.547 | 1.00 | 22.00 | C |
| ATOM                      | 2288 | N   | GLY | E | 162 | 51.221 | 18.396 | 25.603 | 1.00 | 16.53                     | N | ATOM | 2851 | CG2 | VAL | E | 171 | 48.617 | 17.437 | 29.010 | 1.00 | 16.99 | C |
| ATOM                      | 2289 | CA  | GLY | E | 162 | 50.657 | 17.117 | 25.222 | 1.00 | 15.11                     | C | ATOM | 2852 | C   | VAL | E | 171 | 46.074 | 14.808 | 30.137 | 1.00 | 23.54 | C |
| ATOM                      | 2290 | C   | GLY | E | 162 | 51.488 | 16.211 | 24.153 | 1.00 | 22.53                     | C | ATOM | 2853 | O   | VAL | E | 171 | 45.085 | 14.671 | 29.489 | 1.00 | 27.02 | C |
| ATOM                      | 2291 | O   | GLY | E | 162 | 51.265 | 15.249 | 23.843 | 1.00 | 25.71                     | O | ATOM | 2854 | N   | ASP | E | 172 | 46.675 | 14.503 | 31.486 | 1.00 | 18.75 | C |
| ATOM                      | 2292 | N   | LEU | E | 163 | 52.457 | 17.133 | 24.062 | 1.00 | 13.64                     | N | ATOM | 2855 | CA  | ASP | E | 172 | 44.891 | 14.912 | 32.166 | 1.00 | 18.43 | C |
| ATOM                      | 2293 | CA  | LYS | E | 163 | 53.216 | 16.569 | 22.469 | 1.00 | 19.42                     | C | ATOM | 2856 | CB  | ASP | E | 172 | 45.230 | 12.845 | 33.072 | 1.00 | 28.73 | C |
| ATOM                      | 2294 | CB  | LYS | E | 163 | 53.6   |        |        |      |                           |   |      |      |     |     |   |     |        |        |        |      |       |   |

|      |      |     |           | dimer-PDB-coordinates.txt |        |        |      |       |      |      |     | dimer-PDB-coordinates.txt |        |        |        |      |       |      |      |   |           |        |        |        |      |       |
|------|------|-----|-----------|---------------------------|--------|--------|------|-------|------|------|-----|---------------------------|--------|--------|--------|------|-------|------|------|---|-----------|--------|--------|--------|------|-------|
| ATOM | 2986 | C   | GLY E 189 | 57.747                    | 10.595 | 32.681 | 1.00 | 28.85 | ATOM | 3049 | C   | ILE E 297                 | 63.964 | 21.108 | 31.162 | 1.00 | 29.75 | ATOM | 3110 | C | GLY E 206 | 52.633 | 36.295 | 70.318 | 1.00 | 21.33 |
| ATOM | 2987 | D   | GLY E 189 | 58.764                    | 11.279 | 32.573 | 1.00 | 28.38 | ATOM | 3050 | C   | ILE E 197                 | 64.805 | 21.875 | 31.943 | 1.00 | 26.11 | ATOM | 3111 | O | GLY E 206 | 53.585 | 36.661 | 70.644 | 1.00 | 27.03 |
| ATOM | 2988 | N   | VAL E 190 | 58.564                    | 10.984 | 32.210 | 1.00 | 24.34 | ATOM | 3051 | N   | GLY E 198                 | 62.930 | 21.302 | 31.980 | 1.00 | 29.51 | ATOM | 3112 | C | GLY E 206 | 52.633 | 36.295 | 70.318 | 1.00 | 21.33 |
| ATOM | 2989 | CA  | VAL E 190 | 56.416                    | 12.214 | 31.490 | 1.00 | 20.60 | ATOM | 3052 | CA  | GLY E 198                 | 62.930 | 21.302 | 31.980 | 1.00 | 29.51 | ATOM | 3113 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2990 | CB  | VAL E 190 | 55.006                    | 12.340 | 30.846 | 1.00 | 17.15 | ATOM | 3053 | C   | GLY E 198                 | 62.930 | 21.302 | 31.980 | 1.00 | 29.51 | ATOM | 3114 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2991 | CG1 | VAL E 190 | 54.885                    | 13.685 | 30.144 | 1.00 | 15.13 | ATOM | 3054 | D   | GLY E 198                 | 61.468 | 24.425 | 32.707 | 1.00 | 25.55 | ATOM | 3115 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2992 | CG2 | VAL E 190 | 54.744                    | 11.189 | 30.879 | 1.00 | 14.30 | ATOM | 3055 | N   | GLY E 199                 | 62.984 | 24.152 | 33.087 | 1.00 | 25.77 | ATOM | 3116 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2993 | C   | VAL E 190 | 56.729                    | 13.433 | 32.269 | 1.00 | 20.18 | ATOM | 3056 | CA  | GLN E 199                 | 62.637 | 25.417 | 30.448 | 1.00 | 31.47 | ATOM | 3117 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2994 | D   | VAL E 190 | 57.503                    | 14.292 | 31.659 | 1.00 | 22.03 | ATOM | 3057 | CB  | GLN E 199                 | 63.141 | 26.037 | 30.294 | 1.00 | 18.68 | ATOM | 3118 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2995 | N   | ALA E 191 | 56.143                    | 13.490 | 33.461 | 1.00 | 18.69 | ATOM | 3058 | CG  | GLN E 199                 | 64.232 | 26.889 | 31.734 | 1.00 | 14.76 | ATOM | 3119 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2996 | CA  | ALA E 191 | 56.390                    | 14.599 | 34.363 | 1.00 | 20.70 | ATOM | 3059 | CD  | GLN E 199                 | 65.217 | 26.067 | 31.534 | 1.00 | 24.48 | ATOM | 3120 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2997 | CB  | ALA E 191 | 55.606                    | 14.422 | 35.872 | 1.00 | 20.18 | ATOM | 3060 | OE1 | GLN E 199                 | 64.809 | 27.186 | 31.264 | 1.00 | 23.54 | ATOM | 3121 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2998 | C   | ALA E 191 | 57.880                    | 14.755 | 34.655 | 1.00 | 24.88 | ATOM | 3061 | NE2 | GLN E 199                 | 66.204 | 27.811 | 31.833 | 1.00 | 21.69 | ATOM | 3122 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 2999 | D   | ALA E 191 | 58.403                    | 15.867 | 34.668 | 1.00 | 26.72 | ATOM | 3062 | C   | GLN E 199                 | 62.066 | 28.231 | 29.643 | 1.00 | 25.27 | ATOM | 3123 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3000 | N   | GLN E 192 | 58.557                    | 13.645 | 34.895 | 1.00 | 22.28 | ATOM | 3063 | CG  | GLN E 199                 | 62.335 | 34.415 | 28.225 | 1.00 | 22.99 | ATOM | 3124 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3001 | CA  | GLN E 192 | 59.990                    | 13.719 | 35.210 | 1.00 | 27.42 | ATOM | 3064 | N   | PHE E 200                 | 61.027 | 35.900 | 28.723 | 1.00 | 27.72 | ATOM | 3125 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3002 | CB  | GLN E 192 | 60.547                    | 12.365 | 35.674 | 1.00 | 24.25 | ATOM | 3065 | CA  | PHE E 200                 | 60.388 | 25.816 | 27.428 | 1.00 | 20.24 | ATOM | 3126 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3003 | CG  | GLN E 192 | 60.100                    | 13.969 | 37.055 | 1.00 | 34.67 | ATOM | 3066 | CS  | PHE E 200                 | 59.113 | 24.964 | 27.583 | 1.00 | 17.66 | ATOM | 3127 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3004 | CD  | GLN E 192 | 58.592                    | 11.775 | 37.153 | 1.00 | 42.69 | ATOM | 3067 | CG  | PHE E 200                 | 59.447 | 27.468 | 27.409 | 1.00 | 15.37 | ATOM | 3128 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3005 | OE1 | GLN E 192 | 57.938                    | 11.336 | 36.193 | 1.00 | 35.89 | ATOM | 3068 | CD  | PHE E 200                 | 59.666 | 27.249 | 27.966 | 1.00 | 16.90 | ATOM | 3129 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3006 | NE2 | GLN E 192 | 58.032                    | 12.104 | 36.318 | 1.00 | 38.21 | ATOM | 3069 | CZ  | PHE E 200                 | 59.781 | 27.119 | 29.375 | 1.00 | 16.62 | ATOM | 3130 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3007 | C   | GLN E 192 | 60.788                    | 14.216 | 34.924 | 1.00 | 23.53 | ATOM | 3070 | CE1 | PHE E 200                 | 59.694 | 27.280 | 30.171 | 1.00 | 20.81 | ATOM | 3131 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3008 | O   | GLN E 192 | 61.690                    | 15.017 | 34.180 | 1.00 | 26.00 | ATOM | 3071 | CE2 | PHE E 200                 | 59.472 | 27.310 | 29.580 | 1.00 | 15.96 | ATOM | 3132 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3009 | N   | ARG E 193 | 60.457                    | 12.729 | 32.833 | 1.00 | 24.72 | ATOM | 3072 | CD1 | PHE E 200                 | 60.024 | 27.168 | 26.854 | 1.00 | 20.29 | ATOM | 3133 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3010 | CA  | ARG E 193 | 61.131                    | 14.209 | 31.633 | 1.00 | 24.72 | ATOM | 3073 | N   | PHE E 200                 | 59.713 | 26.084 | 27.599 | 1.00 | 22.38 | ATOM | 3134 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3011 | CB  | ARG E 193 | 60.615                    | 13.470 | 30.408 | 1.00 | 21.61 | ATOM | 3074 | O   | PHE E 200                 | 60.037 | 27.290 | 26.836 | 1.00 | 22.60 | ATOM | 3135 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3012 | CG  | ARG E 193 | 61.352                    | 13.844 | 29.146 | 1.00 | 28.44 | ATOM | 3075 | N   | THR E 201                 | 59.464 | 26.467 | 24.908 | 1.00 | 21.67 | ATOM | 3136 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3013 | CD  | ARG E 193 | 60.466                    | 13.974 | 27.853 | 1.00 | 39.54 | ATOM | 3076 | CA  | THR E 201                 | 60.404 | 26.383 | 23.868 | 1.00 | 23.67 | ATOM | 3137 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3014 | NE  | ARG E 193 | 60.251                    | 12.277 | 27.601 | 1.00 | 36.33 | ATOM | 3077 | CB  | THR E 201                 | 61.637 | 29.429 | 24.501 | 1.00 | 23.14 | ATOM | 3138 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3015 | CZ  | ARG E 193 | 59.063                    | 11.746 | 27.311 | 1.00 | 49.38 | ATOM | 3078 | OG1 | THR E 201                 | 59.797 | 30.336 | 24.262 | 1.00 | 21.01 | ATOM | 3139 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3016 | NH1 | ARG E 193 | 57.965                    | 12.485 | 27.355 | 1.00 | 43.33 | ATOM | 3079 | OG2 | THR E 201                 | 58.119 | 26.077 | 24.295 | 1.00 | 15.93 | ATOM | 3140 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3017 | NH2 | ARG E 193 | 58.966                    | 10.471 | 26.974 | 1.00 | 58.54 | ATOM | 3080 | C   | THR E 201                 | 58.038 | 27.168 | 23.489 | 1.00 | 24.20 | ATOM | 3141 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3018 | C   | ARG E 193 | 60.959                    | 15.724 | 31.467 | 1.00 | 29.94 | ATOM | 3081 | O   | THR E 201                 | 57.052 | 26.740 | 24.712 | 1.00 | 12.14 | ATOM | 3142 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3019 | O   | ARG E 193 | 61.934                    | 16.967 | 31.196 | 1.00 | 34.80 | ATOM | 3082 | N   | VAL E 202                 | 55.712 | 28.325 | 24.216 | 1.00 | 20.25 | ATOM | 3143 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3020 | N   | LEU E 194 | 59.716                    | 16.200 | 31.554 | 1.00 | 23.44 | ATOM | 3083 | CA  | VAL E 202                 | 54.903 | 27.809 | 25.535 | 1.00 | 19.38 | ATOM | 3144 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3021 | CA  | LEU E 194 | 59.453                    | 17.634 | 31.384 | 1.00 | 25.19 | ATOM | 3084 | CB  | VAL E 202                 | 53.507 | 27.793 | 25.768 | 1.00 | 15.49 | ATOM | 3145 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3022 | CB  | LEU E 194 | 57.952                    | 17.950 | 31.443 | 1.00 | 16.03 | ATOM | 3085 | CG1 | VAL E 202                 | 55.695 | 26.786 | 26.265 | 1.00 | 22.99 | ATOM | 3146 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3023 | CG  | LEU E 194 | 57.106                    | 17.439 | 30.279 | 1.00 | 23.61 | ATOM | 3086 | CG2 | VAL E 202                 | 54.963 | 29.471 | 23.658 | 1.00 | 22.99 | ATOM | 3147 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3024 | CD1 | LEU E 194 | 55.622                    | 17.762 | 30.509 | 1.00 | 25.13 | ATOM | 3087 | C   | VAL E 202                 | 54.858 | 30.566 | 24.226 | 1.00 | 24.37 | ATOM | 3148 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3025 | CD2 | LEU E 194 | 57.599                    | 18.048 | 28.976 | 1.00 | 21.28 | ATOM | 3088 | O   | VAL E 202                 | 54.453 | 29.225 | 22.441 | 1.00 | 25.29 | ATOM | 3149 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3026 | C   | LEU E 194 | 60.194                    | 16.442 | 32.429 | 1.00 | 23.94 | ATOM | 3089 | N   | PRO E 203                 | 53.644 | 30.249 | 23.759 | 1.00 | 27.60 | ATOM | 3150 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3027 | O   | LEU E 194 | 60.704                    | 19.522 | 32.141 | 1.00 | 20.23 | ATOM | 3090 | CA  | PRO E 203                 | 53.638 | 29.638 | 20.369 | 1.00 | 24.14 | ATOM | 3151 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3028 | N   | CYS E 195 | 60.249                    | 17.905 | 33.642 | 1.00 | 22.21 | ATOM | 3091 | CB  | PRO E 203                 | 54.389 | 28.543 | 20.237 | 1.00 | 27.72 | ATOM | 3152 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3029 | CA  | CYS E 195 | 60.945                    | 18.561 | 34.733 | 1.00 | 24.91 | ATOM | 3092 | CG  | PRO E 203                 | 54.644 | 28.029 | 21.619 | 1.00 | 18.35 | ATOM | 3153 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3030 | CB  | CYS E 195 | 60.590                    | 17.890 | 36.066 | 1.00 | 31.37 | ATOM | 3093 | CD  | PRO E 203                 | 52.321 | 30.457 | 22.497 | 1.00 | 25.43 | ATOM | 3154 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3031 | SG  | CYS E 195 | 61.279                    | 18.680 | 37.322 | 1.00 | 61.47 | ATOM | 3094 | C   | PRO E 203                 | 51.533 | 29.498 | 22.678 | 1.00 | 34.08 | ATOM | 3155 | C | GLN E 207 | 53.076 | 36.565 | 70.721 | 1.00 | 18.31 |
| ATOM | 3032 | C   | CYS E 195 | 62.471                    | 18.604 | 34.483 | 1.00 | 25.21 | ATOM | 3095 | O   | PRO E 203                 | 52.048 | 31.688 | 21.929 | 1.00 | 23.35 | ATOM |      |   |           |        |        |        |      |       |

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|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3238 | CB  | VAL | F | 139 | 38.053 | 16.341 | 11.228 | 1.00 | 16.15 |
| ATOM | 3239 | CG1 | VAL | F | 139 | 37.044 | 16.193 | 11.353 | 1.00 | 16.66 |
| ATOM | 3240 | CG2 | VAL | F | 139 | 39.374 | 15.673 | 11.598 | 1.00 | 16.03 |
| ATOM | 3241 | C   | VAL | F | 139 | 36.276 | 16.339 | 9.485  | 1.00 | 24.77 |
| ATOM | 3242 | O   | VAL | F | 139 | 36.404 | 17.697 | 9.068  | 1.00 | 23.30 |
| ATOM | 3243 | N   | THR | F | 140 | 35.101 | 15.925 | 9.603  | 1.00 | 18.36 |
| ATOM | 3244 | CA  | THR | F | 140 | 33.874 | 16.568 | 9.144  | 1.00 | 27.07 |
| ATOM | 3245 | CB  | THR | F | 140 | 35.428 | 16.078 | 7.781  | 1.00 | 24.33 |
| ATOM | 3246 | CG1 | THR | F | 140 | 31.327 | 14.586 | 7.854  | 1.00 | 23.86 |
| ATOM | 3247 | CG2 | THR | F | 140 | 34.442 | 16.390 | 6.674  | 1.00 | 27.23 |
| ATOM | 3248 | C   | THR | F | 140 | 32.759 | 16.301 | 10.138 | 1.00 | 25.44 |
| ATOM | 3249 | O   | THR | F | 140 | 32.662 | 15.379 | 10.950 | 1.00 | 20.41 |
| ATOM | 3250 | N   | GLY | F | 141 | 31.695 | 17.104 | 10.954 | 1.00 | 31.98 |
| ATOM | 3251 | CA  | GLY | F | 141 | 30.491 | 16.909 | 10.850 | 1.00 | 26.45 |
| ATOM | 3252 | C   | GLY | F | 141 | 30.138 | 18.061 | 11.778 | 1.00 | 27.67 |
| ATOM | 3253 | O   | GLY | F | 141 | 29.285 | 17.909 | 12.650 | 1.00 | 34.54 |
| ATOM | 3254 | N   | PHE | F | 142 | 30.786 | 19.209 | 11.605 | 1.00 | 22.20 |
| ATOM | 3255 | CA  | PHE | F | 142 | 30.551 | 20.344 | 12.488 | 1.00 | 26.33 |
| ATOM | 3256 | CB  | PHE | F | 142 | 31.631 | 21.401 | 12.287 | 1.00 | 26.95 |
| ATOM | 3257 | CG  | PHE | F | 142 | 31.017 | 20.839 | 13.295 | 1.00 | 30.03 |
| ATOM | 3258 | CD1 | PHE | F | 142 | 31.683 | 20.627 | 13.488 | 1.00 | 21.60 |
| ATOM | 3259 | CE1 | PHE | F | 142 | 34.953 | 20.091 | 13.504 | 1.00 | 25.04 |
| ATOM | 3260 | CZ  | PHE | F | 142 | 35.580 | 19.763 | 12.311 | 1.00 | 26.79 |
| ATOM | 3261 | CE2 | PHE | F | 142 | 34.924 | 19.976 | 11.110 | 1.00 | 25.67 |
| ATOM | 3262 | CD2 | PHE | F | 142 | 33.646 | 20.503 | 11.106 | 1.00 | 17.42 |
| ATOM | 3263 | C   | PHE | F | 142 | 29.173 | 20.954 | 12.265 | 1.00 | 28.48 |
| ATOM | 3264 | O   | PHE | F | 142 | 28.786 | 21.213 | 11.134 | 1.00 | 27.72 |
| ATOM | 3265 | N   | PRO | F | 143 | 28.424 | 21.179 | 13.355 | 1.00 | 31.76 |
| ATOM | 3266 | CA  | PRO | F | 143 | 27.097 | 21.801 | 13.236 | 1.00 | 30.16 |
| ATOM | 3267 | CB  | PRO | F | 143 | 26.459 | 21.518 | 14.603 | 1.00 | 25.89 |
| ATOM | 3268 | CG  | PRO | F | 143 | 27.411 | 21.437 | 15.546 | 1.00 | 23.65 |
| ATOM | 3269 | CD  | PRO | F | 143 | 28.741 | 20.789 | 14.744 | 1.00 | 19.96 |
| ATOM | 3270 | C   | PRO | F | 143 | 27.201 | 23.304 | 13.014 | 1.00 | 26.57 |
| ATOM | 3271 | O   | PRO | F | 143 | 28.130 | 23.946 | 13.515 | 1.00 | 29.12 |
| ATOM | 3272 | N   | ALA | F | 144 | 26.244 | 23.956 | 12.292 | 1.00 | 26.96 |
| ATOM | 3273 | CA  | ALA | F | 144 | 25.008 | 25.312 | 12.049 | 1.00 | 26.06 |
| ATOM | 3274 | CB  | ALA | F | 144 | 25.071 | 25.432 | 11.108 | 1.00 | 30.71 |
| ATOM | 3275 | C   | ALA | F | 144 | 26.103 | 26.137 | 13.341 | 1.00 | 31.49 |
| ATOM | 3276 | O   | ALA | F | 144 | 26.466 | 27.313 | 13.373 | 1.00 | 33.78 |
| ATOM | 3277 | N   | SER | F | 145 | 25.612 | 25.514 | 14.406 | 1.00 | 28.42 |
| ATOM | 3278 | CA  | SER | F | 145 | 24.424 | 26.203 | 15.677 | 1.00 | 23.47 |
| ATOM | 3279 | CB  | SER | F | 145 | 24.445 | 25.411 | 16.545 | 1.00 | 27.91 |
| ATOM | 3280 | OG  | SER | F | 145 | 24.967 | 24.135 | 16.865 | 1.00 | 30.70 |
| ATOM | 3281 | C   | SER | F | 145 | 26.703 | 26.439 | 16.478 | 1.00 | 26.84 |
| ATOM | 3282 | O   | SER | F | 145 | 26.665 | 27.127 | 17.487 | 1.00 | 28.63 |
| ATOM | 3283 | N   | LEU | F | 146 | 27.822 | 25.857 | 16.056 | 1.00 | 29.46 |
| ATOM | 3284 | CA  | LEU | F | 146 | 29.112 | 26.091 | 16.729 | 1.00 | 31.13 |
| ATOM | 3285 | CB  | LEU | F | 146 | 30.223 | 25.289 | 16.649 | 1.00 | 35.88 |
| ATOM | 3286 | CG  | LEU | F | 146 | 30.545 | 25.927 | 16.649 | 1.00 | 35.22 |
| ATOM | 3287 | CD1 | LEU | F | 146 | 31.841 | 23.436 | 16.070 | 1.00 | 27.10 |
| ATOM | 3288 | CD2 | LEU | F | 146 | 30.627 | 24.002 | 18.179 | 1.00 | 28.66 |
| ATOM | 3289 | C   | LEU | F | 146 | 29.535 | 27.571 | 16.804 | 1.00 | 33.24 |
| ATOM | 3290 | O   | LEU | F | 146 | 28.422 | 28.422 | 15.786 | 1.00 | 30.71 |
| ATOM | 3291 | N   | ARG | F | 147 | 29.505 | 28.026 | 17.957 | 1.00 | 39.61 |
| ATOM | 3292 | CA  | ARG | F | 147 | 30.217 | 29.435 | 18.243 | 1.00 | 53.20 |
| ATOM | 3293 | CB  | ARG | F | 147 | 29.663 | 29.877 | 19.602 | 1.00 | 60.44 |
| ATOM | 3294 | CG  | ARG | F | 147 | 28.164 | 29.731 | 19.770 | 1.00 | 67.43 |
| ATOM | 3295 | CD  | ARG | F | 147 | 27.411 | 30.211 | 18.916 | 1.00 | 58.42 |
| ATOM | 3296 | NE  | ARG | F | 147 | 26.039 | 30.906 | 19.389 | 1.00 | 85.48 |
| ATOM | 3297 | CZ  | ARG | F | 147 | 25.381 | 32.060 | 19.347 | 1.00 | 92.40 |
| ATOM | 3298 | NH1 | ARG | F | 147 | 15.969 | 31.144 | 18.855 | 1.00 | 88.22 |
| ATOM | 3299 | NH2 | ARG | F | 147 | 24.136 | 31.131 | 19.799 | 1.00 | 81.17 |
| ATOM | 3300 | C   | ARG | F | 147 | 31.714 | 29.698 | 18.295 | 1.00 | 51.41 |

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|   |      |      |     |     |   |     |        |        |        |      |       |
|---|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| C | ATOM | 3301 | O   | ARG | F | 147 | 32.141 | 30.850 | 18.298 | 1.00 | 56.62 |
| C | ATOM | 3302 | N   | LEU | F | 148 | 32.501 | 28.627 | 18.216 | 1.00 | 40.52 |
| C | ATOM | 3303 | CA  | LEU | F | 148 | 33.937 | 28.739 | 18.290 | 1.00 | 37.92 |
| C | ATOM | 3304 | CB  | LEU | F | 148 | 34.160 | 27.314 | 18.305 | 1.00 | 28.10 |
| C | ATOM | 3305 | CG  | LEU | F | 148 | 34.000 | 26.393 | 19.389 | 1.00 | 14.53 |
| C | ATOM | 3306 | CD1 | LEU | F | 148 | 34.612 | 25.017 | 19.279 | 1.00 | 25.63 |
| C | ATOM | 3307 | CD2 | LEU | F | 148 | 34.259 | 26.872 | 20.786 | 1.00 | 33.82 |
| C | ATOM | 3308 | C   | LEU | F | 148 | 34.568 | 29.527 | 17.142 | 1.00 | 28.40 |
| C | ATOM | 3309 | O   | LEU | F | 148 | 34.103 | 29.440 | 16.004 | 1.00 | 32.99 |
| C | ATOM | 3310 | N   | SER | F | 149 | 35.572 | 30.332 | 17.455 | 1.00 | 25.10 |
| C | ATOM | 3311 | CA  | SER | F | 149 | 36.421 | 30.329 | 18.433 | 1.00 | 26.89 |
| C | ATOM | 3312 | CB  | SER | F | 149 | 37.425 | 31.576 | 17.026 | 1.00 | 31.58 |
| C | ATOM | 3313 | CG  | SER | F | 149 | 38.010 | 31.144 | 17.778 | 1.00 | 30.63 |
| C | ATOM | 3314 | C   | SER | F | 149 | 37.191 | 29.809 | 15.745 | 1.00 | 27.97 |
| C | ATOM | 3315 | O   | SER | F | 149 | 37.226 | 28.690 | 16.238 | 1.00 | 30.81 |
| C | ATOM | 3316 | N   | GLU | F | 150 | 37.826 | 30.113 | 14.622 | 1.00 | 28.02 |
| C | ATOM | 3317 | CA  | GLU | F | 150 | 38.548 | 29.080 | 13.869 | 1.00 | 35.00 |
| C | ATOM | 3318 | CB  | GLU | F | 150 | 39.045 | 29.653 | 13.539 | 1.00 | 34.10 |
| C | ATOM | 3319 | CG  | GLU | F | 150 | 37.917 | 29.899 | 11.520 | 1.00 | 46.93 |
| C | ATOM | 3320 | CD  | GLU | F | 150 | 38.382 | 30.605 | 10.247 | 1.00 | 61.68 |
| C | ATOM | 3321 | OE1 | GLU | F | 150 | 39.553 | 31.071 | 10.167 | 1.00 | 51.74 |
| C | ATOM | 3322 | OE2 | GLU | F | 150 | 37.561 | 30.684 | 9.308  | 1.00 | 68.13 |
| C | ATOM | 3323 | C   | GLU | F | 150 | 39.701 | 28.149 | 14.690 | 1.00 | 31.23 |
| C | ATOM | 3324 | O   | GLU | F | 150 | 39.831 | 17.332 | 14.742 | 1.00 | 30.13 |
| C | ATOM | 3325 | N   | GLU | F | 151 | 40.412 | 19.452 | 15.353 | 1.00 | 24.86 |
| C | ATOM | 3326 | CA  | GLU | F | 151 | 41.322 | 19.056 | 16.191 | 1.00 | 20.02 |
| C | ATOM | 3327 | CB  | GLU | F | 151 | 42.239 | 20.280 | 15.737 | 1.00 | 30.77 |
| C | ATOM | 3328 | CG  | GLU | F | 151 | 42.937 | 20.310 | 15.000 | 1.00 | 48.19 |
| C | ATOM | 3329 | CD  | GLU | F | 151 | 44.692 | 30.823 | 17.312 | 1.00 | 68.55 |
| C | ATOM | 3330 | OE1 | GLU | F | 151 | 44.482 | 31.958 | 16.827 | 1.00 | 73.37 |
| C | ATOM | 3331 | OE2 | GLU | F | 151 | 45.843 | 30.402 | 17.822 | 1.00 | 60.02 |
| C | ATOM | 3332 | C   | GLU | F | 151 | 41.080 | 28.149 | 17.337 | 1.00 | 29.46 |
| C | ATOM | 3333 | O   | GLU | F | 151 | 41.758 | 17.171 | 17.642 | 1.00 | 26.84 |
| C | ATOM | 3334 | N   | GLU | F | 152 | 39.957 | 28.467 | 17.980 | 1.00 | 20.91 |
| C | ATOM | 3335 | CA  | GLU | F | 152 | 39.478 | 17.635 | 19.082 | 1.00 | 28.07 |
| C | ATOM | 3336 | CB  | GLU | F | 152 | 38.264 | 28.249 | 19.787 | 1.00 | 25.19 |
| C | ATOM | 3337 | CG  | GLU | F | 152 | 38.501 | 29.585 | 20.444 | 1.00 | 51.66 |
| C | ATOM | 3338 | CD  | GLU | F | 152 | 37.239 | 29.134 | 21.542 | 1.00 | 34.10 |
| C | ATOM | 3339 | OE1 | GLU | F | 152 | 36.290 | 30.590 | 20.394 | 1.00 | 43.20 |
| C | ATOM | 3340 | OE2 | GLU | F | 152 | 37.197 | 30.156 | 22.359 | 1.00 | 62.78 |
| C | ATOM | 3341 | C   | GLU | F | 152 | 29.099 | 26.245 | 18.777 | 1.00 | 23.48 |
| C | ATOM | 3342 | O   | GLU | F | 152 | 39.362 | 25.244 | 19.250 | 1.00 | 21.61 |
| C | ATOM | 3343 | N   | LEU | F | 153 | 38.462 | 26.156 | 17.410 | 1.00 | 17.64 |
| C | ATOM | 3344 | CA  | LEU | F | 153 | 35.047 | 25.824 | 15.826 | 1.00 | 30.81 |
| C | ATOM | 3345 | CB  | LEU | F | 153 | 37.270 | 25.155 | 15.533 | 1.00 | 18.37 |
| C | ATOM | 3346 | CG  | LEU | F | 153 | 36.882 | 23.871 | 14.805 | 1.00 | 25.45 |
| C | ATOM | 3347 | CD1 | LEU | F | 153 | 35.959 | 23.023 | 15.703 | 1.00 | 19.51 |
| C | ATOM | 3348 | CD2 | LEU | F | 153 | 36.184 | 24.165 | 13.474 | 1.00 | 22.42 |
| C | ATOM | 3349 | C   | LEU | F | 153 | 39.274 | 14.063 | 18.557 | 1.00 | 34.10 |
| C | ATOM | 3350 | N   | LEU | F | 153 | 39.321 | 12.874 | 16.901 | 1.00 | 20.77 |
| C | ATOM | 3351 | O   | LEU | F | 154 | 40.281 | 24.687 | 15.971 | 1.00 | 16.27 |
| C | ATOM | 3352 | CA  | LEU | F | 154 | 41.514 | 23.983 | 15.671 | 1.00 | 22.28 |
| C | ATOM | 3353 | CB  | LEU | F | 154 | 42.464 | 24.860 | 14.855 | 1.00 | 15.89 |
| C | ATOM | 3354 | CG  | LEU | F | 154 | 42.918 | 25.075 | 13.398 | 1.00 | 27.05 |
| C | ATOM | 3355 | CD1 | LEU | F | 154 | 42.905 | 26.134 | 12.696 | 1.00 | 21.74 |
| C | ATOM | 3356 | CD2 | LEU | F | 154 | 42.050 | 23.772 | 12.624 | 1.00 | 20.59 |
| C | ATOM | 3357 | C   | LEU | F | 154 | 42.184 | 23.495 | 16.945 | 1.00 | 21.62 |
| C | ATOM | 3358 | O   | LEU | F | 154 | 42.595 | 22.359 | 17.007 | 1.00 | 19.29 |
| C | ATOM | 3359 | N   | ASP | F | 155 | 42.271 | 24.351 | 17.962 | 1.00 | 16.57 |
| C | ATOM | 3360 | CA  | ASP | F | 155 | 42.827 | 13.940 | 19.245 | 1.00 | 20.99 |
| C | ATOM | 3361 | CB  | ASP | F | 155 | 42.866 | 25.109 | 20.    |      |       |

|      |      |     |     |   |     |        |        |        |      |       |      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3490 | CA  | ASP | F | 172 | 51.963 | 16.359 | 17.734 | 1.00 | 22.11 | ATOM | 3553 | CB  | SER | F | 180 | 26.506 | 19.243 | 6.041  | 1.00 | 29.46 |
| ATOM | 3491 | CB  | ASP | F | 172 | 52.812 | 17.471 | 11.817 | 1.00 | 20.25 | ATOM | 3554 | OG  | SER | F | 180 | 37.610 | 19.507 | 5.200  | 1.00 | 39.09 |
| ATOM | 3492 | CG  | ASP | F | 172 | 53.750 | 18.288 | 10.922 | 1.00 | 67.18 | ATOM | 3555 | C   | SER | F | 180 | 37.587 | 20.847 | 7.601  | 1.00 | 30.36 |
| ATOM | 3493 | OD1 | ASP | F | 172 | 54.352 | 18.155 | 11.410 | 1.00 | 28.45 | ATOM | 3556 | O   | SER | F | 180 | 38.111 | 21.913 | 7.770  | 1.00 | 24.63 |
| ATOM | 3494 | OD2 | ASP | F | 172 | 53.887 | 17.900 | 9.726  | 1.00 | 67.14 | ATOM | 3557 | N   | VAL | F | 181 | 38.133 | 20.021 | 6.480  | 1.00 | 22.54 |
| ATOM | 3495 | C   | ASP | F | 172 | 51.275 | 19.461 | 11.915 | 1.00 | 22.12 | ATOM | 3558 | CA  | VAL | F | 181 | 39.455 | 20.297 | 9.015  | 1.00 | 21.00 |
| ATOM | 3496 | O   | ASP | F | 172 | 51.629 | 20.629 | 11.982 | 1.00 | 29.94 | ATOM | 3559 | CB  | VAL | F | 181 | 39.436 | 20.417 | 10.341 | 1.00 | 19.10 |
| ATOM | 3497 | N   | VAL | F | 173 | 50.275 | 19.075 | 11.145 | 1.00 | 21.12 | ATOM | 3560 | CG1 | VAL | F | 181 | 40.856 | 20.430 | 11.090 | 1.00 | 16.37 |
| ATOM | 3498 | CA  | VAL | F | 173 | 49.647 | 19.883 | 10.205 | 1.00 | 15.45 | ATOM | 3561 | CG2 | VAL | F | 181 | 38.676 | 21.685 | 10.951 | 1.00 | 21.38 |
| ATOM | 3499 | CB  | VAL | F | 173 | 49.750 | 19.393 | 8.796  | 1.00 | 21.97 | ATOM | 3562 | C   | VAL | F | 181 | 40.410 | 19.214 | 8.588  | 1.00 | 19.11 |
| ATOM | 3500 | CG3 | VAL | F | 173 | 48.672 | 19.355 | 7.879  | 1.00 | 21.38 | ATOM | 3563 | O   | VAL | F | 181 | 40.179 | 18.040 | 8.748  | 1.00 | 22.15 |
| ATOM | 3501 | CG2 | VAL | F | 173 | 51.139 | 19.626 | 8.240  | 1.00 | 20.65 | ATOM | 3564 | N   | NET | F | 182 | 41.561 | 19.611 | 8.048  | 1.00 | 21.02 |
| ATOM | 3502 | C   | VAL | F | 173 | 48.176 | 20.166 | 10.582 | 1.00 | 16.78 | ATOM | 3565 | CA  | MET | F | 182 | 42.576 | 18.648 | 7.678  | 1.00 | 19.60 |
| ATOM | 3503 | O   | VAL | F | 173 | 47.513 | 15.216 | 11.005 | 1.00 | 16.24 | ATOM | 3566 | CB  | MET | F | 182 | 43.187 | 19.032 | 6.148  | 1.00 | 20.87 |
| ATOM | 3504 | N   | ARG | F | 174 | 47.656 | 21.382 | 10.440 | 1.00 | 18.18 | ATOM | 3567 | CG  | MET | F | 182 | 43.091 | 17.921 | 7.609  | 1.00 | 31.25 |
| ATOM | 3505 | CA  | ARG | F | 174 | 46.324 | 21.584 | 10.671 | 1.00 | 16.67 | ATOM | 3568 | SD  | MET | F | 182 | 43.525 | 18.307 | 5.236  | 1.00 | 61.08 |
| ATOM | 3506 | CB  | ARG | F | 174 | 45.896 | 21.822 | 12.157 | 1.00 | 16.59 | ATOM | 3569 | CE  | MET | F | 182 | 46.199 | 17.896 | 6.790  | 1.00 | 3.23  |
| ATOM | 3507 | CG  | ARG | F | 174 | 46.367 | 23.170 | 12.705 | 1.00 | 23.95 | ATOM | 3570 | C   | MET | F | 182 | 43.654 | 18.580 | 8.756  | 1.00 | 19.34 |
| ATOM | 3508 | CD  | ARG | F | 174 | 46.345 | 23.237 | 14.248 | 1.00 | 18.90 | ATOM | 3571 | O   | MET | F | 182 | 44.210 | 19.611 | 9.155  | 1.00 | 17.14 |
| ATOM | 3509 | NE  | ARG | F | 174 | 46.143 | 24.646 | 14.097 | 1.00 | 24.97 | ATOM | 3572 | N   | LEU | F | 183 | 43.951 | 17.369 | 9.223  | 1.00 | 18.61 |
| ATOM | 3510 | CZ  | ARG | F | 174 | 45.831 | 24.993 | 15.937 | 1.00 | 27.79 | ATOM | 3573 | CA  | LEU | F | 183 | 45.023 | 17.195 | 10.200 | 1.00 | 18.86 |
| ATOM | 3511 | NH1 | ARG | F | 174 | 45.664 | 24.099 | 16.908 | 1.00 | 20.16 | ATOM | 3574 | CB  | LEU | F | 183 | 44.464 | 16.614 | 11.511 | 1.00 | 16.09 |
| ATOM | 3512 | NH2 | ARG | F | 174 | 45.649 | 26.278 | 16.208 | 1.00 | 24.41 | ATOM | 3575 | CG  | LEU | F | 183 | 43.818 | 17.425 | 12.260 | 1.00 | 22.53 |
| ATOM | 3513 | C   | ARG | F | 174 | 45.732 | 22.728 | 9.792  | 1.00 | 20.54 | ATOM | 3576 | CG1 | LEU | F | 183 | 42.899 | 16.645 | 13.454 | 1.00 | 14.36 |
| ATOM | 3514 | O   | ARG | F | 174 | 46.266 | 23.829 | 9.846  | 1.00 | 23.16 | ATOM | 3577 | CD2 | LEU | F | 183 | 43.943 | 18.783 | 12.717 | 1.00 | 12.44 |
| ATOM | 3515 | N   | GLU | F | 175 | 44.723 | 22.452 | 8.962  | 1.00 | 20.30 | ATOM | 3578 | C   | LEU | F | 183 | 46.091 | 18.181 | 9.629  | 1.00 | 17.96 |
| ATOM | 3516 | CA  | GLU | F | 175 | 44.235 | 23.430 | 7.991  | 1.00 | 25.15 | ATOM | 3579 | O   | LEU | F | 183 | 45.781 | 15.299 | 8.964  | 1.00 | 20.49 |
| ATOM | 3517 | CB  | GLU | F | 175 | 44.741 | 23.092 | 6.592  | 1.00 | 26.35 | ATOM | 3580 | N   | GLY | F | 184 | 47.347 | 16.610 | 9.882  | 1.00 | 20.16 |
| ATOM | 3518 | CG  | GLU | F | 175 | 46.169 | 23.395 | 6.314  | 1.00 | 31.37 | ATOM | 3581 | CA  | GLY | F | 184 | 48.161 | 15.768 | 9.481  | 1.00 | 16.23 |
| ATOM | 3519 | CD  | GLU | F | 175 | 46.471 | 23.339 | 4.821  | 1.00 | 35.95 | ATOM | 3582 | C   | GLY | F | 184 | 49.255 | 15.372 | 10.705 | 1.00 | 18.99 |
| ATOM | 3520 | OE1 | GLU | F | 175 | 45.674 | 23.736 | 4.063  | 1.00 | 45.49 | ATOM | 3583 | O   | GLY | F | 184 | 48.592 | 16.723 | 11.528 | 1.00 | 19.62 |
| ATOM | 3521 | OE2 | GLU | F | 175 | 47.503 | 23.906 | 4.402  | 1.00 | 60.95 | ATOM | 3584 | N   | PHE | F | 185 | 49.537 | 14.001 | 10.834 | 1.00 | 15.10 |
| ATOM | 3522 | C   | GLU | F | 175 | 42.718 | 23.461 | 7.904  | 1.00 | 21.63 | ATOM | 3585 | CA  | PHE | F | 185 | 50.218 | 13.571 | 12.015 | 1.00 | 21.40 |
| ATOM | 3523 | O   | GLU | F | 175 | 42.062 | 22.427 | 7.987  | 1.00 | 19.94 | ATOM | 3586 | CB  | PHE | F | 185 | 49.530 | 12.287 | 12.522 | 1.00 | 19.40 |
| ATOM | 3524 | N   | LEU | F | 176 | 42.166 | 24.646 | 7.700  | 1.00 | 20.68 | ATOM | 3587 | CG  | PHE | F | 185 | 48.102 | 12.511 | 12.910 | 1.00 | 18.60 |
| ATOM | 3525 | CA  | LEU | F | 176 | 40.747 | 24.770 | 7.415  | 1.00 | 24.26 | ATOM | 3588 | CD1 | PHE | F | 185 | 47.771 | 12.899 | 14.194 | 1.00 | 15.81 |
| ATOM | 3526 | CB  | LEU | F | 176 | 40.234 | 26.127 | 7.872  | 1.00 | 16.40 | ATOM | 3589 | CE1 | PHE | F | 185 | 48.834 | 13.147 | 15.149 | 1.00 | 16.92 |
| ATOM | 3527 | CG  | LEU | F | 176 | 40.459 | 26.341 | 9.360  | 1.00 | 25.64 | ATOM | 3590 | CZ  | PHE | F | 185 | 45.831 | 13.042 | 13.594 | 1.00 | 14.57 |
| ATOM | 3528 | CD1 | LEU | F | 176 | 40.361 | 27.813 | 9.726  | 1.00 | 34.90 | ATOM | 3591 | CE2 | PHE | F | 185 | 45.763 | 12.675 | 12.307 | 1.00 | 16.91 |
| ATOM | 3529 | CD2 | LEU | F | 176 | 39.459 | 25.511 | 10.140 | 1.00 | 24.51 | ATOM | 3592 | CD2 | PHE | F | 185 | 47.098 | 12.423 | 11.968 | 1.00 | 15.60 |
| ATOM | 3530 | C   | LEU | F | 176 | 40.516 | 24.603 | 9.926  | 1.00 | 27.11 | ATOM | 3593 | C   | PHE | F | 185 | 51.722 | 13.402 | 11.799 | 1.00 | 23.79 |
| ATOM | 3531 | O   | LEU | F | 176 | 41.035 | 25.379 | 9.126  | 1.00 | 26.78 | ATOM | 3594 | O   | PHE | F | 185 | 52.184 | 13.187 | 10.680 | 1.00 | 21.93 |
| ATOM | 3532 | N   | LEU | F | 177 | 39.768 | 23.564 | 5.560  | 1.00 | 25.70 | ATOM | 3595 | N   | ALA | F | 186 | 52.476 | 13.550 | 12.885 | 1.00 | 26.30 |
| ATOM | 3533 | CA  | LEU | F | 177 | 39.298 | 23.379 | 4.185  | 1.00 | 22.05 | ATOM | 3596 | CA  | ALA | F | 186 | 53.923 | 13.416 | 12.856 | 1.00 | 28.80 |
| ATOM | 3534 | CB  | LEU | F | 177 | 39.608 | 21.970 | 3.693  | 1.00 | 24.59 | ATOM | 3597 | CB  | ALA | F | 186 | 54.517 | 13.833 | 14.200 | 1.00 | 21.99 |
| ATOM | 3535 | C   | LEU | F | 177 | 41.010 | 21.691 | 3.143  | 1.00 | 26.76 | ATOM | 3598 | C   | ALA | F | 186 | 54.327 | 11.985 | 12.529 | 1.00 | 30.51 |
| ATOM | 3536 | CD1 | LEU | F | 177 | 42.081 | 22.402 | 3.938  | 1.00 | 39.74 | ATOM | 3599 | O   | ALA | F | 186 | 55.769 | 11.739 | 14.794 | 1.00 | 35.86 |
| ATOM | 3537 | CD2 | LEU | F | 177 | 41.276 | 20.202 | 3.107  | 1.00 | 34.63 | ATOM | 3600 | N   | ARG | F | 187 | 53.609 | 11.016 | 13.079 | 1.00 | 29.94 |
| ATOM | 3538 | C   | LEU | F | 177 | 37.791 | 23.629 | 4.132  | 1.00 | 30.05 | ATOM | 3601 | CA  | ARG | F | 187 | 54.038 | 9.676  | 12.965 | 1.00 | 29.90 |
| ATOM | 3539 | O   | LEU | F | 177 | 37.129 | 23.765 | 5.183  | 1.00 | 31.67 | ATOM | 3602 | CB  | ARG | F | 187 | 54.247 | 9.012  | 14.342 | 1.00 | 32.36 |
| ATOM | 3540 | N   | PRO | F | 178 | 37.230 | 23.706 | 2.815  | 1.00 | 36.40 | ATOM | 3603 | CG  | ARG | F | 187 | 55.443 | 9.646  | 15.089 | 1.00 | 33.94 |
| ATOM | 3541 | CA  | PRO | F | 178 | 35.784 | 23.937 | 2.805  | 1.00 | 39.89 | ATOM | 3604 | CG  | ARG | F | 187 | 56.336 | 8.620  | 15.712 | 1.00 | 76.27 |
| ATOM | 3542 | CB  | PRO | F | 178 | 35.533 | 23.860 | 1.301  | 1.00 | 43.67 | ATOM | 3605 | CE  | ARG | F | 187 | 56.169 | 7.753  | 17.168 | 1.00 | 71.87 |
| ATOM | 3543 | CG  | PRO | F | 178 | 36.845 | 24.273 | 0.694  | 1.00 | 44.51 | ATOM | 3606 | CZ  | ARG | F | 187 | 56.725 | 9.617  | 17.929 | 1.00 | 91.17 |
| ATOM | 3544 | CD  | PRO | F | 178 | 37.869 | 23.684 | 1.598  | 1.00 | 37.08 | ATOM | 3607 | NH1 | ARG | F | 187 | 57.446 | 10.589 | 17.382 | 1.00 | 91.42 |
| ATOM | 3545 | CD2 | PRO | F | 178 | 34.373 | 24.605 | 3.558  | 1.00 | 33.24 | ATOM |      |     |     |   |     |        |        |        |      |       |

| dimer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |            |
|---------------------------|------|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM                      | 3742 | O   | GLY | F | 205 | 23.516 | 23.397 | 24.538 | 1.00 37.66 |
| ATOM                      | 3743 | N   | GLY | F | 206 | 30.594 | 23.397 | 24.538 | 1.00 26.24 |
| ATOM                      | 3744 | CA  | GLY | F | 206 | 29.385 | 22.998 | 25.211 | 1.00 20.98 |
| ATOM                      | 3745 | C   | GLY | F | 206 | 28.653 | 21.828 | 24.585 | 1.00 21.64 |
| ATOM                      | 3746 | C   | GLY | F | 206 | 27.918 | 21.134 | 25.270 | 1.00 24.78 |
| ATOM                      | 3747 | N   | GLN | F | 207 | 29.839 | 23.610 | 23.288 | 1.00 21.66 |
| ATOM                      | 3748 | CA  | GLN | F | 207 | 28.189 | 20.504 | 22.568 | 1.00 20.93 |
| ATOM                      | 3749 | CG  | GLN | F | 207 | 27.839 | 20.921 | 21.148 | 1.00 18.00 |
| ATOM                      | 3750 | CG  | GLN | F | 207 | 27.058 | 22.226 | 21.071 | 1.00 17.07 |
| ATOM                      | 3751 | CD  | GLN | F | 207 | 26.554 | 22.942 | 19.874 | 1.00 22.05 |
| ATOM                      | 3752 | OE1 | GLN | F | 207 | 25.910 | 22.717 | 19.026 | 1.00 21.58 |
| ATOM                      | 3753 | NE2 | GLN | F | 207 | 26.837 | 23.750 | 19.214 | 1.00 21.43 |
| ATOM                      | 3754 | C   | GLN | F | 207 | 29.115 | 19.288 | 22.557 | 1.00 23.38 |
| ATOM                      | 3755 | O   | GLN | F | 207 | 30.328 | 19.427 | 22.700 | 1.00 20.29 |
| ATOM                      | 3756 | N   | GLN | F | 208 | 28.536 | 18.104 | 22.385 | 1.00 20.97 |
| ATOM                      | 3757 | CA  | GLN | F | 208 | 29.306 | 16.884 | 22.159 | 1.00 21.08 |
| ATOM                      | 3758 | CG  | GLN | F | 208 | 29.935 | 15.803 | 21.353 | 1.00 21.22 |
| ATOM                      | 3759 | CG  | GLN | F | 208 | 28.555 | 16.336 | 24.479 | 1.00 37.67 |
| ATOM                      | 3760 | CD  | GLN | F | 208 | 29.691 | 16.310 | 25.434 | 1.00 44.53 |
| ATOM                      | 3761 | OE1 | GLN | F | 208 | 30.823 | 16.002 | 25.054 | 1.00 36.40 |
| ATOM                      | 3762 | NE2 | GLN | F | 208 | 29.406 | 16.133 | 26.699 | 1.00 43.30 |
| ATOM                      | 3763 | C   | GLN | F | 209 | 28.824 | 14.405 | 25.227 | 1.00 39.63 |
| ATOM                      | 3764 | O   | GLN | F | 209 | 27.880 | 15.873 | 20.554 | 1.00 20.55 |
| ATOM                      | 3765 | N   | VAL | F | 209 | 29.902 | 16.565 | 19.864 | 1.00 19.84 |
| ATOM                      | 3766 | CA  | VAL | F | 209 | 29.625 | 16.495 | 18.443 | 1.00 19.40 |
| ATOM                      | 3767 | CG  | VAL | F | 209 | 30.798 | 17.683 | 17.725 | 1.00 21.41 |
| ATOM                      | 3768 | CG2 | VAL | F | 209 | 29.963 | 17.669 | 16.262 | 1.00 21.60 |
| ATOM                      | 3769 | CG2 | VAL | F | 209 | 29.878 | 19.000 | 16.383 | 1.00 17.55 |
| ATOM                      | 3770 | C   | VAL | F | 209 | 30.135 | 15.200 | 17.824 | 1.00 18.78 |
| ATOM                      | 3771 | O   | VAL | F | 209 | 31.301 | 14.857 | 17.973 | 1.00 20.08 |
| ATOM                      | 3772 | N   | PRO | F | 210 | 33.270 | 14.498 | 17.114 | 1.00 22.82 |
| ATOM                      | 3773 | CA  | PRO | F | 210 | 29.702 | 13.112 | 16.386 | 1.00 22.81 |
| ATOM                      | 3774 | CG  | PRO | F | 210 | 28.191 | 12.580 | 16.099 | 1.00 25.33 |
| ATOM                      | 3775 | CG  | PRO | F | 210 | 27.359 | 13.806 | 16.002 | 1.00 23.26 |
| ATOM                      | 3776 | CD  | PRO | F | 210 | 27.816 | 14.771 | 16.944 | 1.00 19.81 |
| ATOM                      | 3777 | OE1 | PRO | F | 210 | 30.416 | 13.732 | 15.088 | 1.00 25.30 |
| ATOM                      | 3778 | O   | PRO | F | 210 | 28.824 | 14.216 | 15.504 | 1.00 22.81 |
| ATOM                      | 3779 | N   | LEU | F | 211 | 31.695 | 13.389 | 14.984 | 1.00 19.95 |
| ATOM                      | 3780 | CA  | LEU | F | 211 | 32.527 | 13.776 | 13.560 | 1.00 19.72 |
| ATOM                      | 3781 | CG  | LEU | F | 211 | 33.750 | 14.573 | 14.349 | 1.00 14.53 |
| ATOM                      | 3782 | CG  | LEU | F | 211 | 32.542 | 15.916 | 15.035 | 1.00 19.71 |
| ATOM                      | 3783 | CD  | LEU | F | 211 | 34.852 | 16.511 | 15.452 | 1.00 17.53 |
| ATOM                      | 3784 | OE1 | LEU | F | 211 | 32.796 | 16.876 | 14.305 | 1.00 19.83 |
| ATOM                      | 3785 | C   | LEU | F | 211 | 33.010 | 12.537 | 13.139 | 1.00 21.23 |
| ATOM                      | 3786 | O   | LEU | F | 211 | 33.155 | 11.475 | 13.746 | 1.00 22.01 |
| ATOM                      | 3787 | N   | ARG | F | 212 | 33.288 | 12.691 | 11.846 | 1.00 24.75 |
| ATOM                      | 3788 | CA  | ARG | F | 212 | 33.270 | 11.652 | 11.023 | 1.00 23.01 |
| ATOM                      | 3789 | CG  | ARG | F | 212 | 33.074 | 11.466 | 9.738  | 1.00 19.38 |
| ATOM                      | 3790 | CG  | ARG | F | 212 | 31.654 | 10.989 | 9.908  | 1.00 21.45 |
| ATOM                      | 3791 | CD  | ARG | F | 212 | 31.587 | 9.504  | 9.678  | 1.00 63.31 |
| ATOM                      | 3792 | OE1 | ARG | F | 212 | 30.218 | 9.810  | 9.675  | 1.00 68.84 |
| ATOM                      | 3793 | CZ  | ARG | F | 212 | 29.909 | 7.720  | 9.677  | 1.00 11.24 |
| ATOM                      | 3794 | NH1 | ARG | F | 212 | 30.880 | 6.815  | 9.691  | 1.00 70.96 |
| ATOM                      | 3795 | NH2 | ARG | F | 212 | 28.640 | 7.338  | 9.673  | 1.00 70.98 |
| ATOM                      | 3796 | C   | ARG | F | 212 | 35.294 | 11.978 | 10.658 | 1.00 17.64 |
| ATOM                      | 3797 | O   | ARG | F | 212 | 36.132 | 13.130 | 10.353 | 1.00 18.49 |
| ATOM                      | 3798 | N   | VAL | F | 213 | 36.139 | 10.964 | 10.653 | 1.00 20.41 |
| ATOM                      | 3799 | CA  | VAL | F | 213 | 37.488 | 11.093 | 10.147 | 1.00 26.17 |
| ATOM                      | 3800 | CG  | VAL | F | 213 | 36.514 | 10.629 | 11.193 | 1.00 25.00 |
| ATOM                      | 3801 | CG1 | VAL | F | 213 | 39.895 | 10.522 | 10.573 | 1.00 16.21 |
| ATOM                      | 3802 | CG2 | VAL | F | 213 | 39.521 | 11.390 | 12.380 | 1.00 20.46 |
| ATOM                      | 3803 | O   | VAL | F | 213 | 37.610 | 10.225 | 8.909  | 1.00 28.13 |
| ATOM                      | 3804 | O   | VAL | F | 213 | 37.283 | 9.077  | 6.942  | 1.00 26.12 |

| dimer-PDB-coordinates.txt |      |   |     |   |     |         |        |        |            |
|---------------------------|------|---|-----|---|-----|---------|--------|--------|------------|
| HETATM                    | 3868 | O | HON | S | 35  | 49.043  | 17.745 | 22.016 | 1.00 25.43 |
| HETATM                    | 3869 | O | HON | S | 40  | 54.167  | 11.388 | 34.397 | 1.00 22.47 |
| HETATM                    | 3870 | O | HON | S | 41  | 39.813  | 13.553 | 24.839 | 1.00 19.48 |
| HETATM                    | 3871 | O | HON | S | 42  | 23.075  | 16.208 | 46.228 | 1.00 20.99 |
| HETATM                    | 3872 | O | HON | S | 43  | 49.166  | 17.109 | 18.761 | 1.00 20.90 |
| HETATM                    | 3873 | O | HON | S | 44  | 42.771  | 27.378 | 42.584 | 1.00 31.77 |
| HETATM                    | 3874 | O | HON | S | 45  | 45.116  | 15.537 | 39.801 | 1.00 31.92 |
| HETATM                    | 3875 | O | HON | S | 46  | 47.039  | 16.033 | 26.100 | 1.00 25.74 |
| HETATM                    | 3876 | O | HON | S | 47  | 9.906   | 22.790 | 46.081 | 1.00 28.01 |
| HETATM                    | 3877 | O | HON | S | 48  | 48.620  | 18.216 | 18.077 | 1.00 26.17 |
| HETATM                    | 3878 | O | HON | S | 49  | 22.323  | 27.499 | 35.852 | 1.00 34.27 |
| HETATM                    | 3879 | O | HON | S | 50  | 5.437   | 35.970 | 30.795 | 1.00 22.65 |
| HETATM                    | 3880 | O | HON | S | 51  | 44.275  | 18.425 | 16.970 | 1.00 24.20 |
| HETATM                    | 3881 | O | HON | S | 52  | 47.778  | 12.773 | 16.342 | 1.00 28.89 |
| HETATM                    | 3882 | O | HON | S | 53  | 8.843   | 21.964 | 31.650 | 1.00 26.17 |
| HETATM                    | 3883 | O | HON | S | 54  | 42.215  | 11.916 | 18.388 | 1.00 33.00 |
| HETATM                    | 3884 | O | HON | S | 55  | 37.896  | 7.365  | 37.790 | 1.00 24.36 |
| HETATM                    | 3885 | O | HON | S | 56  | 4.583   | 32.143 | 48.563 | 1.00 26.04 |
| HETATM                    | 3886 | O | HON | S | 57  | 0.221   | 41.274 | 12.234 | 1.00 28.83 |
| HETATM                    | 3887 | O | HON | S | 58  | 50.639  | 32.772 | 19.398 | 1.00 37.77 |
| HETATM                    | 3888 | O | HON | S | 59  | 11.570  | 8.784  | 8.154  | 1.00 26.04 |
| HETATM                    | 3889 | O | HON | S | 60  | 37.874  | 10.101 | 35.870 | 1.00 23.00 |
| HETATM                    | 3890 | O | HON | S | 61  | 0.647   | 25.621 | 46.121 | 1.00 34.76 |
| HETATM                    | 3891 | O | HON | S | 62  | 41.460  | 12.596 | 41.670 | 1.00 33.36 |
| HETATM                    | 3892 | O | HON | S | 63  | 41.427  | 32.659 | 44.762 | 1.00 27.67 |
| HETATM                    | 3893 | O | HON | S | 64  | 1.316   | 22.453 | 46.044 | 1.00 35.79 |
| HETATM                    | 3894 | O | HON | S | 65  | 9.746   | 14.476 | 44.432 | 1.00 29.77 |
| HETATM                    | 3895 | O | HON | S | 66  | 35.198  | 6.506  | 36.380 | 1.00 27.55 |
| HETATM                    | 3896 | O | HON | S | 67  | 10.496  | 16.892 | 19.136 | 1.00 34.56 |
| HETATM                    | 3897 | O | HON | S | 68  | 7.425   | 10.677 | 60.304 | 1.00 37.73 |
| HETATM                    | 3898 | O | HON | S | 69  | 21.748  | 11.888 | 37.963 | 1.00 21.07 |
| HETATM                    | 3899 | O | HON | S | 70  | 12.710  | 36.452 | 53.880 | 1.00 30.10 |
| HETATM                    | 3900 | O | HON | S | 71  | 95.387  | 6.784  | 19.837 | 1.00 30.37 |
| HETATM                    | 3901 | O | HON | S | 72  | 44.630  | 12.567 | 39.453 | 1.00 30.84 |
| HETATM                    | 3902 | O | HON | S | 73  | 53.314  | 17.824 | 5.518  | 1.00 38.39 |
| HETATM                    | 3903 | O | HON | S | 74  | 16.106  | 21.729 | 13.869 | 1.00 40.25 |
| HETATM                    | 3904 | O | HON | S | 75  | 9.065   | 33.447 | 46.921 | 1.00 31.04 |
| HETATM                    | 3905 | O | HON | S | 76  | 50.320  | 22.238 | 22.455 | 1.00 41.57 |
| HETATM                    | 3906 | O | HON | S | 77  | 54.868  | 10.685 | 55.259 | 1.00 34.57 |
| HETATM                    | 3907 | O | HON | S | 78  | 24.164  | 11.420 | 30.477 | 1.00 26.68 |
| HETATM                    | 3908 | O | HON | S | 79  | 51.485  | 15.437 | 6.407  | 1.00 33.52 |
| HETATM                    | 3909 | O | HON | S | 80  | 8.962   | 10.803 | 49.359 | 1.00 28.86 |
| HETATM                    | 3910 | O | HON | S | 81  | 6.858   | 11.816 | 30.750 | 1.00 34.57 |
| HETATM                    | 3911 | O | HON | S | 82  | -10.563 | 40.219 | 41.170 | 1.00 17.45 |
| HETATM                    | 3912 | O | HON | S | 83  | 18.791  | 18.539 | 39.812 | 1.00 41.73 |
| HETATM                    | 3913 | O | HON | S | 84  | 26.506  | 26.752 | 26.575 | 1.00 34.09 |
| HETATM                    | 3914 | O | HON | S | 85  | 36.829  | 21.160 | 48.125 | 1.00 35.88 |
| HETATM                    | 3915 | O | HON | S | 86  | 60.842  | 20.830 | 24.584 | 1.00 37.60 |
| HETATM                    | 3916 | O | HON | S | 87  | 8.645   | 21.145 | 44.243 | 1.00 30.09 |
| HETATM                    | 3917 | O | HON | S | 88  | -4.684  | 18.553 | 48.964 | 1.00 31.22 |
| HETATM                    | 3918 | O | HON | S | 89  | -0.717  | 19.021 | 29.824 | 1.00 36.77 |
| HETATM                    | 3919 | O | HON | S | 90  | 6.816   | 16.372 | 43.470 | 1.00 32.00 |
| HETATM                    | 3920 | O | HON | S | 91  | 17.260  | 5.101  | 38.902 | 1.00 40.73 |
| HETATM                    | 3921 | O | HON | S | 92  | 20.476  | 16.755 | 28.841 | 1.00 41.35 |
| HETATM                    | 3922 | O | HON | S | 93  | 18.982  | 20.713 | 36.210 | 1.00 31.12 |
| HETATM                    | 3923 | O | HON | S | 94  | 90.668  | 8.218  | 19.473 | 1.00 35.98 |
| HETATM                    | 3924 | O | HON | S | 95  | 40.114  | 31.963 | 37.966 | 1.00 43.20 |
| HETATM                    | 3925 | O | HON | S | 96  | 57.449  | 25.842 | 37.562 | 1.00 29.67 |
| HETATM                    | 3926 | O | HON | S | 97  | 49.281  | 39.253 | 23.932 | 1.00 38.48 |
| HETATM                    | 3927 | O | HON | S | 98  | -1.215  | 25.026 | 49.741 | 1.00 29.51 |
| HETATM                    | 3928 | O | HON | S | 99  | 7.796   | 24.367 | 40.493 | 1.00 32.03 |
| HETATM                    | 3929 | O | HON | S | 100 | -9.520  | 41.020 | 42.439 | 1.00 27.49 |
| HETATM                    | 3930 | O | HON | S | 101 | 21.398  | 22.441 | 34.448 | 1.00 35.79 |

|                           |      |     |     |   |     |         |        |        |            |
|---------------------------|------|-----|-----|---|-----|---------|--------|--------|------------|
| dimer-PDB-coordinates.txt |      |     |     |   |     |         |        |        |            |
| ATOM                      | 3805 | N   | SER | F | 214 | 38.080  | 10.821 | 7.821  | 1.00 22.34 |
| ATOM                      | 3806 | CA  | SER | F | 214 | 38.244  | 10.123 | 6.542  | 1.00 22.66 |
| ATOM                      | 3807 | CB  | SER | F | 214 | 37.253  | 10.651 | 5.504  | 1.00 28.04 |
| ATOM                      | 3808 | OG  | SER | F | 214 | 35.936  | 10.711 | 6.025  | 1.00 28.71 |
| ATOM                      | 3809 | C   | SER | F | 214 | 39.652  | 10.354 | 6.020  | 1.00 20.37 |
| ATOM                      | 3810 | O   | SER | F | 214 | 40.337  | 11.279 | 6.460  | 1.00 23.23 |
| ATOM                      | 3811 | N   | PRO | F | 215 | 40.107  | 9.517  | 5.072  | 1.00 39.92 |
| ATOM                      | 3812 | CA  | PRO | F | 215 | 41.442  | 9.735  | 4.023  | 1.00 37.93 |
| ATOM                      | 3813 | CB  | PRO | F | 215 | 41.646  | 8.514  | 3.595  | 1.00 37.93 |
| ATOM                      | 3814 | CG  | PRO | F | 215 | 40.611  | 7.524  | 4.025  | 1.00 46.15 |
| ATOM                      | 3815 | CD  | PRO | F | 215 | 39.447  | 8.336  | 4.492  | 1.00 37.38 |
| ATOM                      | 3816 | C   | PRO | F | 215 | 41.455  | 11.019 | 3.628  | 1.00 35.17 |
| ATOM                      | 3817 | O   | PRO | F | 215 | 40.411  | 11.389 | 2.640  | 1.00 37.66 |
| ATOM                      | 3818 | O   | TYR | F | 216 | 44.158  | 11.871 | 1.161  | 1.00 42.96 |
| ATOM                      | 3819 | N   | TYR | F | 216 | 42.604  | 11.687 | 3.601  | 1.00 30.60 |
| ATOM                      | 3820 | CA  | TYR | F | 216 | 42.721  | 12.891 | 2.780  | 1.00 40.07 |
| ATOM                      | 3821 | C   | TYR | F | 216 | 43.145  | 12.544 | 1.356  | 1.00 38.96 |
| ATOM                      | 3822 | CG  | TYR | F | 216 | 43.733  | 13.850 | 3.195  | 1.00 36.75 |
| ATOM                      | 3823 | CG  | TYR | F | 216 | 43.820  | 15.102 | 2.640  | 1.00 36.65 |
| ATOM                      | 3824 | CD  | TYR | F | 216 | 42.677  | 15.923 | 2.429  | 1.00 51.23 |
| ATOM                      | 3825 | CDZ | TYR | F | 216 | 45.043  | 15.708 | 2.301  | 1.00 46.98 |
| ATOM                      | 3826 | CE1 | TYR | F | 216 | 42.744  | 17.142 | 1.807  | 1.00 55.07 |
| ATOM                      | 3827 | CE2 | TYR | F | 216 | 45.120  | 16.950 | 1.670  | 1.00 36.44 |
| ATOM                      | 3828 | O   | TYR | F | 216 | 43.966  | 17.645 | 1.878  | 1.00 37.23 |
| ATOM                      | 3829 | OH  | TYR | F | 216 | 44.025  | 18.870 | 0.801  | 1.00 56.33 |
| HETATM                    | 3830 | O   | HOM | S | 1   | 21.221  | 5.609  | 4.647  | 1.00 20.93 |
| HETATM                    | 3831 | O   | HOM | S | 2   | -4.438  | 19.691 | 18.586 | 1.00 18.25 |
| HETATM                    | 3832 | O   | HOM | S | 3   | 23.251  | 9.234  | 12.586 | 1.00 18.61 |
| HETATM                    | 3833 | O   | HOM | S | 4   | 61.109  | 21.153 | 29.786 | 1.00 28.71 |
| HETATM                    | 3834 | O   | HOM | S | 5   | 23.484  | 23.279 | 14.094 | 1.00 38.34 |
| HETATM                    | 3835 | O   | HOM | S | 6   | -7.014  | 21.348 | 13.655 | 1.00 16.31 |
| HETATM                    | 3836 | O   | HOM | S | 7   | 22.295  | 5.464  | 27.076 | 1.00 23.31 |
| HETATM                    | 3837 | O   | HOM | S | 8   | 8.281   | 32.554 | 25.861 | 1.00 34.92 |
| HETATM                    | 3838 | O   | HOM | S | 9   | 28.159  | -1.537 | 43.806 | 1.00 26.96 |
| HETATM                    | 3839 | O   | HOM | S | 10  | 19.831  | 5.949  | 43.009 | 1.00 27.72 |
| HETATM                    | 3840 | O   | HOM | S | 11  | 49.796  | 15.156 | 20.698 | 1.00 20.26 |
| HETATM                    | 3841 | O   | HOM | S | 12  | -3.361  | 20.504 | 25.107 | 1.00 28.66 |
| HETATM                    | 3842 | O   | HOM | S | 13  | 54.832  | 22.462 | 19.827 | 1.00 21.95 |
| HETATM                    | 3843 | O   | HOM | S | 14  | -1.165  | 22.957 | 44.203 | 1.00 19.92 |
| HETATM                    | 3844 | O   | HOM | S | 15  | 49.059  | 4.532  | 11.588 | 1.00 37.64 |
| HETATM                    | 3845 | O   | HOM | S | 16  | 35.659  | 33.051 | 19.260 | 1.00 22.58 |
| HETATM                    | 3846 | O   | HOM | S | 17  | 15.100  | 35.943 | 55.333 | 1.00 42.87 |
| HETATM                    | 3847 | O   | HOM | S | 18  | -0.632  | 20.465 | 15.190 | 1.00 20.99 |
| HETATM                    | 3848 | O   | HOM | S | 19  | 35.508  | 29.253 | 54.114 | 1.00 28.46 |
| HETATM                    | 3849 | O   | HOM | S | 20  | 38.220  | 30.946 | 7.056  | 1.00 35.11 |
| HETATM                    | 3850 | O   | HOM | S | 21  | 41.569  | 47.447 | 19.099 | 1.00 27.81 |
| HETATM                    | 3851 | O   | HOM | S | 22  | 27.416  | 13.273 | 27.836 | 1.00 24.66 |
| HETATM                    | 3852 | O   | HOM | S | 23  | -2.321  | 23.386 | 47.609 | 1.00 21.44 |
| HETATM                    | 3853 | O   | HOM | S | 24  | 51.932  | 15.248 | 8.559  | 1.00 22.64 |
| HETATM                    | 3854 | O   | HOM | S | 25  | 40.714  | 26.555 | 2.331  | 1.00 27.00 |
| HETATM                    | 3855 | O   | HOM | S | 26  | 44.724  | 27.04  | 47.406 | 1.00 23.89 |
| HETATM                    | 3856 | O   | HOM | S | 27  | -4.252  | 17.085 | 67.756 | 1.00 23.27 |
| HETATM                    | 3857 | O   | HOM | S | 28  | 34.400  | 9.250  | 20.834 | 1.00 30.75 |
| HETATM                    | 3858 | O   | HOM | S | 29  | 31.742  | 11.915 | 31.743 | 1.00 23.71 |
| HETATM                    | 3859 | O   | HOM | S | 30  | 19.187  | 3.636  | 31.708 | 1.00 23.48 |
| HETATM                    | 3860 | O   | HOM | S | 31  | 389.044 | 33.929 | 33.929 | 1.00 31.00 |
| HETATM                    | 3861 | O   | HOM | S | 32  | 29.363  | 17.105 | 33.492 | 1.00 31.41 |
| HETATM                    | 3862 | O   | HOM | S | 33  | 52.739  | 10.230 | 17.866 | 1.00 36.70 |
| HETATM                    | 3863 | O   | HOM | S | 34  | 53.627  | 41.622 | 31.045 | 1.00 28.81 |
| HETATM                    | 3864 | O   | HOM | S | 35  | 21.647  | 9.530  | 35.992 | 1.00 19.41 |
| HETATM                    | 3865 | O   | HOM | S | 36  | 9.366   | 34.284 | 44.525 | 1.00 22.24 |
| HETATM                    | 3866 | O   | HOM | S | 37  | -5.063  | 20.358 | 58.099 | 1.00 27.68 |
| HETATM                    | 3867 | O   | HOM | S | 38  | 63.141  | 26.837 | 27.147 | 1.00 35.35 |

| dimer-PDB-coordinates.txt |   |           |                                  | dimer-PDB-coordinates.txt |           |           |                                  |
|---------------------------|---|-----------|----------------------------------|---------------------------|-----------|-----------|----------------------------------|
| HETATM 3994               | O | HOH S 165 | -9.282 40.297 38.848 1.00 36.38  | O                         |           |           |                                  |
| HETATM 3995               | O | HOH S 166 | 11.691 24.052 20.249 1.00 35.48  | O HETATM 4057             | O         | HOH S 228 | -5.071 21.327 64.068 1.00 41.14  |
| HETATM 3996               | O | HOH S 167 | 2.373 39.998 48.812 1.00 41.75   | O HETATM 4058             | O         | HOH S 229 | 54.466 8.266 28.809 1.00 47.02   |
| HETATM 3997               | O | HOH S 168 | 21.518 0.309 28.567 1.00 40.64   | O HETATM 4059             | O         | HOH S 230 | 6.850 39.512 28.760 1.00 44.36   |
| HETATM 3998               | O | HOH S 169 | 43.380 25.963 45.023 1.00 38.11  | O HETATM 4060             | O         | HOH S 231 | 24.868 22.046 56.865 1.00 46.59  |
| HETATM 3999               | O | HOH S 170 | 51.342 12.523 4.323 1.00 43.38   | O HETATM 4061             | O         | HOH S 232 | -3.272 20.128 65.707 1.00 47.63  |
| HETATM 4000               | O | HOH S 171 | 35.530 8.330 34.419 1.00 35.81   | O HETATM 4062             | O         | HOH S 233 | 41.427 11.715 32.489 1.00 42.77  |
| HETATM 4001               | O | HOH S 172 | -8.074 20.470 42.477 1.00 41.00  | O HETATM 4063             | O         | HOH S 234 | -12.962 31.824 43.545 1.00 37.91 |
| HETATM 4002               | O | HOH S 173 | 25.037 1.467 20.547 1.00 50.25   | O HETATM 4064             | O         | HOH S 235 | 23.778 3.245 36.878 1.00 40.08   |
| HETATM 4003               | O | HOH S 174 | 27.164 26.865 32.514 1.00 41.74  | O HETATM 4065             | O         | HOH S 236 | 8.862 23.864 19.184 1.00 39.74   |
| HETATM 4004               | O | HOH S 175 | 6.457 23.954 25.273 1.00 42.09   | O HETATM 4066             | O         | HOH S 237 | 25.789 1.411 37.337 1.00 43.15   |
| HETATM 4005               | O | HOH S 176 | 51.020 25.018 24.036 1.00 37.06  | O HETATM 4067             | O         | HOH S 238 | 36.196 29.450 32.136 1.00 42.17  |
| HETATM 4006               | O | HOH S 177 | 43.687 31.780 22.070 1.00 46.50  | O HETATM 4068             | O         | HOH S 239 | 10.234 9.431 50.535 1.00 43.98   |
| HETATM 4007               | O | HOH S 178 | 37.564 23.178 27.935 1.00 45.76  | O HETATM 4069             | O         | HOH S 240 | 67.550 27.018 29.741 1.00 50.92  |
| HETATM 4008               | O | HOH S 179 | 3.096 32.329 49.262 1.00 34.90   | O HETATM 4070             | O         | HOH S 241 | 32.108 19.069 54.652 1.00 47.45  |
| HETATM 4009               | O | HOH S 180 | 17.681 29.337 26.021 1.00 39.46  | O HETATM 4071             | O         | HOH S 242 | 37.563 6.519 7.374 1.00 47.89    |
| HETATM 4010               | O | HOH S 181 | 35.733 25.359 19.506 1.00 34.29  | O HETATM 4072             | O         | HOH S 243 | 5.096 17.518 26.627 1.00 48.69   |
| HETATM 4011               | O | HOH S 182 | -4.998 35.105 49.055 1.00 40.78  | O HETATM 4073             | O         | HOH S 244 | 14.860 34.963 43.070 1.00 46.92  |
| HETATM 4012               | O | HOH S 183 | 37.092 21.412 30.959 1.00 38.02  | O HETATM 4074             | O         | HOH S 245 | 23.261 6.239 34.676 1.00 38.88   |
| HETATM 4013               | O | HOH S 184 | 19.080 17.105 55.227 1.00 37.80  | O HETATM 4075             | O         | HOH S 246 | 11.807 14.600 44.397 1.00 44.37  |
| HETATM 4014               | O | HOH S 185 | 12.425 16.697 37.200 1.00 34.18  | O HETATM 4076             | O         | HOH S 247 | 26.215 30.639 33.521 1.00 48.82  |
| HETATM 4015               | O | HOH S 186 | 46.800 33.505 39.829 1.00 35.34  | O TER 4077                | HOH S 247 |           |                                  |
| HETATM 4016               | O | HOH S 187 | 14.787 3.578 37.197 1.00 42.00   | O                         | END       |           |                                  |
| HETATM 4017               | O | HOH S 188 | 62.812 21.431 36.641 1.00 42.34  | O                         |           |           |                                  |
| HETATM 4018               | O | HOH S 189 | 27.852 8.907 17.300 1.00 38.92   | O                         |           |           |                                  |
| HETATM 4019               | O | HOH S 190 | 5.894 49.090 36.724 1.00 42.99   | O                         |           |           |                                  |
| HETATM 4020               | O | HOH S 191 | 31.670 17.937 33.299 1.00 39.74  | O                         |           |           |                                  |
| HETATM 4021               | O | HOH S 192 | 33.176 31.837 36.416 1.00 35.80  | O                         |           |           |                                  |
| HETATM 4022               | O | HOH S 193 | 52.452 10.866 20.106 1.00 41.18  | O                         |           |           |                                  |
| HETATM 4023               | O | HOH S 194 | 7.277 17.811 45.829 1.00 39.24   | O                         |           |           |                                  |
| HETATM 4024               | O | HOH S 195 | -1.240 41.881 51.365 1.00 42.32  | O                         |           |           |                                  |
| HETATM 4025               | O | HOH S 196 | 49.106 35.672 17.582 1.00 41.10  | O                         |           |           |                                  |
| HETATM 4026               | O | HOH S 197 | 21.427 2.526 51.935 1.00 36.36   | O                         |           |           |                                  |
| HETATM 4027               | O | HOH S 198 | 51.305 27.098 42.571 1.00 41.01  | O                         |           |           |                                  |
| HETATM 4028               | O | HOH S 199 | -11.704 33.595 31.301 1.00 44.39 | O                         |           |           |                                  |
| HETATM 4029               | O | HOH S 200 | 42.150 25.315 -0.048 1.00 42.65  | O                         |           |           |                                  |
| HETATM 4030               | O | HOH S 201 | 5.984 12.234 46.086 1.00 41.87   | O                         |           |           |                                  |
| HETATM 4031               | O | HOH S 202 | 28.701 27.034 25.782 1.00 49.26  | O                         |           |           |                                  |
| HETATM 4032               | O | HOH S 203 | 23.756 21.507 11.666 1.00 43.30  | O                         |           |           |                                  |
| HETATM 4033               | O | HOH S 204 | 39.879 21.176 25.770 1.00 43.38  | O                         |           |           |                                  |
| HETATM 4034               | O | HOH S 205 | 20.482 -1.034 40.457 1.00 45.26  | O                         |           |           |                                  |
| HETATM 4035               | O | HOH S 206 | -10.007 31.388 45.809 1.00 39.80 | O                         |           |           |                                  |
| HETATM 4036               | O | HOH S 207 | -2.799 15.691 40.979 1.00 50.97  | O                         |           |           |                                  |
| HETATM 4037               | O | HOH S 208 | 11.763 35.466 51.563 1.00 46.85  | O                         |           |           |                                  |
| HETATM 4038               | O | HOH S 209 | -2.852 41.013 25.510 1.00 37.56  | O                         |           |           |                                  |
| HETATM 4039               | O | HOH S 210 | -16.544 26.697 37.367 1.00 26.50 | O                         |           |           |                                  |
| HETATM 4040               | O | HOH S 211 | 35.197 22.163 24.295 1.00 39.11  | O                         |           |           |                                  |
| HETATM 4041               | O | HOH S 212 | 24.036 19.892 56.952 1.00 42.94  | O                         |           |           |                                  |
| HETATM 4042               | O | HOH S 213 | 51.088 26.431 21.988 1.00 43.64  | O                         |           |           |                                  |
| HETATM 4043               | O | HOH S 214 | -1.696 17.105 29.227 1.00 39.75  | O                         |           |           |                                  |
| HETATM 4044               | O | HOH S 215 | 32.262 21.969 24.877 1.00 31.01  | O                         |           |           |                                  |
| HETATM 4045               | O | HOH S 216 | 47.026 20.287 5.338 1.00 49.06   | O                         |           |           |                                  |
| HETATM 4046               | O | HOH S 217 | 19.814 0.487 37.793 1.00 47.56   | O                         |           |           |                                  |
| HETATM 4047               | O | HOH S 218 | 22.763 3.969 29.881 1.00 33.75   | O                         |           |           |                                  |
| HETATM 4048               | O | HOH S 219 | 20.404 13.754 8.768 1.00 37.27   | O                         |           |           |                                  |
| HETATM 4049               | O | HOH S 220 | 9.308 22.277 42.182 1.00 41.67   | O                         |           |           |                                  |
| HETATM 4050               | O | HOH S 221 | 21.616 6.796 52.594 1.00 39.07   | O                         |           |           |                                  |
| HETATM 4051               | O | HOH S 222 | 5.798 6.390 19.316 1.00 54.60    | O                         |           |           |                                  |
| HETATM 4052               | O | HOH S 223 | -6.033 29.948 55.762 1.00 46.80  | O                         |           |           |                                  |
| HETATM 4053               | O | HOH S 224 | 51.961 4.665 35.931 1.00 45.87   | O                         |           |           |                                  |
| HETATM 4054               | O | HOH S 225 | 19.679 9.217 46.387 1.00 41.46   | O                         |           |           |                                  |
| HETATM 4055               | O | HOH S 226 | 22.613 4.644 21.797 1.00 34.09   | O                         |           |           |                                  |
| HETATM 4056               | O | HOH S 227 | 62.226 30.854 35.763 1.00 48.70  | O                         |           |           |                                  |

FIGURE 33

REMARK TOTAL octamer-PDB-coordinates.txt  
REMARK 3 5332 5264.00  
REMARK 3 C\_free\_flags.md5.hexdigest 17e8a21009d4d6f90b3b9cccf760c0  
REMARK 3 IF THIS FILE IS FOR PDB DEPOSITION: REMOVE ALL FROM THIS LINE UP.  
REMARK 3  
REMARK 3 REFINEMENT.  
REMARK 3 PROGRAM : PHENIX (phenix.refine: 1.9-1692)  
REMARK 3 AUTHORS : Adams, Afonine, Burnley, Chen, Davis, Echols, Gildea,  
REMARK 3 : Gopal, Gros, Grosse-Kunstleve, Headd, Hung, Immerino,  
REMARK 3 : Jorgensen, McCoy, McKee, Moriarty, Pai, Read, Richardson,  
REMARK 3 : Rienecker, Romo-Bohmer, Sachdev, Sauter, Smith, Storer,  
REMARK 3 : Terwilliger, Zwart  
REMARK 3  
REMARK 3 REFINEMENT TARGET : ML  
REMARK 3  
REMARK 3 DATA USED IN REFINEMENT.  
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.475  
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 36.714  
REMARK 3 MIN(FOBS, SIGMA\_FOBS) : 0.11  
REMARK 3 COMPLETENESS FOR RANGE (%) : 89.62  
REMARK 3 NUMBER OF REFLECTIONS : 26058  
REMARK 3 NUMBER OF REFLECTIONS (NON-ANOMALOUS) : 26958  
REMARK 3  
REMARK 3 FIT TO DATA USED IN REFINEMENT.  
REMARK 3 R VALUE (WORKING SET) : 0.2236  
REMARK 3 R VALUE (WORKING SET) : 0.2207  
REMARK 3 FREE R VALUE : 0.2638  
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 6.80  
REMARK 3 FREE R VALUE TEST SET COUNT : 1832  
REMARK 3  
REMARK 3 FIT TO DATA USED IN REFINEMENT (IN BINS).  
REMARK 3 BIN RESOLUTION RANGE COMPLETION NWORK NFREE RWORK RFREE  
REMARK 3 1 36.7180 - 5.8113 0.97 2147 157 0.1927 0.2290  
REMARK 3 2 5.8113 - 4.6115 0.99 2149 153 0.1842 0.2123  
REMARK 3 3 4.6115 - 3.8113 0.98 2152 150 0.1773 0.2098  
REMARK 3 4 3.8113 - 3.2625 0.87 1872 139 0.2057 0.2441  
REMARK 3 5 3.2625 - 2.8113 0.88 1905 142 0.2351 0.3294  
REMARK 3 6 2.8113 - 2.4750 0.95 1896 135 0.2500 0.3020  
REMARK 3 7 2.4750 - 2.2000 0.96 2122 150 0.2506 0.2488  
REMARK 3 8 2.2000 - 1.9000 0.95 2009 146 0.2485 0.3158  
REMARK 3 9 1.9000 - 1.7971 0.91 1938 142 0.2579 0.3201  
REMARK 3 10 1.7971 - 1.7006 0.84 1842 134 0.2737 0.3271  
REMARK 3 11 1.7006 - 1.6162 0.85 1786 127 0.3013 0.3053  
REMARK 3 12 1.6162 - 1.5414 0.78 1720 121 0.3072 0.3970  
REMARK 3 13 1.5414 - 1.4745 0.78 1625 132 0.2778 0.3483  
REMARK 3  
REMARK 3 BULK SOLVENT MODELLING.  
REMARK 3 METHOD USED : FLAT BULK SOLVENT MODEL  
REMARK 3 SOLVENT RADIUS : 1.11  
REMARK 3 SHRINKAGE RADIUS : 0.90  
REMARK 3 GRID STEP FACTOR : 4.00  
REMARK 3  
REMARK 3 ERROR ESTIMATES.  
REMARK 3 COORDINATE ERROR (MAXIMUM-LIKELIHOOD BASED) : 0.39  
REMARK 3 PHASE ERROR (DEGREES, MAXIMUM-LIKELIHOOD BASED) : 28.72  
REMARK 3  
REMARK 3 STRUCTURE FACTORS CALCULATION ALGORITHM : FFT  
REMARK 3  
REMARK 3 DEVIATIONS FROM IDEAL VALUES.  
REMARK 3 RMSD MAX COUNT  
REMARK 3 BOND : 0.003 0.035 1099  
REMARK 3 ANGLE : 0.742 5.795 7008

REMARK 3 octamer-PDB-coordinates.txt  
REMARK 3 CHIRALITY : 0.037 0.331 768  
REMARK 3 PLANARITY : 0.003 0.026 933  
REMARK 3 DIHEDRAL : 11.056 74.369 1980  
REMARK 3 MIN NONBONDED DISTANCE : 1.865  
REMARK 3  
REMARK 3 MOLPROBITY STATISTICS.  
REMARK 3 ALL-ATOM CLASHSCORE : 6.95  
REMARK 3 RAMACHANDRAN PLOT:  
REMARK 3 OUTLIERS : 0.00 %  
REMARK 3 ALLOWED : 1.68 %  
REMARK 3 FAVORED : 98.32 %  
REMARK 3 ROTAMER OUTLIERS : 1.45 %  
REMARK 3 CBETA DEVIATIONS : 0  
REMARK 3  
REMARK 3 ATOMIC DISPLACEMENT PARAMETERS.  
REMARK 3 WILSON B : NONE  
REMARK 3 RMS(B\_ISO\_OR\_EQUIVALENT BONDED) : 7.31  
REMARK 3 ATOMS NUMBER OF ATOMS  
REMARK 3 ZSO ANISO  
REMARK 3 ALL (NO H) : 5332 0  
REMARK 3 SOLVENT : 213 0  
REMARK 3 NON-SOLVENT : 5119 0  
REMARK 3 HYDROGENS : 0 0  
REMARK 3  
REMARK 3 TORSION ACS DETAILS.  
REMARK 3 NUMBER OF ACS GROUPS : 1  
REMARK 3 ACS GROUP : 1  
REMARK 3 SELECTION : chain 'A'  
REMARK 3 SELECTION : chain 'B'  
REMARK 3 SELECTION : chain 'C'  
REMARK 3 SELECTION : chain 'D'  
REMARK 3 SELECTION : chain 'E'  
REMARK 3 SELECTION : chain 'F'  
REMARK 3 SELECTION : chain 'G'  
REMARK 3 SELECTION : chain 'H'  
REMARK 3  
REMARK 3 RESTRAINED TORSIONS: 3204  
REMARK 3 BELOW LIMIT RMSD : 1.184  
REMARK 3 ALL RESTRAINT RMSD : 11.643  
REMARK 3 Histogram of differences under limit:  
REMARK 3 1.500 - 3.000: 216  
REMARK 3 3.000 - 4.500: 32  
REMARK 3 4.500 - 6.000: 14  
REMARK 3 6.000 - 7.500: 4  
REMARK 3 7.500 - 9.000: 13  
REMARK 3 9.000 - 10.500: 1  
REMARK 3 10.500 - 12.000: 3  
REMARK 3 12.000 - 13.500: 2  
REMARK 3 13.500 - 15.000: 0  
REMARK 3 Histogram of differences over limit:  
REMARK 3 15.000 - 31.200: 1  
REMARK 3 31.200 - 47.400: 13  
REMARK 3 47.400 - 63.600: 10  
REMARK 3 63.600 - 79.800: 8  
REMARK 3 79.800 - 96.000: 15  
REMARK 3 96.000 - 112.200: 5  
REMARK 3 112.200 - 128.400: 1  
REMARK 3 128.400 - 144.600: 3  
REMARK 3 144.600 - 160.800: 2  
REMARK 3 160.800 - 177.000: 2  
REMARK 3  
CRYST1 44.412 125.316 77.175 90.00 90.32 90.00 P 1 21 1

SCALE1 3 0.022516 0.000000 0.000000 0.000000  
SCALE2 3 0.000000 0.007980 0.000000 0.000000  
SCALE3 3 0.000000 0.000000 0.012958 0.000000  
ATOM 1 N ARG A 135 14.767 -34.173 5.266 1.00 51.47  
ATOM 2 CA ARG A 135 14.641 -34.427 6.697 1.00 45.35  
ATOM 3 C ARG A 135 14.530 -33.110 7.460 1.00 54.02  
ATOM 4 O ARG A 135 14.697 -32.036 6.888 1.00 45.28  
ATOM 5 CB ARG A 135 15.835 -35.245 7.204 1.00 49.06  
ATOM 6 CG ARG A 135 15.526 -36.124 8.407 1.00 62.03  
ATOM 7 CD ARG A 135 14.637 -37.297 9.025 1.00 49.49  
ATOM 8 HE ARG A 135 15.237 -38.105 9.967 1.00 56.43  
ATOM 9 CZ ARG A 135 16.197 -39.002 7.168 1.00 61.27  
ATOM 10 NH2 ARG A 135 16.672 -39.207 8.387 1.00 58.41  
ATOM 11 NH2 ARG A 135 16.686 -39.693 5.144 1.00 43.95  
ATOM 12 N ARG A 136 14.270 -33.200 8.759 1.00 41.92  
ATOM 13 CA ARG A 136 14.017 -32.020 9.575 1.00 30.08  
ATOM 14 C ARG A 136 15.003 -31.919 10.749 1.00 44.28  
ATOM 15 O ARG A 136 15.411 -32.937 11.307 1.00 40.52  
ATOM 16 CB ARG A 136 12.559 -32.073 10.057 1.00 36.54  
ATOM 17 CG ARG A 136 11.596 -32.044 8.877 1.00 57.65  
ATOM 18 CD ARG A 136 10.151 -32.125 9.276 1.00 58.06  
ATOM 19 NE ARG A 136 9.259 -31.950 8.117 1.00 67.51  
ATOM 20 CZ ARG A 136 7.995 -31.549 8.183 1.00 71.90  
ATOM 21 NH2 ARG A 136 7.449 -31.226 9.347 1.00 71.13  
ATOM 22 NH2 ARG A 136 7.287 -31.413 7.079 1.00 65.75  
ATOM 23 N VAL A 137 15.387 -30.695 11.121 1.00 34.33  
ATOM 24 CA VAL A 137 15.367 -30.501 12.197 1.00 34.02  
ATOM 25 C VAL A 137 15.917 -29.547 13.303 1.00 38.16  
ATOM 26 O VAL A 137 14.913 -28.844 13.176 1.00 28.18  
ATOM 27 CB VAL A 137 17.713 -29.959 11.662 1.00 28.97  
ATOM 28 CG VAL A 137 18.347 -30.942 10.698 1.00 24.17  
ATOM 29 CG2 VAL A 137 17.528 -28.596 11.009 1.00 29.15  
ATOM 30 N LEU A 138 16.664 -29.591 14.391 1.00 37.13  
ATOM 31 CA LEU A 138 16.432 -28.626 15.511 1.00 25.86  
ATOM 32 C LEU A 138 17.597 -27.666 15.742 1.00 31.16  
ATOM 33 O LEU A 138 18.745 -26.088 15.885 1.00 36.36  
ATOM 34 CB LEU A 138 16.152 -29.416 16.792 1.00 35.51  
ATOM 35 CG LEU A 138 15.680 -28.602 17.995 1.00 37.63  
ATOM 36 CD LEU A 138 14.275 -28.070 17.757 1.00 40.40  
ATOM 37 CO2 LEU A 138 15.235 -29.433 19.266 1.00 48.51  
ATOM 38 N VAL A 139 17.294 -26.372 15.772 1.00 24.34  
ATOM 39 CA VAL A 139 18.306 -25.349 16.007 1.00 21.27  
ATOM 40 C VAL A 139 18.235 -24.841 17.444 1.00 27.88  
ATOM 41 O VAL A 139 17.221 -24.284 17.864 1.00 28.81  
ATOM 42 CB VAL A 139 16.142 -24.160 15.041 1.00 33.76  
ATOM 43 CG2 VAL A 139 19.354 -23.209 15.163 1.00 20.13  
ATOM 44 CG2 VAL A 139 19.001 -24.656 13.611 1.00 31.69  
ATOM 45 N THR A 140 19.314 -25.042 16.195 1.00 41.75  
ATOM 46 CA THR A 140 19.360 -24.840 19.598 1.00 30.19  
ATOM 47 C THR A 140 20.560 -23.744 19.887 1.00 42.29  
ATOM 48 O THR A 140 21.598 -23.688 19.103 1.00 36.57  
ATOM 49 CB THR A 140 19.423 -25.863 20.534 1.00 31.86  
ATOM 50 CG2 THR A 140 18.240 -26.788 20.291 1.00 34.86  
ATOM 51 OG1 THR A 140 20.643 -26.580 20.306 1.00 32.22  
ATOM 52 N GLY A 141 20.513 -23.043 21.016 1.00 42.58  
ATOM 53 CA GLY A 141 21.639 -22.240 21.456 1.00 35.84  
ATOM 54 C GLY A 141 21.316 -20.751 21.505 1.00 41.20  
ATOM 55 O GLY A 141 22.257 -19.952 21.764 1.00 45.15  
ATOM 56 N PHE A 142 20.108 -20.373 21.249 1.00 48.80  
ATOM 57 CA PHE A 142 19.723 -18.965 21.249 1.00 60.86  
ATOM 58 C PHE A 142 19.823 -18.320 22.629 1.00 59.26  
ATOM 59 O PHE A 142 19.199 -18.717 23.583 1.00 53.61  
ATOM 60 CB PHE A 142 16.397 -18.603 20.719 1.00 51.57

octamer-PDB-coordinates.txt  
ATOM 61 CG PHE A 142 18.084 -19.357 19.359 1.00 45.55  
ATOM 62 CD1 PHE A 142 18.428 -18.658 18.220 1.00 45.59  
ATOM 63 CD2 PHE A 142 17.534 -20.659 19.218 1.00 36.41  
ATOM 64 CE1 PHE A 142 18.233 -19.211 16.966 1.00 39.23  
ATOM 65 CE2 PHE A 142 17.136 -21.206 17.966 1.00 35.84  
ATOM 66 CE3 PHE A 142 17.686 -20.492 16.839 1.00 34.35  
ATOM 67 N PRO A 143 20.618 -17.245 22.739 1.00 64.85  
ATOM 68 CA PRO A 143 20.750 -16.481 23.982 1.00 68.91  
ATOM 69 C PRO A 143 19.556 -15.555 24.205 1.00 75.84  
ATOM 70 PRO A 143 18.935 -15.237 23.218 1.00 84.15  
ATOM 71 CB PRO A 143 22.034 -15.684 23.764 1.00 90.78  
ATOM 72 CG PRO A 143 22.077 -15.471 23.292 1.00 59.80  
ATOM 73 CD PRO A 143 21.505 -16.726 21.681 1.00 59.55  
ATOM 74 N ALA A 144 19.262 -15.243 25.462 1.00 77.28  
ATOM 75 CA ALA A 144 18.267 -14.338 25.806 1.00 51.06  
ATOM 76 C ALA A 144 18.464 -13.656 25.425 1.00 81.64  
ATOM 77 O ALA A 144 17.586 -12.084 25.241 1.00 71.65  
ATOM 78 CB ALA A 144 17.355 -14.377 27.289 1.00 74.47  
ATOM 79 N SER A 145 19.749 -12.560 25.310 1.00 77.87  
ATOM 80 CA SER A 145 20.200 -11.240 24.966 1.00 82.52  
ATOM 81 C SER A 145 19.643 -10.750 23.634 1.00 82.64  
ATOM 82 O SER A 145 18.432 -9.513 23.456 1.00 82.64  
ATOM 83 CB SER A 145 21.730 -11.160 24.932 1.00 83.34  
ATOM 84 OG SER A 145 22.248 -11.973 23.892 1.00 88.67  
ATOM 85 N LEU A 146 19.433 -11.693 22.703 1.00 91.83  
ATOM 86 CA LEU A 146 18.982 -11.296 22.357 1.00 87.75  
ATOM 87 C LEU A 146 17.520 -10.855 21.319 1.00 91.72  
ATOM 88 O LEU A 146 16.662 -11.491 21.952 1.00 79.05  
ATOM 89 CB LEU A 146 19.179 -10.482 20.414 1.00 85.72  
ATOM 90 CG LEU A 146 18.784 -12.220 19.961 1.00 92.02  
ATOM 91 CD1 LEU A 146 19.690 -11.166 18.945 1.00 87.45  
ATOM 92 CD2 LEU A 146 18.313 -13.504 18.152 1.00 87.21  
ATOM 93 N ARG A 147 17.743 -9.763 20.632 1.00 90.66  
ATOM 94 CA ARG A 147 15.884 -9.245 20.533 1.00 84.36  
ATOM 95 C ARG A 147 15.406 -9.185 19.038 1.00 83.13  
ATOM 96 O ARG A 147 15.561 -8.140 18.422 1.00 79.31  
ATOM 97 CB ARG A 147 15.798 -7.852 21.600 1.00 96.07  
ATOM 98 CG ARG A 147 16.143 -7.776 22.634 1.00 77.30  
ATOM 99 CD ARG A 147 15.100 -8.498 23.462 1.00 66.17  
ATOM 100 NE ARG A 147 13.782 -7.891 23.293 1.00 71.67  
ATOM 101 CZ ARG A 147 13.312 -6.893 24.034 1.00 59.78  
ATOM 102 NH2 ARG A 147 14.057 -6.370 24.998 1.00 65.05  
ATOM 103 NH2 ARG A 147 12.099 -6.409 23.004 1.00 70.38  
ATOM 104 N LEU A 148 14.820 -10.262 18.612 1.00 77.18  
ATOM 105 CA LEU A 148 14.237 -10.301 17.284 1.00 68.74  
ATOM 106 C LEU A 148 12.813 -10.845 17.314 1.00 68.94  
ATOM 107 O LEU A 148 12.900 -11.690 18.184 1.00 66.04  
ATOM 108 CB LEU A 148 15.086 -11.152 16.339 1.00 71.01  
ATOM 109 CG LEU A 148 16.457 -10.185 15.960 1.00 78.94  
ATOM 110 CD1 LEU A 148 17.227 -11.566 15.008 1.00 53.71  
ATOM 111 CD2 LEU A 148 16.328 -9.232 15.179 1.00 76.39  
ATOM 112 N SER A 149 11.952 -10.355 16.456 1.00 64.66  
ATOM 113 CA SER A 149 10.607 -10.902 16.313 1.00 61.98  
ATOM 114 C SER A 149 10.701 -12.344 15.823 1.00 56.92  
ATOM 115 O SER A 149 11.738 -12.750 15.296 1.00 63.78  
ATOM 116 CB SER A 149 9.770 -10.058 15.349 1.00 62.03  
ATOM 117 CG SER A 149 10.424 -9.900 14.102 1.00 59.44  
ATOM 118 N GLU A 150 9.636 -13.120 16.009 1.00 43.56  
ATOM 119 CA GLU A 150 9.618 -14.501 15.533 1.00 54.81  
ATOM 120 C GLU A 150 9.859 -14.537 14.036 1.00 61.23  
ATOM 121 O GLU A 150 10.641 -15.358 13.533 1.00 48.62  
ATOM 122 CB GLU A 150 8.278 -15.181 15.821 1.00 34.61  
ATOM 123 CG GLU A 150 9.221 -16.614 15.109 1.00 37.53

| octamer-PDB-coordinates.txt |     |     |           |                                  |
|-----------------------------|-----|-----|-----------|----------------------------------|
| ATOM                        | 124 | CD  | GLU A 150 | 6.822 -17.198 13.295 1.00 60.93  |
| ATOM                        | 125 | OE1 | GLU A 150 | 8.846 -16.419 15.296 1.00 33.82  |
| ATOM                        | 126 | OE2 | GLU A 150 | 6.696 -18.441 15.282 1.00 60.88  |
| ATOM                        | 127 | N   | GLU A 151 | 9.217 -13.616 13.336 1.00 64.00  |
| ATOM                        | 128 | CA  | GLU A 151 | 9.263 -13.569 11.895 1.00 59.30  |
| ATOM                        | 129 | C   | GLU A 151 | 10.667 -13.244 11.399 1.00 51.20 |
| ATOM                        | 130 | CG  | GLU A 151 | 11.152 -13.845 10.443 1.00 44.09 |
| ATOM                        | 131 | CB  | GLU A 151 | 8.268 -12.920 11.362 1.00 64.70  |
| ATOM                        | 132 | CG  | GLU A 151 | 8.000 -12.595 9.866 1.00 50.62   |
| ATOM                        | 133 | CD  | GLU A 151 | 7.187 -13.807 9.469 1.00 75.97   |
| ATOM                        | 134 | OE1 | GLU A 151 | 6.599 -14.452 10.361 1.00 71.32  |
| ATOM                        | 135 | OE2 | GLU A 151 | 7.129 -14.112 10.259 1.00 50.77  |
| ATOM                        | 136 | N   | GLU A 152 | 11.325 -12.308 12.074 1.00 48.19 |
| ATOM                        | 137 | CA  | GLU A 152 | 12.666 -11.894 11.681 1.00 47.76 |
| ATOM                        | 138 | C   | GLU A 152 | 13.705 -12.959 12.022 1.00 51.09 |
| ATOM                        | 139 | CG  | GLU A 152 | 14.621 -13.206 11.241 1.00 48.69 |
| ATOM                        | 140 | CB  | GLU A 152 | 13.031 -10.564 12.344 1.00 59.60 |
| ATOM                        | 141 | CG  | GLU A 152 | 14.343 -9.965 11.864 1.00 63.03  |
| ATOM                        | 142 | CD  | GLU A 152 | 14.596 -8.582 12.434 1.00 82.67  |
| ATOM                        | 143 | OE1 | GLU A 152 | 13.760 -8.104 13.229 1.00 92.40  |
| ATOM                        | 144 | OE2 | GLU A 152 | 15.631 -7.974 12.086 1.00 83.68  |
| ATOM                        | 145 | N   | LEU A 153 | 13.558 -13.590 13.184 1.00 15.64 |
| ATOM                        | 146 | CA  | LEU A 153 | 14.450 -14.675 13.582 1.00 36.95 |
| ATOM                        | 147 | C   | LEU A 153 | 14.366 -15.827 12.588 1.00 42.62 |
| ATOM                        | 148 | CG  | LEU A 153 | 15.385 -16.295 12.065 1.00 42.32 |
| ATOM                        | 149 | CB  | LEU A 153 | 14.111 -15.170 14.990 1.00 43.77 |
| ATOM                        | 150 | CG  | LEU A 153 | 14.060 -16.420 15.460 1.00 50.07 |
| ATOM                        | 151 | CD  | LEU A 153 | 16.336 -16.315 15.686 1.00 36.87 |
| ATOM                        | 152 | CD2 | LEU A 153 | 14.226 -16.993 16.719 1.00 31.04 |
| ATOM                        | 153 | N   | LEU A 154 | 13.140 -16.271 12.326 1.00 36.01 |
| ATOM                        | 154 | CA  | LEU A 154 | 12.900 -17.358 11.386 1.00 42.51 |
| ATOM                        | 155 | C   | LEU A 154 | 13.371 -16.024 9.183 1.00 37.90  |
| ATOM                        | 156 | CG  | LEU A 154 | 13.862 -17.844 9.245 1.00 37.58  |
| ATOM                        | 157 | CB  | LEU A 154 | 11.419 -17.737 11.365 1.00 37.90 |
| ATOM                        | 158 | CG  | LEU A 154 | 10.901 -18.445 12.626 1.00 40.71 |
| ATOM                        | 159 | CD1 | LEU A 154 | 9.409 -18.716 12.499 1.00 47.77  |
| ATOM                        | 160 | CD2 | LEU A 154 | 11.671 -19.593 12.858 1.00 29.02 |
| ATOM                        | 161 | N   | ASP A 155 | 13.740 -15.722 9.633 1.00 31.34  |
| ATOM                        | 162 | CA  | ASP A 155 | 13.671 -15.258 8.311 1.00 35.85  |
| ATOM                        | 163 | C   | ASP A 155 | 15.188 -15.354 8.201 1.00 34.67  |
| ATOM                        | 164 | CG  | ASP A 155 | 15.702 -15.917 7.240 1.00 40.23  |
| ATOM                        | 165 | CB  | ASP A 155 | 13.220 -15.822 6.049 1.00 37.27  |
| ATOM                        | 166 | CG  | ASP A 155 | 11.800 -15.946 7.526 1.00 40.12  |
| ATOM                        | 167 | CD1 | ASP A 155 | 11.244 -14.801 7.180 1.00 26.00  |
| ATOM                        | 168 | CD2 | ASP A 155 | 11.240 -12.628 7.483 1.00 43.39  |
| ATOM                        | 169 | N   | LYS A 156 | 15.495 -14.817 7.192 1.00 36.53  |
| ATOM                        | 170 | CA  | LYS A 156 | 17.355 -14.682 9.206 1.00 34.37  |
| ATOM                        | 171 | C   | LYS A 156 | 18.861 -15.295 9.161 1.00 37.90  |
| ATOM                        | 172 | CG  | LYS A 156 | 18.795 -16.629 8.418 1.00 38.07  |
| ATOM                        | 173 | CB  | LYS A 156 | 17.913 -14.166 10.450 1.00 23.04 |
| ATOM                        | 174 | CG  | LYS A 156 | 17.597 -12.683 10.596 1.00 36.64 |
| ATOM                        | 175 | CD  | LYS A 156 | 16.151 -11.581 9.399 1.00 35.95  |
| ATOM                        | 176 | CD  | LYS A 156 | 17.646 -10.402 9.577 1.00 37.90  |
| ATOM                        | 177 | NZ  | LYS A 156 | 18.127 -9.616 8.345 1.00 60.84   |
| ATOM                        | 178 | N   | LEU A 157 | 17.242 -17.160 9.962 1.00 32.02  |
| ATOM                        | 179 | CA  | LEU A 157 | 17.623 -18.467 10.010 1.00 22.69 |
| ATOM                        | 180 | C   | LEU A 157 | 17.581 -18.264 8.672 1.00 33.84  |
| ATOM                        | 181 | CG  | LEU A 157 | 18.213 -19.028 8.223 1.00 23.65  |
| ATOM                        | 182 | CB  | LEU A 157 | 16.865 -19.285 11.128 1.00 32.44 |
| ATOM                        | 183 | CG  | LEU A 157 | 17.283 -18.882 12.544 1.00 30.64 |
| ATOM                        | 184 | CD1 | LEU A 157 | 16.393 -19.541 13.679 1.00 26.05 |
| ATOM                        | 185 | CD2 | LEU A 157 | 18.743 -19.129 12.792 1.00 22.02 |
| ATOM                        | 186 | N   | GLU A 158 | 16.255 -18.359 9.035 1.00 32.24  |

| octamer-PDB-coordinates.txt |     |     |           |                                  |
|-----------------------------|-----|-----|-----------|----------------------------------|
| ATOM                        | 250 | CG  | ARG A 165 | 27.202 -19.837 1.307 1.00 36.11  |
| ATOM                        | 251 | CD  | ARG A 165 | 27.958 -16.124 1.121 1.00 40.59  |
| ATOM                        | 252 | NE  | ARG A 165 | 27.354 -17.401 1.833 1.00 52.66  |
| ATOM                        | 253 | CZ  | ARG A 165 | 26.565 -16.493 1.267 1.00 57.32  |
| ATOM                        | 254 | NH1 | ARG A 165 | 26.289 -15.568 -0.028 1.00 51.79 |
| ATOM                        | 255 | NH2 | ARG A 165 | 26.063 -15.109 1.993 1.00 60.93  |
| ATOM                        | 256 | N   | ASN A 166 | 26.557 -21.643 4.104 1.00 42.31  |
| ATOM                        | 257 | CA  | ASN A 166 | 26.601 -21.955 4.529 1.00 33.11  |
| ATOM                        | 258 | C   | ASN A 166 | 26.319 -24.433 4.784 1.00 29.70  |
| ATOM                        | 259 | CG  | ASN A 166 | 26.294 -24.663 5.926 1.00 28.72  |
| ATOM                        | 260 | CB  | ASN A 166 | 25.603 -22.092 5.301 1.00 30.48  |
| ATOM                        | 261 | CG  | ASN A 166 | 26.626 -20.641 5.880 1.00 30.76  |
| ATOM                        | 262 | ND1 | ASN A 166 | 25.049 -19.748 5.376 1.00 23.65  |
| ATOM                        | 263 | ND2 | ASN A 166 | 27.215 -20.326 5.429 1.00 35.65  |
| ATOM                        | 264 | N   | GLY A 167 | 26.106 -25.182 3.707 1.00 25.79  |
| ATOM                        | 265 | CA  | GLY A 167 | 25.843 -26.605 3.802 1.00 24.68  |
| ATOM                        | 266 | C   | GLY A 167 | 24.161 -26.919 3.827 1.00 22.32  |
| ATOM                        | 267 | CG  | GLY A 167 | 23.961 -28.066 4.027 1.00 28.79  |
| ATOM                        | 268 | N   | GLY A 168 | 23.143 -25.890 3.621 1.00 39.96  |
| ATOM                        | 269 | CA  | GLY A 168 | 22.101 -26.030 3.705 1.00 28.01  |
| ATOM                        | 270 | C   | GLY A 168 | 21.415 -26.185 2.261 1.00 30.05  |
| ATOM                        | 271 | CG  | GLY A 168 | 21.998 -26.704 1.407 1.00 38.63  |
| ATOM                        | 272 | CB  | GLY A 168 | 20.170 -25.774 2.290 1.00 26.23  |
| ATOM                        | 273 | CA  | GLY A 169 | 19.162 -25.058 1.992 1.00 25.32  |
| ATOM                        | 274 | C   | GLY A 169 | 17.960 -25.325 1.312 1.00 31.24  |
| ATOM                        | 275 | N   | GLY A 169 | 17.662 -24.782 2.376 1.00 22.10  |
| ATOM                        | 276 | N   | ASP A 170 | 17.104 -25.480 0.304 1.00 24.82  |
| ATOM                        | 277 | CA  | ASP A 170 | 15.735 -24.962 0.345 1.00 35.57  |
| ATOM                        | 278 | C   | ASP A 170 | 16.970 -25.416 1.588 1.00 37.19  |
| ATOM                        | 279 | CG  | ASP A 170 | 14.973 -26.597 1.936 1.00 29.31  |
| ATOM                        | 280 | CB  | ASP A 170 | 14.971 -25.384 -0.312 1.00 34.53 |
| ATOM                        | 281 | CG  | ASP A 170 | 15.417 -24.628 -2.152 1.00 28.51 |
| ATOM                        | 282 | OD1 | ASP A 170 | 16.496 -24.000 -2.119 1.00 31.96 |
| ATOM                        | 283 | OD2 | ASP A 170 | 14.891 -24.691 -2.163 1.00 31.16 |
| ATOM                        | 284 | N   | VAL A 171 | 14.318 -24.468 2.251 1.00 28.79  |
| ATOM                        | 285 | CA  | VAL A 171 | 13.575 -24.762 3.469 1.00 36.25  |
| ATOM                        | 286 | C   | VAL A 171 | 12.075 -24.889 3.198 1.00 36.76  |
| ATOM                        | 287 | CG  | VAL A 171 | 11.456 -23.792 2.645 1.00 41.39  |
| ATOM                        | 288 | CB  | VAL A 171 | 13.003 -23.674 4.533 1.00 29.05  |
| ATOM                        | 289 | CG1 | VAL A 171 | 12.941 -23.935 5.763 1.00 24.29  |
| ATOM                        | 290 | CG2 | VAL A 171 | 15.273 -23.609 4.921 1.00 26.46  |
| ATOM                        | 291 | N   | ASP A 172 | 11.513 -26.022 3.601 1.00 36.52  |
| ATOM                        | 292 | CA  | ASP A 172 | 10.092 -26.294 3.414 1.00 36.53  |
| ATOM                        | 293 | C   | ASP A 172 | 9.274 -25.875 4.629 1.00 40.98   |
| ATOM                        | 294 | CG  | ASP A 172 | 8.224 -25.247 4.487 1.00 45.15   |
| ATOM                        | 295 | CB  | ASP A 172 | 9.859 -27.776 3.131 1.00 47.86   |
| ATOM                        | 296 | CG  | ASP A 172 | 10.178 -28.151 1.707 1.00 51.25  |
| ATOM                        | 297 | OD1 | ASP A 172 | 10.397 -27.235 0.864 1.00 45.59  |
| ATOM                        | 298 | OD2 | ASP A 172 | 10.306 -29.362 1.434 1.00 53.74  |
| ATOM                        | 299 | N   | VAL A 173 | 8.219 -26.219 5.820 1.00 38.82   |
| ATOM                        | 300 | CA  | VAL A 173 | 8.988 -25.926 7.040 1.00 39.15   |
| ATOM                        | 301 | C   | VAL A 173 | 9.810 -25.171 8.039 1.00 38.10   |
| ATOM                        | 302 | CG  | VAL A 173 | 11.027 -25.324 8.123 1.00 43.80  |
| ATOM                        | 303 | CB  | VAL A 173 | 8.538 -27.304 7.693 1.00 47.74   |
| ATOM                        | 304 | CG1 | VAL A 173 | 7.645 -27.055 7.811 1.00 49.31   |
| ATOM                        | 305 | CG2 | VAL A 173 | 7.813 -28.165 6.840 1.00 56.86   |
| ATOM                        | 306 | N   | ARG A 174 | 9.127 -24.324 8.802 1.00 36.31   |
| ATOM                        | 307 | CA  | ARG A 174 | 9.775 -23.353 9.670 1.00 39.17   |
| ATOM                        | 308 | C   | ARG A 174 | 8.951 -23.163 10.940 1.00 38.54  |
| ATOM                        | 309 | CG  | ARG A 174 | 7.776 -22.798 10.873 1.00 36.78  |
| ATOM                        | 310 | CB  | ARG A 174 | 9.934 -22.019 8.838 1.00 46.03   |
| ATOM                        | 311 | CG  | ARG A 174 | 11.146 -21.204 9.330 1.00 46.66  |
| ATOM                        | 312 | CD  | ARG A 174 | 11.275 -19.997 8.420 1.00 41.33  |

|                             |      |     |     |           |        |         |        |      |       |     |
|-----------------------------|------|-----|-----|-----------|--------|---------|--------|------|-------|-----|
| octamer-PDB-coordinates.txt |      |     |     |           |        |         |        |      |       |     |
| C                           | ATOM | 187 | CA  | GLU A 158 | 15.937 | -19.548 | 6.739  | 1.00 | 35.43 | C   |
| C                           | ATOM | 188 | C   | GLU A 158 | 16.907 | -19.061 | 5.666  | 1.00 | 27.52 | C   |
| O                           | ATOM | 189 | O   | GLU A 158 | 17.258 | -19.807 | 4.755  | 1.00 | 26.81 | C   |
| O                           | ATOM | 190 | CB  | GLU A 158 | 14.498 | -19.229 | 6.314  | 1.00 | 33.86 | C   |
| N                           | ATOM | 191 | CG  | GLU A 158 | 14.057 | -19.877 | 5.033  | 1.00 | 35.62 | C   |
| C                           | ATOM | 192 | CD  | GLU A 158 | 12.577 | -19.700 | 4.755  | 1.00 | 29.58 | C   |
| C                           | ATOM | 193 | OE1 | GLU A 158 | 12.083 | -20.288 | 3.770  | 1.00 | 30.33 | C   |
| O                           | ATOM | 194 | OE2 | GLU A 158 | 11.909 | -18.968 | 5.515  | 1.00 | 39.84 | O1- |
| C                           | ATOM | 195 | N   | LIE A 159 | 17.327 | -17.804 | 5.774  | 1.00 | 29.92 | N   |
| N                           | ATOM | 196 | CA  | LIE A 159 | 18.149 | -17.256 | 4.891  | 1.00 | 38.75 | N   |
| C                           | ATOM | 197 | C   | LIE A 159 | 19.662 | -16.006 | 5.055  | 1.00 | 50.52 | C   |
| O                           | ATOM | 198 | O   | LIE A 159 | 20.268 | -18.141 | 4.077  | 1.00 | 37.50 | O   |
| O                           | ATOM | 199 | O   | LIE A 159 | 18.606 | -15.759 | 5.149  | 1.00 | 49.76 | O   |
| C                           | ATOM | 200 | CG1 | LIE A 159 | 17.356 | -14.932 | 4.853  | 1.00 | 31.59 | C   |
| C                           | ATOM | 201 | CG2 | LIE A 159 | 19.778 | -15.267 | 4.303  | 1.00 | 20.50 | C   |
| C                           | ATOM | 202 | CD1 | LIE A 159 | 17.060 | -14.786 | 3.394  | 1.00 | 41.54 | C   |
| C                           | ATOM | 203 | N   | PHE A 160 | 20.090 | -15.156 | 6.304  | 1.00 | 28.45 | N   |
| C                           | ATOM | 204 | CA  | PHE A 160 | 21.381 | -18.762 | 5.594  | 1.00 | 30.17 | C   |
| C                           | ATOM | 205 | C   | PHE A 160 | 21.419 | -20.215 | 6.150  | 1.00 | 31.62 | C   |
| C                           | ATOM | 206 | CG  | PHE A 160 | 22.301 | -20.625 | 5.394  | 1.00 | 35.21 | O   |
| O                           | ATOM | 207 | CB  | PHE A 160 | 21.695 | -18.686 | 6.088  | 1.00 | 28.63 | O   |
| O                           | ATOM | 208 | CG  | PHE A 160 | 23.124 | -19.010 | 8.413  | 1.00 | 39.10 | O   |
| C                           | ATOM | 209 | CD1 | PHE A 160 | 24.142 | -18.196 | 7.944  | 1.00 | 28.49 | C   |
| C                           | ATOM | 210 | CD2 | PHE A 160 | 23.457 | -20.149 | 9.132  | 1.00 | 30.17 | C   |
| C                           | ATOM | 211 | CE1 | PHE A 160 | 25.460 | -18.427 | 8.228  | 1.00 | 30.39 | C   |
| C                           | ATOM | 212 | CE2 | PHE A 160 | 21.781 | -20.441 | 9.410  | 1.00 | 32.90 | C   |
| C                           | ATOM | 213 | CZ  | PHE A 160 | 25.782 | -19.604 | 8.956  | 1.00 | 34.50 | C   |
| C                           | ATOM | 214 | N   | PHE A 161 | 20.451 | -20.991 | 6.630  | 1.00 | 20.06 | N   |
| C                           | ATOM | 215 | CA  | PHE A 161 | 20.437 | -22.425 | 6.378  | 1.00 | 28.34 | C   |
| N                           | ATOM | 216 | C   | PHE A 161 | 19.600 | -21.757 | 5.033  | 1.00 | 28.93 | N   |
| C                           | ATOM | 217 | CG  | PHE A 161 | 19.689 | -21.926 | 4.666  | 1.00 | 32.28 | O   |
| C                           | ATOM | 218 | CB  | PHE A 161 | 19.709 | -22.150 | 7.511  | 1.00 | 24.93 | C   |
| O                           | ATOM | 219 | CD  | PHE A 161 | 20.454 | -23.128 | 8.820  | 1.00 | 31.60 | O   |
| C                           | ATOM | 220 | CD1 | PHE A 161 | 21.571 | -23.926 | 9.009  | 1.00 | 25.79 | C   |
| C                           | ATOM | 221 | CD2 | PHE A 161 | 20.039 | -22.309 | 9.857  | 1.00 | 22.73 | C   |
| C                           | ATOM | 222 | CE1 | PHE A 161 | 22.262 | -23.909 | 10.209 | 1.00 | 23.08 | C   |
| C                           | ATOM | 223 | CE2 | PHE A 161 | 20.725 | -22.288 | 11.060 | 1.00 | 20.23 | C   |
| N                           | ATOM | 224 | CZ  | PHE A 161 | 21.838 | -23.088 | 11.235 | 1.00 | 27.82 | N   |
| C                           | ATOM | 225 | N   | GLY A 162 | 19.383 | -21.726 | 4.302  | 1.00 | 27.19 | N   |
| C                           | ATOM | 226 | CA  | GLY A 162 | 18.875 | -21.915 | 2.955  | 1.00 | 22.58 | C   |
| O                           | ATOM | 227 | C   | GLY A 162 | 19.985 | -21.893 | 1.921  | 1.00 | 26.26 | O   |
| C                           | ATOM | 228 | O   | GLY A 162 | 19.801 | -22.339 | 0.788  | 1.00 | 23.64 | O   |
| O                           | ATOM | 229 | N   | LYS A 163 | 22.145 | -21.382 | 2.925  | 1.00 | 22.90 | N   |
| C                           | ATOM | 230 | CA  | LYS A 163 | 22.283 | -21.238 | 1.424  | 1.00 | 32.21 | C   |
| O                           | ATOM | 231 | C   | LYS A 163 | 23.096 | -22.511 | 1.921  | 1.00 | 29.29 | O   |
| C                           | ATOM | 232 | O   | LYS A 163 | 23.416 | -23.134 | 1.355  | 1.00 | 30.80 | O   |
| C                           | ATOM | 233 | CB  | LYS A 163 | 23.186 | -20.088 | 1.876  | 1.00 | 31.18 | C   |
| C                           | ATOM | 234 | CG  | LYS A 163 | 22.533 | -18.712 | 1.780  | 1.00 | 42.95 | C   |
| C                           | ATOM | 235 | CD  | LYS A 163 | 23.464 | -17.656 | 2.390  | 1.00 | 44.88 | C   |
| C                           | ATOM | 236 | CD1 | LYS A 163 | 22.792 | -16.301 | 2.453  | 1.00 | 46.53 | C   |
| C                           | ATOM | 237 | CD2 | LYS A 163 | 22.214 | -15.902 | 2.402  | 1.00 | 40.03 | C   |
| C                           | ATOM | 238 | N   | THR A 164 | 23.430 | -22.920 | 0.116  | 1.00 | 29.87 | N   |
| C                           | ATOM | 239 | CA  | THR A 164 | 24.240 | -24.111 | -0.100 | 1.00 | 30.61 | C   |
| N1+                         | ATOM | 240 | C   | THR A 164 | 25.670 | -23.912 | 0.400  | 1.00 | 42.90 | C   |
| C                           | ATOM | 241 | O   | THR A 164 | 26.388 | -24.978 | 0.773  | 1.00 | 40.90 | O   |
| C                           | ATOM | 242 | CB  | THR A 164 | 24.275 | -24.511 | 0.587  | 1.00 | 30.81 | C   |
| O                           | ATOM | 243 | CG2 | THR A 164 | 22.861 | -24.662 | -2.130 | 1.00 | 26.16 | O   |
| C                           | ATOM | 244 | OG1 | THR A 164 | 24.967 | -23.509 | -2.341 | 1.00 | 52.55 | C   |
| C                           | ATOM | 245 | N   | ARG A 165 | 26.139 | -22.668 | 0.408  | 1.00 | 33.82 | N   |
| C                           | ATOM | 246 | CA  | ARG A 165 | 27.495 | -22.374 | 0.869  | 1.00 | 36.68 | C   |
| C                           | ATOM | 247 | C   | ARG A 165 | 27.665 | -22.811 | 2.370  | 1.00 | 36.91 | C   |
| C                           | ATOM | 248 | O   | ARG A 165 | 28.746 | -21.752 | 2.515  | 1.00 | 33.13 | O   |
| N                           | ATOM | 249 | CB  | ARG A 165 | 27.903 | -20.938 | 0.523  | 1.00 | 42.72 | C   |

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|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|--|
| ATOM | 376 | C   | LEU | A | 183 | 8.784  | -21.539 | 39.519 | 1.00 | 36.52 |  |
| ATOM | 377 | O   | LEU | A | 183 | 8.102  | -22.623 | 39.506 | 1.00 | 39.53 |  |
| ATOM | 378 | CB  | LEU | A | 183 | 7.501  | -19.758 | 38.410 | 1.00 | 38.90 |  |
| ATOM | 379 | CG  | LEU | A | 183 | 7.319  | -18.649 | 37.365 | 1.00 | 41.06 |  |
| ATOM | 380 | CD1 | LEU | A | 183 | 6.062  | -17.892 | 37.579 | 1.00 | 39.99 |  |
| ATOM | 381 | CD2 | LEU | A | 183 | 8.555  | -17.707 | 37.394 | 1.00 | 38.95 |  |
| ATOM | 382 | N   | GLY | A | 184 | 9.577  | -21.271 | 40.532 | 1.00 | 36.90 |  |
| ATOM | 383 | CA  | GLY | A | 184 | 9.649  | -22.084 | 41.730 | 1.00 | 25.56 |  |
| ATOM | 384 | C   | GLY | A | 184 | 9.155  | -21.291 | 42.919 | 1.00 | 32.30 |  |
| ATOM | 385 | O   | GLY | A | 184 | 9.536  | -20.446 | 43.122 | 1.00 | 49.99 |  |
| ATOM | 386 | N   | PHE | A | 185 | 8.281  | -21.905 | 43.706 | 1.00 | 33.48 |  |
| ATOM | 387 | CA  | PHE | A | 185 | 7.641  | -21.213 | 44.818 | 1.00 | 32.89 |  |
| ATOM | 388 | C   | PHE | A | 185 | 8.163  | -21.694 | 46.163 | 1.00 | 37.35 |  |
| ATOM | 389 | O   | PHE | A | 185 | 8.614  | -22.831 | 46.297 | 1.00 | 43.28 |  |
| ATOM | 390 | CB  | PHE | A | 185 | 6.174  | -21.369 | 44.737 | 1.00 | 30.50 |  |
| ATOM | 391 | CG  | PHE | A | 185 | 5.526  | -20.538 | 43.476 | 1.00 | 25.12 |  |
| ATOM | 392 | CD1 | PHE | A | 185 | 5.174  | -19.502 | 43.388 | 1.00 | 24.46 |  |
| ATOM | 393 | CD2 | PHE | A | 185 | 5.336  | -21.649 | 42.371 | 1.00 | 32.90 |  |
| ATOM | 394 | CE  | PHE | A | 185 | 4.634  | -18.968 | 42.227 | 1.00 | 21.96 |  |
| ATOM | 395 | CE2 | PHE | A | 185 | 4.796  | -21.140 | 41.207 | 1.00 | 21.86 |  |
| ATOM | 396 | CZ  | PHE | A | 185 | 4.449  | -18.306 | 41.135 | 1.00 | 20.26 |  |
| ATOM | 397 | N   | ALA | A | 186 | 8.097  | -20.816 | 47.158 | 1.00 | 36.57 |  |
| ATOM | 398 | CA  | ALA | A | 186 | 8.644  | -21.109 | 46.478 | 1.00 | 40.58 |  |
| ATOM | 399 | CB  | ALA | A | 186 | 7.734  | -22.031 | 49.301 | 1.00 | 37.63 |  |
| ATOM | 400 | O   | ALA | A | 186 | 8.202  | -22.957 | 49.938 | 1.00 | 38.8  |  |
| ATOM | 401 | CB  | ALA | A | 186 | 8.906  | -19.813 | 49.226 | 1.00 | 30.02 |  |
| ATOM | 402 | N   | ARG | A | 187 | 6.436  | -21.728 | 49.231 | 1.00 | 42.32 |  |
| ATOM | 403 | CA  | ARG | A | 187 | 5.492  | -22.451 | 50.140 | 1.00 | 50.71 |  |
| ATOM | 404 | CB  | ARG | A | 187 | 4.626  | -23.606 | 49.394 | 1.00 | 49.06 |  |
| ATOM | 405 | O   | ARG | A | 187 | 4.491  | -23.486 | 48.715 | 1.00 | 50.99 |  |
| ATOM | 406 | CB  | ARG | A | 187 | 4.433  | -21.495 | 50.698 | 1.00 | 43.36 |  |
| ATOM | 407 | CG  | ARG | A | 187 | 3.443  | -22.152 | 51.649 | 1.00 | 58.32 |  |
| ATOM | 408 | CD  | ARG | A | 187 | 1.434  | -21.254 | 52.193 | 1.00 | 50.34 |  |
| ATOM | 409 | CE  | ARG | A | 187 | 1.121  | -20.671 | 51.128 | 1.00 | 51.96 |  |
| ATOM | 410 | CZ  | ARG | A | 187 | 0.736  | -19.632 | 51.208 | 0.00 | 50.56 |  |
| ATOM | 411 | NH1 | ARG | A | 187 | 0.753  | -18.909 | 52.413 | 0.00 | 50.49 |  |
| ATOM | 412 | NH2 | ARG | A | 187 | -0.062 | -19.250 | 50.295 | 0.00 | 49.87 |  |
| ATOM | 413 | N   | ASP | A | 188 | 4.644  | -24.725 | 50.089 | 1.00 | 50.17 |  |
| ATOM | 414 | CA  | ASP | A | 188 | 3.978  | -25.892 | 49.532 | 1.00 | 47.21 |  |
| ATOM | 415 | C   | ASP | A | 188 | 2.504  | -25.622 | 49.234 | 1.00 | 53.54 |  |
| ATOM | 416 | O   | ASP | A | 188 | 1.810  | -24.991 | 50.032 | 1.00 | 54.39 |  |
| ATOM | 417 | CB  | ASP | A | 188 | 4.108  | -27.091 | 50.465 | 1.00 | 58.16 |  |
| ATOM | 418 | CG  | ASP | A | 188 | 5.515  | -27.651 | 50.507 | 1.00 | 72.66 |  |
| ATOM | 419 | CD1 | ASP | A | 188 | 6.169  | -27.702 | 49.532 | 1.00 | 70.93 |  |
| ATOM | 420 | CD2 | ASP | A | 188 | 5.967  | -28.042 | 51.604 | 1.00 | 67.33 |  |
| ATOM | 421 | N   | GLY | A | 189 | 2.034  | -26.102 | 48.088 | 1.00 | 42.33 |  |
| ATOM | 422 | CA  | GLY | A | 189 | 0.630  | -26.004 | 47.736 | 1.00 | 39.55 |  |
| ATOM | 423 | C   | GLY | A | 189 | 0.332  | -24.866 | 46.781 | 1.00 | 49.37 |  |
| ATOM | 424 | O   | GLY | A | 189 | -0.707 | -24.400 | 46.320 | 1.00 | 43.54 |  |
| ATOM | 425 | N   | VAL | A | 190 | 1.243  | -23.901 | 46.721 | 1.00 | 50.74 |  |
| ATOM | 426 | CA  | VAL | A | 190 | 1.072  | -22.746 | 45.835 | 1.00 | 53.91 |  |
| ATOM | 427 | C   | VAL | A | 190 | 1.122  | -23.157 | 44.365 | 1.00 | 42.98 |  |
| ATOM | 428 | CB  | VAL | A | 190 | 0.213  | -22.848 | 43.584 | 1.00 | 53.13 |  |
| ATOM | 429 | CG  | VAL | A | 190 | -1.181 | -21.685 | 45.983 | 1.00 | 46.05 |  |
| ATOM | 430 | CD1 | VAL | A | 190 | 1.996  | -20.513 | 45.143 | 1.00 | 42.75 |  |
| ATOM | 431 | CD2 | VAL | A | 190 | 2.090  | -21.212 | 47.546 | 1.00 | 49.99 |  |
| ATOM | 432 | N   | ALA | A | 191 | 2.196  | -23.856 | 44.005 | 1.00 | 47.82 |  |
| ATOM | 433 | CA  | ALA | A | 191 | 2.376  | -24.383 | 42.656 | 1.00 | 54.17 |  |
| ATOM | 434 | C   | ALA | A | 191 | -0.687 | -24.187 | 42.256 | 1.00 | 46.05 |  |
| ATOM | 435 | O   | ALA | A | 191 | 0.649  | -25.116 | 41.155 | 1.00 | 45.30 |  |
| ATOM | 436 | CB  | ALA | A | 191 | 3.660  | -25.182 | 42.568 | 1.00 | 49.06 |  |
| ATOM | 437 | N   | GLN | A | 192 | -0.778 | -26.127 | 43.172 | 1.00 | 47.69 |  |
| ATOM | 438 | CA  | GLN | A | 192 | 0.357  | -26.998 | 42.946 | 1.00 | 52.73 |  |

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|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|--|
| ATOM | 502 | CA  | PHE | A | 200 | -4.446 | -17.267 | 53.694 | 1.00 | 30.67 |  |
| ATOM | 503 | C   | PHE | A | 200 | -4.392 | -16.230 | 52.577 | 1.00 | 43.05 |  |
| ATOM | 504 | O   | PHE | A | 200 | -3.967 | -16.532 | 52.463 | 1.00 | 49.63 |  |
| ATOM | 505 | CB  | PHE | A | 200 | -3.271 | -17.101 | 51.602 | 1.00 | 46.90 |  |
| ATOM | 506 | CG  | PHE | A | 200 | -3.219 | -18.042 | 55.780 | 1.00 | 38.41 |  |
| ATOM | 507 | CD1 | PHE | A | 200 | -2.762 | -19.321 | 55.651 | 1.00 | 28.30 |  |
| ATOM | 508 | CD2 | PHE | A | 200 | -3.731 | -17.651 | 57.006 | 1.00 | 43.35 |  |
| ATOM | 509 | CE1 | PHE | A | 200 | -2.693 | -20.180 | 56.720 | 1.00 | 31.69 |  |
| ATOM | 510 | CE2 | PHE | A | 200 | -3.724 | -18.518 | 58.081 | 1.00 | 47.84 |  |
| ATOM | 511 | CZ  | PHE | A | 200 | -3.204 | -19.769 | 57.936 | 1.00 | 48.76 |  |
| ATOM | 512 | N   | THR | A | 201 | -4.830 | -15.011 | 52.872 | 1.00 | 59.65 |  |
| ATOM | 513 | CA  | THR | A | 201 | -4.671 | -13.836 | 51.941 | 1.00 | 51.22 |  |
| ATOM | 514 | C   | THR | A | 201 | -3.712 | -12.689 | 52.532 | 1.00 | 53.42 |  |
| ATOM | 515 | O   | THR | A | 201 | -4.035 | -12.190 | 53.507 | 1.00 | 58.10 |  |
| ATOM | 516 | CB  | THR | A | 201 | -6.015 | -13.225 | 51.610 | 1.00 | 58.41 |  |
| ATOM | 517 | CG2 | THR | A | 201 | -5.805 | -12.054 | 50.659 | 1.00 | 53.66 |  |
| ATOM | 518 | OG1 | THR | A | 201 | -6.886 | -14.181 | 50.992 | 1.00 | 55.65 |  |
| ATOM | 519 | N   | VAL | A | 202 | -2.531 | -12.763 | 51.992 | 1.00 | 54.64 |  |
| ATOM | 520 | CA  | VAL | A | 202 | -1.470 | -11.913 | 52.455 | 1.00 | 59.91 |  |
| ATOM | 521 | C   | VAL | A | 202 | -1.203 | -10.702 | 51.571 | 1.00 | 56.82 |  |
| ATOM | 522 | O   | VAL | A | 202 | -1.014 | -10.842 | 50.361 | 1.00 | 61.29 |  |
| ATOM | 523 | CB  | VAL | A | 202 | -0.153 | -12.695 | 52.600 | 1.00 | 48.75 |  |
| ATOM | 524 | CG1 | VAL | A | 202 | 0.889  | -11.848 | 53.316 | 1.00 | 37.13 |  |
| ATOM | 525 | CG2 | VAL | A | 202 | 0.388  | -13.940 | 53.351 | 1.00 | 55.88 |  |
| ATOM | 526 | N   | PRO | A | 203 | -1.200 | -9.504  | 52.173 | 1.00 | 64.11 |  |
| ATOM | 527 | CA  | PRO | A | 203 | -0.815 | -8.290  | 51.448 | 1.00 | 59.29 |  |
| ATOM | 528 | C   | PRO | A | 203 | 0.667  | -8.318  | 51.077 | 1.00 | 61.69 |  |
| ATOM | 529 | O   | PRO | A | 203 | 1.525  | -8.160  | 51.945 | 1.00 | 60.20 |  |
| ATOM | 530 | CB  | PRO | A | 203 | -1.118 | -7.171  | 52.451 | 1.00 | 56.90 |  |
| ATOM | 531 | CG  | PRO | A | 203 | -1.054 | -7.839  | 53.788 | 1.00 | 61.66 |  |
| ATOM | 532 | CD  | PRO | A | 203 | -1.508 | -9.213  | 53.559 | 1.00 | 58.60 |  |
| ATOM | 533 | N   | LEU | A | 204 | 0.956  | -8.515  | 52.955 | 1.00 | 62.10 |  |
| ATOM | 534 | CA  | LEU | A | 204 | 2.832  | -8.560  | 52.337 | 1.00 | 61.69 |  |
| ATOM | 535 | C   | LEU | A | 204 | 2.503  | -7.685  | 52.083 | 1.00 | 68.09 |  |
| ATOM | 536 | O   | LEU | A | 204 | 1.817  | -7.949  | 52.978 | 1.00 | 72.27 |  |
| ATOM | 537 | CB  | LEU | A | 204 | 2.744  | -9.999  | 52.994 | 1.00 | 56.08 |  |
| ATOM | 538 | CG  | LEU | A | 204 | 2.719  | -11.023 | 53.130 | 1.00 | 44.86 |  |
| ATOM | 539 | CD1 | LEU | A | 204 | 3.046  | -12.411 | 52.603 | 1.00 | 46.29 |  |
| ATOM | 540 | CD2 | LEU | A | 204 | 3.684  | -10.629 | 51.233 | 1.00 | 40.27 |  |
| ATOM | 541 | N   | GLY | A | 205 | 3.426  | -6.731  | 52.168 | 1.00 | 77.07 |  |
| ATOM | 542 | CA  | GLY | A | 205 | 3.731  | -5.539  | 52.063 | 1.00 | 79.85 |  |
| ATOM | 543 | C   | GLY | A | 205 | 2.519  | -5.122  | 52.513 | 1.00 | 79.60 |  |
| ATOM | 544 | O   | GLY | A | 205 | 2.389  | -4.932  | 52.393 | 1.00 | 77.01 |  |
| ATOM | 545 | N   | GLY | A | 206 | 1.630  | -4.693  | 52.407 | 1.00 | 77.39 |  |
| ATOM | 546 | CA  | GLY | A | 206 | 0.435  | -3.970  | 52.014 | 1.00 | 71.80 |  |
| ATOM | 547 | C   | GLY | A | 206 | -0.686 | -4.858  | 50.506 | 1.00 | 80.47 |  |
| ATOM | 548 | O   | GLY | A | 206 | -1.745 | -4.366  | 50.121 | 1.00 | 84.85 |  |
| ATOM | 549 | N   | GLN | A | 207 | -0.457 | -6.168  | 50.501 | 1.00 | 80.97 |  |
| ATOM | 550 | CA  | GLN | A | 207 | -1.471 | -7.117  | 50.034 | 1.00 | 73.43 |  |
| ATOM | 551 | C   | GLN | A | 207 | -2.061 | -7.927  | 52.197 | 1.00 | 70.10 |  |
| ATOM | 552 | O   | GLN | A | 207 | -1.437 | -8.074  | 52.245 | 1.00 | 65.57 |  |
| ATOM | 553 | CB  | GLN | A | 207 | -0.885 | -8.071  | 52.999 | 1.00 | 69.14 |  |
| ATOM | 554 | CG  | GLN | A | 207 | 0.015  | -7.408  | 53.968 | 1.00 | 65.01 |  |
| ATOM | 555 | CD  | GLN | A | 207 | 0.638  | -8.441  | 53.016 | 1.00 | 69.68 |  |
| ATOM | 556 | CE  | GLN | A | 207 | 1.262  | -7.913  | 52.195 | 1.00 | 79.61 |  |
| ATOM | 557 | CE2 | GLN | A | 207 | 0.570  | -9.149  | 53.240 | 1.00 | 75.35 |  |
| ATOM | 558 | N   | GLN | A | 208 | -3.270 | -8.436  | 52.996 | 1.00 | 60.22 |  |
| ATOM | 559 | CA  | GLN | A | 208 | -3.861 | -9.385  | 52.933 | 1.00 | 61.83 |  |
| ATOM | 560 | C   | GLN | A | 208 | -3.579 | -10.803 | 52.457 | 1.00 | 71.42 |  |
| ATOM | 561 | O   | GLN | A | 208 | -4.386 | -11.407 | 52.749 | 1.00 | 67.87 |  |
| ATOM | 562 | CB  | GLN | A | 208 | -5.965 | -9.184  | 52.073 | 1.00 | 68.06 |  |
| ATOM | 563 | CG  | GLN | A | 208 | -5.736 | -7.833  | 52.824 |      |       |  |

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|-----------------------------|-----|---------------|----------------------------------|-----------------------------|------|-----|---------------|----------------------------------|-----|
| ATOM                        | 628 | CE1 TYR A 216 | 12.342 -27.563 24.324 1.00 53.25 | C                           | ATOM | 691 | N PHE B 142   | 2.956 -18.005 25.514 1.00 45.24  | N   |
| ATOM                        | 629 | CE2 TYR A 216 | 12.231 -28.683 26.243 1.00 60.23 | C                           | ATOM | 692 | CA PHE B 142  | 3.474 -16.703 25.104 1.00 44.28  | N   |
| ATOM                        | 630 | CZ TYR A 216  | 12.436 -28.092 25.011 1.00 68.78 | C                           | ATOM | 693 | C PHE B 142   | 3.396 -16.502 25.593 1.00 58.28  | C   |
| ATOM                        | 631 | OH TYR A 216  | 13.678 -28.031 24.464 1.00 60.99 | C                           | ATOM | 694 | O PHE B 142   | 3.922 -17.309 22.826 1.00 56.68  | O   |
| ATOM                        | 632 | N GLY B 134   | 8.656 -30.371 43.586 1.00 60.92  | N                           | ATOM | 695 | C PHE B 142   | 4.919 -16.526 25.574 1.00 56.96  | C   |
| ATOM                        | 633 | CA GLY B 134  | 7.227 -30.374 43.835 1.00 60.56  | C                           | ATOM | 696 | CG PHE B 142  | 5.102 -16.706 27.054 1.00 66.68  | C   |
| ATOM                        | 634 | C GLY B 134   | 6.657 -28.975 43.968 1.00 64.91  | C                           | ATOM | 697 | CD1 PHE B 142 | 4.844 -15.662 27.939 1.00 48.59  | C   |
| ATOM                        | 635 | O GLY B 134   | 5.456 -28.801 44.171 1.00 64.72  | O                           | ATOM | 698 | CD2 PHE B 142 | 5.544 -17.913 27.569 1.00 51.38  | C   |
| ATOM                        | 636 | N ARG B 135   | 7.534 -27.974 43.834 1.00 59.76  | N                           | ATOM | 699 | CE1 PHE B 142 | 5.014 -15.824 25.291 1.00 39.74  | C   |
| ATOM                        | 637 | CA ARG B 135  | 7.308 -26.580 43.958 1.00 49.30  | C                           | ATOM | 700 | CE2 PHE B 142 | 5.716 -18.078 28.930 1.00 43.76  | C   |
| ATOM                        | 638 | C ARG B 135   | 7.436 -25.791 42.694 1.00 37.66  | C                           | ATOM | 701 | CZ PHE B 142  | 5.453 -15.420 23.163 1.00 62.13  | C   |
| ATOM                        | 639 | O ARG B 135   | 7.640 -24.581 42.746 1.00 38.49  | O                           | ATOM | 702 | N PRO B 143   | 3.881 -14.480 21.170 1.00 70.30  | N   |
| ATOM                        | 640 | CB ARG B 135  | 7.770 -25.931 45.164 1.00 38.77  | C                           | ATOM | 703 | CA PRO B 143  | 2.603 -15.079 21.744 1.00 64.80  | C   |
| ATOM                        | 641 | CG ARG B 135  | 7.416 -26.545 46.498 1.00 53.56  | C                           | ATOM | 704 | C PRO B 143   | 3.881 -14.480 21.170 1.00 70.30  | C   |
| ATOM                        | 642 | CD ARG B 135  | 8.274 -25.914 47.615 1.00 46.69  | C                           | ATOM | 705 | O PRO B 143   | 4.673 -13.580 21.898 1.00 65.49  | O   |
| ATOM                        | 643 | NE ARG B 135  | 9.655 -26.018 47.348 1.00 49.58  | N                           | ATOM | 706 | CB PRO B 143  | 1.477 -14.043 21.738 1.00 71.71  | C   |
| ATOM                        | 644 | CZ ARG B 135  | 10.588 -25.302 47.966 1.00 56.92 | C                           | ATOM | 707 | CG PRO B 143  | 3.600 -13.376 23.057 1.00 63.97  | C   |
| ATOM                        | 645 | NH1 ARG B 135 | 10.245 -24.421 48.895 1.00 70.65 | NH1                         | ATOM | 708 | CD PRO B 143  | 2.031 -14.449 24.023 1.00 64.16  | C   |
| ATOM                        | 646 | NH2 ARG B 135 | 11.666 -25.468 47.654 1.00 59.88 | NH2                         | ATOM | 709 | N ALA B 144   | 4.071 -14.643 19.667 1.00 75.30  | N   |
| ATOM                        | 647 | N ARG B 136   | 7.466 -26.481 41.558 1.00 39.84  | N                           | ATOM | 710 | CA ALA B 144  | 5.227 -14.063 19.183 1.00 72.00  | C   |
| ATOM                        | 648 | CA ARG B 136  | 7.835 -25.847 40.299 1.00 32.81  | C                           | ATOM | 711 | C ALA B 144   | 5.147 -12.557 19.106 1.00 74.68  | C   |
| ATOM                        | 649 | C ARG B 136   | 6.716 -25.961 39.270 1.00 27.68  | C                           | ATOM | 712 | O ALA B 144   | 6.167 -11.882 18.964 1.00 81.31  | O   |
| ATOM                        | 650 | O ARG B 136   | 6.018 -26.971 39.209 1.00 42.31  | O                           | ATOM | 713 | CB ALA B 144  | 5.349 -14.676 17.804 1.00 60.70  | C   |
| ATOM                        | 651 | CB ARG B 136  | 9.109 -26.476 39.734 1.00 39.50  | C                           | ATOM | 714 | N SER B 145   | 3.931 -12.027 19.195 1.00 74.38  | N   |
| ATOM                        | 652 | CG ARG B 136  | 10.357 -26.283 40.877 1.00 37.77 | C                           | ATOM | 715 | CA SER B 145  | 3.686 -10.586 19.153 1.00 76.16  | C   |
| ATOM                        | 653 | CD ARG B 136  | 11.548 -26.952 39.906 1.00 56.98 | C                           | ATOM | 716 | C SER B 145   | 4.415 -9.835 20.268 1.00 81.92   | C   |
| ATOM                        | 654 | NE ARG B 136  | 12.811 -26.662 40.577 1.00 60.87 | N                           | ATOM | 717 | O SER B 145   | 4.815 -8.601 20.100 1.00 82.18   | O   |
| ATOM                        | 655 | CZ ARG B 136  | 13.275 -27.345 41.619 1.00 67.79 | C                           | ATOM | 718 | CB SER B 145  | 2.165 -10.305 19.240 1.00 60.29  | C   |
| ATOM                        | 656 | NH1 ARG B 136 | 12.582 -28.365 42.107 1.00 79.69 | NH1                         | ATOM | 719 | CG SER B 145  | 1.676 -10.694 20.502 1.00 92.36  | C   |
| ATOM                        | 657 | NH2 ARG B 136 | 14.415 -27.013 42.469 1.00 61.11 | NH2                         | ATOM | 720 | N LEU B 146   | 4.576 -10.500 21.406 1.00 84.31  | N   |
| ATOM                        | 658 | N VAL B 137   | 6.546 -24.917 38.466 1.00 37.30  | N                           | ATOM | 721 | C LEU B 146   | 5.157 -9.678 21.587 1.00 83.32   | C   |
| ATOM                        | 659 | CA VAL B 137  | 5.517 -24.913 37.434 1.00 38.55  | C                           | ATOM | 722 | O LEU B 146   | 6.656 -9.630 21.450 1.00 84.18   | O   |
| ATOM                        | 660 | C VAL B 137   | 6.098 -24.528 36.079 1.00 40.36  | C                           | ATOM | 723 | O LEU B 146   | 7.418 -10.527 22.082 1.00 74.84  | C   |
| ATOM                        | 661 | CB VAL B 137  | 7.224 -24.039 35.992 1.00 43.64  | C                           | ATOM | 724 | CB LEU B 146  | 4.682 -10.733 23.822 1.00 72.49  | C   |
| ATOM                        | 662 | CG VAL B 137  | 4.366 -23.941 37.770 1.00 41.99  | C                           | ATOM | 725 | CG LEU B 146  | 5.361 -10.183 25.159 1.00 80.74  | C   |
| ATOM                        | 663 | CD VAL B 137  | 3.653 -24.872 39.040 1.00 47.76  | C                           | ATOM | 726 | CD LEU B 146  | 4.645 -8.908 25.521 1.00 81.94   | C   |
| ATOM                        | 664 | CE1 VAL B 137 | 4.892 -22.518 37.888 1.00 26.22  | C                           | ATOM | 727 | CD2 LEU B 146 | 10.643 -7.465 17.537 1.00 65.89  | C   |
| ATOM                        | 665 | N LEU B 138   | 5.822 -24.756 35.024 1.00 37.25  | N                           | ATOM | 728 | N ARG B 147   | 7.074 -8.405 22.753 1.00 68.61   | N   |
| ATOM                        | 666 | CA LEU B 138  | 5.710 -24.353 33.679 1.00 29.06  | C                           | ATOM | 729 | CA ARG B 147  | 8.481 -8.033 22.706 1.00 72.52   | C   |
| ATOM                        | 667 | C LEU B 138   | 4.687 -23.388 33.099 1.00 32.56  | C                           | ATOM | 730 | C ARG B 147   | 8.915 -7.455 24.044 1.00 71.17   | C   |
| ATOM                        | 668 | O LEU B 138   | 3.487 -23.686 33.044 1.00 47.76  | O                           | ATOM | 731 | N SER B 147   | 8.859 -6.244 24.261 1.00 73.99   | N   |
| ATOM                        | 669 | CB LEU B 138  | 5.859 -22.571 32.766 1.00 49.71  | C                           | ATOM | 732 | CB ARG B 147  | 8.794 -7.034 21.591 1.00 69.41   | C   |
| ATOM                        | 670 | CG LEU B 138  | 7.190 -26.319 32.625 1.00 45.66  | C                           | ATOM | 733 | CG ARG B 147  | 8.414 -7.500 20.190 1.00 77.46   | C   |
| ATOM                        | 671 | CD1 LEU B 138 | 7.144 -27.546 31.930 1.00 44.69  | C                           | ATOM | 734 | CD ARG B 147  | 9.364 -6.610 19.768 1.00 75.86   | C   |
| ATOM                        | 672 | CD2 LEU B 138 | 8.331 -25.599 32.421 1.00 52.92  | C                           | ATOM | 735 | N SER B 147   | 10.750 -6.419 19.727 1.00 82.31  | N   |
| ATOM                        | 673 | N VAL B 139   | 5.150 -22.221 32.667 1.00 47.40  | N                           | ATOM | 736 | CB ARG B 147  | 11.330 -7.610 18.659 1.00 78.11  | C   |
| ATOM                        | 674 | CA VAL B 139  | 4.261 -21.233 32.071 1.00 46.87  | C                           | ATOM | 737 | NH1 ARG B 147 | 10.643 -7.465 17.537 1.00 65.89  | NH1 |
| ATOM                        | 675 | C VAL B 139   | 4.406 -21.222 30.552 1.00 54.48  | C                           | ATOM | 738 | NH2 ARG B 147 | 12.598 -7.221 18.717 1.00 76.79  | NH2 |
| ATOM                        | 676 | O VAL B 139   | 5.479 -20.929 30.025 1.00 48.65  | O                           | ATOM | 739 | N LEU B 148   | 9.362 -8.332 24.937 1.00 68.88   | N   |
| ATOM                        | 677 | CB VAL B 139  | 4.534 -19.819 32.622 1.00 38.93  | C                           | ATOM | 740 | CA LEU B 148  | 9.879 -7.910 26.230 1.00 57.01   | C   |
| ATOM                        | 678 | CG VAL B 139  | 4.464 -18.050 32.144 1.00 38.51  | C                           | ATOM | 741 | C LEU B 148   | 11.260 -6.801 26.489 1.00 54.43  | C   |
| ATOM                        | 679 | CD VAL B 139  | 4.586 -19.845 32.142 1.00 27.94  | C                           | ATOM | 742 | O LEU B 148   | 11.864 -9.603 26.028 1.00 60.18  | O   |
| ATOM                        | 680 | N THR B 140   | 3.325 -21.556 29.636 1.00 54.13  | N                           | ATOM | 743 | CB LEU B 148  | 8.920 -8.327 27.150 1.00 57.41   | C   |
| ATOM                        | 681 | CA THR B 140  | 3.385 -21.613 28.398 1.00 49.48  | C                           | ATOM | 744 | CG LEU B 148  | 7.575 -7.595 27.408 1.00 65.76   | C   |
| ATOM                        | 682 | C THR B 140   | 2.214 -20.759 27.819 1.00 47.30  | C                           | ATOM | 745 | CD1 LEU B 148 | 6.698 -8.174 28.509 1.00 55.49   | C   |
| ATOM                        | 683 | O THR B 140   | 1.268 -20.405 28.523 1.00 46.31  | O                           | ATOM | 746 | CD2 LEU B 148 | 7.765 -6.097 27.596 1.00 64.15   | C   |
| ATOM                        | 684 | CB THR B 140  | 3.188 -20.059 27.883 1.00 46.31  | C                           | ATOM | 747 | N SER B 149   | 12.094 -7.034 27.210 1.00 77.18  | N   |
| ATOM                        | 685 | CG1 THR B 140 | 4.190 -23.946 28.446 1.00 41.42  | C                           | ATOM | 748 | CA SER B 149  | 13.987 -8.285 27.635 1.00 53.64  | C   |
| ATOM                        | 686 | CG2 THR B 140 | 1.293 -23.581 28.276 1.00 52.23  | C                           | ATOM | 749 | C SER B 149   | 13.170 -8.480 28.552 1.00 50.70  | C   |
| ATOM                        | 687 | N GLY B 141   | 2.318 -20.432 26.934 1.00 45.96  | N                           | ATOM | 750 | O SER B 149   | 12.064 -9.649 29.113 1.00 40.60  | O   |
| ATOM                        | 688 | CA GLY B 141  | 1.263 -19.706 25.851 1.00 42.36  | C                           | ATOM | 751 | CB SER B 149  | 14.213 -7.204 28.339 1.00 55.31  | C   |
| ATOM                        | 689 | C GLY B 141   | 1.475 -18.161 25.365 1.00 32.95  | C                           | ATOM | 752 | CG SER B 149  | 15.951 -6.018 28.407 1.00 49.69  | C   |
| ATOM                        | 690 | O GLY B 141   | 0.846 -17.569 24.862 1.00 42.14  | O                           | ATOM | 753 | N GLU B 150   | 14.194 -10.315 28.704 1.00 49.79 | N   |
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| ATOM                        | 754 | CA GLU B 150  | 14.109 -11.472 29.589 1.00 41.30 | C                           | ATOM | 817 | CB LEU B 157  | 6.238 -14.094 34.832 1.00 39.07  | C   |
| ATOM                        | 755 | C GLU B 150   | 13.786 -11.016 31.007 1.00 43.40 | C                           | ATOM | 818 | CG LEU B 157  | 5.962 -14.136 33.124 1.00 38.40  | C   |
| ATOM                        | 756 | O GLU B 150   | 12.937 -11.601 31.692 1.00 41.01 | O                           | ATOM | 819 | CD1 LEU B 157 | 6.877 -15.235 32.689 1.00 27.60  | C   |
| ATOM                        | 757 | CB GLU B 150  | 15.417 -12.263 29.573 1.00 42.92 | C                           | ATOM | 820 | CD2 LEU B 157 | 4.518 -14.486 33.046 1.00 31.71  | C   |
| ATOM                        | 758 | CG GLU B 150  | 15.421 -13.466 30.500 1.00 43.52 | C                           | ATOM | 821 | N GLU B 158   | 6.683 -12.796 37.676 1.00 30.56  | N   |
| ATOM                        | 759 | CD GLU B 150  | 16.799 -14.073 30.666 1.00 43.33 | C                           | ATOM | 822 | CA GLU B 158  | 6.851 -12.928 39.119 1.00 32.80  | C   |
| ATOM                        | 760 | OE1 GLU B 150 | 16.884 -15.249 31.076 1.00 46.55 | O                           | ATOM | 823 | C GLU B 158   | 5.895 -11.995 39.864 1.00 37.72  | C   |
| ATOM                        | 761 | OE2 GLU B 150 | 17.797 -13.372 30.395 1.00 66.84 | O                           | ATOM | 824 | O GLU B 158   | 5.408 -12.326 40.945 1.00 36.99  | O   |
| ATOM                        | 762 | N GLU B 151   | 14.435 -9.967 31.424 1.00 41.49  | N                           | ATOM | 825 | CB GLU B 158  | 8.299 -12.643 39.527 1.00 36.81  | C   |
| ATOM                        | 763 | CA GLU B 151  | 14.316 -9.427 32.774 1.00 45.39  | C                           | ATOM | 826 | CG GLU B 158  | 8.578 -12.867 41.009 1.00 27.09  | C   |
| ATOM                        | 764 | C GLU B 151   | 12.915 -8.881 33.006 1.00 46.51  | C                           | ATOM | 827 | CD GLU B 158  | 10.052 -12.777 41.352 1.00 37.91 | C   |
| ATOM                        | 765 | O GLU B 151   | 12.327 -9.114 34.057 1.00 41.51  | O                           | ATOM | 828 | OE1 GLU B 158 | 10.410 -13.050 42.517 1.00 47.97 | O   |
| ATOM                        | 766 | CB GLU B 151  | 15.317 -8.335 33.036 1.00 37.93  | C                           | ATOM | 829 | OE2 GLU B 158 | 10.854 -12.428 40.460 1.00 30.62 | O   |
| ATOM                        | 767 | CG GLU B 151  | 16.544 -8.796 33.866 1.00 44.95  | C                           | ATOM | 830 | N ILE B 159   | 5.637 -10.827 39.281 1.00 37.70  | N   |
| ATOM                        | 768 | CD GLU B 151  | 16.273 -8.718 35.359 1.00 64.95  | C                           | ATOM | 831 | CA ILE B 159  | 4.633 -9.890 39.815 1.00 34.19   | C   |
| ATOM                        | 769 | OE1 GLU B 151 | 15.952 -7.613 35.847 1.00 61.83  | O                           | ATOM | 832 | C ILE B 159   | 3.278 -10.539 39.843 1.00 39.33  | C   |
| ATOM                        | 770 | OE2 GLU B 151 | 16.380 -9.756 36.042 1.00 72.24  | O                           | ATOM | 833 | O ILE B 159   | 2.591 -10.512 40.862 1.00 40.38  | O   |
| ATOM                        | 771 | N GLU B 152   | 12.373 -8.176 32.043 1.00 49.34  | N                           | ATOM | 834 | CB ILE B 159  | 4.567 -8.586 38.987 1.00 40.68   | C   |
| ATOM                        | 772 | C GLU B 152   | 11.045 -7.594 32.167 1.00 37.10  | C                           | ATOM | 835 | CG1 ILE B 159 | 5.876 -7.000 39.052 1.00 41.11   | C   |
| ATOM                        | 773 | O GLU B 152   | 9.964 -8.666 32.104 1.00 46.47   | O                           | ATOM | 836 | CG2 ILE B 159 | 3.431 -7.711 39.491 1.00 30.50   | C   |
| ATOM                        | 774 | O GLU B 152   | 8.990 -8.602 32.644 1.00 48.37   | O                           | ATOM | 837 | CD1 ILE B 159 | 6.110 -7.109 40.362 1.00 37.01   | C   |
| ATOM                        | 775 | CB GLU B 152  | 10.785 -6.524 31.105 1.00 54.07  | C                           | ATOM | 838 | CD2 ILE B 159 | 2.879 -11.119 39.716 1.00 39.16  | C   |
| ATOM                        | 776 | CG GLU B 152  | 9.476 -6.773 31.320 1.00 61.66   | C                           | ATOM | 839 | CA PHE B 160  | 1.552 -11.710 38.606 1.00 41.85  | C   |
| ATOM                        | 777 | CD GLU B 152  | 9.264 -4.624 30.354 1.00 70.81   | C                           | ATOM | 840 | C PHE B 160   | 1.367 -12.907 39.529 1.00 40.04  | C   |
| ATOM                        | 778 | OE1 GLU B 152 | 10.158 -4.418 29.487 1.00 70.00  | O                           | ATOM | 841 | O PHE B 160   | 0.443 -12.945 40.341 1.00 39.54  | O   |
| ATOM                        | 779 | OE2 GLU B 152 | 8.                               |                             |      |     |               |                                  |     |

| OCTANER-POB-coordinates.txt |     |     |     |   |     |        |         |        |      | OCTANER-POB-coordinates.txt |   |      |     |     |     |   |     |        |         |        |      |       |      |      |     |     |     |   |     |        |         |        |      |       |      |
|-----------------------------|-----|-----|-----|---|-----|--------|---------|--------|------|-----------------------------|---|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|------|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|------|
| ATOM                        | 880 | N   | ARG | B | 165 | -3.856 | -12.948 | 45.447 | 1.00 | 39.07                       | N | ATOM | 943 | C   | ARG | B | 174 | 13.847 | -18.292 | 36.711 | 1.00 | 42.30 | C    | ATOM | 943 | C   | ARG | B | 174 | 13.847 | -18.292 | 36.711 | 1.00 | 42.30 | C    |
| ATOM                        | 881 | CA  | ARG | B | 165 | -5.151 | -12.707 | 44.815 | 1.00 | 44.79                       | C | ATOM | 944 | O   | ARG | B | 174 | 15.041 | -17.097 | 36.723 | 1.00 | 32.73 | C    | ATOM | 944 | O   | ARG | B | 174 | 15.041 | -17.097 | 36.723 | 1.00 | 32.73 | C    |
| ATOM                        | 882 | C   | ARG | B | 165 | -5.254 | -13.409 | 42.463 | 1.00 | 51.92                       | C | ATOM | 945 | CG  | ARG | B | 174 | 12.871 | -16.413 | 38.067 | 1.00 | 36.97 | C    | ATOM | 945 | CG  | ARG | B | 174 | 12.871 | -16.413 | 38.067 | 1.00 | 36.97 | C    |
| ATOM                        | 883 | O   | ARG | B | 165 | -6.352 | -11.639 | 42.947 | 1.00 | 63.42                       | O | ATOM | 946 | CG  | ARG | B | 174 | 11.774 | -15.709 | 37.313 | 1.00 | 32.17 | C    | ATOM | 946 | CG  | ARG | B | 174 | 11.774 | -15.709 | 37.313 | 1.00 | 32.17 | C    |
| ATOM                        | 884 | CB  | ARG | B | 165 | -5.113 | -11.206 | 43.851 | 1.00 | 14.15                       | C | ATOM | 947 | CD  | ARG | B | 174 | 11.723 | -14.258 | 37.772 | 1.00 | 49.94 | C    | ATOM | 947 | CD  | ARG | B | 174 | 11.723 | -14.258 | 37.772 | 1.00 | 49.94 | C    |
| ATOM                        | 885 | CG  | ARG | B | 165 | -4.548 | -10.495 | 43.820 | 0.00 | 43.32                       | C | ATOM | 948 | CE  | ARG | B | 174 | 12.974 | -13.559 | 37.486 | 1.00 | 40.99 | C    | ATOM | 948 | CE  | ARG | B | 174 | 12.974 | -13.559 | 37.486 | 1.00 | 40.99 | C    |
| ATOM                        | 886 | CD  | ARG | B | 165 | -5.132 | -9.120  | 43.316 | 0.00 | 45.36                       | C | ATOM | 949 | CZ  | ARG | B | 174 | 13.117 | -12.238 | 37.511 | 1.00 | 40.59 | C    | ATOM | 949 | CZ  | ARG | B | 174 | 13.117 | -12.238 | 37.511 | 1.00 | 40.59 | C    |
| ATOM                        | 887 | NE  | ARG | B | 165 | -4.350 | -8.363  | 42.343 | 0.00 | 45.07                       | C | ATOM | 950 | NH1 | ARG | B | 174 | 12.084 | -11.462 | 37.806 | 1.00 | 36.42 | C    | ATOM | 950 | NH1 | ARG | B | 174 | 12.084 | -11.462 | 37.806 | 1.00 | 36.42 | C    |
| ATOM                        | 888 | CZ  | ARG | B | 165 | -3.466 | -7.423  | 42.663 | 0.00 | 44.81                       | C | ATOM | 951 | NH2 | ARG | B | 174 | 14.295 | -11.693 | 37.236 | 1.00 | 34.95 | NH1+ | ATOM | 951 | NH2 | ARG | B | 174 | 14.295 | -11.693 | 37.236 | 1.00 | 34.95 | NH1+ |
| ATOM                        | 889 | NH1 | ARG | B | 165 | -3.247 | -7.123  | 42.936 | 0.00 | 49.19                       | N | ATOM | 952 | N   | GLU | B | 175 | 13.278 | -18.929 | 35.693 | 1.00 | 32.92 | C    | ATOM | 952 | N   | GLU | B | 175 | 13.278 | -18.929 | 35.693 | 1.00 | 32.92 | C    |
| ATOM                        | 890 | NH2 | ARG | B | 165 | -2.804 | -6.780  | 41.710 | 0.00 | 45.78                       | C | ATOM | 953 | CA  | GLU | B | 175 | 14.075 | -19.323 | 34.537 | 1.00 | 33.74 | C    | ATOM | 953 | CA  | GLU | B | 175 | 14.075 | -19.323 | 34.537 | 1.00 | 33.74 | C    |
| ATOM                        | 891 | N   | ASN | B | 166 | -4.109 | -13.765 | 42.890 | 1.00 | 49.44                       | C | ATOM | 954 | C   | GLU | B | 175 | 13.298 | -19.284 | 35.228 | 1.00 | 37.83 | C    | ATOM | 954 | C   | GLU | B | 175 | 13.298 | -19.284 | 35.228 | 1.00 | 37.83 | C    |
| ATOM                        | 892 | CA  | ASN | B | 166 | -4.085 | -14.524 | 41.646 | 1.00 | 44.40                       | C | ATOM | 955 | O   | GLU | B | 175 | 12.271 | -18.945 | 33.075 | 1.00 | 31.15 | C    | ATOM | 955 | O   | GLU | B | 175 | 12.271 | -18.945 | 33.075 | 1.00 | 31.15 | C    |
| ATOM                        | 893 | C   | ASN | B | 166 | -3.939 | -16.017 | 41.918 | 1.00 | 45.25                       | C | ATOM | 956 | CB  | GLU | B | 175 | 14.643 | -20.729 | 34.733 | 1.00 | 38.78 | C    | ATOM | 956 | CB  | GLU | B | 175 | 14.643 | -20.729 | 34.733 | 1.00 | 38.78 | C    |
| ATOM                        | 894 | O   | ASN | B | 166 | -3.801 | -16.825 | 40.992 | 1.00 | 47.17                       | C | ATOM | 957 | CG  | GLU | B | 175 | 15.547 | -21.172 | 33.594 | 1.00 | 50.78 | C    | ATOM | 957 | CG  | GLU | B | 175 | 15.547 | -21.172 | 33.594 | 1.00 | 50.78 | C    |
| ATOM                        | 895 | CB  | ASN | B | 166 | -2.947 | -14.090 | 40.749 | 1.00 | 42.11                       | C | ATOM | 958 | CD  | GLU | B | 175 | 16.061 | -22.586 | 33.763 | 1.00 | 53.52 | C    | ATOM | 958 | CD  | GLU | B | 175 | 16.061 | -22.586 | 33.763 | 1.00 | 53.52 | C    |
| ATOM                        | 896 | CG  | ASN | B | 166 | -3.205 | -12.663 | 40.178 | 1.00 | 50.61                       | C | ATOM | 959 | CE  | GLU | B | 175 | 15.700 | -23.239 | 34.765 | 1.00 | 57.67 | C    | ATOM | 959 | CE  | GLU | B | 175 | 15.700 | -23.239 | 34.765 | 1.00 | 57.67 | C    |
| ATOM                        | 897 | ND2 | ASN | B | 166 | -2.141 | -11.890 | 40.004 | 1.00 | 42.34                       | C | ATOM | 960 | OE2 | GLU | B | 175 | 16.824 | -23.044 | 32.866 | 1.00 | 50.24 | O1-  | ATOM | 960 | OE2 | GLU | B | 175 | 16.824 | -23.044 | 32.866 | 1.00 | 50.24 | O1-  |
| ATOM                        | 898 | OD1 | ASN | B | 166 | -4.348 | -12.290 | 39.913 | 1.00 | 54.49                       | C | ATOM | 961 | N   | LEU | B | 176 | 13.609 | -18.409 | 32.287 | 1.00 | 37.81 | C    | ATOM | 961 | N   | LEU | B | 176 | 13.609 | -18.409 | 32.287 | 1.00 | 37.81 | C    |
| ATOM                        | 899 | N   | GLY | B | 167 | -3.872 | -16.372 | 43.187 | 1.00 | 32.46                       | C | ATOM | 962 | CA  | LEU | B | 176 | 13.324 | -18.499 | 30.915 | 1.00 | 37.46 | C    | ATOM | 962 | CA  | LEU | B | 176 | 13.324 | -18.499 | 30.915 | 1.00 | 37.46 | C    |
| ATOM                        | 900 | CA  | GLY | B | 167 | -3.754 | -17.160 | 43.600 | 1.00 | 37.95                       | C | ATOM | 963 | C   | LEU | B | 176 | 14.104 | -19.501 | 30.073 | 1.00 | 36.53 | C    | ATOM | 963 | C   | LEU | B | 176 | 14.104 | -19.501 | 30.073 | 1.00 | 36.53 | C    |
| ATOM                        | 901 | C   | GLY | B | 167 | -2.311 | -18.180 | 43.795 | 1.00 | 45.90                       | C | ATOM | 964 | O   | LEU | B | 176 | 15.290 | -19.302 | 29.811 | 1.00 | 39.06 | C    | ATOM | 964 | O   | LEU | B | 176 | 15.290 | -19.302 | 29.811 | 1.00 | 39.06 | C    |
| ATOM                        | 902 | O   | GLY | B | 167 | -2.021 | -19.356 | 44.021 | 1.00 | 46.56                       | C | ATOM | 965 | CB  | LEU | B | 176 | 13.123 | -16.985 | 28.808 | 1.00 | 48.71 | C    | ATOM | 965 | CB  | LEU | B | 176 | 13.123 | -16.985 | 28.808 | 1.00 | 48.71 | C    |
| ATOM                        | 903 | N   | GLY | B | 168 | -1.403 | -17.214 | 43.711 | 1.00 | 41.93                       | C | ATOM | 966 | CG  | LEU | B | 176 | 11.735 | -17.515 | 28.482 | 1.00 | 36.53 | C    | ATOM | 966 | CG  | LEU | B | 176 | 11.735 | -17.515 | 28.482 | 1.00 | 36.53 | C    |
| ATOM                        | 904 | CA  | GLY | B | 168 | 0.018  | -17.501 | 43.776 | 1.00 | 41.11                       | C | ATOM | 967 | CD  | LEU | B | 176 | 13.267 | -15.545 | 28.345 | 1.00 | 35.35 | C    | ATOM | 967 | CD  | LEU | B | 176 | 13.267 | -15.545 | 28.345 | 1.00 | 35.35 | C    |
| ATOM                        | 905 | C   | GLY | B | 168 | 0.651  | -17.179 | 43.135 | 1.00 | 49.98                       | C | ATOM | 968 | CE  | LEU | B | 176 | 13.490 | -20.581 | 29.657 | 1.00 | 33.82 | C    | ATOM | 968 | CE  | LEU | B | 176 | 13.490 | -20.581 | 29.657 | 1.00 | 33.82 | C    |
| ATOM                        | 906 | O   | GLY | B | 168 | 0.002  | -17.410 | 46.173 | 1.00 | 45.23                       | C | ATOM | 969 | N   | LEU | B | 177 | 14.118 | -21.577 | 28.827 | 1.00 | 51.42 | C    | ATOM | 969 | N   | LEU | B | 177 | 14.118 | -21.577 | 28.827 | 1.00 | 51.42 | C    |
| ATOM                        | 907 | N   | GLY | B | 169 | 1.935  | -16.935 | 45.116 | 1.00 | 40.14                       | C | ATOM | 970 | CA  | LEU | B | 177 | 14.337 | -20.972 | 27.339 | 1.00 | 45.69 | C    | ATOM | 970 | CA  | LEU | B | 177 | 14.337 | -20.972 | 27.339 | 1.00 | 45.69 | C    |
| ATOM                        | 908 | CA  | GLY | B | 169 | 2.706  | -16.756 | 46.333 | 1.00 | 29.40                       | C | ATOM | 971 | C   | LEU | B | 177 | 13.524 | -20.171 | 26.979 | 1.00 | 51.42 | C    | ATOM | 971 | C   | LEU | B | 177 | 13.524 | -20.171 | 26.979 | 1.00 | 51.42 | C    |
| ATOM                        | 909 | C   | GLY | B | 169 | 4.134  | -16.450 | 46.003 | 1.00 | 32.25                       | C | ATOM | 972 | O   | LEU | B | 177 | 13.313 | -22.886 | 28.756 | 1.00 | 38.56 | C    | ATOM | 972 | O   | LEU | B | 177 | 13.313 | -22.886 | 28.756 | 1.00 | 38.56 | C    |
| ATOM                        | 910 | O   | GLY | B | 169 | 4.505  | -16.107 | 44.891 | 1.00 | 25.61                       | C | ATOM | 973 | CB  | LEU | B | 177 | 13.221 | -23.600 | 29.992 | 1.00 | 38.70 | C    | ATOM | 973 | CB  | LEU | B | 177 | 13.221 | -23.600 | 29.992 | 1.00 | 38.70 | C    |
| ATOM                        | 911 | N   | ASP | B | 170 | 4.988  | -16.351 | 44.012 | 1.00 | 29.18                       | C | ATOM | 974 | CG  | LEU | B | 177 | 12.664 | -23.119 | 31.238 | 1.00 | 15.37 | C    | ATOM | 974 | CG  | LEU | B | 177 | 12.664 | -23.119 | 31.238 | 1.00 | 15.37 | C    |
| ATOM                        | 912 | CA  | ASP | B | 170 | 6.397  | -15.994 | 46.879 | 1.00 | 31.71                       | C | ATOM | 975 | CD  | LEU | B | 177 | 10.426 | -25.064 | 29.632 | 1.00 | 35.98 | C    | ATOM | 975 | CD  | LEU | B | 177 | 10.426 | -25.064 | 29.632 | 1.00 | 35.98 | C    |
| ATOM                        | 913 | C   | ASP | B | 170 | 7.134  | -16.362 | 45.671 | 1.00 | 34.71                       | C | ATOM | 976 | CE  | LEU | B | 177 | 15.441 | -21.352 | 26.772 | 1.00 | 57.76 | C    | ATOM | 976 | CE  | LEU | B | 177 | 15.441 | -21.352 | 26.772 | 1.00 | 57.76 | C    |
| ATOM                        | 914 | O   | ASP | B | 170 | 7.115  | -16.067 | 48.229 | 1.00 | 22.66                       | C | ATOM | 977 | N   | PRO | B | 178 | 15.670 | -20.716 | 25.517 | 1.00 | 59.16 | C    | ATOM | 977 | N   | PRO | B | 178 | 15.670 | -20.716 | 25.517 | 1.00 | 59.16 | C    |
| ATOM                        | 915 | CB  | ASP | B | 170 | 6.746  | -14.919 | 49.162 | 1.00 | 29.46                       | C | ATOM | 978 | C   | PRO | B | 178 | 14.821 | -20.705 | 24.417 | 1.00 | 56.95 | C    | ATOM | 978 | C   | PRO | B | 178 | 14.821 | -20.705 | 24.417 | 1.00 | 56.95 | C    |
| ATOM                        | 916 | CG  | ASP | B | 170 | 5.733  | -14.244 | 48.887 | 1.00 | 39.19                       | C | ATOM | 979 | CA  | PRO | B | 178 | 14.615 | -19.652 | 23.765 | 1.00 | 51.05 | C    | ATOM | 979 | CA  | PRO | B | 178 | 14.615 | -19.652 | 23.765 | 1.00 | 51.05 | C    |
| ATOM                        | 917 | OD1 | ASP | B | 170 | 7.475  | -14.707 | 50.142 | 1.00 | 28.91                       | C | ATOM | 980 | CB  | PRO | B | 178 | 12.056 | -21.572 | 25.064 | 1.00 | 35.98 | C    | ATOM | 980 | CB  | PRO | B | 178 | 12.056 | -21.572 | 25.064 | 1.00 | 35.98 | C    |
| ATOM                        | 918 | OD2 | ASP | B | 170 | 7.662  | -16.206 | 44.965 | 1.00 | 32.42                       | C | ATOM | 981 | CG  | PRO | B | 178 | 17.488 | -22.334 | 26.228 | 1.00 | 66.64 | C    | ATOM | 981 | CG  | PRO | B | 178 | 17.488 | -22.334 | 26.228 | 1.00 | 66.64 | C    |
| ATOM                        | 919 | N   | VAL | B | 171 | 8.631  | -16.899 | 43.946 | 1.00 | 29.42                       | C | ATOM | 982 | CD  | PRO | B | 178 | 16.373 | -22.402 | 27.216 | 1.00 | 70.67 | C    | ATOM | 982 | CD  | PRO | B | 178 | 16.373 | -22.402 | 27.216 | 1.00 | 70.67 | C    |
| ATOM                        | 920 | CA  | VAL | B | 171 | 10.106 | -16.924 | 44.161 | 1.00 | 25.13                       | C | ATOM | 983 | C   | GLY | B | 179 | 14.370 | -21.843 | 24.216 | 1.00 | 55.11 | C    | ATOM | 983 | C   | GLY | B | 179 | 14.370 | -21.843 | 24.216 | 1.00 | 55.11 | C    |
| ATOM                        | 921 | C   | VAL | B | 171 | 10.705 | -15.878 | 44.600 | 1.00 | 25.13                       | C | ATOM | 984 |     |     |   |     |        |         |        |      |       |      |      |     |     |     |   |     |        |         |        |      |       |      |

|                             |      |     |     |   |     |        |         |        |            |     |
|-----------------------------|------|-----|-----|---|-----|--------|---------|--------|------------|-----|
| ATOM                        | 1132 | CG  | GLN | B | 199 | 23.066 | -24.417 | 16.810 | 1.00 41.04 | C   |
| ATOM                        | 1133 | CD  | GLN | B | 199 | 30.049 | -24.337 | 17.963 | 1.00 64.13 | C   |
| ATOM                        | 1134 | NE2 | GLN | B | 199 | 30.162 | -23.157 | 18.561 | 1.00 82.00 | C   |
| ATOM                        | 1135 | OE1 | GLN | B | 199 | 30.686 | -25.326 | 18.322 | 1.00 74.89 | C   |
| ATOM                        | 1136 | N   | PHE | B | 200 | 27.359 | -23.790 | 14.097 | 1.00 31.96 | C   |
| ATOM                        | 1137 | CA  | PHE | B | 200 | 27.361 | -22.704 | 13.126 | 1.00 29.18 | C   |
| ATOM                        | 1138 | C   | PHE | B | 200 | 27.461 | -21.361 | 13.332 | 1.00 32.56 | C   |
| ATOM                        | 1139 | O   | PHE | B | 200 | 27.089 | -21.237 | 13.996 | 1.00 31.21 | C   |
| ATOM                        | 1140 | CB  | PHE | B | 200 | 26.132 | -22.731 | 12.238 | 1.00 26.93 | C   |
| ATOM                        | 1141 | CG  | PHE | B | 200 | 25.959 | -24.000 | 11.458 | 1.00 27.56 | C   |
| ATOM                        | 1142 | CD1 | PHE | B | 200 | 25.356 | -25.108 | 12.030 | 1.00 26.59 | C   |
| ATOM                        | 1143 | CD2 | PHE | B | 200 | 26.374 | -24.074 | 10.139 | 1.00 21.26 | C   |
| ATOM                        | 1144 | CE1 | PHE | B | 200 | 25.190 | -26.273 | 11.308 | 1.00 27.84 | C   |
| ATOM                        | 1145 | CE2 | PHE | B | 200 | 26.209 | -25.235 | 9.332  | 1.00 26.13 | C   |
| ATOM                        | 1146 | CZ  | PHE | B | 200 | 25.616 | -26.335 | 9.906  | 1.00 34.99 | C   |
| ATOM                        | 1147 | N   | THR | B | 201 | 27.964 | -20.357 | 13.125 | 1.00 34.48 | N   |
| ATOM                        | 1148 | CA  | THR | B | 201 | 27.941 | -18.993 | 13.627 | 1.00 41.61 | C   |
| ATOM                        | 1149 | C   | THR | B | 201 | 26.999 | -18.159 | 12.769 | 1.00 33.63 | C   |
| ATOM                        | 1150 | O   | THR | B | 201 | 27.287 | -17.870 | 11.607 | 1.00 32.18 | C   |
| ATOM                        | 1151 | CB  | THR | B | 201 | 29.343 | -18.363 | 13.634 | 1.00 40.22 | C   |
| ATOM                        | 1152 | CG2 | THR | B | 201 | 29.277 | -16.936 | 14.140 | 1.00 44.32 | C   |
| ATOM                        | 1153 | OG1 | THR | B | 201 | 30.203 | -19.125 | 14.489 | 1.00 36.69 | C   |
| ATOM                        | 1154 | N   | VAL | B | 202 | 25.871 | -17.773 | 13.353 | 1.00 40.94 | N   |
| ATOM                        | 1155 | CA  | VAL | B | 202 | 24.836 | -17.065 | 12.417 | 1.00 43.78 | C   |
| ATOM                        | 1156 | C   | VAL | B | 202 | 24.739 | -15.613 | 13.065 | 1.00 56.81 | C   |
| ATOM                        | 1157 | O   | VAL | B | 202 | 24.610 | -15.329 | 14.260 | 1.00 48.19 | C   |
| ATOM                        | 1158 | CB  | VAL | B | 202 | 23.460 | -17.735 | 12.793 | 1.00 31.64 | C   |
| ATOM                        | 1159 | CG1 | VAL | B | 202 | 22.419 | -17.066 | 11.910 | 1.00 39.60 | C   |
| ATOM                        | 1160 | CG2 | VAL | B | 202 | 23.552 | -19.235 | 12.478 | 1.00 27.58 | C   |
| ATOM                        | 1161 | N   | PRO | B | 203 | 24.805 | -14.856 | 12.089 | 1.00 56.92 | N   |
| ATOM                        | 1162 | CA  | PRO | B | 203 | 24.610 | -13.265 | 12.385 | 1.00 54.10 | C   |
| ATOM                        | 1163 | C   | PRO | B | 203 | 23.175 | -12.985 | 12.510 | 1.00 50.90 | C   |
| ATOM                        | 1164 | O   | PRO | B | 203 | 22.278 | -13.000 | 11.569 | 1.00 62.67 | C   |
| ATOM                        | 1165 | CB  | PRO | B | 203 | 23.924 | -12.570 | 11.041 | 1.00 55.62 | C   |
| ATOM                        | 1166 | CE  | PRO | B | 203 | 25.719 | -13.592 | 10.274 | 1.00 61.43 | C   |
| ATOM                        | 1167 | CD  | PRO | B | 203 | 25.184 | -14.920 | 10.696 | 1.00 52.91 | C   |
| ATOM                        | 1168 | N   | LEU | B | 204 | 22.960 | -12.722 | 14.094 | 1.00 62.75 | N   |
| ATOM                        | 1169 | CA  | LEU | B | 204 | 21.618 | -12.416 | 14.566 | 1.00 63.03 | C   |
| ATOM                        | 1170 | C   | LEU | B | 204 | 21.639 | -11.180 | 15.442 | 1.00 71.79 | C   |
| ATOM                        | 1171 | O   | LEU | B | 204 | 22.306 | -11.165 | 16.451 | 1.00 69.25 | C   |
| ATOM                        | 1172 | CB  | LEU | B | 204 | 21.028 | -13.602 | 15.336 | 1.00 65.68 | C   |
| ATOM                        | 1173 | CG  | LEU | B | 204 | 20.847 | -14.945 | 14.577 | 1.00 53.38 | C   |
| ATOM                        | 1174 | CD1 | LEU | B | 204 | 20.351 | -15.996 | 15.520 | 1.00 49.06 | C   |
| ATOM                        | 1175 | CD2 | LEU | B | 204 | 19.876 | -15.700 | 13.433 | 1.00 40.52 | C   |
| ATOM                        | 1176 | N   | GLY | B | 205 | 20.865 | -10.462 | 15.042 | 1.00 74.11 | C   |
| ATOM                        | 1177 | CA  | GLY | B | 205 | 20.765 | -9.924  | 15.793 | 1.00 78.63 | C   |
| ATOM                        | 1178 | C   | GLY | B | 205 | 22.118 | -8.314  | 16.110 | 1.00 76.04 | C   |
| ATOM                        | 1179 | O   | GLY | B | 205 | 22.136 | -7.737  | 17.381 | 1.00 73.15 | C   |
| ATOM                        | 1180 | N   | GLY | B | 206 | 23.037 | -8.412  | 15.155 | 1.00 77.57 | C   |
| ATOM                        | 1181 | CA  | GLY | B | 206 | 24.365 | -7.852  | 15.207 | 1.00 75.06 | C   |
| ATOM                        | 1182 | C   | GLY | B | 206 | 25.343 | -8.722  | 16.077 | 1.00 75.06 | C   |
| ATOM                        | 1183 | O   | GLY | B | 206 | 26.495 | -8.341  | 16.296 | 1.00 76.73 | C   |
| ATOM                        | 1184 | N   | GLN | B | 207 | 24.309 | -9.905  | 16.492 | 1.00 85.47 | C   |
| ATOM                        | 1185 | CA  | GLN | B | 207 | 25.835 | -10.777 | 17.210 | 1.00 76.73 | C   |
| ATOM                        | 1186 | C   | GLN | B | 207 | 26.261 | -11.916 | 16.312 | 1.00 64.00 | C   |
| ATOM                        | 1187 | O   | GLN | B | 207 | 25.550 | -12.267 | 15.361 | 1.00 63.27 | C   |
| ATOM                        | 1188 | CB  | GLN | B | 207 | 25.234 | -11.341 | 16.500 | 1.00 67.55 | C   |
| ATOM                        | 1189 | CG  | GLN | B | 207 | 24.421 | -10.432 | 19.391 | 1.00 74.18 | C   |
| ATOM                        | 1190 | CD  | GLN | B | 207 | 23.880 | -11.236 | 20.549 | 1.00 76.34 | C   |
| ATOM                        | 1191 | NE2 | GLN | B | 207 | 23.366 | -10.572 | 21.565 | 1.00 60.88 | C   |
| ATOM                        | 1192 | OE1 | GLN | B | 207 | 23.955 | -12.458 | 20.529 | 1.00 83.18 | C   |
| ATOM                        | 1193 | N   | GLN | B | 208 | 27.427 | -12.487 | 16.597 | 1.00 59.68 | C   |
| ATOM                        | 1194 | CA  | GLN | B | 208 | 27.837 | -13.717 | 15.938 | 1.00 63.20 | C   |
| octamer-PDB-coordinates.txt |      |     |     |   |     |        |         |        |            |     |
| ATOM                        | 1258 | G   | TYR | B | 216 | 13.451 | -35.436 | 14.264 | 1.00 77.61 | C   |
| ATOM                        | 1259 | CB  | TYR | B | 216 | 12.834 | -32.466 | 14.161 | 1.00 47.20 | C   |
| ATOM                        | 1260 | CG  | TYR | B | 216 | 12.530 | -21.996 | 14.779 | 1.00 55.14 | C   |
| ATOM                        | 1261 | CD1 | TYR | B | 216 | 12.525 | -31.124 | 15.858 | 1.00 53.29 | C   |
| ATOM                        | 1262 | CD2 | TYR | B | 216 | 11.307 | -32.439 | 14.287 | 1.00 47.93 | C   |
| ATOM                        | 1263 | CE  | TYR | B | 216 | 11.340 | -30.694 | 16.422 | 1.00 54.71 | C   |
| ATOM                        | 1264 | CE2 | TYR | B | 216 | 10.117 | -32.608 | 14.647 | 1.00 44.33 | C   |
| ATOM                        | 1265 | CZ  | TYR | B | 216 | 10.140 | -31.145 | 15.913 | 1.00 59.40 | C   |
| ATOM                        | 1266 | OH  | TYR | B | 216 | 8.956  | -30.724 | 16.473 | 1.00 50.74 | C   |
| ATOM                        | 1267 | O   | VAL | B | 217 | 10.155 | -35.923 | 16.184 | 1.00 59.75 | C   |
| ATOM                        | 1268 | CB  | VAL | B | 217 | 13.365 | -34.905 | 16.462 | 1.00 68.85 | C   |
| ATOM                        | 1269 | CA  | VAL | B | 217 | 12.471 | -36.071 | 16.765 | 1.00 71.66 | C   |
| ATOM                        | 1270 | C   | VAL | B | 217 | 11.046 | -35.556 | 16.935 | 1.00 70.73 | C   |
| ATOM                        | 1271 | CB  | VAL | B | 217 | 12.909 | -36.816 | 18.063 | 1.00 55.98 | C   |
| ATOM                        | 1272 | CG1 | VAL | B | 217 | 13.430 | -38.195 | 17.713 | 1.00 47.81 | C   |
| ATOM                        | 1273 | CG2 | VAL | B | 217 | 13.961 | -36.018 | 18.815 | 1.00 62.62 | C   |
| ATOM                        | 1274 | N   | GLY | B | 218 | 27.799 | -15.197 | 15.127 | 1.00 46.61 | C   |
| ATOM                        | 1275 | CA  | GLY | B | 218 | 26.376 | -11.268 | 15.490 | 1.00 50.60 | C   |
| ATOM                        | 1276 | C   | GLY | B | 218 | 25.601 | -12.088 | 14.475 | 1.00 61.30 | C   |
| ATOM                        | 1277 | O   | GLY | B | 218 | 24.841 | -12.967 | 14.839 | 1.00 60.37 | C   |
| ATOM                        | 1278 | CB  | ARG | B | 219 | 25.769 | -11.760 | 13.197 | 1.00 48.79 | C   |
| ATOM                        | 1279 | CG  | ARG | B | 219 | 25.065 | -12.471 | 12.138 | 1.00 49.39 | C   |
| ATOM                        | 1280 | C   | ARG | B | 219 | 24.378 | -11.539 | 11.322 | 1.00 48.57 | C   |
| ATOM                        | 1281 | O   | ARG | B | 219 | 23.870 | -11.851 | 10.167 | 1.00 55.37 | C   |
| ATOM                        | 1282 | CB  | ARG | B | 219 | 26.043 | -13.192 | 11.205 | 1.00 54.97 | C   |
| ATOM                        | 1283 | CG  | ARG | B | 219 | 26.923 | -14.236 | 11.874 | 1.00 64.82 | C   |
| ATOM                        | 1284 | CD  | ARG | B | 219 | 37.901 | -14.537 | 10.873 | 1.00 45.23 | C   |
| ATOM                        | 1285 | NE  | ARG | B | 219 | 29.715 | -13.625 | 10.207 | 1.00 64.94 | C   |
| ATOM                        | 1286 | CZ  | ARG | B | 219 | 29.401 | -13.041 | 9.089  | 1.00 68.37 | C   |
| ATOM                        | 1287 | NH2 | ARG | B | 219 | 29.373 | -15.234 | 8.510  | 1.00 75.59 | NH2 |
| ATOM                        | 1288 | NH2 | ARG | B | 219 | 30.114 | -13.063 | 8.546  | 1.00 60.83 | NH2 |
| ATOM                        | 1289 | N   | ARG | B | 219 | 23.821 | -10.398 | 11.901 | 1.00 56.18 | C   |
| ATOM                        | 1290 | CA  | ARG | B | 219 | 22.966 | -9.429  | 11.201 | 1.00 47.93 | C   |
| ATOM                        | 1291 | C   | ARG | B | 219 | 21.704 | -9.192  | 11.982 | 1.00 42.73 | C   |
| ATOM                        | 1292 | O   | ARG | B | 219 | 21.707 | -9.155  | 13.212 | 1.00 42.67 | C   |
| ATOM                        | 1293 | CB  | ARG | B | 219 | 23.718 | -8.103  | 10.982 | 1.00 47.29 | C   |
| ATOM                        | 1294 | CG  | ARG | B | 219 | 24.899 | -8.165  | 10.036 | 1.00 50.24 | C   |
| ATOM                        | 1295 | CD  | ARG | B | 219 | 25.542 | -6.819  | 9.856  | 1.00 43.50 | C   |
| ATOM                        | 1296 | CE  | ARG | B | 219 | 26.555 | -6.828  | 8.805  | 1.00 57.89 | C   |
| ATOM                        | 1297 | CZ  | ARG | B | 219 | 26.963 | -5.738  | 8.180  | 1.00 60.95 | C   |
| ATOM                        | 1298 | NH2 | ARG | B | 219 | 26.498 | -4.548  | 8.500  | 1.00 64.95 | NH2 |
| ATOM                        | 1299 | NH2 | ARG | B | 219 | 27.913 | -5.837  | 7.233  | 1.00 70.25 | NH2 |
| ATOM                        | 1300 | N   | VAL | B | 220 | 20.609 | -9.034  | 11.249 | 1.00 47.62 | C   |
| ATOM                        | 1301 | CA  | VAL | B | 220 | 19.2   |         |        |            |     |

|      |      |     |           | octamer-PDB-coordinates.txt |         |        |            |
|------|------|-----|-----------|-----------------------------|---------|--------|------------|
| ATOM | 1384 | O   | LEU C 148 | 9.256                       | -1.277  | 3.559  | 1.00 55.28 |
| ATOM | 1385 | CB  | LEU C 148 | 8.136                       | -4.092  | 3.537  | 1.00 46.92 |
| ATOM | 1386 | CG  | LEU C 148 | 7.027                       | -5.084  | 3.164  | 1.00 44.79 |
| ATOM | 1387 | CD  | LEU C 148 | 7.198                       | -6.311  | 2.667  | 1.00 39.35 |
| ATOM | 1388 | CD2 | LEU C 148 | 6.580                       | -5.402  | 2.158  | 1.00 34.59 |
| ATOM | 1389 | N   | SER C 149 | 9.953                       | -2.323  | 2.540  | 1.00 37.32 |
| ATOM | 1390 | CA  | SER C 149 | 11.297                      | -1.818  | 5.777  | 1.00 46.41 |
| ATOM | 1391 | C   | SER C 149 | 12.235                      | -2.402  | 4.729  | 1.00 44.24 |
| ATOM | 1392 | O   | SER C 149 | 11.936                      | -3.436  | 4.130  | 1.00 45.26 |
| ATOM | 1393 | CB  | SER C 149 | 11.775                      | -2.173  | 7.186  | 1.00 41.59 |
| ATOM | 1394 | OG  | SER C 149 | 11.667                      | -3.565  | 7.423  | 1.00 43.61 |
| ATOM | 1395 | N   | GLU C 150 | 13.361                      | -1.736  | 4.500  | 1.00 41.74 |
| ATOM | 1396 | CA  | GLU C 150 | 14.337                      | -2.217  | 3.531  | 1.00 43.92 |
| ATOM | 1397 | C   | GLU C 150 | 14.929                      | -3.609  | 9.719  | 1.00 41.92 |
| ATOM | 1398 | O   | GLU C 150 | 14.347                      | -4.192  | 9.761  | 1.00 45.84 |
| ATOM | 1399 | CB  | GLU C 150 | 15.536                      | -1.251  | 3.414  | 1.00 28.37 |
| ATOM | 1400 | CG  | GLU C 150 | 16.575                      | -1.710  | 2.426  | 1.00 44.99 |
| ATOM | 1401 | CD  | GLU C 150 | 17.844                      | -0.886  | 2.500  | 1.00 52.34 |
| ATOM | 1402 | OE1 | GLU C 150 | 18.616                      | -0.899  | 1.531  | 1.00 40.77 |
| ATOM | 1403 | OE2 | GLU C 150 | 18.069                      | -0.234  | 3.139  | 1.00 63.36 |
| ATOM | 1404 | N   | GLU C 151 | 15.099                      | -3.804  | 5.199  | 1.00 49.91 |
| ATOM | 1405 | CA  | GLU C 151 | 15.650                      | -5.066  | 5.677  | 1.00 50.04 |
| ATOM | 1406 | C   | GLU C 151 | 14.651                      | -6.210  | 5.514  | 1.00 37.61 |
| ATOM | 1407 | O   | GLU C 151 | 15.092                      | -7.310  | 5.116  | 1.00 41.92 |
| ATOM | 1408 | CB  | GLU C 151 | 16.077                      | -4.948  | 7.143  | 1.00 39.36 |
| ATOM | 1409 | CG  | GLU C 151 | 16.908                      | -6.122  | 7.636  | 1.00 61.19 |
| ATOM | 1410 | CD  | GLU C 151 | 17.180                      | -6.056  | 9.126  | 1.00 71.90 |
| ATOM | 1411 | OE1 | GLU C 151 | 17.065                      | -4.954  | 9.703  | 1.00 77.87 |
| ATOM | 1412 | OE2 | GLU C 151 | 17.513                      | -7.119  | 9.719  | 1.00 64.37 |
| ATOM | 1413 | N   | GLU C 152 | 13.384                      | -5.947  | 9.806  | 1.00 42.32 |
| ATOM | 1414 | CA  | GLU C 152 | 12.359                      | -6.980  | 5.694  | 1.00 35.13 |
| ATOM | 1415 | C   | GLU C 152 | 12.047                      | -7.293  | 4.237  | 1.00 36.16 |
| ATOM | 1416 | CB  | GLU C 152 | 11.859                      | -8.452  | 3.573  | 1.00 31.30 |
| ATOM | 1417 | CG  | GLU C 152 | 11.077                      | -6.412  | 5.566  | 1.00 40.33 |
| ATOM | 1418 | CD  | GLU C 152 | 10.021                      | -7.653  | 6.464  | 1.00 44.18 |
| ATOM | 1419 | CD  | GLU C 152 | 8.804                       | -7.263  | 7.279  | 1.00 65.03 |
| ATOM | 1420 | OE1 | GLU C 152 | 8.763                       | -6.122  | 7.784  | 1.00 66.71 |
| ATOM | 1421 | OE2 | GLU C 152 | 7.858                       | -8.099  | 7.403  | 1.00 65.52 |
| ATOM | 1422 | N   | LEU C 153 | 12.003                      | -6.251  | 3.406  | 1.00 41.51 |
| ATOM | 1423 | CA  | LEU C 153 | 11.775                      | -6.424  | 1.978  | 1.00 39.30 |
| ATOM | 1424 | C   | LEU C 153 | 12.879                      | -7.274  | 1.362  | 1.00 38.00 |
| ATOM | 1425 | O   | LEU C 153 | 12.613                      | -8.275  | 0.690  | 1.00 29.92 |
| ATOM | 1426 | CB  | LEU C 153 | 11.644                      | -9.060  | 1.282  | 1.00 42.37 |
| ATOM | 1427 | CG  | LEU C 153 | 11.644                      | -9.060  | 1.282  | 1.00 40.64 |
| ATOM | 1428 | CD  | LEU C 153 | 10.310                      | -5.627  | -0.729 | 1.00 28.44 |
| ATOM | 1429 | CD2 | LEU C 153 | 11.900                      | -3.691  | -0.812 | 1.00 46.29 |
| ATOM | 1430 | N   | LEU C 154 | 14.121                      | -6.873  | 1.615  | 1.00 32.60 |
| ATOM | 1431 | CA  | LEU C 154 | 15.281                      | -7.587  | 1.404  | 1.00 27.88 |
| ATOM | 1432 | C   | LEU C 154 | 15.343                      | -9.014  | 1.682  | 1.00 41.28 |
| ATOM | 1433 | O   | LEU C 154 | 15.725                      | -9.944  | 0.924  | 1.00 31.37 |
| ATOM | 1434 | CB  | LEU C 154 | 16.565                      | -6.832  | 1.444  | 1.00 35.95 |
| ATOM | 1435 | CG  | LEU C 154 | 16.812                      | -5.509  | 0.721  | 1.00 40.02 |
| ATOM | 1436 | CD  | LEU C 154 | 18.093                      | -4.854  | 1.205  | 1.00 37.30 |
| ATOM | 1437 | CD2 | LEU C 154 | 16.051                      | -10.457 | -0.795 | 1.00 42.77 |
| ATOM | 1438 | N   | ASP C 155 | 14.961                      | -9.192  | 2.805  | 1.00 25.81 |
| ATOM | 1439 | CA  | ASP C 155 | 14.945                      | -10.524 | 3.502  | 1.00 32.84 |
| ATOM | 1440 | C   | ASP C 155 | 13.933                      | -11.424 | 2.805  | 1.00 29.70 |
| ATOM | 1441 | O   | ASP C 155 | 14.268                      | -12.539 | 2.421  | 1.00 23.67 |
| ATOM | 1442 | CB  | ASP C 155 | 14.644                      | -10.457 | 5.002  | 1.00 37.50 |
| ATOM | 1443 | CG  | ASP C 155 | 15.887                      | -10.175 | 5.830  | 1.00 49.36 |
| ATOM | 1444 | CD  | ASP C 155 | 17.004                      | -10.248 | 5.275  | 1.00 29.74 |
| ATOM | 1445 | OE1 | ASP C 155 | 15.745                      | -9.886  | 7.038  | 1.00 44.78 |
| ATOM | 1446 | N   | LYS C 156 | 12.703                      | -10.943 | 2.644  | 1.00 32.84 |

|      |      |     |           | octamer-PDB-coordinates.txt |         |         |            |
|------|------|-----|-----------|-----------------------------|---------|---------|------------|
| ATOM | 1510 | CB  | LYS C 163 | 13.961                      | -21.242 | -2.870  | 1.00 25.25 |
| ATOM | 1511 | CG  | LYS C 163 | 13.737                      | -20.991 | -1.391  | 1.00 28.96 |
| ATOM | 1512 | CD  | LYS C 163 | 12.287                      | -21.013 | -1.011  | 1.00 47.45 |
| ATOM | 1513 | CD  | LYS C 163 | 12.087                      | -20.589 | 0.436   | 1.00 51.38 |
| ATOM | 1514 | N2  | LYS C 163 | 12.950                      | -21.156 | 1.275   | 1.00 35.86 |
| ATOM | 1515 | N   | THR C 164 | 16.193                      | -22.773 | -4.911  | 1.00 33.64 |
| ATOM | 1516 | CA  | THR C 164 | 16.415                      | -23.321 | -6.227  | 1.00 30.97 |
| ATOM | 1517 | C   | THR C 164 | 15.108                      | -21.741 | -6.693  | 1.00 31.81 |
| ATOM | 1518 | CB  | THR C 164 | 15.010                      | -23.768 | -8.120  | 1.00 34.20 |
| ATOM | 1519 | CG  | THR C 164 | 17.353                      | -24.514 | -6.147  | 1.00 46.93 |
| ATOM | 1520 | CD  | THR C 164 | 18.650                      | -24.168 | -5.449  | 1.00 33.12 |
| ATOM | 1521 | OE1 | THR C 164 | 16.709                      | -25.592 | -5.417  | 1.00 52.03 |
| ATOM | 1522 | N   | ARG C 165 | 14.104                      | -24.064 | -6.083  | 1.00 30.41 |
| ATOM | 1523 | CA  | ARG C 165 | 13.805                      | -24.014 | -6.614  | 1.00 31.12 |
| ATOM | 1524 | C   | ARG C 165 | 13.100                      | -23.304 | -7.315  | 1.00 31.22 |
| ATOM | 1525 | O   | ARG C 165 | 11.184                      | -23.517 | -8.107  | 1.00 33.04 |
| ATOM | 1526 | CB  | ARG C 165 | 11.920                      | -25.045 | -5.507  | 1.00 31.57 |
| ATOM | 1527 | CG  | ARG C 165 | 11.445                      | -24.060 | -4.451  | 1.00 39.95 |
| ATOM | 1528 | CD  | ARG C 165 | 10.319                      | -24.680 | -3.632  | 1.00 41.64 |
| ATOM | 1529 | OE  | ARG C 165 | 9.835                       | -24.060 | -2.565  | 1.00 40.06 |
| ATOM | 1530 | CZ  | ARG C 165 | 10.212                      | -23.912 | -1.293  | 1.00 51.76 |
| ATOM | 1531 | NH1 | ARG C 165 | 11.061                      | -24.863 | -0.929  | 1.00 40.38 |
| ATOM | 1532 | NH2 | ARG C 165 | 9.727                       | -23.078 | -0.382  | 1.00 45.21 |
| ATOM | 1533 | N   | ASN C 166 | 12.530                      | -22.080 | -7.024  | 1.00 24.74 |
| ATOM | 1534 | CA  | ASN C 166 | 11.004                      | -20.907 | -7.713  | 1.00 30.70 |
| ATOM | 1535 | C   | ASN C 166 | 12.895                      | -20.512 | -6.656  | 1.00 29.27 |
| ATOM | 1536 | O   | ASN C 166 | 12.633                      | -19.526 | -9.575  | 1.00 26.85 |
| ATOM | 1537 | CB  | ASN C 166 | 11.861                      | -19.731 | -6.748  | 1.00 26.50 |
| ATOM | 1538 | CG  | ASN C 166 | 10.731                      | -19.922 | -5.762  | 1.00 32.43 |
| ATOM | 1539 | CD  | ASN C 166 | 10.901                      | -19.189 | -4.559  | 1.00 34.59 |
| ATOM | 1540 | OE1 | ASN C 166 | 9.716                       | -20.544 | -6.076  | 1.00 30.49 |
| ATOM | 1541 | N   | GLY C 167 | 13.954                      | -21.287 | -9.100  | 1.00 40.06 |
| ATOM | 1542 | CA  | GLY C 167 | 14.875                      | -21.046 | -10.193 | 1.00 31.96 |
| ATOM | 1543 | C   | GLY C 167 | 16.060                      | -20.199 | -9.778  | 1.00 32.77 |
| ATOM | 1544 | O   | GLY C 167 | 16.871                      | -19.794 | -10.612 | 1.00 35.56 |
| ATOM | 1545 | N   | GLY C 168 | 16.159                      | -19.926 | -8.482  | 1.00 25.32 |
| ATOM | 1546 | CA  | GLY C 168 | 17.197                      | -19.054 | -7.866  | 1.00 32.22 |
| ATOM | 1547 | C   | GLY C 168 | 18.388                      | -19.791 | -7.386  | 1.00 26.68 |
| ATOM | 1548 | O   | GLY C 168 | 18.715                      | -20.900 | -7.409  | 1.00 42.20 |
| ATOM | 1549 | N   | GLY C 169 | 19.034                      | -19.165 | -6.407  | 1.00 33.61 |
| ATOM | 1550 | CA  | GLY C 169 | 20.227                      | -19.713 | -5.786  | 1.00 37.04 |
| ATOM | 1551 | C   | GLY C 169 | 20.803                      | -18.755 | -4.759  | 1.00 31.22 |
| ATOM | 1552 | O   | GLY C 169 | 20.215                      | -17.707 | -4.490  | 1.00 32.91 |
| ATOM | 1553 | N   | ASP C 170 | 21.946                      | -19.120 | -4.181  | 1.00 28.97 |
| ATOM | 1554 | CA  | ASP C 170 | 22.490                      | -18.318 | -3.141  | 1.00 31.84 |
| ATOM | 1555 | C   | ASP C 170 | 22.607                      | -16.874 | -3.583  | 1.00 37.80 |
| ATOM | 1556 | O   | ASP C 170 | 23.290                      | -16.617 | -4.685  | 1.00 41.57 |
| ATOM | 1557 | CB  | ASP C 170 | 23.925                      | -18.940 | -2.731  | 1.00 40.32 |
| ATOM | 1558 | CG  | ASP C 170 | 23.753                      | -19.206 | -1.915  | 1.00 44.01 |
| ATOM | 1559 | CD  | ASP C 170 | 22.635                      | -20.783 | -1.907  | 1.00 42.47 |
| ATOM | 1560 | OE1 | ASP C 170 | 24.747                      | -20.457 | -1.299  | 1.00 41.15 |
| ATOM | 1561 | N   | VAL C 171 | 22.446                      | -15.941 | -2.708  | 1.00 40.04 |
| ATOM | 1562 | CA  | VAL C 171 | 22.551                      | -14.513 | -2.988  | 1.00 34.35 |
| ATOM | 1563 | C   | VAL C 171 | 21.793                      | -13.814 | -2.152  | 1.00 36.56 |
| ATOM | 1564 | O   | VAL C 171 | 24.026                      | -14.039 | -1.153  | 1.00 44.23 |
| ATOM | 1565 | CB  | VAL C 171 | 21.299                      | -13.762 | -2.490  | 1.00 37.23 |
| ATOM | 1566 | CG  | VAL C 171 | 21.465                      | -12.263 | -2.671  | 1.00 40.55 |
| ATOM | 1567 | CD  | VAL C 171 | 20.058                      | -14.261 | -3.225  | 1.00 27.19 |
| ATOM | 1568 | N   | ASP C 172 | 24.589                      | -13.194 | -3.162  | 1.00 48.82 |
| ATOM | 1569 | CA  | ASP C 172 | 25.813                      | -12.560 | -2.678  | 1.00 50.06 |
| ATOM | 1570 | C   | ASP C 172 | 25.592                      | -11.115 | -2.236  | 1.00 49.03 |
| ATOM | 1571 | O   | ASP C 172 | 26.030                      | -10.715 | -1.157  | 1.00 45.41 |
| ATOM | 1572 | CB  | ASP C 172 | 26.893                      | -12.584 | -3.765  | 1.00 46.15 |

|   |      |      |     |                             |        |         |        |      |       |   |  |
|---|------|------|-----|-----------------------------|--------|---------|--------|------|-------|---|--|
|   |      |      |     | octamer-PDB-coordinates.txt |        |         |        |      |       |   |  |
| O | ATOM | 1447 | CA  | LYS C 156                   | 11.667 | -11.709 | 4.951  | 1.00 | 30.61 | C |  |
| C | ATOM | 1448 | C   | LYS C 156                   | 12.090 | -12.054 | 0.525  | 1.00 | 37.13 | C |  |
| C | ATOM | 1449 | O   | LYS C 156                   | 11.913 | -13.191 | 0.072  | 1.00 | 41.13 | C |  |
| C | ATOM | 1450 | CB  | LYS C 156                   | 10.346 | -10.937 | 1.927  | 1.00 | 29.39 | C |  |
| C | ATOM | 1451 | CG  | LYS C 156                   | 9.722  | -10.695 | 3.293  | 1.00 | 49.03 | C |  |
| C | ATOM | 1452 | CD  | LYS C 156                   | 9.384  | -12.003 | 3.991  | 1.00 | 33.12 | C |  |
| C | ATOM | 1453 | CD2 | LYS C 156                   | 8.727  | -11.759 | 5.392  | 1.00 | 14.25 | C |  |
| C | ATOM | 1454 | NZ  | LYS C 156                   | 8.648  | -12.009 | 6.136  | 1.00 | 59.07 | C |  |
| C | ATOM | 1455 | N   | LEU C 157                   | 12.661 | -11.076 | -0.173 | 1.00 | 33.27 | N |  |
| C | ATOM | 1456 | CA  | LEU C 157                   | 13.112 | -11.290 | -1.545 | 1.00 | 31.68 | C |  |
| C | ATOM | 1457 | C   | LEU C 157                   | 14.209 | -12.346 | -1.616 | 1.00 | 23.46 | C |  |
| C | ATOM | 1458 | O   | LEU C 157                   | 14.212 | -13.180 | -0.892 | 1.00 | 27.12 | C |  |
| C | ATOM | 1459 | CB  | LEU C 157                   | 13.608 | -9.982  | -2.164 | 1.00 | 20.68 | C |  |
| C | ATOM | 1460 | CG  | LEU C 157                   | 12.533 | -8.937  | -2.466 | 1.00 | 22.11 | C |  |
| C | ATOM | 1461 | CD  | LEU C 157                   | 13.166 | -7.648  | -2.952 | 1.00 | 25.44 | C |  |
| C | ATOM | 1462 | CD2 | LEU C 157                   | 11.543 | -9.463  | -3.488 | 1.00 | 21.37 | C |  |
| C | ATOM | 1463 | N   | GLU C 158                   | 15.143 | -12.309 | 0.670  | 1.00 | 36.60 | C |  |
| C | ATOM | 1464 | CA  | GLU C 158                   | 16.218 | -13.292 | -0.680 | 1.00 | 32.50 | C |  |
| C | ATOM | 1465 | C   | GLU C 158                   | 15.672 | -14.674 | -0.267 | 1.00 | 34.63 | C |  |
| C | ATOM | 1466 | O   | GLU C 158                   | 16.184 | -15.890 | -0.735 | 1.00 | 33.69 | C |  |
| C | ATOM | 1467 | CB  | GLU C 158                   | 17.316 | -12.869 | 0.347  | 1.00 | 37.71 | C |  |
| C | ATOM | 1468 | CG  | GLU C 158                   | 18.525 | -13.799 | 0.836  | 1.00 | 40.75 | C |  |
| C | ATOM | 1469 | CD  | GLU C 158                   | 19.697 | -13.249 | 1.125  | 1.00 | 40.95 | C |  |
| C | ATOM | 1470 | OE1 | GLU C 158                   | 20.763 | -13.864 | 1.050  | 1.00 | 53.32 | C |  |
| C | ATOM | 1471 | OE2 | GLU C 158                   | 19.536 | -12.200 | 1.782  | 1.00 | 48.94 | C |  |
| C | ATOM | 1472 | C   | GLU C 158                   | 18.641 | -11.706 | 0.573  | 1.00 | 40.34 | C |  |
| C | ATOM | 1473 | CA  | ILE C 159                   | 13.954 | -13.950 | 0.195  | 1.00 | 34.77 | C |  |
| C | ATOM | 1474 | C   | ILE C 159                   | 13.392 | -16.559 | -0.377 | 1.00 | 44.25 | C |  |
| C | ATOM | 1475 | O   | ILE C 159                   | 13.566 | -17.741 | -0.653 | 1.00 | 44.77 | C |  |
| C | ATOM | 1476 | CB  | ILE C 159                   | 12.800 | -16.754 | 1.907  | 1.00 | 36.10 | C |  |
| C | ATOM | 1477 | CG  | ILE C 159                   | 12.328 | -15.723 | 3.173  | 1.00 | 38.21 | C |  |
| C | ATOM | 1478 | CG2 | ILE C 159                   | 12.025 | -17.049 | 3.007  | 1.00 | 30.88 | C |  |
| C | ATOM | 1479 | CD1 | ILE C 159                   | 13.969 | -16.406 | 4.060  | 1.00 | 43.61 | C |  |
| C | ATOM | 1480 | N   | PHE C 160                   | 12.675 | -15.751 | -1.152 | 1.00 | 36.96 | C |  |
| C | ATOM | 1481 | CA  | PHE C 160                   | 12.024 | -16.264 | -2.367 | 1.00 | 38.35 | C |  |
| C | ATOM | 1482 | C   | PHE C 160                   | 13.057 | -16.695 | -3.418 | 1.00 | 31.67 | C |  |
| C | ATOM | 1483 | O   | PHE C 160                   | 13.066 | -17.041 | -3.870 | 1.00 | 27.65 | C |  |
| C | ATOM | 1484 | CB  | PHE C 160                   | 11.143 | -15.221 | -3.907 | 1.00 | 38.67 | C |  |
| C | ATOM | 1485 | CG  | PHE C 160                   | 10.295 | -15.775 | -4.106 | 1.00 | 31.94 | C |  |
| C | ATOM | 1486 | CD2 | PHE C 160                   | 10.511 | -15.405 | -5.425 | 1.00 | 26.32 | C |  |
| C | ATOM | 1487 | CD1 | PHE C 160                   | 9.339  | -16.733 | -5.173 | 1.00 | 33.47 | C |  |
| C | ATOM | 1488 | CE2 | PHE C 160                   | 9.743  | -15.935 | -6.142 | 1.00 | 25.52 | C |  |
| C | ATOM | 1489 | CE1 | PHE C 160                   | 8.562  | -17.266 | -6.342 | 1.00 | 35.46 | C |  |
| C | ATOM | 1490 | CZ  | PHE C 160                   | 8.768  | -16.872 | -6.145 | 1.00 | 29.44 | C |  |
| C | ATOM | 1491 | N   | PHE C 162                   | 13.935 | -15.761 | -3.792 | 1.00 | 21.57 | C |  |
| C | ATOM | 1492 | CA  | PHE C 162                   | 14.863 | -15.998 | -4.000 | 1.00 | 20.74 | C |  |
| C | ATOM | 1493 | C   | PHE C 161                   | 16.135 | -16.697 | -4.490 | 1.00 | 34.08 | C |  |
| C | ATOM | 1494 | O   | PHE C 161                   | 17.015 | -16.925 | -5.318 | 1.00 | 28.59 | C |  |
| C | ATOM | 1495 | CB  | PHE C 161                   | 15.228 | -14.607 | -5.321 | 1.00 | 24.59 | C |  |
| C | ATOM | 1496 | CG  | PHE C 161                   | 14.083 | -13.934 | -6.280 | 1.00 | 28.09 | C |  |
| C | ATOM | 1497 | CG2 | PHE C 161                   | 13.646 | -14.395 | -6.61  | 1.00 | 30.31 | C |  |
| C | ATOM | 1498 | CD2 | PHE C 161                   | 13.433 | -17.834 | -5.671 | 1.00 | 25.78 | C |  |
| C | ATOM | 1499 | CE1 | PHE C 161                   | 12.595 | -13.778 | -8.117 | 1.00 | 27.29 | C |  |
| C | ATOM | 1500 | CE2 | PHE C 161                   | 12.402 | -12.721 | -6.323 | 1.00 | 26.65 | C |  |
| C | ATOM | 1501 | CZ  | PHE C 161                   | 11.973 | -12.684 | -7.547 | 1.00 | 25.36 | C |  |
| C | ATOM | 1502 | N   | PHE C 162                   | 16.230 | -17.068 | -3.218 | 1.00 | 24.62 | C |  |
| C | ATOM | 1503 | CA  | GLY C 152                   | 17.348 | -17.869 | -2.748 | 1.00 | 25.15 | C |  |
| C | ATOM | 1504 | C   | GLY C 152                   | 17.090 | -19.348 | -2.939 | 1.00 | 29.49 | C |  |
| C | ATOM | 1505 | O   | GLY C 152                   | 18.006 | -20.167 | -2.872 | 1.00 | 31.54 | C |  |
| C | ATOM | 1506 | N   | LYS C 163                   | 15.827 | -19.687 | -3.177 | 1.00 | 26.88 | C |  |
| C | ATOM | 1507 | CA  | LYS C 163                   | 15.413 | -21.075 | -3.233 | 1.00 | 26.87 | C |  |
| C | ATOM | 1508 | C   | LYS C 163                   | 15.596 | -21.557 | -4.780 | 1.00 | 31.19 | C |  |
| C | ATOM | 1509 | O   | LYS C 163                   | 15.203 | -20.871 | -5.703 | 1.00 | 32.14 | C |  |

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|-----------------------------|------|-----|-----------|----------------------------------|
| ATOM                        | 1636 | N   | VAL C 181 | 9.623 9.240 -7.866 1.00 41.70    |
| ATOM                        | 1637 | CA  | VAL C 181 | 8.587 10.151 -7.366 1.00 36.76   |
| ATOM                        | 1638 | N   | VAL C 181 | 7.498 10.468 -8.408 1.00 29.15   |
| ATOM                        | 1639 | O   | VAL C 181 | 7.786 10.769 -9.556 1.00 38.66   |
| ATOM                        | 1640 | CB  | VAL C 181 | 9.220 11.477 -6.910 1.00 31.64   |
| ATOM                        | 1641 | CE1 | VAL C 181 | 8.159 12.546 -6.686 1.00 33.20   |
| ATOM                        | 1642 | CG2 | VAL C 181 | 10.019 11.245 -5.642 1.00 34.07  |
| ATOM                        | 1643 | N   | MET C 182 | 6.243 10.394 -7.971 1.00 30.25   |
| ATOM                        | 1644 | CA  | MET C 182 | 5.117 10.774 -8.813 1.00 28.52   |
| ATOM                        | 1645 | C   | MET C 182 | 4.552 12.123 -6.357 1.00 31.91   |
| ATOM                        | 1646 | O   | MET C 182 | 4.414 12.382 -7.160 1.00 33.32   |
| ATOM                        | 1647 | CB  | MET C 182 | 4.042 9.677 -8.810 1.00 36.56    |
| ATOM                        | 1648 | CG  | MET C 182 | 2.846 9.902 -7.897 1.00 42.72    |
| ATOM                        | 1649 | SD  | MET C 182 | 1.512 10.829 -6.684 1.00 38.74   |
| ATOM                        | 1650 | CE  | MET C 182 | 0.190 10.537 -7.515 1.00 37.00   |
| ATOM                        | 1651 | N   | LEU C 183 | 4.272 12.994 -9.323 1.00 40.76   |
| ATOM                        | 1652 | CA  | LEU C 183 | 3.680 14.300 -9.050 1.00 33.03   |
| ATOM                        | 1653 | C   | LEU C 183 | 2.384 14.495 -9.849 1.00 40.35   |
| ATOM                        | 1654 | O   | LEU C 183 | 2.333 14.150 -11.028 1.00 37.08  |
| ATOM                        | 1655 | CB  | LEU C 183 | 4.666 15.423 -9.379 1.00 37.46   |
| ATOM                        | 1656 | CG  | LEU C 183 | 5.976 15.509 -8.569 1.00 32.12   |
| ATOM                        | 1657 | CD2 | LEU C 183 | 6.804 16.686 -9.079 1.00 25.11   |
| ATOM                        | 1658 | CD2 | LEU C 183 | 5.704 15.629 -7.098 1.00 31.20   |
| ATOM                        | 1659 | N   | GLY C 184 | 1.365 15.044 -9.104 1.00 42.07   |
| ATOM                        | 1660 | CA  | GLY C 184 | 0.116 15.338 -9.879 1.00 29.42   |
| ATOM                        | 1661 | C   | GLY C 184 | -0.193 16.823 -9.888 1.00 37.22  |
| ATOM                        | 1662 | O   | GLY C 184 | -0.094 17.493 -8.859 1.00 35.53  |
| ATOM                        | 1663 | N   | PHE C 185 | -0.574 17.339 -11.053 1.00 30.55 |
| ATOM                        | 1664 | CA  | PHE C 185 | -0.769 18.009 -10.588 1.00 47.79 |
| ATOM                        | 1665 | C   | PHE C 185 | -2.268 19.127 -11.372 1.00 47.35 |
| ATOM                        | 1666 | O   | PHE C 185 | -3.071 18.100 -11.823 1.00 44.69 |
| ATOM                        | 1667 | CB  | PHE C 185 | 0.011 19.274 -12.423 1.00 34.51  |
| ATOM                        | 1668 | CG  | PHE C 185 | 1.490 19.047 -12.292 1.00 33.40  |
| ATOM                        | 1669 | CD2 | PHE C 185 | 2.289 19.969 -11.627 1.00 36.51  |
| ATOM                        | 1670 | CD2 | PHE C 185 | 2.077 17.907 -12.614 1.00 37.39  |
| ATOM                        | 1671 | CE1 | PHE C 185 | 3.648 19.747 -11.495 1.00 39.04  |
| ATOM                        | 1672 | CE2 | PHE C 185 | 3.433 17.686 -12.695 1.00 36.24  |
| ATOM                        | 1673 | C   | PHE C 185 | 4.213 18.605 -12.021 1.00 32.54  |
| ATOM                        | 1674 | N   | ALA C 186 | -2.617 20.352 -10.988 1.00 47.79 |
| ATOM                        | 1675 | CA  | ALA C 186 | -4.007 20.801 -10.992 1.00 45.21 |
| ATOM                        | 1676 | C   | ALA C 186 | -4.534 21.175 -12.367 1.00 50.12 |
| ATOM                        | 1677 | O   | ALA C 186 | -5.616 20.828 -12.723 1.00 60.27 |
| ATOM                        | 1678 | CB  | ALA C 186 | -4.164 21.977 -10.727 1.00 43.56 |
| ATOM                        | 1679 | N   | ARG C 187 | -3.719 21.898 -13.143 1.00 59.85 |
| ATOM                        | 1680 | CA  | ARG C 187 | -4.179 22.434 -14.433 1.00 59.12 |
| ATOM                        | 1681 | C   | ARG C 187 | -3.808 21.457 -15.561 1.00 60.14 |
| ATOM                        | 1682 | O   | ARG C 187 | -2.740 20.844 -15.548 1.00 48.53 |
| ATOM                        | 1683 | N   | ARG C 187 | -1.596 21.809 -14.695 1.00 58.54 |
| ATOM                        | 1684 | CG  | ARG C 187 | -1.076 24.441 -15.987 1.00 63.91 |
| ATOM                        | 1685 | CD  | ARG C 187 | -3.500 25.354 -16.208 1.00 72.07 |
| ATOM                        | 1686 | CE  | ARG C 187 | -2.062 25.611 -16.459 1.00 77.79 |
| ATOM                        | 1687 | CZ  | ARG C 187 | -1.278 26.883 -16.406 1.00 83.36 |
| ATOM                        | 1688 | NH1 | ARG C 187 | -1.793 28.069 -16.112 1.00 85.42 |
| ATOM                        | 1689 | NH2 | ARG C 187 | 0.010 26.717 -16.650 1.00 77.00  |
| ATOM                        | 1690 | N   | ASP C 188 | -4.703 21.323 -16.539 1.00 59.96 |
| ATOM                        | 1691 | CA  | ASP C 188 | -4.466 20.470 -17.699 1.00 51.80 |
| ATOM                        | 1692 | C   | ASP C 188 | -3.313 20.959 -18.554 1.00 43.50 |
| ATOM                        | 1693 | O   | ASP C 188 | -3.196 22.191 -18.791 1.00 46.47 |
| ATOM                        | 1694 | N   | ASP C 188 | -5.731 20.369 -18.154 1.00 54.10 |
| ATOM                        | 1695 | CG  | ASP C 188 | -6.622 19.546 -17.894 1.00 80.40 |
| ATOM                        | 1696 | CD1 | ASP C 188 | -6.497 18.527 -17.254 1.00 86.10 |
| ATOM                        | 1697 | DD2 | ASP C 188 | -8.006 19.925 -18.013 1.00 91.01 |
| ATOM                        | 1698 | N   | GLY C 189 | -2.466 20.076 -19.019 1.00 40.43 |

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|-----------------------------|------|-----|-----------|----------------------------------|
| ATOM                        | 1762 | CG1 | ILE C 197 | 9.931 21.127 -21.027 1.00 36.53  |
| ATOM                        | 1763 | CG2 | ILE C 197 | 12.183 20.227 -20.337 1.00 37.03 |
| ATOM                        | 1764 | CD1 | ILE C 197 | 9.808 22.118 -19.811 1.00 30.87  |
| ATOM                        | 1765 | N   | GLY C 198 | 10.964 16.736 -20.704 1.00 45.75 |
| ATOM                        | 1766 | CA  | GLY C 198 | 11.569 15.444 -20.436 1.00 34.55 |
| ATOM                        | 1767 | C   | GLY C 198 | 12.689 15.415 -19.413 1.00 43.30 |
| ATOM                        | 1768 | O   | GLY C 198 | 12.983 14.801 -18.370 1.00 39.67 |
| ATOM                        | 1769 | N   | GLN C 199 | 12.758 16.477 -19.707 1.00 46.83 |
| ATOM                        | 1770 | CA  | GLN C 199 | 12.593 16.471 -18.688 1.00 38.68 |
| ATOM                        | 1771 | C   | GLN C 199 | 15.103 17.481 -18.105 1.00 44.12 |
| ATOM                        | 1772 | O   | GLN C 199 | 14.925 16.561 -18.666 1.00 45.39 |
| ATOM                        | 1773 | CB  | GLN C 199 | 16.152 15.914 -19.730 1.00 44.97 |
| ATOM                        | 1774 | CG  | GLN C 199 | 17.525 15.877 -19.986 1.00 55.96 |
| ATOM                        | 1775 | CD  | GLN C 199 | 17.635 14.710 -16.002 1.00 41.12 |
| ATOM                        | 1776 | NE2 | GLN C 199 | 17.639 13.505 -18.518 1.00 74.22 |
| ATOM                        | 1777 | OE1 | GLN C 199 | 17.716 14.941 -16.793 1.00 50.62 |
| ATOM                        | 1778 | N   | PHE C 200 | 15.430 17.381 -16.820 1.00 41.73 |
| ATOM                        | 1779 | CA  | PHE C 200 | 15.607 18.566 -15.997 1.00 44.03 |
| ATOM                        | 1780 | C   | PHE C 200 | 16.847 18.437 -15.114 1.00 43.28 |
| ATOM                        | 1781 | O   | PHE C 200 | 17.280 17.332 -14.803 1.00 32.54 |
| ATOM                        | 1782 | CB  | PHE C 200 | 14.361 18.801 -15.097 1.00 43.27 |
| ATOM                        | 1783 | CG  | PHE C 200 | 13.097 18.979 -15.855 1.00 34.40 |
| ATOM                        | 1784 | CD1 | PHE C 200 | 12.357 17.990 -16.260 1.00 36.77 |
| ATOM                        | 1785 | CD2 | PHE C 200 | 12.618 20.241 -16.144 1.00 29.46 |
| ATOM                        | 1786 | CE1 | PHE C 200 | 11.179 18.040 -16.951 1.00 43.32 |
| ATOM                        | 1787 | CE2 | PHE C 200 | 11.432 20.413 -16.834 1.00 29.67 |
| ATOM                        | 1788 | CZ  | PHE C 200 | 10.709 19.306 -17.236 1.00 41.34 |
| ATOM                        | 1789 | N   | THR C 201 | 17.418 19.568 -14.720 1.00 37.66 |
| ATOM                        | 1790 | CA  | THR C 201 | 18.497 19.554 -13.742 1.00 29.71 |
| ATOM                        | 1791 | C   | THR C 201 | 18.026 20.326 -12.462 1.00 35.64 |
| ATOM                        | 1792 | O   | THR C 201 | 17.850 21.446 -17.420 1.00 43.46 |
| ATOM                        | 1793 | CB  | THR C 201 | 19.761 20.258 -14.265 1.00 47.00 |
| ATOM                        | 1794 | CG2 | THR C 201 | 20.834 20.258 -13.205 1.00 36.79 |
| ATOM                        | 1795 | OG1 | THR C 201 | 20.252 19.585 -15.442 1.00 45.14 |
| ATOM                        | 1796 | N   | VAL C 202 | 17.826 19.429 -11.619 1.00 34.40 |
| ATOM                        | 1797 | CA  | VAL C 202 | 17.783 19.928 -10.264 1.00 33.69 |
| ATOM                        | 1798 | C   | VAL C 202 | 18.333 19.894 -9.059 1.00 40.12  |
| ATOM                        | 1799 | O   | VAL C 202 | 18.941 18.852 -8.808 1.00 35.95  |
| ATOM                        | 1800 | CB  | VAL C 202 | 16.056 19.588 -9.718 1.00 33.72  |
| ATOM                        | 1801 | CG1 | VAL C 202 | 15.434 19.755 -9.487 1.00 27.23  |
| ATOM                        | 1802 | CG2 | VAL C 202 | 15.050 19.003 -10.850 1.00 32.49 |
| ATOM                        | 1803 | N   | PRO C 203 | 18.596 21.038 -8.393 1.00 38.35  |
| ATOM                        | 1804 | CA  | PRO C 203 | 19.446 21.111 -7.238 1.00 35.53  |
| ATOM                        | 1805 | C   | PRO C 203 | 18.903 20.520 -6.053 1.00 46.30  |
| ATOM                        | 1806 | O   | PRO C 203 | 17.940 20.743 -5.413 1.00 38.34  |
| ATOM                        | 1807 | CB  | PRO C 203 | 19.497 22.611 -6.921 1.00 40.88  |
| ATOM                        | 1808 | CG  | PRO C 203 | 19.043 23.290 -8.174 1.00 45.05  |
| ATOM                        | 1809 | CD  | PRO C 203 | 18.038 22.365 -8.780 1.00 47.76  |
| ATOM                        | 1810 | N   | LEU C 204 | 19.525 19.179 -5.772 1.00 46.02  |
| ATOM                        | 1811 | CA  | LEU C 204 | 19.129 18.375 -4.661 1.00 46.89  |
| ATOM                        | 1812 | C   | LEU C 204 | 20.331 17.699 -3.643 1.00 43.93  |
| ATOM                        | 1813 | O   | LEU C 204 | 21.278 17.322 -4.383 1.00 39.53  |
| ATOM                        | 1814 | CB  | LEU C 204 | 18.360 17.100 -5.169 1.00 37.18  |
| ATOM                        | 1815 | CG  | LEU C 204 | 17.059 17.141 -5.938 1.00 33.61  |
| ATOM                        | 1816 | CD  | LEU C 204 | 16.491 16.031 -6.464 1.00 34.76  |
| ATOM                        | 1817 | CD2 | LEU C 204 | 16.043 18.051 -5.063 1.00 31.39  |
| ATOM                        | 1818 | N   | GLY C 205 | 20.294 18.179 -2.544 1.00 44.49  |
| ATOM                        | 1819 | CA  | GLY C 205 | 21.349 17.761 -1.627 1.00 47.36  |
| ATOM                        | 1820 | C   | GLY C 205 | 22.745 18.229 -2.017 1.00 50.11  |
| ATOM                        | 1821 | O   | GLY C 205 | 23.711 17.481 -1.864 1.00 52.84  |
| ATOM                        | 1822 | N   | GLY C 206 | 22.852 19.451 -2.528 1.00 45.12  |
| ATOM                        | 1823 | CA  | GLY C 206 | 24.133 20.004 -2.918 1.00 36.90  |
| ATOM                        | 1824 | C   | GLY C 206 | 24.607 19.512 -4.273 1.00 55.19  |

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|-----------------------------|------|------|-----|--------------------------------------------|
| N                           | ATOM | 1699 | CA  | GLY C 189 1.368 19.435 -19.923 1.00 37.56  |
| C                           | ATOM | 1700 | C   | GLY C 189 -0.027 20.576 -19.265 1.00 39.31 |
| C                           | ATOM | 1701 | O   | GLY C 189 0.939 20.534 -19.944 1.00 48.57  |
| C                           | ATOM | 1702 | N   | VAL C 190 -0.013 20.738 -17.945 1.00 46.13 |
| C                           | ATOM | 1703 | CA  | VAL C 190 1.234 20.913 -17.206 1.00 51.08  |
| C                           | ATOM | 1704 | C   | VAL C 190 2.099 19.680 -17.275 1.00 32.42  |
| C                           | ATOM | 1705 | O   | VAL C 190 3.279 19.723 -17.635 1.00 41.40  |
| C                           | ATOM | 1706 | CB  | VAL C 190 0.965 21.260 -15.729 1.00 42.85  |
| C                           | ATOM | 1707 | CG1 | VAL C 190 2.271 21.372 -14.959 1.00 40.52  |
| C                           | ATOM | 1708 | CG2 | VAL C 190 0.161 22.547 -13.625 1.00 40.01  |
| C                           | ATOM | 1709 | N   | ALA C 191 7.503 18.126 -11.912 1.00 31.57  |
| C                           | ATOM | 1710 | CA  | ALA C 191 3.172 17.235 -17.006 1.00 35.01  |
| C                           | ATOM | 1711 | C   | ALA C 191 2.701 16.957 -18.411 1.00 37.21  |
| C                           | ATOM | 1712 | O   | ALA C 191 3.532 16.536 -18.589 1.00 44.39  |
| C                           | ATOM | 1713 | CB  | ALA C 191 1.233 16.128 -16.596 1.00 33.84  |
| C                           | ATOM | 1714 | N   | GLN C 192 2.096 17.267 -19.405 1.00 35.68  |
| C                           | ATOM | 1715 | CA  | GLN C 192 2.243 17.110 -20.803 1.00 44.40  |
| C                           | ATOM | 1716 | C   | GLN C 192 3.440 17.980 -21.167 1.00 39.21  |
| C                           | ATOM | 1717 | O   | GLN C 192 4.325 17.544 -21.699 1.00 45.68  |
| C                           | ATOM | 1718 | CB  | GLN C 192 1.065 17.433 -21.728 1.00 43.27  |
| C                           | ATOM | 1719 | CG  | GLN C 192 0.009 18.839 -21.823 1.00 39.32  |
| C                           | ATOM | 1720 | CD  | GLN C 192 -0.793 16.132 -20.547 1.00 53.00 |
| C                           | ATOM | 1721 | NEZ | GLN C 192 -1.374 15.004 -20.354 1.00 49.67 |
| C                           | ATOM | 1722 | QE1 | GLN C 192 -0.893 17.111 -19.744 1.00 49.06 |
| C                           | ATOM | 1723 | N   | ARG C 193 3.456 19.210 -20.662 1.00 40.10  |
| C                           | ATOM | 1724 | CA  | ARG C 193 5.000 20.130 -20.926 1.00 38.77  |
| C                           | ATOM | 1725 | C   | ARG C 193 5.684 19.635 -20.106 1.00 41.14  |
| C                           | ATOM | 1726 | O   | ARG C 193 6.914 19.634 -20.957 1.00 47.07  |
| C                           | ATOM | 1727 | CB  | ARG C 193 4.239 21.527 -20.392 1.00 34.23  |
| C                           | ATOM | 1728 | CG  | ARG C 193 5.232 22.593 -20.831 1.00 43.46  |
| C                           | ATOM | 1729 | CD  | ARG C 193 5.000 23.913 -20.107 1.00 47.79  |
| C                           | ATOM | 1730 | NE  | ARG C 193 3.596 24.277 -20.023 1.00 49.90  |
| C                           | ATOM | 1731 | CZ  | ARG C 193 3.030 24.813 -18.945 1.00 52.00  |
| C                           | ATOM | 1732 | NH1 | ARG C 193 3.756 25.042 -17.859 1.00 42.59  |
| C                           | ATOM | 1733 | NH2 | ARG C 193 1.240 25.116 -18.950 1.00 72.32  |
| C                           | ATOM | 1734 | N   | LEU C 194 5.794 19.215 -19.049 1.00 37.79  |
| C                           | ATOM | 1735 | CA  | LEU C 194 6.960 18.734 -18.346 1.00 40.04  |
| C                           | ATOM | 1736 | C   | LEU C 194 7.519 17.444 -18.956 1.00 37.61  |
| C                           | ATOM | 1737 | O   | LEU C 194 8.732 17.241 -19.022 1.00 36.24  |
| C                           | ATOM | 1738 | CB  | LEU C 194 6.677 18.536 -16.662 1.00 30.53  |
| C                           | ATOM | 1739 | CG  | LEU C 194 6.447 19.648 -16.739 1.00 27.79  |
| C                           | ATOM | 1740 | CD1 | LEU C 194 6.037 19.592 -14.683 1.00 25.24  |
| C                           | ATOM | 1741 | CD2 | LEU C 19                                   |

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|-----------------------------|------|-----|-----------|---------|--------|---------|------|-------|--|
| ATOM                        | 1886 | CB  | SER C 214 | 5.073   | 9.353  | -18.218 | 1.00 | 41.87 |  |
| ATOM                        | 1889 | OG  | SER C 214 | 5.480   | 9.461  | -18.348 | 1.00 | 55.74 |  |
| ATOM                        | 1890 | N   | PRO C 215 | 9.045   | 10.331 | -18.363 | 1.00 | 32.84 |  |
| ATOM                        | 1891 | CA  | PRO C 215 | 3.660   | 10.237 | -17.890 | 1.00 | 38.22 |  |
| ATOM                        | 1892 | C   | PRO C 215 | 3.443   | 9.066  | -16.909 | 1.00 | 44.70 |  |
| ATOM                        | 1893 | O   | PRO C 215 | 4.079   | 8.019  | -17.038 | 1.00 | 51.21 |  |
| ATOM                        | 1894 | CB  | PRO C 215 | 2.876   | 9.964  | -19.162 | 1.00 | 39.80 |  |
| ATOM                        | 1895 | CG  | PRO C 215 | 3.727   | 10.542 | -20.262 | 1.00 | 28.12 |  |
| ATOM                        | 1896 | CD  | PRO C 215 | 5.135   | 10.271 | -19.831 | 1.00 | 26.06 |  |
| ATOM                        | 1897 | N   | TYR C 216 | 2.590   | 9.268  | -15.935 | 1.00 | 44.10 |  |
| ATOM                        | 1898 | CA  | TYR C 216 | 2.272   | 6.132  | -14.951 | 1.00 | 46.80 |  |
| ATOM                        | 1899 | C   | TYR C 216 | 0.917   | 7.583  | -15.238 | 1.00 | 54.27 |  |
| ATOM                        | 1900 | O   | TYR C 216 | -0.052  | 8.286  | -15.388 | 1.00 | 54.56 |  |
| ATOM                        | 1901 | CB  | TYR C 216 | 2.297   | 8.820  | -13.540 | 1.00 | 42.38 |  |
| ATOM                        | 1902 | CG  | TYR C 216 | 2.208   | 7.789  | -12.441 | 1.00 | 40.17 |  |
| ATOM                        | 1903 | CD1 | TYR C 216 | 9.752   | 5.959  | -12.441 | 1.00 | 49.87 |  |
| ATOM                        | 1904 | CD2 | TYR C 216 | 1.063   | 7.655  | -11.669 | 1.00 | 39.50 |  |
| ATOM                        | 1905 | CE1 | TYR C 216 | 3.220   | 6.009  | -11.169 | 1.00 | 37.77 |  |
| ATOM                        | 1906 | CE2 | TYR C 216 | 0.990   | 6.711  | -10.459 | 1.00 | 48.08 |  |
| ATOM                        | 1907 | CZ  | TYR C 216 | 2.074   | 5.891  | -10.434 | 1.00 | 47.31 |  |
| ATOM                        | 1908 | OH  | TYR C 216 | 2.013   | 4.949  | -9.414  | 1.00 | 50.85 |  |
| ATOM                        | 1909 | O   | VAL C 217 | -1.924  | 4.260  | -14.215 | 1.00 | 59.11 |  |
| ATOM                        | 1910 | N   | VAL C 217 | 0.875   | 6.258  | -15.335 | 1.00 | 55.85 |  |
| ATOM                        | 1911 | CA  | VAL C 217 | -0.397  | 5.567  | -15.539 | 1.00 | 57.38 |  |
| ATOM                        | 1912 | C   | VAL C 217 | 4.786   | 4.746  | -14.312 | 1.00 | 60.45 |  |
| ATOM                        | 1913 | CB  | VAL C 217 | -0.364  | 4.672  | -16.782 | 1.00 | 61.95 |  |
| ATOM                        | 1914 | CG1 | VAL C 217 | -0.268  | 5.537  | -18.043 | 1.00 | 51.19 |  |
| ATOM                        | 1915 | CG2 | VAL C 217 | 0.763   | 3.684  | -16.724 | 1.00 | 52.01 |  |
| ATOM                        | 1916 | N   | ARG D 135 | -1.747  | 15.266 | -16.710 | 1.00 | 51.71 |  |
| ATOM                        | 1917 | CA  | ARG D 135 | -2.371  | 14.415 | -15.711 | 1.00 | 48.75 |  |
| ATOM                        | 1918 | C   | ARG D 135 | -14.387 | 14.223 | -14.561 | 1.00 | 51.96 |  |
| ATOM                        | 1919 | O   | ARG D 135 | -2.134  | 15.128 | -13.757 | 1.00 | 40.39 |  |
| ATOM                        | 1920 | CB  | ARG D 135 | -2.778  | 13.002 | -16.338 | 1.00 | 53.57 |  |
| ATOM                        | 1921 | CG  | ARG D 135 | -4.038  | 12.481 | -15.752 | 1.00 | 69.20 |  |
| ATOM                        | 1922 | CH  | ARG D 135 | 5.226   | 13.315 | -14.230 | 1.00 | 78.68 |  |
| ATOM                        | 1923 | NE  | ARG D 135 | -2.253  | 12.513 | -16.890 | 1.00 | 41.18 |  |
| ATOM                        | 1924 | CZ  | ARG D 135 | -7.276  | 11.809 | -16.245 | 1.00 | 79.92 |  |
| ATOM                        | 1925 | NH1 | ARG D 135 | -7.124  | 11.826 | -14.920 | 1.00 | 79.66 |  |
| ATOM                        | 1926 | NH2 | ARG D 135 | -8.074  | 11.105 | -16.922 | 1.00 | 70.41 |  |
| ATOM                        | 1927 | N   | ARG D 136 | -0.760  | 13.041 | -14.499 | 1.00 | 46.60 |  |
| ATOM                        | 1928 | CA  | ARG D 136 | 0.227   | 14.710 | -13.469 | 1.00 | 31.96 |  |
| ATOM                        | 1929 | C   | ARG D 136 | 1.542   | 12.287 | -14.123 | 1.00 | 36.76 |  |
| ATOM                        | 1930 | O   | ARG D 136 | 1.535   | 11.693 | -15.200 | 1.00 | 32.47 |  |
| ATOM                        | 1931 | CB  | ARG D 136 | -0.283  | 11.611 | -12.532 | 1.00 | 36.92 |  |
| ATOM                        | 1932 | CG  | ARG D 136 | -1.021  | 10.912 | -11.672 | 1.00 | 35.56 |  |
| ATOM                        | 1933 | CD  | ARG D 136 | -1.921  | 10.912 | -10.753 | 1.00 | 45.12 |  |
| ATOM                        | 1934 | NE  | ARG D 136 | -2.924  | 11.378 | -9.798  | 1.00 | 69.00 |  |
| ATOM                        | 1935 | CZ  | ARG D 136 | -3.226  | 10.753 | -8.664  | 1.00 | 62.85 |  |
| ATOM                        | 1936 | NH1 | ARG D 136 | -2.612  | 9.621  | -8.341  | 1.00 | 62.46 |  |
| ATOM                        | 1937 | NH2 | ARG D 136 | -4.157  | 11.512 | -7.855  | 1.00 | 58.13 |  |
| ATOM                        | 1938 | N   | VAL D 137 | 2.667   | 12.599 | -13.484 | 1.00 | 41.85 |  |
| ATOM                        | 1939 | CA  | VAL D 137 | 3.972   | 12.261 | -14.049 | 1.00 | 31.73 |  |
| ATOM                        | 1940 | C   | VAL D 137 | 4.840   | 11.466 | -13.087 | 1.00 | 34.45 |  |
| ATOM                        | 1941 | O   | VAL D 137 | 4.539   | 11.362 | -11.899 | 1.00 | 35.84 |  |
| ATOM                        | 1942 | CB  | VAL D 137 | 4.767   | 13.511 | -14.448 | 1.00 | 39.99 |  |
| ATOM                        | 1943 | CG1 | VAL D 137 | 4.030   | 11.295 | -15.541 | 1.00 | 34.27 |  |
| ATOM                        | 1944 | CG2 | VAL D 137 | 5.021   | 14.388 | -18.227 | 1.00 | 33.50 |  |
| ATOM                        | 1945 | N   | LEU D 138 | 5.916   | 10.898 | -13.621 | 1.00 | 34.20 |  |
| ATOM                        | 1946 | CA  | LEU D 138 | 6.895   | 10.172 | -12.625 | 1.00 | 32.68 |  |
| ATOM                        | 1947 | C   | LEU D 138 | 8.272   | 10.808 | -12.839 | 1.00 | 38.27 |  |
| ATOM                        | 1948 | O   | LEU D 138 | 8.772   | 10.996 | -14.066 | 1.00 | 45.85 |  |
| ATOM                        | 1949 | CB  | LEU D 138 | 6.952   | 8.700  | -13.235 | 1.00 | 30.13 |  |
| ATOM                        | 1950 | CG  | LEU D 138 | 7.806   | 7.818  | -12.321 | 1.00 | 31.81 |  |

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|-----------------------------|------|-----|-----------|--------|--------|--------|------|-------|--|
| ATOM                        | 2014 | CD  | ARG D 147 | 20.650 | 8.038  | 1.148  | 0.00 | 66.77 |  |
| ATOM                        | 2015 | NE  | ARG D 147 | 19.665 | 7.690  | 2.333  | 0.00 | 71.14 |  |
| ATOM                        | 2016 | CZ  | ARG D 147 | 20.162 | 6.701  | 3.169  | 0.00 | 76.16 |  |
| ATOM                        | 2017 | NH1 | ARG D 147 | 17.128 | 5.933  | 2.956  | 0.00 | 77.36 |  |
| ATOM                        | 2018 | NH2 | ARG D 147 | 19.181 | 6.463  | 4.216  | 0.00 | 85.57 |  |
| ATOM                        | 2019 | N   | LEU D 148 | 18.196 | 12.356 | 1.128  | 1.00 | 69.00 |  |
| ATOM                        | 2020 | CA  | LEU D 148 | 17.324 | 13.367 | 1.699  | 1.00 | 66.13 |  |
| ATOM                        | 2021 | C   | LEU D 148 | 16.107 | 12.647 | 2.245  | 1.00 | 56.06 |  |
| ATOM                        | 2022 | CB  | LEU D 148 | 15.713 | 11.606 | 1.719  | 1.00 | 64.78 |  |
| ATOM                        | 2023 | CG  | LEU D 148 | 16.014 | 10.405 | 1.656  | 1.00 | 57.74 |  |
| ATOM                        | 2024 | CH  | LEU D 148 | 17.993 | 15.366 | 0.150  | 1.00 | 59.26 |  |
| ATOM                        | 2025 | CD1 | LEU D 148 | 17.439 | 16.259 | -0.949 | 1.00 | 45.61 |  |
| ATOM                        | 2026 | CD2 | LEU D 148 | 18.555 | 16.199 | 1.291  | 1.00 | 59.60 |  |
| ATOM                        | 2027 | N   | SER D 149 | 15.519 | 13.191 | 1.304  | 1.00 | 57.95 |  |
| ATOM                        | 2028 | CA  | SER D 149 | 14.631 | 12.657 | 2.812  | 1.00 | 53.08 |  |
| ATOM                        | 2029 | C   | SER D 149 | 13.195 | 12.657 | 2.812  | 1.00 | 53.08 |  |
| ATOM                        | 2030 | O   | SER D 149 | 13.245 | 13.450 | 1.871  | 1.00 | 51.43 |  |
| ATOM                        | 2031 | CB  | SER D 149 | 19.677 | 13.366 | 5.121  | 1.00 | 46.77 |  |
| ATOM                        | 2032 | CG  | SER D 149 | 13.763 | 14.759 | 4.834  | 1.00 | 53.22 |  |
| ATOM                        | 2033 | N   | GLU D 150 | 12.202 | 11.792 | 0.984  | 1.00 | 52.36 |  |
| ATOM                        | 2034 | CA  | GLU D 150 | 11.079 | 11.721 | 2.061  | 1.00 | 52.73 |  |
| ATOM                        | 2035 | C   | GLU D 150 | 10.373 | 13.070 | 1.980  | 1.00 | 51.62 |  |
| ATOM                        | 2036 | O   | GLU D 150 | 10.045 | 13.552 | 0.937  | 1.00 | 48.73 |  |
| ATOM                        | 2037 | CB  | GLU D 150 | 10.206 | 10.623 | 2.497  | 1.00 | 40.95 |  |
| ATOM                        | 2038 | CG  | GLU D 150 | 8.874  | 10.480 | 1.622  | 1.00 | 43.94 |  |
| ATOM                        | 2039 | CH  | GLU D 150 | 7.831  | 9.560  | 2.335  | 1.00 | 57.08 |  |
| ATOM                        | 2040 | OE1 | GLU D 150 | 6.969  | 9.058  | 1.490  | 1.00 | 66.53 |  |
| ATOM                        | 2041 | OE2 | GLU D 150 | 7.851  | 9.342  | 3.464  | 1.00 | 64.70 |  |
| ATOM                        | 2042 | N   | GLU D 151 | 10.177 | 13.689 | 3.138  | 1.00 | 56.48 |  |
| ATOM                        | 2043 | CA  | GLU D 151 | 10.177 | 13.689 | 3.138  | 1.00 | 56.48 |  |
| ATOM                        | 2044 | C   | GLU D 151 | 10.227 | 16.078 | 2.538  | 1.00 | 47.62 |  |
| ATOM                        | 2045 | O   | GLU D 151 | 9.650  | 16.891 | 1.817  | 1.00 | 38.29 |  |
| ATOM                        | 2046 | CB  | GLU D 151 | 9.138  | 15.322 | 4.659  | 1.00 | 50.65 |  |
| ATOM                        | 2047 | CG  | GLU D 151 | 8.147  | 16.472 | 4.847  | 1.00 | 53.63 |  |
| ATOM                        | 2048 | CH  | GLU D 151 | 6.730  | 16.089 | 4.429  | 1.00 | 69.37 |  |
| ATOM                        | 2049 | OE1 | GLU D 151 | 6.455  | 14.880 | 4.279  | 1.00 | 76.88 |  |
| ATOM                        | 2050 | OE2 | GLU D 151 | 5.890  | 16.999 | 4.272  | 1.00 | 73.14 |  |
| ATOM                        | 2051 | N   | GLU D 152 | 11.537 | 16.120 | 2.766  | 1.00 | 51.64 |  |
| ATOM                        | 2052 | CA  | GLU D 152 | 12.356 | 17.178 | 2.185  | 1.00 | 50.53 |  |
| ATOM                        | 2053 | C   | GLU D 152 | 12.547 | 16.969 | 0.686  | 1.00 | 49.07 |  |
| ATOM                        | 2054 | O   | GLU D 152 | 12.540 | 17.390 | -0.078 | 1.00 | 44.75 |  |
| ATOM                        | 2055 | CB  | GLU D 152 | 13.718 | 17.274 | 2.874  | 1.00 | 40.16 |  |
| ATOM                        | 2056 | CG  | GLU D 152 | 14.530 | 18.469 | 2.195  | 1.00 | 53.45 |  |
| ATOM                        | 2057 | CH  | GLU D 152 | 15.822 | 18.657 | 3.157  | 1.00 | 72.05 |  |
| ATOM                        | 2058 | OE1 | GLU D 152 | 16.113 | 17.038 | 4.055  | 1.00 | 85.96 |  |
| ATOM                        | 2059 | OE2 | GLU D 152 | 16.550 | 19.625 | 2.853  | 1.00 | 67.86 |  |
| ATOM                        | 2060 | N   | LEU D 153 | 12.722 | 15.718 | 0.272  | 1.00 | 45.00 |  |
| ATOM                        | 2061 | CA  | LEU D 153 | 12.842 | 15.399 | -1.147 | 1.00 | 37.51 |  |
| ATOM                        | 2062 | C   | LEU D 153 | 11.576 | 15.828 | -1.880 | 1.00 | 37.20 |  |
| ATOM                        | 2063 | O   | LEU D 153 | 11.640 | 16.545 | -2.885 | 1.00 | 40.41 |  |
| ATOM                        | 2064 | CB  | LEU D 153 | 13.095 | 13.905 | -1.353 | 1.00 | 42.69 |  |
| ATOM                        | 2065 | CG  | LEU D 153 | 13.078 | 13.420 | -2.804 | 1.00 | 42.36 |  |
| ATOM                        | 2066 | CH  | LEU D 153 | 14.278 | 13.967 | -3.572 | 1.00 | 27.60 |  |
| ATOM                        | 2067 | CD1 | LEU D 153 | 13.033 | 11.901 | -2.864 | 1.00 | 48.15 |  |
| ATOM                        | 2068 | N   | LEU D 154 | 10.475 | 15.399 | 1.361  | 1.00 | 33.45 |  |
| ATOM                        | 2069 | CA  | LEU D 154 | 9.140  | 15.755 | -1.950 | 1.00 | 35.96 |  |
| ATOM                        | 2070 | C   | LEU D 154 | 8.924  | 17.269 | -1.932 | 1.00 | 37.40 |  |
| ATOM                        | 2071 | O   | LEU D 154 | 8.350  | 17.832 | -2.867 | 1.00 | 41.00 |  |
| ATOM                        | 2072 | CB  | LEU D 154 | 7.996  | 15.047 | -1.219 | 1.00 | 36.61 |  |
| ATOM                        | 2073 | CG  | LEU D 154 | 7.893  | 13.515 | -1.440 | 1.00 | 42.81 |  |
| ATOM                        | 2074 | CH  | LEU D 154 | 6.764  | 12.931 | -0.626 | 1.00 | 42.81 |  |
| ATOM                        | 2075 | CD2 | LEU D 154 | 7.713  | 13.218 | -2.916 | 1.00 | 29.87 |  |
| ATOM                        | 2076 | N   | ASP D 155 | 9.391  | 17.923 | -0.872 | 1.00 | 37.58 |  |

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|-----------------------------|------|-----|-----------|--------|--------|---------|------|-------|----|
| ATOM                        | 1951 | CD1 | LEU D 138 | 7.153  | 7.871  | -10.956 | 1.00 | 30.82 |    |
| ATOM                        | 1952 | CD2 | LEU D 138 | 8.052  | 6.456  | -12.948 | 1.00 | 35.33 |    |
| ATOM                        | 1953 | N   | VAL D 139 | 8.882  | 11.135 | -11.825 | 1.00 | 35.61 |    |
| ATOM                        | 1954 | CA  | VAL D 139 | 10.211 | 11.730 | -11.818 | 1.00 | 35.42 |    |
| ATOM                        | 1955 | C   | VAL D 139 | 11.241 | 10.662 | -11.472 | 1.00 | 35.09 | </ |

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|-----------------------------|------|-----|-----|-----|-------|--------|---------|------------|------------|
| ATOM                        | 2140 | N   | GLY | D   | 162   | 6.709  | 22.990  | -9.273     | 1.00 30.29 |
| ATOM                        | 2141 | CG  | ARG | D   | 162   | 5.549  | 23.826  | -9.015     | 1.00 36.75 |
| ATOM                        | 2142 | C   | GLY | D   | 162   | 5.702  | 25.172  | -9.899     | 1.00 36.44 |
| ATOM                        | 2143 | O   | GLY | D   | 162   | 4.746  | 25.935  | -9.837     | 1.00 32.31 |
| ATOM                        | 2144 | N   | LYS | D   | 162   | 6.929  | 25.455  | -10.124    | 1.00 29.59 |
| ATOM                        | 2145 | CA  | LYS | D   | 163   | 7.276  | 26.731  | -10.739    | 1.00 33.64 |
| ATOM                        | 2146 | LYS | D   | 163 | 6.888 | 26.766 | -12.237 | 1.00 34.60 |            |
| ATOM                        | 2147 | O   | LYS | D   | 163   | 7.366  | 25.885  | -12.986    | 1.00 41.83 |
| ATOM                        | 2148 | CB  | LYS | D   | 163   | 8.755  | 27.034  | -10.492    | 1.00 29.66 |
| ATOM                        | 2149 | CG  | LYS | D   | 163   | 9.092  | 27.289  | -3.024     | 1.00 34.32 |
| ATOM                        | 2150 | CD  | LYS | D   | 163   | 10.579 | 27.143  | -8.808     | 1.00 42.15 |
| ATOM                        | 2151 | CE  | LYS | D   | 163   | 10.963 | 27.548  | -7.320     | 1.00 48.17 |
| ATOM                        | 2152 | NZ  | LYS | D   | 163   | 10.101 | 26.595  | -6.613     | 1.00 38.09 |
| ATOM                        | 2153 | N   | THR | D   | 164   | 6.334  | 27.862  | -12.669    | 1.00 36.70 |
| ATOM                        | 2154 | CA  | THR | D   | 164   | 6.016  | 28.056  | -14.081    | 1.00 35.44 |
| ATOM                        | 2155 | C   | THR | D   | 164   | 7.263  | 28.321  | -14.916    | 1.00 31.74 |
| ATOM                        | 2156 | O   | THR | D   | 164   | 7.309  | 28.022  | -16.107    | 1.00 36.04 |
| ATOM                        | 2157 | CB  | THR | D   | 164   | 5.023  | 29.221  | -14.289    | 1.00 37.12 |
| ATOM                        | 2158 | CG2 | THR | D   | 164   | 3.780  | 29.024  | -13.438    | 1.00 35.85 |
| ATOM                        | 2159 | OG1 | THR | D   | 164   | 5.647  | 30.460  | -13.935    | 1.00 61.93 |
| ATOM                        | 2160 | NH1 | ARG | D   | 165   | 8.281  | 28.698  | -14.286    | 1.00 29.93 |
| ATOM                        | 2161 | CA  | ARG | D   | 165   | 8.537  | 29.189  | -14.964    | 1.00 36.85 |
| ATOM                        | 2162 | C   | ARG | D   | 165   | 10.277 | 27.907  | -15.135    | 1.00 35.37 |
| ATOM                        | 2163 | O   | ARG | D   | 165   | 11.343 | 27.958  | -16.209    | 1.00 32.91 |
| ATOM                        | 2164 | CB  | ARG | D   | 165   | 10.421 | 30.075  | -14.088    | 1.00 32.16 |
| ATOM                        | 2165 | CG  | ARG | D   | 165   | 10.919 | 29.394  | -12.856    | 1.00 35.04 |
| ATOM                        | 2166 | CD  | ARG | D   | 165   | 12.082 | 30.463  | -12.260    | 1.00 36.79 |
| ATOM                        | 2167 | NE  | ARG | D   | 165   | 12.693 | 29.701  | -11.058    | 0.00 37.92 |
| ATOM                        | 2168 | CG2 | ARG | D   | 165   | 12.351 | 30.041  | -9.820     | 0.00 38.64 |
| ATOM                        | 2169 | NH1 | ARG | D   | 165   | 11.376 | 30.916  | -9.616     | 0.00 36.34 |
| ATOM                        | 2170 | NH2 | ARG | D   | 165   | 12.668 | 29.493  | -6.783     | 0.00 39.19 |
| ATOM                        | 2171 | N   | ASN | D   | 166   | 9.930  | 26.815  | -14.661    | 1.00 34.62 |
| ATOM                        | 2172 | CA  | ASN | D   | 166   | 10.489 | 25.512  | -14.987    | 1.00 36.18 |
| ATOM                        | 2173 | C   | ASN | D   | 166   | 9.560  | 24.736  | -15.915    | 1.00 40.74 |
| ATOM                        | 2174 | CB  | ASN | D   | 166   | 8.859  | 23.608  | -16.308    | 1.00 34.15 |
| ATOM                        | 2175 | CG  | ASN | D   | 166   | 10.750 | 24.705  | -13.715    | 1.00 38.58 |
| ATOM                        | 2176 | CG2 | ASN | D   | 166   | 11.905 | 25.252  | -12.904    | 1.00 26.75 |
| ATOM                        | 2177 | ND2 | ASN | D   | 166   | 11.826 | 25.097  | -11.588    | 0.00 29.50 |
| ATOM                        | 2178 | OD1 | ASN | D   | 166   | 12.859 | 25.802  | -13.451    | 1.00 27.72 |
| ATOM                        | 2179 | N   | GLY | D   | 167   | 8.434  | 25.352  | -16.266    | 1.00 33.70 |
| ATOM                        | 2180 | CA  | GLY | D   | 167   | 7.467  | 24.726  | -17.150    | 1.00 25.53 |
| ATOM                        | 2181 | C   | GLY | D   | 167   | 6.376  | 23.999  | -16.390    | 1.00 35.32 |
| ATOM                        | 2182 | O   | GLY | D   | 167   | 5.531  | 23.305  | -16.956    | 1.00 40.03 |
| ATOM                        | 2183 | N   | GLY | D   | 168   | 6.365  | 24.159  | -15.071    | 1.00 21.42 |
| ATOM                        | 2184 | CA  | GLY | D   | 168   | 5.443  | 23.427  | -14.327    | 1.00 31.44 |
| ATOM                        | 2185 | C   | GLY | D   | 168   | 4.186  | 24.187  | -13.627    | 1.00 33.39 |
| ATOM                        | 2186 | O   | GLY | D   | 168   | 3.705  | 23.051  | -14.558    | 1.00 41.13 |
| ATOM                        | 2187 | N   | GLY | D   | 169   | 3.661  | 23.654  | -12.652    | 1.00 35.24 |
| ATOM                        | 2188 | CA  | GLY | D   | 169   | 2.427  | 24.436  | -12.160    | 1.00 31.01 |
| ATOM                        | 2189 | C   | GLY | D   | 169   | 2.030  | 23.820  | -10.832    | 1.00 37.52 |
| ATOM                        | 2190 | O   | GLY | D   | 169   | 2.773  | 23.009  | -10.278    | 1.00 40.70 |
| ATOM                        | 2191 | N   | ASP | D   | 170   | 0.663  | 24.208  | -10.323    | 1.00 32.41 |
| ATOM                        | 2192 | CA  | ASP | D   | 170   | 0.382  | 23.752  | -9.019     | 1.00 34.11 |
| ATOM                        | 2193 | C   | ASP | D   | 170   | 0.386  | 22.252  | -8.887     | 1.00 29.13 |
| ATOM                        | 2194 | O   | ASP | D   | 170   | -0.084 | 21.533  | -9.772     | 1.00 32.26 |
| ATOM                        | 2195 | CB  | ASP | D   | 170   | -1.031 | 23.261  | -8.760     | 1.00 27.79 |
| ATOM                        | 2196 | CG  | ASP | D   | 170   | -1.053 | 25.768  | -3.467     | 1.00 16.37 |
| ATOM                        | 2197 | OD1 | ASP | D   | 170   | -0.046 | 26.446  | -5.754     | 1.00 33.91 |
| ATOM                        | 2198 | OD2 | ASP | D   | 170   | -2.079 | 26.256  | -7.949     | 1.00 40.49 |
| ATOM                        | 2199 | N   | VAL | D   | 171   | 0.937  | 24.776  | -7.776     | 1.00 33.11 |
| ATOM                        | 2200 | CA  | VAL | D   | 171   | 0.952  | 20.305  | -7.667     | 1.00 38.49 |
| ATOM                        | 2201 | C   | VAL | D   | 171   | -0.127 | 19.892  | -6.575     | 1.00 40.69 |
| ATOM                        | 2202 | O   | VAL | D   | 171   | -0.251 | 20.439  | -5.479     | 1.00 49.68 |

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|-----------------------------|------|-----|-----|---|-----|--------|---------|---------|------------|
| ATOM                        | 2266 | C   | GLY | D | 173 | 12.582 | 0.130   | -5.695  | 1.00 47.05 |
| ATOM                        | 2267 | O   | GLY | D | 173 | 12.274 | -0.804  | -4.944  | 1.00 49.60 |
| ATOM                        | 2268 | N   | SER | D | 180 | 13.106 | -0.051  | -6.894  | 1.00 46.48 |
| ATOM                        | 2269 | CA  | SER | D | 180 | 11.390 | -1.387  | -7.405  | 1.00 44.08 |
| ATOM                        | 2270 | C   | SER | D | 180 | 12.517 | -2.070  | -6.602  | 1.00 43.87 |
| ATOM                        | 2271 | O   | SER | D | 180 | 15.293 | -1.321  | -5.939  | 1.00 31.31 |
| ATOM                        | 2272 | CB  | SER | D | 180 | 13.743 | -1.335  | -8.892  | 1.00 41.70 |
| ATOM                        | 2273 | CG  | SER | D | 180 | 12.597 | -1.044  | -9.673  | 1.00 55.71 |
| ATOM                        | 2274 | N   | VAL | D | 181 | 14.823 | -3.344  | -5.653  | 1.00 44.53 |
| ATOM                        | 2275 | CA  | VAL | D | 181 | 14.667 | -4.068  | -5.913  | 1.00 38.43 |
| ATOM                        | 2276 | C   | VAL | D | 181 | 16.611 | -4.837  | -6.658  | 1.00 26.48 |
| ATOM                        | 2277 | O   | VAL | D | 181 | 16.168 | -5.503  | -7.793  | 1.00 44.76 |
| ATOM                        | 2278 | CB  | VAL | D | 181 | 15.043 | -5.047  | -4.912  | 1.00 35.98 |
| ATOM                        | 2279 | CG1 | VAL | D | 181 | 16.088 | -6.023  | -4.370  | 1.00 26.71 |
| ATOM                        | 2280 | CG2 | VAL | D | 181 | 14.391 | -4.274  | -3.772  | 1.00 38.29 |
| ATOM                        | 2281 | N   | MET | D | 182 | 17.912 | -4.736  | -6.597  | 1.00 40.76 |
| ATOM                        | 2282 | CA  | MET | D | 182 | 18.904 | -5.505  | -7.342  | 1.00 42.42 |
| ATOM                        | 2283 | C   | MET | D | 182 | 19.398 | -6.678  | -6.498  | 1.00 48.10 |
| ATOM                        | 2284 | O   | MET | D | 182 | 19.684 | -6.522  | -5.310  | 1.00 41.58 |
| ATOM                        | 2285 | CB  | MET | D | 182 | 19.086 | -4.627  | -7.758  | 1.00 38.43 |
| ATOM                        | 2286 | CG  | MET | D | 182 | 21.200 | -5.394  | -8.464  | 1.00 42.51 |
| ATOM                        | 2287 | SD  | MET | D | 182 | 22.643 | -5.085  | -7.786  | 1.00 70.99 |
| ATOM                        | 2288 | CE  | MET | D | 182 | 22.735 | -5.914  | -6.204  | 1.00 45.95 |
| ATOM                        | 2289 | N   | LEU | D | 183 | 19.485 | -7.852  | -7.117  | 1.00 43.67 |
| ATOM                        | 2290 | CA  | LEU | D | 183 | 19.987 | -9.045  | -6.443  | 1.00 36.45 |
| ATOM                        | 2291 | C   | LEU | D | 183 | 21.160 | -9.664  | -7.201  | 1.00 42.36 |
| ATOM                        | 2292 | O   | LEU | D | 183 | 21.131 | -9.779  | -8.428  | 1.00 34.20 |
| ATOM                        | 2293 | CB  | LEU | D | 183 | 18.864 | -10.072 | -6.274  | 1.00 43.88 |
| ATOM                        | 2294 | CG  | LEU | D | 183 | 17.685 | -9.641  | -5.397  | 1.00 39.16 |
| ATOM                        | 2295 | CD1 | LEU | D | 183 | 16.642 | -10.742 | -5.318  | 1.00 25.63 |
| ATOM                        | 2296 | CD2 | LEU | D | 183 | 18.166 | -9.253  | -4.007  | 1.00 22.66 |
| ATOM                        | 2297 | N   | GLY | D | 184 | 22.191 | -10.061 | -6.460  | 1.00 40.80 |
| ATOM                        | 2298 | CA  | GLY | D | 184 | 23.356 | -10.708 | -7.041  | 1.00 50.49 |
| ATOM                        | 2299 | C   | GLY | D | 184 | 23.561 | -12.127 | -6.534  | 1.00 36.32 |
| ATOM                        | 2300 | O   | GLY | D | 184 | 23.474 | -12.391 | -5.346  | 1.00 43.44 |
| ATOM                        | 2301 | N   | PHE | D | 185 | 23.820 | -13.043 | -7.468  | 1.00 41.52 |
| ATOM                        | 2302 | CA  | PHE | D | 185 | 23.935 | -14.458 | -7.135  | 1.00 46.48 |
| ATOM                        | 2303 | C   | PHE | D | 185 | 25.368 | -14.980 | -7.214  | 1.00 51.57 |
| ATOM                        | 2304 | O   | PHE | D | 185 | 26.200 | -14.447 | -7.942  | 1.00 60.06 |
| ATOM                        | 2305 | CB  | PHE | D | 185 | 23.016 | -15.262 | -8.051  | 1.00 37.92 |
| ATOM                        | 2306 | CG  | PHE | D | 185 | 21.576 | -14.872 | -7.930  | 1.00 43.81 |
| ATOM                        | 2307 | CD1 | PHE | D | 185 | 20.771 | -15.438 | -6.957  | 1.00 33.23 |
| ATOM                        | 2308 | CD2 | PHE | D | 185 | 21.036 | -13.912 | -8.769  | 1.00 38.40 |
| ATOM                        | 2309 | CE1 | PHE | D | 185 | 19.447 | -15.070 | -6.838  | 1.00 36.90 |
| ATOM                        | 2310 | CE2 | PHE | D | 185 | 19.717 | -13.540 | -8.655  | 1.00 40.51 |
| ATOM                        | 2311 | CZ  | PHE | D | 185 | 18.922 | -14.115 | -7.685  | 1.00 37.77 |
| ATOM                        | 2312 | N   | ALA | D | 186 | 25.644 | -16.031 | -6.449  | 1.00 49.64 |
| ATOM                        | 2313 | CA  | ALA | D | 186 | 26.988 | -16.590 | -6.354  | 1.00 52.96 |
| ATOM                        | 2314 | C   | ALA | D | 186 | 27.335 | -17.436 | -7.673  | 1.00 49.37 |
| ATOM                        | 2315 | O   | ALA | D | 186 | 28.453 | -17.384 | -8.066  | 1.00 54.18 |
| ATOM                        | 2316 | CB  | ALA | D | 186 | 27.119 | -17.420 | -1.087  | 1.00 57.68 |
| ATOM                        | 2317 | N   | ARG | D | 187 | 26.370 | -18.218 | -8.027  | 1.00 55.80 |
| ATOM                        | 2318 | CA  | ARG | D | 187 | 26.590 | -19.180 | -9.096  | 1.00 52.36 |
| ATOM                        | 2319 | C   | ARG | D | 187 | 26.272 | -18.601 | -10.479 | 1.00 54.42 |
| ATOM                        | 2320 | CG  | ARG | D | 187 | 25.292 | -17.479 | -10.650 | 1.00 51.93 |
| ATOM                        | 2321 | CB  | ARG | D | 187 | 25.731 | -20.418 | -8.825  | 1.00 49.28 |
| ATOM                        | 2322 | CG2 | ARG | D | 187 | 26.250 | -21.311 | -7.693  | 1.00 70.58 |
| ATOM                        | 2323 | CD  | ARG | D | 187 | 25.406 | -22.574 | -7.554  | 1.00 86.78 |
| ATOM                        | 2324 | NE  | ARG | D | 187 | 24.006 | -22.222 | -7.326  | 1.00 84.26 |
| ATOM                        | 2325 | OG1 | ARG | D | 187 | 23.007 | -23.095 | -7.528  | 1.00 87.78 |
| ATOM                        | 2326 | NH1 | ARG | D | 187 | 23.238 | -24.384 | -7.328  | 1.00 92.40 |
| ATOM                        | 2327 | NH2 | ARG | D | 187 | 21.773 | -22.660 | -6.998  | 1.00 71.61 |
| ATOM                        | 2328 | N   | ASP | D | 188 | 27.117 | -18.925 | -11.450 | 1.00 61.12 |

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|-----------------------------|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| N                           | ATOM | 2203 | CB  | VAL | D | 171 | 2.354  | 19.699 | -6.937 | 1.00 | 30.96 |
| C                           | ATOM | 2204 | CG1 | VAL | D | 171 | 2.365  | 18.418 | -6.589 | 1.00 | 26.56 |
| O                           | ATOM | 2205 | CG2 | VAL | D | 171 | 3.477  | 20.730 | -7.391 | 1.00 | 33.91 |
| C                           | ATOM | 2206 | N   | ASP | D | 172 | -0.937 | 18.924 | -6.996 | 1.00 | 39.01 |
| N                           | ATOM | 2207 | CA  | ASP | D | 172 | -2.067 | 18.469 | -6.191 | 1.00 | 40.70 |
| C                           | ATOM | 2208 | C   | ASP | D | 172 | -1.725 | 17.276 | -5.304 | 1.00 | 41.91 |
| O                           | ATOM | 2209 | CD  | ASP | D | 172 | -2.058 | 17.260 | -4.121 | 1.00 | 51.46 |
| C                           | ATOM | 2210 | CB  | ASP | D | 172 | 1.24   | 18.105 | -5.851 | 1.00 | 40.00 |
| N                           | ATOM | 2211 | CG  | ASP | D | 172 | -4.003 | 19.128 | -7.582 | 1.00 | 66.48 |
| C                           | ATOM | 2212 | OD1 | ASP | D | 172 | -3.813 | 20.419 | -7.003 | 1.00 | 65.18 |
| O                           | ATOM | 2213 | OD2 | ASP | D | 172 | -4.788 | 19.195 | -8.544 | 1.00 | 73.10 |
| C                           | ATOM | 2214 | CA  | VAL | D | 173 | 1.067  | 16.677 | -5.881 | 1.00 | 44.07 |
| N                           | ATOM | 2215 | C   | VAL | D | 173 | -0.767 | 15.037 | -5.859 | 1.00 | 49.09 |
| M                           | ATOM | 2216 | C   | VAL | D | 173 | 0.707  | 14.708 | -5.256 | 1.00 | 37.58 |
| C                           | ATOM | 2217 | O   | VAL | D | 173 | 1.365  | 15.031 | -6.246 | 1.00 | 35.70 |
| C                           | ATOM | 2218 | CG  | VAL | D | 173 | -1.860 | 19.874 | -5.709 | 1.00 | 36.36 |
| O                           | ATOM | 2219 | CG1 | VAL | D | 173 | -1.48  | 19.721 | -5.721 | 1.00 | 37.24 |
| C                           | ATOM | 2220 | CG2 | VAL | D | 173 | -1.368 | 12.567 | -4.992 | 1.00 | 42.11 |
| N                           | ATOM | 2221 | N   | ARG | D | 174 | 1.233  | 14.069 | -4.213 | 1.00 | 44.94 |
| C                           | ATOM | 2222 | CA  | ARG | D | 174 | 2.659  | 13.866 | -4.049 | 1.00 | 40.39 |
| O                           | ATOM | 2223 | ARG | ARG | D | 174 | 2.963  | 12.519 | -3.731 | 1.00 | 39.21 |
| C                           | ATOM | 2224 | O   | ARG | D | 174 | -2.463 | 12.243 | -3.303 | 1.00 | 49.03 |
| N                           | ATOM | 2225 | CB  | ARG | D | 174 | 3.245  | 14.994 | -3.129 | 1.00 | 52.35 |
| O                           | ATOM | 2226 | CG  | ARG | D | 174 | 4.676  | 15.381 | -3.476 | 1.00 | 57.54 |
| C                           | ATOM | 2227 | CD  | ARG | D | 174 | 5.015  | 16.623 | -2.668 | 1.00 | 55.38 |
| C                           | ATOM | 2228 | NE  | ARG | D | 174 | 4.91   | 16.361 | -2.677 | 1.00 | 55.38 |
| N                           | ATOM | 2229 | Z   | ARG | D | 174 | 5.399  | 17.167 | -0.391 | 1.00 | 73.91 |
| C                           | ATOM | 2230 | NH1 | ARG | D | 174 | 6.016  | 18.290 | -0.627 | 1.00 | 37.32 |
| N                           | ATOM | 2231 | NH2 | ARG | D | 174 | 5.359  | 16.449 | 0.989  | 1.00 | 29.17 |
| C                           | ATOM | 2232 | GLU | LEU | D | 175 | 3.747  | 14.688 | -1.479 | 1.00 | 47.59 |
| N                           | ATOM | 2233 | CA  | GLU | D | 175 | 4.036  | 10.316 | -3.542 | 1.00 | 7.71  |
| C                           | ATOM | 2234 | C   | GLU | D | 175 | 5.416  | 9.819  | -3.944 | 1.00 | 39.25 |
| O                           | ATOM | 2235 | O   | GLU | D | 175 | 5.757  | 9.797  | -5.127 | 1.00 | 45.53 |
| C                           | ATOM | 2236 | LEU | LEU | D | 175 | 2.947  | 9.370  | -3.989 | 1.00 | 43.55 |
| N                           | ATOM | 2237 | CG  | GLU | D | 175 | 7.925  | 10.074 | -6.090 | 1.00 | 74.74 |
| C                           | ATOM | 2238 | CD  | GLU | D | 175 | 2.002  | 7.037  | -3.905 | 1.00 | 58.15 |
| O                           | ATOM | 2239 | OE1 | LEU | D | 175 | 1.158  | 7.472  | -4.717 | 1.00 | 59.90 |
| C                           | ATOM | 2240 | OE2 | LEU | D | 175 | 1.988  | 8.666  | -3.471 | 1.00 | 64.58 |
| N                           | ATOM | 2241 | LEU | LEU | D | 175 | 4.707  | 9.400  | -6.073 | 1.00 | 66.07 |
| C                           | ATOM | 2242 | CA  | LEU | D | 176 | 7.463  | 8.703  | -3.237 | 1.00 | 41.15 |
| O                           | ATOM | 2243 | C   | LEU | D | 176 | 7.219  | 7.204  | -3.394 | 1.00 | 50.01 |
| C                           | ATOM | 2244 | O   | LEU | D | 176 | 6.940  | 6.498  | -2.425 | 1.00 | 48.88 |
| N                           | ATOM | 2245 | LEU | LEU | D | 176 | 8.468  | 8.954  | -2.123 | 1.00 | 37.95 |
| C                           | ATOM | 2246 | CG  | LEU | D | 176 | 3.785  | 3.339  | -3.275 | 1.00 | 30.60 |
| O                           | ATOM | 2247 | CD1 | LEU | D | 176 | 10.514 | 8.348  | -3.491 | 1.00 | 29.75 |
| C                           | ATOM | 2248 | CD2 | LEU | D | 176 | 10.688 | 8.474  | -1.000 | 1.00 | 24.63 |
| O                           | ATOM | 2249 | N   | LEU | D | 177 | 7.324  | 6.734  | -4.693 | 1.00 | 47.76 |
| C                           | ATOM | 2250 | LEU | LEU | D | 177 | 8.102  | 6.073  | -5.753 | 1.00 | 41.57 |
| N                           | ATOM | 2251 | C   | LEU | D | 177 | 8.250  | 4.410  | -4.561 | 1.00 | 48.23 |
| C                           | ATOM | 2252 | O   | LEU | D | 177 | 9.411  | 4.827  | -4.568 | 1.00 | 48.93 |
| O                           | ATOM | 2253 | CB  | LEU | D | 177 | 6.588  | 5.211  | -6.478 | 1.00 | 47.67 |
| C                           | ATOM | 2254 | CD  | LEU | D | 177 | 6.860  | 5.856  | -6.984 | 1.00 | 46.32 |
| N                           | ATOM | 2255 | CD2 | LEU | D | 177 | 6.672  | 4.900  | -6.860 | 1.00 | 40.07 |
| C                           | ATOM | 2256 | CD3 | LEU | D | 177 | 4.362  | 5.303  | -6.217 | 1.00 | 44.77 |
| O                           | ATOM | 2257 | N   | PRO | D | 178 | 7.923  | 3.159  | -4.139 | 1.00 | 42.09 |
| C                           | ATOM | 2258 | CA  | PRO | D | 178 | 9.913  | 2.177  | -3.731 | 1.00 | 30.38 |
| N                           | ATOM | 2259 | C   | PRO | D | 178 | 9.889  | 1.911  | -3.667 | 1.00 | 30.23 |
| O                           | ATOM | 2260 | O   | PRO | D | 178 | 9.867  | 1.882  | -3.977 | 1.00 | 35.93 |
| C                           | ATOM | 2261 | CG  | PRO | D | 178 | 8.032  | 0.920  | -3.471 | 1.00 | 36.70 |
| N                           | ATOM | 2262 | CG  | PRO | D | 178 | 6.813  | 1.131  | -4.246 | 1.00 | 48.83 |
| C                           | ATOM | 2263 | CD  | PRO | D | 178 | 6.561  | 2.660  | -4.172 | 1.00 | 53.68 |
| O                           | ATOM | 2264 | N   | GLY | D | 179 | 11.226 | 1.700  | -4.445 | 1.00 | 34.84 |
| C                           | ATOM | 2265 | CA  | GLY | D | 179 | 12.344 | 1.565  | -3.757 | 1.00 | 29.93 |

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|-----------------------------|------|-----|-----------|
| ATOM                        | Z392 | CD  | GLN D 196 |
| ATOM                        | Z393 | NE2 | GLN D 196 |
| ATOM                        | Z394 | OE1 | GLN D 196 |
| ATOM                        | Z395 | N   | TLE D 197 |
| ATOM                        | Z396 | CA  | TLE D 197 |
| ATOM                        | Z397 | C   | TLE D 197 |
| ATOM                        | Z398 | O   | TLE D 197 |
| ATOM                        | Z399 | CB  | TLE D 197 |
| ATOM                        | Z400 | CG  | TLE D 197 |
| ATOM                        | Z401 | CG2 | TLE D 197 |
| ATOM                        | Z402 | CD1 | TLE D 197 |
| ATOM                        | Z403 | N   | GLY D 198 |
| ATOM                        | Z404 | CA  | GLY D 198 |
| ATOM                        | Z405 | C   | GLY D 198 |
| ATOM                        | Z406 | O   | GLY D 198 |
| ATOM                        | Z407 | N   | GLN D 199 |
| ATOM                        | Z408 | CA  | GLN D 199 |
| ATOM                        | Z409 | C   | GLN D 199 |
| ATOM                        | Z410 | O   | GLN D 199 |
| ATOM                        | Z411 | CB  | GLN D 199 |
| ATOM                        | Z412 | CG  | GLN D 199 |
| ATOM                        | Z413 | CG2 | GLN D 199 |
| ATOM                        | Z414 | NE2 | GLN D 199 |
| ATOM                        | Z415 | O   | GLN D 199 |
| ATOM                        | Z416 | N   | PHE D 200 |
| ATOM                        | Z417 | CA  | PHE D 200 |
| ATOM                        | Z418 | C   | PHE D 200 |
| ATOM                        | Z419 | O   | PHE D 200 |
| ATOM                        | Z420 | CB  | PHE D 200 |
| ATOM                        | Z421 | CG  | PHE D 200 |
| ATOM                        | Z422 | CG2 | PHE D 200 |
| ATOM                        | Z423 | CD2 | PHE D 200 |
| ATOM                        | Z424 | CE1 | PHE D 200 |
| ATOM                        | Z425 | CE2 | PHE D 200 |
| ATOM                        | Z426 | CZ  | PHE D 200 |
| ATOM                        | Z427 | N   | THR D 201 |
| ATOM                        | Z428 | CA  | THR D 201 |
| ATOM                        | Z429 | C   | THR D 201 |
| ATOM                        | Z430 | O   | THR D 201 |
| ATOM                        | Z431 | CB  | THR D 201 |
| ATOM                        | Z432 | CG2 | THR D 201 |
| ATOM                        | Z433 | OG1 | THR D 201 |
| ATOM                        | Z434 | N   | VAL D 202 |
| ATOM                        | Z435 | CA  | VAL D 202 |
| ATOM                        | Z436 | C   | VAL D 202 |
| ATOM                        | Z437 | O   | VAL D 202 |
| ATOM                        | Z438 | CB  | VAL D 202 |
| ATOM                        | Z439 | CG1 | VAL D 202 |
| ATOM                        | Z440 | CG2 | VAL D 202 |
| ATOM                        | Z441 | V   | PRO D 203 |
| ATOM                        | Z442 | CA  | PRO D 203 |
| ATOM                        | Z443 | C   | PRO D 203 |
| ATOM                        | Z444 | O   | PRO D 203 |
| ATOM                        | Z445 | CB  | PRO D 203 |
| ATOM                        | Z446 | CG  | PRO D 203 |
| ATOM                        | Z447 | CD  | PRO D 203 |
| ATOM                        | Z448 | V   | LEU D 204 |
| ATOM                        | Z449 | CA  | LEU D 204 |
| ATOM                        | Z450 | C   | LEU D 204 |
| ATOM                        | Z451 | O   | LEU D 204 |
| ATOM                        | Z452 | CB  | LEU D 204 |
| ATOM                        | Z453 | CG  | LEU D 204 |
| ATOM                        | Z454 | CD1 | LEU D 204 |

| octamer-PDB-coordinates.txt |      |     |           |
|-----------------------------|------|-----|-----------|
| ATOM                        | Z518 | O   | VAL D 213 |
| ATOM                        | Z519 | CB  | VAL D 213 |
| ATOM                        | Z520 | CG1 | VAL D 213 |
| ATOM                        | Z521 | CG2 | VAL D 213 |
| ATOM                        | Z522 | N   | SER D 214 |
| ATOM                        | Z523 | CA  | SER D 214 |
| ATOM                        | Z524 | C   | SER D 214 |
| ATOM                        | Z525 | O   | SER D 214 |
| ATOM                        | Z526 | CB  | SER D 214 |
| ATOM                        | Z527 | CG  | SER D 214 |
| ATOM                        | Z528 | V   | PRO D 215 |
| ATOM                        | Z529 | CA  | PRO D 215 |
| ATOM                        | Z530 | C   | PRO D 215 |
| ATOM                        | Z531 | O   | PRO D 215 |
| ATOM                        | Z532 | CB  | PRO D 215 |
| ATOM                        | Z533 | CG  | PRO D 215 |
| ATOM                        | Z534 | CD  | PRO D 215 |
| ATOM                        | Z535 | N   | TYR D 216 |
| ATOM                        | Z536 | CA  | TYR D 216 |
| ATOM                        | Z537 | C   | TYR D 216 |
| ATOM                        | Z538 | O   | TYR D 216 |
| ATOM                        | Z539 | CB  | TYR D 216 |
| ATOM                        | Z540 | CG  | TYR D 216 |
| ATOM                        | Z541 | CD1 | TYR D 216 |
| ATOM                        | Z542 | CD2 | TYR D 216 |
| ATOM                        | Z543 | CE1 | TYR D 216 |
| ATOM                        | Z544 | CE2 | TYR D 216 |
| ATOM                        | Z545 | CZ  | TYR D 216 |
| ATOM                        | Z546 | OH  | TYR D 216 |
| ATOM                        | Z547 | O   | VAL D 217 |
| ATOM                        | Z548 | N   | VAL D 217 |
| ATOM                        | Z549 | CA  | VAL D 217 |
| ATOM                        | Z550 | C   | VAL D 217 |
| ATOM                        | Z551 | CB  | VAL D 217 |
| ATOM                        | Z552 | CG1 | VAL D 217 |
| ATOM                        | Z553 | CG2 | VAL D 217 |
| ATOM                        | Z554 | N   | GLY E 134 |
| ATOM                        | Z555 | CA  | GLY E 134 |
| ATOM                        | Z556 | C   | GLY E 134 |
| ATOM                        | Z557 | O   | GLY E 134 |
| ATOM                        | Z558 | N   | ARG E 135 |
| ATOM                        | Z559 | CA  | ARG E 135 |
| ATOM                        | Z560 | C   | ARG E 135 |
| ATOM                        | Z561 | O   | ARG E 135 |
| ATOM                        | Z562 | CB  | ARG E 135 |
| ATOM                        | Z563 | CG  | ARG E 135 |
| ATOM                        | Z564 | CD  | ARG E 135 |
| ATOM                        | Z565 | NE  | ARG E 135 |
| ATOM                        | Z566 | CZ  | ARG E 135 |
| ATOM                        | Z567 | NH2 | ARG E 135 |
| ATOM                        | Z568 | NH  | ARG E 135 |
| ATOM                        | Z569 | N   | ARG E 136 |
| ATOM                        | Z570 | CA  | ARG E 136 |
| ATOM                        | Z571 | C   | ARG E 136 |
| ATOM                        | Z572 | O   | ARG E 136 |
| ATOM                        | Z573 | CB  | ARG E 136 |
| ATOM                        | Z574 | CG  | ARG E 136 |
| ATOM                        | Z575 | CD  | ARG E 136 |
| ATOM                        | Z576 | NE  | ARG E 136 |
| ATOM                        | Z577 | CZ  | ARG E 136 |
| ATOM                        | Z578 | NH2 | ARG E 136 |
| ATOM                        | Z579 | NH  | ARG E 136 |
| ATOM                        | Z580 | N   | VAL E 137 |

| octamer-PDB-coordinates.txt |      |     |           |
|-----------------------------|------|-----|-----------|
| ATOM                        | Z455 | CD2 | LEU D 204 |
| ATOM                        | Z456 | N   | GLY D 205 |
| ATOM                        | Z457 | CA  | GLY D 205 |
| ATOM                        | Z458 | C   | GLY D 205 |
| ATOM                        | Z459 | O   | GLY D 205 |
| ATOM                        | Z460 | N   | GLY D 206 |
| ATOM                        | Z461 | CA  | GLY D 206 |
| ATOM                        | Z462 | C   | GLY D 206 |
| ATOM                        | Z463 | O   | GLY D 206 |
| ATOM                        | Z464 | N   | GLN D 207 |
| ATOM                        | Z465 | CA  | GLN D 207 |
| ATOM                        | Z466 | C   | GLN D 207 |
| ATOM                        | Z467 | O   | GLN D 207 |
| ATOM                        | Z468 | CB  | GLN D 207 |
| ATOM                        | Z469 | CG  | GLN D 207 |
| ATOM                        | Z470 | CD  | GLN D 207 |
| ATOM                        | Z471 | NE2 | GLN D 207 |
| ATOM                        | Z472 | OE1 | GLN D 207 |
| ATOM                        | Z473 | N   | GLN D 208 |
| ATOM                        | Z474 | CA  | GLN D 208 |
| ATOM                        | Z475 | C   | GLN D 208 |
| ATOM                        | Z476 | O   | GLN D 208 |
| ATOM                        | Z477 | CB  | GLN D 208 |
| ATOM                        | Z478 | CG  | GLN D 208 |
| ATOM                        | Z479 | CG2 | GLN D 208 |
| ATOM                        | Z480 | NE2 | GLN D 208 |
| ATOM                        | Z481 | OE1 | GLN D 208 |
| ATOM                        | Z482 | N   | VAL D 209 |
| ATOM                        | Z483 | CA  | VAL D 209 |
| ATOM                        | Z484 | C   | VAL D 209 |
| ATOM                        | Z485 | O   | VAL D 209 |
| ATOM                        | Z486 | CB  | VAL D 209 |
| ATOM                        | Z487 | CG1 | VAL D 209 |
| ATOM                        | Z488 | CG2 | VAL D 209 |
| ATOM                        | Z489 | N   | PRO D 210 |
| ATOM                        | Z490 | CA  | PRO D 210 |
| ATOM                        | Z491 | C   | PRO D 210 |
| ATOM                        | Z492 | O   | PRO D 210 |
| ATOM                        | Z493 | CB  | PRO D 210 |
| ATOM                        | Z494 | CG  | PRO D 210 |
| ATOM                        | Z495 | CG2 | PRO D 210 |
| ATOM                        | Z496 | N   | LEU D 211 |
| ATOM                        | Z497 | CA  | LEU D 211 |
| ATOM                        | Z498 | C   | LEU D 211 |
| ATOM                        | Z499 | O   | LEU D 211 |
| ATOM                        | Z500 | CB  | LEU D 211 |
| ATOM                        | Z501 | CG  | LEU D 211 |
| ATOM                        | Z502 | CD1 | LEU D 211 |
| ATOM                        | Z503 | CD2 | LEU D 211 |
| ATOM                        | Z504 | N   | ARG D 212 |
| ATOM                        | Z505 | CA  | ARG D 212 |
| ATOM                        | Z506 | C   | ARG D 212 |
| ATOM                        | Z507 | O   | ARG D 212 |
| ATOM                        | Z508 | CB  | ARG D 212 |
| ATOM                        | Z509 | CG  | ARG D 212 |
| ATOM                        | Z510 | CG2 | ARG D 212 |
| ATOM                        | Z511 | NE  | ARG D 212 |
| ATOM                        | Z512 | CZ  | ARG D 212 |
| ATOM                        | Z513 | NH2 | ARG D 212 |
| ATOM                        | Z514 | NH  | ARG D 212 |
| ATOM                        | Z515 | N   | VAL D 213 |
| ATOM                        | Z516 | CA  | VAL D 213 |
| ATOM                        | Z517 | C   | VAL D 213 |

| octamer-PDB-coordinates.txt |      |     |           |
|-----------------------------|------|-----|-----------|
| ATOM                        | Z581 | CA  | VAL E 137 |
| ATOM                        | Z582 | C   | VAL E 137 |
| ATOM                        | Z583 | O   | VAL E 137 |
| ATOM                        | Z584 | CB  | VAL E 137 |
| ATOM                        | Z585 | CG1 | VAL E 137 |
| ATOM                        | Z586 | CG2 | VAL E 137 |
| ATOM                        | Z587 | N   | LEU E 138 |
| ATOM                        | Z588 | CA  | LEU E 138 |
| ATOM                        | Z589 | C   | LEU E 138 |
| ATOM                        | Z590 | O   | LEU E 138 |
| ATOM                        | Z591 | CB  | LEU E 138 |
| ATOM                        | Z592 | CG  | LEU E 138 |
| ATOM                        | Z593 | CD1 | LEU E 138 |
| ATOM                        | Z594 | CD2 | LEU E 138 |
| ATOM                        | Z595 | CE1 | LEU E 138 |
| ATOM                        | Z596 | CE2 | LEU E 138 |
| ATOM                        | Z597 | CZ  | LEU E 138 |
| ATOM                        | Z598 | N   | VAL E 139 |
| ATOM                        | Z599 | CA  | VAL E 139 |
| ATOM                        | Z600 | C   | VAL E 139 |
| ATOM                        | Z601 | O   | VAL E 139 |
| ATOM                        | Z602 | N   | TYR E 140 |
| ATOM                        | Z603 | CA  | TYR E 140 |
| ATOM                        | Z604 | C   | TYR E 140 |
| ATOM                        | Z605 | O   | TYR E 140 |
| ATOM                        | Z606 | CB  | TYR E 140 |
| ATOM                        | Z607 | CG  | TYR E 140 |
| ATOM                        | Z608 | CG2 | TYR E 140 |
| ATOM                        | Z609 | N   | GLY E 141 |
| ATOM                        | Z610 | CA  | GLY E 141 |
| ATOM                        | Z611 | C   | GLY E 141 |
| ATOM                        | Z612 | O   | GLY E 141 |
| ATOM                        | Z613 | N   | PHE E 142 |
| ATOM                        | Z614 | CA  | PHE E 142 |
| ATOM                        | Z615 | C   | PHE E 142 |
| ATOM                        | Z616 | O   | PHE E 142 |
| ATOM                        | Z617 | CB  | PHE E 142 |
| ATOM                        | Z618 | CG  | PHE E 142 |
| ATOM                        | Z619 | CD1 | PHE E 142 |
| ATOM                        | Z620 | CD2 | PHE E 142 |
| ATOM                        | Z621 | CE1 | PHE E 142 |
| ATOM                        | Z622 | CE2 | PHE E 142 |
| ATOM                        | Z623 | CZ  | PHE E 142 |
| ATOM                        | Z624 | N   | PRO E 143 |
| ATOM                        | Z625 | CA  | PRO E 143 |
| ATOM                        | Z626 | C   | PRO E 143 |
| ATOM                        | Z627 | O   | PRO E 143 |
| ATOM                        | Z628 | CB  | PRO E 143 |
| ATOM                        | Z629 | CG  | PRO E 143 |
| ATOM                        | Z630 | CD  | PRO E 143 |
| ATOM                        | Z631 | N   | ALA E 144 |
| ATOM                        | Z632 | CA  | ALA E 144 |
| ATOM                        | Z633 | C   | ALA E 144 |
| ATOM                        | Z634 | O   | ALA E 144 |
| ATOM                        | Z635 | CB  | ALA E 144 |
| ATOM                        | Z636 | N   | SER E 145 |
| ATOM                        | Z637 | CA  | SER E 145 |
| ATOM                        | Z638 | C   | SER E 145 |
| ATOM                        | Z639 | O   | SER E 145 |
| ATOM                        | Z640 | CB  | SER E 145 |
| ATOM                        | Z641 | CG  | SER E 145 |
| ATOM                        | Z642 | N   | LEU E 146 |
| ATOM                        | Z643 | CA  | LEU E 146 |

| octamer-PDB-coordinates.txt |      |     |           |
|-----------------------------|------|-----|-----------|
| ATOM                        | Z581 | CA  | VAL E 137 |
| ATOM                        | Z582 | C   | VAL E 137 |
| ATOM                        | Z583 | O   | VAL E 137 |
| ATOM                        | Z584 | CB  | VAL E 137 |
| ATOM                        | Z585 | CG1 | VAL E 137 |
| ATOM                        | Z586 | CG2 | VAL E 137 |
| ATOM                        | Z587 | N   | LEU E 138 |
| ATOM                        | Z588 | CA  | LEU E 138 |
| ATOM                        | Z589 | C   | LEU E 138 |
| ATOM                        | Z590 | O   | LEU E 138 |
| ATOM                        | Z591 | CB  | LEU E 138 |
| ATOM                        | Z592 | CG  | LEU E 138 |
| ATOM                        | Z593 | CD1 | LEU E 138 |
| ATOM                        | Z594 | CD2 | LEU E 138 |
| ATOM                        | Z595 | CE1 | LEU E 138 |
| ATOM                        | Z596 | CE2 | LEU E 138 |
| ATOM                        | Z597 | CZ  | LEU E 138 |
| ATOM                        | Z598 | N   | VAL E 139 |
| ATOM                        | Z599 | CA  | VAL E 139 |
| ATOM                        | Z600 | C   | VAL E 139 |
| ATOM                        | Z601 | O   | VAL E 139 |
| ATOM                        | Z602 | N   | TYR E 140 |
| ATOM                        | Z603 | CA  | TYR E 140 |
| ATOM                        | Z604 | C   | TYR E 140 |
| ATOM                        | Z605 | O   | TYR E 140 |
| ATOM                        | Z606 | CB  | TYR E 140 |
| ATOM                        | Z607 | CG  | TYR E 140 |
| ATOM                        | Z608 | CG2 | TYR E 140 |
| ATOM                        | Z609 | N   | GLY E 141 |
| ATOM                        | Z610 | CA  | GLY E 141 |
| ATOM                        | Z611 | C   | GLY E 141 |
| ATOM                        | Z612 | O   | GLY E 141 |
| ATOM                        | Z613 | N   | PHE E 142 |
| ATOM                        | Z614 | CA  | PHE E 142 |
| ATOM                        | Z615 | C   | PHE E 142 |
| ATOM                        | Z616 | O   | PHE E 142 |
| ATOM                        | Z617 | CB  | PHE E 142 |
| ATOM                        | Z618 | CG  | PHE E 142 |
| ATOM                        | Z619 | CD1 | PHE E 142 |
| ATOM                        | Z620 | CD2 | PHE E 142 |
| ATOM                        | Z621 | CE1 | PHE E 142 |
| ATOM                        | Z622 | CE2 | PHE E 142 |
| ATOM                        | Z623 | CZ  | PHE E 142 |
| ATOM                        | Z624 | N   | PRO E 143 |
| ATOM                        | Z625 | CA  | PRO E 143 |
| ATOM                        | Z626 | C   | PRO E 143 |
| ATOM                        | Z627 | O   | PRO E 143 |
| ATOM                        | Z628 | CB  | PRO E 143 |
| ATOM                        | Z629 | CG  | PRO E 143 |
| ATOM                        | Z630 | CD  | PRO E 143 |
| ATOM                        | Z631 | N   | ALA E 144 |
| ATOM                        | Z632 | CA  | ALA E 144 |
| ATOM                        | Z633 | C   | ALA E 144 |
| ATOM                        | Z634 | O   | ALA E 144 |
| ATOM                        | Z635 | CB  | ALA E 144 |
| ATOM                        | Z636 | N   | SER E 145 |
| ATOM                        | Z637 | CA  | SER E 145 |
| ATOM                        | Z638 | C   | SER E 145 |
| ATOM                        | Z639 | O   | SER E 145 |
| ATOM                        | Z640 | CB  | SER E 145 |
| ATOM                        | Z641 | CG  | SER E 145 |
| ATOM                        | Z642 | N   | LEU E 146 |
| ATOM                        | Z643 | CA  | LEU E 146 |

| octamer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |            |
|-----------------------------|------|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM                        | 2644 | C   | LEU | E | 146 | 17.986 | 26.608 | 16.805 | 1.00 87.26 |
| ATOM                        | 2645 | O   | LEU | E | 146 | 17.210 | 27.514 | 15.414 | 1.00 80.02 |
| ATOM                        | 2646 | CB  | LEU | E | 146 | 19.940 | 27.892 | 17.334 | 1.00 87.60 |
| ATOM                        | 2647 | CG  | LEU | E | 146 | 19.582 | 27.398 | 19.333 | 1.00 89.50 |
| ATOM                        | 2648 | CD  | LEU | E | 146 | 20.148 | 26.115 | 19.638 | 1.00 87.61 |
| ATOM                        | 2649 | CD2 | LEU | E | 146 | 19.910 | 26.458 | 20.348 | 1.00 89.14 |
| ATOM                        | 2650 | N   | ARG | E | 147 | 17.577 | 25.566 | 17.484 | 1.00 86.42 |
| ATOM                        | 2651 | CA  | ARG | E | 147 | 16.789 | 25.176 | 17.581 | 1.00 81.58 |
| ATOM                        | 2652 | C   | ARG | E | 147 | 15.676 | 24.970 | 19.015 | 1.00 82.26 |
| ATOM                        | 2653 | O   | ARG | E | 147 | 15.958 | 25.066 | 19.554 | 1.00 87.64 |
| ATOM                        | 2654 | CB  | ARG | E | 147 | 15.957 | 23.681 | 16.797 | 1.00 85.33 |
| ATOM                        | 2655 | CG  | ARG | E | 147 | 16.217 | 23.968 | 15.304 | 1.00 67.44 |
| ATOM                        | 2656 | CD  | ARG | E | 147 | 15.140 | 22.845 | 14.584 | 1.00 68.75 |
| ATOM                        | 2657 | HE  | ARG | E | 147 | 14.046 | 22.807 | 14.854 | 1.00 57.90 |
| ATOM                        | 2658 | CZ  | ARG | E | 147 | 13.772 | 21.913 | 14.320 | 1.00 67.51 |
| ATOM                        | 2659 | NH1 | ARG | E | 147 | 13.669 | 20.984 | 13.458 | 1.00 70.90 |
| ATOM                        | 2660 | NH2 | ARG | E | 147 | 11.927 | 21.934 | 14.617 | 1.00 76.97 |
| ATOM                        | 2661 | N   | LEU | E | 148 | 14.572 | 26.095 | 19.626 | 1.00 77.63 |
| ATOM                        | 2662 | CA  | LEU | E | 148 | 14.572 | 25.958 | 20.964 | 1.00 68.15 |
| ATOM                        | 2663 | C   | LEU | E | 148 | 13.154 | 26.531 | 20.900 | 1.00 63.97 |
| ATOM                        | 2664 | O   | LEU | E | 148 | 12.838 | 27.459 | 20.245 | 1.00 53.24 |
| ATOM                        | 2665 | CB  | LEU | E | 148 | 15.442 | 26.493 | 21.990 | 1.00 70.33 |
| ATOM                        | 2666 | CG  | LEU | E | 148 | 16.789 | 26.066 | 22.362 | 1.00 76.00 |
| ATOM                        | 2667 | CD  | LEU | E | 148 | 17.568 | 26.067 | 23.319 | 1.00 60.89 |
| ATOM                        | 2668 | CD2 | LEU | E | 148 | 16.802 | 24.693 | 22.872 | 1.00 76.32 |
| ATOM                        | 2669 | N   | SER | E | 149 | 12.309 | 25.976 | 21.856 | 1.00 64.90 |
| ATOM                        | 2670 | CA  | SER | E | 149 | 10.955 | 26.492 | 22.061 | 1.00 57.70 |
| ATOM                        | 2671 | C   | SER | E | 149 | 10.972 | 27.913 | 22.617 | 1.00 55.87 |
| ATOM                        | 2672 | O   | SER | E | 149 | 11.969 | 26.337 | 23.205 | 1.00 62.12 |
| ATOM                        | 2673 | CG  | SER | E | 149 | 10.171 | 23.975 | 22.000 | 1.00 59.66 |
| ATOM                        | 2674 | OC  | SER | E | 149 | 10.875 | 25.364 | 24.206 | 1.00 61.73 |
| ATOM                        | 2675 | N   | GLU | E | 150 | 9.873  | 26.844 | 22.440 | 1.00 48.26 |
| ATOM                        | 2676 | CA  | GLU | E | 150 | 9.793  | 30.007 | 22.951 | 1.00 52.91 |
| ATOM                        | 2677 | C   | GLU | E | 150 | 9.981  | 30.094 | 24.157 | 1.00 58.43 |
| ATOM                        | 2678 | O   | GLU | E | 150 | 10.717 | 30.904 | 24.869 | 1.00 57.91 |
| ATOM                        | 2679 | CB  | GLU | E | 150 | 8.451  | 30.646 | 22.614 | 1.00 45.52 |
| ATOM                        | 2680 | CG  | GLU | E | 150 | 8.336  | 32.056 | 23.172 | 1.00 52.53 |
| ATOM                        | 2681 | CD  | GLU | E | 150 | 8.951  | 32.603 | 23.125 | 1.00 47.41 |
| ATOM                        | 2682 | CD2 | GLU | E | 150 | 6.772  | 33.843 | 23.163 | 1.00 47.45 |
| ATOM                        | 2683 | OE2 | GLU | E | 150 | 5.386  | 31.797 | 23.055 | 1.00 47.45 |
| ATOM                        | 2684 | N   | GLU | E | 151 | 9.308  | 29.159 | 25.160 | 1.00 53.12 |
| ATOM                        | 2685 | CA  | GLU | E | 151 | 9.311  | 29.165 | 26.642 | 1.00 47.08 |
| ATOM                        | 2686 | C   | GLU | E | 151 | 10.715 | 28.825 | 27.117 | 1.00 51.86 |
| ATOM                        | 2687 | O   | GLU | E | 151 | 11.186 | 29.403 | 28.092 | 1.00 48.63 |
| ATOM                        | 2688 | CB  | GLU | E | 151 | 8.298  | 28.194 | 27.183 | 1.00 52.91 |
| ATOM                        | 2689 | CG  | GLU | E | 151 | 8.075  | 28.378 | 28.674 | 1.00 62.39 |
| ATOM                        | 2690 | CD  | GLU | E | 151 | 7.170  | 27.372 | 29.271 | 1.00 74.41 |
| ATOM                        | 2691 | CD2 | GLU | E | 151 | 7.684  | 26.426 | 29.972 | 1.00 69.70 |
| ATOM                        | 2692 | OE2 | GLU | E | 151 | 5.943  | 27.395 | 29.049 | 1.00 99.78 |
| ATOM                        | 2693 | N   | GLU | E | 152 | 11.390 | 27.855 | 26.454 | 1.00 57.91 |
| ATOM                        | 2694 | CA  | GLU | E | 152 | 12.726 | 27.481 | 26.867 | 1.00 41.73 |
| ATOM                        | 2695 | C   | GLU | E | 152 | 13.753 | 28.563 | 26.545 | 1.00 44.08 |
| ATOM                        | 2696 | CB  | GLU | E | 152 | 14.611 | 28.824 | 27.338 | 1.00 34.71 |
| ATOM                        | 2697 | CG  | GLU | E | 152 | 13.827 | 26.261 | 26.107 | 1.00 55.81 |
| ATOM                        | 2698 | CD  | GLU | E | 152 | 14.440 | 25.585 | 26.688 | 1.00 57.91 |
| ATOM                        | 2699 | CD2 | GLU | E | 152 | 14.725 | 24.220 | 26.096 | 1.00 81.23 |
| ATOM                        | 2700 | OE1 | GLU | E | 152 | 13.920 | 23.744 | 25.276 | 1.00 65.79 |
| ATOM                        | 2701 | OE2 | GLU | E | 152 | 15.761 | 23.622 | 26.439 | 1.00 44.16 |
| ATOM                        | 2702 | N   | LEU | E | 153 | 13.616 | 23.978 | 25.302 | 1.00 41.03 |
| ATOM                        | 2703 | CA  | LEU | E | 153 | 14.497 | 30.294 | 25.008 | 1.00 57.91 |
| ATOM                        | 2704 | C   | LEU | E | 153 | 14.369 | 31.438 | 26.008 | 1.00 37.04 |
| ATOM                        | 2705 | O   | LEU | E | 153 | 15.365 | 31.923 | 26.547 | 1.00 43.56 |
| ATOM                        | 2706 | CB  | LEU | E | 153 | 14.186 | 30.769 | 23.595 | 1.00 37.96 |

| octamer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |            |
|-----------------------------|------|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM                        | 2770 | CZ  | PHE | E | 160 | 25.626 | 35.360 | 29.685 | 1.00 39.39 |
| ATOM                        | 2771 | N   | PHE | E | 161 | 20.279 | 36.680 | 31.972 | 1.00 22.55 |
| ATOM                        | 2772 | CA  | PHE | E | 161 | 20.245 | 38.100 | 31.207 | 1.00 25.29 |
| ATOM                        | 2773 | C   | PHE | E | 161 | 19.579 | 38.431 | 31.540 | 1.00 25.69 |
| ATOM                        | 2774 | O   | PHE | E | 161 | 19.454 | 39.598 | 31.908 | 1.00 27.73 |
| ATOM                        | 2775 | CB  | PHE | E | 161 | 19.520 | 38.814 | 31.060 | 1.00 28.48 |
| ATOM                        | 2776 | CG  | PHE | E | 161 | 20.283 | 38.800 | 29.784 | 1.00 32.67 |
| ATOM                        | 2777 | CD  | PHE | E | 161 | 22.389 | 39.623 | 29.587 | 1.00 30.37 |
| ATOM                        | 2778 | CD2 | PHE | E | 161 | 19.904 | 37.963 | 28.726 | 1.00 24.67 |
| ATOM                        | 2779 | CE1 | PHE | E | 161 | 22.092 | 39.615 | 28.999 | 1.00 31.23 |
| ATOM                        | 2780 | CE2 | PHE | E | 161 | 20.608 | 37.950 | 27.536 | 1.00 22.97 |
| ATOM                        | 2781 | CZ  | PHE | E | 162 | 21.704 | 38.777 | 27.373 | 1.00 31.97 |
| ATOM                        | 2782 | N   | GLY | E | 162 | 19.159 | 37.396 | 34.261 | 1.00 27.96 |
| ATOM                        | 2783 | CA  | GLY | E | 162 | 18.633 | 37.563 | 35.602 | 1.00 24.03 |
| ATOM                        | 2784 | C   | GLY | E | 162 | 19.740 | 37.533 | 36.640 | 1.00 31.60 |
| ATOM                        | 2785 | O   | GLY | E | 162 | 19.553 | 37.955 | 37.782 | 1.00 28.32 |
| ATOM                        | 2786 | N   | LYS | E | 163 | 20.903 | 37.035 | 36.232 | 1.00 27.11 |
| ATOM                        | 2787 | CA  | LYS | E | 163 | 22.037 | 36.884 | 37.137 | 1.00 28.78 |
| ATOM                        | 2788 | C   | LYS | E | 163 | 22.682 | 38.175 | 37.253 | 1.00 34.93 |
| ATOM                        | 2789 | O   | LYS | E | 163 | 23.152 | 38.811 | 36.248 | 1.00 37.91 |
| ATOM                        | 2790 | CB  | LYS | E | 163 | 22.959 | 35.757 | 36.667 | 1.00 34.13 |
| ATOM                        | 2791 | CG  | LYS | E | 163 | 22.353 | 34.866 | 36.725 | 1.00 40.36 |
| ATOM                        | 2792 | CD  | LYS | E | 163 | 23.291 | 33.347 | 36.095 | 1.00 46.26 |
| ATOM                        | 2793 | CD2 | LYS | E | 163 | 22.641 | 31.978 | 35.926 | 1.00 57.12 |
| ATOM                        | 2794 | NZ  | LYS | E | 163 | 22.068 | 31.519 | 37.274 | 1.00 53.01 |
| ATOM                        | 2795 | N   | THR | E | 164 | 23.146 | 38.559 | 38.484 | 1.00 27.55 |
| ATOM                        | 2796 | CA  | THR | E | 164 | 23.937 | 39.757 | 38.728 | 1.00 33.60 |
| ATOM                        | 2797 | C   | THR | E | 164 | 25.381 | 39.588 | 38.256 | 1.00 37.71 |
| ATOM                        | 2798 | O   | THR | E | 164 | 26.039 | 40.568 | 37.904 | 1.00 36.56 |
| ATOM                        | 2799 | CB  | THR | E | 164 | 23.935 | 40.211 | 40.218 | 1.00 39.78 |
| ATOM                        | 2800 | CG  | THR | E | 164 | 22.508 | 40.273 | 40.730 | 1.00 31.99 |
| ATOM                        | 2801 | OG1 | THR | E | 164 | 24.616 | 39.133 | 40.374 | 1.00 61.97 |
| ATOM                        | 2802 | N   | ARG | E | 165 | 25.873 | 38.350 | 38.249 | 1.00 32.62 |
| ATOM                        | 2803 | CA  | ARG | E | 165 | 27.241 | 38.067 | 37.809 | 1.00 43.75 |
| ATOM                        | 2804 | C   | ARG | E | 165 | 27.423 | 38.351 | 36.320 | 1.00 39.78 |
| ATOM                        | 2805 | O   | ARG | E | 165 | 28.547 | 38.504 | 35.840 | 1.00 46.05 |
| ATOM                        | 2806 | CB  | ARG | E | 165 | 27.670 | 36.657 | 38.162 | 1.00 46.10 |
| ATOM                        | 2807 | CG  | ARG | E | 165 | 26.999 | 35.947 | 37.366 | 1.00 45.77 |
| ATOM                        | 2808 | CD  | ARG | E | 165 | 27.761 | 34.240 | 37.564 | 1.00 47.67 |
| ATOM                        | 2809 | CD2 | ARG | E | 165 | 27.175 | 33.116 | 36.879 | 1.00 59.39 |
| ATOM                        | 2810 | CZ  | ARG | E | 165 | 26.375 | 32.207 | 37.386 | 1.00 64.62 |
| ATOM                        | 2811 | NH1 | ARG | E | 165 | 26.066 | 32.262 | 38.674 | 1.00 44.16 |
| ATOM                        | 2812 | NH2 | ARG | E | 165 | 25.891 | 31.217 | 36.648 | 1.00 60.60 |
| ATOM                        | 2813 | N   | ASN | E | 166 | 26.321 | 38.336 | 35.564 | 1.00 39.05 |
| ATOM                        | 2814 | CA  | ASN | E | 166 | 26.363 | 36.619 | 34.110 | 1.00 64.99 |
| ATOM                        | 2815 | C   | ASN | E | 166 | 26.035 | 40.129 | 33.886 | 1.00 36.49 |
| ATOM                        | 2816 | O   | ASN | E | 166 | 25.980 | 40.574 | 32.740 | 1.00 33.39 |
| ATOM                        | 2817 | CB  | ASN | E | 166 | 25.407 | 37.762 | 33.349 | 1.00 29.17 |
| ATOM                        | 2818 | CG  | ASN | E | 166 | 25.902 | 36.332 | 33.241 | 1.00 34.71 |
| ATOM                        | 2819 | CD  | ASN | E | 166 | 24.972 | 35.386 | 33.189 | 1.00 31.14 |
| ATOM                        | 2820 | OD1 | ASN | E | 166 | 27.107 | 36.082 | 33.197 | 1.00 50.24 |
| ATOM                        | 2821 | N   | GLY | E | 167 | 25.807 | 40.876 | 34.962 | 1.00 26.29 |
| ATOM                        | 2822 | CA  | GLY | E | 167 | 25.515 | 42.294 | 34.863 | 1.00 24.93 |
| ATOM                        | 2823 | C   | GLY | E | 167 | 24.023 | 42.603 | 34.896 | 1.00 36.89 |
| ATOM                        | 2824 | O   | GLY | E | 167 | 23.623 | 43.750 | 34.693 | 1.00 33.14 |
| ATOM                        | 2825 | N   | GLY | E | 168 | 23.214 | 41.577 | 35.052 | 1.00 37.10 |
| ATOM                        | 2826 | CA  | GLY | E | 168 | 21.773 | 41.216 | 34.970 | 1.00 28.57 |
| ATOM                        | 2827 | C   | GLY | E | 168 | 21.092 | 41.887 | 35.315 | 1.00 32.55 |
| ATOM                        | 2828 | O   | GLY | E | 168 | 21.671 | 42.430 | 37.236 | 1.00 39.00 |
| ATOM                        | 2829 | N   | GLY | E | 169 | 19.552 | 41.158 | 36.389 | 1.00 24.14 |
| ATOM                        | 2830 | CA  | GLY | E | 169 | 19.048 | 41.561 | 37.594 | 1.00 35.50 |
| ATOM                        | 2831 | C   | GLY | E | 169 | 17.656 | 41.003 | 37.375 | 1.00 37.31 |
| ATOM                        | 2832 | O   | GLY | E | 169 | 17.380 | 40.439 | 36.315 | 1.00 26.27 |

|   |      |      |     |     |   |     |        |        |        |            |
|---|------|------|-----|-----|---|-----|--------|--------|--------|------------|
| C | ATOM | 2707 | CG  | LEU | E | 153 | 14.940 | 32.050 | 23.167 | 1.00 47.32 |
| O | ATOM | 2708 | CD1 | LEU | E | 153 | 16.421 | 31.756 | 22.993 | 1.00 41.39 |
| C | ATOM | 2709 | CD2 | LEU | E | 153 | 14.351 | 32.631 | 21.892 | 1.00 35.39 |
| C | ATOM | 2710 | N   | LEU | E | 154 | 13.130 | 31.955 | 26.253 | 1.00 33.30 |

| octamer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |      | octamer-PDB-coordinates.txt |      |      |     |     |   |     |        |        |         |      |       |      |      |     |     |   |     |        |        |         |      |       |
|-----------------------------|------|-----|-----|---|-----|--------|--------|--------|------|-----------------------------|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM                        | 2896 | CG  | LEU | E | 177 | 9.920  | 41.534 | 19.699 | 1.00 | 42.82                       | ATOM | 2959 | N   | ARG | E | 187 | 6.759  | 37.437 | -10.815 | 1.00 | 45.14 | ATOM | 2960 | CA  | ARG | E | 187 | 6.759  | 37.437 | -10.815 | 1.00 | 45.14 |
| ATOM                        | 2897 | CD1 | LEU | E | 177 | 10.762 | 42.741 | 19.153 | 1.00 | 52.02                       | ATOM | 2961 | CB  | ARG | E | 187 | 4.896  | 37.206 | -12.340 | 1.00 | 50.18 | ATOM | 2962 | O   | ARG | E | 187 | 4.754  | 39.137 | -9.740  | 1.00 | 44.96 |
| ATOM                        | 2898 | CD2 | LEU | E | 177 | 8.558  | 42.092 | 20.154 | 1.00 | 44.55                       | ATOM | 2963 | CG  | ARG | E | 187 | 3.894  | 37.890 | -13.327 | 1.00 | 79.41 | ATOM | 2964 | CH  | ARG | E | 187 | 2.939  | 36.921 | -14.010 | 1.00 | 73.01 |
| ATOM                        | 2899 | N   | PRO | E | 178 | 7.187  | 38.412 | 17.300 | 1.00 | 60.14                       | ATOM | 2965 | CI  | ARG | E | 187 | 1.948  | 36.355 | -13.103 | 1.00 | 61.10 | ATOM | 2966 | NE  | ARG | E | 187 | 1.150  | 35.903 | -13.393 | 1.00 | 95.23 |
| ATOM                        | 2900 | CA  | PRO | E | 178 | 7.095  | 37.392 | 16.355 | 1.00 | 66.01                       | ATOM | 2967 | CZ  | ARG | E | 187 | 1.307  | 34.707 | -14.572 | 1.00 | 87.31 | ATOM | 2968 | NH1 | ARG | E | 187 | 0.309  | 34.851 | -12.510 | 1.00 | 89.52 |
| ATOM                        | 2901 | C   | PRO | E | 178 | 8.111  | 36.919 | 15.323 | 1.00 | 69.12                       | ATOM | 2969 | CO  | ASP | E | 188 | 4.942  | 40.424 | -11.627 | 1.00 | 53.75 | ATOM | 2970 | CD  | ASP | E | 188 | 4.243  | 41.569 | -11.058 | 1.00 | 44.94 |
| ATOM                        | 2902 | O   | PRO | E | 178 | 8.197  | 35.720 | 15.040 | 1.00 | 52.79                       | ATOM | 2971 | CA  | ASP | E | 188 | 2.769  | 41.283 | -10.793 | 1.00 | 57.02 | ATOM | 2972 | O   | ASP | E | 188 | 2.090  | 40.640 | -11.589 | 1.00 | 65.78 |
| ATOM                        | 2903 | CG  | PRO | E | 178 | 5.935  | 38.096 | 15.637 | 1.00 | 59.84                       | ATOM | 2973 | CB  | ASP | E | 188 | 4.358  | 42.764 | -12.018 | 1.00 | 65.22 | ATOM | 2974 | CG  | ASP | E | 188 | 5.752  | 43.353 | -12.054 | 1.00 | 79.72 |
| ATOM                        | 2904 | CG  | PRO | E | 178 | 5.561  | 39.248 | 15.478 | 1.00 | 57.16                       | ATOM | 2975 | CO1 | ASP | E | 188 | 6.197  | 43.428 | -10.918 | 1.00 | 79.13 | ATOM | 2976 | CO2 | ASP | E | 188 | 6.202  | 43.741 | -13.152 | 1.00 | 75.68 |
| ATOM                        | 2905 | CD  | PRO | E | 178 | 6.706  | 39.596 | 17.366 | 1.00 | 53.79                       | ATOM | 2977 | N   | GLY | E | 189 | 2.284  | 41.776 | -9.616  | 1.00 | 39.34 | ATOM | 2978 | N   | GLY | E | 189 | 0.876  | 41.660 | -9.317  | 1.00 | 41.93 |
| ATOM                        | 2906 | N   | GLY | E | 179 | 8.471  | 37.353 | 14.769 | 1.00 | 45.06                       | ATOM | 2979 | CA  | GLY | E | 189 | 0.555  | 40.555 | -8.355  | 1.00 | 48.72 | ATOM | 2980 | CB  | GLY | E | 189 | -0.491 | 40.566 | -7.704  | 1.00 | 44.94 |
| ATOM                        | 2907 | CA  | GLY | E | 179 | 9.768  | 37.566 | 13.667 | 1.00 | 60.66                       | ATOM | 2981 | N   | VAL | E | 190 | 1.458  | 39.584 | -8.264  | 1.00 | 50.09 | ATOM | 2982 | CA  | VAL | E | 190 | 1.271  | 38.443 | -7.376  | 1.00 | 47.06 |
| ATOM                        | 2908 | C   | GLY | E | 179 | 8.976  | 37.348 | 12.392 | 1.00 | 61.36                       | ATOM | 2983 | CB  | VAL | E | 190 | 1.306  | 38.904 | -5.926  | 1.00 | 43.98 | ATOM | 2984 | CG  | VAL | E | 190 | 1.402  | 38.556 | -5.138  | 1.00 | 42.04 |
| ATOM                        | 2909 | O   | GLY | E | 179 | 7.906  | 36.738 | 13.302 | 1.00 | 38.87                       | ATOM | 2985 | CH  | VAL | E | 190 | 2.351  | 37.369 | -7.596  | 1.00 | 39.95 | ATOM | 2986 | CI  | VAL | E | 190 | 2.152  | 36.214 | -6.628  | 1.00 | 29.01 |
| ATOM                        | 2910 | N   | SER | E | 180 | 9.526  | 37.849 | 11.292 | 1.00 | 54.76                       | ATOM | 2987 | CG2 | VAL | E | 190 | 2.322  | 36.876 | -9.033  | 1.00 | 46.25 | ATOM | 2988 | CG1 | VAL | E | 190 | 2.261  | 36.640 | -5.590  | 1.00 | 29.62 |
| ATOM                        | 2911 | CA  | SER | E | 180 | 8.864  | 37.751 | 10.005 | 1.00 | 42.97                       | ATOM | 2989 | CH2 | VAL | E | 190 | 2.151  | 36.211 | -4.262  | 1.00 | 45.43 | ATOM | 2990 | CA  | ALA | E | 191 | 1.284  | 41.032 | -7.900  | 1.00 | 45.43 |
| ATOM                        | 2912 | C   | SER | E | 180 | 9.493  | 36.855 | 8.982  | 1.00 | 36.97                       | ATOM | 2991 | O   | ALA | E | 191 | 0.733  | 40.831 | -2.816  | 1.00 | 41.41 | ATOM | 2992 | CB  | ALA | E | 191 | 3.775  | 41.066 | -4.193  | 1.00 | 37.93 |
| ATOM                        | 2913 | O   | SER | E | 180 | 10.654 | 36.467 | 9.106  | 1.00 | 48.23                       | ATOM | 2993 | CG  | ALA | E | 191 | 0.839  | 41.366 | -4.834  | 1.00 | 55.72 | ATOM | 2994 | CH  | ALA | E | 191 | -0.337 | 42.705 | -4.616  | 1.00 | 45.44 |
| ATOM                        | 2914 | CB  | SER | E | 180 | 8.802  | 39.101 | 9.427  | 1.00 | 55.64                       | ATOM | 2995 | CI  | ALA | E | 191 | -1.610 | 41.836 | -4.427  | 1.00 | 51.07 | ATOM | 2996 | CG  | ALA | E | 191 | -2.446 | 42.752 | -3.612  | 1.00 | 50.63 |
| ATOM                        | 2915 | OG  | SER | E | 180 | 7.883  | 40.000 | 10.149 | 1.00 | 54.69                       | ATOM | 2997 | CH2 | ALA | E | 191 | -0.522 | 43.658 | -5.819  | 1.00 | 49.32 | ATOM | 2998 | CH  | ALA | E | 191 | -0.405 | 44.866 | -5.792  | 1.00 | 52.69 |
| ATOM                        | 2916 | N   | VAL | E | 181 | 8.708  | 36.469 | 7.975  | 1.00 | 40.65                       | ATOM | 2999 | CO  | GLN | E | 192 | 1.855  | 44.506 | -16.043 | 1.00 | 65.31 | ATOM | 3000 | CO1 | GLN | E | 192 | 2.767  | 45.354 | -15.579 | 1.00 | 62.63 |
| ATOM                        | 2917 | CA  | VAL | E | 181 | 9.230  | 35.755 | 6.831  | 1.00 | 30.18                       | ATOM | 3001 | CO2 | GLN | E | 192 | 2.154  | 43.474 | -6.645  | 1.00 | 57.02 | ATOM | 3002 | CO3 | GLN | E | 192 | -1.762 | 40.794 | -5.123  | 1.00 | 46.64 |
| ATOM                        | 2918 | C   | VAL | E | 181 | 9.027  | 36.661 | 5.633  | 1.00 | 20.75                       | ATOM | 3003 | N   | ARG | E | 193 | -2.937 | 39.931 | -5.039  | 1.00 | 52.32 | ATOM | 3004 | CA  | ARG | E | 193 | -2.992 | 38.279 | -5.665  | 1.00 | 54.84 |
| ATOM                        | 2919 | O   | VAL | E | 181 | 7.934  | 37.185 | 5.413  | 1.00 | 37.28                       | ATOM | 3005 | CB  | ARG | E | 193 | -2.930 | 38.845 | -6.116  | 1.00 | 47.16 | ATOM | 3006 | CG  | ARG | E | 193 | -4.707 | 38.026 | -6.170  | 1.00 | 53.91 |
| ATOM                        | 2920 | CG  | VAL | E | 181 | 8.536  | 34.108 | 6.606  | 1.00 | 37.28                       | ATOM | 3007 | CH  | ARG | E | 193 | -3.066 | 36.852 | -7.110  | 1.00 | 51.63 | ATOM | 3008 | CH2 | ARG | E | 193 | -3.427 | 37.938 | -6.369  | 1.00 | 60.30 |
| ATOM                        | 2921 | CG1 | VAL | E | 181 | 8.909  | 33.852 | 5.240  | 1.00 | 37.02                       | ATOM | 3009 | CH  | ARG | E | 193 | -2.516 | 36.503 | -9.002  | 1.00 | 60.14 | ATOM | 3010 | CH1 | ARG | E | 193 | -2.143 | 35.335 | -8.499  | 1.00 | 52.27 |
| ATOM                        | 2922 | CG2 | VAL | E | 181 | 8.909  | 33.428 | 7.706  | 1.00 | 31.74                       | ATOM | 3011 | NH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3012 | NH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2923 | N   | MET | E | 182 | 10.073 | 36.842 | 4.823  | 1.00 | 37.74                       | ATOM | 3013 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3014 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2924 | N   | MET | E | 182 | 9.917  | 37.636 | 3.617  | 1.00 | 27.57                       | ATOM | 3015 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3016 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2925 | C   | MET | E | 182 | 9.943  | 36.759 | 2.374  | 1.00 | 27.57                       | ATOM | 3017 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3018 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2926 | O   | MET | E | 182 | 10.760 | 35.848 | 2.324  | 1.00 | 32.87                       | ATOM | 3019 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3020 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2927 | CB  | MET | E | 182 | 11.093 | 36.663 | 3.554  | 1.00 | 32.90                       | ATOM | 3021 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3022 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2928 | CG  | MET | E | 182 | 11.152 | 39.474 | 2.271  | 1.00 | 37.60                       | ATOM | 3023 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3024 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2929 | SO  | MET | E | 182 | 12.314 | 38.774 | 1.103  | 1.00 | 58.66                       | ATOM | 3025 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3026 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2930 | CE  | MET | E | 182 | 11.705 | 39.366 | -0.143 | 1.00 | 61.18                       | ATOM | 3027 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3028 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2931 | N   | LEU | E | 183 | 9.009  | 37.040 | 1.463  | 1.00 | 41.06                       | ATOM | 3029 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3030 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2932 | CA  | LEU | E | 183 | 8.921  | 36.328 | 0.201  | 1.00 | 30.77                       | ATOM | 3031 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3032 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2933 | C   | LEU | E | 183 | 8.959  | 37.307 | -0.962 | 1.00 | 29.34                       | ATOM | 3033 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3034 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2934 | O   | LEU | E | 183 | 8.301  | 38.347 | -0.191 | 1.00 | 31.09                       | ATOM | 3035 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3036 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2935 | CB  | LEU | E | 183 | 7.645  | 35.486 | 0.129  | 1.00 | 27.77                       | ATOM | 3037 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3038 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2936 | CG  | LEU | E | 183 | 7.478  | 34.346 | 1.135  | 1.00 | 35.05                       | ATOM | 3039 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3040 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2937 | CD1 | LEU | E | 183 | 6.156  | 33.631 | 0.904  | 1.00 | 30.37                       | ATOM | 3041 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3042 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2938 | CD2 | LEU | E | 183 | 8.642  | 33.368 | 1.054  | 1.00 | 29.51                       | ATOM | 3043 | CH  | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 | ATOM | 3044 | CH1 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |
| ATOM                        | 2939 | N   | GLY | E | 184 | 9.736  | 37.974 | -3.186 | 1.00 | 37.99                       | ATOM | 3045 | CH2 | ARG | E | 193 | -1.979 | 36.936 | -10.135 | 1.00 | 67.57 |      |      |     |     |   |     |        |        |         |      |       |

| octamer-PDB-coordinates.txt |      |     |     |     |       |        |        |         |       | octamer-PDB-coordinates.txt |      |      |      |     |     |     |       |        |        |        |       |       |   |
|-----------------------------|------|-----|-----|-----|-------|--------|--------|---------|-------|-----------------------------|------|------|------|-----|-----|-----|-------|--------|--------|--------|-------|-------|---|
| ATOM                        | 3146 | C   | ARG | E   | 212   | -0.106 | 37.999 | 6.643   | 1.00  | 45.73                       | C    | ATOM | 3211 | NE  | ARG | F   | 136   | 12.946 | 42.530 | -2.172 | 1.00  | 64.76 | N |
| ATOM                        | 3149 | O   | ARG | E   | 212   | 1.054  | 37.669 | 6.880   | 1.00  | 44.52                       | O    | ATOM | 3212 | CZ  | ARG | F   | 136   | 13.437 | 43.496 | -3.213 | 1.00  | 63.94 | N |
| ATOM                        | 3150 | CB  | ARG | E   | 212   | -1.456 | 38.814 | 5.576   | 1.00  | 54.97                       | O    | ATOM | 3213 | WH  | ARG | F   | 136   | 12.753 | 44.139 | -1.747 | 1.00  | 65.06 | C |
| ATOM                        | 3151 | CD  | ARG | E   | 212   | -2.318 | 38.888 | 9.243   | 0.00  | 55.20                       | O    | ATOM | 3214 | NH2 | ARG | F   | 136   | 14.616 | 42.884 | -3.718 | 1.00  | 61.63 | N |
| ATOM                        | 3152 | CG  | ARG | E   | 212   | -2.489 | 40.000 | 10.154  | 0.00  | 51.65                       | C    | ATOM | 3215 | N   | VAL | F   | 137   | 6.668  | 40.602 | -0.137 | 1.00  | 28.94 | N |
| ATOM                        | 3153 | NE  | ARG | E   | 212   | -1.957 | 40.004 | 11.269  | 0.00  | 55.81                       | C    | ATOM | 3216 | CA  | VAL | F   | 137   | 5.630  | 40.601 | 0.086  | 1.00  | 36.41 | C |
| ATOM                        | 3154 | CZ  | ARG | E   | 212   | -2.246 | 39.471 | 12.450  | 0.00  | 57.13                       | C    | ATOM | 3217 | C   | VAL | F   | 137   | 6.230  | 40.309 | 2.231  | 1.00  | 43.33 | C |
| ATOM                        | 3155 | NH1 | ARG | E   | 212   | -3.453 | 38.972 | 12.674  | 0.00  | 57.24                       | N1+  | ATOM | 3218 | O   | VAL | F   | 137   | 3.353  | 39.513 | 0.180  | 1.00  | 37.93 | O |
| ATOM                        | 3156 | NH2 | ARG | E   | 212   | -1.351 | 39.442 | 13.408  | 0.00  | 57.80                       | N    | ATOM | 3219 | CB  | VAL | F   | 137   | 4.490  | 39.699 | 0.980  | 1.00  | 36.04 | C |
| ATOM                        | 3157 | N   | VAL | E   | 213   | -0.452 | 37.669 | 5.540   | 1.00  | 42.45                       | N    | ATOM | 3220 | CG1 | VAL | F   | 137   | 3.778  | 40.107 | -0.718 | 1.00  | 43.27 | C |
| ATOM                        | 3158 | CA  | VAL | E   | 213   | -0.518 | 39.041 | 4.531   | 1.00  | 35.55                       | C    | ATOM | 3221 | CG2 | VAL | F   | 137   | 5.025  | 38.278 | 0.467  | 1.00  | 26.41 | C |
| ATOM                        | 3159 | C   | VAL | E   | 213   | 0.419  | 40.535 | 4.244   | 1.00  | 39.70                       | C    | ATOM | 3222 | N   | LEU | F   | 138   | 5.478  | 40.549 | 3.299  | 1.00  | 34.84 | N |
| ATOM                        | 3161 | G   | VAL | E   | 213   | -0.653 | 41.036 | 3.901   | 1.00  | 52.79                       | O    | ATOM | 3223 | CA  | LEU | F   | 138   | 5.926  | 40.168 | 4.027  | 1.00  | 33.37 | C |
| ATOM                        | 3162 | CG1 | VAL | E   | 213   | 0.318  | 38.243 | 3.217   | 1.00  | 35.95                       | C    | ATOM | 3224 | C   | LEU | F   | 138   | 4.897  | 39.324 | 3.253  | 1.00  | 33.24 | C |
| ATOM                        | 3163 | CG2 | VAL | E   | 213   | 0.583  | 36.778 | 3.456   | 1.00  | 31.53                       | C    | ATOM | 3225 | O   | LEU | F   | 138   | 3.719  | 39.567 | 5.348  | 1.00  | 47.00 | O |
| ATOM                        | 3164 | N   | SER | E   | 214   | 1.530  | 41.252 | 4.386   | 1.00  | 50.31                       | N    | ATOM | 3226 | CB  | LEU | F   | 138   | 6.133  | 41.414 | 5.487  | 1.00  | 44.42 | C |
| ATOM                        | 3165 | CA  | SER | E   | 214   | 1.538  | 42.657 | 4.121   | 1.00  | 41.10                       | C    | ATOM | 3227 | CG  | LEU | F   | 138   | 6.883  | 41.231 | 6.799  | 1.00  | 54.17 | C |
| ATOM                        | 3166 | O   | SER | E   | 214   | 2.719  | 43.019 | 3.222   | 1.00  | 41.96                       | C    | ATOM | 3228 | CD1 | LEU | F   | 138   | 4.454  | 39.650 | 6.462  | 1.00  | 39.49 | C |
| ATOM                        | 3167 | O   | SER | E   | 214   | 3.713  | 42.250 | 3.195   | 1.00  | 45.69                       | C    | ATOM | 3229 | CD2 | LEU | F   | 138   | 6.774  | 42.476 | 7.659  | 1.00  | 52.19 | C |
| ATOM                        | 3168 | CB  | SER | E   | 214   | 1.594  | 43.481 | 5.423   | 1.00  | 42.50                       | C    | ATOM | 3230 | N   | VAL | F   | 139   | 5.312  | 38.041 | 5.676  | 1.00  | 31.70 | N |
| ATOM                        | 3169 | OG  | SER | E   | 214   | 2.612  | 42.934 | 6.266   | 1.00  | 47.22                       | C    | ATOM | 3231 | CA  | VAL | F   | 139   | 4.422  | 37.071 | 6.289  | 1.00  | 41.64 | C |
| ATOM                        | 3170 | N   | PRO | E   | 215   | 2.641  | 44.127 | 2.470   | 1.00  | 46.26                       | N    | ATOM | 3232 | C   | VAL | F   | 139   | 4.561  | 37.009 | 7.311  | 1.00  | 50.00 | C |
| ATOM                        | 3171 | C   | PRO | E   | 215   | 3.751  | 44.514 | 1.589   | 1.00  | 48.33                       | C    | ATOM | 3233 | O   | VAL | F   | 139   | 5.822  | 36.465 | 8.132  | 1.00  | 41.80 | C |
| ATOM                        | 3172 | C   | PRO | E   | 215   | 1.039  | 44.841 | 2.348   | 1.00  | 55.61                       | C    | ATOM | 3234 | CB  | VAL | F   | 139   | 4.637  | 35.655 | 5.742  | 1.00  | 37.83 | C |
| ATOM                        | 3173 | O   | PRO | E   | 215   | 4.996  | 45.271 | 3.500   | 1.00  | 52.11                       | O    | ATOM | 3235 | CG1 | VAL | F   | 139   | 3.558  | 34.768 | 6.216  | 1.00  | 37.65 | C |
| ATOM                        | 3174 | CB  | PRO | E   | 215   | 3.210  | 45.743 | 0.848   | 1.00  | 45.91                       | C    | ATOM | 3236 | CG2 | VAL | F   | 139   | 4.646  | 35.695 | 5.191  | 1.00  | 20.10 | C |
| ATOM                        | 3175 | CG  | PRO | E   | 215   | 2.048  | 46.202 | 1.633   | 1.00  | 39.17                       | C    | ATOM | 3237 | C   | THR | F   | 140   | 3.462  | 37.341 | 6.514  | 1.00  | 49.18 | N |
| ATOM                        | 3176 | CD  | PRO | E   | 215   | 1.469  | 45.000 | 2.297   | 1.00  | 39.89                       | C    | ATOM | 3238 | CA  | THR | F   | 140   | 3.481  | 37.367 | 3.976  | 1.00  | 47.10 | C |
| ATOM                        | 3177 | N   | TYR | E   | 216   | 6.172  | 44.837 | 1.682   | 1.00  | 47.16                       | C    | ATOM | 3239 | C   | THR | F   | 140   | 2.355  | 36.513 | 10.559 | 1.00  | 47.17 | C |
| ATOM                        | 3178 | CA  | TYR | E   | 216   | 7.486  | 44.537 | 2.256   | 1.00  | 47.27                       | C    | ATOM | 3240 | O   | THR | F   | 140   | 1.413  | 36.153 | 9.854  | 1.00  | 52.43 | O |
| ATOM                        | 3179 | C   | TYR | E   | 216   | 8.054  | 46.223 | 1.992   | 1.00  | 60.80                       | C    | ATOM | 3241 | CB  | THR | F   | 140   | 3.341  | 38.804 | 10.513 | 1.00  | 54.11 | C |
| ATOM                        | 3180 | O   | TYR | E   | 216   | 8.029  | 46.634 | 0.655   | 1.00  | 69.86                       | D    | ATOM | 3242 | CG  | THR | F   | 140   | 4.954  | 39.690 | 9.972  | 1.00  | 46.33 | C |
| ATOM                        | 3181 | CB  | TYR | E   | 216   | 8.452  | 43.760 | 1.785   | 1.00  | 58.19                       | C    | ATOM | 3243 | OG1 | THR | F   | 140   | 2.072  | 39.341 | 10.113 | 1.00  | 57.79 | C |
| ATOM                        | 3182 | CG  | TYR | E   | 216   | 9.823  | 43.784 | 2.424   | 1.00  | 57.16                       | C    | ATOM | 3244 | N   | GLY | F   | 141   | 2.458  | 36.191 | 11.846 | 1.00  | 46.65 | N |
| ATOM                        | 3183 | CD1 | TYR | E   | 216   | 10.005 | 43.387 | 3.742   | 1.00  | 51.70                       | C    | ATOM | 3245 | CA  | GLY | F   | 141   | 1.401  | 35.472 | 12.537 | 1.00  | 44.46 | C |
| ATOM                        | 3184 | CD2 | TYR | E   | 216   | 10.938 | 44.193 | 1.703   | 1.00  | 64.06                       | C    | ATOM | 3246 | O   | GLY | F   | 141   | 1.778  | 34.097 | 13.082 | 1.00  | 58.75 | C |
| ATOM                        | 3185 | OE1 | TYR | E   | 216   | 11.259 | 43.401 | 4.325   | 1.00  | 55.11                       | C    | ATOM | 3247 | C   | THR | F   | 142   | 0.924  | 33.345 | 12.552 | 1.00  | 61.71 | C |
| ATOM                        | 3186 | OE2 | TYR | E   | 216   | 12.191 | 44.211 | 1.277   | 1.00  | 67.07                       | C    | ATOM | 3248 | N   | PHE | F   | 142   | 3.053  | 33.742 | 12.946 | 1.00  | 53.80 | C |
| ATOM                        | 3187 | CZ  | TYR | E   | 216   | 12.350 | 43.815 | 1.568   | 1.00  | 61.92                       | C    | ATOM | 3249 | CA  | PHE | F   | 142   | 3.537  | 32.436 | 13.390 | 1.00  | 51.67 | C |
| ATOM                        | 3188 | OH  | TYR | E   | 216   | 13.601 | 43.833 | 4.163   | 1.00  | 68.36                       | O    | ATOM | 3250 | C   | PHE | F   | 142   | 3.433  | 32.256 | 14.906 | 1.00  | 54.26 | C |
| ATOM                        | 3189 | N   | GLY | F   | 134   | 8.339  | 46.330 | -6.436  | 1.00  | 78.86                       | N    | ATOM | 3251 | C   | PHE | F   | 142   | 3.367  | 31.000 | 15.669 | 1.00  | 54.49 | C |
| ATOM                        | 3190 | CA  | GLY | F   | 134   | 7.244  | 36.968 | -5.520  | 1.00  | 10.29                       | N    | ATOM | 3252 | CB  | PHE | F   | 142   | 4.965  | 32.211 | 12.944 | 1.00  | 62.15 | C |
| ATOM                        | 3191 | GLY | F   | 134 | 6.710 | 44.655 | -2.637 | 1.00    | 18.83 | C                           | ATOM | 3253 | CG   | PHE | F   | 142 | 5.194 | 32.060 | 11.467 | 1.00   | 59.62 | C     |   |
| ATOM                        | 3192 | O   | GLY | F   | 134   | 5.508  | 44.611 | -1.805  | 1.00  | 67.02                       | C    | ATOM | 3254 | CD1 | PHE | F   | 142   | 4.937  | 31.357 | 10.592 | 1.00  | 60.42 | C |
| ATOM                        | 3193 | N   | ARG | F   | 135   | 7.606  | 43.679 | -5.529  | 1.00  | 52.33                       | N    | ATOM | 3255 | CD2 | PHE | F   | 142   | 5.648  | 33.604 | 10.953 | 1.00  | 59.29 | C |
| ATOM                        | 3194 | CA  | ARG | F   | 135   | 7.252  | 42.275 | -5.620  | 1.00  | 50.04                       | C    | ATOM | 3256 | CG  | PHE | F   | 142   | 5.128  | 31.513 | 9.232  | 1.00  | 58.37 | C |
| ATOM                        | 3195 | O   | ARG | F   | 135   | 7.381  | 41.718 | -4.351  | 1.00  | 41.16                       | C    | ATOM | 3257 | CE2 | PHE | F   | 142   | 5.841  | 33.765 | 9.594  | 1.00  | 53.90 | C |
| ATOM                        | 3196 | O   | ARG | F   | 135   | 7.836  | 40.128 | -4.360  | 1.00  | 40.61                       | C    | ATOM | 3258 | CZ  | PHE | F   | 142   | 5.561  | 32.719 | 8.732  | 1.00  | 40.10 | C |
| ATOM                        | 3197 | CB  | ARG | F   | 135   | 7.899  | 41.607 | -6.829  | 1.00  | 40.18                       | C    | ATOM | 3259 | N   | PRO | F   | 143   | 2.734  | 31.195 | 15.343 | 1.00  | 66.88 | N |
| ATOM                        | 3198 | CG  | ARG | F   | 135   | 7.539  | 42.204 | -8.163  | 1.00  | 44.39                       | C    | ATOM | 3260 | CA  | PRO | F   | 143   | 2.572  | 30.854 | 16.760 | 1.00  | 70.08 | C |
| ATOM                        | 3199 | CD  | ARG | F   | 135   | 8.354  | 41.548 | -9.261  | 1.00  | 47.70                       | C    | ATOM | 3261 | C   | PRO | F   | 143   | 4.863  | 30.285 | 17.359 | 1.00  | 75.50 | C |
| ATOM                        | 3200 | NE  | ARG | F   | 135   | 9.785  | 41.660 | -6.998  | 1.00  | 57.96                       | N    | ATOM | 3262 | CB  | PRO | F   | 143   | 4.959  | 29.545 | 16.637 | 1.00  | 74.73 | C |
| ATOM                        | 3201 | CZ  | ARG | F   | 135   | 10.716 | 42.921 | -9.587  | 1.00  | 60.11                       | N    | ATOM | 3263 | CG  | PRO | F   | 143   | 1.404  | 29.867 | 16.746 | 1.00  | 75.68 | C |
| ATOM                        | 3202 | NH1 | ARG | F   | 135   | 10.170 | 40.019 | -10.500 | 1.00  | 66.85                       | N1+  | ATOM | 3264 | CG  | PRO | F   | 143   | 1.523  | 29.195 | 15.426 | 1.00  | 66.89 | C |
| ATOM                        | 3203 | NH2 | ARG | F   | 135   | 11.995 | 41.099 | -9.292  | 1.00  | 66.03                       | N    | ATOM | 3265 | CD  | PRO | F   | 143   | 2.033  | 29.252 | 14.470 | 1.00  | 74.78 | C |
| ATOM                        | 3204 | N   | ARG | F   | 136   | 7.591  | 42.221 | -3.225  | 1.00  | 41.63                       | N    | ATOM | 3266 | C   | ALA | F   | 144   | 10.395 | 29.600 | 14.669 | 1.00  | 77.45 | N |
| ATOM                        | 3205 | O   | ARG | F   | 136   | 7.577  | 41.612 | -1.960  | 1.00  | 32.59                       | C    | ATOM | 3267 | CA  | ALA | F   | 144   | 5.021  | 29.748 | 19.374 | 1.00  | 73.50 | C |
| ATOM                        | 3206 | C   | ARG | F   | 136   | 6.841  | 40.915 | -0.315  | 1.00  | 41.22                       | C    | ATOM | 3268 | C   | ALA | F   | 144   | 4.595  | 28.231 | 19.442 | 1.00  | 61.79 | C |
| ATOM                        | 3207 | O   | ARG | F   | 136   | 6.139  | 42.731 | -0.894  | 1.00  | 40.25                       | C    | ATOM | 3269 | O   | ALA | F   | 144   | 5.389  | 27.520 | 19.599 | 1.00  | 76.18 | C |
| ATOM                        | 3208 | CB  | ARG | F   | 136   | 9.229  | 42.281 | -1.397  | 1.00  | 37.62                       | C    | ATOM | 3270 | CB  | ALA | F   | 144   | 5.232  | 30.321 | 20.744 | 1.00  | 61.83 | C |
| ATOM                        | 3209 | CG  | ARG | F   | 136   | 10.490 | 42.110 | -2.227  | 1.00  | 41.45                       | C    | ATOM | 3271 | CD  | ALA | F   | 144   | 4.765  | 27.747 | 19.315 | 1.00  | 62.43 | C |
| ATOM                        | 3210 | CD  | ARG | F   | 136   | 11.659 | 42.813 | -1.543  | 1.00  | 59.34                       | C    | ATOM | 3272 | CA  | SER | F   | 145   | 3.471  | 26.317 | 19.360 | 1.00  | 74.32 | C |
|                             |      |     |     |     |       |        |        |         |       |                             |      |      |      |     |     |     |       |        |        |        |       |       |   |

SUBSTITUTE SHEET (RULE 26)

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|-----------------------------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM                        | 3652 | O   | LEU F 194 | 24.571 | 45.535 | 27.468 | 1.00 | 30.51 | O |
| ATOM                        | 3653 | CB  | LEU F 194 | 22.420 | 44.624 | 29.978 | 1.00 | 32.12 | C |
| ATOM                        | 3654 | CG  | LEU F 194 | 22.259 | 43.790 | 31.249 | 1.00 | 25.75 | C |
| ATOM                        | 3655 | CD1 | LEU F 194 | 20.901 | 43.128 | 31.274 | 1.00 | 24.31 | C |
| ATOM                        | 3656 | CD2 | LEU F 194 | 23.362 | 43.752 | 31.353 | 1.00 | 31.40 | C |
| ATOM                        | 3657 | N   | CGV F 195 | 23.357 | 47.154 | 28.217 | 1.00 | 35.10 | N |
| ATOM                        | 3658 | CA  | CVS F 195 | 23.545 | 47.814 | 26.932 | 1.00 | 32.15 | C |
| ATOM                        | 3659 | C   | CVS F 195 | 24.997 | 48.268 | 26.762 | 1.00 | 42.94 | C |
| ATOM                        | 3660 | O   | CVS F 195 | 25.567 | 48.153 | 25.676 | 1.00 | 33.06 | O |
| ATOM                        | 3661 | CB  | CVS F 195 | 22.601 | 49.006 | 26.784 | 1.00 | 20.16 | C |
| ATOM                        | 3662 | CG  | CVS F 195 | 20.889 | 48.549 | 26.548 | 1.00 | 35.40 | C |
| ATOM                        | 3663 | N   | GLN F 196 | 25.586 | 48.786 | 27.838 | 1.00 | 45.81 | N |
| ATOM                        | 3664 | CA  | GLN F 196 | 26.983 | 49.216 | 27.829 | 1.00 | 39.31 | C |
| ATOM                        | 3665 | C   | GLN F 196 | 27.930 | 48.048 | 27.573 | 1.00 | 32.55 | C |
| ATOM                        | 3666 | O   | GLN F 196 | 28.927 | 48.185 | 26.666 | 1.00 | 51.48 | O |
| ATOM                        | 3667 | CB  | GLN F 196 | 27.354 | 49.908 | 29.144 | 1.00 | 39.65 | C |
| ATOM                        | 3668 | CG  | GLN F 196 | 26.634 | 51.226 | 29.397 | 0.00 | 42.21 | C |
| ATOM                        | 3669 | CD  | GLN F 196 | 26.851 | 52.227 | 28.269 | 0.00 | 40.03 | C |
| ATOM                        | 3670 | NE2 | GLN F 196 | 25.771 | 52.859 | 27.823 | 0.00 | 41.15 | N |
| ATOM                        | 3671 | OE1 | GLN F 196 | 27.976 | 52.432 | 27.814 | 0.00 | 37.30 | O |
| ATOM                        | 3672 | N   | ILE F 197 | 27.619 | 46.892 | 26.454 | 1.00 | 36.35 | N |
| ATOM                        | 3673 | CA  | ILE F 197 | 28.406 | 45.687 | 27.912 | 1.00 | 34.61 | C |
| ATOM                        | 3674 | C   | ILE F 197 | 28.256 | 45.232 | 26.455 | 1.00 | 37.88 | C |
| ATOM                        | 3675 | O   | ILE F 197 | 29.229 | 44.869 | 25.806 | 1.00 | 30.36 | O |
| ATOM                        | 3676 | CG1 | ILE F 197 | 27.584 | 44.535 | 25.844 | 1.00 | 36.13 | C |
| ATOM                        | 3677 | CG2 | ILE F 197 | 28.216 | 44.919 | 30.311 | 1.00 | 43.33 | C |
| ATOM                        | 3678 | CG2 | ILE F 197 | 28.734 | 43.257 | 28.506 | 1.00 | 28.15 | C |
| ATOM                        | 3679 | CD1 | ILE F 197 | 27.684 | 42.901 | 31.307 | 1.00 | 30.34 | C |
| ATOM                        | 3680 | N   | THR F 198 | 27.029 | 45.319 | 25.949 | 1.00 | 27.42 | N |
| ATOM                        | 3681 | CA  | GLY F 198 | 25.167 | 45.113 | 24.761 | 1.00 | 47.43 | C |
| ATOM                        | 3682 | C   | GLY F 198 | 26.743 | 43.672 | 24.063 | 1.00 | 34.68 | C |
| ATOM                        | 3683 | O   | GLY F 198 | 25.723 | 43.192 | 23.574 | 1.00 | 39.13 | O |
| ATOM                        | 3684 | N   | GLN F 199 | 27.670 | 42.978 | 24.202 | 1.00 | 33.48 | N |
| ATOM                        | 3685 | CA  | GLN F 199 | 27.987 | 41.620 | 25.681 | 1.00 | 33.96 | C |
| ATOM                        | 3686 | C   | GLN F 199 | 28.036 | 40.547 | 24.403 | 1.00 | 34.74 | C |
| ATOM                        | 3687 | D   | GLN F 199 | 28.700 | 40.754 | 25.821 | 1.00 | 33.94 | D |
| ATOM                        | 3688 | CG  | GLN F 199 | 29.233 | 41.490 | 27.791 | 1.00 | 41.31 | C |
| ATOM                        | 3689 | CD  | GLN F 199 | 30.554 | 41.754 | 23.500 | 1.00 | 47.37 | C |
| ATOM                        | 3690 | NE2 | GLN F 199 | 31.750 | 41.750 | 21.537 | 1.00 | 27.94 | N |
| ATOM                        | 3691 | NE2 | GLN F 199 | 32.950 | 41.731 | 23.125 | 1.00 | 69.41 | N |
| ATOM                        | 3692 | OE1 | GLN F 199 | 31.608 | 41.296 | 21.846 | 1.00 | 78.21 | O |
| ATOM                        | 3693 | N   | PHE F 200 | 27.311 | 39.491 | 24.618 | 1.00 | 29.39 | N |
| ATOM                        | 3694 | CA  | PHE F 200 | 27.275 | 38.431 | 25.617 | 1.00 | 34.06 | C |
| ATOM                        | 3695 | C   | PHE F 200 | 27.403 | 37.142 | 24.863 | 1.00 | 35.09 | C |
| ATOM                        | 3696 | O   | PHE F 200 | 27.081 | 36.894 | 23.793 | 1.00 | 35.09 | O |
| ATOM                        | 3697 | CB  | PHE F 200 | 25.979 | 34.456 | 26.432 | 1.00 | 33.30 | C |
| ATOM                        | 3698 | CG  | PHE F 200 | 25.767 | 39.784 | 27.157 | 1.00 | 35.10 | C |
| ATOM                        | 3699 | CD  | PHE F 200 | 25.162 | 40.866 | 26.517 | 1.00 | 31.26 | C |
| ATOM                        | 3700 | CD2 | PHE F 200 | 25.143 | 39.918 | 28.463 | 1.00 | 40.47 | C |
| ATOM                        | 3701 | CE1 | PHE F 200 | 24.983 | 42.059 | 27.184 | 1.00 | 35.43 | C |
| ATOM                        | 3702 | CE2 | PHE F 200 | 25.946 | 41.109 | 29.156 | 1.00 | 34.02 | C |
| ATOM                        | 3703 | CZ  | PHE F 200 | 25.364 | 42.180 | 28.505 | 1.00 | 34.10 | C |
| ATOM                        | 3704 | N   | THR F 201 | 27.887 | 36.091 | 25.725 | 1.00 | 32.53 | N |
| ATOM                        | 3705 | CA  | THR F 201 | 27.689 | 34.713 | 21.761 | 1.00 | 47.43 | C |
| ATOM                        | 3706 | C   | THR F 201 | 26.943 | 33.883 | 26.104 | 1.00 | 43.10 | C |
| ATOM                        | 3707 | D   | THR F 201 | 27.201 | 33.620 | 27.279 | 1.00 | 44.13 | D |
| ATOM                        | 3708 | CH  | THR F 201 | 29.304 | 34.097 | 25.317 | 1.00 | 42.26 | C |
| ATOM                        | 3709 | CG2 | THR F 201 | 29.167 | 32.632 | 24.850 | 1.00 | 59.76 | C |
| ATOM                        | 3710 | OG1 | THR F 201 | 30.185 | 34.842 | 24.466 | 1.00 | 44.26 | C |
| ATOM                        | 3711 | N   | VAL F 202 | 25.835 | 33.474 | 25.498 | 1.00 | 37.93 | N |
| ATOM                        | 3712 | CA  | VAL F 202 | 24.809 | 32.746 | 26.225 | 1.00 | 48.50 | C |
| ATOM                        | 3713 | C   | VAL F 202 | 24.758 | 31.299 | 25.759 | 1.00 | 54.59 | C |
| ATOM                        | 3714 | O   | VAL F 202 | 24.647 | 31.028 | 24.560 | 1.00 | 47.06 | O |

| octamer-PDB-coordinates.txt |      |     |           |        |        |        |      |       |   |
|-----------------------------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM                        | 3715 | CG  | LEU F 211 | 22.404 | 35.988 | 22.143 | 1.00 | 44.96 | C |
| ATOM                        | 3716 | CD1 | LEU F 211 | 22.483 | 35.551 | 23.271 | 1.00 | 43.96 | C |
| ATOM                        | 3717 | CD2 | LEU F 211 | 21.688 | 35.926 | 20.806 | 1.00 | 40.21 | C |
| ATOM                        | 3718 | N   | ARG F 212 | 23.552 | 40.232 | 21.248 | 1.00 | 40.88 | N |
| ATOM                        | 3719 | CA  | ARG F 212 | 22.752 | 41.665 | 21.457 | 1.00 | 35.81 | C |
| ATOM                        | 3720 | C   | ARG F 212 | 22.752 | 42.258 | 22.205 | 1.00 | 35.81 | C |
| ATOM                        | 3721 | O   | ARG F 212 | 21.426 | 41.841 | 22.025 | 1.00 | 30.37 | O |
| ATOM                        | 3722 | CB  | ARG F 212 | 23.945 | 42.663 | 20.117 | 1.00 | 32.51 | C |
| ATOM                        | 3723 | CG  | ARG F 212 | 25.121 | 43.314 | 20.078 | 1.00 | 40.67 | C |
| ATOM                        | 3724 | CD  | ARG F 212 | 25.969 | 43.281 | 20.466 | 1.00 | 37.03 | C |
| ATOM                        | 3725 | NE  | ARG F 212 | 26.636 | 41.769 | 18.835 | 1.00 | 39.85 | N |
| ATOM                        | 3726 | CZ  | ARG F 212 | 26.239 | 40.740 | 18.119 | 1.00 | 48.31 | C |
| ATOM                        | 3727 | NH1 | ARG F 212 | 25.372 | 40.831 | 17.338 | 1.00 | 41.52 | N |
| ATOM                        | 3728 | NH2 | ARG F 212 | 26.913 | 39.599 | 18.154 | 1.00 | 43.05 | N |
| ATOM                        | 3729 | N   | VAL F 213 | 22.864 | 43.243 | 23.041 | 1.00 | 24.14 | N |
| ATOM                        | 3730 | CA  | VAL F 213 | 21.833 | 43.907 | 23.820 | 1.00 | 24.04 | C |
| ATOM                        | 3731 | C   | VAL F 213 | 21.878 | 45.409 | 23.597 | 1.00 | 30.70 | C |
| ATOM                        | 3732 | O   | VAL F 213 | 22.909 | 46.034 | 23.794 | 1.00 | 29.19 | O |
| ATOM                        | 3733 | CG1 | VAL F 213 | 21.383 | 43.607 | 23.634 | 1.00 | 34.14 | C |
| ATOM                        | 3734 | CG2 | VAL F 213 | 21.018 | 44.416 | 24.446 | 1.00 | 38.13 | C |
| ATOM                        | 3735 | CG  | VAL F 213 | 21.755 | 42.126 | 25.007 | 1.00 | 18.76 | C |
| ATOM                        | 3736 | N   | SER F 214 | 20.748 | 45.954 | 23.169 | 1.00 | 33.09 | N |
| ATOM                        | 3737 | CA  | SER F 214 | 20.634 | 47.368 | 22.857 | 1.00 | 33.46 | C |
| ATOM                        | 3738 | C   | SER F 214 | 19.370 | 47.900 | 23.514 | 1.00 | 30.36 | C |
| ATOM                        | 3739 | O   | SER F 214 | 18.482 | 47.117 | 23.852 | 1.00 | 34.91 | O |
| ATOM                        | 3740 | CB  | SER F 214 | 20.604 | 47.587 | 21.340 | 1.00 | 42.46 | C |
| ATOM                        | 3741 | CG  | SER F 214 | 19.667 | 46.727 | 20.717 | 1.00 | 35.78 | C |
| ATOM                        | 3742 | N   | PRO F 215 | 19.283 | 49.227 | 23.706 | 1.00 | 11.65 | N |
| ATOM                        | 3743 | CA  | PRO F 215 | 18.086 | 49.810 | 24.319 | 1.00 | 32.34 | C |
| ATOM                        | 3744 | C   | PRO F 215 | 16.854 | 49.474 | 23.491 | 1.00 | 40.64 | C |
| ATOM                        | 3745 | O   | PRO F 215 | 16.983 | 49.244 | 22.240 | 1.00 | 49.61 | O |
| ATOM                        | 3746 | CG  | PRO F 215 | 16.375 | 51.314 | 24.304 | 1.00 | 26.12 | C |
| ATOM                        | 3747 | CD  | PRO F 215 | 19.859 | 51.406 | 24.289 | 1.00 | 33.35 | C |
| ATOM                        | 3748 | N   | PRO F 215 | 20.312 | 50.249 | 23.448 | 1.00 | 34.22 | N |
| ATOM                        | 3749 | CA  | TYR F 216 | 15.681 | 49.441 | 24.110 | 1.00 | 42.21 | C |
| ATOM                        | 3750 | C   | TYR F 216 | 14.489 | 49.041 | 23.382 | 1.00 | 42.21 | C |
| ATOM                        | 3751 | O   | TYR F 216 | 13.869 | 50.268 | 22.721 | 1.00 | 64.53 | O |
| ATOM                        | 3752 | CB  | TYR F 216 | 13.613 | 51.267 | 23.386 | 1.00 | 59.51 | C |
| ATOM                        | 3753 | CG  | TYR F 216 | 13.485 | 48.364 | 24.334 | 1.00 | 46.89 | C |
| ATOM                        | 3754 | CD  | TYR F 216 | 12.243 | 47.822 | 22.679 | 1.00 | 36.37 | C |
| ATOM                        | 3755 | NE  | TYR F 216 | 12.299 | 46.676 | 22.897 | 1.00 | 55.07 | N |
| ATOM                        | 3756 | CG2 | TYR F 216 | 11.000 | 48.433 | 23.859 | 1.00 | 56.67 | C |
| ATOM                        | 3757 | CD1 | TYR F 216 | 11.159 | 46.159 | 22.303 | 1.00 | 58.41 | C |
| ATOM                        | 3758 | CZ  | TYR F 216 | 9.365  | 47.926 | 21.270 | 1.00 | 62.30 | C |
| ATOM                        | 3759 | OH  | TYR F 216 | 9.945  | 46.789 | 22.493 | 1.00 | 66.19 | O |
| ATOM                        | 3760 | OH  | TYR F 216 | 9.808  | 46.780 | 21.906 | 1.00 | 55.62 | O |
| ATOM                        | 3761 | O   | VAL F 217 | 12.450 | 53.479 | 20.623 | 1.00 | 72.62 | O |
| ATOM                        | 3762 | N   | VAL F 217 | 13.679 | 50.142 | 21.408 | 1.00 | 60.26 | N |
| ATOM                        | 3763 | CA  | VAL F 217 | 13.149 | 51.181 | 20.512 | 1.00 | 64.24 | C |
| ATOM                        | 3764 | C   | VAL F 217 | 13.189 | 52.604 | 21.070 | 1.00 | 57.27 | C |
| ATOM                        | 3765 | CB  | VAL F 217 | 11.696 | 50.867 | 20.093 | 1.00 | 69.06 | C |
| ATOM                        | 3766 | CG1 | VAL F 217 | 11.650 | 49.573 | 19.290 | 1.00 | 62.51 | C |
| ATOM                        | 3767 | CG2 | VAL F 217 | 10.789 | 50.791 | 21.309 | 1.00 | 67.00 | C |
| ATOM                        | 3768 | N   | SER F 218 | -8.763 | 1.878  | 51.689 | 1.00 | 89.15 | N |
| ATOM                        | 3769 | CA  | SER F 218 | -7.780 | 1.840  | 51.402 | 1.00 | 91.45 | C |
| ATOM                        | 3770 | C   | SER F 218 | -6.645 | 2.855  | 51.433 | 1.00 | 90.16 | C |
| ATOM                        | 3771 | O   | SER F 218 | -6.749 | 2.258  | 55.493 | 1.00 | 84.02 | O |
| ATOM                        | 3772 | N   | SER F 218 | -7.220 | 3.009  | 51.987 | 1.00 | 94.32 | N |
| ATOM                        | 3773 | C   | SER F 218 | -6.113 | 4.097  | 51.918 | 1.00 | 86.30 | C |
| ATOM                        | 3774 | O   | SER F 218 | -5.161 | 3.145  | 44.989 | 1.00 | 91.45 | O |
| ATOM                        | 3775 | N   | GLY F 134 | -4.365 | 3.578  | 54.900 | 1.00 | 79.16 | N |
| ATOM                        | 3776 | C   | GLY F 134 | -3.586 | 2.283  | 54.777 | 1.00 | 69.33 | C |
| ATOM                        | 3777 | O   | GLY F 134 | -3.196 | 1.667  | 55.770 | 1.00 | 50.11 | O |

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|-----------------------------|------|-----|-----------|--------|--------|--------|------|-------|--|
| ATOM                        | 3715 | CB  | VAL F 202 | 23.420 | 33.392 | 26.044 | 1.00 | 39.36 |  |
| ATOM                        | 3716 | CG1 | VAL F 202 | 22.868 | 33.690 | 26.912 | 1.00 | 37.42 |  |
| ATOM                        | 3717 | CG2 | VAL F 202 | 23.463 | 34.020 | 26.372 | 1.00 | 36.95 |  |
| ATOM                        | 3718 | N   | PRO F 203 | 24.357 | 30.361 | 26.101 | 1.00 | 38.81 |  |
| ATOM                        | 3719 | CA  | PRO F 203 | 24.702 | 28.937 | 26.410 | 1.00 | 54.77 |  |
| ATOM                        | 3720 | C   | PRO F 203 | 23.270 | 28.618 | 26.001 | 1.00 | 50.79 |  |
| ATOM                        | 3721 | CG  | PRO F 203 | 22.371 | 28.599 | 26.847 | 1.00 | 65.08 |  |
| ATOM                        | 3722 | CB  | PRO F 203 | 25.072 | 28.153 | 26.772 | 1.00 | 59.59 |  |
| ATOM                        | 3723 | CG  | PRO F 203 | 24.810 | 29.292 | 26.736 | 1.00 | 65.26 |  |
| ATOM                        | 3724 | CD  | PRO F 203 | 25.186 | 30.391 | 26.130 | 1.00 | 59.69 |  |
| ATOM                        | 3725 | N   | LEU F 204 | 23.066 | 23.368 | 24.714 | 1.00 | 54.70 |  |
| ATOM                        | 3726 | CA  | LEU F 204 | 21.267 | 24.000 | 24.205 | 1.00 | 59.84 |  |
| ATOM                        | 3727 | C   | LEU F 204 | 21.809 | 26.831 | 23.780 | 1.00 | 61.87 |  |
| ATOM                        | 3728 | D   | LEU F 204 | 22.532 | 26.841 | 22.283 | 1.00 | 68.87 |  |
| ATOM                        | 3729 | CB  | LEU F 204 | 21.142 | 29.238 | 23.467 | 1.00 | 55.26 |  |
| ATOM                        | 3730 | CG  | LEU F 204 | 26.908 | 30.539 | 24.236 | 1.00 | 66.12 |  |
| ATOM                        | 3731 | CD1 | LEU F 204 | 26.411 | 31.632 | 23.346 | 1.00 | 60.66 |  |
| ATOM                        | 3732 | CD2 | LEU F 204 | 19.924 | 30.321 | 25.366 | 1.00 | 46.84 |  |
| ATOM                        | 3733 | N   | GLY F 205 | 21.041 | 25.798 | 23.614 | 1.00 | 69.74 |  |
| ATOM                        | 3734 | CA  | GLY F 205 | 20.971 | 24.590 | 22.811 | 1.00 | 75.81 |  |
| ATOM                        | 3735 | GL1 | GLY F 205 | 21.920 | 23.948 | 22.546 | 1.00 | 70.76 |  |
| ATOM                        | 3736 | O   | GLY F 205 | 22.569 | 21.474 | 22.103 | 1.00 | 74.35 |  |
| ATOM                        | 3737 | N   | GLY F 206 | 23.181 | 23.944 | 23.558 | 1.00 | 67.12 |  |
| ATOM                        | 3738 | CA  | GLY F 206 | 24.495 | 23.340 | 23.432 | 1.00 | 59.94 |  |
| ATOM                        | 3739 | C   | GLY F 206 | 26.649 | 24.290 | 22.726 | 1.00 | 66.80 |  |
| ATOM                        | 3740 | O   | GLY F 206 | 26.647 | 23.738 | 22.728 | 1.00 | 66.80 |  |
| ATOM                        | 3741 | N   | GLM F 207 | 25.070 | 25.432 | 22.355 | 1.00 | 79.30 |  |
| ATOM                        | 3742 | CA  | GLN F 207 | 25.947 | 26.370 | 21.664 | 1.00 | 73.42 |  |
| ATOM                        | 3743 | C   | GLN F 207 | 26.155 | 27.532 | 22.961 | 1.00 | 68.71 |  |
| ATOM                        | 3744 | GL1 | GLN F 207 | 25.651 | 27.875 | 23.509 | 1.00 | 74.07 |  |
| ATOM                        | 3745 | CB  | GLN F 207 | 25.258 | 26.919 | 23.067 | 1.00 | 69.88 |  |
| ATOM                        | 3746 | CG  | GLN F 207 | 24.485 | 25.885 | 19.607 | 1.00 | 69.89 |  |
| ATOM                        | 3747 | CD  | GLN F 207 | 23.735 | 26.504 | 18.441 | 1.00 | 78.47 |  |
| ATOM                        | 3748 | OE1 | GLN F 207 | 23.212 | 25.662 | 17.958 | 1.00 | 86.18 |  |
| ATOM                        | 3749 | OE1 | GLN F 207 | 23.627 | 27.735 | 17.755 | 1.00 | 86.18 |  |
| ATOM                        | 3750 | N   | GLN F 208 | 27.498 | 28.134 | 22.255 | 1.00 | 73.02 |  |
| ATOM                        | 3751 | CA  | GLN F 208 | 27.397 | 29.384 | 22.886 | 1.00 | 66.56 |  |
| ATOM                        | 3752 | C   | GLN F 208 | 27.487 | 30.527 | 21.970 | 1.00 | 67.53 |  |
| ATOM                        | 3753 | GL1 | GLN F 208 | 28.381 | 30.963 | 21.155 | 1.00 | 78.91 |  |
| ATOM                        | 3754 | CB  | GLN F 208 | 29.403 | 29.413 | 20.643 | 1.00 | 64.42 |  |
| ATOM                        | 3755 | CG  | GLN F 208 | 29.872 | 28.400 | 24.185 | 1.00 | 74.69 |  |
| ATOM                        | 3756 | CD  | GLN F 208 | 29.243 | 28.624 | 25.542 | 1.00 | 71.55 |  |
| ATOM                        | 3757 | O   | GLN F 208 | 28.267 | 27.700 | 25.965 | 1.00 | 73.57 |  |
| ATOM                        | 3758 | OE1 | GLN F 208 | 29.570 | 29.636 | 25.963 | 1.00 | 73.57 |  |
| ATOM                        | 3759 | N   | VAL F 209 | 26.243 | 30.974 | 22.107 | 1.00 | 61.32 |  |
| ATOM                        | 3760 | CA  | VAL F 209 | 25.680 | 31.938 | 21.160 | 1.00 | 56.14 |  |
| ATOM                        | 3761 | C   | VAL F 209 | 26.095 | 33.379 | 21.544 | 1.00 | 57.10 |  |
| ATOM                        | 3762 | GL1 | VAL F 209 | 25.645 | 33.645 | 23.621 | 1.00 | 46.81 |  |
| ATOM                        | 3763 | CB  | VAL F 209 | 24.154 | 34.785 | 21.651 | 1.00 | 64.16 |  |
| ATOM                        | 3764 | CG1 | VAL F 209 | 23.586 | 32.838 | 20.126 | 1.00 | 52.03 |  |
| ATOM                        | 3765 | CG2 | VAL F 209 | 23.795 | 30.390 | 20.577 | 1.00 | 52.54 |  |
| ATOM                        | 3766 | N   | PRO F 210 | 26.693 | 34.095 | 20.645 | 1.00 | 48.58 |  |
| ATOM                        | 3767 | CA  | PRO F 210 | 26.905 | 35.867 | 20.968 | 1.00 | 47.53 |  |
| ATOM                        | 3768 | C   | PRO F 210 | 25.734 | 36.372 | 20.568 | 1.00 | 48.01 |  |
| ATOM                        | 3769 | O   | PRO F 210 | 25.264 | 36.425 | 19.431 | 1.00 | 46.31 |  |
| ATOM                        | 3770 | CB  | PRO F 210 | 28.093 | 35.817 | 19.871 | 1.00 | 37.07 |  |
| ATOM                        | 3771 | CG  | PRO F 210 | 27.911 | 34.817 | 18.787 | 1.00 | 55.84 |  |
| ATOM                        | 3772 | CD  | PRO F 210 | 27.387 | 33.580 | 18.000 | 1.00 | 49.49 |  |
| ATOM                        | 3773 | N   | LEU F 211 | 25.234 | 27.034 | 21.597 | 1.00 | 47.55 |  |
| ATOM                        | 3774 | CA  | LEU F 211 | 24.046 | 27.851 | 21.461 | 1.00 | 39.08 |  |
| ATOM                        | 3775 | C   | LEU F 211 | 21.363 | 39.331 | 21.759 | 1.00 | 36.89 |  |
| ATOM                        | 3776 | O   | LEU F 211 | 19.633 | 39.361 | 21.759 | 1.00 | 36.89 |  |
| ATOM                        | 3777 | CB  | LEU F 211 | 27.926 | 37.493 | 22.186 | 1.00 | 31.43 |  |

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|-----------------------------|------|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM                        | 3904 | CE1 | PHE | G | 142 | 14.124 | 2.361  | 45.708 | 1.00 38.43 |
| ATOM                        | 3905 | CE2 | PHE | G | 142 | 12.930 | 4.834  | 46.591 | 1.00 39.22 |
| ATOM                        | 3906 | CZ  | PHE | G | 142 | 12.965 | 3.502  | 46.129 | 1.00 32.83 |
| ATOM                        | 3907 | N   | PRO | G | 143 | 18.816 | 6.215  | 46.393 | 1.00 55.13 |
| ATOM                        | 3908 | CA  | PRO | G | 143 | 20.998 | 7.031  | 46.101 | 1.00 55.45 |
| ATOM                        | 3909 | C   | PRO | G | 143 | 20.973 | 7.560  | 44.676 | 1.00 55.06 |
| ATOM                        | 3910 | O   | PRO | G | 143 | 20.354 | 6.975  | 43.801 | 1.00 57.96 |
| ATOM                        | 3911 | CB  | PRO | G | 143 | 22.153 | 8.047  | 46.291 | 1.00 63.73 |
| ATOM                        | 3912 | CG  | PRO | G | 143 | 21.561 | 4.727  | 45.934 | 1.00 65.09 |
| ATOM                        | 3913 | CD  | PRO | G | 143 | 20.137 | 5.075  | 46.415 | 1.00 57.96 |
| ATOM                        | 3914 | N   | ALA | G | 144 | 21.638 | 6.740  | 44.452 | 1.00 65.40 |
| ATOM                        | 3915 | CA  | ALA | G | 144 | 21.703 | 9.307  | 43.122 | 1.00 58.75 |
| ATOM                        | 3916 | C   | ALA | G | 144 | 22.544 | 8.441  | 42.192 | 1.00 61.40 |
| ATOM                        | 3917 | O   | ALA | G | 144 | 22.390 | 8.490  | 40.971 | 1.00 65.44 |
| ATOM                        | 3918 | CB  | ALA | G | 144 | 22.274 | 10.745 | 43.195 | 1.00 43.96 |
| ATOM                        | 3919 | N   | SER | G | 145 | 23.436 | 7.654  | 42.735 | 1.00 62.55 |
| ATOM                        | 3920 | CA  | SER | G | 145 | 24.267 | 6.732  | 42.041 | 1.00 67.22 |
| ATOM                        | 3921 | C   | SER | G | 145 | 23.438 | 5.731  | 41.262 | 1.00 69.80 |
| ATOM                        | 3922 | O   | SER | G | 145 | 23.821 | 5.281  | 40.181 | 1.00 72.67 |
| ATOM                        | 3923 | CB  | SER | G | 145 | 25.246 | 6.000  | 42.981 | 1.00 59.41 |
| ATOM                        | 3924 | OG  | SER | G | 145 | 24.545 | 5.159  | 43.880 | 1.00 65.99 |
| ATOM                        | 3925 | N   | LEU | G | 146 | 22.284 | 5.383  | 41.023 | 1.00 65.51 |
| ATOM                        | 3926 | CA  | LEU | G | 146 | 21.414 | 4.382  | 41.271 | 1.00 63.65 |
| ATOM                        | 3927 | C   | LEU | G | 146 | 20.726 | 4.925  | 39.974 | 1.00 62.68 |
| ATOM                        | 3928 | O   | LEU | G | 146 | 20.107 | 5.986  | 40.007 | 1.00 63.49 |
| ATOM                        | 3929 | CB  | LEU | G | 146 | 20.363 | 3.916  | 42.293 | 1.00 61.56 |
| ATOM                        | 3930 | CG  | LEU | G | 146 | 19.370 | 2.842  | 41.769 | 1.00 62.43 |
| ATOM                        | 3931 | CD  | LEU | G | 146 | 20.076 | 1.524  | 41.510 | 1.00 58.27 |
| ATOM                        | 3932 | CE  | LEU | G | 146 | 18.275 | 2.661  | 42.831 | 1.00 55.49 |
| ATOM                        | 3933 | N   | ARG | G | 147 | 20.843 | 4.184  | 38.651 | 1.00 58.80 |
| ATOM                        | 3934 | CA  | ARG | G | 147 | 20.205 | 4.553  | 37.620 | 1.00 58.45 |
| ATOM                        | 3935 | C   | ARG | G | 147 | 19.373 | 3.423  | 37.037 | 1.00 51.62 |
| ATOM                        | 3936 | O   | ARG | G | 147 | 19.866 | 2.601  | 36.265 | 1.00 70.78 |
| ATOM                        | 3937 | CB  | ARG | G | 147 | 21.246 | 5.021  | 36.601 | 1.00 57.96 |
| ATOM                        | 3938 | CG  | ARG | G | 147 | 21.386 | 6.270  | 37.031 | 1.00 70.12 |
| ATOM                        | 3939 | CD  | ARG | G | 147 | 21.007 | 7.433  | 37.058 | 1.00 67.94 |
| ATOM                        | 3940 | NE  | ARG | G | 147 | 21.612 | 8.689  | 37.486 | 1.00 63.64 |
| ATOM                        | 3941 | CZ  | ARG | G | 147 | 20.931 | 9.802  | 37.711 | 1.00 81.45 |
| ATOM                        | 3942 | NH1 | ARG | G | 147 | 19.604 | 9.810  | 37.549 | 1.00 84.36 |
| ATOM                        | 3943 | NH2 | ARG | G | 147 | 21.543 | 10.907 | 38.093 | 1.00 89.86 |
| ATOM                        | 3944 | N   | LEU | G | 148 | 18.103 | 3.398  | 37.415 | 1.00 55.60 |
| ATOM                        | 3945 | CA  | LEU | G | 148 | 17.159 | 2.436  | 36.869 | 1.00 66.78 |
| ATOM                        | 3946 | C   | LEU | G | 148 | 15.962 | 3.131  | 36.317 | 1.00 55.61 |
| ATOM                        | 3947 | O   | LEU | G | 148 | 15.600 | 4.250  | 35.829 | 1.00 55.96 |
| ATOM                        | 3948 | CB  | LEU | G | 148 | 16.718 | 1.428  | 37.932 | 1.00 54.95 |
| ATOM                        | 3949 | CG  | LEU | G | 148 | 17.772 | 0.423  | 38.400 | 1.00 59.40 |
| ATOM                        | 3950 | CD  | LEU | G | 148 | 17.275 | -0.445 | 39.522 | 1.00 61.38 |
| ATOM                        | 3951 | CE  | LEU | G | 148 | 18.251 | -0.134 | 39.239 | 1.00 58.10 |
| ATOM                        | 3952 | N   | SER | G | 149 | 15.353 | 2.649  | 35.270 | 1.00 52.17 |
| ATOM                        | 3953 | CA  | SER | G | 149 | 14.136 | 3.230  | 34.726 | 1.00 42.11 |
| ATOM                        | 3954 | C   | SER | G | 149 | 13.025 | 3.105  | 35.771 | 1.00 45.62 |
| ATOM                        | 3955 | O   | SER | G | 149 | 13.087 | 2.397  | 36.715 | 1.00 45.73 |
| ATOM                        | 3956 | CB  | SER | G | 149 | 13.707 | 2.496  | 33.453 | 1.00 39.29 |
| ATOM                        | 3957 | CG  | SER | G | 149 | 13.897 | 1.403  | 33.685 | 1.00 34.44 |
| ATOM                        | 3958 | N   | GLU | G | 150 | 12.026 | 4.040  | 35.600 | 1.00 42.88 |
| ATOM                        | 3959 | CA  | GLU | G | 150 | 10.592 | 4.085  | 36.511 | 1.00 51.78 |
| ATOM                        | 3960 | C   | GLU | G | 150 | 10.210 | 2.722  | 36.564 | 1.00 47.88 |
| ATOM                        | 3961 | O   | GLU | G | 150 | 9.872  | 2.213  | 37.640 | 1.00 39.15 |
| ATOM                        | 3962 | CB  | GLU | G | 150 | 9.903  | 5.470  | 36.071 | 1.00 46.85 |
| ATOM                        | 3963 | CG  | GLU | G | 150 | 8.661  | 5.289  | 36.937 | 1.00 47.66 |
| ATOM                        | 3964 | CD  | GLU | G | 150 | 7.610  | 6.191  | 36.318 | 1.00 52.63 |
| ATOM                        | 3965 | CE  | GLU | G | 150 | 6.730  | 6.679  | 37.057 | 1.00 55.65 |
| ATOM                        | 3966 | OE2 | GLU | G | 150 | 7.661  | 6.409  | 35.089 | 1.00 65.32 |

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|-----------------------------|------|-----|-----|---|-----|--------|---------|--------|------------|
| ATOM                        | 4030 | CB  | GLU | G | 158 | 6.074  | -4.338  | 42.730 | 1.00 30.27 |
| ATOM                        | 4031 | CG  | GLU | G | 158 | 4.711  | -5.035  | 42.889 | 1.00 30.28 |
| ATOM                        | 4032 | CD  | GLU | G | 158 | 3.754  | -4.687  | 41.784 | 1.00 32.11 |
| ATOM                        | 4033 | OE1 | GLU | G | 158 | 2.584  | -5.117  | 41.868 | 1.00 34.93 |
| ATOM                        | 4034 | OE2 | GLU | G | 158 | 4.155  | -3.990  | 40.829 | 1.00 33.61 |
| ATOM                        | 4035 | N   | ILE | G | 159 | 8.169  | -6.464  | 39.549 | 1.00 32.75 |
| ATOM                        | 4036 | CA  | ILE | G | 159 | 8.846  | -7.826  | 41.707 | 1.00 27.94 |
| ATOM                        | 4037 | C   | ILE | G | 159 | 9.270  | -6.007  | 45.158 | 1.00 32.33 |
| ATOM                        | 4038 | O   | ILE | G | 159 | 8.654  | -6.955  | 45.822 | 1.00 25.09 |
| ATOM                        | 4039 | CB  | ILE | G | 159 | 10.044 | -6.183  | 42.796 | 1.00 37.33 |
| ATOM                        | 4040 | CG  | ILE | G | 159 | 9.637  | -6.170  | 41.324 | 1.00 34.44 |
| ATOM                        | 4041 | CD  | ILE | G | 159 | 10.593 | -9.556  | 43.158 | 1.00 18.56 |
| ATOM                        | 4042 | CE  | ILE | G | 159 | 8.799  | -9.341  | 40.114 | 1.00 40.45 |
| ATOM                        | 4043 | N   | PHE | G | 160 | 10.096 | -7.084  | 45.646 | 1.00 26.87 |
| ATOM                        | 4044 | CA  | PHE | G | 160 | 10.629 | -7.183  | 46.996 | 1.00 29.75 |
| ATOM                        | 4045 | C   | PHE | G | 160 | 9.166  | -7.087  | 46.077 | 1.00 24.68 |
| ATOM                        | 4046 | O   | PHE | G | 160 | 9.449  | -7.967  | 48.927 | 1.00 40.06 |
| ATOM                        | 4047 | CB  | PHE | G | 160 | 11.670 | -6.986  | 47.248 | 1.00 24.76 |
| ATOM                        | 4048 | CG  | PHE | G | 160 | 12.445 | -6.271  | 48.513 | 1.00 28.44 |
| ATOM                        | 4049 | CD  | PHE | G | 160 | 12.061 | -5.610  | 49.677 | 1.00 27.98 |
| ATOM                        | 4050 | CE  | PHE | G | 160 | 13.103 | -7.163  | 48.541 | 1.00 20.14 |
| ATOM                        | 4051 | OE1 | PHE | G | 160 | 12.750 | -5.793  | 50.858 | 1.00 20.75 |
| ATOM                        | 4052 | OE2 | PHE | G | 160 | 14.205 | -7.142  | 49.759 | 1.00 23.49 |
| ATOM                        | 4053 | CZ  | PHE | G | 160 | 13.824 | -6.659  | 50.900 | 1.00 25.86 |
| ATOM                        | 4054 | N   | PHE | G | 161 | 8.786  | -6.011  | 48.042 | 1.00 28.20 |
| ATOM                        | 4055 | CA  | PHE | G | 161 | 7.616  | -5.765  | 49.100 | 1.00 31.19 |
| ATOM                        | 4056 | C   | PHE | G | 161 | 6.520  | -6.126  | 48.853 | 1.00 23.56 |
| ATOM                        | 4057 | O   | PHE | G | 161 | 5.578  | -6.429  | 49.636 | 1.00 30.72 |
| ATOM                        | 4058 | CB  | PHE | G | 161 | 7.512  | -4.264  | 49.243 | 1.00 28.16 |
| ATOM                        | 4059 | CG  | PHE | G | 161 | 8.729  | -3.494  | 49.775 | 1.00 27.17 |
| ATOM                        | 4060 | CD  | PHE | G | 161 | 9.074  | -3.571  | 51.115 | 1.00 26.19 |
| ATOM                        | 4061 | CE  | PHE | G | 161 | 8.496  | -2.703  | 48.635 | 1.00 26.55 |
| ATOM                        | 4062 | CE1 | PHE | G | 161 | 10.159 | -2.869  | 51.609 | 1.00 30.73 |
| ATOM                        | 4063 | CE2 | PHE | G | 161 | 10.583 | -1.997  | 49.423 | 1.00 25.00 |
| ATOM                        | 4064 | CZ  | PHE | G | 161 | 10.214 | -2.982  | 50.768 | 1.00 25.73 |
| ATOM                        | 4065 | N   | GLY | G | 162 | 6.479  | -7.282  | 47.760 | 1.00 35.44 |
| ATOM                        | 4066 | CA  | GLY | G | 162 | 5.354  | -8.156  | 47.479 | 1.00 28.19 |
| ATOM                        | 4067 | C   | GLY | G | 162 | 5.517  | -9.520  | 48.124 | 1.00 29.94 |
| ATOM                        | 4068 | O   | GLY | G | 162 | 4.354  | -10.279 | 48.257 | 1.00 28.13 |
| ATOM                        | 4069 | N   | LYS | G | 163 | 6.742  | -9.925  | 45.540 | 1.00 35.39 |
| ATOM                        | 4070 | CA  | LYS | G | 163 | 7.061  | -11.127 | 48.139 | 1.00 36.36 |
| ATOM                        | 4071 | C   | LYS | G | 163 | 6.742  | -11.208 | 50.605 | 1.00 40.93 |
| ATOM                        | 4072 | O   | LYS | G | 163 | 7.067  | -10.302 | 51.376 | 1.00 37.58 |
| ATOM                        | 4073 | CB  | LYS | G | 163 | 8.538  | -11.474 | 48.907 | 1.00 31.94 |
| ATOM                        | 4074 | CG  | LYS | G | 163 | 8.948  | -11.727 | 47.466 | 1.00 40.02 |
| ATOM                        | 4075 | CD  | LYS | G | 163 | 10.455 | -11.929 | 47.371 | 1.00 26.17 |
| ATOM                        | 4076 | CE  | LYS | G | 163 | 10.922 | -12.032 | 45.931 | 1.00 31.24 |
| ATOM                        | 4077 | NZ  | LYS | G | 163 | 10.154 | -13.052 | 45.165 | 1.00 31.20 |
| ATOM                        | 4078 | N   | THR | G | 164 | 6.100  | -12.307 | 50.994 | 1.00 35.75 |
| ATOM                        | 4079 | CA  | THR | G | 164 | 5.761  | -12.559 | 52.388 | 1.00 32.42 |
| ATOM                        | 4080 | C   | THR | G | 164 | 7.042  | -12.791 | 51.193 | 1.00 34.47 |
| ATOM                        | 4081 | O   | THR | G | 164 | 7.103  | -12.495 | 54.387 | 1.00 31.09 |
| ATOM                        | 4082 | CB  | THR | G | 164 | 4.815  | -13.776 | 52.522 | 1.00 30.48 |
| ATOM                        | 4083 | CG  | THR | G | 164 | 4.460  | -14.048 | 53.980 | 1.00 29.02 |
| ATOM                        | 4084 | OG1 | THR | G | 164 | 7.612  | -15.135 | 51.781 | 1.00 40.36 |
| ATOM                        | 4085 | N   | ARG | G | 165 | 8.077  | -13.289 | 52.521 | 1.00 26.69 |
| ATOM                        | 4086 | CA  | ARG | G | 165 | 9.361  | -13.537 | 51.171 | 1.00 31.54 |
| ATOM                        | 4087 | C   | ARG | G | 165 | 10.043 | -12.244 | 53.606 | 1.00 29.55 |
| ATOM                        | 4088 | O   | ARG | G | 165 | 10.904 | -12.546 | 54.485 | 1.00 29.31 |
| ATOM                        | 4089 | N   | ARG | G | 165 | 10.296 | -14.309 | 52.138 | 1.00 32.42 |
| ATOM                        | 4090 | CG  | ARG | G | 165 | 10.011 | -15.796 | 52.132 | 0.00 33.36 |
| ATOM                        | 4091 | CD  | ARG | G | 165 | 11.009 | -16.466 | 51.201 | 0.00 34.90 |
| ATOM                        | 4092 | NE  | ARG | G | 165 | 11.028 | -17.927 | 51.354 | 0.00 38.19 |

| octamer-PDB-coordinates.txt |      |    |     |   |     |        |       |        |            |
|-----------------------------|------|----|-----|---|-----|--------|-------|--------|------------|
| ATOM                        | 3967 | N  | GLU | G | 151 | 10.045 | 2.116 | 35.393 | 1.00 53.94 |
| ATOM                        | 3968 | CA | GLU | G | 151 | 9.341  | 0.847 | 35.277 | 1          |

| octamer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |      | octamer-PDB-coordinates.txt |   |      |      |     |     |   |     |        |        |        |      |       |     |
|-----------------------------|------|-----|-----|---|-----|--------|--------|--------|------|-----------------------------|---|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|-----|
| ATOM                        | 4156 | NH2 | ARG | G | 174 | 5.621  | -1.488 | 37.021 | 1.00 | 50.50                       | N | ATOM | 4219 | CG  | LEU | G | 183 | 17.369 | 25.370 | 43.985 | 1.00 | 31.28 | C   |
| ATOM                        | 4157 | N   | GLU | G | 175 | 3.603  | 4.039  | 42.688 | 1.00 | 41.56                       | N | ATOM | 4220 | CD1 | LEU | G | 183 | 18.360 | 26.409 | 44.000 | 1.00 | 19.45 | C   |
| ATOM                        | 4158 | CA  | GLU | G | 175 | 3.570  | 5.333  | 42.067 | 1.00 | 43.09                       | C | ATOM | 4221 | CD2 | LEU | G | 183 | 17.804 | 24.962 | 42.562 | 1.00 | 22.77 | C   |
| ATOM                        | 4159 | C   | GLU | G | 175 | 5.224  | 5.923  | 42.476 | 1.00 | 41.92                       | C | ATOM | 4222 | N   | GLY | G | 184 | 21.901 | 25.695 | 45.036 | 1.00 | 38.93 | N   |
| ATOM                        | 4160 | OE1 | GLU | G | 175 | 5.139  | 6.000  | 42.704 | 1.00 | 42.93                       | O | ATOM | 4223 | CA  | GLY | G | 184 | 23.050 | 26.247 | 45.649 | 1.00 | 39.15 | C   |
| ATOM                        | 4161 | CB  | GLU | G | 175 | 9.751  | 6.319  | 42.410 | 1.00 | 42.08                       | C | ATOM | 4224 | C   | GLY | G | 184 | 24.755 | 27.352 | 47.687 | 1.00 | 42.14 | C   |
| ATOM                        | 4162 | CG  | GLU | G | 175 | 2.884  | 7.673  | 41.733 | 1.00 | 50.23                       | C | ATOM | 4225 | O   | GLY | G | 184 | 23.201 | 27.948 | 48.973 | 1.00 | 46.46 | O   |
| ATOM                        | 4163 | CD  | GLU | G | 175 | 1.779  | 8.632  | 42.131 | 1.00 | 61.70                       | C | ATOM | 4226 | N   | PHE | G | 185 | 23.468 | 28.586 | 46.111 | 1.00 | 46.54 | N   |
| ATOM                        | 4164 | OE2 | GLU | G | 175 | 0.921  | 8.246  | 42.952 | 1.00 | 53.86                       | O | ATOM | 4227 | CA  | PHE | G | 185 | 22.607 | 29.993 | 45.791 | 1.00 | 45.40 | C   |
| ATOM                        | 4165 | OE1 | GLU | G | 175 | 1.767  | 9.772  | 41.432 | 1.00 | 38.14                       | O | ATOM | 4228 | C   | PHE | G | 185 | 23.044 | 30.489 | 45.926 | 1.00 | 50.73 | C   |
| ATOM                        | 4166 | N   | LEU | G | 176 | 6.025  | 6.990  | 41.945 | 1.00 | 46.49                       | N | ATOM | 4229 | O   | PHE | G | 185 | 24.258 | 31.947 | 47.911 | 1.00 | 53.85 | O   |
| ATOM                        | 4167 | CA  | LEU | G | 176 | 7.267  | 7.020  | 41.754 | 1.00 | 48.74                       | C | ATOM | 4230 | CB  | PHE | G | 185 | 22.653 | 30.804 | 46.655 | 1.00 | 40.64 | C   |
| ATOM                        | 4168 | C   | LEU | G | 176 | 6.994  | 8.514  | 41.885 | 1.00 | 53.18                       | C | ATOM | 4231 | CG  | PHE | G | 185 | 21.217 | 30.409 | 46.483 | 1.00 | 48.23 | C   |
| ATOM                        | 4169 | O   | LEU | G | 176 | 6.700  | 9.201  | 40.906 | 1.00 | 47.41                       | O | ATOM | 4232 | CD1 | PHE | G | 185 | 20.446 | 30.966 | 45.476 | 1.00 | 42.61 | C   |
| ATOM                        | 4170 | CB  | LEU | G | 176 | 6.291  | 12.103 | 40.453 | 1.00 | 44.16                       | C | ATOM | 4233 | CD2 | PHE | G | 185 | 20.648 | 29.447 | 47.303 | 1.00 | 42.47 | C   |
| ATOM                        | 4171 | CG  | LEU | G | 176 | 9.579  | 7.598  | 40.685 | 1.00 | 34.52                       | C | ATOM | 4234 | CE1 | PHE | G | 185 | 19.128 | 30.588 | 45.305 | 1.00 | 37.66 | C   |
| ATOM                        | 4172 | CD1 | LEU | G | 176 | 10.316 | 7.401  | 42.000 | 1.00 | 38.62                       | C | ATOM | 4235 | CE2 | PHE | G | 185 | 19.332 | 29.065 | 47.137 | 1.00 | 36.19 | C   |
| ATOM                        | 4173 | CD2 | LEU | G | 176 | 10.461 | 7.263  | 39.507 | 1.00 | 44.45                       | C | ATOM | 4236 | CZ  | PHE | G | 185 | 18.573 | 29.633 | 46.139 | 1.00 | 32.29 | C   |
| ATOM                        | 4174 | N   | LEU | G | 177 | 7.090  | 8.999  | 43.116 | 1.00 | 52.02                       | N | ATOM | 4237 | N   | ALA | G | 186 | 25.362 | 31.521 | 45.160 | 1.00 | 51.13 | N   |
| ATOM                        | 4175 | CA  | LEU | G | 177 | 6.848  | 10.131 | 42.864 | 1.00 | 44.79                       | C | ATOM | 4238 | CA  | ALA | G | 186 | 26.740 | 32.054 | 45.119 | 1.00 | 58.01 | C   |
| ATOM                        | 4176 | C   | LEU | G | 177 | 7.942  | 11.325 | 43.013 | 1.00 | 44.20                       | C | ATOM | 4239 | C   | ALA | G | 186 | 27.047 | 32.393 | 46.332 | 1.00 | 55.12 | C   |
| ATOM                        | 4177 | O   | LEU | G | 177 | 9.144  | 10.936 | 42.992 | 1.00 | 44.43                       | O | ATOM | 4240 | O   | ALA | G | 186 | 28.143 | 32.857 | 46.896 | 1.00 | 60.56 | O   |
| ATOM                        | 4178 | CB  | LEU | G | 177 | 6.625  | 10.536 | 44.951 | 1.00 | 45.71                       | C | ATOM | 4241 | CB  | ALA | G | 186 | 26.953 | 32.839 | 47.831 | 1.00 | 50.36 | C   |
| ATOM                        | 4179 | CG  | LEU | G | 177 | 5.130  | 9.594  | 44.469 | 1.00 | 43.69                       | C | ATOM | 4242 | N   | ARG | G | 187 | 26.094 | 33.766 | 48.695 | 1.00 | 52.40 | N   |
| ATOM                        | 4180 | CD1 | LEU | G | 177 | 4.196  | 10.111 | 44.864 | 1.00 | 44.79                       | C | ATOM | 4243 | N   | ASP | G | 187 | 26.292 | 34.779 | 47.751 | 1.00 | 49.22 | C   |
| ATOM                        | 4181 | CD2 | LEU | G | 177 | 4.118  | 10.429 | 44.732 | 1.00 | 43.36                       | C | ATOM | 4244 | C   | ARG | G | 187 | 25.889 | 34.267 | 49.100 | 1.00 | 55.16 | C   |
| ATOM                        | 4182 | N   | PRO | G | 178 | 7.641  | 12.572 | 42.645 | 1.00 | 45.21                       | N | ATOM | 4245 | D   | ARG | G | 187 | 24.875 | 33.608 | 49.269 | 1.00 | 51.56 | O   |
| ATOM                        | 4183 | CA  | PRO | G | 178 | 8.626  | 13.550 | 42.166 | 1.00 | 38.44                       | C | ATOM | 4246 | CB  | ARG | G | 187 | 25.497 | 36.027 | 47.332 | 1.00 | 53.79 | C   |
| ATOM                        | 4184 | C   | PRO | G | 178 | 5.722  | 13.703 | 43.204 | 1.00 | 37.89                       | C | ATOM | 4247 | CB  | ARG | G | 187 | 25.599 | 37.235 | 48.260 | 1.00 | 62.51 | C   |
| ATOM                        | 4185 | O   | PRO | G | 178 | 9.440  | 13.416 | 44.403 | 1.00 | 44.79                       | O | ATOM | 4248 | CD  | ARG | G | 187 | 24.766 | 38.352 | 49.100 | 1.00 | 55.94 | C   |
| ATOM                        | 4186 | CB  | PRO | G | 178 | 7.788  | 14.614 | 41.938 | 1.00 | 46.42                       | C | ATOM | 4249 | NE  | ARG | G | 187 | 24.629 | 39.472 | 48.609 | 1.00 | 51.23 | N   |
| ATOM                        | 4187 | CG  | PRO | G | 178 | 6.548  | 14.608 | 42.744 | 1.00 | 50.55                       | C | ATOM | 4250 | CZ  | ARG | G | 187 | 23.906 | 40.560 | 48.364 | 1.00 | 99.16 | C   |
| ATOM                        | 4188 | CD  | PRO | G | 178 | 6.283  | 13.142 | 42.667 | 1.00 | 57.45                       | C | ATOM | 4251 | NH1 | ARG | G | 187 | 23.200 | 40.679 | 47.218 | 1.00 | 99.36 | N1+ |
| ATOM                        | 4189 | N   | GLY | G | 179 | 10.553 | 13.978 | 42.744 | 1.00 | 34.25                       | N | ATOM | 4252 | NH2 | ARG | G | 187 | 23.841 | 41.531 | 49.265 | 1.00 | 91.05 | N   |
| ATOM                        | 4190 | CA  | GLY | G | 179 | 12.085 | 14.102 | 43.453 | 1.00 | 42.82                       | C | ATOM | 4253 | N   | ASP | G | 188 | 25.694 | 42.535 | 50.111 | 1.00 | 58.13 | C   |
| ATOM                        | 4191 | C   | GLY | G | 179 | 12.335 | 15.527 | 44.093 | 1.00 | 52.73                       | C | ATOM | 4254 | CA  | ASP | G | 188 | 26.413 | 44.271 | 51.498 | 1.00 | 51.04 | C   |
| ATOM                        | 4192 | O   | GLY | G | 179 | 12.037 | 16.476 | 43.367 | 1.00 | 46.57                       | O | ATOM | 4255 | C   | ASP | G | 188 | 25.757 | 44.980 | 52.035 | 1.00 | 43.22 | C   |
| ATOM                        | 4193 | N   | SER | G | 180 | 12.865 | 15.681 | 45.303 | 1.00 | 51.32                       | N | ATOM | 4256 | O   | ASP | G | 188 | 24.965 | 36.167 | 51.741 | 1.00 | 41.79 | O   |
| ATOM                        | 4194 | CA  | SER | G | 180 | 13.159 | 17.005 | 45.835 | 1.00 | 48.26                       | C | ATOM | 4257 | CB  | ASP | G | 188 | 27.616 | 34.581 | 52.392 | 1.00 | 49.34 | C   |
| ATOM                        | 4195 | C   | SER | G | 180 | 14.239 | 17.463 | 44.998 | 1.00 | 50.44                       | C | ATOM | 4258 | CG  | ASP | G | 188 | 28.779 | 33.649 | 53.111 | 1.00 | 55.94 | C   |
| ATOM                        | 4196 | O   | SER | G | 180 | 15.003 | 16.985 | 44.298 | 1.00 | 44.56                       | O | ATOM | 4259 | CD1 | ASP | G | 188 | 28.537 | 32.431 | 51.983 | 1.00 | 70.11 | O   |
| ATOM                        | 4197 | CB  | SER | G | 180 | 13.588 | 16.925 | 47.302 | 1.00 | 41.97                       | C | ATOM | 4260 | CD2 | ASP | G | 188 | 29.938 | 34.104 | 52.203 | 1.00 | 71.62 | O1+ |
| ATOM                        | 4198 | CG  | SER | G | 180 | 12.491 | 16.604 | 48.139 | 1.00 | 54.39                       | C | ATOM | 4261 | N   | GLY | G | 189 | 24.351 | 34.246 | 52.776 | 1.00 | 39.76 | C   |
| ATOM                        | 4199 | N   | VAL | G | 181 | 14.233 | 18.985 | 45.074 | 1.00 | 38.35                       | N | ATOM | 4262 | CA  | GLY | G | 189 | 23.195 | 34.850 | 53.432 | 1.00 | 42.86 | C   |
| ATOM                        | 4200 | CA  | VAL | G | 181 | 15.349 | 19.219 | 44.335 | 1.00 | 49.75                       | C | ATOM | 4263 | CB  | GLY | G | 189 | 24.606 | 32.652 | 53.147 | 1.00 | 40.62 | C   |
| ATOM                        | 4201 | C   | VAL | G | 181 | 16.306 | 20.434 | 45.277 | 1.00 | 39.91                       | C | ATOM | 4264 | O   | GLY | G | 189 | 20.814 | 34.728 | 53.281 | 1.00 | 41.41 | O   |
| ATOM                        | 4202 | O   | VAL | G | 181 | 15.865 | 21.073 | 46.241 | 1.00 | 49.71                       | O | ATOM | 4265 | N   | VAL | G | 190 | 22.002 | 34.285 | 51.398 | 1.00 | 37.06 | N   |
| ATOM                        | 4203 | CB  | VAL | G | 181 | 14.711 | 20.736 | 43.367 | 1.00 | 49.37                       | C | ATOM | 4266 | CA  | VAL | G | 190 | 20.827 | 34.052 | 50.565 | 1.00 | 99.36 | C   |
| ATOM                        | 4204 | CD1 | VAL | G | 181 | 12.787 | 21.708 | 42.832 | 1.00 | 32.62                       | C | ATOM | 4267 | C   | VAL | G | 190 | 20.081 | 32.805 | 51.016 | 1.00 | 42.46 | C   |
| ATOM                        | 4205 | CG2 | VAL | G | 181 | 14.016 | 20.098 | 42.827 | 1.00 | 38.31                       | C | ATOM | 4268 | CB  | VAL | G | 190 | 18.689 | 32.843 | 51.238 | 1.00 | 42.24 | C   |
| ATOM                        | 4206 | N   | MET | G | 182 | 17.598 | 20.314 | 44.994 | 1.00 | 42.62                       | N | ATOM | 4269 | CB  | VAL | G | 190 | 21.200 | 33.901 | 49.060 | 1.00 | 38.33 | C   |
| ATOM                        | 4207 | CA  | MET | G | 182 | 18.609 | 21.017 | 45.763 | 1.00 | 47.63                       | C | ATOM | 4270 | CG1 | VAL | G | 190 | 19.960 | 33.599 | 48.251 | 1.00 | 99.36 | C   |
| ATOM                        | 4208 | C   | MET | G | 182 | 19.113 | 22.214 | 44.954 | 1.00 | 46.25                       | C | ATOM | 4271 | CG2 | VAL | G | 190 | 21.893 | 35.155 | 48.577 | 1.00 | 29.02 | C   |
| ATOM                        | 4209 | O   | MET | G | 182 | 19.388 | 22.103 | 43.757 | 1.00 | 46.49                       | O | ATOM | 4272 | N   | GLN | G | 191 | 20.615 | 31.700 | 53.852 | 1.00 | 35.64 | N   |
| ATOM                        | 4210 | CB  | MET | G | 182 | 19.745 | 20.056 | 46.135 | 1.00 | 49.26                       | C | ATOM | 4273 | CA  | ALA | G | 191 | 20.245 | 30.450 | 51.622 | 1.00 | 45.24 | C   |
| ATOM                        | 4211 | CG  | MET | G | 182 | 21.133 | 20.507 | 45.744 | 1.00 | 50.37                       | C | ATOM | 4274 | C   | ALA | G | 191 | 19.539 | 30.676 | 51.954 | 1.00 | 45.25 | C   |
| ATOM                        | 4212 | SD  | MET | G | 182 | 21.788 | 21.779 | 46.830 | 1.00 | 53.24                       | S | ATOM | 4275 | O   | ALA | G | 191 | 10.417 | 30.721 | 53.151 | 1.00 | 36.91 | O   |
| ATOM                        | 4213 | CE  | MET | G | 182 | 23.126 | 22.366 | 45.809 | 1.00 | 51.33                       | C | ATOM | 4276 | CB  | ALA | G | 191 | 21.326 | 29.383 | 51.757 | 1.00 | 43.21 | C   |
| ATOM                        | 4214 | N   | MET | G | 182 | 19.206 | 22.103 | 45.615 | 1.00 | 41.74                       | N | ATOM | 4277 | N   | GLN | G | 191 | 20.194 | 31.403 | 53.852 | 1.00 | 43.17 | N   |
| ATOM                        | 4215 | CA  | LEU | G | 183 | 19.701 | 24.584 | 44.983 | 1.00 | 36.30                       | C | ATOM | 4278 | CA  | GLN | G | 192 | 19.621 | 31.715 | 55.155 | 1.00 | 44.44 | C   |
| ATOM                        | 4216 | C   | LEU | G | 183 | 20.869 | 25.184 | 45.759 | 1.00 | 36.57                       | C | ATOM | 4279 | C   | GLN | G | 192 | 18.343 | 32.539 | 55.044 | 1.00 | 40.26 | C   |
| ATOM                        | 4217 | O   | LEU |   |     |        |        |        |      |                             |   |      |      |     |     |   |     |        |        |        |      |       |     |

| octamer-PDB-coordinates.txt |      |     |     |     |       |        |        |            |            |
|-----------------------------|------|-----|-----|-----|-------|--------|--------|------------|------------|
| ATOM                        | 4408 | CA  | VAL | G   | 209   | 2.567  | 24.840 | 43.824     | 1.00 43.00 |
| ATOM                        | 4409 | C   | VAL | G   | 209   | 3.233  | 25.458 | 45.047     | 1.00 42.15 |
| ATOM                        | 4410 | VAL | G   | 209 | 4.201 | 26.203 | 44.321 | 1.00 42.49 |            |
| ATOM                        | 4411 | CB  | VAL | G   | 209   | 3.593  | 23.950 | 43.101     | 1.00 34.88 |
| ATOM                        | 4412 | CG1 | VAL | G   | 209   | 4.214  | 32.967 | 44.075     | 1.00 40.71 |
| ATOM                        | 4413 | CG2 | VAL | G   | 209   | 2.939  | 23.226 | 41.935     | 1.00 41.83 |
| ATOM                        | 4414 | N   | PRO | G   | 210   | 2.717  | 21.137 | 46.243     | 1.00 50.02 |
| ATOM                        | 4415 | C   | PRO | G   | 210   | 3.137  | 21.582 | 47.496     | 1.00 44.56 |
| ATOM                        | 4416 | C   | PRO | G   | 210   | 4.560  | 24.749 | 47.489     | 1.00 35.98 |
| ATOM                        | 4417 | O   | PRO | G   | 210   | 4.454  | 23.541 | 48.063     | 1.00 47.61 |
| ATOM                        | 4418 | CB  | PRO | G   | 210   | 2.217  | 23.386 | 48.525     | 1.00 41.13 |
| ATOM                        | 4419 | CG  | PRO | G   | 210   | 1.375  | 24.297 | 47.964     | 1.00 40.85 |
| ATOM                        | 4420 | CD  | PRO | G   | 210   | 1.443  | 24.432 | 46.489     | 1.00 39.10 |
| ATOM                        | 4421 | N   | LEU | G   | 211   | 5.719  | 25.393 | 47.902     | 1.00 34.32 |
| ATOM                        | 4422 | CA  | LEU | G   | 211   | 6.955  | 24.694 | 49.215     | 1.00 31.12 |
| ATOM                        | 4423 | C   | LEU | G   | 211   | 7.573  | 25.200 | 49.510     | 1.00 37.40 |
| ATOM                        | 4424 | O   | LEU | G   | 211   | 7.319  | 26.330 | 49.940     | 1.00 45.05 |
| ATOM                        | 4425 | CB  | LEU | G   | 211   | 7.961  | 24.847 | 47.071     | 1.00 33.62 |
| ATOM                        | 4426 | CG  | LEU | G   | 211   | 7.571  | 24.904 | 45.697     | 1.00 34.23 |
| ATOM                        | 4427 | CD1 | LEU | G   | 211   | 8.567  | 24.766 | 46.645     | 1.00 27.20 |
| ATOM                        | 4428 | CD2 | LEU | G   | 211   | 7.493  | 22.787 | 45.730     | 1.00 31.08 |
| ATOM                        | 4429 | N   | ARG | G   | 212   | 8.402  | 24.354 | 50.115     | 1.00 35.78 |
| ATOM                        | 4430 | CA  | ARG | G   | 212   | 9.108  | 24.696 | 51.342     | 1.00 44.36 |
| ATOM                        | 4431 | C   | ARG | G   | 212   | 10.411 | 24.628 | 51.085     | 1.00 44.16 |
| ATOM                        | 4432 | O   | ARG | G   | 212   | 11.073 | 23.837 | 50.264     | 1.00 37.84 |
| ATOM                        | 4433 | CB  | ARG | G   | 212   | 8.719  | 23.760 | 52.495     | 1.00 51.95 |
| ATOM                        | 4434 | CG  | ARG | G   | 212   | 7.381  | 24.094 | 53.150     | 1.00 48.75 |
| ATOM                        | 4435 | CD  | ARG | G   | 212   | 7.469  | 25.297 | 54.084     | 1.00 44.14 |
| ATOM                        | 4436 | NE  | ARG | G   | 212   | 8.400  | 25.993 | 55.048     | 1.00 41.39 |
| ATOM                        | 4437 | CZ  | ARG | G   | 212   | 8.287  | 25.902 | 56.323     | 1.00 53.57 |
| ATOM                        | 4438 | NH1 | ARG | G   | 212   | 7.482  | 26.955 | 56.337     | 1.00 57.01 |
| ATOM                        | 4439 | NH2 | ARG | G   | 212   | 9.071  | 25.660 | 57.365     | 1.00 53.02 |
| ATOM                        | 4440 | CA  | VAL | G   | 213   | 11.363 | 25.478 | 51.776     | 1.00 37.80 |
| ATOM                        | 4441 | C   | VAL | G   | 213   | 12.913 | 25.532 | 51.627     | 1.00 43.28 |
| ATOM                        | 4442 | O   | VAL | G   | 213   | 13.889 | 25.373 | 52.981     | 1.00 44.40 |
| ATOM                        | 4443 | D   | VAL | G   | 213   | 13.221 | 26.141 | 53.908     | 1.00 47.72 |
| ATOM                        | 4444 | CB  | VAL | G   | 213   | 13.262 | 26.857 | 50.976     | 1.00 41.34 |
| ATOM                        | 4445 | CG1 | VAL | G   | 213   | 14.775 | 26.973 | 50.961     | 1.00 41.89 |
| ATOM                        | 4446 | CG2 | VAL | G   | 213   | 15.129 | 26.941 | 49.545     | 1.00 45.16 |
| ATOM                        | 4447 | N   | SER | G   | 214   | 14.361 | 24.381 | 53.092     | 1.00 48.42 |
| ATOM                        | 4448 | CA  | SER | G   | 214   | 15.038 | 24.108 | 54.347     | 1.00 43.36 |
| ATOM                        | 4449 | C   | SER | G   | 214   | 16.520 | 23.923 | 54.092     | 1.00 47.86 |
| ATOM                        | 4450 | O   | SER | G   | 214   | 16.917 | 23.638 | 52.963     | 1.00 49.32 |
| ATOM                        | 4451 | CB  | SER | G   | 214   | 16.441 | 22.870 | 55.035     | 1.00 43.13 |
| ATOM                        | 4452 | CG  | SER | G   | 214   | 14.341 | 21.826 | 54.057     | 1.00 51.67 |
| ATOM                        | 4453 | N   | PRO | G   | 215   | 17.345 | 24.099 | 55.134     | 1.00 47.04 |
| ATOM                        | 4454 | CA  | PRO | G   | 215   | 18.787 | 23.330 | 54.945     | 1.00 38.22 |
| ATOM                        | 4455 | C   | PRO | G   | 215   | 19.138 | 22.137 | 54.494     | 1.00 42.97 |
| ATOM                        | 4456 | O   | PRO | G   | 215   | 18.455 | 21.560 | 54.859     | 1.00 48.46 |
| ATOM                        | 4457 | CB  | PRO | G   | 215   | 19.356 | 24.229 | 56.333     | 1.00 33.35 |
| ATOM                        | 4458 | CG  | PRO | G   | 215   | 18.334 | 25.135 | 56.973     | 1.00 45.41 |
| ATOM                        | 4459 | CD  | PRO | G   | 215   | 17.020 | 24.601 | 56.481     | 1.00 45.79 |
| ATOM                        | 4460 | N   | TYR | G   | 216   | 20.210 | 22.998 | 53.717     | 1.00 39.94 |
| ATOM                        | 4461 | CA  | TYR | G   | 216   | 20.610 | 21.137 | 53.148     | 1.00 47.62 |
| ATOM                        | 4462 | C   | TYR | G   | 216   | 21.695 | 20.434 | 53.978     | 1.00 39.45 |
| ATOM                        | 4463 | O   | TYR | G   | 216   | 22.188 | 20.990 | 54.960     | 1.00 41.37 |
| ATOM                        | 4464 | CB  | TYR | G   | 216   | 21.094 | 21.138 | 51.712     | 1.00 40.09 |
| ATOM                        | 4465 | CG1 | TYR | G   | 216   | 22.193 | 20.039 | 50.964     | 1.00 50.80 |
| ATOM                        | 4466 | CG2 | TYR | G   | 216   | 20.348 | 19.200 | 50.552     | 1.00 52.38 |
| ATOM                        | 4467 | CD1 | TYR | G   | 216   | 22.684 | 19.669 | 50.655     | 1.00 58.71 |
| ATOM                        | 4468 | CD2 | TYR | G   | 216   | 20.603 | 18.041 | 49.360     | 1.00 59.63 |
| ATOM                        | 4469 | CE1 | TYR | G   | 216   | 22.949 | 18.504 | 49.963     | 1.00 68.78 |
| ATOM                        | 4470 | CE2 | TYR | G   | 216   | 21.905 | 17.693 | 49.568     | 1.00 64.49 |

| octamer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |            |
|-----------------------------|------|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM                        | 4534 | CA  | GLY | H | 141 | 6.566  | 20.026 | 48.326 | 1.00 39.06 |
| ATOM                        | 4535 | C   | GLY | H | 141 | 6.004  | 19.728 | 46.945 | 1.00 40.92 |
| ATOM                        | 4536 | O   | GLY | H | 141 | 6.343  | 20.056 | 46.477 | 1.00 44.35 |
| ATOM                        | 4537 | N   | PHE | H | 142 | 6.827  | 19.275 | 46.062 | 1.00 42.82 |
| ATOM                        | 4538 | CA  | PHE | H | 142 | 6.364  | 18.926 | 44.708 | 1.00 40.93 |
| ATOM                        | 4539 | C   | PHE | H | 142 | 5.292  | 17.864 | 44.763 | 1.00 54.85 |
| ATOM                        | 4540 | O   | PHE | H | 142 | 5.501  | 16.780 | 45.308 | 1.00 53.69 |
| ATOM                        | 4541 | CB  | PHE | H | 142 | 7.532  | 18.464 | 43.835 | 1.00 37.93 |
| ATOM                        | 4542 | CG  | PHE | H | 142 | 8.839  | 19.434 | 43.793 | 1.00 34.92 |
| ATOM                        | 4543 | CD1 | PHE | H | 142 | 8.675  | 20.522 | 42.934 | 1.00 40.39 |
| ATOM                        | 4544 | CD2 | PHE | H | 142 | 9.805  | 19.256 | 44.607 | 1.00 37.73 |
| ATOM                        | 4545 | CE1 | PHE | H | 142 | 9.724  | 21.417 | 42.893 | 1.00 30.37 |
| ATOM                        | 4546 | CE2 | PHE | H | 142 | 10.862 | 20.146 | 44.563 | 1.00 40.17 |
| ATOM                        | 4547 | N   | PRO | H | 143 | 10.823 | 21.728 | 43.711 | 1.00 33.48 |
| ATOM                        | 4548 | C   | PRO | H | 143 | 4.119  | 18.180 | 44.197 | 1.00 52.91 |
| ATOM                        | 4549 | CA  | PRO | H | 143 | 2.971  | 17.271 | 43.169 | 1.00 50.08 |
| ATOM                        | 4550 | C   | PRO | H | 143 | 3.154  | 16.150 | 43.156 | 1.00 65.12 |
| ATOM                        | 4551 | O   | PRO | H | 143 | 3.591  | 16.327 | 43.166 | 1.00 66.45 |
| ATOM                        | 4552 | CB  | PRO | H | 143 | 4.816  | 18.187 | 43.763 | 1.00 54.40 |
| ATOM                        | 4553 | CG  | PRO | H | 143 | 2.464  | 19.223 | 42.916 | 1.00 40.85 |
| ATOM                        | 4554 | CD  | PRO | H | 143 | 3.824  | 19.456 | 43.522 | 1.00 48.90 |
| ATOM                        | 4555 | N   | ALA | H | 144 | 2.463  | 15.024 | 42.379 | 1.00 68.26 |
| ATOM                        | 4556 | CA  | ALA | H | 144 | 2.584  | 13.900 | 42.456 | 1.00 63.65 |
| ATOM                        | 4557 | C   | ALA | H | 144 | 1.900  | 14.272 | 41.138 | 1.00 66.47 |
| ATOM                        | 4558 | O   | ALA | H | 144 | 2.217  | 15.712 | 40.069 | 1.00 70.51 |
| ATOM                        | 4559 | CB  | ALA | H | 144 | 1.907  | 12.671 | 43.056 | 1.00 59.27 |
| ATOM                        | 4560 | N   | SER | H | 145 | 0.974  | 15.221 | 41.211 | 1.00 64.10 |
| ATOM                        | 4561 | CA  | SER | H | 145 | 0.278  | 15.780 | 40.037 | 1.00 58.45 |
| ATOM                        | 4562 | C   | SER | H | 145 | 1.234  | 16.365 | 39.030 | 1.00 63.60 |
| ATOM                        | 4563 | O   | SER | H | 145 | 1.013  | 16.290 | 37.822 | 1.00 69.27 |
| ATOM                        | 4564 | CB  | SER | H | 145 | -0.785 | 16.748 | 40.453 | 1.00 61.41 |
| ATOM                        | 4565 | CG  | SER | H | 145 | -1.348 | 16.987 | 39.321 | 1.00 73.01 |
| ATOM                        | 4566 | N   | LEU | H | 146 | 2.298  | 16.387 | 39.512 | 1.00 66.26 |
| ATOM                        | 4567 | C   | LEU | H | 146 | 3.211  | 17.724 | 38.674 | 1.00 72.38 |
| ATOM                        | 4568 | O   | LEU | H | 146 | 4.098  | 16.911 | 37.830 | 1.00 62.69 |
| ATOM                        | 4569 | CB  | LEU | H | 146 | 4.761  | 15.912 | 38.349 | 1.00 62.33 |
| ATOM                        | 4570 | CG  | LEU | H | 146 | 4.108  | 18.639 | 39.520 | 1.00 76.65 |
| ATOM                        | 4571 | CD  | LEU | H | 146 | 5.112  | 19.105 | 38.755 | 1.00 59.91 |
| ATOM                        | 4572 | CD1 | LEU | H | 146 | 4.392  | 20.518 | 37.877 | 1.00 61.52 |
| ATOM                        | 4573 | CD2 | LEU | H | 146 | 6.065  | 20.198 | 39.716 | 1.00 60.72 |
| ATOM                        | 4574 | N   | ARG | H | 147 | 4.100  | 17.053 | 36.523 | 1.00 58.34 |
| ATOM                        | 4575 | CA  | ARG | H | 147 | 4.923  | 16.281 | 35.604 | 1.00 66.73 |
| ATOM                        | 4576 | C   | ARG | H | 147 | 5.733  | 17.221 | 34.710 | 1.00 62.59 |
| ATOM                        | 4577 | O   | ARG | H | 147 | 5.266  | 17.626 | 33.646 | 1.00 62.61 |
| ATOM                        | 4578 | CB  | ARG | H | 147 | 4.054  | 15.348 | 34.760 | 1.00 66.77 |
| ATOM                        | 4579 | CG  | ARG | H | 147 | 3.197  | 14.399 | 35.590 | 1.00 71.14 |
| ATOM                        | 4580 | CD  | ARG | H | 147 | 4.021  | 13.407 | 36.395 | 1.00 74.98 |
| ATOM                        | 4581 | NE  | ARG | H | 147 | 3.161  | 12.550 | 37.208 | 1.00 84.49 |
| ATOM                        | 4582 | CZ  | ARG | H | 147 | 3.601  | 11.692 | 38.124 | 1.00 82.55 |
| ATOM                        | 4583 | NH1 | ARG | H | 147 | 4.901  | 11.576 | 38.318 | 1.00 71.79 |
| ATOM                        | 4584 | NH2 | ARG | H | 147 | 2.739  | 10.956 | 38.813 | 1.00 84.71 |
| ATOM                        | 4585 | N   | LEU | H | 148 | 6.941  | 17.568 | 35.140 | 1.00 59.47 |
| ATOM                        | 4586 | CA  | LEU | H | 148 | 7.823  | 18.413 | 34.339 | 1.00 55.89 |
| ATOM                        | 4587 | C   | LEU | H | 148 | 9.161  | 17.740 | 34.114 | 1.00 16.12 |
| ATOM                        | 4588 | O   | LEU | H | 148 | 9.624  | 16.965 | 34.952 | 1.00 57.67 |
| ATOM                        | 4589 | CB  | LEU | H | 148 | 8.043  | 19.774 | 35.008 | 1.00 47.76 |
| ATOM                        | 4590 | CG  | LEU | H | 148 | 6.891  | 20.777 | 35.064 | 1.00 46.72 |
| ATOM                        | 4591 | CD1 | LEU | H | 148 | 7.304  | 22.006 | 35.856 | 1.00 39.10 |
| ATOM                        | 4592 | CD2 | LEU | H | 148 | 6.461  | 21.168 | 33.658 | 1.00 58.69 |
| ATOM                        | 4593 | N   | SER | H | 149 | 9.786  | 18.028 | 32.975 | 1.00 36.96 |
| ATOM                        | 4594 | CA  | SER | H | 149 | 11.330 | 17.530 | 32.709 | 1.00 48.50 |
| ATOM                        | 4595 | C   | SER | H | 149 | 12.065 | 16.099 | 33.748 | 1.00 40.85 |
| ATOM                        | 4596 | O   | SER | H | 149 | 11.793 | 19.127 | 34.362 | 1.00 45.05 |

| octamer-PDB-coordinates.txt |      |       |     |   |     |        |        |        |            |   |
|-----------------------------|------|-------|-----|---|-----|--------|--------|--------|------------|---|
| ATOM                        | 4471 | OH    | TYR | G | 216 | 12.165 | 16.532 | 48.872 | 1.00 53.07 | O |
| ATOM                        | 4472 | N     | SER | H | 133 | 30.106 | 24.904 | 53.323 | 1.00 62.22 | O |
| ATOM                        | 4473 | CA    | SER | H | 133 | 29.125 | 25.477 | 52.410 | 1.00 75.44 | N |
| ATOM                        | 4474 | C     | SER | H | 133 | 28.260 | 26.514 | 53.118 | 1.00 70.70 | C |
| ATOM                        | 4475 | O     | SER | H | 133 | 28.623 | 27.872 | 53.087 | 1.00 77.75 | O |
| ATOM                        | 4476 | CB    | SER | H | 133 | 28.247 | 24.379 | 51.903 | 1.00 77.75 | C |
| ATOM                        | 4477 | OG    | SER | H | 133 | 27.308 | 23.892 | 52.747 | 1.00 66.86 | O |
| ATOM                        | 4478 | N     | GLY | H | 134 | 27.102 | 26.076 | 53.604 | 1.00 67.78 | N |
| ATOM                        | 4479 | CA    | GLY | H | 134 | 26.147 | 26.972 | 54.225 | 1.00 50.78 | C |
| ATOM                        | 4480 | C     | GLY | H | 134 | 25.361 | 27.793 | 53.177 | 1.00 50.78 | C |
| ATOM                        | 4481 | O     | GLY | H | 134 | 24.623 | 28.975 | 53.589 | 1.00 54.82 | O |
| ATOM                        | 4482 | N     | ARG | H | 135 | 25.512 | 27.467 | 51.916 | 1.00 55.31 | N |
| ATOM                        | 4483 | CA    | ARG | H | 135 | 24.757 | 26.183 | 50.856 | 1.00 47.47 | C |
| ATOM                        | 4484 | C     | ARG | H | 135 | 23.901 | 27.163 | 50.905 | 1.00 47.47 | C |
| ATOM                        | 4485 | O     | ARG | H | 135 | 23.542 | 27.591 | 45.533 | 1.00 59.68 | O |
| ATOM                        | 4486 | CB    | ARG | H | 135 | 25.772 | 28.900 | 49.949 | 1.00 39.36 | C |
| ATOM                        | 4487 | CG    | ARG | H | 135 | 26.662 | 29.937 | 50.609 | 1.00 58.58 | C |
| ATOM                        | 4488 | CH    | ARG | H | 135 | 27.638 | 30.507 | 50.805 | 1.00 58.58 | C |
| ATOM                        | 4489 | NE    | ARG | H | 135 | 28.420 | 29.455 | 48.945 | 1.00 58.64 | N |
| ATOM                        | 4490 | CZ    | ARG | H | 135 | 29.103 | 29.620 | 47.317 | 1.00 71.14 | C |
| ATOM                        | 4491 | NH1   | ARG | H | 135 | 29.102 | 30.796 | 47.204 | 1.00 75.92 | N |
| ATOM                        | 4492 | OH2   | ARG | H | 135 | 29.785 | 28.607 | 48.137 | 1.00 75.92 | O |
| ATOM                        | 4493 | N     | ARG | H | 136 | 23.593 | 26.117 | 49.828 | 1.00 57.76 | N |
| ATOM                        | 4494 | CA    | ARG | H | 136 | 22.709 | 25.155 | 49.903 | 1.00 48.50 | C |
| ATOM                        | 4495 | C     | ARG | H | 136 | 21.400 | 24.836 | 50.632 | 1.00 47.52 | C |
| ATOM                        | 4496 | O     | ARG | H | 136 | 21.359 | 24.819 | 51.661 | 1.00 40.92 | O |
| ATOM                        | 4497 | CB    | ARG | H | 136 | 23.458 | 23.839 | 48.907 | 1.00 52.32 | C |
| ATOM                        | 4498 | CG    | ARG | H | 136 | 24.653 | 23.947 | 48.750 | 1.00 53.67 | C |
| ATOM                        | 4499 | CD    | ARG | H | 136 | 25.216 | 22.992 | 48.559 | 1.00 55.77 | C |
| ATOM                        | 4500 | NE    | ARG | H | 136 | 26.327 | 22.626 | 47.706 | 1.00 52.16 | N |
| ATOM                        | 4501 | CZ    | ARG | H | 136 | 26.776 | 22.957 | 47.706 | 1.00 52.16 | C |
| ATOM                        | 4502 | NH1   | ARG | H | 136 | 26.268 | 30.352 | 47.162 | 1.00 74.19 | N |
| ATOM                        | 4503 | NH2   | ARG | H | 136 | 27.689 | 21.673 | 45.914 | 1.00 69.33 | N |
| ATOM                        | 4504 | N     | VAL | H | 137 | 20.333 | 24.728 | 49.656 | 1.00 39.59 | N |
| ATOM                        | 4505 | CA    | VAL | H | 137 | 19.605 | 24.505 | 50.055 | 1.00 35.98 | C |
| ATOM                        | 4506 | C     | VAL | H | 137 | 18.313 | 23.900 | 50.783 | 1.00 35.44 | C |
| ATOM                        | 4507 | O     | VAL | H | 137 | 18.758 | 22.765 | 48.766 | 1.00 35.48 | O |
| ATOM                        | 4508 | CB    | VAL | H | 137 | 18.101 | 25.737 | 50.201 | 1.00 43.09 | C |
| ATOM                        | 4509 | CG1   | VAL | H | 137 | 18.661 | 26.942 | 50.935 | 1.00 34.67 | C |
| ATOM                        | 4510 | CG2   | VAL | H | 137 | 19.594 | 26.035 | 50.935 | 1.00 34.67 | C |
| ATOM                        | 4511 | N     | LEU | H | 138 | 17.316 | 22.886 | 50.420 | 1.00 41.34 | N |
| ATOM                        | 4512 | CA    | LEU | H | 138 | 16.387 | 21.809 | 49.898 | 1.00 46.14 | C |
| ATOM                        | 4513 | C     | LEU | H | 138 | 14.978 | 22.316 | 49.832 | 1.00 41.74 | C |
| ATOM                        | 4514 | LEU1A | LEU | H | 138 | 14.338 | 22.465 | 49.832 | 1.00 41.74 | C |
| ATOM                        | 4515 | CB    | LEU | H | 138 | 16.347 | 20.641 | 50.834 | 1.00 47.46 | C |
| ATOM                        | 4516 | CG    | LEU | H | 138 | 15.657 | 19.376 | 50.373 | 1.00 39.59 | C |
| ATOM                        | 4517 | CD1   | LEU | H | 138 | 16.475 | 18.729 | 49.271 | 1.00 36.26 | C |
| ATOM                        | 4518 | CD2   | LEU | H | 138 | 15.418 | 18.401 | 49.271 | 1.00 36.26 | C |
| ATOM                        | 4519 | N     | VAL | H | 139 | 14.508 | 22.127 | 48.405 | 1.00 37.87 | N |
| ATOM                        | 4520 | CA    | VAL | H | 139 | 13.62  | 21.540 | 48.633 | 1.00 46.86 | C |
| ATOM                        | 4521 | C     | VAL | H | 139 | 12.241 | 21.328 | 47.994 | 1.00 43.31 | C |
| ATOM                        | 4522 | O     | VAL | H | 139 | 12.455 | 20.402 | 47.212 | 1.00 40.14 | O |
| ATOM                        | 4523 | CB    | VAL | H | 139 | 13.133 | 23.258 | 46.677 | 1.00 40.14 | C |
| ATOM                        | 4524 | CG1   | VAL | H | 139 | 11.753 | 23.832 | 46.198 | 1.00 29.65 | C |
| ATOM                        | 4525 | CG2   | VAL | H | 139 | 14.195 | 24.342 | 46.325 | 1.00 30.61 | C |
| ATOM                        | 4526 | N     | THR | H | 140 | 11.224 | 21.334 | 48.847 | 1.00 34.94 | N |
| ATOM                        | 4527 | CA    | THR | H | 140 | 10.307 | 20.232 | 48.847 | 1.00 34.94 | C |
| ATOM                        | 4528 | C     | THR | H | 140 | 8.864  | 20.672 | 48.739 | 1.00 42.57 | C |
| ATOM                        | 4529 | O     | THR | H | 140 | 8.563  | 21.460 | 48.648 | 1.00 50.86 | O |
| ATOM                        | 4530 | CB    | THR | H | 140 | 10.414 | 19.487 | 50.297 | 1.00 42.57 | C |
| ATOM                        | 4531 | CG2   | THR | H | 140 | 11.845 | 19.013 | 50.371 | 1.00 42.57 | C |
| ATOM                        | 4532 | CG1   | THR | H | 140 | 10.372 | 19.351 | 50.371 | 1.00 43.85 | C |
| ATOM                        | 4533 | N     | GLY | H | 141 | 7.978  | 19.725 | 48.452 | 1.00 41.14 | N |

|                             |      |     |     |   |     |        |        |        |      |                             |      |      |     |     |   |     |        |        |        |      |       |
|-----------------------------|------|-----|-----|---|-----|--------|--------|--------|------|-----------------------------|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| octamer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |      | octamer-PDB-coordinates.txt |      |      |     |     |   |     |        |        |        |      |       |
| ATOM                        | 4660 | CA  | LEU | H | 157 | 12.867 | 26.969 | 40.069 | 1.00 | 31.11                       | ATOM | 4723 | CB  | THR | H | 164 | 16.998 | 40.191 | 44.743 | 1.00 | 37.82 |
| ATOM                        | 4661 | C   | LEU | H | 157 | 13.974 | 28.009 | 40.171 | 1.00 | 32.42                       | ATOM | 4724 | CG2 | THR | H | 164 | 18.323 | 39.823 | 44.091 | 1.00 | 35.10 |
| ATOM                        | 4662 | O   | LEU | H | 157 | 13.975 | 28.830 | 41.086 | 1.00 | 33.87                       | ATOM | 4725 | OG1 | THR | H | 164 | 16.327 | 41.247 | 41.001 | 1.00 | 48.42 |
| ATOM                        | 4663 | CB  | LEU | H | 157 | 13.334 | 25.645 | 40.674 | 1.00 | 24.81                       | ATOM | 4726 | CA  | ARG | H | 165 | 13.747 | 39.713 | 44.591 | 1.00 | 29.31 |
| ATOM                        | 4664 | CG  | LEU | H | 157 | 12.235 | 24.616 | 40.381 | 1.00 | 24.76                       | ATOM | 4727 | CA  | ARG | H | 165 | 12.442 | 40.130 | 45.102 | 1.00 | 29.85 |
| ATOM                        | 4665 | CD1 | LEU | H | 157 | 12.537 | 23.313 | 41.406 | 1.00 | 30.42                       | ATOM | 4728 | C   | ARG | H | 165 | 11.726 | 38.986 | 45.513 | 1.00 | 27.71 |
| ATOM                        | 4666 | CD2 | LEU | H | 157 | 11.232 | 25.146 | 41.940 | 1.00 | 26.01                       | ATOM | 4729 | O   | ARG | H | 165 | 10.810 | 39.213 | 46.602 | 1.00 | 25.94 |
| ATOM                        | 4667 | N   | GLU | H | 158 | 14.921 | 27.967 | 39.236 | 1.00 | 34.73                       | ATOM | 4730 | CB  | ARG | H | 165 | 11.556 | 40.678 | 43.979 | 1.00 | 27.03 |
| ATOM                        | 4668 | CA  | GLU | H | 158 | 16.007 | 28.940 | 39.225 | 1.00 | 37.40                       | ATOM | 4731 | CG  | ARG | H | 165 | 11.061 | 39.643 | 42.978 | 1.00 | 26.10 |
| ATOM                        | 4669 | CG  | GLU | H | 158 | 15.479 | 30.331 | 38.875 | 1.00 | 35.96                       | ATOM | 4732 | CD  | ARG | H | 165 | 9.923  | 40.217 | 42.141 | 1.00 | 32.05 |
| ATOM                        | 4670 | O   | GLU | H | 158 | 15.996 | 31.335 | 39.360 | 1.00 | 42.03                       | ATOM | 4733 | NE  | ARG | H | 165 | 9.420  | 39.274 | 44.145 | 1.00 | 40.28 |
| ATOM                        | 4671 | CB  | GLU | H | 158 | 17.110 | 28.519 | 38.253 | 1.00 | 33.28                       | ATOM | 4734 | CZ  | ARG | H | 165 | 9.766  | 39.288 | 39.861 | 1.00 | 50.97 |
| ATOM                        | 4672 | CG  | GLU | H | 158 | 18.331 | 29.429 | 38.285 | 1.00 | 39.46                       | ATOM | 4735 | NH2 | ARG | H | 165 | 10.609 | 40.207 | 39.411 | 1.00 | 42.48 |
| ATOM                        | 4673 | CD  | GLU | H | 158 | 19.498 | 28.676 | 37.491 | 1.00 | 36.84                       | ATOM | 4736 | NH2 | ARG | H | 165 | 9.260  | 38.391 | 39.024 | 1.00 | 44.42 |
| ATOM                        | 4674 | CE  | GLU | H | 158 | 20.592 | 29.476 | 37.546 | 1.00 | 42.63                       | ATOM | 4737 | N   | ASN | H | 166 | 12.149 | 37.757 | 45.535 | 1.00 | 30.04 |
| ATOM                        | 4675 | OE2 | GLU | H | 158 | 19.324 | 27.640 | 36.817 | 1.00 | 45.43                       | ATOM | 4738 | CA  | ASN | H | 166 | 11.605 | 36.593 | 46.220 | 1.00 | 27.83 |
| ATOM                        | 4676 | N   | ILE | H | 159 | 14.455 | 30.384 | 38.026 | 1.00 | 32.77                       | ATOM | 4739 | C   | ASN | H | 166 | 12.487 | 38.209 | 47.404 | 1.00 | 39.00 |
| ATOM                        | 4677 | CA  | ILE | H | 159 | 13.792 | 31.645 | 37.706 | 1.00 | 38.97                       | ATOM | 4740 | O   | ASN | H | 166 | 12.256 | 35.235 | 48.107 | 1.00 | 24.63 |
| ATOM                        | 4678 | C   | ILE | H | 159 | 13.118 | 32.268 | 38.988 | 1.00 | 40.80                       | ATOM | 4741 | CB  | ASN | H | 166 | 11.475 | 35.416 | 45.254 | 1.00 | 26.99 |
| ATOM                        | 4679 | O   | ILE | H | 159 | 13.461 | 33.440 | 39.255 | 1.00 | 50.90                       | ATOM | 4742 | CG  | ASN | H | 166 | 10.368 | 35.622 | 44.237 | 1.00 | 30.90 |
| ATOM                        | 4680 | CB  | ILE | H | 159 | 12.648 | 31.468 | 36.683 | 1.00 | 40.16                       | ATOM | 4743 | ND2 | ASN | H | 166 | 10.557 | 35.075 | 43.041 | 1.00 | 31.17 |
| ATOM                        | 4681 | CG1 | ILE | H | 159 | 13.167 | 31.014 | 35.327 | 1.00 | 37.03                       | ATOM | 4744 | OD1 | ASN | H | 166 | 9.317  | 35.254 | 44.520 | 1.00 | 26.37 |
| ATOM                        | 4682 | CG2 | ILE | H | 159 | 11.893 | 32.775 | 36.505 | 1.00 | 33.49                       | ATOM | 4745 | N   | GLY | H | 167 | 12.544 | 36.989 | 47.614 | 1.00 | 33.62 |
| ATOM                        | 4683 | CD1 | ILE | H | 159 | 13.888 | 32.093 | 34.555 | 1.00 | 42.11                       | ATOM | 4746 | CA  | GLY | H | 167 | 14.466 | 36.764 | 48.711 | 1.00 | 29.38 |
| ATOM                        | 4684 | C   | PHE | H | 160 | 12.453 | 31.482 | 39.750 | 1.00 | 32.28                       | ATOM | 4747 | C   | GLY | H | 167 | 11.667 | 35.930 | 48.308 | 1.00 | 26.36 |
| ATOM                        | 4685 | CA  | PHE | H | 160 | 11.821 | 32.009 | 40.928 | 1.00 | 33.27                       | ATOM | 4748 | O   | GLY | H | 167 | 16.478 | 35.546 | 49.148 | 1.00 | 33.36 |
| ATOM                        | 4686 | C   | PHE | H | 160 | 12.847 | 32.368 | 42.001 | 1.00 | 30.58                       | ATOM | 4749 | N   | GLY | H | 168 | 13.776 | 35.643 | 49.016 | 1.00 | 28.58 |
| ATOM                        | 4687 | O   | PHE | H | 160 | 12.066 | 33.496 | 42.945 | 1.00 | 28.08                       | ATOM | 4750 | CA  | GLY | H | 168 | 12.831 | 34.743 | 48.429 | 1.00 | 29.36 |
| ATOM                        | 4688 | CB  | PHE | H | 160 | 10.617 | 30.897 | 41.487 | 1.00 | 24.33                       | ATOM | 4751 | C   | GLY | H | 168 | 18.016 | 35.531 | 45.940 | 1.00 | 29.13 |
| ATOM                        | 4689 | CG  | PHE | H | 160 | 9.914  | 31.560 | 42.595 | 1.00 | 29.01                       | ATOM | 4752 | O   | GLY | H | 168 | 18.329 | 36.647 | 46.355 | 1.00 | 42.65 |
| ATOM                        | 4690 | CD1 | PHE | H | 160 | 10.386 | 31.556 | 43.913 | 1.00 | 20.29                       | ATOM | 4753 | N   | GLY | H | 168 | 18.675 | 34.901 | 44.973 | 1.00 | 30.44 |
| ATOM                        | 4691 | CD2 | PHE | H | 160 | 8.708  | 32.095 | 42.308 | 1.00 | 32.07                       | ATOM | 4754 | CA  | GLY | H | 169 | 19.863 | 34.476 | 43.342 | 1.00 | 43.20 |
| ATOM                        | 4692 | CE1 | PHE | H | 160 | 9.599  | 32.078 | 44.921 | 1.00 | 26.09                       | ATOM | 4755 | O   | GLY | H | 169 | 19.863 | 33.415 | 43.099 | 1.00 | 42.15 |
| ATOM                        | 4693 | CE2 | PHE | H | 160 | 7.915  | 32.615 | 43.213 | 1.00 | 26.13                       | ATOM | 4756 | N   | ASP | H | 170 | 21.580 | 34.838 | 42.753 | 1.00 | 31.86 |
| ATOM                        | 4694 | C   | PHE | H | 160 | 8.359  | 32.606 | 44.621 | 1.00 | 27.06                       | ATOM | 4757 | CA  | ASP | H | 170 | 22.227 | 34.025 | 41.723 | 1.00 | 36.69 |
| ATOM                        | 4695 | N   | PHE | H | 161 | 13.896 | 31.409 | 42.354 | 1.00 | 22.84                       | ATOM | 4758 | C   | ASP | H | 170 | 22.471 | 32.536 | 41.126 | 1.00 | 49.86 |
| ATOM                        | 4696 | CA  | PHE | H | 161 | 14.631 | 31.579 | 43.483 | 1.00 | 25.95                       | ATOM | 4759 | O   | ASP | H | 170 | 22.468 | 32.444 | 40.179 | 1.00 | 49.86 |
| ATOM                        | 4697 | C   | PHE | H | 161 | 15.909 | 32.314 | 43.053 | 1.00 | 30.48                       | ATOM | 4760 | CB  | ASP | H | 170 | 23.542 | 34.676 | 41.286 | 1.00 | 27.63 |
| ATOM                        | 4698 | CG  | PHE | H | 161 | 16.769 | 32.513 | 43.894 | 1.00 | 31.82                       | ATOM | 4761 | CG  | ASP | H | 170 | 23.326 | 35.912 | 40.493 | 1.00 | 41.57 |
| ATOM                        | 4699 | CD  | PHE | H | 161 | 14.984 | 30.213 | 44.059 | 1.00 | 24.47                       | ATOM | 4762 | OD1 | ASP | H | 170 | 22.193 | 36.441 | 40.493 | 1.00 | 47.87 |
| ATOM                        | 4700 | CG  | PHE | H | 161 | 13.832 | 29.541 | 44.751 | 1.00 | 25.62                       | ATOM | 4763 | OD2 | ASP | H | 170 | 24.264 | 36.160 | 39.779 | 1.00 | 50.93 |
| ATOM                        | 4701 | CD1 | PHE | H | 161 | 13.407 | 29.974 | 45.199 | 1.00 | 26.73                       | ATOM | 4764 | N   | VAL | H | 171 | 22.615 | 31.640 | 41.316 | 1.00 | 39.13 |
| ATOM                        | 4702 | CD2 | PHE | H | 161 | 13.165 | 28.485 | 44.949 | 1.00 | 25.24                       | ATOM | 4765 | CA  | VAL | H | 171 | 22.238 | 30.215 | 41.607 | 1.00 | 39.36 |
| ATOM                        | 4703 | CE  | PHE | H | 161 | 12.342 | 29.363 | 44.632 | 1.00 | 22.11                       | ATOM | 4766 | CA  | VAL | H | 171 | 23.483 | 29.607 | 40.961 | 1.00 | 40.19 |
| ATOM                        | 4704 | CE2 | PHE | H | 161 | 12.099 | 27.869 | 44.780 | 1.00 | 25.73                       | ATOM | 4767 | C   | VAL | H | 171 | 23.697 | 29.753 | 39.758 | 1.00 | 45.15 |
| ATOM                        | 4705 | CZ  | PHE | H | 161 | 11.666 | 28.309 | 46.023 | 1.00 | 20.84                       | ATOM | 4768 | CB  | VAL | H | 171 | 20.992 | 29.442 | 41.123 | 1.00 | 38.96 |
| ATOM                        | 4706 | N   | GLY | H | 162 | 16.007 | 32.698 | 41.795 | 1.00 | 32.52                       | ATOM | 4769 | CG  | VAL | H | 171 | 21.274 | 27.947 | 41.328 | 1.00 | 41.94 |
| ATOM                        | 4707 | CA  | GLY | H | 162 | 17.122 | 33.501 | 41.936 | 1.00 | 24.55                       | ATOM | 4770 | CG1 | VAL | H | 171 | 19.746 | 29.938 | 41.841 | 1.00 | 27.15 |
| ATOM                        | 4708 | CG  | GLY | H | 162 | 16.815 | 34.909 | 41.514 | 1.00 | 25.88                       | ATOM | 4771 | N   | ASP | H | 172 | 24.302 | 28.931 | 41.763 | 1.00 | 46.25 |
| ATOM                        | 4709 | O   | GLY | H | 162 | 17.771 | 35.811 | 41.460 | 1.00 | 32.58                       | ATOM | 4772 | CA  | ASP | H | 172 | 25.759 | 28.316 | 41.260 | 1.00 | 57.88 |
| ATOM                        | 4710 | N   | LYS | H | 163 | 15.587 | 35.327 | 41.720 | 1.00 | 22.75                       | ATOM | 4773 | C   | ASP | H | 172 | 25.328 | 26.669 | 40.825 | 1.00 | 59.97 |
| ATOM                        | 4711 | CA  | LYS | H | 163 | 15.164 | 36.715 | 41.859 | 1.00 | 32.45                       | ATOM | 4774 | CB  | ASP | H | 172 | 25.757 | 26.472 | 39.742 | 1.00 | 48.11 |
| ATOM                        | 4712 | C   | LYS | H | 163 | 15.301 | 37.200 | 43.298 | 1.00 | 38.87                       | ATOM | 4775 | O   | ASP | H | 172 | 26.626 | 28.355 | 42.328 | 1.00 | 60.46 |
| ATOM                        | 4713 | O   | LYS | H | 163 | 14.585 | 36.519 | 44.255 | 1.00 | 30.59                       | ATOM | 4776 | CG  | ASP | H |     |        |        |        |      |       |

| octamer-PDB-coordinates.txt |      |     |     |   |     |        |        |        |      | octamer-PDB-coordinates.txt |   |      |      |     |     |   |     |        |        |        |      |       |   |
|-----------------------------|------|-----|-----|---|-----|--------|--------|--------|------|-----------------------------|---|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM                        | 4912 | CG2 | VAL | H | 190 | -0.303 | -6.737 | 54.058 | 1.00 | 45.00                       | C | ATOM | 4975 | C   | GLN | H | 199 | 14.769 | -1.761 | 56.644 | 1.00 | 46.23 | C |
| ATOM                        | 4913 | N   | ALA | H | 191 | 1.064  | -2.738 | 55.369 | 1.00 | 35.09                       | N | ATOM | 4976 | O   | GLN | H | 199 | 14.585 | -2.830 | 57.228 | 1.00 | 47.18 | C |
| ATOM                        | 4914 | CA  | ALA | H | 191 | 1.723  | -1.481 | 55.448 | 1.00 | 38.67                       | C | ATOM | 4977 | CB  | GLN | H | 199 | 15.859 | -0.145 | 58.236 | 1.00 | 51.34 | C |
| ATOM                        | 4915 | C   | ALA | H | 191 | 2.276  | -1.204 | 56.844 | 1.00 | 40.43                       | C | ATOM | 4978 | CD  | GLN | H | 199 | 17.182 | 0.087  | 59.087 | 1.00 | 57.40 | C |
| ATOM                        | 4916 | O   | ALA | H | 191 | 3.417  | -0.770 | 57.032 | 1.00 | 41.17                       | O | ATOM | 4979 | CD  | GLN | H | 199 | 17.282 | 1.060  | 56.502 | 0.00 | 69.86 | C |
| ATOM                        | 4917 | CB  | ALA | H | 191 | 0.756  | -0.333 | 55.064 | 1.00 | 36.06                       | C | ATOM | 4980 | NE2 | GLN | H | 199 | 17.266 | 3.286  | 57.032 | 0.00 | 70.36 | C |
| ATOM                        | 4918 | N   | GLN | H | 192 | 1.418  | -1.530 | 57.650 | 1.00 | 42.25                       | N | ATOM | 4981 | OE1 | GLN | H | 199 | 17.367 | 0.645  | 55.294 | 0.00 | 64.86 | C |
| ATOM                        | 4919 | CA  | GLN | H | 192 | 1.551  | -1.350 | 59.245 | 1.00 | 40.97                       | C | ATOM | 4982 | N   | PHE | H | 200 | 15.097 | -1.685 | 55.359 | 1.00 | 61.99 | N |
| ATOM                        | 4920 | CZ  | ARG | H | 192 | 3.042  | -2.238 | 59.587 | 1.00 | 40.26                       | C | ATOM | 4983 | CA  | PHE | H | 200 | 15.267 | -1.874 | 54.331 | 1.00 | 42.40 | C |
| ATOM                        | 4921 | O   | GLN | H | 192 | 3.938  | -1.908 | 60.316 | 1.00 | 42.65                       | O | ATOM | 4984 | C   | PHE | H | 200 | 16.510 | -2.754 | 53.667 | 1.00 | 39.37 | C |
| ATOM                        | 4922 | CB  | GLN | H | 192 | 0.682  | -1.677 | 60.184 | 1.00 | 47.88                       | C | ATOM | 4985 | C   | PHE | H | 200 | 16.960 | -1.853 | 52.379 | 1.00 | 36.50 | C |
| ATOM                        | 4923 | CG  | GLN | H | 192 | -0.360 | -0.576 | 60.305 | 1.00 | 43.94                       | C | ATOM | 4986 | CB  | PHE | H | 200 | 14.047 | -3.103 | 53.632 | 1.00 | 41.87 | C |
| ATOM                        | 4924 | CD  | GLN | H | 192 | -1.172 | -0.390 | 59.038 | 1.00 | 52.25                       | C | ATOM | 4987 | CG  | PHE | H | 200 | 12.758 | -3.285 | 54.377 | 1.00 | 34.70 | C |
| ATOM                        | 4925 | NE2 | GLN | H | 192 | -1.737 | 0.799  | 58.668 | 1.00 | 41.40                       | N | ATOM | 4988 | CD1 | PHE | H | 200 | 12.018 | -2.191 | 54.793 | 1.00 | 28.61 | C |
| ATOM                        | 4926 | OE1 | GLN | H | 192 | -1.288 | -1.304 | 58.222 | 1.00 | 50.18                       | C | ATOM | 4989 | CD2 | PHE | H | 200 | 12.274 | -4.557 | 54.638 | 1.00 | 31.15 | C |
| ATOM                        | 4927 | N   | ARG | H | 193 | 3.054  | -3.451 | 59.066 | 1.00 | 39.42                       | N | ATOM | 4990 | CE3 | PHE | H | 200 | 10.827 | -2.363 | 55.472 | 1.00 | 40.22 | C |
| ATOM                        | 4928 | CA  | ARG | H | 193 | 4.146  | -4.388 | 59.319 | 1.00 | 42.00                       | C | ATOM | 4991 | CE2 | PHE | H | 200 | 11.085 | -4.735 | 59.315 | 1.00 | 20.44 | C |
| ATOM                        | 4929 | C   | ARG | H | 193 | 5.462  | -3.932 | 58.710 | 1.00 | 36.89                       | C | ATOM | 4992 | CZ  | PHE | H | 200 | 10.360 | -2.636 | 55.731 | 1.00 | 40.96 | C |
| ATOM                        | 4930 | O   | ARG | H | 193 | 6.508  | -3.901 | 59.369 | 1.00 | 45.01                       | O | ATOM | 4993 | N   | THR | H | 201 | 17.065 | -3.890 | 53.265 | 1.00 | 31.50 | N |
| ATOM                        | 4931 | CB  | ARG | H | 193 | 3.801  | -5.765 | 58.755 | 1.00 | 35.02                       | C | ATOM | 4994 | CA  | THR | H | 201 | 18.145 | -3.885 | 52.292 | 1.00 | 27.17 | C |
| ATOM                        | 4932 | CG  | ARG | H | 193 | 4.750  | -6.878 | 59.172 | 1.00 | 43.75                       | C | ATOM | 4995 | C   | THR | H | 201 | 17.858 | -4.532 | 51.004 | 1.00 | 32.60 | C |
| ATOM                        | 4933 | CD  | ARG | H | 193 | 4.469  | -6.148 | 58.394 | 1.00 | 46.00                       | C | ATOM | 4996 | O   | THR | H | 201 | 17.438 | -5.742 | 50.947 | 1.00 | 40.60 | C |
| ATOM                        | 4934 | NE  | ARG | H | 193 | 5.001  | -8.478 | 58.275 | 1.00 | 45.86                       | N | ATOM | 4997 | CG  | THR | H | 201 | 19.393 | -4.624 | 52.807 | 1.00 | 43.15 | C |
| ATOM                        | 4935 | CZ  | ARG | H | 193 | 2.853  | -9.882 | 57.427 | 1.00 | 52.47                       | C | ATOM | 4998 | CG3 | THR | H | 201 | 20.486 | -4.619 | 51.749 | 1.00 | 35.19 | C |
| ATOM                        | 4936 | NH1 | ARG | H | 193 | 3.191  | -9.103 | 56.030 | 1.00 | 43.99                       | N | ATOM | 4999 | OG1 | THR | H | 201 | 19.880 | -3.975 | 53.988 | 1.00 | 36.32 | C |
| ATOM                        | 4937 | NH2 | ARG | H | 193 | 1.157  | -9.110 | 57.141 | 1.00 | 65.86                       | C | ATOM | 5000 | N   | VAL | H | 202 | 17.445 | -3.712 | 59.971 | 1.00 | 28.40 | N |
| ATOM                        | 4938 | N   | LEU | H | 194 | 5.403  | -3.483 | 57.450 | 1.00 | 30.71                       | N | ATOM | 5001 | CA  | VAL | H | 202 | 16.949 | -4.177 | 48.704 | 1.00 | 27.90 | C |
| ATOM                        | 4939 | CA  | LEU | H | 194 | 6.597  | -3.050 | 56.754 | 1.00 | 34.68                       | C | ATOM | 5002 | O   | VAL | H | 202 | 21.123 | -4.187 | 47.631 | 1.00 | 49.03 | C |
| ATOM                        | 4940 | C   | LEU | H | 194 | 7.126  | -2.728 | 56.315 | 1.00 | 34.87                       | C | ATOM | 5003 | C   | VAL | H | 202 | 18.676 | -3.104 | 47.425 | 1.00 | 44.36 | C |
| ATOM                        | 4941 | O   | LEU | H | 194 | 8.340  | -2.514 | 57.439 | 1.00 | 39.03                       | O | ATOM | 5004 | CB  | VAL | H | 202 | 15.745 | -3.322 | 48.251 | 1.00 | 24.53 | C |
| ATOM                        | 4942 | CB  | LEU | H | 194 | 6.305  | -2.822 | 55.265 | 1.00 | 26.45                       | C | ATOM | 5005 | CG1 | VAL | H | 202 | 15.115 | -3.908 | 46.994 | 1.00 | 32.23 | C |
| ATOM                        | 4943 | CG  | LEU | H | 194 | 6.090  | -4.151 | 54.535 | 1.00 | 30.03                       | C | ATOM | 5006 | CG2 | VAL | H | 202 | 14.717 | -2.217 | 49.365 | 1.00 | 30.10 | C |
| ATOM                        | 4944 | CD1 | LEU | H | 194 | 5.693  | -3.926 | 53.086 | 1.00 | 27.36                       | C | ATOM | 5007 | N   | GLY | H | 205 | 20.153 | -2.473 | 46.351 | 1.00 | 37.83 | C |
| ATOM                        | 4945 | CD2 | LEU | H | 194 | 7.347  | -5.017 | 54.614 | 1.00 | 21.47                       | C | ATOM | 5008 | CA  | PRO | H | 203 | 19.176 | -5.355 | 45.820 | 1.00 | 41.69 | C |
| ATOM                        | 4946 | N   | CYS | H | 195 | 6.219  | -0.857 | 57.609 | 1.00 | 39.74                       | C | ATOM | 5009 | C   | PRO | H | 203 | 18.681 | -4.552 | 44.622 | 1.00 | 43.72 | C |
| ATOM                        | 4947 | CA  | CYS | H | 195 | 6.606  | 0.366  | 58.501 | 1.00 | 42.18                       | C | ATOM | 5010 | O   | PRO | H | 203 | 17.726 | -4.958 | 43.959 | 1.00 | 40.47 | C |
| ATOM                        | 4948 | C   | CYS | H | 195 | 7.253  | 0.035  | 59.836 | 1.00 | 38.31                       | C | ATOM | 5011 | CB  | PRO | H | 203 | 19.217 | -6.854 | 45.499 | 1.00 | 38.12 | C |
| ATOM                        | 4949 | O   | CYS | H | 195 | 8.223  | 0.843  | 60.264 | 1.00 | 38.31                       | O | ATOM | 5012 | C   | PRO | H | 203 | 21.990 | -7.528 | 46.738 | 1.00 | 47.39 | C |
| ATOM                        | 4950 | CB  | CYS | H | 195 | 5.296  | -1.274 | 58.729 | 1.00 | 30.45                       | C | ATOM | 5013 | CD  | PRO | H | 203 | 17.719 | -6.594 | 47.323 | 1.00 | 45.62 | C |
| ATOM                        | 4951 | SG  | CYS | H | 195 | 4.771  | -2.029 | 57.206 | 1.00 | 46.46                       | S | ATOM | 5014 | N   | LEU | H | 204 | 19.325 | -3.421 | 44.356 | 1.00 | 49.94 | N |
| ATOM                        | 4952 | N   | GLN | H | 196 | 6.700  | -1.007 | 60.481 | 1.00 | 37.27                       | N | ATOM | 5015 | CA  | LEU | H | 204 | 18.952 | -2.571 | 43.230 | 1.00 | 44.20 | C |
| ATOM                        | 4953 | CA  | GLN | H | 196 | 7.200  | -1.530 | 61.752 | 1.00 | 39.23                       | C | ATOM | 5016 | C   | LEU | H | 204 | 20.175 | -2.132 | 42.430 | 1.00 | 43.67 | C |
| ATOM                        | 4954 | C   | GLN | H | 196 | 8.632  | -2.028 | 61.657 | 1.00 | 44.46                       | C | ATOM | 5017 | N   | GLY | H | 204 | 21.123 | -1.570 | 42.430 | 1.00 | 43.67 | C |
| ATOM                        | 4955 | O   | GLN | H | 196 | 9.955  | -1.768 | 62.515 | 1.00 | 43.86                       | O | ATOM | 5018 | CB  | LEU | H | 204 | 18.177 | -1.343 | 43.716 | 1.00 | 43.68 | C |
| ATOM                        | 4956 | CB  | GLN | H | 196 | 6.284  | -3.227 | 62.253 | 1.00 | 41.66                       | C | ATOM | 5019 | CG  | LEU | H | 204 | 16.849 | -1.586 | 44.438 | 1.00 | 36.29 | C |
| ATOM                        | 4957 | CG  | GLN | H | 196 | 6.684  | -3.266 | 63.564 | 1.00 | 54.06                       | C | ATOM | 5020 | CD1 | LEU | H | 204 | 16.270 | -0.278 | 44.951 | 1.00 | 30.54 | C |
| ATOM                        | 4958 | CD  | GLN | H | 196 | 5.708  | -4.150 | 63.978 | 1.00 | 63.98                       | C | ATOM | 5021 | CD2 | LEU | H | 204 | 15.816 | -2.284 | 43.520 | 1.00 | 37.74 | C |
| ATOM                        | 4959 | NE2 | GLN | H | 196 | 6.214  | -5.101 | 64.370 | 1.00 | 58.15                       | C | ATOM | 5022 | N   | GLY | H | 205 | 20.153 | -2.473 | 46.351 | 1.00 | 37.83 | C |
| ATOM                        | 4960 | OE1 | GLN | H | 196 | 4.493  | -4.358 | 63.927 | 1.00 | 54.04                       | O | ATOM | 5023 | CA  | GLY | H | 205 | 21.216 | -2.056 | 40.725 | 1.00 | 47.49 | C |
| ATOM                        | 4961 | N   | ILE | H | 197 | 8.930  | -2.725 | 60.549 | 1.00 | 40.62                       | C | ATOM | 5024 | C   | GLY | H | 205 | 22.609 | -2.448 | 40.635 | 1.00 | 45.82 | C |
| ATOM                        | 4962 | CA  | ILE | H | 197 | 10.303 | -3.149 | 60.296 | 1.00 | 41.74                       | C | ATOM | 5025 | O   | GLY | H | 205 | 23.573 | -1.697 | 40.494 | 1.00 | 54.58 | O |
| ATOM                        | 4963 | C   | ILE | H | 197 | 11.119 | -1.924 | 59.971 | 1.00 | 39.60                       | C | ATOM | 5026 | N   | GLY | H | 206 | 22.712 | -3.469 | 41.145 | 1.00 | 46.84 | C |
| ATOM                        | 4964 | O   | ILE | H | 197 | 12.819 | -1.799 | 60.444 | 1.00 | 41.07                       | O | ATOM | 5027 | C   | GLY | H | 206 | 23.990 | -4.327 | 41.558 | 1.00 | 47.04 | C |
| ATOM                        | 4965 | CB  | ILE | H | 197 | 10.385 | -4.179 | 59.158 | 1.00 | 41.92                       | C | ATOM | 5028 | C   | GLY | H | 206 | 24.440 | -3.745 | 42.925 | 1.00 | 49.36 | C |
| ATOM                        | 4966 | CG1 | ILE | H | 197 | 9.617  | -5.447 | 59.539 | 1.00 | 33.04                       | C | ATOM | 5029 | O   | GLY | H | 206 | 25.522 | -4.129 | 43.388 | 1.00 | 50.61 | C |
| ATOM                        | 4967 | CG2 | ILE | H | 197 | 11.835 | -4.513 | 58.842 | 1.00 | 38.70                       | C | ATOM | 5030 | N   | GLN | H | 207 | 23.642 | -2.909 | 43.573 | 1.00 | 52.33 | N |
| ATOM                        | 4968 | CD1 | ILE | H | 197 | 9.518  | -6.467 | 58.424 | 1.00 | 32.33                       | C | ATOM | 5031 | CA  | GLN | H | 207 | 23.972 | -2.431 | 44.912 | 1.00 | 39.68 | C |
| ATOM                        | 4969 | N   | GLY | H | 198 | 10.601 | -1.021 | 59.168 | 1.00 | 42.78                       | C | ATOM | 5032 | C   | GLN | H | 207 | 23.050 | -1.050 | 45.948 | 1.00 | 49.93 | C |
| ATOM                        | 4970 | CA  | GLY | H | 198 | 11.216 | 0.752  | 58.909 | 1.00 | 35.82                       | C | ATOM | 5033 | O   | GLN | H | 207 | 23.933 | -3.469 | 45.636 | 1.00 | 50.69 | O |
| ATOM                        | 4971 | C   | GLY | H | 198 | 12.351 | 0.281  | 57.903 | 1.00 | 45.75                       | C | ATOM | 5034 | CB  | GLN | H | 207 | 23.888 | -0.905 | 45.004 | 1.00 | 56.50 | C |
| ATOM                        | 4972 | O   | GLY | H | 198 | 12.258 | 0.931  | 56.862 | 1.00 | 48.65                       | O | ATOM | 5035 | CG  | GLN | H | 207 | 24.477 | -0.153 | 43.830 | 1.00 | 71.25 | C |
| ATOM                        | 4973 | N   | GLN | H | 199 | 13.423 | -0.442 | 58.210 | 1.00 | 46.78                       | N | ATOM | 5036 | CD  | GLN | H | 207 | 2      |        |        |      |       |   |

| octamer-PDB-coordinates.txt |   |     |   |     |        |         |         |      |       | octamer-PDB-coordinates.txt |             |   |     |   |     |        |         |         |      |       |   |
|-----------------------------|---|-----|---|-----|--------|---------|---------|------|-------|-----------------------------|-------------|---|-----|---|-----|--------|---------|---------|------|-------|---|
| HETATM 5164                 | O | HOH | 5 | 45  | 2.618  | 19.645  | 0.155   | 1.00 | 35.19 | O                           | HETATM 5227 | O | HOH | 5 | 108 | 17.882 | 13.301  | 47.029  | 1.00 | 41.25 | O |
| HETATM 5165                 | O | HOH | 5 | 46  | 4.725  | 6.150   | 38.933  | 1.00 | 31.47 | O                           | HETATM 5228 | O | HOH | 5 | 109 | 17.344 | 30.167  | -4.373  | 1.00 | 38.62 | O |
| HETATM 5166                 | O | HOH | 5 | 47  | 23.957 | -15.863 | -11.812 | 1.00 | 35.83 | O                           | HETATM 5229 | O | HOH | 5 | 110 | 17.540 | 43.252  | 41.118  | 1.00 | 45.04 | O |
| HETATM 5167                 | O | HOH | 5 | 48  | 20.282 | -14.249 | 7.528   | 1.00 | 37.39 | O                           | HETATM 5230 | O | HOH | 5 | 111 | 28.058 | -2.618  | 47.294  | 1.00 | 46.80 | O |
| HETATM 5168                 | O | HOH | 5 | 49  | 10.744 | 45.078  | -5.535  | 1.00 | 28.18 | O                           | HETATM 5231 | O | HOH | 5 | 112 | 9.074  | 35.573  | 57.721  | 1.00 | 45.16 | O |
| HETATM 5169                 | O | HOH | 5 | 50  | 4.427  | 44.290  | 35.752  | 1.00 | 42.06 | O                           | HETATM 5232 | O | HOH | 5 | 113 | -9.165 | 42.400  | -2.214  | 1.00 | 60.78 | O |
| HETATM 5170                 | O | HOH | 5 | 51  | 16.606 | -11.738 | 8.017   | 1.00 | 31.22 | O                           | HETATM 5233 | O | HOH | 5 | 114 | 9.230  | 8.918   | 55.215  | 1.00 | 40.33 | O |
| HETATM 5171                 | O | HOH | 5 | 52  | 14.028 | -15.380 | 45.567  | 1.00 | 35.18 | O                           | HETATM 5234 | O | HOH | 5 | 115 | 22.589 | 1.623   | 39.518  | 1.00 | 52.68 | O |
| HETATM 5172                 | O | HOH | 5 | 53  | 18.437 | 19.379  | -1.489  | 1.00 | 46.92 | O                           | HETATM 5235 | O | HOH | 5 | 116 | 11.224 | 11.488  | -20.299 | 1.00 | 41.02 | O |
| HETATM 5173                 | O | HOH | 5 | 54  | 10.850 | 10.882  | 40.469  | 1.00 | 37.47 | O                           | HETATM 5236 | O | HOH | 5 | 117 | 27.821 | -4.673  | 48.712  | 1.00 | 53.08 | O |
| HETATM 5174                 | O | HOH | 5 | 55  | 14.231 | -9.178  | 54.155  | 1.00 | 40.97 | O                           | HETATM 5237 | O | HOH | 5 | 118 | 24.265 | -7.317  | -5.943  | 1.00 | 47.47 | O |
| HETATM 5175                 | O | HOH | 5 | 56  | 16.476 | -21.861 | -16.351 | 1.00 | 36.89 | O                           | HETATM 5238 | O | HOH | 5 | 119 | 2.634  | -5.449  | 30.299  | 1.00 | 56.26 | O |
| HETATM 5176                 | O | HOH | 5 | 57  | 4.711  | 9.136   | -0.253  | 1.00 | 36.20 | O                           | HETATM 5239 | O | HOH | 5 | 120 | 24.792 | 8.325   | 45.307  | 1.00 | 45.39 | O |
| HETATM 5177                 | O | HOH | 5 | 58  | 25.420 | -36.707 | 10.825  | 1.00 | 38.77 | O                           | HETATM 5240 | O | HOH | 5 | 121 | 24.417 | 48.318  | 72.713  | 1.00 | 36.96 | O |
| HETATM 5178                 | O | HOH | 5 | 59  | 7.420  | -21.920 | -4.863  | 1.00 | 42.30 | O                           | HETATM 5241 | O | HOH | 5 | 122 | 22.918 | -16.817 | 10.386  | 1.00 | 30.92 | O |
| HETATM 5179                 | O | HOH | 5 | 60  | -0.299 | 14.080  | -1.805  | 1.00 | 35.11 | O                           | HETATM 5242 | O | HOH | 5 | 123 | 30.129 | 50.096  | 36.353  | 1.00 | 35.13 | O |
| HETATM 5180                 | O | HOH | 5 | 61  | 20.158 | 25.600  | 32.093  | 1.00 | 37.98 | O                           | HETATM 5243 | O | HOH | 5 | 124 | 23.922 | 32.518  | 28.798  | 1.00 | 49.49 | O |
| HETATM 5181                 | O | HOH | 5 | 62  | 11.739 | 2.194   | -1.839  | 1.00 | 33.51 | O                           | HETATM 5244 | O | HOH | 5 | 125 | 27.500 | 23.266  | 55.457  | 1.00 | 42.15 | O |
| HETATM 5182                 | O | HOH | 5 | 63  | 7.262  | 33.641  | 50.137  | 1.00 | 30.59 | O                           | HETATM 5245 | O | HOH | 5 | 126 | 19.183 | 11.356  | 39.823  | 1.00 | 46.71 | O |
| HETATM 5183                 | O | HOH | 5 | 64  | 4.012  | 36.921  | 13.045  | 1.00 | 47.77 | O                           | HETATM 5246 | O | HOH | 5 | 127 | 26.820 | 10.982  | 54.219  | 1.00 | 49.96 | O |
| HETATM 5184                 | O | HOH | 5 | 65  | 18.220 | -1.985  | 40.009  | 1.00 | 45.69 | O                           | HETATM 5247 | O | HOH | 5 | 128 | 0.411  | -4.111  | 41.112  | 1.00 | 56.67 | O |
| HETATM 5185                 | O | HOH | 5 | 66  | 14.016 | 1.041   | -8.997  | 1.00 | 42.45 | O                           | HETATM 5248 | O | HOH | 5 | 129 | 28.398 | 31.996  | 32.402  | 1.00 | 46.72 | O |
| HETATM 5186                 | O | HOH | 5 | 67  | 17.939 | 32.783  | 2.392   | 1.00 | 40.23 | O                           | HETATM 5249 | O | HOH | 5 | 130 | 8.302  | 52.517  | 11.128  | 1.00 | 49.79 | O |
| HETATM 5187                 | O | HOH | 5 | 68  | 17.563 | -38.804 | 10.532  | 1.00 | 37.86 | O                           | HETATM 5250 | O | HOH | 5 | 131 | 12.533 | 46.905  | -6.451  | 1.00 | 44.90 | O |
| HETATM 5188                 | O | HOH | 5 | 69  | 11.549 | 25.921  | 3.663   | 1.00 | 41.36 | O                           | HETATM 5251 | O | HOH | 5 | 132 | -7.628 | -8.784  | 19.961  | 1.00 | 46.02 | O |
| HETATM 5189                 | O | HOH | 5 | 70  | 11.102 | -30.831 | 5.030   | 1.00 | 43.96 | O                           | HETATM 5252 | O | HOH | 5 | 133 | -9.621 | 44.381  | 0.035   | 1.00 | 43.25 | O |
| HETATM 5190                 | O | HOH | 5 | 71  | 9.931  | 51.075  | 31.778  | 1.00 | 54.34 | O                           | HETATM 5253 | O | HOH | 5 | 134 | -6.485 | 28.884  | 0.182   | 1.00 | 50.97 | O |
| HETATM 5191                 | O | HOH | 5 | 72  | 25.172 | -15.712 | -14.293 | 1.00 | 36.64 | O                           | HETATM 5254 | O | HOH | 5 | 135 | 22.663 | 39.049  | 51.662  | 1.00 | 50.82 | O |
| HETATM 5192                 | O | HOH | 5 | 73  | 28.872 | 40.243  | 19.577  | 1.00 | 32.11 | O                           | HETATM 5255 | O | HOH | 5 | 136 | 14.595 | -20.681 | -16.554 | 1.00 | 44.13 | O |
| HETATM 5193                 | O | HOH | 5 | 74  | 18.472 | -34.048 | 18.797  | 1.00 | 41.57 | O                           | HETATM 5256 | O | HOH | 5 | 137 | 1.454  | -19.418 | 47.668  | 1.00 | 39.46 | O |
| HETATM 5194                 | O | HOH | 5 | 75  | 5.762  | 31.018  | 47.574  | 1.00 | 36.70 | O                           | HETATM 5257 | O | HOH | 5 | 138 | -1.663 | -3.548  | 40.024  | 1.00 | 49.99 | O |
| HETATM 5195                 | O | HOH | 5 | 76  | 14.441 | 27.980  | 15.832  | 1.00 | 53.42 | O                           | HETATM 5258 | O | HOH | 5 | 139 | -0.211 | 1.278   | 40.084  | 1.00 | 35.64 | O |
| HETATM 5196                 | O | HOH | 5 | 77  | 24.102 | 35.506  | 17.232  | 1.00 | 45.64 | O                           | HETATM 5259 | O | HOH | 5 | 140 | 6.069  | -11.893 | 3.078   | 1.00 | 45.98 | O |
| HETATM 5197                 | O | HOH | 5 | 78  | 13.494 | 5.818   | 38.441  | 1.00 | 42.32 | O                           | HETATM 5260 | O | HOH | 5 | 141 | 25.292 | -2.046  | -3.599  | 1.00 | 43.15 | O |
| HETATM 5198                 | O | HOH | 5 | 79  | 9.664  | -29.385 | -1.699  | 1.00 | 43.86 | O                           | HETATM 5261 | O | HOH | 5 | 142 | 8.585  | -26.953 | 28.059  | 1.00 | 45.11 | O |
| HETATM 5199                 | O | HOH | 5 | 80  | 10.495 | 12.478  | 48.858  | 1.00 | 39.91 | O                           | HETATM 5262 | O | HOH | 5 | 143 | 23.038 | -24.235 | -13.472 | 1.00 | 54.16 | O |
| HETATM 5200                 | O | HOH | 5 | 81  | 0.402  | -11.496 | 49.895  | 1.00 | 36.43 | O                           | HETATM 5263 | O | HOH | 5 | 144 | 2.373  | 29.773  | -9.966  | 1.00 | 33.18 | O |
| HETATM 5201                 | O | HOH | 5 | 82  | -0.107 | -11.341 | 61.207  | 1.00 | 40.21 | O                           | HETATM 5264 | O | HOH | 5 | 145 | 26.196 | 32.545  | 33.815  | 1.00 | 36.09 | O |
| HETATM 5202                 | O | HOH | 5 | 83  | 5.091  | 31.773  | 21.013  | 1.00 | 30.13 | O                           | HETATM 5265 | O | HOH | 5 | 146 | 21.289 | -15.690 | -0.348  | 1.00 | 32.10 | O |
| HETATM 5203                 | O | HOH | 5 | 84  | 31.231 | -10.690 | -7.654  | 1.00 | 50.03 | O                           | HETATM 5266 | O | HOH | 5 | 147 | 17.594 | 48.808  | 34.303  | 1.00 | 46.77 | O |
| HETATM 5204                 | O | HOH | 5 | 85  | 13.124 | -9.496  | 8.063   | 1.00 | 37.68 | O                           | HETATM 5267 | O | HOH | 5 | 148 | -4.353 | 2.241   | 50.813  | 1.00 | 65.32 | O |
| HETATM 5205                 | O | HOH | 5 | 86  | -8.052 | -15.837 | 49.496  | 1.00 | 46.81 | O                           | HETATM 5268 | O | HOH | 5 | 149 | 11.264 | 27.767  | -2.583  | 1.00 | 36.40 | O |
| HETATM 5206                 | O | HOH | 5 | 87  | 10.664 | -33.786 | 2.816   | 1.00 | 43.17 | O                           | HETATM 5269 | O | HOH | 5 | 150 | 11.648 | 9.198   | -15.694 | 1.00 | 42.19 | O |
| HETATM 5207                 | O | HOH | 5 | 88  | 5.149  | -12.840 | 46.744  | 1.00 | 25.58 | O                           | HETATM 5270 | O | HOH | 5 | 151 | 3.708  | -16.205 | 49.767  | 1.00 | 31.38 | O |
| HETATM 5208                 | O | HOH | 5 | 89  | 10.417 | 12.452  | 5.835   | 1.00 | 38.84 | O                           | HETATM 5271 | O | HOH | 5 | 152 | 20.748 | -20.317 | -1.387  | 1.00 | 41.95 | O |
| HETATM 5209                 | O | HOH | 5 | 90  | 17.603 | -8.074  | 51.752  | 1.00 | 33.55 | O                           | HETATM 5272 | O | HOH | 5 | 153 | -1.950 | 19.571  | -2.141  | 1.00 | 47.10 | O |
| HETATM 5210                 | O | HOH | 5 | 91  | 9.521  | 35.944  | 48.873  | 1.00 | 39.11 | O                           | HETATM 5273 | O | HOH | 5 | 154 | 0.268  | -16.997 | 48.767  | 1.00 | 43.14 | O |
| HETATM 5211                 | O | HOH | 5 | 92  | 12.536 | -15.535 | 47.667  | 1.00 | 35.03 | O                           | HETATM 5274 | O | HOH | 5 | 155 | -3.240 | -1.957  | 56.892  | 1.00 | 46.11 | O |
| HETATM 5212                 | O | HOH | 5 | 93  | 8.454  | -31.290 | 2.769   | 1.00 | 48.47 | O                           | HETATM 5275 | O | HOH | 5 | 156 | 9.702  | -29.527 | 41.390  | 1.00 | 52.69 | O |
| HETATM 5213                 | O | HOH | 5 | 94  | 22.872 | 24.388  | 25.815  | 1.00 | 45.72 | O                           | HETATM 5276 | O | HOH | 5 | 157 | 20.010 | -1.815  | -0.315  | 1.00 | 50.51 | O |
| HETATM 5214                 | O | HOH | 5 | 95  | 11.098 | -31.422 | -1.370  | 1.00 | 43.62 | O                           | HETATM 5277 | O | HOH | 5 | 158 | 28.601 | -2.940  | 45.091  | 1.00 | 45.56 | O |
| HETATM 5215                 | O | HOH | 5 | 96  | 7.521  | 33.552  | 56.068  | 1.00 | 28.77 | O                           | HETATM 5278 | O | HOH | 5 | 159 | 14.813 | 2.883   | -2.462  | 1.00 | 44.99 | O |
| HETATM 5216                 | O | HOH | 5 | 97  | 13.649 | 27.440  | -5.484  | 1.00 | 34.11 | O                           | HETATM 5279 | O | HOH | 5 | 160 | 29.542 | -33.205 | 14.739  | 1.00 | 41.98 | O |
| HETATM 5217                 | O | HOH | 5 | 98  | -6.467 | -24.402 | 27.828  | 1.00 | 44.44 | O                           | HETATM 5280 | O | HOH | 5 | 161 | 21.346 | 0.836   | 41.053  | 1.00 | 52.07 | O |
| HETATM 5218                 | O | HOH | 5 | 99  | -2.216 | -18.660 | 51.247  | 1.00 | 41.94 | O                           | HETATM 5281 | O | HOH | 5 | 162 | 10.764 | 48.052  | 19.115  | 1.00 | 43.17 | O |
| HETATM 5219                 | O | HOH | 5 | 100 | 6.440  | -22.951 | 7.866   | 1.00 | 32.96 | O                           | HETATM 5282 | O | HOH | 5 | 163 | 26.424 | 0.272   | -15.472 | 1.00 | 43.20 | O |
| HETATM 5220                 | O | HOH | 5 | 101 | 29.979 | 27.683  | 44.383  | 1.00 | 57.33 | O                           | HETATM 5283 | O | HOH | 5 | 164 | 19.194 | 8.821   | -2.906  | 1.00 | 45.75 | O |
| HETATM 5221                 | O | HOH | 5 | 102 | 8.509  | 42.717  | 10.972  | 1.00 | 45.45 | O                           | HETATM 5284 | O | HOH | 5 | 165 | 9.969  | -1.159  | 8.832   | 1.00 | 43.44 | O |
| HETATM 5222                 | O | HOH | 5 | 103 | 5.880  | 6.854   | -15.901 | 1.00 | 44.46 | O                           | HETATM 5285 | O | HOH | 5 | 166 | 14.272 | 9.143   | 48.237  | 1.00 | 41.96 | O |
| HETATM 5223                 | O | HOH | 5 | 104 | -8.286 | 43.723  | -4.963  | 1.00 | 32.43 | O                           | HETATM 5286 | O | HOH | 5 | 167 | 11.387 | 13.560  | 40.035  | 1.00 | 38.98 | O |
| HETATM 5224                 | O | HOH | 5 | 105 | 27.174 | -6.506  | 45.778  | 1.00 | 38.09 | O                           | HETATM 5287 | O | HOH | 5 | 168 | 2.460  | -7.589  | 44.291  | 1.00 | 47.11 | O |
| HETATM 5225                 | O | HOH | 5 | 106 | 13.108 | -34.187 | 1.287   | 1.00 | 47.17 | O                           | HETATM 5288 | O | HOH | 5 | 169 | 11.884 | 2.594   | -9.742  | 1.00 | 48.87 | O |
| HETATM 5226                 | O | HOH | 5 | 107 | 15.260 | 41.609  | 5.458   | 1.00 | 35.25 | O                           | HETATM 5289 |   |     |   |     |        |         |         |      |       |   |

## INTERNATIONAL SEARCH REPORT

International application No.

PCT/CN2015/000602

**A. CLASSIFICATION OF SUBJECT MATTER**

A61K 38/17(2006.01)i; A61K 39/395(2006.01)i; A61P 37/04(2006.01)i; A61P 29/00(2006.01)i; A61P 35/00(2006.01)i;  
A61P 37/06(2006.01)i; A61P 31/04(2006.01)i; C07K 14/47(2006.01)i; C12N 15/70(2006.01)i; C07K 1/22(2006.01)i;  
C07K 1/18(2006.01)i; C07K 1/16(2006.01)i

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

**B. FIELDS SEARCHED**

Minimum documentation searched (classification system followed by classification symbols)

A61K; A61P; C12N; C07K

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

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

DWPI, SIPOABS, CNABS, CNKI, Google scholar, Pubmed: IFP35, IFI35, NMI, interferon induc+, disease, disorder, high level, activity, highly expressed, modulat+, inhibit+, suppress+, stimulat+, antibody, siRNA, cytokine, immuno+, sequence search based on SEQ ID NOs: 9-12

**C. DOCUMENTS CONSIDERED TO BE RELEVANT**

| Category* | Citation of document, with indication, where appropriate, of the relevant passages                                                                                                                                                                                          | Relevant to claim No.                             |
|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------|
| X         | Anshuman Das et al. "Interferon-Inducible Protein IFI35 Negatively Regulates RIG-I Antiviral Signaling and Supports Vesicular Stomatitis Virus Replication"<br><i>Journal of Virology</i> , Vol. Volume 88, No. No.6, 31 March 2014 (2014-03-31),<br>see the whole document | 88-90                                             |
| A         | Anshuman Das et al. "Interferon-Inducible Protein IFI35 Negatively Regulates RIG-I Antiviral Signaling and Supports Vesicular Stomatitis Virus Replication"<br><i>Journal of Virology</i> , Vol. Volume 88, No. No.6, 31 March 2014 (2014-03-31),<br>see the whole document | 1-28, 34, 35,<br>36-45(part), 46-53, 74-87, 91-93 |
| A         | WO 9928460 A2 (LEADD BVET AL.) 10 June 1999 (1999-06-10)<br>see the whole document                                                                                                                                                                                          | 1-28, 34, 35,<br>36-45(part),<br>46-53, 74-93     |



Further documents are listed in the continuation of Box C.



See patent family annex.

\* Special categories of cited documents:

“A” document defining the general state of the art which is not considered to be of particular relevance  
“E” earlier application or patent but published on or after the international filing date  
“L” document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)  
“O” document referring to an oral disclosure, use, exhibition or other means  
“P” document published prior to the international filing date but later than the priority date claimed

“T” later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention  
“X” document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone  
“Y” document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art  
“&” document member of the same patent family

Date of the actual completion of the international search

13 November 2015

Date of mailing of the international search report

25 November 2015

Name and mailing address of the ISA/CN

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## INTERNATIONAL SEARCH REPORT

International application No.

PCT/CN2015/000602

### C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category* | Citation of document, with indication, where appropriate, of the relevant passages                                                                                                                                                     | Relevant to claim No.                         |
|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------|
| A         | Lingqiang Zhang et al. "The PH domain containing protein CKIP-1 binds to IFP35 and Nmi and is involved in cytokine signaling"<br><i>Cellular Signalling</i> , Vol. volume 19, 17 November 2006 (2006-11-17),<br>see the whole document | 1-28, 34, 35,<br>36-45(part),<br>46-53, 74-93 |

## INTERNATIONAL SEARCH REPORT

International application No.

PCT/CN2015/000602

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

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

1. ☒ Claims Nos.: **1-24, 40-45, 64-69**  
because they relate to subject matter not required to be searched by this Authority, namely:
  - [1] Claims 1-24 relate to methods for treating or preventing diseases associated with abnormally high level or activity of IFP35 and/or NMI with an effective amount of agents that prevent or reduce production or an activity of IFP35 and/or NMI; claims 40-45 relate to methods for treating or preventing diseases associated with abnormally high level or activity of IFP35 and/or NMI with antibodies; claims 64-69 relate to methods for stimulating an immune response in a subject with polypeptides or pharmaceutical compositions.
  - [2] Thus claims 1-24, 40-45 and 64-69 may be excluded from international search according to Rule 39.1(iv).
  - [4] Claims 1-24 might be reasonably expected to be direct to the alleged uses of agents that prevent or reduce production or an activity of IFP35 and/or NMI for the manufacture of pharmaceutical compositions for treating or preventing diseases associated with abnormally high level or activity of IFP35 and/or NMI; claims 40-45 might be reasonably expected to be direct to the alleged uses of antibodies for the manufacture of pharmaceutical compositions for treating or preventing diseases associated with abnormally high level or activity of IFP35 and/or NMI; claims 64-69 might be reasonably expected to be direct to the alleged uses of polypeptides or pharmaceutical compositions for the manufacture of pharmaceutical compositions for stimulating an immune response in a subject.
  - [5] The international search is carried out on the basis of said condition.
2. ☒ Claims Nos.: **29-33, 36-45(part), 54-73**  
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:
  - [1] The technical solutions of claims 29-33, 54-73, and the part of 36-45 citing claims 29-33, refer to sequences of SEQ ID NOs:2, 4, 6 and 8, which are not disclosed in the description. Either, there is not any form of sequence listing filed. Therefore, no meaningful international search on claims 29-33, 54-73, and the part of 36-45 citing claims 29-33 could be carried out.
3. ☐ Claims Nos.:  
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

**INTERNATIONAL SEARCH REPORT**  
**Information on patent family members**

International application No.

**PCT/CN2015/000602**

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