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Supplemental Data

Allosteric Inhibition of the Protein-Protein Interaction between the Leukemia-Associated Proteins Runx1 and CBFβ

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NMR-Based Modeling

Table S1. Results of SDILICON Calculations for Seven Clusters of Compound **10**

Cluster	Final shift deviation (ppm)	Shift penalty energy contribution (kcal/mol)	Final energy of the system (kcal/mol)
1	0.033 +/- 0.029	3.86	-11.87
2	**0.026 +/- 0.018**	**1.97**	**-12.04**
3	0.031 +/- 0.029	3.72	-8.13
4	**0.035 +/- 0.015**	**2.90**	**-12.29**
5	0.035 +/- 0.025	3.73	-8.41
6	0.029 +/- 0.032	3.78	-7.57
7	0.042 +/- 0.028	5.10	-5.17

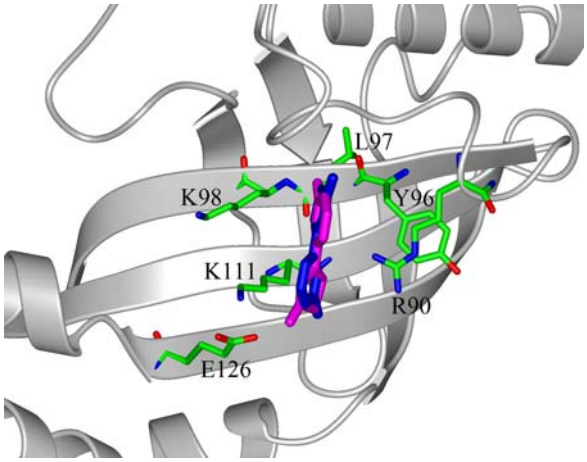


Figure S1. Two Binding Modes of 10 (Cluster 2 in Magenta, Cluster 4 in Blue) to CBFβ Calculated using SDILICON

Sidechains of CBFβ residues interacting with **10** are shown in stick representation (C, green; O, red; N, blue).

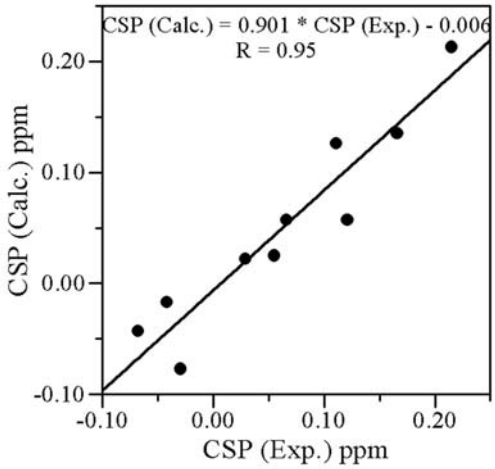
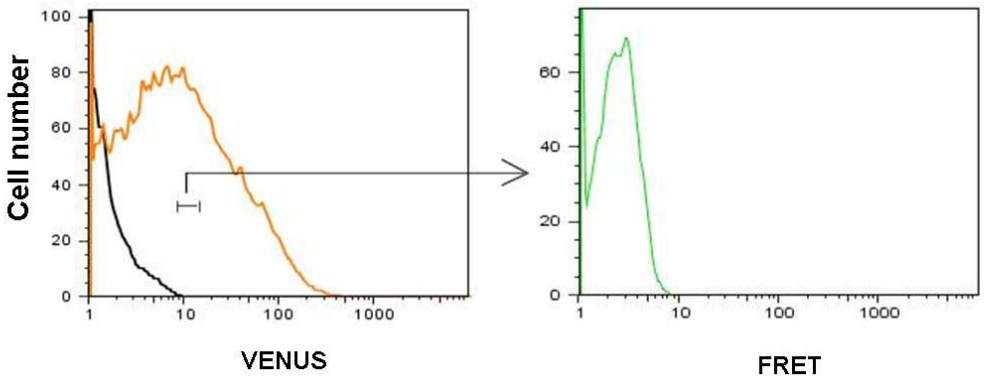
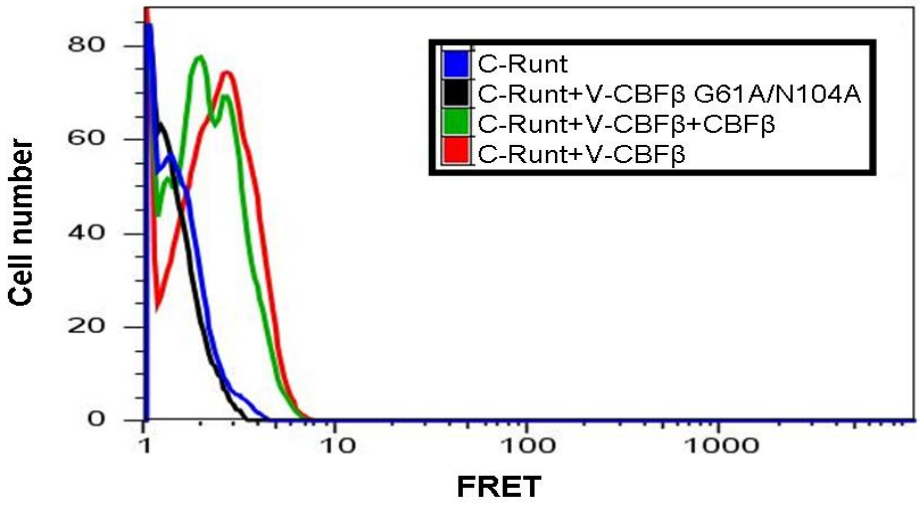


Figure S2. The Correlation of NMR Chemical Shift Perturbations (CSP) for the Amide Protons of CBFβ Observed upon the Binding of 10 with the CSP Calculated with the SDILICON Approach



A.



B.

Figure S3. FACS/FRET Analysis Strategy

(**A**) C-Runt and V-CBFβ transfected HEK293 cells (■ line) were gated on cells expressing a uniform level of Venus fluorescence (488 nm laser; 530 nm/30 filter). Control untransfected cells are represented by the ■ line. Subsequently, the FRET profile of gated cells (horizontal bar) is analyzed using the geometric mean parameter in the histogram on the right (407 nm laser; 530 nm/30 filter).

(**B**) Overlay of FRET (407 nm laser; 530 nm/30 filter) profiles from cells emitting uniform Venus signal (as shown in panel A) in the positive control (C-Runt + V-CBFβ), 50% competition (C-Runt + V-CBFβ + CBFβ) and absolute (C-Runt + V-CBFβ G61A/N104A) negative controls. The background FRET signal from cells transfected with C-Runt only is also shown (a fraction of Cerulean emission extends into the FRET channel).

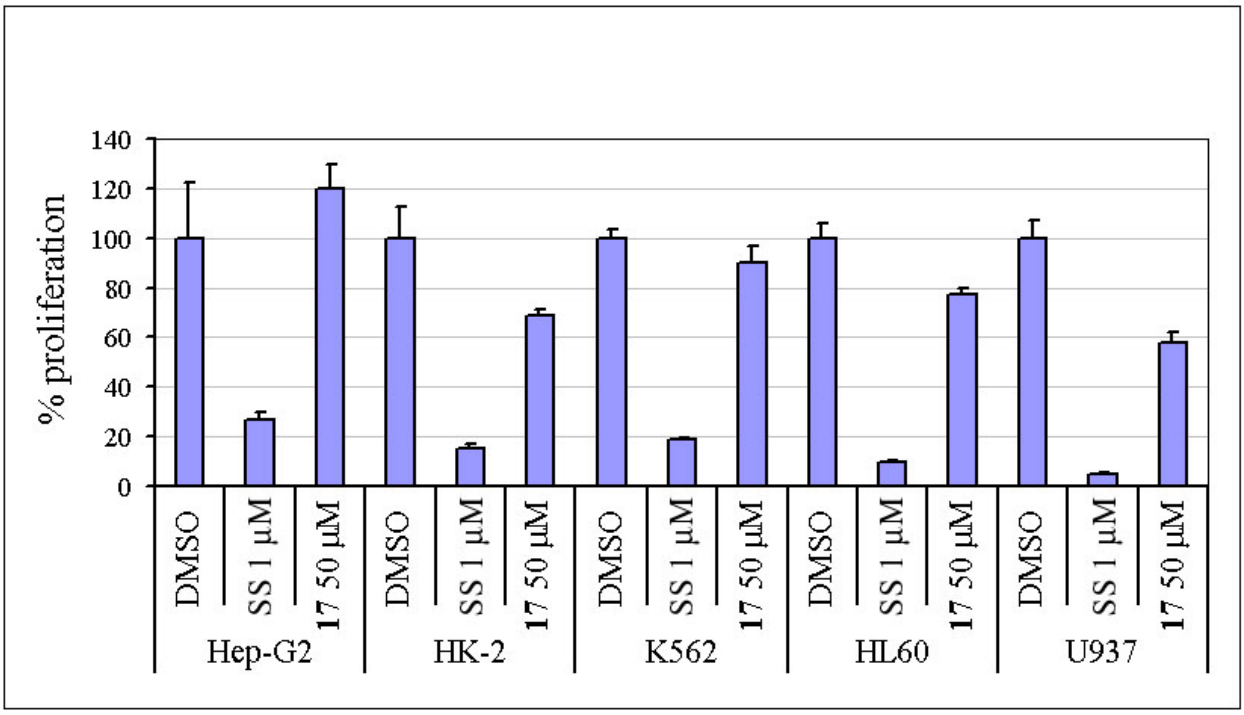


Figure S4. MTT Assays of the Effects of 17 on the Proliferation of Hep-G2, HK-2, K562, HL60, and U937 Cells

All five cell lines were purchased from American Type Culture Collection (Manassas, VA) and grown as described below. An MTT assay was performed as described for the ME-1 cell line in Materials and Methods. Data shown represents the mean ± s.d. of 4 independent measurements.

Virtual Screening

The 20 conformers of CBFβ used to represent the solution structure of the protein were employed for virtual screening, by combining the molecular mechanics energies computed for the docked compounds to each conformer, using an approximation to the previously described K* method of computing binding affinities (K_d) from conformational ensembles of structures [1]. The top-scoring 35 compounds were then selected for experimental screening using NMR spectroscopy.

ELISA Assay

His_6-CBFβ (1-141) was expressed and purified in the same way as CBFβ for NMR with the exception of the protease cleavage step, which was omitted during the preparation of the protein for ELISA. Cerulean-Runt domain fusion protein was prepared as for the FRET assay. Both proteins were dialyzed into ELISA buffer (1x PBS with 0.01% BSA, PBSA). His_6-CBFβ (0.6 μM) was adsorbed onto Ni^{2+} coated 96-wells High Sensitivity plates (ELISA plates, Sigma-Aldrich) at room temperature for 1.5 h and subsequently washed three times with 200 μl of PBSA. A 200 μl aliquot of Cerulean-Runt domain (1.2 μM) and 10.5 μl of 100% DMSO solutions of the compounds (usually 0.1μM – 2000 μM) were mixed on 96-well clear v-bottom plate and 200 μl of the mixture was added to the ELISA plate and incubated for 1.5h. A mixture of Cerulean-Runt domain and 100% DMSO served as a positive control, while PBSA with DMSO was used as a negative control. After washing, plates were incubated for 1h with 200 μl of anti-GFP-horseradish peroxidase conjugates (Miltenyi Biotec) diluted 1:1000 with 1x PBSB followed by washing and addition of 100 μl of Super Aqua Blue ELISA substrate (eBioscience). The enzyme activity was controlled by measurement of absorbance at 405 nm using PHERAstar microplate reader. Absorbance was plotted versus the log of compound concentration and the resulting curve was fit to a sigmodial curve using Origin7.0 (MicroCal, Inc.). Mean values of IC_{50} originating from two independent measurements performed in duplicates together with the standard deviations are reported.

NMR Spectroscopy

Expression, labeling, and purification of ^{15}N-labeled CBFβ was carried out as described previously.[2] NMR samples were prepared by mixing a 340 μl aliquot of CBFβ (0.235 mM) with 20 μl of 20 mM DTT in D_2O and 40 μl of a 10 mM DMSO solution of the various

compounds. The solution was gently pipetted up and down for mixing and then placed into a Shigemi NMR tube. ^{15}N-^{1}H HSQC spectra were recorded on a 500 MHz NMR Varian Inova spectrometer at 20 °C. NMR spectra were processed in NMRPipe and analyzed in Sparky (Goddard, T.D. and Kneller, J. M. University of California, San Francisco).

NMR-Based Docking

^{1}H-^{15}N HSQC spectra for 0.2 mM ^{15}N labeled CBFβ and for the protein mixed with **10** and **8** (up to 5% final DMSO concentration) in molar ratios of 1:2 and 1:6 were collected on a 500 MHz NMR Varian Inova spectrometer at 20 °C. Quantification of ^{1}HN and ^{15}N chemical shift perturbations (CSP) was obtained from the comparison of the ^{15}N-^{1}H HSQC spectra for unliganded CBFβ and its complex with each ligand, collected for the 1:6 molar ratio. The X-ray structure of CBFβ originating from its complex with the Runt domain (PDB code 1E50) was used to guide docking of two compounds (**10** and **8**). The hydrogen atoms were added to the protein using the Insight II/Builder (Accelrys) program. The starting conformations of **10** and **8** were built in the InsightII/Builder program. The structures of the ligands were optimized in an *ab initio* LCAO MO SCF approach at the 6-31G* basis set using the Gaussian98 program. These structures were subjected to flexible docking to the CBFβ binding site employing LigandFit/Cerius2 (Accelrys) approach [3] and using the Dreiding force field [4]. The CBFβ binding site employed for the docking experiments was defined by mapping the experimentally measured chemical shift perturbations observed during ligand binding onto the CBFβ structure. Flexible docking, employing Monte Carlo simulations (100,000 trials), was performed with LigandFit. One hundred of the lowest energy and diverse docking conformations were saved and clustered using the Leader method with an RMS distance threshold of 1.5 Å. The best member from each cluster was saved for further analysis. This resulted in seven clusters for **10** and five

clusters for **8**, representing different possible orientations of the ligands in the protein binding site. The best scored conformer from each cluster was used as a starting ligand 'pose' for its further optimization with the SDILICON (Shift Directed Ligand Conformation) program (http://tonga.usip.edu/gmoyna/sdilicon/sdilicon.c), which requires a pre-docked ligand molecule in the protein binding site. Experimentally measured CSP from ^{15}N-^{1}H HSQC spectra have been used for the calculation of binding modes for **10** and **8** by SDILICON. In this procedure the expected CSP of the protein, resulting from the particular ligand orientation, are calculated and the differences between experimental and simulated CSP are minimized by optimizing ligand position in the protein binding site to best fit the NMR data. The resulting ligand binding modes, with the best agreement of experimentally measured and calculated CSP, were selected and compared between the two compounds. The final ligand binding mode was chosen based on analysis of the potential interactions of all ligands considered in the paper.

Analysis of Compound Inhibition in HEK293 Cells by FACS/FRET

Suspension HEK 293 cells were kindly provided by Dr. Ta Yuan Chang (Dartmouth Medical School, Hanover, NH). Cells were grown in DMEM/F-12 50:50 media (Cellgro) supplemented with 5% FBS (HyClone) and 2.5 mM L-glutamine in T-75 flasks. Upon 60% confluence, cells were transfected using Fugene 6 reagent (Roche) with 5.3 μg each of Cerulean-Runt pcDNA3.1 and Venus-CBFβ pcDNA-3.1 (or Venus-CBFβ G61A/N104A pcDNA-3.1) and CBFβ-pcDNA3.1 plasmids. Cells transfected with Venus-CBFβ pcDNA3.1 or Cerulean-Runt pcDNA3.1 alone were used as additional controls to adjust inter-laser compensation. Empty pcDNA3.1 plasmid was used to normalize total DNA quantities transfected. 36 to 48 hours post-transfection, cells were resuspended in serum-free, phenol-red free DMEM:F-12 medium (Sigma) and split into 5mL falcon tubes. Compounds were dissolved in DMSO and added to the cells at 25 μM or 100 μM concentrations for a final 1% DMSO concentration for 5 hours at 37 ºC. All controls were

treated with 1% DMSO alone. Venus, Cerulean and FRET emission from individual cells were collected on the FACSDiVa flow cytometer, equipped with Coherent® Sapphire™ solid state (488 nm) and Point Source Violet (407 nm) lasers. Venus (530 nm/30 filter) and Cerulean (450 nm/40 filter) emissions were collected upon excitation with 488 nm or 407 nm laser, respectively. FRET refers to Venus emission (530 nm/30 filter) upon excitation at 407nm. FACS and statistical data analyses were performed using FlowJo7 (Treestar) and GraphPad Prism 4 software programs, respectively. FRET output was defined as the geometric mean of FRET signals from a population of cells gated based on a uniform Venus expression level in each treatment. Subsequently, a regression line was determined based on measurements of the FRET for three protein combinations: Cerulean-Runt + Venus-CBFβ, Cerulean-Runt + Venus-CBFβ + CBFβ, and Cerulean-Runt + Venus-CBFβ (G61A/N104A)), defined as 100%, 50% and 0% FRET, respectively. The FRET signal from each treatment was converted to relative percent FRET based on the regression line.

MTT Assays of the Effects of 17 on the Proliferation of Hep-G2, HK-2, K562, HL60, and U937 Cells

All five cell lines were purchased from American Type Culture Collection (Manassas, VA) and cultured in RPMI with 10% fetal bovine serum, 1% penicillin/streptomycin, and 2 mg/ml sodium bicarbonate (Hep-G2), DMEM with 10% FBS, 1% P/S, and 15 mmol/l HEPES (HK-2), DMEM with 10% FBS and 1% P/S (K562), and RPMI with 10% FBS and 1% P/S (HL60, U937). Ninety µl of cells at $1.7 * 10^5$ cells/ml (Hep-G2), $1.2 * 10^5$ cells/ml (HK-2), and $2 * 10^5$ cells/ml (K562, HL60, U937) were placed in 96 well plates and treated with **17** or DMSO control for 72 hours. An MTT assay was then performed as previously described for the ME-1 cell line in Materials and Methods.

Chemical Synthesis

All chemicals were obtained from Aldrich Chemical Company, Milwaukee, Wisconsin or Lancaster Synthesis Inc., Windham, New Hampshire. Compounds **1-3** were purchased from Sigma. Melting points were measured on an Electrothermal Mel-Temp and are uncorrected. Carbon and proton NMR spectra were recorded on a General Electric 300 MHz spectrometer. Chemical shifts are expressed in ppm and coupling constants (J) are in hertz (Hz). Peak multiplicities are abbreviated: broad, br; singlet, s; doublet, d; triplet, t; quartet, q; multiplet, m. Mass spectra were obtained on a Finnagan LcQ Classic spectrometer. High resolution (EI) mass spectra were obtained from the University of Illinois, Urbana-Champaign. Combustion analyses were performed by Atlantic Microlabs Inc.

Naphtho[1,2-d]-thiazol-2-ylamine (4) [[i]Chem Pharm Bull 1991, 39, 11, 2888]

[i] Benzoyl chloride (70.4 mmol) was added drop wise to a solution of ammonium thiocyanate (75 mmol) in acetone (50 mL) and the mixture was stirred for 20 minutes at 50 °C. A solution of α-naphthylamine (65 mmol) in acetone (50 mL) was added drop wise and the mixture was stirred for an additional 1 h at the same temperature. The mixture was diluted with water (50 mL) and the precipitate was collected by filtration and washed with water. The solid was added to 2 N aq. NaOH (100 mL), refluxed for 1 h, and then poured into water. The precipitate was collected by filtration and recrystallized from MeOH to give 1-naphthylthiourea as a purple solid (5.34 g, 41%). mp 195 – 196 °C (lit.[4] 204 – 205 °C); ^{1}H NMR (DMSO-d^{6}) δ 7.48 – 7.57 (m, 5H), 7.82 – 7.98 (m, 4H), 9.73 (s, 1H); ^{13}C NMR (DMSO-d^{6}) δ 123.8, 126.0, 126.7, 127.2, 127.8, 129.1, 130.6, 134.9, 135.3, 183.3; ESI *m/z* 203 (M^{+}).

Bromine (14.85 mmol) was added to a suspension of 1-naphthylthiourea (14.85 mmol) in acetic acid (30 mL) at 0 °C. After stirring at room temperature for 30 minutes, Et_2O was added and the precipitate was collected by filtration and washed with Et_2O. The precipitate was treated

with 25% aq. NH_4OH at room temperature for 1 h. The mixture was filtered and the precipitate was recrystallized from CH_2Cl_2 / MeOH to give a purple solid (1.48 g, 50%). mp 186 – 189 °C (lit.[4] 183 – 186 °C); ^{1}H NMR (DMSO-d^6) δ 7.38 – 7.51 (m, 3H), 7.59 (s, 2H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 8.30 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (DMSO-d^6) δ 120.2, 121.6, 124.3, 126.0, 126.5, 126.8, 128.9, 132.6, 133.4, 153.2, 168.5; APCI *m/z* 201 $[M+H]^+$. Anal. ($C_{11}H_8N_2S$) C, H, N.

Method A: General Procedure for Synthesis of 2-Aminothiazolium Salts (**5-20**)

Thiourea (30 mmol) and iodine (11 mmol) were added to a stirring solution of the appropriate ketone (10 mmol) in absolute ethanol (20 mL). The mixture was heated at 100 °C for 2-3 h in an open vessel and cooled to room temperature. Water was added to the crude residue and the precipitate was collected by filtration and washed with ether.

4-(4'-Trifluoromethylphenyl)-thiazol-2-yl ammonium iodide (5)

Compound **5** was prepared from 4'-(trifluoromethyl)acetophenone (1.12 mmol) using method A and was isolated as a yellow solid (0.75 g, 39%). mp 123-125 °C; ^{1}H NMR (DMSO-d^6) δ 7.36 (s, 1H), 7.80 (d, *J* = 7.9 Hz, 2H), 7.88 (d, *J* = 7.5 Hz, 2H); ^{13}C NMR δ 106.4, 126.6, 126.8, 127.4, 127.6, 127.7, 127.8, 134.9, 141.1, 170.9; EI HRMS calcd for $C_{10}H_8F_3IN_2S$ (M^+-HI) *m/z* 245.035900, found *m/z* 245.036030.

4-(4'-Methoxyphenyl)-thiazol-2-yl ammonium iodide (**6**)

Compound **6** was prepared from 4'-methoxyacetophenone (10 mmol) using method A and was isolated as a white solid (3.16 g, 94%). mp 189-191 °C; ^{1}H NMR (DMSO-d^6) δ 3.74 (s, 3H), 6.99 (d, *J* = 8 Hz, 2H), 7.04 (s, 1H), 7.57 (d, *J* = 8 Hz, 2H), 8.92 (br s); ^{13}C NMR δ 56.4, 101.8, 115.4, 121.9, 128.3, 139.5, 161.1, 171.1; APCI *m/z* 206 $[M+H]^+$-HI; Anal. ($C_{10}H_{11}IN_2OS$) C, H, N.

4-(3',4'-Dimethoxyphenyl)-thiazol-2-yl ammonium iodide (7)

Compound **7** was prepared from 3',4'-dimethoxyacetophenone (10 mmol) using method A and was isolated as a white solid (3.40 g, 93%). mp 251 – 253 °C; ^{1}H NMR (DMSO-d^{6}) δ 3.74 (s, 3H), 3.77 (s, 3H), 7.02 (d, *J* = 8.5 Hz, 1H), 7.12 (s, 1H), 7.14 – 7.28 (m, 2H); ^{13}C NMR (DMSO-d^{6}) δ 56.6, 56.8, 102.0, 110.5, 112.8, 120.0, 122.3, 140.1, 149.9, 150.8, 171.0; APCI *m/z* 237 $[M+H]^{+}$-HI.

4-(3',4'-Methylenedioxyphenyl)-thiazol-2-yl ammonium iodide (8)

Compound **8** was prepared from 3',4'-(methylenedioxy)acetophenone (10 mmol) using method A and was isolated as a gray solid (2.65 g, 76%). mp 198 – 200 °C; ^{1}H NMR (DMSO-d^{6}) δ 6.04 (s, 2H), 6.99 (d, *J* = 8.1 Hz, 1H), 7.05 (s, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.27 (s, 1H); ^{13}C NMR (DMSO-d^{6}) δ 102.3, 102.6, 107.2, 109.5, 121.0, 124.1, 140.6, 148.8, 149.1, 170.9; APCI *m/z* 221 $[M+H]^{+}$-HI.

4-(3'-Chlorophenyl)-thiazol-2-yl ammonium iodide (**9**)

Compound **9** was prepared from 3'-chloroacetophenone (10 mmol) using method A and was isolated as a yellow solid (1.83 g, 54%). mp 166-169 °C; ^{1}H NMR (DMSO-d^{6}) δ 7.31 (s, 1H), 7.43 (m, 2H), 7.62 (d, *J* = 6.2 Hz, 1H), 7.74 (s, 1H); ^{13}C NMR δ 105.5, 125.4, 126.4, 129.9, 131.8, 132.2, 134.6, 139.6, 170.9; APCI *m/z* 211 $[M+H]^{+}$-HI; Anal. ($C_9H_8ClIN_2S$): C, H, N.

4-(3'-Methylphenyl)-thiazol-2-yl ammonium iodide (10)

Compound **10** was prepared from 3'-methylacetophenone (10 mmol) using method A and was isolated as a white solid (2.67 g, 84%). mp 158 – 160 °C; ^{1}H NMR (DMSO-d$_6$) δ 2.33 (s, 3H), 7.19 – 7.51 (m, 5H); ^{13}C NMR (DMSO-d$_6$) δ 21.7, 103.5, 123.7, 127.0, 129.3, 129.7, 130.9, 139.1, 139.8, 170.9; APCI *m/z* 191 $[M+H]^{+}$-HI.

4-(3'-Methoxyphenyl)-thiazol-2-yl ammonium iodide (**11**)

Compound **11** was prepared from 3'-methoxyacetophenone (10 mmol) using method A and was isolated as a white solid (2.58 g, 77%). mp 236-238 °C; ^{1}H NMR (DMSO-d^{6}) δ 3.76 (s, 3H), 6.96 (d, *J* = 7.7 Hz, 1H), 7.21 (m, 2H), 7.23 (s, 1H), 7.36 (t, *J* = 7.9 Hz, 1H); ^{13}C NMR δ 56.4, 104.2, 112.4, 115.9, 119.0, 131.2, 131.3, 140.3, 160.5, 171.0; APCI *m/z* 206 $[M+H]^{+}$-HI.

4-(3'-Trifluoromethoxyphenyl)-thiazol-2-yl ammonium iodide (12)

Compound **12** was prepared from 3'-(trifluoromethoxy)acetophenone (4.9 mmol) using method A and was isolated as a white solid (0.83 g, 44%). mp 158 – 160 °C; ^{1}H NMR (DMSO-d_6) δ 7.36 (s, 1H), 7.40 (s, 1H), 7.59 (t, *J* = 8.1 Hz, 1H), 7.73 – 7.78 (m, 2H); ^{13}C NMR (DMSO-d_6) δ 105.3, 119.1, 121.8, 125.5, 126.3, 130.4, 131.7, 132.8, 149.4, 170.5; APCI *m/z* 260 $[M+H]^{+}$-HI; Anal. ($C_{10}H_8F_3IN_2OS$) C, H, N.

4-(2'-Methylphenyl)-thiazol-2-yl ammonium iodide (13)

Compound **13** was prepared from 2'-methylacetophenone (10 mmol) using method A and was recrystallized from MeOH / Et_2O to give a yellow solid (2.09 g, 66%). mp 174 – 176 °C; ^{1}H NMR (DMSO-d_6) δ 2.06 (s, 3H), 6.90 (s, 1H), 7.02 – 7.09 (m, 2H), 7.27 – 7.35 (m, 2H); ^{13}C NMR (DMSO-d_6) δ 20.7, 106.1, 126.8, 129.8, 130.3, 131.4, 137.1, 158.3, 170.2; APCI *m/z* 191 $[M+H]^{+}$-HI.

4-(2'-Chlorophenyl)-thiazol-2-yl ammonium iodide (**14**)

Compound **14** was prepared from 2'-chloroacetophenone (10 mmol) using method A and was isolated as a yellow solid (1.98 g, 59%). mp 82-84 °C; ^{1}H NMR (DMSO-d^{6}) δ 7.06 (s, 1H), 7.40-7.60 (m, 4H); ^{13}C NMR δ 108.5, 128.6, 129.0, 131.0, 132.5, 132.7, 132.8, 136.6, 170.3; APCI *m/z* 211 $[M+H]^{+}$-HI; Anal. ($C_9H_8ClIN_2S$) C, H, N.

4-(2'-Methoxyphenyl)-thiazol-2-yl ammonium iodide (**15**)

Compound **15** was prepared from 2'-methoxyacetophenone using method A and was isolated as a white solid (2.74 g, 82%). mp 220-221 °C; ^{1}H NMR δ 3.83 (s, 3H), 7.02 (t, *J* = 7.5 Hz, 1H), 7.10 (s, 1H), 7.14 (d, *J* = 8.5 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 7.4 Hz, 1H); ^{13}C NMR δ 56.9, 106.3, 113.0, 118.0, 121.8, 130.0, 132.2, 136.4, 157.1, 170.2; APCI *m/z* 206 $[M+H]^{+}$-HI.

4-(2',4'-Dichlorophenyl)-thiazol-2-yl ammonium iodide (16)

Compound **16** was prepared from 2',4'-dichloroacetophenone (10 mmol) using method A and was isolated as a yellow solid (1.88 g, 50%). mp 174-176 °C; ^{1}H NMR (DMSO-d^{6}) δ 7.06 (s, 1H), 7.45 (d, *J* = 8.3 Hz, 1H), 7.64 (s, 1H), 7.73 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR δ 108.3, 128.4, 130.6, 131.4, 132.8, 133.5, 134.1, 142.5, 169.0; EI HRMS calcd for $C_9H_7Cl_2IN_2S$ (M^{+}-HI) *m/z* 244.970600, found *m/z* 244.970701.

5-Ethyl-4-(4'-methoxyphenyl)-thiazol-2-yl ammonium iodide (17)

Compound **17** was prepared from 4'-methoxybutyrophenone (1.4 mmol) using method A and was isolated as a light yellow solid (1.21 g, 60%). mp 127 – 130 °C; ^{1}H NMR (DMSO-d^{6}) δ 1.10 (t, *J* = 7.3 Hz, 3H), 2.59 (q, J_1 = 7.3 Hz, J_2 = 7.7 Hz, 2H), 3.76 (s, 3H), 7.03 (d, *J* = 8.5 Hz, 2H), 7.37 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (DMSO-d^{6}) δ 16.3, 20.2, 56.3, 100.5, 114.8, 115.2, 121.7, 131.0, 160.9, 168.4, 174.6; APCI *m/z* 235 $[M+H]^{+}$-HI.

5-Propyl-4-(4'-methoxyphenyl)-thiazol-2-yl ammonium iodide (18)

Compound **18** was prepared from 4'-methoxyvalerophenone (5.21 mmol) using method A and was isolated as a white solid (0.77 g, 39%). mp 141 – 143 °C; ^{1}H NMR (DMSO-d^{6}) δ 0.81 (t, *J* = 6.9 Hz, 3H), 1.48 (m, 2H), 2.54 (t, *J* = 7.4 Hz, 2H), 3.76 (s, 3H), 7.03 (d, *J* = 8.1 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (DMSO-d^{6}) δ 14.2, 24.6, 28.3, 56.3, 115.3, 120.2, 121.8, 131.1, 160.9, 168.4, 175.2; APCI *m/z* 249 $[M+H]^{+}$-HI.

***m*-Tolyl-butan-1-one**

Ground magnesium turnings (10.25 mmol) and iodine (2 crystals) were heated with a heat gun until iodine vapor was produced, cooled to room temperature, and a solution of 1-bromopropane (9.39 mmol) in Et_2O (10 mL) was added drop wise. The mixture was stirred for 30 minutes at room temperature and *m*-tolunitrile (8.54 mmol) in Et_2O (20 mL) and $Cu^{(I)}Br$ (0.17 mmol) were added. The mixture was refluxed for 1 h, cooled to room temperature, and water was added slowly followed by the addition of 1 M aq. H_2SO_4 (20 mL). The mixture was stirred at room temperature overnight, extracted with EtOAc, dried, and concentrated. The residue was purified by column chromatography (silica gel, 20% EtOAc/hexanes, $R_f = 0.64$) to give a pale yellow oil (1.05 g, 76%). ^{1}H NMR ($CDCl_3$) δ 1.01 (t, J = 5.7 Hz, 3H), 1.73 – 1.80 (m, 2H), 2.41 (s, 3H), 2.91 – 2.96 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 13.9, 17.8, 21.3, 40.5, 125.2, 128.4, 128.5, 133.6, 137.1, 138.3, 200.6; APCI *m/z* 163 $[M+H]^+$.

5-Ethyl-4-*m*-tolyl-thiazol-2-yl ammonium iodide (19)

Compound **19** was prepared from *m*-tolyl-butan-1-one (1.85 mmol) using method A and was isolated as a yellow solid (0.17 g, 27%). mp 140 – 143 °C; ^{1}H NMR (DMSO-d_6) δ 1.13 (t, J = 6.6 Hz, 3H), 2.37 (s, 3H), 2.66 (q, J_1 = 8.1 Hz, J_2 = 6.6 Hz, 2H), 7.30 – 7.43 (m, 4H); ^{13}C NMR (DMSO-d_6) δ 15.4, 19.2, 20.9, 121.9, 125.7, 128.8, 129.0, 130.1, 131.0, 133.4, 138.2, 157.7, 167.5; APCI *m/z* 219 $[M+H]^+$-HI.

2-Methoxyphenyl-butan-1-one

Ground magnesium turnings (9.01 mmol) and iodine (2 crystals) were heated with a heat gun until iodine vapor was produced, cooled to room temperature, and a solution of 1-bromopropane (8.26 mmol) in Et_2O (10 mL) was added drop wise. The mixture was stirred for 30 minutes at room temperature and 2-methoxybenzonitrile (7.51 mmol) in Et_2O (20 mL) and $Cu^{(I)}Br$ (0.15

mmol) were added. The mixture was refluxed for 1 h, cooled to room temperature, and water was added slowly followed by the addition of 1 M aq. H_2SO_4 (20 mL). The mixture was stirred at room temperature overnight, extracted with EtOAc, dried, and concentrated. The residue was purified by column chromatography (silica gel, 20% EtOAc/hexanes, R_f = 0.45) to give a colorless oil (0.39 g, 29%). ^{1}H NMR ($CDCl_3$) δ 0.95 (t, *J* = 7.5 Hz, 3H), 1.69 (sextet, *J* = 7.5 Hz, 2H), 2.93 (t, *J* = 7.5 Hz, 2H), 3.88 (s, 3H), 6.93 – 7.00 (m, 2H), 7.42 (t, *J* = 6.9 Hz, 1H), 7.63 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 14.2, 18.0, 45.9, 55.7, 111.7, 120.8, 129.0, 130.3, 133.3, 158.6, 203.4; APCI *m/z* 179 $[M+H]^+$.

5-Ethyl-4-(2-methoxyphenyl)-thiazol-2-yl ammonium iodide (20)

Compound **20** was prepared from 2-methoxyphenyl-butan-1-one (2.17 mmol) using method A and was isolated as a yellow solid (0.60 g, 76%). mp 108 – 110 °C; ^{1}H NMR (DMSO-d_6) δ 1.01 (t, *J* = 7.4 Hz, 3H), 2.39 (m, 2H), 3.73 (s, 3H), 7.00 (m, 1H), 7.10 (m, 1H), 7.25 (m, 1H), 7.42 (t, *J* = 5.4 Hz, 1H), 8.94 (br s, 2H); ^{13}C NMR (DMSO-d_6) δ 15.1, 19.3, 55.7, 111.8, 116.7, 120.5, 123.0, 130.0, 131.3, 131.7, 157.1, 167.2; APCI *m/z* 235 $[M+H]^+$-HI; Anal. ($C_{12}H_{15}IN_2OS \cdot 0.5\ H_2O$) C, H, N.

4-(4-Ethoxyphenyl)-5-ethyl-1,3-thiazol-2-yl ammonium iodide (21)

4-Ethoxybenzonitrile (2.0 g, 13.60 mmol) and $Cu^{(I)}Br$ (39.0 mg, 0.27 mmol) were added to a solution of propylmagnesium chloride (8.2 ml, 16.4 mmol, 2.0 M in diethyl ether) in THF (30 ml). The mixture was stirred at room temperature for 1 h, water (10 ml) was added slowly followed by the addition of 15 % H_2SO_4 (20 mL). The mixture was stirred at room temperature for 2 h, extracted with ether, dried over Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography to give 1-(4-ethoxyphenyl)butan-1-one as a clear oil (2.61 g, 100 %). ^{1}H NMR ($CDCl_3$) δ 0.99 (t, J = 7.5, 7.5 Hz, 3H), 1.43 (t, J = 6.9, 7.2 Hz, 3H), 1.67 - 1.81 (m, 2H), 2.89 (t, J = 7.5, 7.2 Hz, 2H), 4.09 (dd, J = 6.9, 7.2 Hz, 2H), 6.88 - 6.93 (m, 2H),

7.90 - 7.95 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 14.10, 14.83, 18.15, 40.29, 63.84, 114.22, 130.42, 162.90, 199.06.

Compound **21** was prepared from 1-(4-ethoxyphenyl)pentan-1-one (2.6 g, 13.5 mmol) using method A and was isolated as a yellow solid (4.01 g, 79 %). mp 168 - 169 °C; ^{1}H NMR (DMSO-d_6) δ 1.15 (t, J = 7.5, 7.2 Hz, 3H), 1.34 (t, J = 6.9, 7.2 Hz, 3H), 2.64 (dd, J = 7.5, 7.5 Hz), 4.08 (dd, J = 7.2, 6.9 Hz, 2H), 7.07 (d, J = 8.7 Hz, 2H), 7.41 (d, J = 8.7 Hz, 2H), 8.94 (br s, 2H); APCI *m/z* 249 $[M+H]^+$ - HI; Anal. ($C_{13}H_{17}IN_2OS$) C, H, N.

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REMARK   4
REMARK   4 P_1E COMPLIES WITH FORMAT V. 2.0,  8-MAY-2007
ATOM      1  N   PRO B   2       3.707  32.624  52.122  1.00 46.68           N
ATOM      2  CA  PRO B   2       2.248  32.739  52.389  1.00 47.03           C
ATOM      3  C   PRO B   2       1.525  31.385  52.299  1.00 49.17           C
ATOM      4  O   PRO B   2       1.634  30.582  53.228  1.00 57.29           O
ATOM      5  CB  PRO B   2       1.704  33.746  51.391  1.00 51.37           C
ATOM      6  CG  PRO B   2       2.975  34.624  51.130  1.00 47.14           C
ATOM      7  CD  PRO B   2       4.124  33.610  51.106  1.00 42.93           C
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ATOM      9  CA  ARG B   3       0.106  29.806  51.112  1.00 37.36           C
ATOM     10  C   ARG B   3       0.467  28.905  49.938  1.00 33.95           C
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ATOM     12  CB  ARG B   3      -1.396  29.995  51.089  1.00 41.19           C
ATOM     13  CG  ARG B   3      -2.154  28.763  51.439  1.00 32.87           C
ATOM     14  CD  ARG B   3      -1.905  28.479  52.900  1.00 39.71           C
ATOM     15  NE  ARG B   3      -2.576  27.269  53.355  1.00 42.69           N
ATOM     16  CZ  ARG B   3      -3.879  27.059  53.218  1.00 47.47           C
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ATOM     18  NH2 ARG B   3      -4.417  25.934  53.659  1.00 52.05           N
ATOM     19  N   VAL B   4       0.745  27.658  50.269  1.00 29.62           N
ATOM     20  CA  VAL B   4       1.125  26.673  49.280  1.00 30.00           C
ATOM     21  C   VAL B   4       0.421  25.351  49.577  1.00 32.33           C
ATOM     22  O   VAL B   4      -0.105  25.142  50.677  1.00 28.39           O
ATOM     23  CB  VAL B   4       2.649  26.437  49.316  1.00 28.28           C
ATOM     24  CG1 VAL B   4       3.386  27.689  48.872  1.00 25.05           C
ATOM     25  CG2 VAL B   4       3.080  26.066  50.740  1.00 23.79           C
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ATOM     27  CA  VAL B   5      -0.217  23.164  48.779  1.00 37.71           C
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ATOM     29  O   VAL B   5       2.004  22.701  49.605  1.00 46.11           O
ATOM     30  CB  VAL B   5      -0.495  22.469  47.439  1.00 33.30           C
ATOM     31  CG1 VAL B   5      -1.448  23.307  46.612  1.00 31.18           C
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ATOM     70  C   SER B  10       3.467  17.583  42.171  1.00 46.30           C
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ATOM    164  C   LYS B  20       2.907  24.157  29.731  1.00 54.73           C
ATOM    165  O   LYS B  20       2.880  24.936  28.775  1.00 54.70           O
ATOM    166  CB  LYS B  20       0.710  23.013  29.414  1.00 58.95           C
ATOM    167  CG  LYS B  20      -0.044  21.729  29.020  1.00 67.63           C
ATOM    168  CD  LYS B  20      -1.489  22.009  28.577  1.00 70.01           C
ATOM    169  CE  LYS B  20      -1.553  22.848  27.299  1.00 70.75           C
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ATOM    170  NZ  LYS B  20      -2.966  23.224  26.968  1.00 71.97           N
ATOM    171  N   LEU B  21       3.541  24.420  30.869  1.00 53.90           N
ATOM    172  CA  LEU B  21       4.220  25.686  31.109  1.00 50.67           C
ATOM    173  C   LEU B  21       5.677  25.538  31.543  1.00 49.81           C
ATOM    174  O   LEU B  21       6.390  26.527  31.673  1.00 49.46           O
ATOM    175  CB  LEU B  21       3.445  26.455  32.174  1.00 47.68           C
ATOM    176  CG  LEU B  21       2.623  27.669  31.756  1.00 48.20           C
ATOM    177  CD1 LEU B  21       1.913  27.431  30.438  1.00 46.96           C
ATOM    178  CD2 LEU B  21       1.643  27.979  32.874  1.00 43.18           C
ATOM    179  N   SER B  22       6.126  24.310  31.759  1.00 51.01           N
ATOM    180  CA  SER B  22       7.497  24.088  32.195  1.00 54.78           C
ATOM    181  C   SER B  22       8.517  24.009  31.055  1.00 55.09           C
ATOM    182  O   SER B  22       9.706  23.831  31.298  1.00 54.31           O
ATOM    183  CB  SER B  22       7.576  22.825  33.057  1.00 54.35           C
ATOM    184  OG  SER B  22       7.204  21.679  32.315  1.00 64.24           O
ATOM    185  N   ARG B  23       8.056  24.146  29.816  1.00 57.71           N
ATOM    186  CA  ARG B  23       8.958  24.108  28.664  1.00 61.06           C
ATOM    187  C   ARG B  23       8.855  25.397  27.859  1.00 60.39           C
ATOM    188  O   ARG B  23       7.753  25.890  27.597  1.00 60.04           O
ATOM    189  CB  ARG B  23       8.632  22.923  27.754  1.00 66.29           C
ATOM    190  CG  ARG B  23       8.818  21.556  28.396  1.00 75.02           C
ATOM    191  CD  ARG B  23       8.332  20.455  27.460  1.00 80.95           C
ATOM    192  NE  ARG B  23       8.320  19.143  28.103  1.00 86.75           N
ATOM    193  CZ  ARG B  23       7.817  18.043  27.548  1.00 89.85           C
ATOM    194  NH1 ARG B  23       7.282  18.095  26.330  1.00 90.15           N
ATOM    195  NH2 ARG B  23       7.841  16.888  28.208  1.00 91.01           N
ATOM    196  N   GLU B  24      10.003  25.933  27.460  1.00 59.15           N
ATOM    197  CA  GLU B  24      10.036  27.166  26.692  1.00 60.62           C
ATOM    198  C   GLU B  24       8.913  27.268  25.677  1.00 59.15           C
ATOM    199  O   GLU B  24       8.815  26.460  24.767  1.00 62.30           O
ATOM    200  CB  GLU B  24      11.376  27.317  25.974  1.00 64.33           C
ATOM    201  CG  GLU B  24      12.530  27.675  26.896  1.00 70.41           C
ATOM    202  CD  GLU B  24      13.718  28.255  26.146  1.00 74.05           C
ATOM    203  OE1 GLU B  24      13.525  29.247  25.405  1.00 75.70           O
ATOM    204  OE2 GLU B  24      14.840  27.724  26.302  1.00 75.92           O
ATOM    205  N   CYS B  25       8.060  28.267  25.844  1.00 58.10           N
ATOM    206  CA  CYS B  25       6.954  28.474  24.929  1.00 57.85           C
ATOM    207  C   CYS B  25       6.722  29.958  24.678  1.00 57.06           C
ATOM    208  O   CYS B  25       7.177  30.805  25.447  1.00 55.95           O
ATOM    209  CB  CYS B  25       5.687  27.799  25.464  1.00 60.03           C
ATOM    210  SG  CYS B  25       5.358  28.036  27.215  1.00 61.13           S
ATOM    211  N   GLU B  26       6.021  30.267  23.590  1.00 58.23           N
ATOM    212  CA  GLU B  26       5.763  31.651  23.212  1.00 58.37           C
ATOM    213  C   GLU B  26       5.127  32.486  24.304  1.00 55.99           C
ATOM    214  O   GLU B  26       4.069  32.140  24.839  1.00 57.60           O
ATOM    215  CB  GLU B  26       4.886  31.722  21.954  1.00 61.65           C
ATOM    216  CG  GLU B  26       4.787  33.137  21.370  1.00 68.53           C
ATOM    217  CD  GLU B  26       4.099  33.192  20.006  1.00 71.58           C
ATOM    218  OE1 GLU B  26       4.415  32.340  19.142  1.00 74.81           O
ATOM    219  OE2 GLU B  26       3.257  34.099  19.795  1.00 69.49           O
ATOM    220  N   ILE B  27       5.792  33.592  24.620  1.00 51.55           N
ATOM    221  CA  ILE B  27       5.328  34.538  25.625  1.00 50.63           C
ATOM    222  C   ILE B  27       5.255  35.895  24.933  1.00 49.12           C
ATOM    223  O   ILE B  27       5.983  36.146  23.972  1.00 49.14           O
ATOM    224  CB  ILE B  27       6.307  34.629  26.822  1.00 49.59           C
ATOM    225  CG1 ILE B  27       7.676  35.115  26.343  1.00 52.71           C
ATOM    226  CG2 ILE B  27       6.429  33.270  27.494  1.00 50.01           C
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ATOM    227  CD1 ILE B  27       8.689  35.300  27.452  1.00 52.75           C
ATOM    228  N   LYS B  28       4.381  36.770  25.413  1.00 47.55           N
ATOM    229  CA  LYS B  28       4.240  38.073  24.796  1.00 47.10           C
ATOM    230  C   LYS B  28       3.829  39.145  25.792  1.00 45.80           C
ATOM    231  O   LYS B  28       2.898  38.961  26.571  1.00 46.71           O
ATOM    232  CB  LYS B  28       3.209  37.996  23.663  1.00 50.06           C
ATOM    233  CG  LYS B  28       3.036  39.295  22.896  1.00 54.17           C
ATOM    234  CD  LYS B  28       1.925  39.192  21.862  1.00 58.46           C
ATOM    235  CE  LYS B  28       2.225  38.145  20.797  1.00 61.39           C
ATOM    236  NZ  LYS B  28       1.160  38.114  19.745  1.00 63.10           N
ATOM    237  N   TYR B  29       4.544  40.261  25.766  1.00 45.23           N
ATOM    238  CA  TYR B  29       4.239  41.389  26.639  1.00 46.09           C
ATOM    239  C   TYR B  29       2.803  41.792  26.319  1.00 47.27           C
ATOM    240  O   TYR B  29       2.393  41.745  25.160  1.00 50.29           O
ATOM    241  CB  TYR B  29       5.205  42.528  26.333  1.00 44.31           C
ATOM    242  CG  TYR B  29       4.890  43.842  26.991  1.00 45.78           C
ATOM    243  CD1 TYR B  29       4.747  43.944  28.375  1.00 46.26           C
ATOM    244  CD2 TYR B  29       4.777  45.001  26.230  1.00 47.30           C
ATOM    245  CE1 TYR B  29       4.504  45.175  28.976  1.00 46.71           C
ATOM    246  CE2 TYR B  29       4.534  46.229  26.817  1.00 46.59           C
ATOM    247  CZ  TYR B  29       4.398  46.315  28.186  1.00 48.77           C
ATOM    248  OH  TYR B  29       4.155  47.546  28.756  1.00 53.53           O
ATOM    249  N   THR B  30       2.034  42.177  27.331  1.00 46.62           N
ATOM    250  CA  THR B  30       0.644  42.541  27.096  1.00 45.73           C
ATOM    251  C   THR B  30       0.278  43.925  27.620  1.00 47.81           C
ATOM    252  O   THR B  30      -0.888  44.315  27.616  1.00 46.96           O
ATOM    253  CB  THR B  30      -0.303  41.491  27.721  1.00 45.73           C
ATOM    254  OG1 THR B  30      -0.319  41.635  29.147  1.00 48.35           O
ATOM    255  CG2 THR B  30       0.173  40.076  27.375  1.00 44.37           C
ATOM    256  N   GLY B  31       1.280  44.672  28.060  1.00 50.42           N
ATOM    257  CA  GLY B  31       1.023  46.003  28.576  1.00 55.15           C
ATOM    258  C   GLY B  31       0.614  46.963  27.480  1.00 58.60           C
ATOM    259  O   GLY B  31       1.027  46.809  26.332  1.00 59.10           O
ATOM    260  N   PHE B  32      -0.200  47.954  27.835  1.00 62.41           N
ATOM    261  CA  PHE B  32      -0.677  48.958  26.882  1.00 65.03           C
ATOM    262  C   PHE B  32      -1.048  48.347  25.558  1.00 69.34           C
ATOM    263  O   PHE B  32      -0.707  48.805  24.477  1.00 69.35           O
ATOM    264  CB  PHE B  32       0.396  50.011  26.667  1.00 62.41           C
ATOM    265  CG  PHE B  32       0.889  50.633  27.940  1.00 62.88           C
ATOM    266  CD1 PHE B  32       1.792  49.954  28.758  1.00 62.69           C
ATOM    267  CD2 PHE B  32       0.437  51.891  28.336  1.00 62.42           C
ATOM    268  CE1 PHE B  32       2.244  50.521  29.958  1.00 60.30           C
ATOM    269  CE2 PHE B  32       0.879  52.470  29.532  1.00 60.33           C
ATOM    270  CZ  PHE B  32       1.786  51.782  30.345  1.00 60.12           C
ATOM    271  N   ARG B  33      -1.761  47.224  25.680  1.00 76.28           N
ATOM    272  CA  ARG B  33      -2.219  46.479  24.550  1.00 82.01           C
ATOM    273  C   ARG B  33      -2.724  47.401  23.394  1.00 84.15           C
ATOM    274  O   ARG B  33      -2.350  47.207  22.260  1.00 83.56           O
ATOM    275  CB  ARG B  33      -3.351  45.557  24.993  1.00 83.97           C
ATOM    276  CG  ARG B  33      -3.876  44.654  23.884  1.00 88.71           C
ATOM    277  CD  ARG B  33      -2.845  43.622  23.425  1.00 91.21           C
ATOM    278  NE  ARG B  33      -3.402  42.654  22.468  1.00 95.66           N
ATOM    279  CZ  ARG B  33      -4.005  41.505  22.824  1.00 98.40           C
ATOM    280  NH1 ARG B  33      -4.124  41.179  24.098  1.00100.78           N
ATOM    281  NH2 ARG B  33      -4.506  40.662  21.926  1.00100.06           N
ATOM    282  N   ASP B  34      -3.600  48.353  23.685  1.00 85.85           N
ATOM    283  CA  ASP B  34      -4.116  49.263  22.635  1.00 87.35           C
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ATOM    284  C   ASP B  34      -3.336  50.577  22.654  1.00 87.45           C
ATOM    285  O   ASP B  34      -3.769  51.556  23.274  1.00 88.66           O
ATOM    286  CB  ASP B  34      -5.553  49.619  22.914  1.00 89.16           C
ATOM    287  CG  ASP B  34      -5.681  50.507  24.123  1.00 92.50           C
ATOM    288  OD1 ASP B  34      -4.727  50.497  24.948  1.00 91.03           O
ATOM    289  OD2 ASP B  34      -6.687  51.219  24.258  1.00 94.84           O
ATOM    290  N   ARG B  35      -2.218  50.591  21.956  1.00 85.93           N
ATOM    291  CA  ARG B  35      -1.360  51.773  21.839  1.00 84.55           C
ATOM    292  C   ARG B  35      -0.310  51.568  20.740  1.00 81.90           C
ATOM    293  O   ARG B  35      -0.043  50.436  20.322  1.00 82.28           O
ATOM    294  CB  ARG B  35      -0.671  52.080  23.178  1.00 85.93           C
ATOM    295  CG  ARG B  35      -1.574  52.780  24.191  1.00 90.30           C
ATOM    296  CD  ARG B  35      -2.064  54.122  23.650  1.00 94.87           C
ATOM    297  NE  ARG B  35      -3.342  54.546  24.226  1.00 97.58           N
ATOM    298  CZ  ARG B  35      -3.951  55.695  23.934  1.00 97.81           C
ATOM    299  NH1 ARG B  35      -3.396  56.542  23.075  1.00 96.86           N
ATOM    300  NH2 ARG B  35      -5.121  55.993  24.488  1.00 95.97           N
ATOM    301  N   PRO B  36       0.284  52.670  20.243  1.00 77.48           N
ATOM    302  CA  PRO B  36       1.303  52.587  19.191  1.00 73.94           C
ATOM    303  C   PRO B  36       2.471  51.677  19.581  1.00 71.91           C
ATOM    304  O   PRO B  36       3.087  51.863  20.631  1.00 69.34           O
ATOM    305  CB  PRO B  36       1.734  54.044  19.019  1.00 73.28           C
ATOM    306  CG  PRO B  36       0.477  54.800  19.328  1.00 72.53           C
ATOM    307  CD  PRO B  36      -0.030  54.078  20.553  1.00 74.89           C
ATOM    308  N   HIS B  37       2.767  50.697  18.731  1.00 70.54           N
ATOM    309  CA  HIS B  37       3.861  49.762  18.979  1.00 69.70           C
ATOM    310  C   HIS B  37       5.136  50.478  19.441  1.00 70.87           C
ATOM    311  O   HIS B  37       5.870  49.961  20.283  1.00 71.04           O
ATOM    312  CB  HIS B  37       4.161  48.955  17.714  1.00 67.03           C
ATOM    313  CG  HIS B  37       5.213  47.906  17.901  1.00 65.39           C
ATOM    314  ND1 HIS B  37       4.942  46.668  18.443  1.00 64.30           N
ATOM    315  CD2 HIS B  37       6.542  47.918  17.640  1.00 65.76           C
ATOM    316  CE1 HIS B  37       6.059  45.964  18.507  1.00 65.22           C
ATOM    317  NE2 HIS B  37       7.044  46.700  18.026  1.00 65.27           N
ATOM    318  N   GLU B  38       5.401  51.655  18.887  1.00 74.32           N
ATOM    319  CA  GLU B  38       6.587  52.418  19.268  1.00 77.97           C
ATOM    320  C   GLU B  38       6.565  52.730  20.763  1.00 76.43           C
ATOM    321  O   GLU B  38       7.565  52.542  21.458  1.00 76.58           O
ATOM    322  CB  GLU B  38       6.665  53.718  18.462  1.00 83.32           C
ATOM    323  CG  GLU B  38       5.610  54.749  18.827  1.00 91.90           C
ATOM    324  CD  GLU B  38       5.583  55.921  17.867  1.00 97.74           C
ATOM    325  OE1 GLU B  38       6.399  55.933  16.920  1.00102.01           O
ATOM    326  OE2 GLU B  38       4.744  56.828  18.058  1.00100.15           O
ATOM    327  N   GLU B  39       5.421  53.195  21.246  1.00 74.62           N
ATOM    328  CA  GLU B  39       5.236  53.526  22.655  1.00 72.35           C
ATOM    329  C   GLU B  39       5.320  52.266  23.530  1.00 69.41           C
ATOM    330  O   GLU B  39       6.035  52.243  24.539  1.00 67.68           O
ATOM    331  CB  GLU B  39       3.880  54.222  22.848  1.00 74.20           C
ATOM    332  CG  GLU B  39       3.470  54.430  24.296  1.00 79.11           C
ATOM    333  CD  GLU B  39       2.176  55.218  24.443  1.00 82.32           C
ATOM    334  OE1 GLU B  39       2.198  56.449  24.223  1.00 82.04           O
ATOM    335  OE2 GLU B  39       1.136  54.604  24.775  1.00 84.67           O
ATOM    336  N   ARG B  40       4.595  51.221  23.137  1.00 63.76           N
ATOM    337  CA  ARG B  40       4.598  49.970  23.882  1.00 60.46           C
ATOM    338  C   ARG B  40       6.030  49.501  24.112  1.00 60.50           C
ATOM    339  O   ARG B  40       6.374  49.045  25.206  1.00 61.18           O
ATOM    340  CB  ARG B  40       3.810  48.891  23.132  1.00 57.59           C
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ATOM    341  CG  ARG B  40       2.355  49.249  22.882  1.00 55.17           C
ATOM    342  CD  ARG B  40       1.579  48.056  22.361  1.00 54.49           C
ATOM    343  NE  ARG B  40       1.345  47.063  23.401  1.00 55.63           N
ATOM    344  CZ  ARG B  40       1.666  45.779  23.297  1.00 56.18           C
ATOM    345  NH1 ARG B  40       2.236  45.328  22.190  1.00 56.64           N
ATOM    346  NH2 ARG B  40       1.424  44.948  24.303  1.00 55.36           N
ATOM    347  N   GLN B  41       6.865  49.617  23.083  1.00 58.61           N
ATOM    348  CA  GLN B  41       8.261  49.210  23.191  1.00 58.10           C
ATOM    349  C   GLN B  41       8.955  49.986  24.299  1.00 56.59           C
ATOM    350  O   GLN B  41       9.745  49.419  25.049  1.00 57.68           O
ATOM    351  CB  GLN B  41       8.999  49.435  21.869  1.00 60.15           C
ATOM    352  CG  GLN B  41       8.624  48.458  20.747  1.00 65.11           C
ATOM    353  CD  GLN B  41       9.380  48.740  19.442  1.00 67.67           C
ATOM    354  OE1 GLN B  41       9.196  49.792  18.822  1.00 68.61           O
ATOM    355  NE2 GLN B  41      10.237  47.803  19.030  1.00 65.14           N
ATOM    356  N   ALA B  42       8.661  51.280  24.406  1.00 56.46           N
ATOM    357  CA  ALA B  42       9.271  52.111  25.447  1.00 57.81           C
ATOM    358  C   ALA B  42       8.714  51.726  26.816  1.00 58.54           C
ATOM    359  O   ALA B  42       9.462  51.537  27.775  1.00 58.82           O
ATOM    360  CB  ALA B  42       9.007  53.588  25.175  1.00 56.35           C
ATOM    361  N   ARG B  43       7.393  51.614  26.896  1.00 58.97           N
ATOM    362  CA  ARG B  43       6.734  51.235  28.137  1.00 59.78           C
ATOM    363  C   ARG B  43       7.402  49.977  28.683  1.00 59.43           C
ATOM    364  O   ARG B  43       7.812  49.935  29.844  1.00 60.04           O
ATOM    365  CB  ARG B  43       5.255  50.932  27.886  1.00 61.27           C
ATOM    366  CG  ARG B  43       4.457  52.061  27.262  1.00 63.33           C
ATOM    367  CD  ARG B  43       4.248  53.202  28.230  1.00 63.84           C
ATOM    368  NE  ARG B  43       3.236  54.123  27.726  1.00 66.34           N
ATOM    369  CZ  ARG B  43       2.761  55.164  28.403  1.00 68.52           C
ATOM    370  NH1 ARG B  43       3.211  55.425  29.627  1.00 67.29           N
ATOM    371  NH2 ARG B  43       1.828  55.941  27.858  1.00 67.78           N
ATOM    372  N   PHE B  44       7.508  48.959  27.829  1.00 58.23           N
ATOM    373  CA  PHE B  44       8.103  47.681  28.209  1.00 56.95           C
ATOM    374  C   PHE B  44       9.486  47.795  28.839  1.00 59.35           C
ATOM    375  O   PHE B  44       9.749  47.185  29.884  1.00 58.27           O
ATOM    376  CB  PHE B  44       8.198  46.736  27.009  1.00 50.55           C
ATOM    377  CG  PHE B  44       8.856  45.419  27.336  1.00 47.57           C
ATOM    378  CD1 PHE B  44       8.203  44.474  28.124  1.00 45.60           C
ATOM    379  CD2 PHE B  44      10.144  45.139  26.894  1.00 43.82           C
ATOM    380  CE1 PHE B  44       8.821  43.271  28.465  1.00 41.38           C
ATOM    381  CE2 PHE B  44      10.771  43.938  27.231  1.00 43.24           C
ATOM    382  CZ  PHE B  44      10.104  43.004  28.019  1.00 41.98           C
ATOM    383  N   GLN B  45      10.376  48.554  28.206  1.00 60.21           N
ATOM    384  CA  GLN B  45      11.720  48.698  28.745  1.00 63.36           C
ATOM    385  C   GLN B  45      11.771  49.526  30.021  1.00 62.79           C
ATOM    386  O   GLN B  45      12.542  49.220  30.933  1.00 63.02           O
ATOM    387  CB  GLN B  45      12.670  49.292  27.705  1.00 65.85           C
ATOM    388  CG  GLN B  45      13.484  48.241  26.975  1.00 70.11           C
ATOM    389  CD  GLN B  45      14.837  48.762  26.529  1.00 73.12           C
ATOM    390  OE1 GLN B  45      15.649  49.201  27.351  1.00 75.59           O
ATOM    391  NE2 GLN B  45      15.090  48.712  25.224  1.00 73.01           N
ATOM    392  N   ASN B  46      10.962  50.578  30.085  1.00 62.60           N
ATOM    393  CA  ASN B  46      10.927  51.421  31.273  1.00 62.85           C
ATOM    394  C   ASN B  46      10.415  50.584  32.434  1.00 61.07           C
ATOM    395  O   ASN B  46      10.953  50.648  33.542  1.00 61.69           O
ATOM    396  CB  ASN B  46      10.010  52.623  31.051  1.00 66.55           C
ATOM    397  CG  ASN B  46      10.552  53.578  30.007  1.00 70.63           C
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ATOM    398  OD1 ASN B  46      11.658  54.103  30.149  1.00 71.82           O
ATOM    399  ND2 ASN B  46       9.778  53.807  28.949  1.00 71.67           N
ATOM    400  N   ALA B  47       9.379  49.792  32.165  1.00 56.50           N
ATOM    401  CA  ALA B  47       8.795  48.923  33.173  1.00 54.27           C
ATOM    402  C   ALA B  47       9.810  47.860  33.582  1.00 54.10           C
ATOM    403  O   ALA B  47       9.904  47.510  34.757  1.00 54.14           O
ATOM    404  CB  ALA B  47       7.528  48.267  32.636  1.00 53.08           C
ATOM    405  N   CYS B  48      10.564  47.343  32.615  1.00 53.41           N
ATOM    406  CA  CYS B  48      11.576  46.335  32.911  1.00 54.44           C
ATOM    407  C   CYS B  48      12.649  46.915  33.819  1.00 56.45           C
ATOM    408  O   CYS B  48      13.156  46.236  34.710  1.00 54.39           O
ATOM    409  CB  CYS B  48      12.222  45.813  31.627  1.00 54.27           C
ATOM    410  SG  CYS B  48      11.304  44.484  30.837  1.00 56.34           S
ATOM    411  N   ARG B  49      12.994  48.176  33.592  1.00 58.29           N
ATOM    412  CA  ARG B  49      14.000  48.818  34.414  1.00 60.67           C
ATOM    413  C   ARG B  49      13.460  49.073  35.814  1.00 60.73           C
ATOM    414  O   ARG B  49      14.233  49.203  36.762  1.00 61.75           O
ATOM    415  CB  ARG B  49      14.472  50.122  33.770  1.00 63.56           C
ATOM    416  CG  ARG B  49      15.370  49.906  32.562  1.00 68.95           C
ATOM    417  CD  ARG B  49      16.050  51.189  32.097  1.00 74.18           C
ATOM    418  NE  ARG B  49      15.100  52.178  31.591  1.00 82.34           N
ATOM    419  CZ  ARG B  49      14.385  53.002  32.355  1.00 85.96           C
ATOM    420  NH1 ARG B  49      14.507  52.969  33.679  1.00 86.54           N
ATOM    421  NH2 ARG B  49      13.543  53.861  31.793  1.00 85.34           N
ATOM    422  N   ASP B  50      12.137  49.142  35.948  1.00 59.59           N
ATOM    423  CA  ASP B  50      11.517  49.353  37.256  1.00 58.04           C
ATOM    424  C   ASP B  50      11.279  47.991  37.897  1.00 55.78           C
ATOM    425  O   ASP B  50      10.812  47.901  39.033  1.00 53.75           O
ATOM    426  CB  ASP B  50      10.177  50.086  37.132  1.00 63.45           C
ATOM    427  CG  ASP B  50      10.311  51.456  36.489  1.00 68.86           C
ATOM    428  OD1 ASP B  50      11.335  52.131  36.742  1.00 72.63           O
ATOM    429  OD2 ASP B  50       9.386  51.861  35.745  1.00 71.15           O
ATOM    430  N   GLY B  51      11.586  46.936  37.143  1.00 52.89           N
ATOM    431  CA  GLY B  51      11.426  45.584  37.642  1.00 50.29           C
ATOM    432  C   GLY B  51      10.049  44.958  37.519  1.00 50.31           C
ATOM    433  O   GLY B  51       9.779  43.948  38.165  1.00 48.19           O
ATOM    434  N   ARG B  52       9.157  45.542  36.728  1.00 51.14           N
ATOM    435  CA  ARG B  52       7.839  44.931  36.568  1.00 56.02           C
ATOM    436  C   ARG B  52       7.396  44.817  35.119  1.00 55.57           C
ATOM    437  O   ARG B  52       7.873  45.546  34.247  1.00 57.82           O
ATOM    438  CB  ARG B  52       6.754  45.654  37.396  1.00 59.33           C
ATOM    439  CG  ARG B  52       7.050  47.077  37.827  1.00 68.21           C
ATOM    440  CD  ARG B  52       6.918  48.100  36.683  1.00 76.50           C
ATOM    441  NE  ARG B  52       5.540  48.350  36.241  1.00 80.34           N
ATOM    442  CZ  ARG B  52       5.198  49.326  35.396  1.00 82.95           C
ATOM    443  NH1 ARG B  52       6.133  50.140  34.909  1.00 83.47           N
ATOM    444  NH2 ARG B  52       3.930  49.490  35.024  1.00 83.11           N
ATOM    445  N   SER B  53       6.502  43.868  34.863  1.00 54.02           N
ATOM    446  CA  SER B  53       5.979  43.657  33.525  1.00 52.90           C
ATOM    447  C   SER B  53       4.804  42.692  33.548  1.00 51.90           C
ATOM    448  O   SER B  53       4.547  42.024  34.551  1.00 51.65           O
ATOM    449  CB  SER B  53       7.080  43.119  32.606  1.00 55.03           C
ATOM    450  OG  SER B  53       6.646  43.087  31.257  1.00 55.62           O
ATOM    451  N   GLU B  54       4.080  42.639  32.437  1.00 53.21           N
ATOM    452  CA  GLU B  54       2.934  41.750  32.294  1.00 52.56           C
ATOM    453  C   GLU B  54       3.183  40.953  31.036  1.00 50.20           C
ATOM    454  O   GLU B  54       3.134  41.488  29.931  1.00 50.78           O
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ATOM    455  CB  GLU B  54       1.644  42.543  32.134  1.00 56.30           C
ATOM    456  CG  GLU B  54       1.495  43.669  33.120  1.00 66.67           C
ATOM    457  CD  GLU B  54       0.108  44.270  33.102  1.00 72.99           C
ATOM    458  OE1 GLU B  54      -0.435  44.491  31.989  1.00 74.90           O
ATOM    459  OE2 GLU B  54      -0.430  44.526  34.203  1.00 75.33           O
ATOM    460  N   ILE B  55       3.460  39.673  31.207  1.00 46.71           N
ATOM    461  CA  ILE B  55       3.740  38.818  30.080  1.00 47.54           C
ATOM    462  C   ILE B  55       2.839  37.604  30.147  1.00 48.97           C
ATOM    463  O   ILE B  55       2.851  36.855  31.120  1.00 49.43           O
ATOM    464  CB  ILE B  55       5.223  38.368  30.083  1.00 47.67           C
ATOM    465  CG1 ILE B  55       6.144  39.591  30.000  1.00 46.82           C
ATOM    466  CG2 ILE B  55       5.496  37.455  28.901  1.00 48.57           C
ATOM    467  CD1 ILE B  55       7.616  39.286  30.243  1.00 44.90           C
ATOM    468  N   ALA B  56       2.053  37.419  29.097  1.00 51.91           N
ATOM    469  CA  ALA B  56       1.137  36.291  29.019  1.00 53.22           C
ATOM    470  C   ALA B  56       1.708  35.178  28.150  1.00 52.02           C
ATOM    471  O   ALA B  56       2.482  35.431  27.226  1.00 51.24           O
ATOM    472  CB  ALA B  56      -0.198  36.750  28.448  1.00 52.72           C
ATOM    473  N   PHE B  57       1.356  33.940  28.477  1.00 52.35           N
ATOM    474  CA  PHE B  57       1.780  32.806  27.670  1.00 51.63           C
ATOM    475  C   PHE B  57       0.697  32.796  26.597  1.00 51.68           C
ATOM    476  O   PHE B  57      -0.464  32.524  26.890  1.00 51.78           O
ATOM    477  CB  PHE B  57       1.741  31.502  28.468  1.00 49.12           C
ATOM    478  CG  PHE B  57       2.866  31.352  29.451  1.00 48.34           C
ATOM    479  CD1 PHE B  57       4.113  30.903  29.032  1.00 47.73           C
ATOM    480  CD2 PHE B  57       2.680  31.641  30.798  1.00 50.21           C
ATOM    481  CE1 PHE B  57       5.164  30.739  29.941  1.00 49.35           C
ATOM    482  CE2 PHE B  57       3.725  31.481  31.718  1.00 49.13           C
ATOM    483  CZ  PHE B  57       4.970  31.027  31.285  1.00 48.15           C
ATOM    484  N   VAL B  58       1.082  33.131  25.368  1.00 53.57           N
ATOM    485  CA  VAL B  58       0.157  33.209  24.242  1.00 53.16           C
ATOM    486  C   VAL B  58      -0.648  31.949  23.934  1.00 52.51           C
ATOM    487  O   VAL B  58      -1.850  32.024  23.693  1.00 54.48           O
ATOM    488  CB  VAL B  58       0.899  33.617  22.960  1.00 53.75           C
ATOM    489  CG1 VAL B  58      -0.104  33.794  21.812  1.00 48.63           C
ATOM    490  CG2 VAL B  58       1.700  34.897  23.211  1.00 49.99           C
ATOM    491  N   ALA B  59       0.010  30.798  23.933  1.00 51.94           N
ATOM    492  CA  ALA B  59      -0.671  29.549  23.629  1.00 52.70           C
ATOM    493  C   ALA B  59      -1.877  29.277  24.525  1.00 53.82           C
ATOM    494  O   ALA B  59      -2.942  28.891  24.038  1.00 55.64           O
ATOM    495  CB  ALA B  59       0.312  28.379  23.710  1.00 50.64           C
ATOM    496  N   THR B  60      -1.727  29.486  25.829  1.00 53.63           N
ATOM    497  CA  THR B  60      -2.827  29.206  26.745  1.00 52.49           C
ATOM    498  C   THR B  60      -3.563  30.440  27.250  1.00 51.46           C
ATOM    499  O   THR B  60      -4.581  30.331  27.944  1.00 49.42           O
ATOM    500  CB  THR B  60      -2.336  28.400  27.955  1.00 51.76           C
ATOM    501  OG1 THR B  60      -1.336  27.465  27.534  1.00 53.36           O
ATOM    502  CG2 THR B  60      -3.493  27.620  28.561  1.00 54.06           C
ATOM    503  N   GLY B  61      -3.060  31.612  26.891  1.00 50.29           N
ATOM    504  CA  GLY B  61      -3.692  32.835  27.337  1.00 50.95           C
ATOM    505  C   GLY B  61      -3.543  33.042  28.835  1.00 50.90           C
ATOM    506  O   GLY B  61      -4.338  33.748  29.456  1.00 47.84           O
ATOM    507  N   THR B  62      -2.531  32.416  29.428  1.00 52.26           N
ATOM    508  CA  THR B  62      -2.291  32.576  30.859  1.00 53.31           C
ATOM    509  C   THR B  62      -1.511  33.873  31.086  1.00 52.59           C
ATOM    510  O   THR B  62      -0.325  33.967  30.759  1.00 49.99           O
ATOM    511  CB  THR B  62      -1.468  31.410  31.440  1.00 54.22           C
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ATOM    512  OG1 THR B  62      -2.080  30.162  31.087  1.00 56.20           O
ATOM    513  CG2 THR B  62      -1.397  31.527  32.963  1.00 51.35           C
ATOM    514  N   ASN B  63      -2.191  34.876  31.629  1.00 52.88           N
ATOM    515  CA  ASN B  63      -1.559  36.158  31.900  1.00 53.75           C
ATOM    516  C   ASN B  63      -0.856  36.148  33.246  1.00 52.22           C
ATOM    517  O   ASN B  63      -1.317  35.519  34.198  1.00 53.06           O
ATOM    518  CB  ASN B  63      -2.602  37.277  31.891  1.00 57.62           C
ATOM    519  CG  ASN B  63      -2.983  37.705  30.493  1.00 59.43           C
ATOM    520  OD1 ASN B  63      -2.300  38.521  29.875  1.00 61.56           O
ATOM    521  ND2 ASN B  63      -4.071  37.150  29.982  1.00 59.40           N
ATOM    522  N   LEU B  64       0.273  36.842  33.312  1.00 48.39           N
ATOM    523  CA  LEU B  64       1.034  36.946  34.546  1.00 41.45           C
ATOM    524  C   LEU B  64       1.551  38.360  34.725  1.00 40.81           C
ATOM    525  O   LEU B  64       1.973  39.007  33.769  1.00 41.71           O
ATOM    526  CB  LEU B  64       2.221  35.983  34.541  1.00 36.38           C
ATOM    527  CG  LEU B  64       1.924  34.502  34.776  1.00 38.87           C
ATOM    528  CD1 LEU B  64       3.240  33.733  34.856  1.00 35.24           C
ATOM    529  CD2 LEU B  64       1.121  34.325  36.059  1.00 31.82           C
ATOM    530  N   SER B  65       1.473  38.861  35.949  1.00 39.49           N
ATOM    531  CA  SER B  65       2.023  40.172  36.248  1.00 37.47           C
ATOM    532  C   SER B  65       3.315  39.734  36.930  1.00 36.62           C
ATOM    533  O   SER B  65       3.286  38.902  37.841  1.00 35.05           O
ATOM    534  CB  SER B  65       1.125  40.936  37.208  1.00 37.46           C
ATOM    535  OG  SER B  65       1.638  42.233  37.429  1.00 44.83           O
ATOM    536  N   LEU B  66       4.449  40.251  36.478  1.00 35.38           N
ATOM    537  CA  LEU B  66       5.712  39.825  37.055  1.00 35.35           C
ATOM    538  C   LEU B  66       6.535  40.902  37.745  1.00 38.20           C
ATOM    539  O   LEU B  66       6.561  42.071  37.330  1.00 33.85           O
ATOM    540  CB  LEU B  66       6.565  39.171  35.973  1.00 37.04           C
ATOM    541  CG  LEU B  66       5.908  38.047  35.171  1.00 38.90           C
ATOM    542  CD1 LEU B  66       6.819  37.650  34.020  1.00 36.74           C
ATOM    543  CD2 LEU B  66       5.619  36.862  36.093  1.00 38.05           C
ATOM    544  N   GLN B  67       7.216  40.479  38.807  1.00 38.14           N
ATOM    545  CA  GLN B  67       8.085  41.353  39.570  1.00 39.59           C
ATOM    546  C   GLN B  67       9.486  40.762  39.505  1.00 38.10           C
ATOM    547  O   GLN B  67       9.741  39.663  39.996  1.00 41.00           O
ATOM    548  CB  GLN B  67       7.594  41.451  41.010  1.00 42.65           C
ATOM    549  CG  GLN B  67       6.114  41.787  41.085  1.00 49.18           C
ATOM    550  CD  GLN B  67       5.792  42.764  42.191  1.00 52.54           C
ATOM    551  OE1 GLN B  67       6.000  42.478  43.376  1.00 54.01           O
ATOM    552  NE2 GLN B  67       5.284  43.928  41.815  1.00 50.71           N
ATOM    553  N   PHE B  68      10.386  41.496  38.874  1.00 34.48           N
ATOM    554  CA  PHE B  68      11.751  41.051  38.707  1.00 38.30           C
ATOM    555  C   PHE B  68      12.637  41.402  39.901  1.00 40.14           C
ATOM    556  O   PHE B  68      13.549  42.232  39.814  1.00 41.79           O
ATOM    557  CB  PHE B  68      12.295  41.640  37.407  1.00 35.42           C
ATOM    558  CG  PHE B  68      11.409  41.372  36.227  1.00 37.04           C
ATOM    559  CD1 PHE B  68      11.042  40.068  35.899  1.00 38.54           C
ATOM    560  CD2 PHE B  68      10.926  42.415  35.447  1.00 34.27           C
ATOM    561  CE1 PHE B  68      10.205  39.810  34.807  1.00 37.74           C
ATOM    562  CE2 PHE B  68      10.090  42.166  34.354  1.00 34.71           C
ATOM    563  CZ  PHE B  68       9.730  40.862  34.034  1.00 33.69           C
ATOM    564  N   PHE B  69      12.348  40.751  41.023  1.00 39.06           N
ATOM    565  CA  PHE B  69      13.089  40.959  42.251  1.00 39.40           C
ATOM    566  C   PHE B  69      13.127  39.659  43.027  1.00 39.36           C
ATOM    567  O   PHE B  69      12.284  38.782  42.836  1.00 39.36           O
ATOM    568  CB  PHE B  69      12.415  42.020  43.131  1.00 41.33           C
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ATOM    569  CG  PHE B  69      12.277  43.359  42.481  1.00 43.66           C
ATOM    570  CD1 PHE B  69      13.324  44.277  42.525  1.00 45.50           C
ATOM    571  CD2 PHE B  69      11.097  43.712  41.836  1.00 43.17           C
ATOM    572  CE1 PHE B  69      13.197  45.528  41.941  1.00 44.24           C
ATOM    573  CE2 PHE B  69      10.955  44.963  41.247  1.00 44.52           C
ATOM    574  CZ  PHE B  69      12.007  45.874  41.299  1.00 46.54           C
ATOM    575  N   PRO B  70      14.110  39.516  43.921  1.00 38.69           N
ATOM    576  CA  PRO B  70      14.209  38.292  44.716  1.00 38.60           C
ATOM    577  C   PRO B  70      12.933  38.168  45.547  1.00 37.90           C
ATOM    578  O   PRO B  70      12.430  39.167  46.055  1.00 32.76           O
ATOM    579  CB  PRO B  70      15.440  38.546  45.584  1.00 37.36           C
ATOM    580  CG  PRO B  70      16.270  39.466  44.728  1.00 38.21           C
ATOM    581  CD  PRO B  70      15.245  40.416  44.182  1.00 36.41           C
ATOM    582  N   ALA B  71      12.414  36.950  45.682  1.00 38.59           N
ATOM    583  CA  ALA B  71      11.196  36.727  46.453  1.00 43.19           C
ATOM    584  C   ALA B  71      11.264  37.434  47.810  1.00 48.57           C
ATOM    585  O   ALA B  71      10.240  37.902  48.331  1.00 47.37           O
ATOM    586  CB  ALA B  71      10.970  35.245  46.647  1.00 39.03           C
ATOM    587  N   SER B  72      12.469  37.509  48.376  1.00 51.95           N
ATOM    588  CA  SER B  72      12.670  38.178  49.657  1.00 56.30           C
ATOM    589  C   SER B  72      12.215  39.630  49.532  1.00 58.88           C
ATOM    590  O   SER B  72      11.477  40.118  50.385  1.00 62.81           O
ATOM    591  CB  SER B  72      14.143  38.114  50.066  1.00 58.03           C
ATOM    592  N   TRP B  73      12.644  40.313  48.470  1.00 59.05           N
ATOM    593  CA  TRP B  73      12.245  41.699  48.246  1.00 61.67           C
ATOM    594  C   TRP B  73      13.185  42.442  47.294  1.00 64.01           C
ATOM    595  O   TRP B  73      14.375  42.629  47.582  1.00 65.05           O
ATOM    596  CB  TRP B  73      12.194  42.432  49.572  1.00 66.59           C
ATOM    597  CG  TRP B  73      10.919  43.148  49.845  1.00 72.25           C
ATOM    598  CD1 TRP B  73      10.425  44.237  49.180  1.00 72.29           C
ATOM    599  CD2 TRP B  73      10.017  42.893  50.926  1.00 74.78           C
ATOM    600  NE1 TRP B  73       9.276  44.681  49.788  1.00 73.57           N
ATOM    601  CE2 TRP B  73       9.000  43.873  50.861  1.00 75.60           C
ATOM    602  CE3 TRP B  73       9.968  41.928  51.946  1.00 75.00           C
ATOM    603  CZ2 TRP B  73       7.943  43.918  51.781  1.00 78.20           C
ATOM    604  CZ3 TRP B  73       8.919  41.970  52.859  1.00 78.33           C
ATOM    605  CH2 TRP B  73       7.918  42.961  52.768  1.00 79.44           C
ATOM    606  N   ARG B  78      10.485  50.921  45.920  1.00 76.51           N
ATOM    607  CA  ARG B  78      11.202  51.031  44.655  1.00 77.64           C
ATOM    608  C   ARG B  78      12.700  50.796  44.840  1.00 78.85           C
ATOM    609  O   ARG B  78      13.276  51.144  45.878  1.00 79.86           O
ATOM    610  CB  ARG B  78      10.964  52.406  44.031  1.00 75.55           C
ATOM    611  N   GLN B  79      13.314  50.199  43.822  1.00 78.03           N
ATOM    612  CA  GLN B  79      14.747  49.899  43.808  1.00 76.34           C
ATOM    613  C   GLN B  79      15.044  49.128  42.522  1.00 73.25           C
ATOM    614  O   GLN B  79      14.378  48.146  42.212  1.00 71.49           O
ATOM    615  CB  GLN B  79      15.140  49.068  45.039  1.00 76.90           C
ATOM    616  N   THR B  80      16.042  49.585  41.776  1.00 71.72           N
ATOM    617  CA  THR B  80      16.406  48.959  40.514  1.00 68.50           C
ATOM    618  C   THR B  80      16.822  47.505  40.674  1.00 64.85           C
ATOM    619  O   THR B  80      17.550  47.151  41.597  1.00 63.84           O
ATOM    620  CB  THR B  80      17.532  49.763  39.817  1.00 69.72           C
ATOM    621  OG1 THR B  80      17.004  51.027  39.394  1.00 69.97           O
ATOM    622  CG2 THR B  80      18.073  49.017  38.599  1.00 68.63           C
ATOM    623  N   PRO B  81      16.349  46.639  39.766  1.00 62.72           N
ATOM    624  CA  PRO B  81      16.661  45.209  39.792  1.00 59.85           C
ATOM    625  C   PRO B  81      18.087  44.914  39.339  1.00 56.32           C
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ATOM    626  O   PRO B  81      18.652  45.647  38.533  1.00 56.40           O
ATOM    627  CB  PRO B  81      15.627  44.629  38.837  1.00 62.00           C
ATOM    628  CG  PRO B  81      15.517  45.701  37.805  1.00 58.16           C
ATOM    629  CD  PRO B  81      15.435  46.951  38.649  1.00 60.87           C
ATOM    630  N   SER B  82      18.667  43.844  39.869  1.00 51.57           N
ATOM    631  CA  SER B  82      20.015  43.453  39.494  1.00 49.69           C
ATOM    632  C   SER B  82      19.988  42.787  38.114  1.00 51.89           C
ATOM    633  O   SER B  82      18.925  42.427  37.617  1.00 52.01           O
ATOM    634  CB  SER B  82      20.590  42.486  40.529  1.00 43.55           C
ATOM    635  OG  SER B  82      19.765  41.350  40.669  1.00 39.05           O
ATOM    636  N   ARG B  83      21.155  42.631  37.499  1.00 55.30           N
ATOM    637  CA  ARG B  83      21.253  42.010  36.185  1.00 58.93           C
ATOM    638  C   ARG B  83      20.818  40.550  36.236  1.00 58.92           C
ATOM    639  O   ARG B  83      20.646  39.907  35.205  1.00 59.07           O
ATOM    640  CB  ARG B  83      22.690  42.117  35.668  1.00 63.97           C
ATOM    641  CG  ARG B  83      23.195  43.548  35.644  1.00 71.47           C
ATOM    642  CD  ARG B  83      24.643  43.623  35.219  1.00 80.05           C
ATOM    643  NE  ARG B  83      25.156  44.987  35.327  1.00 87.26           N
ATOM    644  CZ  ARG B  83      26.399  45.338  35.020  1.00 90.04           C
ATOM    645  NH1 ARG B  83      27.258  44.420  34.585  1.00 92.24           N
ATOM    646  NH2 ARG B  83      26.788  46.602  35.150  1.00 91.30           N
ATOM    647  N   GLU B  84      20.620  40.035  37.443  1.00 58.45           N
ATOM    648  CA  GLU B  84      20.198  38.656  37.609  1.00 59.64           C
ATOM    649  C   GLU B  84      18.714  38.493  37.279  1.00 59.72           C
ATOM    650  O   GLU B  84      18.282  37.419  36.855  1.00 60.44           O
ATOM    651  CB  GLU B  84      20.454  38.192  39.047  1.00 62.57           C
ATOM    652  CG  GLU B  84      20.387  36.686  39.229  1.00 65.41           C
ATOM    653  CD  GLU B  84      20.407  36.262  40.681  1.00 68.49           C
ATOM    654  OE1 GLU B  84      21.282  36.738  41.437  1.00 73.10           O
ATOM    655  OE2 GLU B  84      19.550  35.443  41.068  1.00 70.34           O
ATOM    656  N   TYR B  85      17.933  39.553  37.475  1.00 56.95           N
ATOM    657  CA  TYR B  85      16.504  39.495  37.192  1.00 54.26           C
ATOM    658  C   TYR B  85      16.111  40.260  35.939  1.00 53.85           C
ATOM    659  O   TYR B  85      15.019  40.079  35.404  1.00 54.21           O
ATOM    660  CB  TYR B  85      15.702  39.998  38.396  1.00 51.71           C
ATOM    661  CG  TYR B  85      15.814  39.079  39.584  1.00 50.56           C
ATOM    662  CD1 TYR B  85      16.999  39.003  40.319  1.00 51.90           C
ATOM    663  CD2 TYR B  85      14.765  38.237  39.939  1.00 47.92           C
ATOM    664  CE1 TYR B  85      17.138  38.110  41.373  1.00 49.35           C
ATOM    665  CE2 TYR B  85      14.895  37.337  40.992  1.00 50.47           C
ATOM    666  CZ  TYR B  85      16.085  37.278  41.704  1.00 50.06           C
ATOM    667  OH  TYR B  85      16.234  36.380  42.731  1.00 48.87           O
ATOM    668  N   VAL B  86      17.000  41.126  35.476  1.00 54.16           N
ATOM    669  CA  VAL B  86      16.749  41.900  34.272  1.00 56.30           C
ATOM    670  C   VAL B  86      18.089  42.105  33.590  1.00 58.25           C
ATOM    671  O   VAL B  86      18.886  42.948  33.989  1.00 59.26           O
ATOM    672  CB  VAL B  86      16.077  43.259  34.600  1.00 54.70           C
ATOM    673  CG1 VAL B  86      15.986  44.128  33.354  1.00 49.87           C
ATOM    674  CG2 VAL B  86      14.676  43.013  35.149  1.00 51.32           C
ATOM    675  N   ASP B  87      18.332  41.298  32.566  1.00 61.45           N
ATOM    676  CA  ASP B  87      19.577  41.339  31.816  1.00 65.27           C
ATOM    677  C   ASP B  87      19.382  41.886  30.400  1.00 66.46           C
ATOM    678  O   ASP B  87      18.682  41.288  29.582  1.00 65.70           O
ATOM    679  CB  ASP B  87      20.157  39.928  31.737  1.00 68.13           C
ATOM    680  CG  ASP B  87      21.630  39.922  31.402  1.00 73.07           C
ATOM    681  OD1 ASP B  87      22.046  40.695  30.510  1.00 74.51           O
ATOM    682  OD2 ASP B  87      22.373  39.136  32.030  1.00 74.29           O
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ATOM    683  N   LEU B  88      20.006  43.023  30.116  1.00 68.81           N
ATOM    684  CA  LEU B  88      19.922  43.638  28.797  1.00 72.49           C
ATOM    685  C   LEU B  88      21.166  43.361  27.943  1.00 74.29           C
ATOM    686  O   LEU B  88      21.246  43.663  26.798  1.00 74.51           O
ATOM    687  CB  LEU B  88      19.730  45.144  28.918  1.00 71.87           C
ATOM    688  CG  LEU B  88      18.336  45.642  29.289  1.00 72.31           C
ATOM    689  CD1 LEU B  88      18.396  47.115  29.671  1.00 71.86           C
ATOM    690  CD2 LEU B  88      17.401  45.423  28.113  1.00 71.54           C
ATOM    691  N   GLU B  89      22.176  42.726  28.541  1.00 75.90           N
ATOM    692  CA  GLU B  89      23.377  42.410  27.807  1.00 78.55           C
ATOM    693  C   GLU B  89      23.389  40.972  27.275  1.00 78.62           C
ATOM    694  O   GLU B  89      23.717  40.709  26.137  1.00 79.44           O
ATOM    695  CB  GLU B  89      24.571  42.523  28.770  1.00 81.02           C
ATOM    696  CG  GLU B  89      24.431  43.673  29.764  1.00 85.93           C
ATOM    697  CD  GLU B  89      25.198  43.431  31.083  1.00 89.14           C
ATOM    698  OE1 GLU B  89      26.462  43.420  31.061  1.00 89.47           O
ATOM    699  OE2 GLU B  89      24.541  43.249  32.150  1.00 90.88           O
ATOM    700  N   ARG B  90      23.271  40.027  28.192  1.00 78.43           N
ATOM    701  CA  ARG B  90      23.316  38.636  27.757  1.00 77.57           C
ATOM    702  C   ARG B  90      23.089  38.408  26.249  1.00 77.93           C
ATOM    703  O   ARG B  90      23.687  37.510  25.658  1.00 78.33           O
ATOM    704  CB  ARG B  90      22.327  37.812  28.566  1.00 78.07           C
ATOM    705  CG  ARG B  90      22.323  36.338  28.231  1.00 78.24           C
ATOM    706  CD  ARG B  90      21.489  35.560  29.224  1.00 79.74           C
ATOM    707  NE  ARG B  90      21.248  34.194  28.770  1.00 83.47           N
ATOM    708  CZ  ARG B  90      20.601  33.271  29.477  1.00 85.26           C
ATOM    709  NH1 ARG B  90      20.128  33.562  30.684  1.00 84.17           N
ATOM    710  NH2 ARG B  90      20.421  32.055  28.972  1.00 85.50           N
ATOM    711  N   GLU B  91      22.219  39.209  25.636  1.00 77.28           N
ATOM    712  CA  GLU B  91      21.945  39.099  24.206  1.00 76.44           C
ATOM    713  C   GLU B  91      21.329  40.369  23.645  1.00 75.11           C
ATOM    714  O   GLU B  91      20.135  40.613  23.814  1.00 76.33           O
ATOM    715  CB  GLU B  91      21.013  37.924  23.915  1.00 79.17           C
ATOM    716  CG  GLU B  91      21.726  36.603  23.732  1.00 84.24           C
ATOM    717  CD  GLU B  91      20.930  35.635  22.879  1.00 88.35           C
ATOM    718  OE1 GLU B  91      20.558  36.009  21.742  1.00 87.88           O
ATOM    719  OE2 GLU B  91      20.681  34.501  23.345  1.00 90.20           O
ATOM    720  N   ALA B  92      22.144  41.172  22.971  1.00 73.16           N
ATOM    721  CA  ALA B  92      21.675  42.421  22.387  1.00 71.42           C
ATOM    722  C   ALA B  92      20.311  42.232  21.738  1.00 69.68           C
ATOM    723  O   ALA B  92      20.002  41.155  21.229  1.00 68.80           O
ATOM    724  CB  ALA B  92      22.676  42.922  21.362  1.00 71.02           C
ATOM    725  N   GLY B  93      19.489  43.275  21.772  1.00 68.38           N
ATOM    726  CA  GLY B  93      18.171  43.185  21.168  1.00 69.27           C
ATOM    727  C   GLY B  93      17.075  42.682  22.090  1.00 68.71           C
ATOM    728  O   GLY B  93      15.914  43.088  21.971  1.00 68.98           O
ATOM    729  N   LYS B  94      17.422  41.785  23.005  1.00 66.67           N
ATOM    730  CA  LYS B  94      16.421  41.278  23.928  1.00 64.92           C
ATOM    731  C   LYS B  94      16.833  41.337  25.394  1.00 61.29           C
ATOM    732  O   LYS B  94      17.980  41.641  25.722  1.00 59.83           O
ATOM    733  CB  LYS B  94      16.002  39.855  23.536  1.00 66.40           C
ATOM    734  CG  LYS B  94      17.116  38.896  23.175  1.00 64.90           C
ATOM    735  CD  LYS B  94      16.491  37.662  22.529  1.00 68.54           C
ATOM    736  CE  LYS B  94      17.511  36.631  22.076  1.00 71.67           C
ATOM    737  NZ  LYS B  94      16.832  35.448  21.470  1.00 72.00           N
ATOM    738  N   VAL B  95      15.872  41.069  26.272  1.00 57.23           N
ATOM    739  CA  VAL B  95      16.118  41.102  27.704  1.00 51.21           C
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ATOM    740  C   VAL B  95      15.694  39.812  28.380  1.00 49.64           C
ATOM    741  O   VAL B  95      14.607  39.297  28.131  1.00 48.67           O
ATOM    742  CB  VAL B  95      15.370  42.275  28.374  1.00 48.42           C
ATOM    743  CG1 VAL B  95      13.864  42.106  28.213  1.00 48.05           C
ATOM    744  CG2 VAL B  95      15.748  42.350  29.842  1.00 49.12           C
ATOM    745  N   TYR B  96      16.570  39.289  29.231  1.00 47.72           N
ATOM    746  CA  TYR B  96      16.282  38.075  29.970  1.00 46.56           C
ATOM    747  C   TYR B  96      15.697  38.463  31.320  1.00 45.95           C
ATOM    748  O   TYR B  96      16.245  39.316  32.017  1.00 46.06           O
ATOM    749  CB  TYR B  96      17.551  37.247  30.128  1.00 48.72           C
ATOM    750  CG  TYR B  96      17.886  36.479  28.874  1.00 53.31           C
ATOM    751  CD1 TYR B  96      18.266  37.140  27.701  1.00 55.83           C
ATOM    752  CD2 TYR B  96      17.780  35.090  28.843  1.00 55.38           C
ATOM    753  CE1 TYR B  96      18.530  36.429  26.527  1.00 57.55           C
ATOM    754  CE2 TYR B  96      18.041  34.371  27.681  1.00 58.34           C
ATOM    755  CZ  TYR B  96      18.415  35.043  26.530  1.00 60.07           C
ATOM    756  OH  TYR B  96      18.673  34.317  25.392  1.00 65.42           O
ATOM    757  N   LEU B  97      14.578  37.833  31.678  1.00 45.60           N
ATOM    758  CA  LEU B  97      13.868  38.141  32.916  1.00 41.63           C
ATOM    759  C   LEU B  97      13.651  36.963  33.847  1.00 40.21           C
ATOM    760  O   LEU B  97      13.378  35.847  33.413  1.00 41.46           O
ATOM    761  CB  LEU B  97      12.510  38.745  32.574  1.00 39.40           C
ATOM    762  CG  LEU B  97      12.587  39.908  31.588  1.00 41.65           C
ATOM    763  CD1 LEU B  97      11.209  40.169  30.983  1.00 39.62           C
ATOM    764  CD2 LEU B  97      13.135  41.136  32.304  1.00 40.54           C
ATOM    765  N   LYS B  98      13.769  37.234  35.141  1.00 38.67           N
ATOM    766  CA  LYS B  98      13.568  36.230  36.175  1.00 37.36           C
ATOM    767  C   LYS B  98      12.522  36.803  37.142  1.00 35.47           C
ATOM    768  O   LYS B  98      12.633  37.950  37.580  1.00 33.11           O
ATOM    769  CB  LYS B  98      14.886  35.944  36.907  1.00 35.86           C
ATOM    770  CG  LYS B  98      14.781  34.834  37.938  1.00 36.98           C
ATOM    771  CD  LYS B  98      16.099  34.593  38.649  1.00 44.72           C
ATOM    772  CE  LYS B  98      15.923  33.603  39.788  1.00 50.00           C
ATOM    773  NZ  LYS B  98      17.170  33.416  40.571  1.00 51.69           N
ATOM    774  N   ALA B  99      11.498  36.020  37.461  1.00 33.06           N
ATOM    775  CA  ALA B  99      10.456  36.511  38.353  1.00 34.24           C
ATOM    776  C   ALA B  99       9.897  35.428  39.257  1.00 32.60           C
ATOM    777  O   ALA B  99       9.298  34.471  38.786  1.00 34.31           O
ATOM    778  CB  ALA B  99       9.332  37.137  37.542  1.00 31.43           C
ATOM    779  N   PRO B 100      10.085  35.570  40.579  1.00 32.99           N
ATOM    780  CA  PRO B 100       9.592  34.595  41.562  1.00 32.60           C
ATOM    781  C   PRO B 100       8.128  34.862  41.913  1.00 30.53           C
ATOM    782  O   PRO B 100       7.659  35.999  41.810  1.00 32.08           O
ATOM    783  CB  PRO B 100      10.492  34.827  42.786  1.00 29.73           C
ATOM    784  CG  PRO B 100      11.488  35.942  42.346  1.00 33.45           C
ATOM    785  CD  PRO B 100      10.802  36.667  41.249  1.00 31.42           C
ATOM    786  N   MET B 101       7.413  33.821  42.326  1.00 27.32           N
ATOM    787  CA  MET B 101       6.020  33.975  42.738  1.00 28.42           C
ATOM    788  C   MET B 101       5.482  32.662  43.242  1.00 26.93           C
ATOM    789  O   MET B 101       6.136  31.633  43.125  1.00 28.33           O
ATOM    790  CB  MET B 101       5.144  34.443  41.568  1.00 30.72           C
ATOM    791  CG  MET B 101       4.880  33.366  40.513  1.00 34.34           C
ATOM    792  SD  MET B 101       4.548  34.032  38.853  1.00 40.60           S
ATOM    793  CE  MET B 101       2.950  33.441  38.606  1.00 43.54           C
ATOM    794  N   ILE B 102       4.298  32.702  43.839  1.00 26.61           N
ATOM    795  CA  ILE B 102       3.656  31.474  44.275  1.00 27.62           C
ATOM    796  C   ILE B 102       2.464  31.383  43.322  1.00 28.05           C
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ATOM    797  O   ILE B 102       1.569  32.225  43.355  1.00 28.89           O
ATOM    798  CB  ILE B 102       3.187  31.537  45.740  1.00 23.92           C
ATOM    799  CG1 ILE B 102       4.391  31.746  46.664  1.00 25.87           C
ATOM    800  CG2 ILE B 102       2.503  30.225  46.122  1.00 23.18           C
ATOM    801  CD1 ILE B 102       4.080  31.481  48.175  1.00 24.78           C
ATOM    802  N   LEU B 103       2.493  30.396  42.435  1.00 27.66           N
ATOM    803  CA  LEU B 103       1.430  30.200  41.452  1.00 28.50           C
ATOM    804  C   LEU B 103       0.607  28.967  41.802  1.00 28.01           C
ATOM    805  O   LEU B 103       1.142  27.870  41.908  1.00 28.82           O
ATOM    806  CB  LEU B 103       2.047  30.051  40.063  1.00 28.23           C
ATOM    807  CG  LEU B 103       1.159  29.662  38.877  1.00 37.61           C
ATOM    808  CD1 LEU B 103      -0.029  30.627  38.734  1.00 36.45           C
ATOM    809  CD2 LEU B 103       2.028  29.651  37.604  1.00 35.52           C
ATOM    810  N   ASN B 104      -0.695  29.152  41.987  1.00 29.55           N
ATOM    811  CA  ASN B 104      -1.590  28.056  42.347  1.00 30.61           C
ATOM    812  C   ASN B 104      -0.987  27.180  43.434  1.00 32.02           C
ATOM    813  O   ASN B 104      -0.918  25.953  43.302  1.00 32.81           O
ATOM    814  CB  ASN B 104      -1.937  27.183  41.133  1.00 32.13           C
ATOM    815  CG  ASN B 104      -2.794  27.913  40.117  1.00 35.89           C
ATOM    816  OD1 ASN B 104      -3.556  28.818  40.466  1.00 34.24           O
ATOM    817  ND2 ASN B 104      -2.681  27.515  38.850  1.00 34.94           N
ATOM    818  N   GLY B 105      -0.538  27.832  44.501  1.00 31.42           N
ATOM    819  CA  GLY B 105       0.019  27.134  45.642  1.00 32.13           C
ATOM    820  C   GLY B 105       1.409  26.542  45.548  1.00 30.97           C
ATOM    821  O   GLY B 105       1.836  25.845  46.479  1.00 30.24           O
ATOM    822  N   VAL B 106       2.124  26.793  44.458  1.00 28.72           N
ATOM    823  CA  VAL B 106       3.457  26.235  44.361  1.00 31.30           C
ATOM    824  C   VAL B 106       4.486  27.304  44.037  1.00 31.51           C
ATOM    825  O   VAL B 106       4.283  28.109  43.141  1.00 32.01           O
ATOM    826  CB  VAL B 106       3.521  25.048  43.320  1.00 32.73           C
ATOM    827  CG1 VAL B 106       2.116  24.538  43.012  1.00 28.08           C
ATOM    828  CG2 VAL B 106       4.247  25.452  42.065  1.00 28.81           C
ATOM    829  N   CYS B 107       5.578  27.330  44.799  1.00 30.84           N
ATOM    830  CA  CYS B 107       6.628  28.311  44.556  1.00 33.12           C
ATOM    831  C   CYS B 107       7.319  28.049  43.237  1.00 32.02           C
ATOM    832  O   CYS B 107       7.908  26.995  43.038  1.00 36.57           O
ATOM    833  CB  CYS B 107       7.675  28.281  45.666  1.00 30.42           C
ATOM    834  SG  CYS B 107       7.022  28.791  47.247  1.00 33.94           S
ATOM    835  N   VAL B 108       7.253  29.011  42.332  1.00 30.98           N
ATOM    836  CA  VAL B 108       7.907  28.844  41.054  1.00 30.93           C
ATOM    837  C   VAL B 108       8.717  30.075  40.699  1.00 32.30           C
ATOM    838  O   VAL B 108       8.678  31.096  41.389  1.00 32.26           O
ATOM    839  CB  VAL B 108       6.887  28.587  39.906  1.00 28.02           C
ATOM    840  CG1 VAL B 108       5.996  27.414  40.252  1.00 26.10           C
ATOM    841  CG2 VAL B 108       6.062  29.834  39.647  1.00 24.44           C
ATOM    842  N   ILE B 109       9.460  29.951  39.611  1.00 33.35           N
ATOM    843  CA  ILE B 109      10.255  31.033  39.090  1.00 35.94           C
ATOM    844  C   ILE B 109       9.950  31.095  37.596  1.00 38.90           C
ATOM    845  O   ILE B 109      10.033  30.092  36.889  1.00 39.17           O
ATOM    846  CB  ILE B 109      11.761  30.787  39.276  1.00 36.59           C
ATOM    847  CG1 ILE B 109      12.097  30.679  40.761  1.00 42.85           C
ATOM    848  CG2 ILE B 109      12.545  31.927  38.659  1.00 32.42           C
ATOM    849  CD1 ILE B 109      13.572  30.426  41.044  1.00 46.36           C
ATOM    850  N   TRP B 110       9.576  32.274  37.130  1.00 39.01           N
ATOM    851  CA  TRP B 110       9.282  32.488  35.728  1.00 40.13           C
ATOM    852  C   TRP B 110      10.576  33.004  35.088  1.00 41.59           C
ATOM    853  O   TRP B 110      11.130  34.010  35.527  1.00 42.60           O
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ATOM    854  CB  TRP B 110       8.178  33.540  35.609  1.00 35.97           C
ATOM    855  CG  TRP B 110       7.719  33.851  34.226  1.00 36.92           C
ATOM    856  CD1 TRP B 110       6.577  33.417  33.631  1.00 37.79           C
ATOM    857  CD2 TRP B 110       8.351  34.731  33.285  1.00 39.24           C
ATOM    858  NE1 TRP B 110       6.446  33.976  32.384  1.00 38.29           N
ATOM    859  CE2 TRP B 110       7.520  34.788  32.145  1.00 37.79           C
ATOM    860  CE3 TRP B 110       9.537  35.482  33.298  1.00 38.35           C
ATOM    861  CZ2 TRP B 110       7.834  35.568  31.024  1.00 39.30           C
ATOM    862  CZ3 TRP B 110       9.849  36.257  32.181  1.00 39.81           C
ATOM    863  CH2 TRP B 110       8.996  36.294  31.059  1.00 38.03           C
ATOM    864  N   LYS B 111      11.066  32.305  34.073  1.00 43.95           N
ATOM    865  CA  LYS B 111      12.277  32.727  33.362  1.00 45.97           C
ATOM    866  C   LYS B 111      11.973  32.820  31.870  1.00 45.29           C
ATOM    867  O   LYS B 111      11.286  31.968  31.313  1.00 49.12           O
ATOM    868  CB  LYS B 111      13.424  31.737  33.578  1.00 44.17           C
ATOM    869  CG  LYS B 111      13.778  31.518  35.032  1.00 49.79           C
ATOM    870  CD  LYS B 111      15.062  30.724  35.176  1.00 53.57           C
ATOM    871  CE  LYS B 111      15.349  30.410  36.640  1.00 60.48           C
ATOM    872  NZ  LYS B 111      16.601  29.620  36.820  1.00 62.26           N
ATOM    873  N   GLY B 112      12.473  33.861  31.226  1.00 44.48           N
ATOM    874  CA  GLY B 112      12.233  34.009  29.808  1.00 45.94           C
ATOM    875  C   GLY B 112      12.886  35.256  29.269  1.00 47.49           C
ATOM    876  O   GLY B 112      13.467  36.038  30.027  1.00 48.16           O
ATOM    877  N   TRP B 113      12.812  35.441  27.955  1.00 46.48           N
ATOM    878  CA  TRP B 113      13.388  36.624  27.336  1.00 47.11           C
ATOM    879  C   TRP B 113      12.379  37.233  26.375  1.00 48.61           C
ATOM    880  O   TRP B 113      11.471  36.553  25.885  1.00 48.48           O
ATOM    881  CB  TRP B 113      14.695  36.289  26.596  1.00 47.44           C
ATOM    882  CG  TRP B 113      14.564  35.191  25.582  1.00 50.25           C
ATOM    883  CD1 TRP B 113      14.845  33.863  25.763  1.00 50.02           C
ATOM    884  CD2 TRP B 113      14.052  35.314  24.249  1.00 48.96           C
ATOM    885  NE1 TRP B 113      14.533  33.154  24.626  1.00 50.98           N
ATOM    886  CE2 TRP B 113      14.044  34.020  23.684  1.00 50.82           C
ATOM    887  CE3 TRP B 113      13.598  36.393  23.479  1.00 49.90           C
ATOM    888  CZ2 TRP B 113      13.598  33.776  22.381  1.00 51.59           C
ATOM    889  CZ3 TRP B 113      13.152  36.149  22.182  1.00 52.23           C
ATOM    890  CH2 TRP B 113      13.156  34.849  21.648  1.00 50.44           C
ATOM    891  N   ILE B 114      12.529  38.524  26.117  1.00 48.67           N
ATOM    892  CA  ILE B 114      11.631  39.205  25.213  1.00 51.07           C
ATOM    893  C   ILE B 114      12.399  40.122  24.279  1.00 55.21           C
ATOM    894  O   ILE B 114      13.313  40.838  24.696  1.00 58.18           O
ATOM    895  CB  ILE B 114      10.562  39.999  25.988  1.00 51.44           C
ATOM    896  CG1 ILE B 114       9.419  39.055  26.368  1.00 52.23           C
ATOM    897  CG2 ILE B 114      10.057  41.163  25.163  1.00 44.81           C
ATOM    898  CD1 ILE B 114       8.226  39.753  26.947  1.00 57.77           C
ATOM    899  N   ASP B 115      12.026  40.071  23.006  1.00 56.26           N
ATOM    900  CA  ASP B 115      12.650  40.876  21.974  1.00 55.45           C
ATOM    901  C   ASP B 115      12.220  42.328  22.151  1.00 55.15           C
ATOM    902  O   ASP B 115      11.036  42.643  22.080  1.00 55.90           O
ATOM    903  CB  ASP B 115      12.229  40.342  20.601  1.00 58.41           C
ATOM    904  CG  ASP B 115      12.989  40.989  19.468  1.00 58.68           C
ATOM    905  OD1 ASP B 115      12.598  42.097  19.045  1.00 60.29           O
ATOM    906  OD2 ASP B 115      13.983  40.391  19.014  1.00 57.11           O
ATOM    907  N   LEU B 116      13.186  43.210  22.384  1.00 55.45           N
ATOM    908  CA  LEU B 116      12.889  44.622  22.592  1.00 57.59           C
ATOM    909  C   LEU B 116      12.193  45.247  21.392  1.00 60.18           C
ATOM    910  O   LEU B 116      11.582  46.315  21.500  1.00 62.00           O
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ATOM    911  CB  LEU B 116      14.176  45.390  22.888  1.00 54.93           C
ATOM    912  CG  LEU B 116      14.986  44.894  24.084  1.00 56.44           C
ATOM    913  CD1 LEU B 116      16.259  45.721  24.205  1.00 55.39           C
ATOM    914  CD2 LEU B 116      14.151  44.991  25.352  1.00 55.92           C
ATOM    915  N   GLN B 117      12.287  44.575  20.248  1.00 61.57           N
ATOM    916  CA  GLN B 117      11.682  45.061  19.016  1.00 62.20           C
ATOM    917  C   GLN B 117      10.267  44.521  18.890  1.00 60.19           C
ATOM    918  O   GLN B 117       9.293  45.277  18.866  1.00 59.99           O
ATOM    919  CB  GLN B 117      12.511  44.597  17.811  1.00 68.12           C
ATOM    920  CG  GLN B 117      12.479  45.528  16.609  1.00 74.32           C
ATOM    921  CD  GLN B 117      13.285  46.801  16.838  1.00 79.08           C
ATOM    922  OE1 GLN B 117      12.938  47.633  17.684  1.00 80.87           O
ATOM    923  NE2 GLN B 117      14.374  46.952  16.088  1.00 80.66           N
ATOM    924  N   ARG B 118      10.170  43.198  18.828  1.00 58.08           N
ATOM    925  CA  ARG B 118       8.896  42.506  18.671  1.00 58.62           C
ATOM    926  C   ARG B 118       7.981  42.519  19.903  1.00 57.96           C
ATOM    927  O   ARG B 118       6.754  42.550  19.769  1.00 56.31           O
ATOM    928  CB  ARG B 118       9.167  41.059  18.257  1.00 61.27           C
ATOM    929  CG  ARG B 118      10.233  40.913  17.177  1.00 61.95           C
ATOM    930  CD  ARG B 118      10.419  39.457  16.804  1.00 65.96           C
ATOM    931  NE  ARG B 118       9.145  38.859  16.409  1.00 72.21           N
ATOM    932  CZ  ARG B 118       8.986  37.588  16.048  1.00 75.15           C
ATOM    933  NH1 ARG B 118      10.027  36.760  16.025  1.00 76.29           N
ATOM    934  NH2 ARG B 118       7.779  37.142  15.709  1.00 74.16           N
ATOM    935  N   LEU B 119       8.582  42.494  21.094  1.00 55.46           N
ATOM    936  CA  LEU B 119       7.843  42.473  22.353  1.00 50.60           C
ATOM    937  C   LEU B 119       7.190  41.109  22.539  1.00 51.84           C
ATOM    938  O   LEU B 119       6.143  40.981  23.176  1.00 52.38           O
ATOM    939  CB  LEU B 119       6.782  43.579  22.394  1.00 46.21           C
ATOM    940  CG  LEU B 119       7.309  45.006  22.242  1.00 43.77           C
ATOM    941  CD1 LEU B 119       6.237  46.007  22.661  1.00 39.03           C
ATOM    942  CD2 LEU B 119       8.540  45.187  23.102  1.00 42.87           C
ATOM    943  N   ASP B 120       7.821  40.093  21.959  1.00 53.51           N
ATOM    944  CA  ASP B 120       7.354  38.711  22.054  1.00 56.55           C
ATOM    945  C   ASP B 120       8.604  37.964  22.471  1.00 56.24           C
ATOM    946  O   ASP B 120       9.690  38.547  22.487  1.00 55.64           O
ATOM    947  CB  ASP B 120       6.910  38.161  20.692  1.00 64.20           C
ATOM    948  CG  ASP B 120       6.138  39.170  19.870  1.00 71.41           C
ATOM    949  OD1 ASP B 120       4.993  39.514  20.246  1.00 75.22           O
ATOM    950  OD2 ASP B 120       6.686  39.621  18.841  1.00 74.15           O
ATOM    951  N   GLY B 121       8.470  36.679  22.785  1.00 53.26           N
ATOM    952  CA  GLY B 121       9.640  35.926  23.184  1.00 51.37           C
ATOM    953  C   GLY B 121       9.335  34.532  23.671  1.00 52.85           C
ATOM    954  O   GLY B 121       8.273  33.976  23.381  1.00 53.15           O
ATOM    955  N   MET B 122      10.278  33.972  24.423  1.00 53.61           N
ATOM    956  CA  MET B 122      10.145  32.630  24.970  1.00 53.57           C
ATOM    957  C   MET B 122      10.411  32.626  26.479  1.00 53.58           C
ATOM    958  O   MET B 122      11.313  33.314  26.963  1.00 53.03           O
ATOM    959  CB  MET B 122      11.135  31.692  24.270  1.00 54.51           C
ATOM    960  CG  MET B 122      10.947  31.593  22.759  1.00 56.69           C
ATOM    961  SD  MET B 122       9.378  30.812  22.283  1.00 63.29           S
ATOM    962  CE  MET B 122       9.818  29.087  22.486  1.00 55.42           C
ATOM    963  N   GLY B 123       9.630  31.840  27.214  1.00 52.58           N
ATOM    964  CA  GLY B 123       9.811  31.746  28.653  1.00 48.83           C
ATOM    965  C   GLY B 123       9.084  30.548  29.225  1.00 49.19           C
ATOM    966  O   GLY B 123       8.313  29.894  28.520  1.00 48.49           O
ATOM    967  N   CYS B 124       9.316  30.260  30.502  1.00 47.75           N
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ATOM    968  CA  CYS B 124       8.668  29.125  31.151  1.00 47.92           C
ATOM    969  C   CYS B 124       8.673  29.226  32.683  1.00 46.76           C
ATOM    970  O   CYS B 124       9.189  30.183  33.260  1.00 44.52           O
ATOM    971  CB  CYS B 124       9.359  27.833  30.726  1.00 45.60           C
ATOM    972  SG  CYS B 124      11.096  27.764  31.219  1.00 55.20           S
ATOM    973  N   LEU B 125       8.103  28.217  33.327  1.00 44.50           N
ATOM    974  CA  LEU B 125       8.030  28.161  34.777  1.00 44.71           C
ATOM    975  C   LEU B 125       8.973  27.106  35.349  1.00 46.50           C
ATOM    976  O   LEU B 125       9.100  26.014  34.804  1.00 48.88           O
ATOM    977  CB  LEU B 125       6.594  27.851  35.206  1.00 42.59           C
ATOM    978  CG  LEU B 125       5.675  28.973  35.697  1.00 42.83           C
ATOM    979  CD1 LEU B 125       6.192  30.343  35.294  1.00 41.92           C
ATOM    980  CD2 LEU B 125       4.287  28.726  35.148  1.00 39.58           C
ATOM    981  N   GLU B 126       9.628  27.438  36.453  1.00 48.39           N
ATOM    982  CA  GLU B 126      10.551  26.527  37.121  1.00 48.80           C
ATOM    983  C   GLU B 126      10.146  26.336  38.575  1.00 48.80           C
ATOM    984  O   GLU B 126       9.721  27.282  39.232  1.00 50.71           O
ATOM    985  CB  GLU B 126      11.967  27.097  37.105  1.00 52.96           C
ATOM    986  CG  GLU B 126      12.776  26.824  35.864  1.00 57.75           C
ATOM    987  CD  GLU B 126      14.171  27.435  35.950  1.00 63.25           C
ATOM    988  OE1 GLU B 126      14.792  27.376  37.042  1.00 61.13           O
ATOM    989  OE2 GLU B 126      14.647  27.967  34.921  1.00 64.35           O
ATOM    990  N   PHE B 127      10.276  25.119  39.086  1.00 46.84           N
ATOM    991  CA  PHE B 127       9.950  24.875  40.477  1.00 46.78           C
ATOM    992  C   PHE B 127      11.081  25.479  41.310  1.00 48.76           C
ATOM    993  O   PHE B 127      12.253  25.176  41.077  1.00 49.75           O
ATOM    994  CB  PHE B 127       9.853  23.379  40.752  1.00 43.52           C
ATOM    995  CG  PHE B 127       9.608  23.045  42.199  1.00 44.15           C
ATOM    996  CD1 PHE B 127       8.430  23.450  42.832  1.00 42.71           C
ATOM    997  CD2 PHE B 127      10.556  22.343  42.933  1.00 38.74           C
ATOM    998  CE1 PHE B 127       8.202  23.153  44.173  1.00 41.90           C
ATOM    999  CE2 PHE B 127      10.337  22.042  44.273  1.00 40.62           C
ATOM   1000  CZ  PHE B 127       9.156  22.449  44.895  1.00 41.64           C
ATOM   1001  N   ASP B 128      10.734  26.337  42.270  1.00 49.34           N
ATOM   1002  CA  ASP B 128      11.730  26.979  43.123  1.00 50.94           C
ATOM   1003  C   ASP B 128      11.915  26.164  44.401  1.00 52.38           C
ATOM   1004  O   ASP B 128      11.289  26.448  45.422  1.00 51.39           O
ATOM   1005  CB  ASP B 128      11.281  28.404  43.472  1.00 52.76           C
ATOM   1006  CG  ASP B 128      12.410  29.265  44.056  1.00 56.23           C
ATOM   1007  OD1 ASP B 128      13.235  28.745  44.846  1.00 55.89           O
ATOM   1008  OD2 ASP B 128      12.459  30.477  43.735  1.00 56.18           O
ATOM   1009  N   GLU B 129      12.774  25.151  44.339  1.00 55.49           N
ATOM   1010  CA  GLU B 129      13.031  24.293  45.490  1.00 59.27           C
ATOM   1011  C   GLU B 129      13.316  25.069  46.776  1.00 58.16           C
ATOM   1012  O   GLU B 129      12.684  24.834  47.800  1.00 56.62           O
ATOM   1013  CB  GLU B 129      14.235  23.381  45.225  1.00 65.05           C
ATOM   1014  CG  GLU B 129      13.987  22.256  44.233  1.00 75.49           C
ATOM   1015  CD  GLU B 129      15.273  21.541  43.819  1.00 80.49           C
ATOM   1016  OE1 GLU B 129      16.074  21.186  44.714  1.00 82.78           O
ATOM   1017  OE2 GLU B 129      15.479  21.330  42.600  1.00 82.40           O
ATOM   1018  N   GLU B 130      14.347  25.918  46.712  1.00 57.16           N
ATOM   1019  CA  GLU B 130      14.819  26.751  47.825  1.00 57.89           C
ATOM   1020  C   GLU B 130      13.612  27.483  48.522  1.00 56.99           C
ATOM   1021  O   GLU B 130      13.366  27.247  49.672  1.00 56.09           O
ATOM   1022  CB  GLU B 130      15.861  27.760  47.328  1.00 60.14           C
ATOM   1023  CG  GLU B 130      16.751  28.328  48.437  1.00 65.19           C
ATOM   1024  CD  GLU B 130      17.874  29.257  47.910  1.00 71.24           C
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ATOM   1025  OE1 GLU B 130      18.579  28.880  46.928  1.00 70.81           O
ATOM   1026  OE2 GLU B 130      18.065  30.371  48.480  1.00 73.16           O
ATOM   1027  N   ARG B 131      12.818  28.254  47.775  1.00 55.31           N
ATOM   1028  CA  ARG B 131      11.653  29.033  48.302  1.00 52.91           C
ATOM   1029  C   ARG B 131      10.565  28.136  48.867  1.00 52.24           C
ATOM   1030  O   ARG B 131       9.992  28.395  49.925  1.00 48.92           O
ATOM   1031  CB  ARG B 131      11.063  29.873  47.153  1.00 55.86           C
ATOM   1032  CG  ARG B 131      11.584  31.308  47.112  1.00 61.66           C
ATOM   1033  CD  ARG B 131      10.465  32.342  47.236  1.00 70.69           C
ATOM   1034  NE  ARG B 131       9.345  31.897  48.080  1.00 77.71           N
ATOM   1035  CZ  ARG B 131       8.094  32.392  47.993  1.00 80.55           C
ATOM   1036  NH1 ARG B 131       7.811  33.327  47.116  1.00 83.70           N
ATOM   1037  NH2 ARG B 131       7.104  31.961  48.770  1.00 81.38           N
ATOM   1038  N   ALA B 132      10.324  27.046  48.143  1.00 53.42           N
ATOM   1039  CA  ALA B 132       9.306  26.069  48.473  1.00 56.15           C
ATOM   1040  C   ALA B 132       9.468  25.477  49.863  1.00 58.73           C
ATOM   1041  O   ALA B 132       8.487  25.293  50.588  1.00 57.18           O
ATOM   1042  CB  ALA B 132       9.314  24.962  47.427  1.00 55.58           C
ATOM   1043  N   GLN B 133      10.704  25.189  50.247  1.00 63.37           N
ATOM   1044  CA  GLN B 133      10.961  24.599  51.558  1.00 67.45           C
ATOM   1045  C   GLN B 133      10.838  25.553  52.738  1.00 68.51           C
ATOM   1046  O   GLN B 133      10.513  25.129  53.845  1.00 67.02           O
ATOM   1047  CB  GLN B 133      12.335  23.935  51.572  1.00 68.44           C
ATOM   1048  CG  GLN B 133      12.389  22.662  50.750  1.00 71.81           C
ATOM   1049  CD  GLN B 133      13.795  22.123  50.591  1.00 75.37           C
ATOM   1050  OE1 GLN B 133      13.996  21.066  49.992  1.00 76.78           O
ATOM   1051  NE2 GLN B 133      14.782  22.849  51.122  1.00 75.52           N
ATOM   1052  N   GLN B 134      11.086  26.838  52.517  1.00 70.86           N
ATOM   1053  CA  GLN B 134      10.987  27.779  53.622  1.00 75.31           C
ATOM   1054  C   GLN B 134       9.546  28.212  53.860  1.00 75.59           C
ATOM   1055  O   GLN B 134       9.249  28.912  54.824  1.00 76.63           O
ATOM   1056  CB  GLN B 134      11.896  28.991  53.384  1.00 77.92           C
ATOM   1057  CG  GLN B 134      11.474  29.922  52.269  1.00 83.84           C
ATOM   1058  CD  GLN B 134      12.589  30.879  51.887  1.00 87.63           C
ATOM   1059  OE1 GLN B 134      12.378  31.842  51.144  1.00 89.86           O
ATOM   1060  NE2 GLN B 134      13.792  30.608  52.389  1.00 89.21           N
ATOM   1061  N   GLU B 135       8.649  27.781  52.981  1.00 76.64           N
ATOM   1062  CA  GLU B 135       7.234  28.102  53.114  1.00 76.61           C
ATOM   1063  C   GLU B 135       6.606  27.098  54.074  1.00 78.04           C
ATOM   1064  O   GLU B 135       5.657  26.404  53.652  1.00 78.42           O
ATOM   1065  CB  GLU B 135       6.534  28.011  51.758  1.00 74.83           C
ATOM   1066  CG  GLU B 135       6.699  29.224  50.856  1.00 73.33           C
ATOM   1067  CD  GLU B 135       5.882  30.419  51.318  1.00 71.77           C
ATOM   1068  OE1 GLU B 135       4.826  30.216  51.958  1.00 69.41           O
ATOM   1069  OE2 GLU B 135       6.287  31.561  51.022  1.00 71.08           O
ATOM   1070  OXT GLU B 135       7.076  27.008  55.230  1.00 78.65           O
ATOM   1071  C1  MON1  131      17.877  35.989  34.051  0.00  0.00           C
ATOM   1072  C2  MON1  131      16.921  37.153  34.182  0.00  0.00           C
ATOM   1073  C3  MON1  131      19.249  36.184  34.188  0.00  0.00           C
ATOM   1074  C4  MON1  131      20.124  35.121  34.074  0.00  0.00           C
ATOM   1075  C5  MON1  131      19.650  33.845  33.817  0.00  0.00           C
ATOM   1076  C6  MON1  131      18.287  33.628  33.667  0.00  0.00           C
ATOM   1077  C7  MON1  131      17.782  32.269  33.369  0.00  0.00           C
ATOM   1078  C8  MON1  131      16.802  31.956  32.505  0.00  0.00           C
ATOM   1079  S9  MON1  131      16.563  30.232  32.469  0.00  0.00           S
ATOM   1080  C10 MON1  131      17.834  30.088  33.654  0.00  0.00           C
ATOM   1081  N11 MON1  131      18.247  28.861  34.101  0.00  0.00           N
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ATOM   1082  N12 MON1  131      18.364  31.190  34.019  0.00  0.00           N
ATOM   1083  C13 MON1  131      17.415  34.709  33.795  0.00  0.00           C
END
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