## Supporting Information for:

# The Solution Structure of a Nonribosomal Peptide Synthetase Carrier Protein Loaded with its Substrate Reveals Transient, Well-defined Contacts.

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**Cloning of ArCP 14-93 and Sfp into pET-Duet-1.**

Sfp and GB1-TEV-ArCP14-93 were cloned into multiple cloning sites 1 and 2 of the dual expression vector pET-Duet-1, respectively, in two steps. The fragment coding for GB1-TEV-14-93 was PCR amplified from pETRP1B-GB1-TEV-ArCP14-93 using primers ArCP_NdeI_Nterm (5'-GGAGATATACATATGCAGTACAAACTGATCC-3') and ArCP_XhoI_Cterm-2(5'-GGTGCTCGAGCCGCCTACTCAG GCGACC-3') to generate a DNA fragment containing XhoI and NdeI cut sites. The PCR product and target vector pET-Duet1 were digested with XhoI and NdeI, gel purified, and extracted. The fragment coding for GB1-TEV-ArCP14-93 was ligated into pET-Duet-1 to yield pET-Duet-MCS1-GB1-TEV-ArCP14-93. The fragment coding for Sfp-His6 was PCR amplified from pET24a-SfpHis6 using primers Sfp_NcoI_Nterm-2 (5'-GAAGGAGATATACCCAT GGAGATTTACGGAA-3') and Sfp_EcoRI_Cterm-2(5'-AGCGTTGAATTCGATCTCCAGTGGTGGTGGTGGTGGTGCT CCAGTAAAGCTC-3') to generate a DNA fragment containing NcoI and EcoRI cut sites. The PCR product and target vector pET-Duet-MCS1-GB1-TEV-ArCP14-93 were digested with NcoI and EcoRI, gel purified, and extracted. The fragment coding for Sfp-His6 was ligated into pET-Duet-MCS1-GB1-TEV-ArCP14-93 to yield pET-Duet-SfpHis6-GB1-TEV-ArCP14-93. Site-directed mutagenesis using the vector pET-Duet-SfpHis6-GB1-TEV-ArCP14-93 and primers pET-Duet-Sfp_AddT_For (5'TGGTCTCGT ACGAAGAGCTTTACTGGAG-3') and pET_Duet-Sfp_AddT_Rev (5'TGGTGGTGGTGGTGGTGCTCCA GTAAAA-3') was performed to correct a frame-shift mutation that occurred during cloning. The DNA sequence of pET-Duet-SfpHis6-GB1-TEV-ArCP14-93 was confirmed by DNA sequencing. This plasmid directs production of Sfp containing a C-terminal hexahistidine tag and residues 14-93 of HMWP2 with an N-terminal GB1 tag followed by a hexahistidine tag and a TEV cleavage site. Following TEV cleavage of GB1-TEV-ArCP14-93, a GT sequence remains at the N-terminus of ArCP14-93.

Cloning of YbtE, ArCP 14-93 (without Sfp), Sfp, their expression and purification were performed as previously described [1].

**NMR data collection**

**$^{15}$N-Holo ArCP and $^{15}$N-loaded ArCP.** 3D-NOESY-HN-HSQCs (16 scans, 2048 (1H, 16.019 ppm at 4.696 ppm) × 40 (15N, 26 ppm at 117 ppm) × 120 (1H, 11 ppm at 4.696 ppm) complex points, mixing time of 90 ms, 4 days 12 hrs) were recorded for 15N samples of apo, holo, and loaded ArCP. All 3D spectra were linear predicted once and zero-filled to the nearest power of two.

**$^{13}$C,$^{15}$N-Holo ArCP in $H_2O$.** The following experiments were run on a 320 μM sample in 90% H2O/10% D2O: HNCO (16 scans, 2048 (1H, 16.019 ppm at 4.698 ppm) × 64 (15N, 26 ppm at 117 ppm) × 75 (13C, 11 ppm at 174 ppm) complex points, 10h20m), HNCA (16 scans, 2048 (1H, 16.019 ppm at 4.698 ppm) × 64 (15N, 26 ppm at 117 ppm) × 100 (13C, 30 ppm at 52 ppm) complex points, 13h44m), HNCACB (32 scans, 2048(1H, 16.109 ppm at 4.698 ppm) × 64 (15N, 26 ppm at 117 ppm) × 150 (13C, 60 ppm at 42 ppm) complex points, 1d18h14m), HNCACO (32 scans, 2048 (1H, 16.019 ppm at 4.698 ppm) × 64 (15N, 26 ppm at 117 ppm) × 75(13C, 11 ppm at 75 ppm) complex points, 20h55m), and HcccoNH (16 scans, 2048 (1H, 16.019 ppm at 4.698 ppm) × 28 (15N, 26 ppm at 117 ppm) × 50(1H, 7 ppm at 4.698 ppm) complex points, 1d7h25m).

**$^{13}$C,$^{15}$N-Holo ArCP in $D_2O$.** The following experiments were run: 2D-hbCBcgcdHD (192 scans, 2048 (1H, 16.0192 ppm at 4.696 ppm) × 52 (13C, 22.0002 ppm at 30 ppm) complex points, 3h18m) and 3D-HC-HSQC-NOESY (16 scans, 2048 (1H, 16.0192 ppm at 4.696 ppm) × 100 (1H, 13 ppm at 4.696 ppm) × 50 (13C, 50.0003 at 69.5 ppm) complex points, mixing time of 90 ms, 4d15h29m).

**$^{13}$C,$^{15}$N-Loaded ArCP in $H_2O$.** The following experiments performed: HNCO (16 scans, 2048 (1H, 16.019 ppm at 4.698 ppm) × 64 (15N, 26 ppm at 117 ppm) × 75 (13C, 11 ppm at 174 ppm) complex points, 10h20m), HNCA (16 scans, 2048 (1H, 16.019 ppm at 4.698 ppm) × 64 (15N, 26 ppm at 117 ppm) × 100(13C, 30 ppm at 52 ppm) complex points, 13h44m), HNCACB (32 scans, 2048(1H, 16.109 ppm at 4.698 ppm) × 64 (15N, 26 ppm at 117 ppm) × 150 (13C, 60 ppm at 42 ppm) complex points, 1d18h14m), HNCACO (32 scans, 2048 (1H, 16.019 ppm at 4.698 ppm) × 64 (15N, 26 ppm at 117 ppm) × 75(13C, 11 ppm at 75 ppm) complex points, 20h55m). Following the HNCACO, the sample was buffer exchanged 150-fold into identical buffer as before to remove AMP and PPi and concentrated to 400 μM and the following experiment performed: HcccoNH (16 scans, 2048 (1H, 16.019 ppm at 4.698 ppm) × 28 (15N, 26 ppm at 117 ppm) × 60(1H, 7 ppm at 4.698 ppm) complex points, 1d14h7m).

**$^{13}$C,$^{15}$N-Loaded ArCP in $D_2O$.** 2D-hbCBcgcdHD (800 scans, 2048 (1H, 16.0192 ppm at 4.696 ppm) × 52 (13C, 22.0002 ppm at 30 ppm) complex points, 13h39m) and 3D-NOESY-HC-HSQC (16 scans, 2048 (1H, 16.0192 ppm at 4.696 ppm) × 100 (1H, 13 ppm at 4.696 ppm) × 50 (13C, 50.0003 at 69.5 ppm) complex points, mixing time of 90 ms, 4d15h54m) were run with this sample.

**$^{15}$N-Holo ArCP relaxation.** T1 and {HN}-heteronuclear-NOESY experiments were run on 300 μM (T1 and het-NOE) and 380 μM (T2) holo samples with the following parameters: T1: 24 scans, 2048 (1H, 16.1092 ppm at 4.700 ppm) × 128 (15N, 26 ppm at 117 ppm) complex points, 3s recycling delay, and relaxation delays of 0, 0.510, 1.02, and 1.53 seconds, collected in that order; T2: 16 scans, 2048 (1H 16.0192 ppm at 4.696 ppm) × 128 (15N, 26 ppm at 117 ppm) complex points, 4s recycling delay, and relaxation delays of 0.0, 0.140, 0.350, 0.210, 0.070, and 0.280 seconds collected in that order; {HN}-heteronuclear-NOESY: 100 scans, 2048 (1H, 16.0192 ppm at 4.700 ppm) × 78 (15N, 26 ppm at 117 ppm) complex points, 5s recycling delay for reference experiment and 2s recycling delay followed by 3s saturation by 120° 1H pulses every 5 ms for saturation experiment.

**$^{15}$N-Loaded ArCP relaxation.** T1, T2, and {HN}-heteronuclear-NOESY experiments were run with the following parameters: T1: 24 scans, 2048 (1H, 16.1092 ppm at 4.697 ppm) × 128 (15N, 26 ppm at 117 ppm) complex points, 3s recycling delay, and relaxation delays of 0, 1.53, 0.510, and 1.02 seconds, collected in that order; T2: 16 scans, 2048 (1H 16.0192 ppm at 4.696 ppm) × 128 (15N, 26 ppm at 117 ppm) complex points, 4s recycling delay, and relaxation delays of 0.140, 0.350, 0.210, 0.070, 0.280 and 0.0 seconds collected in that order; {HN}-heteronuclear-NOESY: 100 scans, 2048 (1H, 16.0192 ppm at 4.696 ppm) × 110 (15N, 26 ppm at 117 ppm) complex points, 5s recycling delay for reference experiment and 2s recycling delay followed by 3s saturation by 120° 1H pulses every 5 ms for saturation experiment with saturation and reference experiments collected in an interleaved manner.

| NMR structure statistics for holo-ArCP | |
|---|---|
| Violations (mean and s.d.)[a] | |
| Distance constraints (Å) | 0.32 +/- 0.07 |
| Dihedral angle constraints (º) | 1.88 +/- 0.41 |
| Max. dihedral angle violation (º) | 3.12 |
| Max. distance constraint violation (Å) | 0.43 |
| R. m. s. deviations geometry [c] | |
| Bond lengths (Å) | 0.017 |
| Bond angles (º) | 1.4 |
| Average pairwise r.m.s.d. [residues 19–88] (Å) [a] | |
| Heavy | 0.88 +/- 0.07 |
| Backbone | 0.37 +/- 0.06 |
| Ramachandran Statistics [b] | |
| Most favoured | 92.5 |
| Additionally allowed | 7.5 |
| Generously allowed | 0.0 |
| Disallowed | 0.0 |

**Table S1**: NMR structure statistics for holo-ArCP. a from CYANA 2.1[2], b from PROCHECK_NMR[3] residues 17-90. c From PSVS[4].

| NMR structure statistics for loaded-ArCP | |
|---|---|
| Violations (mean and s.d.)[a] | |
| Distance constraints (Å) | 0.30 +/- 0.07 |
| Dihedral angle constraints (º) | 2.81 +/- 0.27 |
| Max. dihedral angle violation (º) | 3.38 |
| Max. distance constraint violation (Å) | 0.47 |
| R. m. s. deviations geometry [c] | |
| Bond lengths (Å) | 0.017 |
| Bond angles (º) | 1.6 |
| Average pairwise r.m.s.d. [residues 19–88] (Å) [a] | |
| Heavy | 0.85 +/- 0.09 |
| Backbone | 0.36 +/- 0.08 |
| Ramachandran Statistics [b] | |
| Most favoured | 89.4 |
| Additionally allowed | 10.6 |
| Generously allowed | 0.0 |
| Disallowed | 0.0 |

**Table S2**: NMR structure statistics for loaded-ArCP. a from CYANA 2.1[2], b from PROCHECK_NMR [3], residues 16-89. c From PSVS[4].

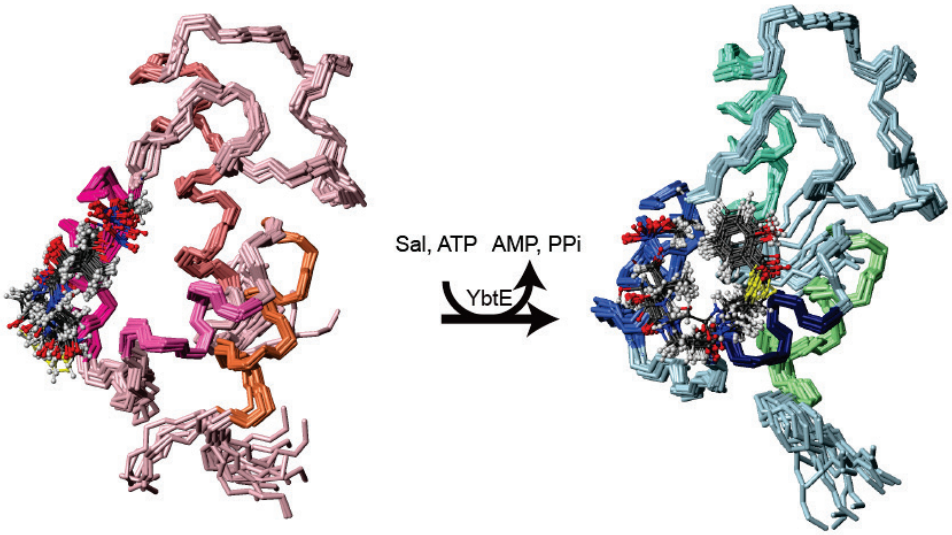


**Figure S1.** NMR bundles for holo-ArCP (left) and loaded-ArCP (blue). In holo-ArCP, alpha helices are colored as follows: α1: brown, α2:magenta, α3:pink, α4:beige. The corresponding colors for loaded-ArCP are: α1:cyan, α2:skye blue, α3:royal blue, α4:green. Alignments made with $C^{\alpha}$ of residues in helices only (r.m.s.d of 0.33 for holo and 0.37 for loaded). Figure generated with molmol[5]. A compact fold in ArCP gives rise to a large number of NMR constraints and, hence, to high resolution structures with low root-mean-squared-standard-deviation (rmsd). Thus, the NMR structure of the holo-ArCP protein core is defined by 1636 distance constraints (20 per residues) leading to an rmsd of 0.88 Å for heavy atoms and 0.37 Å for backbone atoms (see Table S1). $C^{\alpha}$ in helices align with an rmsd of 0.33 Å. This number increases to only 0.38 Å when loops are included (residues 19-89), indicating that the loops are well defined by interactions with the helical core. The protein core of loaded ArCP provides 1314 distance constraints (16 per residue) resulting in an rmsd of 0.86 Å for heavy atoms and 0.35 Å for backbone atoms (Table S2). The rmsd for $C^{\alpha}$ is 0.37 Å when calculated with helices only and 0.4 Å when all residues from 19-89 are included. Thus, the NMR structures of holo- and loaded ArCP are well defined for the entire range of residues excluding N- and C-termini and lead to tight NMR ensembles. The residues masked by PP in holo-ArCP are S52, I53, M56, and L59 on α2, and L71, R72, and Y75 on loopII and α3. In loaded-ArCP, Sal and PP cover a surface involving residues L50-I53, M56, R72, Y75, A76 and I46.

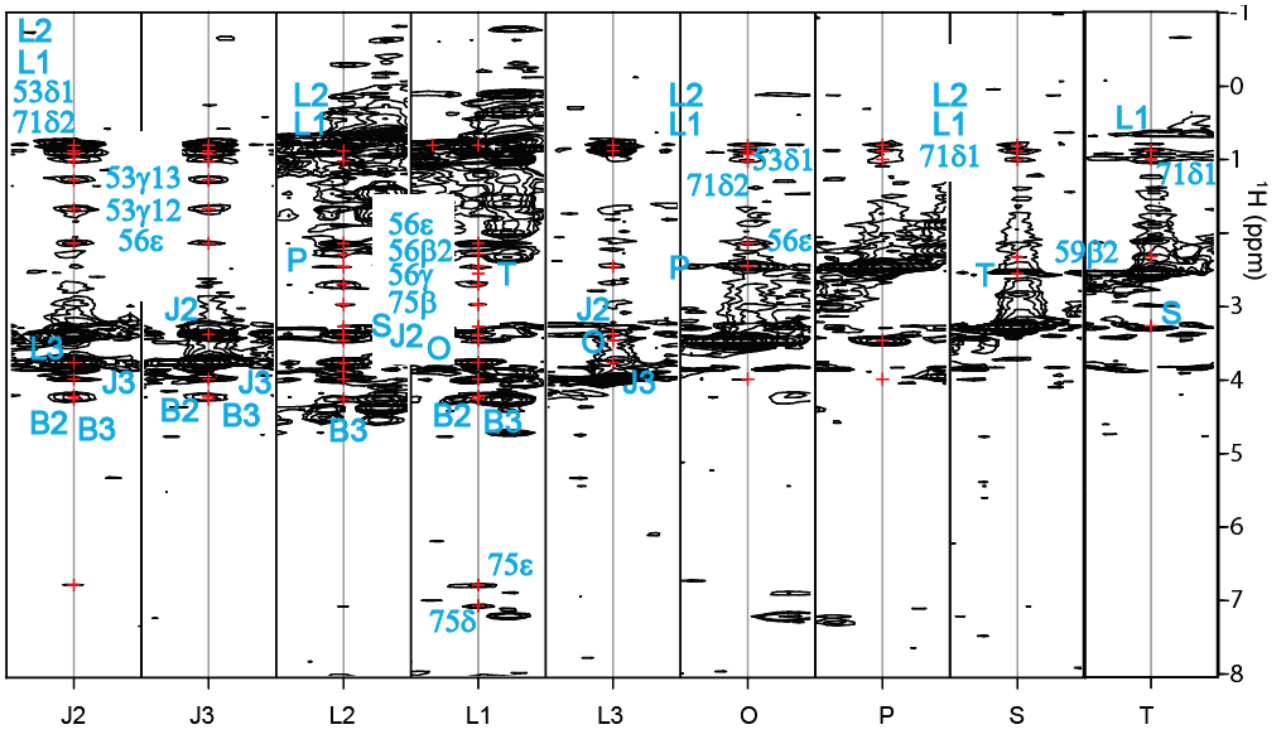


**Figure S2**. NOESY strips involving PP in holo-ArCP. The labels for PP moieties (Roman alphabet) are defined in Figure 1. Labels are positioned between two strips when the corresponding signals are observed in both. For crowded regions, the order of the labels from top to bottom refers to the nearest series of signals, again from top to bottom.

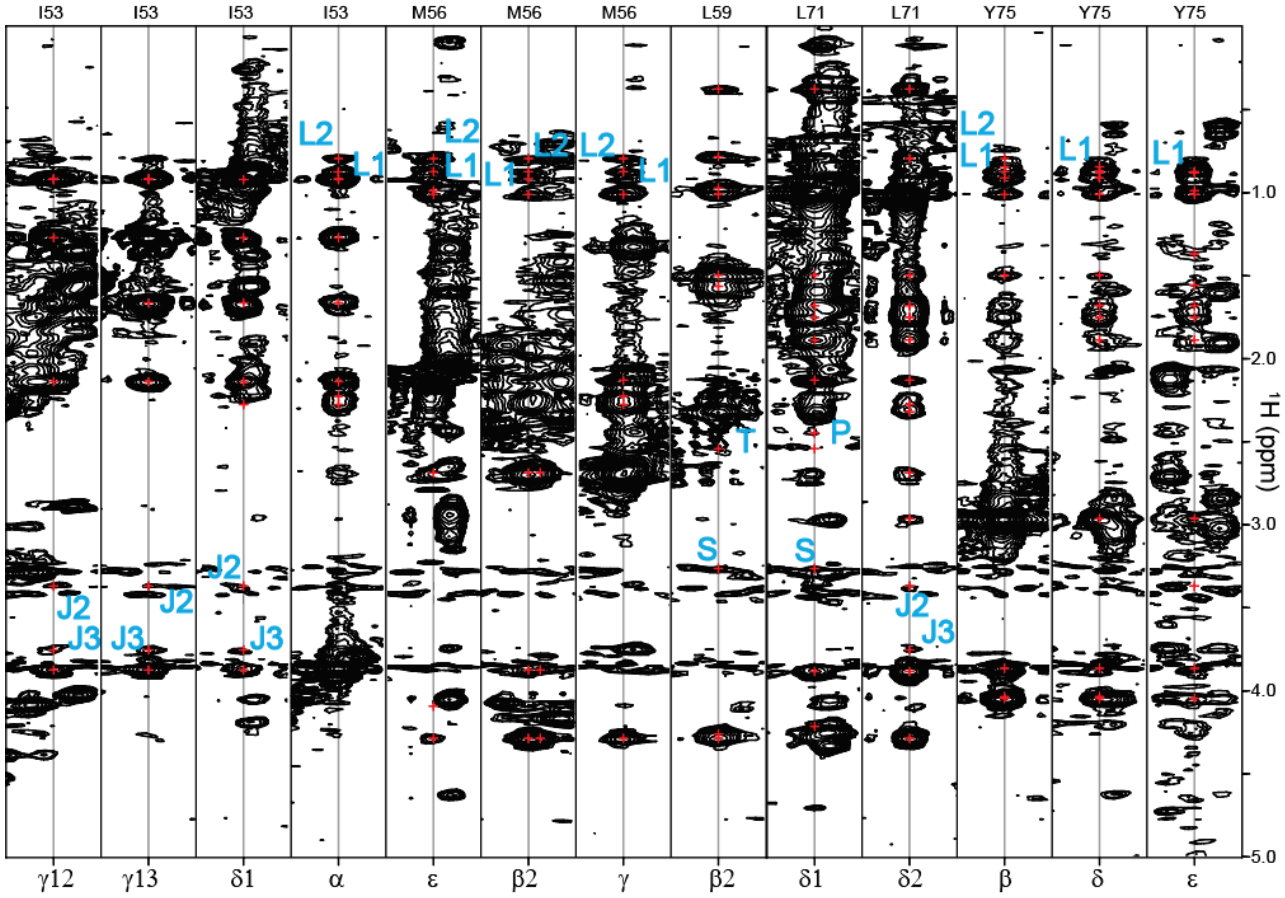


**Figure S3**. NOESY strips of residues in holo-ArCP displaying NOESY cross-peaks with PP. Unlabeled cross-peaks denote cross-peaks within the protein core. A total of 50 cross-peaks involving PP could be assigned unambiguously from peaks seen in Figures S2 and S3. They include 14 nOe's within the PP arm and 36 nOe's between the protein core and PP.

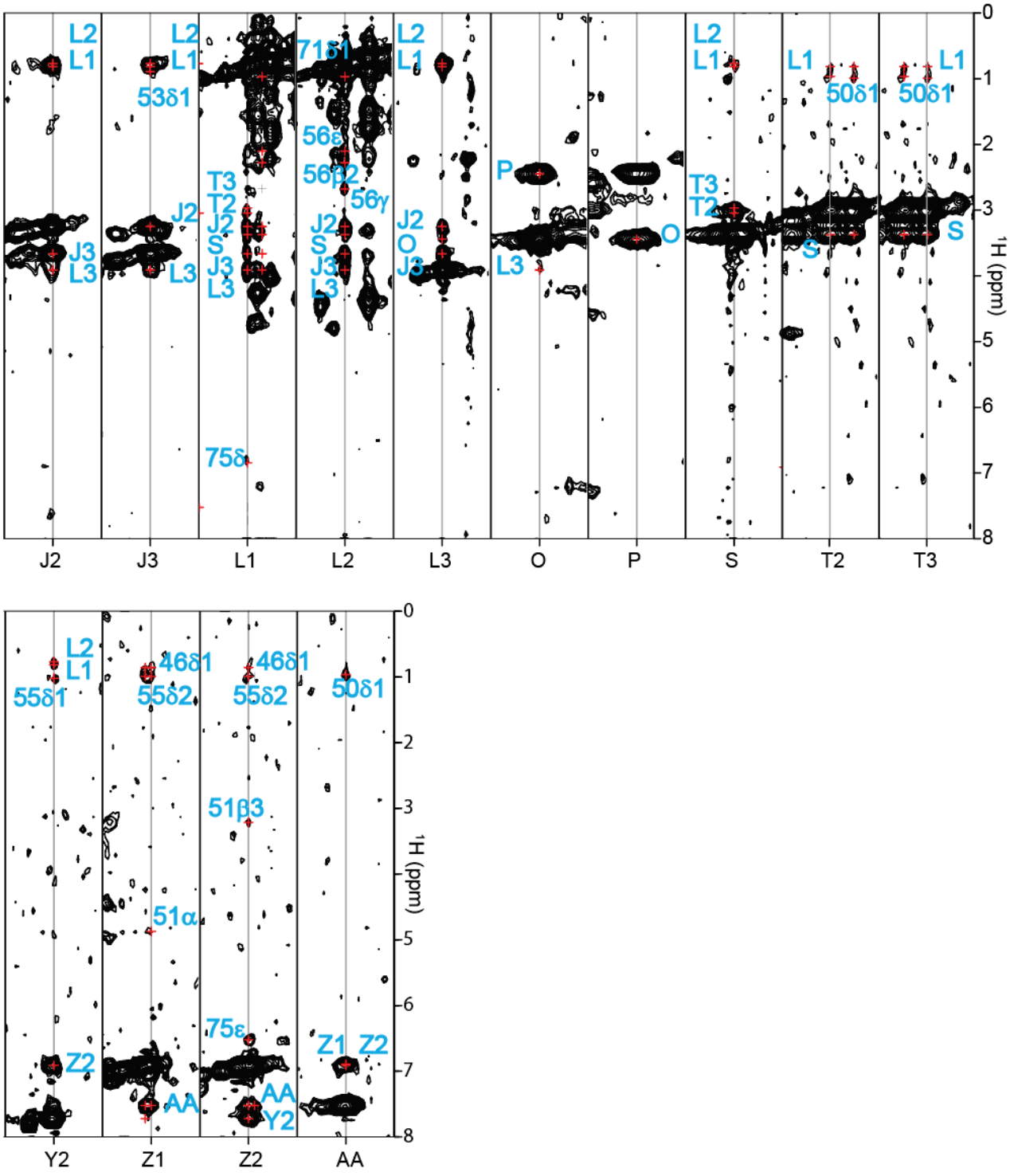


**Figure S4**. NOESY strips involving salicylate and PP in loaded-ArCP. The labels for PP moieties (Roman alphabet) are defined in Figure 1. For crowded regions, the order of the labels from top to bottom refers to the nearest series of signals, again from top to bottom.

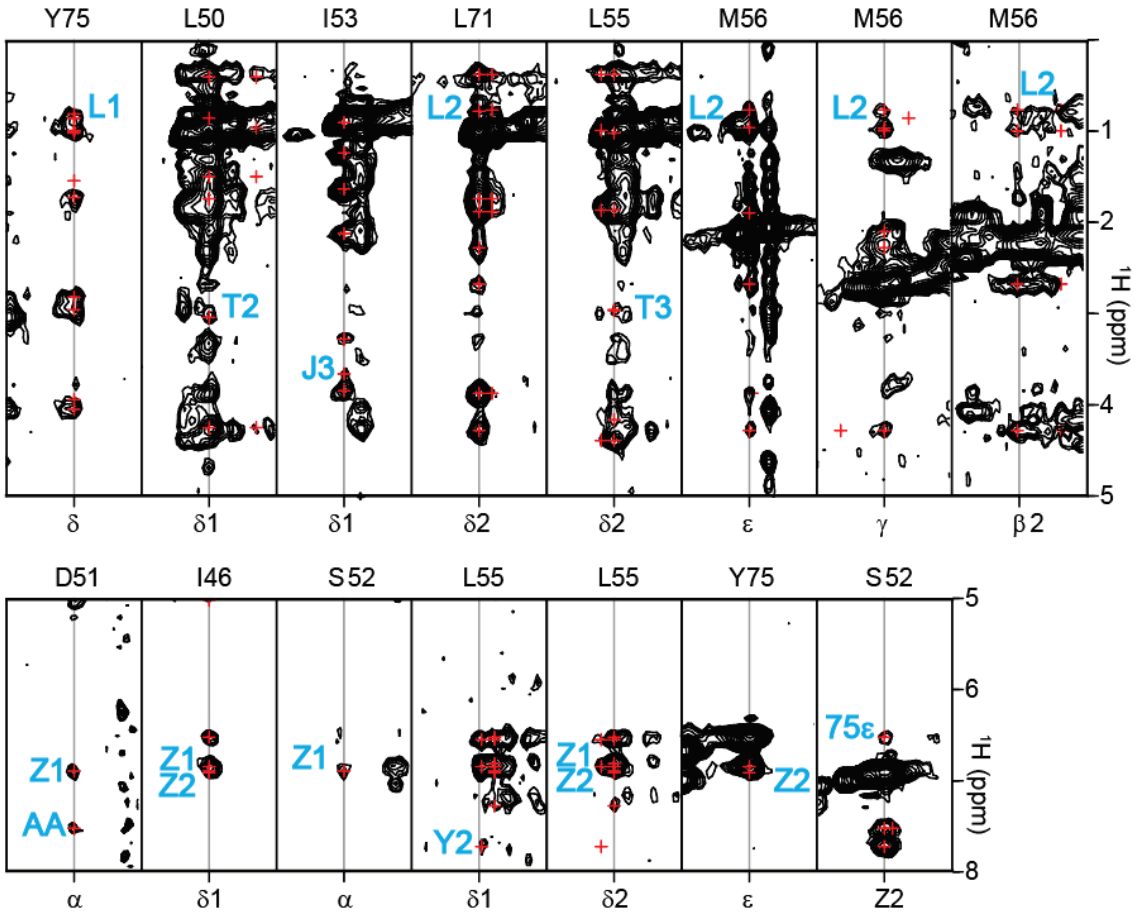


**Figure S5.** NOESY strips of residues in loaded-ArCP displaying NOESY cross-peaks with PP (top) and Sal (bottom). Unlabeled cross-peaks denote cross-peaks within the protein core. The strip of Z2 (in salicylate) is shown to confirm the assignment of a NOESY cross-peak in Y75ε that overlaps with another cross-peak. 12 nOe's were observed between loaded-ArCP and Sal and 8 with PP. In addition, 9 constraints could be determined within the Sal-PP moiety.

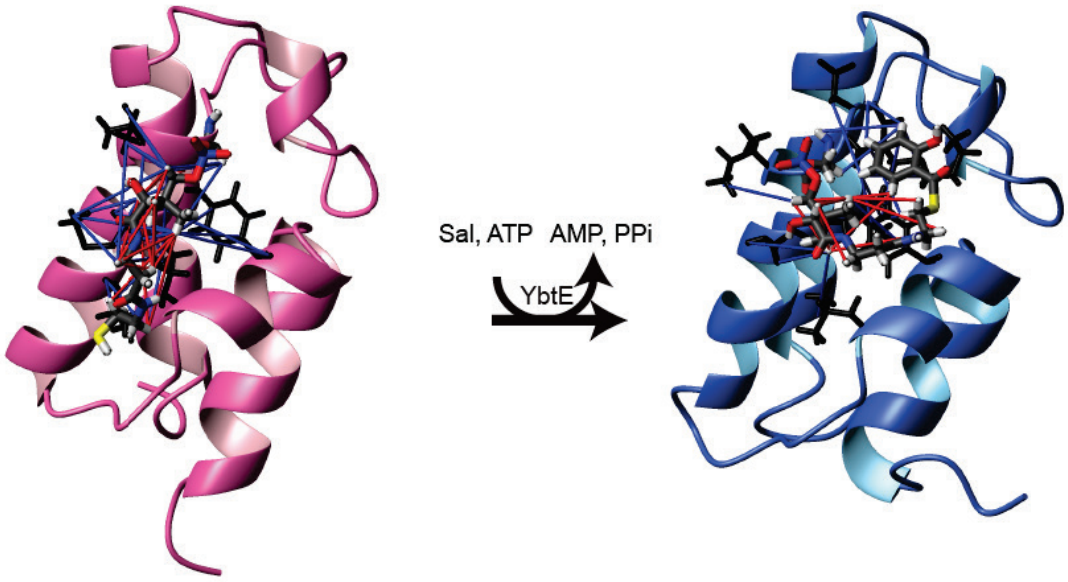


**Figure S6.** Visualization of distance constraints involving prosthetic groups in holo-ArCP (left) and loaded-ArCP (right). Lines in blue denote distances between the core protein and the prosthetic group, those in red denote distances within the prosthetic groups. Side chains of residues involved are shown in black neon. The lowest energy conformers were selected for display.

**Relaxation rates and Model-Free Parameters**

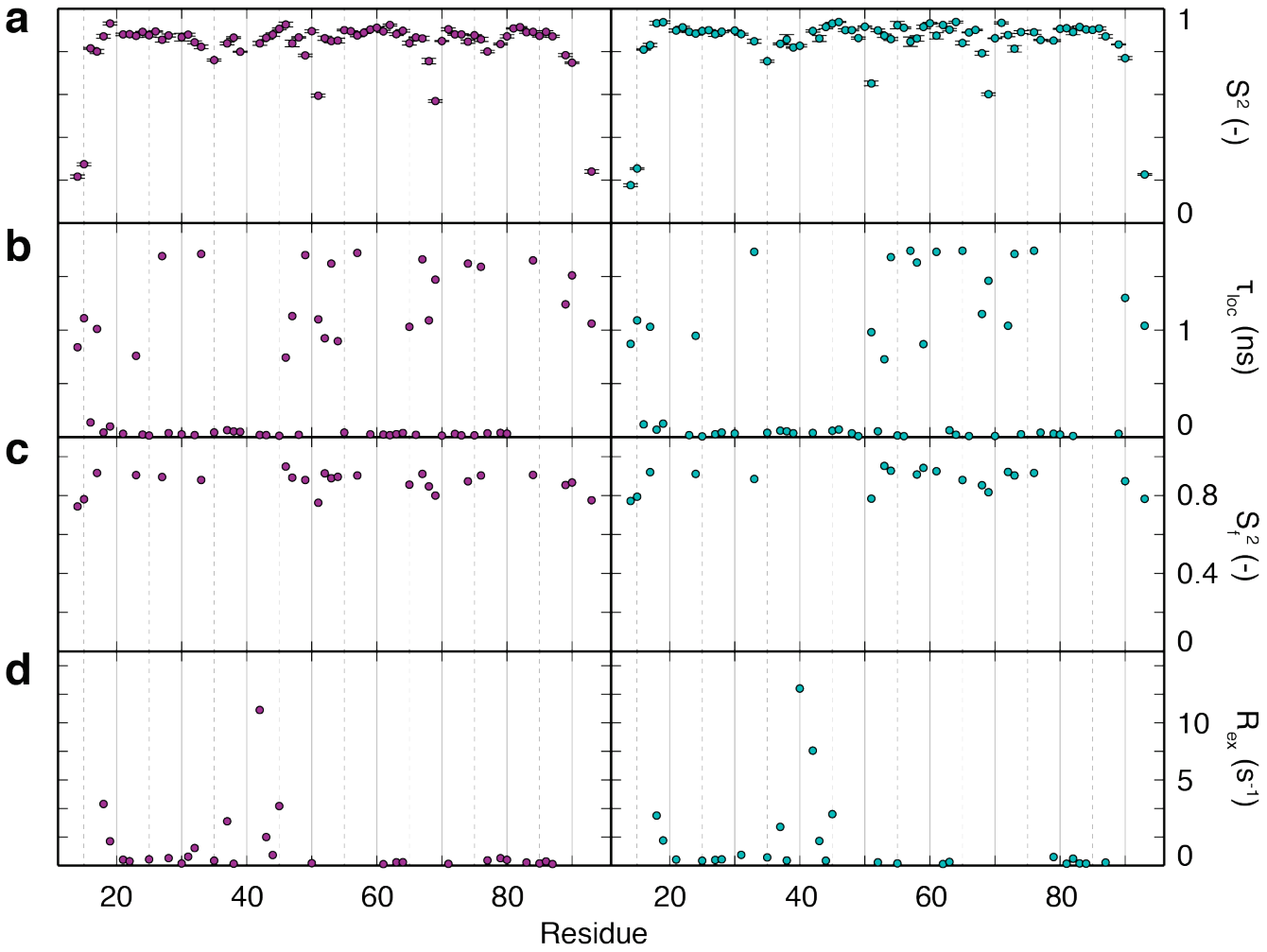


**Figure S7.** Model-free analysis of holo (left, pink) and loaded (right, cyan) ArCP. The analysis was performed using the software ROTDIF[6,7]. ROTDIF selects which parameters to use when fitting based on the Akaike Information Criterion. For a given residue, parameters not selected have not been plotted. (a) Overall ($S^2$) or slow time-scale ($S_s^2$, when $S_f^2$ is present) order parameter (b) Effective correlation time $\tau_{loc}$ (c) Fast time scale order parameter ($S_f^2$) (d) Exchange contribution to transverse relaxation ($R_{ex}$)

| Residue | R1 | σR1 | R2 | σR2 | NOE | σNOE | $S^2$ | σ$S^2$ | $T_{loc}$ | $S_f^2$ | $R_{ex}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **D14** | 1.380 | 0.016 | 2.970 | 0.046 | -0.1324 | 0.0119 | 0.216 | 0.008 | 0.84 | 0.74 | - |
| **N15** | 1.590 | 0.007 | 3.600 | 0.024 | 0.1854 | 0.0037 | 0.274 | 0.007 | 1.11 | 0.78 | - |
| **R16** | 1.890 | 0.011 | 7.090 | 0.036 | 0.5295 | 0.0073 | 0.815 | 0.004 | 0.14 | - | - |
| **H17** | 1.890 | 0.010 | 7.400 | 0.034 | 0.6726 | 0.0065 | 0.800 | 0.010 | 1.01 | 0.92 | - |
| **A18** | 1.870 | 0.014 | 12.010 | 0.079 | 0.7287 | 0.0086 | 0.871 | 0.009 | 0.04 | - | 4.31 |
| **A19** | 1.980 | 0.011 | 10.040 | 0.038 | 0.7245 | 0.0132 | 0.931 | 0.007 | 0.10 | - | 1.70 |
| **Y21** | 1.870 | 0.007 | 8.220 | 0.036 | 0.7524 | 0.0034 | 0.880 | 0.006 | 0.03 | - | 0.41 |
| **Q22** | 1.840 | 0.011 | 8.150 | 0.035 | 0.7815 | 0.0058 | 0.881 | 0.007 | - | - | 0.30 |
| **Q23** | 1.880 | 0.009 | 7.830 | 0.034 | 0.7566 | 0.0063 | 0.873 | 0.008 | 0.76 | 0.90 | - |
| **L24** | 1.880 | 0.010 | 7.950 | 0.043 | 0.7671 | 0.0058 | 0.892 | 0.003 | 0.02 | - | - |
| **R25** | 1.850 | 0.012 | 8.200 | 0.058 | 0.7767 | 0.0078 | 0.876 | 0.008 | 0.01 | - | 0.43 |
| **E26** | 1.870 | 0.009 | 7.960 | 0.040 | 0.8048 | 0.0060 | 0.894 | 0.003 | - | - | - |
| **R27** | 1.890 | 0.006 | 7.690 | 0.052 | 0.7770 | 0.0069 | 0.855 | 0.011 | 1.69 | 0.89 | - |
| **L28** | 1.890 | 0.007 | 8.170 | 0.026 | 0.7398 | 0.0058 | 0.875 | 0.007 | 0.04 | - | 0.52 |
| **Q30** | 1.830 | 0.009 | 7.900 | 0.035 | 0.7549 | 0.0061 | 0.867 | 0.018 | 0.03 | - | 0.15 |
| **E31** | 1.840 | 0.010 | 8.430 | 0.045 | 0.7960 | 0.0064 | 0.879 | 0.007 | - | - | 0.62 |
| **L32** | 1.800 | 0.009 | 8.640 | 0.036 | 0.7595 | 0.0046 | 0.843 | 0.007 | 0.02 | - | 1.23 |
| **N33** | 1.850 | 0.007 | 7.530 | 0.029 | 0.7738 | 0.0112 | 0.822 | 0.008 | 1.71 | 0.88 | - |
| **T35** | 1.630 | 0.005 | 7.260 | 0.024 | 0.6485 | 0.0037 | 0.760 | 0.005 | 0.04 | - | 0.34 |
| **Q37** | 1.830 | 0.008 | 10.520 | 0.045 | 0.6665 | 0.0097 | 0.838 | 0.007 | 0.06 | - | 3.10 |
| **Q38** | 1.860 | 0.005 | 7.810 | 0.026 | 0.7081 | 0.0041 | 0.865 | 0.004 | 0.05 | - | 0.13 |
| **L39** | 1.720 | 0.007 | 7.210 | 0.027 | 0.6630 | 0.0032 | 0.799 | 0.002 | 0.05 | - | - |
| **E42** | 1.800 | 0.007 | 18.220 | 0.076 | 0.7546 | 0.0069 | 0.838 | 0.009 | 0.02 | - | 10.89 |
| **S43** | 1.810 | 0.013 | 9.750 | 0.070 | 0.7674 | 0.0051 | 0.864 | 0.008 | 0.02 | - | 1.99 |
| **N44** | 1.880 | 0.006 | 8.350 | 0.035 | 0.7961 | 0.0042 | 0.879 | 0.008 | - | - | 0.74 |
| **L45** | 1.900 | 0.008 | 12.240 | 0.061 | 0.7855 | 0.0058 | 0.906 | 0.005 | 0.01 | - | 4.16 |
| **I46** | 1.980 | 0.009 | 8.260 | 0.030 | 0.7693 | 0.0048 | 0.926 | 0.011 | 0.74 | 0.95 | - |
| **Q47** | 1.880 | 0.011 | 7.490 | 0.039 | 0.7454 | 0.0144 | 0.838 | 0.015 | 1.13 | 0.89 | - |
| **A48** | 1.810 | 0.010 | 7.800 | 0.041 | 0.7602 | 0.0058 | 0.866 | 0.003 | 0.02 | - | - |
| **G49** | 1.880 | 0.007 | 7.200 | 0.032 | 0.7461 | 0.0035 | 0.782 | 0.006 | 1.70 | 0.88 | - |
| **L50** | 1.950 | 0.011 | 7.730 | 0.060 | 0.9168 | 0.0173 | 0.895 | 0.007 | - | - | 0.17 |
| **D51** | 1.580 | 0.007 | 5.670 | 0.030 | 0.5928 | 0.0042 | 0.594 | 0.007 | 1.10 | 0.76 | - |
| **S52** | 1.880 | 0.013 | 7.870 | 0.048 | 0.7393 | 0.0095 | 0.862 | 0.010 | 0.92 | 0.91 | - |
| **I53** | 1.860 | 0.009 | 7.720 | 0.035 | 0.7729 | 0.0064 | 0.849 | 0.008 | 1.62 | 0.89 | - |
| **R54** | 1.860 | 0.009 | 7.670 | 0.035 | 0.7453 | 0.0065 | 0.851 | 0.011 | 0.90 | 0.90 | - |
| **L55** | 1.890 | 0.010 | 8.120 | 0.047 | 0.7484 | 0.0053 | 0.900 | 0.004 | 0.04 | - | - |
| **M56** | 1.860 | 0.009 | 8.030 | 0.040 | 0.8017 | 0.0149 | 0.895 | 0.003 | - | - | - |
| **R57** | 1.890 | 0.009 | 7.930 | 0.030 | 0.7883 | 0.0052 | 0.875 | 0.006 | 1.72 | 0.90 | - |
| **W58** | 1.840 | 0.011 | 7.990 | 0.042 | 0.7970 | 0.0054 | 0.888 | 0.004 | - | - | - |
| **L59** | 1.870 | 0.012 | 8.200 | 0.047 | 0.7675 | 0.0071 | 0.903 | 0.004 | 0.03 | - | - |
| **H60** | 1.890 | 0.010 | 8.190 | 0.045 | 0.8126 | 0.0071 | 0.911 | 0.004 | - | - | - |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **W61** | 1.880 | 0.009 | 8.100 | 0.043 | 0.7686 | 0.0068 | 0.894 | 0.005 | 0.02 | - | 0.10 |
| **F62** | 1.910 | 0.012 | 8.380 | 0.050 | 0.7813 | 0.0110 | 0.924 | 0.004 | 0.02 | - | - |
| **R63** | 1.850 | 0.009 | 8.140 | 0.041 | 0.7578 | 0.0053 | 0.881 | 0.006 | 0.03 | - | 0.23 |
| **K64** | 1.900 | 0.011 | 8.230 | 0.061 | 0.7498 | 0.0053 | 0.897 | 0.006 | 0.04 | - | 0.23 |
| **N65** | 1.790 | 0.004 | 7.500 | 0.031 | 0.7812 | 0.0030 | 0.839 | 0.009 | 1.03 | 0.86 | - |
| **G66** | 1.840 | 0.006 | 7.670 | 0.027 | 0.7623 | 0.0032 | 0.866 | 0.002 | 0.02 | - | - |
| **Y67** | 1.950 | 0.006 | 7.660 | 0.027 | 0.7799 | 0.0051 | 0.861 | 0.010 | 1.66 | 0.91 | - |
| **R68** | 1.790 | 0.007 | 6.780 | 0.027 | 0.6983 | 0.0031 | 0.755 | 0.013 | 1.09 | 0.85 | - |
| **L69** | 1.730 | 0.006 | 5.610 | 0.025 | 0.6070 | 0.0041 | 0.569 | 0.006 | 1.47 | 0.80 | - |
| **T70** | 1.870 | 0.004 | 7.150 | 0.023 | 0.7681 | 0.0030 | 0.849 | 0.002 | 0.01 | - | - |
| **L71** | 1.960 | 0.014 | 7.820 | 0.055 | 0.7896 | 0.0072 | 0.904 | 0.007 | - | - | 0.12 |
| **R72** | 1.920 | 0.013 | 7.580 | 0.044 | 0.7548 | 0.0085 | 0.880 | 0.004 | 0.03 | - | - |
| **E73** | 1.850 | 0.009 | 7.820 | 0.037 | 0.7710 | 0.0042 | 0.880 | 0.003 | 0.02 | - | - |
| **L74** | 1.890 | 0.009 | 7.320 | 0.035 | 0.7807 | 0.0036 | 0.846 | 0.008 | 1.62 | 0.87 | - |
| **Y75** | 1.900 | 0.009 | 7.530 | 0.032 | 0.7720 | 0.0041 | 0.876 | 0.003 | 0.02 | - | - |
| **A76** | 1.910 | 0.009 | 7.710 | 0.043 | 0.7673 | 0.0057 | 0.857 | 0.010 | 1.59 | 0.90 | - |
| **A77** | 1.750 | 0.006 | 7.340 | 0.032 | 0.7003 | 0.0032 | 0.800 | 0.006 | 0.04 | - | 0.36 |
| **T79** | 1.800 | 0.005 | 7.900 | 0.027 | 0.7125 | 0.0053 | 0.835 | 0.004 | 0.04 | - | 0.51 |
| **L80** | 1.860 | 0.008 | 8.100 | 0.034 | 0.7454 | 0.0046 | 0.871 | 0.007 | 0.03 | - | 0.40 |
| **A81** | 1.880 | 0.010 | 8.170 | 0.046 | 0.7955 | 0.0061 | 0.908 | 0.003 | - | - | - |
| **A82** | 1.910 | 0.009 | 8.160 | 0.037 | 0.7989 | 0.0080 | 0.914 | 0.003 | - | - | - |
| **W83** | 1.860 | 0.009 | 8.140 | 0.039 | 0.7926 | 0.0049 | 0.890 | 0.005 | - | - | 0.21 |
| **N84** | 1.910 | 0.009 | 7.930 | 0.041 | 0.7908 | 0.0056 | 0.892 | 0.006 | 1.65 | 0.91 | - |
| **Q85** | 1.820 | 0.010 | 7.960 | 0.039 | 0.7883 | 0.0059 | 0.873 | 0.005 | - | - | 0.15 |
| **L86** | 1.860 | 0.012 | 8.260 | 0.052 | 0.8219 | 0.0051 | 0.892 | 0.006 | - | - | 0.29 |
| **M87** | 1.850 | 0.010 | 7.720 | 0.031 | 0.7912 | 0.0055 | 0.871 | 0.005 | - | - | 0.10 |
| **S89** | 1.780 | 0.006 | 7.180 | 0.027 | 0.7315 | 0.0086 | 0.783 | 0.007 | 1.24 | 0.85 | - |
| **R90** | 1.870 | 0.005 | 6.760 | 0.028 | 0.7377 | 0.0033 | 0.748 | 0.004 | 1.51 | 0.87 | - |
| **G93** | 1.550 | 0.005 | 3.360 | 0.027 | 0.1075 | 0.0032 | 0.240 | 0.008 | 1.06 | 0.78 | - |
| **NN** | 1.480 | 0.008 | 2.450 | 0.026 | -0.1610 | 0.0050 | | | | | |
| **NR** | 0.820 | 0.004 | 1.370 | 0.019 | -0.6591 | 0.0089 | | | | | |

**Table S3.** Relaxation parameters and model-free parameters for holo-ArCP. The experimental error for a given parameter is indicated with the σ symbol. ROTDIF[6,7] does not provide experimental errors for $\tau_{loc}$, $S_f^2$, nor $R_{ex}$. Dashes indicate when a given model-free parameter was not included in the fit. Due to limitations of the Lipari-Szabo model, the NN and NR positions of the PP arm were not fit with the model free formalism.

| Residue | R1 | σR1 | R2 | σR2 | NOE | σNOE | $S^2$ | σ$S^2$ | $T_{loc}$ | $S_f^2$ | $R_{ex}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **D14** | 1.430 | 0.013 | 2.800 | 0.037 | -0.1846 | 0.0110 | 0.176 | 0.007 | 0.87 | 0.77 | - |
| **N15** | 1.600 | 0.007 | 3.540 | 0.020 | 0.1449 | 0.0041 | 0.254 | 0.004 | 1.09 | 0.79 | - |
| **R16** | 1.810 | 0.013 | 7.250 | 0.030 | 0.5372 | 0.0062 | 0.809 | 0.003 | 0.12 | - | - |
| **H17** | 1.930 | 0.011 | 7.480 | 0.032 | 0.7035 | 0.0065 | 0.830 | 0.008 | 1.03 | 0.92 | - |
| **A18** | 1.980 | 0.018 | 11.800 | 0.068 | 0.7458 | 0.0077 | 0.932 | 0.009 | 0.07 | - | 3.50 |
| **A19** | 1.970 | 0.013 | 10.290 | 0.044 | 0.7197 | 0.0078 | 0.937 | 0.006 | 0.13 | - | 1.76 |
| **Y21** | 1.880 | 0.011 | 8.410 | 0.031 | 0.8009 | 0.0078 | 0.898 | 0.007 | - | - | 0.42 |
| **Q22** | 1.870 | 0.016 | 8.310 | 0.063 | 0.7946 | 0.0084 | 0.913 | 0.005 | - | - | - |
| **Q23** | 1.860 | 0.009 | 8.030 | 0.041 | 0.7753 | 0.0058 | 0.892 | 0.003 | 0.02 | - | - |
| **L24** | 1.880 | 0.012 | 8.020 | 0.036 | 0.7711 | 0.0057 | 0.884 | 0.007 | 0.95 | 0.91 | - |
| **R25** | 1.860 | 0.010 | 8.410 | 0.039 | 0.7926 | 0.0066 | 0.896 | 0.005 | 0.01 | - | 0.34 |
| **E26** | 1.860 | 0.010 | 8.130 | 0.039 | 0.8064 | 0.0057 | 0.900 | 0.003 | - | - | - |
| **R27** | 1.850 | 0.010 | 8.310 | 0.038 | 0.7590 | 0.0045 | 0.881 | 0.011 | 0.03 | - | 0.39 |
| **L28** | 1.900 | 0.009 | 8.360 | 0.024 | 0.7423 | 0.0049 | 0.893 | 0.005 | 0.04 | - | 0.43 |
| **Q30** | 1.870 | 0.010 | 8.140 | 0.035 | 0.7582 | 0.0048 | 0.898 | 0.003 | 0.03 | - | - |
| **E31** | 1.850 | 0.008 | 8.540 | 0.028 | 0.8073 | 0.0052 | 0.881 | 0.005 | - | - | 0.75 |
| **N33** | 1.830 | 0.008 | 7.830 | 0.025 | 0.7780 | 0.0059 | 0.848 | 0.009 | 1.73 | 0.88 | - |
| **T35** | 1.610 | 0.005 | 7.470 | 0.018 | 0.6551 | 0.0035 | 0.755 | 0.005 | 0.04 | - | 0.57 |
| **Q37** | 1.830 | 0.008 | 10.070 | 0.036 | 0.6743 | 0.0049 | 0.836 | 0.004 | 0.06 | - | 2.71 |
| **Q38** | 1.850 | 0.007 | 7.940 | 0.024 | 0.7002 | 0.0038 | 0.856 | 0.023 | 0.05 | - | 0.35 |
| **L39** | 1.750 | 0.008 | 7.300 | 0.026 | 0.7094 | 0.0048 | 0.819 | 0.003 | 0.04 | - | - |
| **H40** | 1.790 | 0.009 | 19.480 | 0.139 | 0.7872 | 0.0061 | 0.827 | 0.006 | - | - | 12.40 |
| **E42** | 1.910 | 0.010 | 15.980 | 0.087 | 0.7491 | 0.0062 | 0.896 | 0.005 | 0.04 | - | 8.05 |
| **S43** | 1.850 | 0.027 | 9.140 | 0.094 | 0.7968 | 0.0089 | 0.861 | 0.014 | - | - | 1.72 |
| **N44** | 1.900 | 0.011 | 8.550 | 0.035 | 0.8094 | 0.0058 | 0.915 | 0.008 | - | - | 0.34 |
| **L45** | 1.960 | 0.011 | 11.950 | 0.063 | 0.7526 | 0.0050 | 0.931 | 0.005 | 0.06 | - | 3.60 |
| **I46** | 1.990 | 0.008 | 8.330 | 0.026 | 0.7488 | 0.0036 | 0.938 | 0.002 | 0.07 | - | - |
| **Q47** | 1.880 | 0.019 | 7.970 | 0.062 | 0.8018 | 0.0101 | 0.900 | 0.006 | - | - | - |
| **A48** | 1.830 | 0.014 | 8.270 | 0.049 | 0.7544 | 0.0051 | 0.900 | 0.004 | 0.04 | - | - |
| **G49** | 1.880 | 0.017 | 7.370 | 0.045 | 0.7812 | 0.0078 | 0.863 | 0.005 | 0.01 | - | - |
| **L50** | 1.920 | 0.011 | 8.110 | 0.059 | 0.8028 | 0.0122 | 0.916 | 0.004 | - | - | - |
| **D51** | 1.620 | 0.008 | 6.040 | 0.028 | 0.6241 | 0.0047 | 0.651 | 0.011 | 0.98 | 0.78 | - |
| **S52** | 1.940 | 0.014 | 8.110 | 0.046 | 0.7324 | 0.0077 | 0.899 | 0.006 | 0.05 | - | 0.22 |
| **I53** | 1.940 | 0.009 | 8.010 | 0.028 | 0.6934 | 0.0060 | 0.874 | 0.008 | 0.73 | 0.95 | - |
| **R54** | 1.930 | 0.009 | 7.990 | 0.037 | 0.7571 | 0.0063 | 0.858 | 0.007 | 1.68 | 0.93 | - |
| **L55** | 1.940 | 0.013 | 8.360 | 0.051 | 0.7862 | 0.0084 | 0.923 | 0.017 | 0.02 | - | 0.15 |
| **M56** | 1.900 | 0.011 | 8.160 | 0.043 | 0.7918 | 0.0070 | 0.911 | 0.004 | 0.01 | - | - |
| **R57** | 2.230 | 0.032 | 8.160 | 0.060 | 0.8509 | 0.0354 | 0.846 | 0.022 | 1.74 | - | - |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **W58** | 1.880 | 0.022 | 7.960 | 0.071 | 0.7701 | 0.0145 | 0.861 | 0.013 | 1.63 | 0.91 | - |
| **L59** | 1.940 | 0.012 | 8.310 | 0.048 | 0.7695 | 0.0059 | 0.915 | 0.008 | 0.87 | 0.94 | - |
| **H60** | 2.000 | 0.013 | 8.130 | 0.051 | 0.8375 | 0.0066 | 0.932 | 0.004 | - | - | - |
| **W61** | 1.960 | 0.015 | 7.940 | 0.055 | 0.8032 | 0.0090 | 0.874 | 0.015 | 1.73 | 0.93 | - |
| **F62** | 1.920 | 0.013 | 8.400 | 0.044 | 0.8643 | 0.0073 | 0.924 | 0.007 | - | - | 0.11 |
| **R63** | 1.890 | 0.011 | 8.470 | 0.035 | 0.7254 | 0.0073 | 0.902 | 0.006 | 0.06 | - | 0.25 |
| **K64** | 1.960 | 0.014 | 8.430 | 0.048 | 0.7856 | 0.0075 | 0.938 | 0.004 | 0.02 | - | - |
| **N65** | 1.840 | 0.007 | 7.680 | 0.030 | 0.7898 | 0.0043 | 0.840 | 0.009 | 1.74 | 0.88 | - |
| **G66** | 1.850 | 0.006 | 8.010 | 0.021 | 0.7878 | 0.0033 | 0.889 | 0.002 | 0.01 | - | - |
| **Y67** | 1.920 | 0.009 | 7.870 | 0.027 | 0.8005 | 0.0049 | 0.901 | 0.003 | - | - | - |
| **R68** | 1.780 | 0.006 | 7.200 | 0.025 | 0.7366 | 0.0025 | 0.792 | 0.009 | 1.15 | 0.85 | - |
| **L69** | 1.760 | 0.006 | 5.850 | 0.021 | 0.6175 | 0.0043 | 0.601 | 0.006 | 1.46 | 0.82 | - |
| **T70** | 1.840 | 0.005 | 7.530 | 0.021 | 0.7810 | 0.0042 | 0.862 | 0.002 | 0.01 | - | - |
| **L71** | 2.010 | 0.017 | 8.020 | 0.032 | 0.8225 | 0.0125 | 0.934 | 0.005 | - | - | - |
| **R72** | 1.930 | 0.010 | 7.850 | 0.032 | 0.7531 | 0.0042 | 0.877 | 0.008 | 1.04 | 0.92 | - |
| **E73** | 1.940 | 0.028 | 7.500 | 0.071 | 0.7624 | 0.0126 | 0.813 | 0.015 | 1.71 | 0.90 | - |
| **L74** | 1.920 | 0.025 | 7.740 | 0.072 | 0.7615 | 0.0085 | 0.891 | 0.007 | 0.03 | - | - |
| **A76** | 1.900 | 0.013 | 8.150 | 0.042 | 0.7978 | 0.0088 | 0.890 | 0.010 | 1.74 | 0.92 | - |
| **A77** | 1.800 | 0.008 | 7.730 | 0.030 | 0.7203 | 0.0042 | 0.854 | 0.003 | 0.04 | - | - |
| **T79** | 1.800 | 0.007 | 8.230 | 0.034 | 0.7380 | 0.0043 | 0.851 | 0.004 | 0.03 | - | 0.60 |
| **L80** | 1.910 | 0.010 | 8.090 | 0.032 | 0.7733 | 0.0040 | 0.906 | 0.003 | 0.02 | - | - |
| **A81** | 1.870 | 0.012 | 8.380 | 0.043 | 0.8145 | 0.0073 | 0.909 | 0.006 | - | - | 0.13 |
| **A82** | 1.860 | 0.018 | 8.470 | 0.069 | 0.7861 | 0.0107 | 0.891 | 0.013 | 0.01 | - | 0.48 |
| **W83** | 1.890 | 0.010 | 8.420 | 0.037 | 0.8081 | 0.0050 | 0.915 | 0.005 | - | - | 0.15 |
| **N84** | 1.870 | 0.012 | 8.270 | 0.044 | 0.7933 | 0.0087 | 0.903 | 0.007 | - | - | 0.14 |
| **Q85** | 1.840 | 0.013 | 8.220 | 0.043 | 0.7954 | 0.0070 | 0.901 | 0.004 | - | - | - |
| **L86** | 1.880 | 0.025 | 8.200 | 0.086 | 0.8387 | 0.0150 | 0.908 | 0.008 | - | - | - |
| **M87** | 1.830 | 0.016 | 7.910 | 0.062 | 0.8112 | 0.0081 | 0.871 | 0.008 | - | - | 0.21 |
| **S89** | 1.780 | 0.007 | 7.380 | 0.022 | 0.7288 | 0.0034 | 0.833 | 0.002 | 0.03 | - | - |
| **R90** | 1.870 | 0.005 | 6.920 | 0.018 | 0.7050 | 0.0038 | 0.769 | 0.007 | 1.30 | 0.87 | - |
| **G93** | 1.550 | 0.005 | 3.290 | 0.020 | 0.0700 | 0.0033 | 0.226 | 0.004 | 1.04 | 0.78 | - |
| **NN** | 1.740 | 0.007 | 3.920 | 0.020 | 0.3687 | 0.0035 | | | | | |
| **NR** | 1.530 | 0.005 | 3.350 | 0.023 | 0.1834 | 0.0025 | | | | | |

**Table S4.** Relaxation parameters and model-free parameters for loaded-ArCP. The experimental error for a given parameter is indicated with the σ symbol. ROTDIF[6,7] does not provide experimental errors for $\tau_{loc}$, $S_f^2$, nor $R_{ex}$. Dashes indicate when a given model-free parameter was not included in the fit. Due to limitations of the Lipari-Szabo model, the NN and NR positions of the PP arm were not fit with the model free formalism.

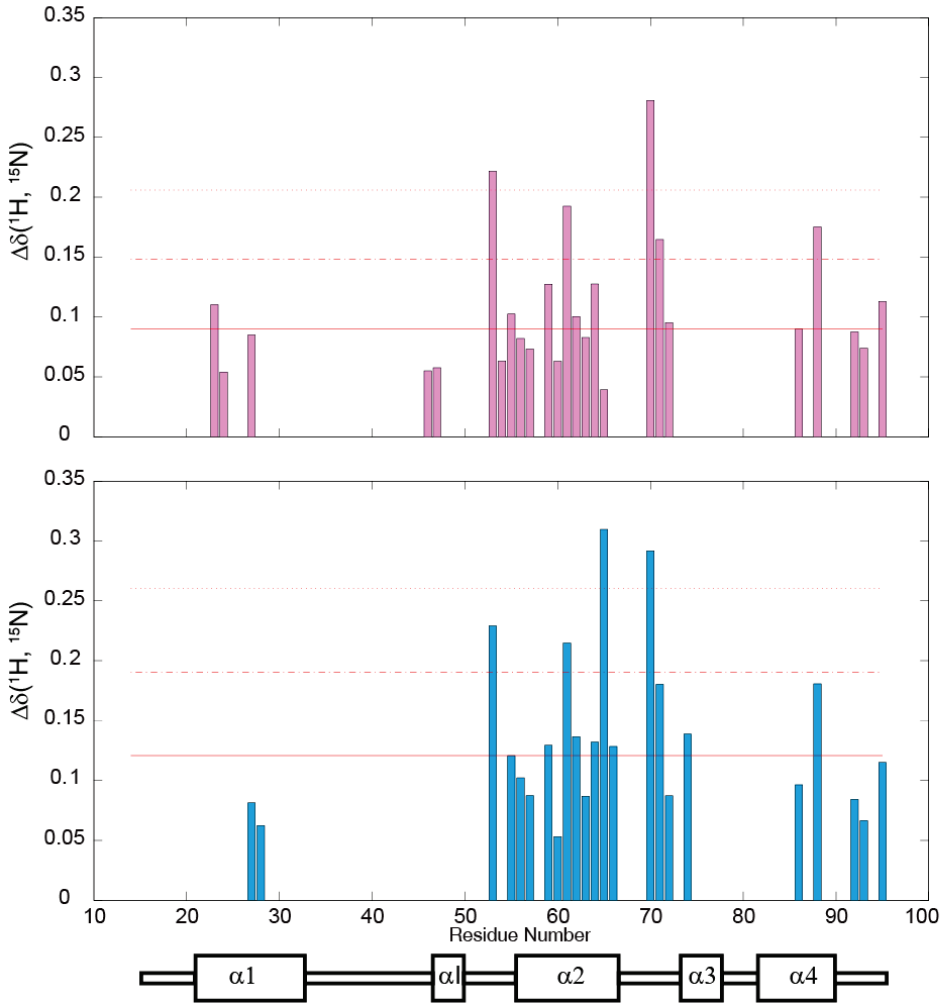


**Figure S8.** Chemical shift perturbations between major and minor forms in holo (top) and loaded (bottom) ArCP. The solid horizontal lines indicate the median (0.09 for holo, 0.12 for loaded) and the median with one standard deviation (std = 0.06 for holo, std = 0.07 for loaded). The reported chemical shift differences are calculated with $\Delta\delta(^{1}H, ^{15}N) = ((\Delta\delta H)^2 + (1/5(\Delta\delta N))^2)^{1/2}$ where $\Delta\delta i$ is the chemical shift difference between the two species for nucleus i.

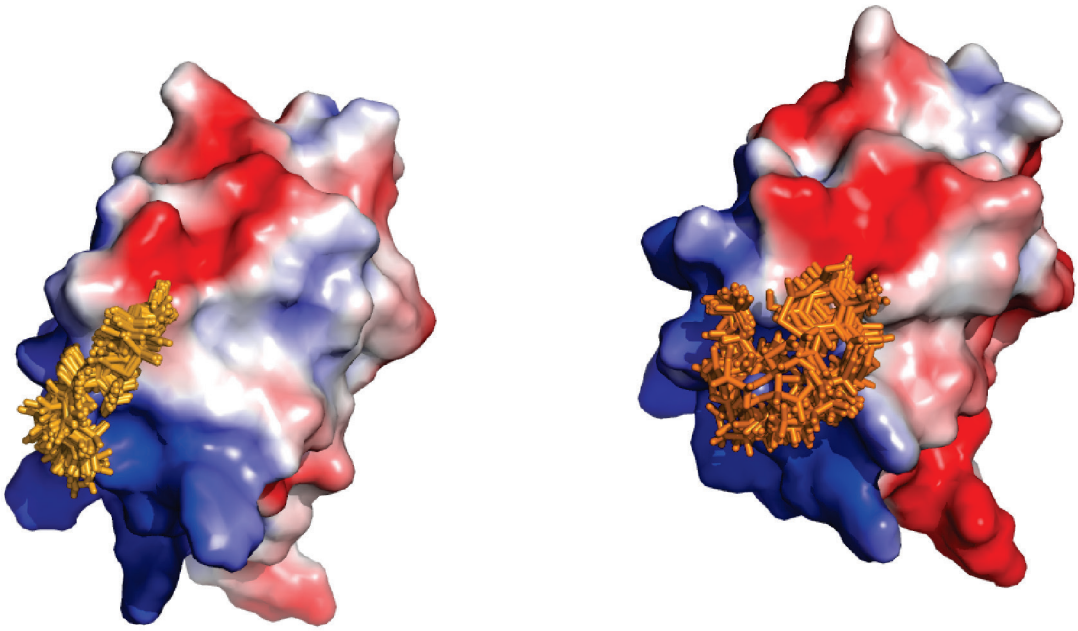

**Figure S9.** Interference between the conformation of the prosthetic groups and interaction surfaces. Blue, positive charges; red, negative charges. Upon substrate loading, the change of conformation in PP modifies access to the positively charged surface as well as the negatively charged surface. Surface potentials were generated using the APBS Tools2.1 plugin[8] for PyMOL[9].

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**NMR chemical shift assignments (BMRB 25786):**

**Holo-ArCP (residues after 100 belong to the second minor conformer)**

| residue number | Nucleus | Chemical Shift (ppm) |
|---|---|---|
| 14 | H | 8.569 |
| 14 | N | 122.9 |
| 14 | CA | 54.25 |
| 14 | CB | 41.083 |
| 14 | C | 176.031 |
| 14 | HB2 | 2.749 |
| 14 | HB3 | 2.68 |
| 14 | HA | 4.645 |
| 15 | H | 8.425 |
| 15 | N | 119.857 |
| 15 | CA | 53.556 |
| 15 | CB | 38.731 |
| 15 | C | 175.735 |
| 15 | HA | 4.719 |
| 15 | HB2 | 2.88 |
| 15 | HB3 | 2.82 |
| 16 | H | 8.347 |
| 16 | CA | 57.735 |
| 16 | HA | 4.211 |
| 16 | CD | 43.039 |
| 16 | CB | 30.224 |
| 16 | CG | 26.684 |
| 16 | HB | 1.849 |
| 16 | HG | 1.628 |
| 16 | HD | 3.206 |
| 16 | N | 122.03 |
| 16 | C | 176.669 |
| 17 | H | 8.395 |
| 17 | N | 118.59 |
| 17 | CA | 58.394 |
| 17 | CB | 30.362 |
| 17 | HA | 4.563 |

| | | |
|---|---|---|
| 17 | HB3 | 3.147 |
| 17 | HB2 | 3.261 |
| 17 | C | 176.284 |
| 17 | CD2 | 118.396 |
| 17 | HD2 | 6.998 |
| 18 | H | 8.436 |
| 18 | N | 122.047 |
| 18 | CA | 54.294 |
| 18 | C | 180.003 |
| 18 | CB | 18.849 |
| 18 | HB | 1.581 |
| 18 | HA | 4.182 |
| 19 | H | 8.402 |
| 19 | N | 122.607 |
| 19 | CA | 55.04 |
| 19 | CB | 18.267 |
| 19 | HB | 1.571 |
| 19 | HA | 4.275 |
| 19 | C | 180.295 |
| 20 | H | 8.317 |
| 20 | N | 118.796 |
| 20 | HB | 2.925 |
| 20 | CB | 40.189 |
| 20 | CA | 56.725 |
| 20 | HA | 4.837 |
| 20 | C | 177.313 |
| 21 | H | 8.679 |
| 21 | N | 120.958 |
| 21 | CA | 61.892 |
| 21 | CB | 38.655 |
| 21 | C | 176.282 |
| 21 | HA | 4.058 |
| 21 | HB3 | 3.003 |
| 21 | HB2 | 3.059 |
| 21 | CD | 133.064 |
| 21 | HE | 6.67 |
| 21 | HD | 7.006 |
| 21 | CE | 118.183 |
| 22 | H | 8.236 |
| 22 | N | 117.715 |
| 22 | CA | 59.11 |
| 22 | C | 178.197 |
| 22 | CB | 27.43 |
| 22 | CG | 33.273 |
| 22 | HA | 3.826 |
| 22 | HG | 2.494 |
| 22 | HB | 2.227 |

| | | |
|---|---|---|
| 23 | H | 8.003 |
| 23 | N | 118.526 |
| 23 | CA | 58.915 |
| 23 | C | 177.521 |
| 23 | CB | 29.032 |
| 23 | CG | 34.938 |
| 23 | HA | 4.1 |
| 23 | HG | 2.67 |
| 23 | HB3 | 2.454 |
| 23 | HB2 | 2.372 |
| 24 | H | 8.031 |
| 24 | N | 121.914 |
| 24 | CA | 58.115 |
| 24 | CB | 41.704 |
| 24 | CD1 | 26.981 |
| 24 | HD1 | 0.975 |
| 24 | CD2 | 23.617 |
| 24 | HD2 | 0.059 |
| 24 | HA | 3.444 |
| 24 | C | 176.882 |
| 24 | HB2 | 1.908 |
| 24 | HB3 | 1.335 |
| 25 | H | 7.981 |
| 25 | N | 116.645 |
| 25 | CA | 60.246 |
| 25 | CB | 29.925 |
| 25 | C | 177.469 |
| 25 | CG | 27.902 |
| 25 | CD | 43.155 |
| 25 | HG | 1.211 |
| 25 | HD | 3.025 |
| 25 | HA | 3.395 |
| 25 | HB2 | 1.577 |
| 25 | HB3 | 1.293 |
| 26 | H | 8.16 |
| 26 | N | 115.943 |
| 26 | CA | 59.517 |
| 26 | CB | 29.439 |
| 26 | HA | 3.832 |
| 26 | CG | 36.563 |
| 26 | C | 179.682 |
| 26 | HB3 | 2.104 |
| 26 | HB2 | 2.002 |
| 26 | HG3 | 2.264 |
| 26 | HG2 | 2.449 |
| 27 | H | 8.283 |
| 27 | N | 118.766 |

| | | |
|---|---|---|
| 27 | CA | 58.855 |
| 27 | CB | 29.996 |
| 27 | C | 179.241 |
| 27 | CG | 27.803 |
| 27 | CD | 42.978 |
| 27 | HA | 4.144 |
| 27 | HG2 | 1.649 |
| 27 | HD2 | 3.001 |
| 27 | HD3 | 2.782 |
| 27 | HB | 1.996 |
| 27 | HG3 | 1.847 |
| 28 | H | 8.389 |
| 28 | N | 122.077 |
| 28 | CA | 58.558 |
| 28 | CB | 42.514 |
| 28 | C | 178.766 |
| 28 | HD1 | 0.312 |
| 28 | CD1 | 26.726 |
| 28 | HA | 4.106 |
| 28 | CD2 | 24.237 |
| 28 | HD2 | 0.438 |
| 28 | HG | 1.325 |
| 28 | HB2 | 0.932 |
| 28 | HB3 | 1.74 |
| 28 | CG | 26.881 |
| 29 | H | 7.914 |
| 29 | N | 117.586 |
| 29 | CA | 66.203 |
| 29 | CB | 37.823 |
| 29 | C | 177.927 |
| 29 | CG2 | 17.235 |
| 29 | HG2 | 0.76 |
| 29 | HB | 1.872 |
| 29 | HA | 3.339 |
| 29 | CD1 | 14.135 |
| 29 | CG1 | 30.527 |
| 29 | HD1 | 0.724 |
| 29 | HG1 | 1.717 |
| 30 | H | 7.287 |
| 30 | N | 116.395 |
| 30 | CA | 58.41 |
| 30 | CB | 28.804 |
| 30 | C | 179.4 |
| 30 | HA | 4.157 |
| 30 | CG | 33.599 |
| 30 | HB | 2.192 |
| 30 | HG2 | 2.418 |

| | | |
|---|---|---|
| 30 | HG3 | 2.551 |
| 31 | H | 8.814 |
| 31 | N | 120.336 |
| 31 | CA | 59.377 |
| 31 | CB | 30.436 |
| 31 | C | 178.395 |
| 31 | CG | 36.933 |
| 31 | HA | 4.023 |
| 31 | HG3 | 2.449 |
| 31 | HG2 | 2.234 |
| 31 | HB3 | 2.108 |
| 31 | HB2 | 2.231 |
| 32 | H | 8.109 |
| 32 | N | 115.139 |
| 32 | CA | 54.101 |
| 32 | C | 176.033 |
| 32 | CD1 | 21.557 |
| 32 | HD1 | 0.675 |
| 32 | HA | 4.377 |
| 32 | HG | 1.497 |
| 32 | CD2 | 25.912 |
| 32 | CB | 41.354 |
| 32 | HD2 | 0.664 |
| 32 | HB3 | 1.678 |
| 32 | HB2 | 1.763 |
| 33 | H | 7.796 |
| 33 | N | 116.751 |
| 33 | CA | 54.024 |
| 33 | CB | 36.929 |
| 33 | C | 174.288 |
| 33 | HB2 | 2.734 |
| 33 | HA | 4.453 |
| 33 | HB3 | 3.151 |
| 34 | H | 7.728 |
| 34 | N | 117.139 |
| 34 | CA | 53.079 |
| 34 | CB | 44.673 |
| 34 | C | 176.521 |
| 34 | HA | 4.787 |
| 34 | CG | 26.865 |
| 34 | HD1 | 0.708 |
| 34 | HD2 | 0.802 |
| 34 | CD2 | 22.457 |
| 34 | CD1 | 26.793 |
| 34 | HB2 | 1.408 |
| 34 | HB3 | 1.54 |
| 35 | H | 8.001 |

| | | |
|---|---|---|
| 35 | N | 110.751 |
| 35 | CA | 59.445 |
| 35 | CB | 68.651 |
| 35 | HG2 | 1.254 |
| 35 | CG2 | 21.746 |
| 35 | HB | 4.563 |
| 35 | HA | 4.803 |
| 35 | C | 174.438 |
| 36 | CA | 65.645 |
| 36 | HA | 4.077 |
| 36 | CB | 31.632 |
| 36 | CG | 28.311 |
| 36 | HB2 | 2.378 |
| 36 | HB3 | 1.928 |
| 36 | HG3 | 2.206 |
| 36 | HG2 | 2.016 |
| 36 | CD | 50.289 |
| 36 | HD | 3.87 |
| 37 | H | 8.005 |
| 37 | N | 112.874 |
| 37 | CA | 57.891 |
| 37 | CB | 27.902 |
| 37 | CG | 34.167 |
| 37 | HA | 4.105 |
| 37 | HB | 2.039 |
| 37 | HG2 | 2.382 |
| 37 | HG3 | 2.479 |
| 37 | C | 176.96 |
| 38 | H | 7.663 |
| 38 | N | 116.477 |
| 38 | CA | 56.398 |
| 38 | C | 175.508 |
| 38 | CB | 31.126 |
| 38 | CG | 34.803 |
| 38 | HG | 2.349 |
| 38 | HB | 2.156 |
| 38 | HA | 4.187 |
| 39 | H | 7.286 |
| 39 | N | 120.726 |
| 39 | HD1 | 0.627 |
| 39 | CD1 | 26.467 |
| 39 | CD2 | 22.953 |
| 39 | HD2 | 0.64 |
| 39 | CA | 53.959 |
| 39 | CB | 41.61 |
| 39 | HB3 | 0.993 |
| 39 | HB2 | 1.719 |

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|---|---|---|
| 39 | HA | 4.371 |
| 39 | C | 174.277 |
| 39 | HG | 1.259 |
| 39 | CG | 26.798 |
| 40 | H | 8.158 |
| 40 | N | 124.68 |
| 40 | CA | 54.762 |
| 40 | HB2 | 3.16 |
| 40 | HB3 | 3.254 |
| 40 | CB | 31.521 |
| 40 | C | 176.727 |
| 40 | HE1 | 8.106 |
| 40 | CE1 | 137.409 |
| 40 | HA | 4.808 |
| 41 | HA | 4.029 |
| 41 | HB | 2.072 |
| 41 | HG | 2.345 |
| 42 | H | 8.808 |
| 42 | N | 113.813 |
| 42 | CA | 55.313 |
| 42 | CG | 36.154 |
| 42 | CB | 29.165 |
| 42 | HG | 2.205 |
| 42 | HA | 4.547 |
| 42 | C | 176.68 |
| 42 | HB3 | 1.909 |
| 42 | HB2 | 2.296 |
| 43 | H | 7.485 |
| 43 | N | 118.066 |
| 43 | CA | 60.156 |
| 43 | CB | 62.827 |
| 43 | HA | 4.088 |
| 43 | C | 173.663 |
| 43 | HB2 | 3.641 |
| 43 | HB3 | 3.713 |
| 44 | H | 8.811 |
| 44 | N | 123.218 |
| 44 | CA | 53.987 |
| 44 | C | 176.926 |
| 44 | CB | 38.433 |
| 44 | HA | 4.392 |
| 44 | HB2 | 2.721 |
| 44 | HB3 | 2.816 |
| 45 | H | 9.385 |
| 45 | N | 128.735 |
| 45 | CA | 57.149 |
| 45 | CB | 42.25 |

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|---|---|---|
| 45 | HA | 3.722 |
| 45 | HD1 | 0.397 |
| 45 | HB3 | 1.07 |
| 45 | CG | 26.677 |
| 45 | HG | 1.368 |
| 45 | CD1 | 22.644 |
| 45 | CD2 | 23.644 |
| 45 | HD2 | -0.631 |
| 45 | C | 178.143 |
| 45 | HB2 | 1.018 |
| 46 | H | 7.659 |
| 46 | N | 119.379 |
| 46 | CA | 63.814 |
| 46 | CB | 36.709 |
| 46 | C | 180.926 |
| 46 | CG1 | 28.02 |
| 46 | CG2 | 16.768 |
| 46 | HG2 | 0.984 |
| 46 | HA | 4.187 |
| 46 | HB | 2.211 |
| 46 | CD1 | 12.594 |
| 46 | HD1 | 0.879 |
| 46 | HG12 | 1.371 |
| 46 | HG13 | 1.557 |
| 47 | H | 8.161 |
| 47 | N | 121.737 |
| 47 | CA | 58.033 |
| 47 | CB | 27.985 |
| 47 | C | 177.739 |
| 47 | CG | 33.839 |
| 47 | HG | 2.385 |
| 47 | HA | 3.989 |
| 47 | HB2 | 2.144 |
| 47 | HB3 | 1.948 |
| 48 | H | 7.448 |
| 48 | N | 117.777 |
| 48 | CA | 52.71 |
| 48 | CB | 18.601 |
| 48 | C | 176.582 |
| 48 | HB | 1.403 |
| 48 | HA | 4.26 |
| 49 | H | 7.445 |
| 49 | N | 102.932 |
| 49 | CA | 44.967 |
| 49 | C | 174.451 |
| 49 | HA2 | 3.683 |
| 49 | HA3 | 4.551 |

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|---|---|---|
| 50 | H | 8.545 |
| 50 | N | 123.058 |
| 50 | CA | 55.909 |
| 50 | CB | 41.454 |
| 50 | C | 173.46 |
| 50 | HD2 | 0.832 |
| 50 | CD1 | 25.838 |
| 50 | CD2 | 26.681 |
| 50 | HA | 4.257 |
| 50 | HD1 | 0.917 |
| 50 | HB2 | 1.452 |
| 50 | HB3 | 1.677 |
| 51 | H | 7.411 |
| 51 | N | 123.238 |
| 51 | CA | 52.325 |
| 51 | CB | 42.256 |
| 51 | HA | 4.83 |
| 51 | C | 176.212 |
| 51 | HB2 | 2.792 |
| 51 | HB3 | 3.24 |
| 52 | H | 9.001 |
| 52 | N | 113.44 |
| 52 | CA | 61.016 |
| 52 | HA | 4.265 |
| 52 | CB | 65.748 |
| 52 | C | 175.8 |
| 52 | HB2 | 4.214 |
| 52 | HB3 | 4.257 |
| 52 | HJ2 | 3.374 |
| 52 | HJ3 | 3.763 |
| 52 | CJ | 74.026 |
| 52 | HL2 | 0.798 |
| 52 | CL2 | 21.384 |
| 52 | HL1 | 0.881 |
| 52 | CL1 | 23.595 |
| 52 | HL3 | 3.993 |
| 52 | CL3 | 76.726 |
| 52 | HO | 3.459 |
| 52 | CO | 38.076 |
| 52 | HP | 2.455 |
| 52 | CP | 38.169 |
| 52 | HS | 3.275 |
| 52 | CS | 45.084 |
| 52 | HT | 2.558 |
| 52 | CT | 26.012 |
| 53 | H | 7.799 |
| 53 | N | 123.207 |

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|---|---|---|
| 53 | CA | 64.432 |
| 53 | C | 179.241 |
| 53 | CB | 37.154 |
| 53 | CD1 | 12.459 |
| 53 | CG2 | 17.301 |
| 53 | CG1 | 28.91 |
| 53 | HG2 | 0.924 |
| 53 | HA | 3.876 |
| 53 | HB | 2.142 |
| 53 | HD1 | 0.923 |
| 53 | HG12 | 1.676 |
| 53 | HG13 | 1.273 |
| 54 | H | 8.412 |
| 54 | N | 121.407 |
| 54 | CA | 59.615 |
| 54 | C | 179.647 |
| 54 | CG | 28.908 |
| 54 | CB | 30.633 |
| 54 | CD | 43.436 |
| 54 | HA | 4.088 |
| 54 | HD | 3.293 |
| 54 | HG2 | 1.757 |
| 54 | HB2 | 2.057 |
| 54 | HB3 | 1.967 |
| 54 | HG3 | 2.135 |
| 55 | H | 9.05 |
| 55 | N | 121.118 |
| 55 | CA | 59.035 |
| 55 | CB | 41.718 |
| 55 | CD1 | 25.54 |
| 55 | CG | 27.968 |
| 55 | HD1 | 0.917 |
| 55 | HA | 4.332 |
| 55 | HD2 | 0.849 |
| 55 | CD2 | 25.139 |
| 55 | C | 178.416 |
| 55 | HB2 | 1.837 |
| 55 | HB3 | 1.714 |
| 56 | H | 7.875 |
| 56 | N | 117.969 |
| 56 | CA | 57.927 |
| 56 | HA | 4.284 |
| 56 | HB2 | 2.276 |
| 56 | HG | 2.698 |
| 56 | CB | 31.317 |
| 56 | CG | 32.369 |
| 56 | C | 178.301 |

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|---|---|---|
| 56 | HE | 2.136 |
| 56 | CE | 17.028 |
| 56 | HB3 | 2.226 |
| 57 | H | 7.609 |
| 57 | N | 119.532 |
| 57 | CA | 59.77 |
| 57 | CB | 29.52 |
| 57 | CG | 27.597 |
| 57 | CD | 43.29 |
| 57 | HA | 4.096 |
| 57 | HD | 3.022 |
| 57 | C | 180.458 |
| 57 | HG | 1.472 |
| 57 | HB2 | 1.776 |
| 57 | HB3 | 1.892 |
| 58 | H | 8.207 |
| 58 | N | 121.82 |
| 58 | CA | 61.063 |
| 58 | HE1 | 11.047 |
| 58 | NE1 | 131.242 |
| 58 | CB | 28.348 |
| 58 | HA | 4.465 |
| 58 | HB3 | 3.463 |
| 58 | HB2 | 3.249 |
| 58 | C | 177.973 |
| 58 | HD1 | 7.173 |
| 58 | HZ2 | 6.892 |
| 58 | CZ2 | 114.081 |
| 58 | CD1 | 126.072 |
| 58 | CH2 | 123.433 |
| 58 | HH2 | 6.497 |
| 59 | H | 8.599 |
| 59 | N | 121.654 |
| 59 | CA | 59.044 |
| 59 | CB | 40.851 |
| 59 | HA | 4.274 |
| 59 | HD1 | 0.782 |
| 59 | CD1 | 23.472 |
| 59 | CD2 | 25.843 |
| 59 | HD2 | 0.988 |
| 59 | C | 178.823 |
| 59 | HG | 1.564 |
| 59 | HB3 | 1.493 |
| 59 | HB2 | 2.322 |
| 60 | H | 7.909 |
| 60 | N | 116.952 |
| 60 | CA | 59.755 |

| | | |
|---|---|---|
| 60 | CB | 30.083 |
| 60 | HA | 4.389 |
| 60 | HB | 3.273 |
| 60 | C | 177.635 |
| 60 | HD2 | 7.11 |
| 60 | CD2 | 119.426 |
| 61 | H | 8.142 |
| 61 | N | 123.194 |
| 61 | CA | 62.541 |
| 61 | HE1 | 9.936 |
| 61 | NE1 | 128.398 |
| 61 | CB | 28.839 |
| 61 | HA | 4.032 |
| 61 | C | 179.298 |
| 61 | HB2 | 3.005 |
| 61 | HB3 | 3.724 |
| 61 | HZ2 | 7.339 |
| 61 | CZ2 | 113.508 |
| 61 | CE3 | 120.243 |
| 61 | HE3 | 6.648 |
| 61 | HD1 | 7.104 |
| 61 | HH2 | 7.092 |
| 61 | CD1 | 126.577 |
| 61 | CH2 | 124.097 |
| 61 | CZ3 | 122.068 |
| 61 | HZ3 | 6.431 |
| 62 | H | 9.447 |
| 62 | N | 120.038 |
| 62 | CA | 63.629 |
| 62 | CB | 38.664 |
| 62 | HA | 4.205 |
| 62 | C | 179.08 |
| 62 | HB3 | 3.368 |
| 62 | HB2 | 3.29 |
| 62 | HE | 6.893 |
| 62 | HZ | 7.008 |
| 62 | CD | 131.994 |
| 62 | CE | 131.336 |
| 62 | HD | 7.2 |
| 62 | CZ | 129.923 |
| 63 | H | 8.665 |
| 63 | N | 118.56 |
| 63 | CA | 59.257 |
| 63 | CB | 29.697 |
| 63 | C | 181.328 |
| 63 | CG | 27.801 |
| 63 | CD | 43.124 |

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|---|---|---|
| 63 | HA | 4.258 |
| 63 | HD | 3.332 |
| 63 | HG | 1.844 |
| 63 | HB | 1.988 |
| 64 | H | 8.69 |
| 64 | N | 122.759 |
| 64 | CA | 58.651 |
| 64 | C | 177.595 |
| 64 | CB | 31.51 |
| 64 | CG | 24.38 |
| 64 | CD | 29.156 |
| 64 | HA | 4.019 |
| 64 | HG | 1.348 |
| 64 | HD2 | 1.576 |
| 64 | HB3 | 1.73 |
| 64 | HB2 | 1.837 |
| 64 | CE | 42.01 |
| 64 | HE | 2.894 |
| 64 | HD3 | 1.547 |
| 65 | H | 7.246 |
| 65 | N | 115.681 |
| 65 | CA | 53.685 |
| 65 | CB | 39.038 |
| 65 | C | 173.405 |
| 65 | HA | 4.532 |
| 65 | HB2 | 2.723 |
| 65 | HB3 | 2.139 |
| 66 | H | 7.603 |
| 66 | N | 105.186 |
| 66 | CA | 45.539 |
| 66 | HA2 | 4.007 |
| 66 | HA3 | 3.578 |
| 66 | C | 173.869 |
| 67 | H | 8.248 |
| 67 | N | 119.699 |
| 67 | CA | 57.858 |
| 67 | CB | 38.564 |
| 67 | HA | 4.542 |
| 67 | HB3 | 2.994 |
| 67 | HB2 | 2.607 |
| 67 | C | 175.838 |
| 67 | CD | 133.519 |
| 67 | HD | 7.288 |
| 67 | HE | 6.88 |
| 67 | CE | 118.34 |
| 68 | H | 8.55 |
| 68 | N | 125.588 |

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|---|---|---|
| 68 | CA | 55.649 |
| 68 | CB | 28.357 |
| 68 | C | 174.479 |
| 68 | CG | 27.198 |
| 68 | CD | 43.577 |
| 68 | HA | 4.389 |
| 68 | HD | 3.199 |
| 68 | HB3 | 1.873 |
| 68 | HG3 | 1.638 |
| 68 | HB2 | 1.714 |
| 68 | HG2 | 1.533 |
| 69 | H | 7.421 |
| 69 | N | 122.034 |
| 69 | CA | 53.367 |
| 69 | CB | 44.286 |
| 69 | C | 175.63 |
| 69 | HD1 | 0.302 |
| 69 | HB2 | 1.408 |
| 69 | HG | 1.242 |
| 69 | CD1 | 25.219 |
| 69 | CG | 26.91 |
| 69 | CD2 | 24.607 |
| 69 | HB3 | 1.282 |
| 69 | HD2 | 0.109 |
| 69 | HA | 4.711 |
| 70 | H | 8.163 |
| 70 | N | 109.789 |
| 70 | CA | 59.377 |
| 70 | CB | 72.18 |
| 70 | CG2 | 21.557 |
| 70 | HG2 | 1.154 |
| 70 | HB | 4.566 |
| 70 | HA | 4.721 |
| 70 | C | 174.636 |
| 71 | H | 8.825 |
| 71 | N | 122.563 |
| 71 | CA | 58.196 |
| 71 | C | 178.632 |
| 71 | CB | 41.94 |
| 71 | HA | 3.885 |
| 71 | HB2 | 1.887 |
| 71 | HB3 | 1.678 |
| 71 | HD1 | 1.003 |
| 71 | CD1 | 25.842 |
| 71 | CG | 26.942 |
| 71 | HD2 | 1.012 |
| 71 | CD2 | 24.186 |

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|---|---|---|
| 71 | HG | 1.751 |
| 72 | H | 8.244 |
| 72 | N | 115.949 |
| 72 | CA | 59.147 |
| 72 | CB | 29.631 |
| 72 | C | 178.893 |
| 72 | CD | 43.139 |
| 72 | CG | 26.998 |
| 72 | HA | 3.876 |
| 72 | HD | 3.188 |
| 72 | HB2 | 1.868 |
| 72 | HG | 1.671 |
| 72 | HB3 | 1.749 |
| 73 | H | 7.461 |
| 73 | N | 117.665 |
| 73 | CA | 59.092 |
| 73 | CB | 29.739 |
| 73 | CG | 37.997 |
| 73 | HG | 2.221 |
| 73 | HA | 3.951 |
| 73 | C | 178.762 |
| 73 | HB3 | 2.23 |
| 73 | HB2 | 1.896 |
| 74 | H | 7.413 |
| 74 | N | 117.724 |
| 74 | CA | 57.469 |
| 74 | CB | 41.619 |
| 74 | C | 179.355 |
| 74 | HA | 3.898 |
| 74 | HG | 1.377 |
| 74 | CD2 | 25.441 |
| 74 | HD1 | -0.776 |
| 74 | HD2 | 0.376 |
| 74 | CD1 | 19.863 |
| 74 | HB3 | 1.896 |
| 74 | HB2 | 1.194 |
| 74 | CG | 25.793 |
| 75 | H | 8.086 |
| 75 | N | 114.976 |
| 75 | CA | 60.638 |
| 75 | CB | 39.688 |
| 75 | C | 176.656 |
| 75 | HA | 4.054 |
| 75 | HB | 2.964 |
| 75 | CE | 118.139 |
| 75 | HE | 6.795 |
| 75 | CD | 133.053 |

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|---|---|---|
| 75 | HD | 7.115 |
| 76 | H | 7.776 |
| 76 | N | 119.116 |
| 76 | CA | 54.468 |
| 76 | CB | 18.535 |
| 76 | C | 178.156 |
| 76 | HA | 4.052 |
| 76 | HB | 1.505 |
| 77 | H | 6.706 |
| 77 | N | 116.862 |
| 77 | CA | 49.713 |
| 77 | CB | 19.226 |
| 77 | C | 173.737 |
| 77 | HB | 1.322 |
| 78 | HA | 5.018 |
| 78 | CA | 61.523 |
| 78 | CB | 28.845 |
| 78 | HB2 | 2.083 |
| 78 | HB3 | 1.921 |
| 78 | HD | 3.566 |
| 78 | CD | 48.3 |
| 78 | HG | 2.113 |
| 78 | CG | 27.319 |
| 79 | H | 7.664 |
| 79 | N | 111.947 |
| 79 | CA | 58.059 |
| 79 | CB | 72.247 |
| 79 | C | 173 |
| 79 | HB | 4.496 |
| 79 | HG2 | 0.85 |
| 79 | HA | 4.396 |
| 79 | CG2 | 21.176 |
| 80 | H | 9.609 |
| 80 | N | 123.227 |
| 80 | CA | 58.209 |
| 80 | CB | 41.579 |
| 80 | HA | 3.747 |
| 80 | HG | 1.616 |
| 80 | CG | 27.005 |
| 80 | CD1 | 24.943 |
| 80 | HD1 | 0.643 |
| 80 | HD2 | 0.587 |
| 80 | CD2 | 23.965 |
| 80 | C | 179.028 |
| 80 | HB3 | 1.918 |
| 80 | HB2 | 1.602 |
| 81 | H | 8.831 |

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|---|---|---|
| 81 | N | 119.663 |
| 81 | CA | 54.876 |
| 81 | CB | 18.428 |
| 81 | C | 181.038 |
| 81 | HB | 1.308 |
| 81 | HA | 4.141 |
| 82 | H | 8.272 |
| 82 | N | 122.181 |
| 82 | CA | 54.808 |
| 82 | CB | 19.088 |
| 82 | C | 181.868 |
| 82 | HA | 4.225 |
| 82 | HB | 1.672 |
| 83 | H | 9.378 |
| 83 | N | 123.399 |
| 83 | CA | 59.562 |
| 83 | C | 178.633 |
| 83 | HE1 | 10.016 |
| 83 | NE1 | 127.824 |
| 83 | CB | 28.301 |
| 83 | HB3 | 3.117 |
| 83 | HB2 | 3.32 |
| 83 | HA | 4.543 |
| 83 | HE3 | 7.266 |
| 83 | HZ2 | 6.798 |
| 83 | HZ3 | 5.96 |
| 83 | CH2 | 123.41 |
| 83 | HH2 | 6.577 |
| 83 | CZ2 | 112.348 |
| 83 | CZ3 | 120.07 |
| 83 | HD1 | 7.274 |
| 83 | CD1 | 124.608 |
| 83 | CE3 | 119.972 |
| 84 | H | 9.136 |
| 84 | N | 118.25 |
| 84 | CA | 57.096 |
| 84 | CB | 39.229 |
| 84 | C | 177.231 |
| 84 | HA | 4.616 |
| 84 | HB3 | 2.828 |
| 84 | HB2 | 2.96 |
| 85 | H | 7.511 |
| 85 | N | 116.261 |
| 85 | CA | 58.748 |
| 85 | CB | 27.84 |
| 85 | C | 179.455 |
| 85 | CG | 33.444 |

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|---|---|---|
| 85 | HA | 4.011 |
| 85 | HB2 | 2.514 |
| 85 | HB3 | 2.24 |
| 86 | H | 8.172 |
| 86 | N | 121.554 |
| 86 | CA | 57.804 |
| 86 | CB | 41.915 |
| 86 | C | 179.171 |
| 86 | HA | 4.041 |
| 86 | CD1 | 25.688 |
| 86 | HG | 1.769 |
| 86 | HD2 | 0.744 |
| 86 | CD2 | 23.026 |
| 86 | HD1 | 0.685 |
| 86 | HB2 | 1.22 |
| 86 | HB3 | 1.945 |
| 86 | CG | 26.63 |
| 87 | H | 8.197 |
| 87 | N | 117.874 |
| 87 | CA | 59.481 |
| 87 | C | 178.221 |
| 87 | HA | 3.752 |
| 87 | CB | 34.875 |
| 87 | CG | 32.651 |
| 87 | HG | 2.637 |
| 87 | HB2 | 2.157 |
| 87 | HB3 | 2.443 |
| 87 | HE | 2.053 |
| 87 | CE | 16.956 |
| 88 | H | 7.902 |
| 88 | N | 117.598 |
| 88 | CA | 57.076 |
| 88 | CB | 42.395 |
| 88 | C | 179.237 |
| 88 | CG | 26.598 |
| 88 | CD1 | 25.324 |
| 88 | HA | 4.054 |
| 88 | HB3 | 1.763 |
| 88 | HD1 | 0.721 |
| 88 | HB2 | 1.482 |
| 88 | CD2 | 22.626 |
| 88 | HD2 | 0.59 |
| 88 | HG | 1.59 |
| 89 | H | 7.958 |
| 89 | N | 113.195 |
| 89 | CA | 59.901 |
| 89 | CB | 63.834 |

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|---|---|---|
| 89 | C | 175.09 |
| 89 | HA | 4.038 |
| 89 | HB | 4.462 |
| 90 | H | 7.923 |
| 90 | N | 122.031 |
| 90 | CA | 53.905 |
| 90 | CB | 29.631 |
| 90 | C | 175.695 |
| 90 | CG | 26.798 |
| 90 | CD | 42.219 |
| 90 | HD | 3.168 |
| 90 | HA | 4.701 |
| 90 | HG3 | 1.694 |
| 90 | HG2 | 1.845 |
| 90 | HB2 | 1.844 |
| 90 | HB3 | 2.063 |
| 91 | H | 7.752 |
| 91 | N | 117.191 |
| 91 | CA | 57.104 |
| 91 | CB | 63.437 |
| 91 | C | 172.914 |
| 92 | CA | 63.414 |
| 92 | HA | 4.42 |
| 92 | HB2 | 2.14 |
| 92 | CB | 31.895 |
| 92 | CG | 27.278 |
| 92 | CD | 50.689 |
| 92 | HD2 | 3.59 |
| 92 | HB3 | 1.948 |
| 92 | HG2 | 1.737 |
| 92 | HG3 | 1.869 |
| 92 | HD3 | 3.378 |
| 93 | H | 8.068 |
| 93 | N | 126.257 |
| 93 | CA | 58.086 |
| 93 | CB | 31.203 |
| 93 | C | 181.226 |
| 93 | CG | 36.519 |
| 93 | HA | 4.237 |
| 93 | HB | 2.227 |
| 93 | HG2 | 2.035 |
| 93 | HG3 | 1.889 |
| 21 | H 1 | 8.569 |
| 21 | N 1 | 120.916 |
| 22 | H 1 | 8.29 |
| 22 | N 1 | 117.73 |
| 25 | H 1 | 8.066 |

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|---|---|---|---|
| 25 | N | 1 | 116.66 |
| 29 | H | 1 | 7.978 |
| 29 | N | 1 | 117.707 |
| 44 | H | 1 | 8.756 |
| 44 | N | 1 | 123.214 |
| 45 | H | 1 | 9.441 |
| 45 | N | 1 | 128.805 |
| 51 | H | 1 | 7.21 |
| 51 | N | 1 | 122.77 |
| 52 | H | 1 | 8.952 |
| 52 | N | 1 | 113.24 |
| 53 | H | 1 | 7.874 |
| 53 | N | 1 | 122.857 |
| 54 | H | 1 | 8.484 |
| 54 | N | 1 | 121.605 |
| 55 | H | 1 | 9.109 |
| 55 | N | 1 | 120.901 |
| 57 | H | 1 | 7.698 |
| 57 | N | 1 | 119.988 |
| 58 | H | 1 | 8.27 |
| 58 | N | 1 | 121.808 |
| 59 | H | 1 | 8.467 |
| 59 | N | 1 | 120.953 |
| 60 | H | 1 | 8.006 |
| 60 | N | 1 | 116.822 |
| 61 | H | 1 | 8.104 |
| 61 | N | 1 | 122.826 |
| 62 | H | 1 | 9.342 |
| 62 | N | 1 | 119.676 |
| 63 | H | 1 | 8.626 |
| 63 | N | 1 | 118.583 |
| 68 | H | 1 | 8.819 |
| 68 | N | 1 | 125.992 |
| 69 | H | 1 | 7.47 |
| 69 | N | 1 | 122.82 |
| 70 | H | 1 | 8.069 |
| 70 | N | 1 | 109.71 |
| 84 | H | 1 | 9.08 |
| 84 | N | 1 | 117.898 |
| 86 | H | 1 | 8.088 |
| 86 | N | 1 | 120.785 |
| 90 | H | 1 | 7.865 |
| 90 | N | 1 | 122.359 |
| 91 | H | 1 | 7.678 |
| 91 | N | 1 | 117.189 |
| 93 | H | 1 | 8.181 |
| 93 | N | 1 | 126.248 |

**Loaded-ArCP (BMRB 25787 ; residues after 100 belong to the second minor conformer)**

| residue number | Nucleus | Chemical Shift (ppm) |
|---|---|---|
| 14 | H | 8.561 |
| 14 | N | 122.878 |
| 14 | CA | 54.291 |
| 14 | CB | 41.082 |
| 14 | C | 176.262 |
| 14 | HB2 | 2.746 |
| 14 | HB3 | 2.676 |
| 14 | HA | 4.646 |
| 15 | H | 8.415 |
| 15 | N | 119.829 |
| 15 | CA | 53.57 |
| 15 | CB | 38.66 |
| 15 | C | 175.877 |
| 15 | HA | 4.728 |
| 15 | HB2 | 2.874 |
| 15 | HB3 | 2.808 |
| 16 | H | 8.338 |
| 16 | CA | 57.723 |
| 16 | HA | 4.218 |
| 16 | CD | 43.359 |
| 16 | CB | 30.262 |
| 16 | CG | 26.882 |
| 16 | HB | 1.851 |
| 16 | HG | 1.625 |
| 16 | HD | 3.202 |
| 16 | N | 122.04 |
| 17 | H | 8.39 |
| 17 | N | 118.569 |
| 17 | CA | 58.376 |
| 17 | CB | 30.352 |
| 17 | HA | 4.575 |
| 17 | HB3 | 3.149 |
| 17 | HB2 | 3.272 |
| 17 | HD2 | 7.026 |
| 17 | CD2 | 119.256 |
| 18 | H | 8.427 |
| 18 | N | 122.055 |
| 18 | CA | 54.286 |
| 18 | C | 179.956 |
| 18 | CB | 18.815 |
| 18 | HB | 1.581 |
| 18 | HA | 4.188 |

| | | |
|---|---|---|
| 19 | H | 8.397 |
| 19 | N | 122.616 |
| 19 | CA | 55.05 |
| 19 | CB | 18.336 |
| 19 | HB | 1.571 |
| 19 | HA | 4.276 |
| 20 | H | 8.305 |
| 20 | N | 118.761 |
| 20 | HB | 2.923 |
| 20 | CB | 40.145 |
| 20 | CA | 56.649 |
| 20 | HA | 4.832 |
| 21 | H | 8.662 |
| 21 | N | 120.921 |
| 21 | CA | 61.89 |
| 21 | CB | 38.556 |
| 21 | C | 176.215 |
| 21 | HA | 4.055 |
| 21 | HB | 3.009 |
| 21 | CD | 132.817 |
| 21 | HE | 7.009 |
| 21 | HD | 6.672 |
| 21 | CE | 117.803 |
| 22 | H | 8.23 |
| 22 | N | 117.709 |
| 22 | CA | 59.121 |
| 22 | C | 178.263 |
| 22 | CB | 27.518 |
| 22 | CG | 33.242 |
| 22 | HA | 3.83 |
| 22 | HG | 2.496 |
| 22 | HB | 2.226 |
| 23 | H | 7.998 |
| 23 | N | 118.536 |
| 23 | CA | 59.071 |
| 23 | C | 177.48 |
| 23 | CB | 28.888 |
| 23 | CG | 34.783 |
| 23 | HA | 4.098 |
| 23 | HG | 2.661 |
| 23 | HB2 | 2.446 |
| 23 | HB3 | 2.364 |
| 24 | H | 8.015 |
| 24 | N | 121.913 |
| 24 | CA | 58.095 |
| 24 | CB | 41.718 |
| 24 | HB2 | 1.904 |

| | | |
|---|---|---|
| 24 | CD1 | 27.113 |
| 24 | HD1 | 0.977 |
| 24 | CD2 | 23.616 |
| 24 | HD2 | 0.064 |
| 24 | HA | 3.439 |
| 24 | HB3 | 1.338 |
| 25 | H | 7.973 |
| 25 | N | 116.667 |
| 25 | CA | 60.24 |
| 25 | CB | 29.861 |
| 25 | C | 177.48 |
| 25 | CG | 29.942 |
| 25 | CD | 43.643 |
| 25 | HB | 1.579 |
| 25 | HG | 1.21 |
| 25 | HD | 3.028 |
| 25 | HA | 3.397 |
| 26 | H | 8.145 |
| 26 | N | 115.926 |
| 26 | CA | 59.525 |
| 26 | CB | 29.41 |
| 26 | HA | 3.83 |
| 26 | CG | 36.652 |
| 26 | HB2 | 2.008 |
| 26 | HB3 | 2.111 |
| 26 | HG2 | 2.271 |
| 26 | HG3 | 2.459 |
| 27 | H | 8.265 |
| 27 | N | 118.785 |
| 27 | CA | 59.03 |
| 27 | CB | 30.091 |
| 27 | C | 179.27 |
| 27 | CG | 28.063 |
| 27 | CD | 43.037 |
| 27 | HA | 4.141 |
| 27 | HG2 | 1.837 |
| 27 | HB | 1.979 |
| 27 | HD2 | 2.757 |
| 27 | HD3 | 2.989 |
| 27 | HG3 | 1.647 |
| 28 | H | 8.384 |
| 28 | N | 122.113 |
| 28 | CA | 58.589 |
| 28 | CB | 42.536 |
| 28 | C | 178.766 |
| 28 | HD1 | 0.321 |
| 28 | CD1 | 26.662 |

| | | |
|---|---|---|
| 28 | HA | 4.101 |
| 28 | CD2 | 24.212 |
| 28 | HD2 | 0.446 |
| 28 | HB3 | 1.737 |
| 28 | HB2 | 0.952 |
| 28 | HG | 1.338 |
| 28 | CG | 26.94 |
| 29 | H | 7.905 |
| 29 | N | 117.57 |
| 29 | CA | 66.197 |
| 29 | CB | 37.796 |
| 29 | C | 177.984 |
| 29 | CG2 | 17.23 |
| 29 | HG2 | 0.758 |
| 29 | HA | 3.34 |
| 29 | CD1 | 14.147 |
| 29 | CG1 | 30.628 |
| 29 | HD1 | 0.722 |
| 29 | HB | 1.868 |
| 30 | H | 7.282 |
| 30 | N | 116.386 |
| 30 | CA | 58.432 |
| 30 | CB | 28.722 |
| 30 | C | 179.376 |
| 30 | HA | 4.161 |
| 30 | CG | 33.619 |
| 30 | HB | 2.199 |
| 30 | HG2 | 2.429 |
| 30 | HG3 | 2.551 |
| 31 | H | 8.811 |
| 31 | N | 120.289 |
| 31 | CA | 59.393 |
| 31 | CB | 30.477 |
| 31 | C | 178.395 |
| 31 | CG | 36.662 |
| 31 | HA | 4.03 |
| 31 | HG2 | 2.449 |
| 31 | HG3 | 2.231 |
| 31 | HB | 2.117 |
| 32 | H | 8.104 |
| 32 | N | 115.14 |
| 32 | CA | 54.115 |
| 32 | C | 176.138 |
| 32 | CD1 | 21.576 |
| 32 | HD1 | 0.688 |
| 32 | HA | 4.382 |
| 32 | HG | 1.511 |

| | | |
|---|---|---|
| 32 | CD2 | 26.066 |
| 32 | CB | 41.35 |
| 32 | HD2 | 0.678 |
| 32 | HB3 | 1.693 |
| 32 | HB2 | 1.772 |
| 33 | H | 7.79 |
| 33 | N | 116.74 |
| 33 | CA | 53.952 |
| 33 | CB | 36.926 |
| 33 | C | 174.288 |
| 33 | HB2 | 2.743 |
| 33 | HA | 4.451 |
| 33 | HB3 | 3.151 |
| 34 | H | 7.743 |
| 34 | N | 117.167 |
| 34 | CA | 53.113 |
| 34 | CB | 44.723 |
| 34 | C | 176.54 |
| 34 | HA | 4.807 |
| 34 | HB2 | 1.425 |
| 34 | CG | 26.614 |
| 34 | HD1 | 0.71 |
| 34 | HD2 | 0.803 |
| 34 | CD2 | 22.477 |
| 34 | CD1 | 26.954 |
| 34 | HB3 | 1.537 |
| 35 | H | 7.991 |
| 35 | N | 110.801 |
| 35 | CA | 59.532 |
| 35 | CB | 68.634 |
| 35 | HG2 | 1.251 |
| 35 | CG2 | 21.759 |
| 35 | HB | 4.564 |
| 35 | HA | 4.806 |
| 36 | CA | 65.653 |
| 36 | HA | 4.077 |
| 36 | CB | 31.762 |
| 36 | CG | 27.782 |
| 36 | HB2 | 2.378 |
| 36 | HB3 | 1.935 |
| 36 | HG2 | 2.216 |
| 36 | HG3 | 2.016 |
| 36 | CD | 50.23 |
| 36 | HD | 3.875 |
| 37 | H | 7.998 |
| 37 | N | 112.861 |
| 37 | CA | 57.896 |

| | | |
|---|---|---|
| 37 | CB | 27.971 |
| 37 | CG | 34.244 |
| 37 | HA | 4.097 |
| 37 | HB | 2.043 |
| 37 | HG2 | 2.39 |
| 37 | HG3 | 2.483 |
| 38 | H | 7.654 |
| 38 | N | 116.463 |
| 38 | CA | 56.42 |
| 38 | C | 175.595 |
| 38 | CB | 31.149 |
| 38 | CG | 34.691 |
| 38 | HG | 2.358 |
| 38 | HA | 4.184 |
| 38 | HB | 2.153 |
| 39 | H | 7.268 |
| 39 | N | 120.715 |
| 39 | HD1 | 0.634 |
| 39 | CD1 | 26.458 |
| 39 | CD2 | 22.995 |
| 39 | HD2 | 0.641 |
| 39 | CA | 53.979 |
| 39 | CB | 41.823 |
| 39 | HB3 | 1.001 |
| 39 | HA | 4.379 |
| 39 | HB2 | 1.72 |
| 39 | HG | 1.255 |
| 39 | CG | 26.879 |
| 40 | H | 8.17 |
| 40 | N | 124.732 |
| 40 | CA | 54.768 |
| 40 | HB3 | 3.156 |
| 40 | HB2 | 3.263 |
| 40 | CB | 31.33 |
| 40 | HE1 | 8.073 |
| 40 | CE1 | 137.492 |
| 40 | HA | 4.83 |
| 42 | H | 8.805 |
| 42 | N | 113.74 |
| 42 | CA | 55.317 |
| 42 | CG | 36.047 |
| 42 | CB | 29.196 |
| 42 | HG | 1.91 |
| 42 | HA | 4.543 |
| 42 | HB2 | 2.248 |
| 42 | HB3 | 1.908 |
| 43 | H | 7.472 |

| | | |
|---|---|---|
| 43 | N | 118.02 |
| 43 | CA | 60.206 |
| 43 | CB | 62.807 |
| 43 | HA | 4.088 |
| 43 | HB2 | 3.724 |
| 43 | HB3 | 3.64 |
| 44 | H | 8.8 |
| 44 | N | 123.274 |
| 44 | CA | 54.003 |
| 44 | C | 176.885 |
| 44 | CB | 38.449 |
| 44 | HA | 4.394 |
| 44 | HB3 | 2.716 |
| 44 | HB2 | 2.815 |
| 45 | H | 9.382 |
| 45 | N | 128.761 |
| 45 | CA | 57.144 |
| 45 | CB | 42.295 |
| 45 | HA | 3.745 |
| 45 | HD1 | 0.4 |
| 45 | HB2 | 1.101 |
| 45 | CG | 26.405 |
| 45 | HG | 1.379 |
| 45 | CD1 | 22.645 |
| 45 | CD2 | 23.71 |
| 45 | HD2 | -0.618 |
| 45 | HB3 | 1.026 |
| 46 | H | 7.672 |
| 46 | N | 119.381 |
| 46 | CA | 63.686 |
| 46 | CB | 36.706 |
| 46 | C | 180.905 |
| 46 | CG1 | 28.032 |
| 46 | CG2 | 16.843 |
| 46 | HG2 | 1.001 |
| 46 | HA | 4.263 |
| 46 | HB | 2.222 |
| 46 | CD1 | 12.474 |
| 46 | HD1 | 0.856 |
| 46 | HG12 | 1.397 |
| 46 | HG13 | 1.54 |
| 47 | H | 8.157 |
| 47 | N | 121.8 |
| 47 | CA | 58.241 |
| 47 | CB | 28.03 |
| 47 | C | 177.706 |
| 47 | CG | 34.056 |

| | | |
|---|---|---|
| 47 | HG | 2.393 |
| 47 | HA | 4.003 |
| 47 | HB2 | 2.151 |
| 47 | HB3 | 1.955 |
| 48 | H | 7.441 |
| 48 | N | 117.705 |
| 48 | CA | 52.724 |
| 48 | CB | 18.615 |
| 48 | C | 176.646 |
| 48 | HB | 1.41 |
| 48 | HA | 4.267 |
| 49 | H | 7.459 |
| 49 | N | 102.97 |
| 49 | CA | 44.972 |
| 49 | C | 174.493 |
| 49 | HA2 | 3.707 |
| 49 | HA3 | 4.567 |
| 50 | H | 8.543 |
| 50 | N | 123.062 |
| 50 | CA | 56.214 |
| 50 | CB | 41.778 |
| 50 | C | 173.497 |
| 50 | HB | 1.494 |
| 50 | HD2 | 0.969 |
| 50 | CD1 | 26.723 |
| 50 | CD2 | 26.931 |
| 50 | HA | 4.251 |
| 50 | HD1 | 0.862 |
| 50 | HG | 1.76 |
| 51 | H | 7.377 |
| 51 | N | 123.093 |
| 51 | CA | 52.208 |
| 51 | CB | 42.248 |
| 51 | HB2 | 2.782 |
| 51 | HA | 4.872 |
| 51 | C | 176.23 |
| 51 | HB3 | 3.214 |
| 52 | H | 8.968 |
| 52 | N | 113.882 |
| 52 | CA | 60.898 |
| 52 | HA | 4.001 |
| 52 | CB | 67.836 |
| 52 | C | 176.643 |
| 52 | HZ1 | 6.898 |
| 52 | CL1 | 23.086 |
| 52 | HL3 | 3.911 |
| 52 | CL3 | 77.045 |

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|---|---|---|
| 52 | HO | 3.442 |
| 52 | HL1 | 0.814 |
| 52 | CO | 37.959 |
| 52 | CT | 31.029 |
| 52 | HT2 | 3.042 |
| 52 | CS | 40.999 |
| 52 | HP | 2.447 |
| 52 | HS | 3.371 |
| 52 | CP | 37.961 |
| 52 | HL2 | 0.768 |
| 52 | CL2 | 21.835 |
| 52 | CJ | 73.754 |
| 52 | HJ2 | 3.25 |
| 52 | HJ3 | 3.662 |
| 52 | CZ1 | 120.156 |
| 52 | HAA | 7.522 |
| 52 | CAA | 139.025 |
| 52 | HZ2 | 6.912 |
| 52 | CZ2 | 122.547 |
| 52 | HY2 | 7.722 |
| 52 | CY2 | 131.827 |
| 52 | HB3 | 4.224 |
| 52 | HT3 | 2.969 |
| 52 | HB2 | 4.264 |
| 53 | H | 7.623 |
| 53 | N | 123.399 |
| 53 | CA | 64.365 |
| 53 | C | 179.524 |
| 53 | CB | 37.098 |
| 53 | CD1 | 12.426 |
| 53 | CG2 | 17.304 |
| 53 | CG1 | 28.755 |
| 53 | HG2 | 0.907 |
| 53 | HA | 3.847 |
| 53 | HB | 2.122 |
| 53 | HD1 | 0.892 |
| 53 | HG12 | 1.646 |
| 53 | HG13 | 1.245 |
| 54 | H | 8.456 |
| 54 | N | 121.206 |
| 54 | CA | 59.59 |
| 54 | C | 179.604 |
| 54 | CG | 28.829 |
| 54 | CB | 30.619 |
| 54 | CD | 43.09 |
| 54 | HA | 4.091 |
| 54 | HD | 3.293 |

| | | |
|---|---|---|
| 54 | HG | 1.769 |
| 54 | HB | 1.974 |
| 55 | H | 9.057 |
| 55 | N | 121.118 |
| 55 | CA | 59.006 |
| 55 | CB | 41.668 |
| 55 | CD1 | 25.839 |
| 55 | CG | 27.968 |
| 55 | HD1 | 1.016 |
| 55 | HA | 4.39 |
| 55 | HB | 1.857 |
| 55 | HG | 1.671 |
| 55 | HD2 | 0.993 |
| 55 | CD2 | 25.318 |
| 56 | H | 7.954 |
| 56 | N | 118.071 |
| 56 | CA | 58.015 |
| 56 | HA | 4.282 |
| 56 | HB | 2.279 |
| 56 | HG | 2.681 |
| 56 | CB | 31.403 |
| 56 | CG | 32.408 |
| 56 | HE | 2.101 |
| 56 | CE | 17.017 |
| 57 | H | 7.616 |
| 57 | N | 119.697 |
| 57 | CA | 59.793 |
| 57 | CB | 29.477 |
| 57 | CG | 27.597 |
| 57 | CD | 43.325 |
| 57 | HA | 4.098 |
| 57 | HD | 3.022 |
| 57 | HB3 | 1.801 |
| 57 | HB2 | 1.893 |
| 57 | HG2 | 1.463 |
| 57 | HG3 | 1.727 |
| 58 | H | 8.228 |
| 58 | N | 121.853 |
| 58 | CA | 61.003 |
| 58 | HE1 | 11.027 |
| 58 | NE1 | 131.116 |
| 58 | CB | 28.28 |
| 58 | HA | 4.469 |
| 58 | HB2 | 3.495 |
| 58 | HB3 | 3.257 |
| 58 | HH2 | 6.517 |
| 58 | CH2 | 123.106 |

| | | |
|---|---|---|
| 58 | CD1 | 125.879 |
| 58 | CZ2 | 113.928 |
| 58 | HZ2 | 6.901 |
| 58 | HD1 | 7.19 |
| 59 | H | 8.654 |
| 59 | N | 121.724 |
| 59 | CA | 58.987 |
| 59 | CB | 40.871 |
| 59 | HA | 4.263 |
| 59 | HD1 | 0.779 |
| 59 | HB2 | 1.494 |
| 59 | CD1 | 23.488 |
| 59 | CD2 | 26.06 |
| 59 | HD2 | 0.962 |
| 59 | HB3 | 2.334 |
| 60 | H | 7.916 |
| 60 | N | 117.03 |
| 60 | CA | 59.804 |
| 60 | CB | 29.929 |
| 60 | HA | 4.377 |
| 60 | HB | 3.281 |
| 60 | HD2 | 7.132 |
| 60 | CD2 | 119.415 |
| 61 | H | 8.12 |
| 61 | N | 123.142 |
| 61 | CA | 62.607 |
| 61 | HE1 | 9.936 |
| 61 | NE1 | 128.434 |
| 61 | CB | 28.767 |
| 61 | HA | 4.013 |
| 61 | HB3 | 3.021 |
| 61 | HB2 | 3.745 |
| 61 | HH2 | 7.089 |
| 61 | HZ2 | 7.344 |
| 61 | CH2 | 123.788 |
| 61 | HZ3 | 6.391 |
| 61 | CE3 | 120.176 |
| 61 | CD1 | 126.497 |
| 61 | CZ2 | 113.351 |
| 61 | HE3 | 6.657 |
| 61 | HD1 | 7.109 |
| 61 | CZ3 | 121.919 |
| 62 | H | 9.446 |
| 62 | N | 120.033 |
| 62 | CA | 63.686 |
| 62 | CB | 38.673 |
| 62 | HA | 4.195 |

| | | |
|---|---|---|
| 62 | HB2 | 3.287 |
| 62 | HE | 6.89 |
| 62 | HD | 7.203 |
| 62 | HZ | 7.047 |
| 62 | CZ | 129.859 |
| 62 | CD | 131.514 |
| 62 | CE | 131.579 |
| 62 | HB3 | 3.382 |
| 63 | H | 8.681 |
| 63 | N | 118.582 |
| 63 | CA | 59.341 |
| 63 | CB | 29.657 |
| 63 | C | 181.343 |
| 63 | CG | 27.997 |
| 63 | CD | 43.31 |
| 63 | HA | 4.254 |
| 63 | HD | 3.306 |
| 63 | HG | 1.842 |
| 63 | HB | 1.988 |
| 64 | H | 8.676 |
| 64 | N | 122.757 |
| 64 | CA | 58.695 |
| 64 | C | 177.573 |
| 64 | CB | 31.428 |
| 64 | CG | 24.534 |
| 64 | CD | 28.956 |
| 64 | HA | 4.029 |
| 64 | HG | 1.353 |
| 64 | HD | 1.575 |
| 64 | HB2 | 1.737 |
| 64 | HB3 | 1.837 |
| 64 | CE | 41.948 |
| 64 | HE | 2.878 |
| 65 | H | 7.234 |
| 65 | N | 115.716 |
| 65 | CA | 53.719 |
| 65 | CB | 39 |
| 65 | C | 173.44 |
| 65 | HA | 4.538 |
| 65 | HB2 | 2.725 |
| 65 | HB3 | 2.144 |
| 66 | H | 7.596 |
| 66 | N | 105.195 |
| 66 | CA | 45.537 |
| 66 | HA2 | 4.001 |
| 66 | HA3 | 3.586 |
| 67 | H | 8.237 |

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|---|---|---|
| 67 | N | 119.719 |
| 67 | CA | 57.807 |
| 67 | CB | 38.5 |
| 67 | HA | 4.554 |
| 67 | HB2 | 3.004 |
| 67 | HB3 | 2.603 |
| 67 | HD | 7.296 |
| 67 | CD | 133.288 |
| 67 | HE | 6.888 |
| 67 | CE | 118.149 |
| 68 | H | 8.53 |
| 68 | N | 125.606 |
| 68 | CA | 55.676 |
| 68 | CB | 28.482 |
| 68 | C | 174.559 |
| 68 | CG | 27.198 |
| 68 | CD | 43.064 |
| 68 | HA | 4.389 |
| 68 | HD | 3.197 |
| 68 | HB2 | 1.875 |
| 68 | HG2 | 1.715 |
| 68 | HB3 | 1.635 |
| 68 | HG3 | 1.534 |
| 69 | H | 7.407 |
| 69 | N | 122.142 |
| 69 | CA | 53.341 |
| 69 | CB | 44.311 |
| 69 | C | 175.706 |
| 69 | HD1 | 0.321 |
| 69 | HB2 | 1.418 |
| 69 | HG | 1.257 |
| 69 | CD1 | 25.174 |
| 69 | CD2 | 24.687 |
| 69 | HB3 | 1.275 |
| 69 | HD2 | 0.103 |
| 69 | HA | 4.713 |
| 70 | H | 8.152 |
| 70 | N | 109.735 |
| 70 | CA | 59.424 |
| 70 | CB | 72.076 |
| 70 | CG2 | 21.553 |
| 70 | HG2 | 1.15 |
| 70 | HB | 4.578 |
| 70 | HA | 4.722 |
| 71 | H | 8.82 |
| 71 | N | 122.488 |
| 71 | CA | 58.343 |

| | | |
|---|---|---|
| 71 | C | 178.622 |
| 71 | CB | 41.866 |
| 71 | HA | 3.876 |
| 71 | HB2 | 1.883 |
| 71 | HB3 | 1.678 |
| 71 | HD1 | 0.966 |
| 71 | CD1 | 25.696 |
| 71 | CG | 25.258 |
| 71 | HD2 | 0.995 |
| 71 | CD2 | 24.332 |
| 72 | H | 8.268 |
| 72 | N | 115.907 |
| 72 | CA | 59.258 |
| 72 | CB | 29.615 |
| 72 | C | 178.98 |
| 72 | CD | 43.125 |
| 72 | CG | 26.998 |
| 72 | HA | 3.779 |
| 72 | HD | 3.162 |
| 72 | HB2 | 1.843 |
| 72 | HG | 1.649 |
| 72 | HB3 | 1.727 |
| 73 | H | 7.438 |
| 73 | N | 117.413 |
| 73 | CA | 59.103 |
| 73 | CB | 29.75 |
| 73 | CG | 37.646 |
| 73 | HG | 2.224 |
| 73 | HA | 3.929 |
| 73 | HB2 | 1.875 |
| 73 | HB3 | 2.229 |
| 74 | H | 7.358 |
| 74 | N | 117.442 |
| 74 | CA | 57.395 |
| 74 | CB | 41.861 |
| 74 | C | 179.405 |
| 74 | HA | 3.906 |
| 74 | HG | 1.358 |
| 74 | CD2 | 25.502 |
| 74 | HD1 | -0.8 |
| 74 | HB3 | 1.208 |
| 74 | HD2 | 0.374 |
| 74 | CD1 | 19.857 |
| 74 | HB2 | 1.365 |
| 74 | CG | 25.656 |
| 75 | H | 8.088 |
| 75 | N | 115.237 |

| | | |
|---|---|---|
| 75 | CA | 60.229 |
| 75 | CB | 39.484 |
| 75 | C | 176.882 |
| 75 | HA | 4.036 |
| 75 | HB3 | 2.825 |
| 75 | HB2 | 2.957 |
| 75 | CD | 132.673 |
| 75 | CE | 118.099 |
| 75 | HE | 6.523 |
| 75 | HD | 6.845 |
| 76 | H | 7.793 |
| 76 | N | 118.861 |
| 76 | CA | 54.27 |
| 76 | CB | 18.494 |
| 76 | C | 178.17 |
| 76 | HA | 3.948 |
| 76 | HB | 1.462 |
| 77 | H | 6.639 |
| 77 | N | 116.989 |
| 77 | CA | 49.652 |
| 77 | CB | 19.173 |
| 77 | C | 173.807 |
| 77 | HB | 1.306 |
| 78 | HA | 5.017 |
| 78 | CA | 61.518 |
| 78 | CB | 26.471 |
| 78 | HB2 | 2.07 |
| 78 | CD | 48.115 |
| 78 | HB3 | 1.912 |
| 78 | HD | 3.523 |
| 79 | H | 7.665 |
| 79 | N | 111.926 |
| 79 | CA | 58.065 |
| 79 | CB | 72.268 |
| 79 | C | 172.978 |
| 79 | HB | 4.497 |
| 79 | HG2 | 0.845 |
| 79 | HA | 4.384 |
| 79 | CG2 | 21.105 |
| 80 | H | 9.616 |
| 80 | N | 123.225 |
| 80 | CA | 58.162 |
| 80 | CB | 41.569 |
| 80 | HA | 3.742 |
| 80 | HB2 | 1.918 |
| 80 | HG | 1.607 |
| 80 | CG | 26.913 |

| | | |
|---|---|---|
| 80 | CD1 | 24.948 |
| 80 | HD1 | 0.64 |
| 80 | HD2 | 0.581 |
| 80 | CD2 | 23.885 |
| 80 | HB3 | 1.611 |
| 81 | H | 8.82 |
| 81 | N | 119.691 |
| 81 | CA | 54.95 |
| 81 | CB | 18.381 |
| 81 | C | 181.058 |
| 81 | HB | 1.301 |
| 81 | HA | 4.145 |
| 82 | H | 8.251 |
| 82 | N | 122.226 |
| 82 | CA | 54.843 |
| 82 | CB | 19.041 |
| 82 | C | 181.84 |
| 82 | HA | 4.22 |
| 82 | HB | 1.66 |
| 83 | H | 9.365 |
| 83 | N | 123.378 |
| 83 | CA | 59.569 |
| 83 | C | 178.554 |
| 83 | HE1 | 10.062 |
| 83 | NE1 | 128.06 |
| 83 | CB | 28.215 |
| 83 | HB2 | 3.129 |
| 83 | HB3 | 3.33 |
| 83 | HA | 4.535 |
| 83 | HZ3 | 5.99 |
| 83 | CZ3 | 119.584 |
| 83 | CD1 | 124.599 |
| 83 | HD1 | 7.282 |
| 83 | CE3 | 120.21 |
| 83 | CZ2 | 112.159 |
| 83 | HE3 | 7.276 |
| 83 | HH2 | 6.55 |
| 83 | CH2 | 123.184 |
| 83 | HZ2 | 6.812 |
| 84 | H | 9.144 |
| 84 | N | 118.259 |
| 84 | CA | 57.11 |
| 84 | CB | 39.23 |
| 84 | C | 177.349 |
| 84 | HA | 4.617 |
| 84 | HB2 | 2.841 |
| 84 | HB3 | 2.959 |

| | | |
|---|---|---|
| 85 | H | 7.498 |
| 85 | N | 116.239 |
| 85 | CA | 58.775 |
| 85 | CB | 27.824 |
| 85 | C | 179.442 |
| 85 | HA | 4.005 |
| 85 | HG | 2.52 |
| 85 | HB2 | 2.244 |
| 85 | HB3 | 2.501 |
| 86 | H | 8.166 |
| 86 | N | 121.605 |
| 86 | CA | 57.983 |
| 86 | CB | 41.896 |
| 86 | C | 179.299 |
| 86 | HA | 4.04 |
| 86 | HB2 | 1.947 |
| 86 | CD1 | 25.733 |
| 86 | HG | 1.763 |
| 86 | HD2 | 0.739 |
| 86 | CD2 | 23.043 |
| 86 | HD1 | 0.687 |
| 86 | HB3 | 1.212 |
| 86 | CG | 26.57 |
| 87 | H | 8.212 |
| 87 | N | 117.886 |
| 87 | CA | 59.509 |
| 87 | C | 177.891 |
| 87 | HA | 3.75 |
| 87 | HB2 | 2.149 |
| 87 | CB | 34.881 |
| 87 | CG | 32.651 |
| 87 | HG2 | 2.647 |
| 87 | HB3 | 2.443 |
| 87 | HE | 2.048 |
| 87 | CE | 16.986 |
| 87 | HG3 | 1.356 |
| 88 | H | 7.893 |
| 88 | N | 117.541 |
| 88 | CA | 57.182 |
| 88 | CB | 42.4 |
| 88 | C | 179.033 |
| 88 | CD1 | 25.343 |
| 88 | HA | 4.059 |
| 88 | HB2 | 1.775 |
| 88 | HD1 | 0.72 |
| 88 | HB3 | 1.475 |
| 88 | CD2 | 22.627 |

| | | |
|---|---|---|
| 88 | HD2 | 0.59 |
| 88 | HG | 1.599 |
| 89 | H | 7.951 |
| 89 | N | 113.194 |
| 89 | CA | 59.957 |
| 89 | CB | 63.956 |
| 89 | C | 174.88 |
| 89 | HA | 4.036 |
| 89 | HB | 4.727 |
| 90 | H | 7.913 |
| 90 | N | 121.967 |
| 90 | CA | 53.937 |
| 90 | CB | 29.589 |
| 90 | C | 175.626 |
| 90 | CG | 26.798 |
| 90 | CD | 42.207 |
| 90 | HD | 3.17 |
| 90 | HA | 4.705 |
| 90 | HB2 | 2.072 |
| 90 | HG2 | 1.724 |
| 90 | HB3 | 1.839 |
| 90 | HG3 | 1.648 |
| 91 | H | 7.731 |
| 91 | N | 117.139 |
| 91 | CA | 57.077 |
| 91 | CB | 63.455 |
| 91 | C | 173.346 |
| 92 | CA | 63.392 |
| 92 | HA | 4.423 |
| 92 | HB2 | 2.149 |
| 92 | CB | 31.895 |
| 92 | CG | 27.278 |
| 92 | CD | 50.806 |
| 92 | HD2 | 3.386 |
| 92 | HB3 | 1.873 |
| 92 | HG3 | 1.79 |
| 92 | HG2 | 1.869 |
| 92 | HD3 | 3.595 |
| 93 | H | 8.056 |
| 93 | N | 126.242 |
| 93 | CA | 56.856 |
| 93 | CB | 31.192 |
| 93 | C | 176.315 |
| 93 | CG | 36.519 |
| 93 | HB2 | 2.225 |
| 93 | HG2 | 2.026 |
| 93 | HG3 | 1.877 |

| | | |
|---|---|---|
| 93 | HB3 | 2.039 |
| 25 | H 1 | 8.054 |
| 25 | N 1 | 116.632 |
| 26 | H 1 | 8.083 |
| 26 | N 1 | 115.895 |
| 51 | H 1 | 7.167 |
| 51 | N 1 | 122.636 |
| 53 | H 1 | 7.741 |
| 53 | N 1 | 123.271 |
| 54 | H 1 | 8.539 |
| 54 | N 1 | 121.504 |
| 55 | H 1 | 9.111 |
| 55 | N 1 | 120.775 |
| 57 | H 1 | 7.706 |
| 57 | N 1 | 120.162 |
| 58 | H 1 | 8.281 |
| 58 | N 1 | 121.837 |
| 59 | H 1 | 8.5 |
| 59 | N 1 | 120.976 |
| 60 | H 1 | 8.049 |
| 60 | N 1 | 116.875 |
| 61 | H 1 | 8.081 |
| 61 | N 1 | 122.754 |
| 62 | H 1 | 9.338 |
| 62 | N 1 | 119.653 |
| 63 | H 1 | 8.703 |
| 63 | N 1 | 120.126 |
| 64 | H 1 | 8.596 |
| 64 | N 1 | 122.255 |
| 68 | H 1 | 8.808 |
| 68 | N 1 | 126.047 |
| 69 | H 1 | 7.454 |
| 69 | N 1 | 123.012 |
| 70 | H 1 | 8.065 |
| 70 | N 1 | 109.703 |
| 72 | H 1 | 8.187 |
| 72 | N 1 | 116.47 |
| 84 | H 1 | 9.095 |
| 84 | N 1 | 117.844 |
| 86 | H 1 | 8.086 |
| 86 | N 1 | 120.795 |
| 90 | H 1 | 7.85 |
| 90 | N 1 | 122.246 |
| 91 | H 1 | 7.665 |
| 91 | N 1 | 117.178 |
| 93 | H 1 | 8.171 |
| 93 | N 1 | 126.238 |

**PDB coordinates as outputs from CYANA. In this format the post-translational modification is a side-chain of S52. The coordinates deposited in the PDB are those of the water-refined conformers. Only the coordinates of the low energy conformers are provided here.**

**HOLO (PDB 2N6Y):**

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HEADER      STRUCTURE FROM CYANA 2.1                25-Jun-15      1PDB
EXPDTA      NMR, 20 STRUCTURES
REMARK      99 B-FACTOR COLUMN STORES ADDITIONAL COORDINATE    DIGITS.
MODEL       1
ATOM      1  N   ASP A  14       1.328   0.000   0.000  1.00  4.00
ATOM      2  CA  ASP A  14       2.093  -0.001  -1.242  1.00  0.02
ATOM      3  C   ASP A  14       1.305  -0.669  -2.364  1.00 64.43
ATOM      4  O   ASP A  14       1.150  -0.106  -3.447  1.00 33.41
ATOM      5  CB  ASP A  14       3.429  -0.718  -1.042  1.00 62.14
ATOM      6  CG  ASP A  14       4.140  -0.993  -2.353  1.00 73.30
ATOM      7  OD1 ASP A  14       4.856  -0.094  -2.841  1.00 12.54
ATOM      8  OD2 ASP A  14       3.981  -2.109  -2.891  1.00 15.12
ATOM      9  H   ASP A  14       1.806  -0.000   0.856  1.00 64.11
ATOM     10  HA  ASP A  14       2.283   1.026  -1.515  1.00 24.11
ATOM     11 2HB  ASP A  14       4.072  -0.104  -0.428  1.00 51.03
ATOM     12 3HB  ASP A  14       3.254  -1.660  -0.544  1.00 11.25
ATOM     13  N   ASN A  15       0.812  -1.874  -2.098  1.00 31.41
ATOM     14  CA  ASN A  15       0.042  -2.621  -3.086  1.00 53.53
ATOM     15  C   ASN A  15      -1.349  -2.953  -2.555  1.00 11.35
ATOM     16  O   ASN A  15      -1.711  -2.560  -1.445  1.00 63.21
ATOM     17  CB  ASN A  15       0.775  -3.908  -3.469  1.00 33.04
ATOM     18  CG  ASN A  15       1.369  -3.843  -4.862  1.00 51.03
ATOM     19  ND2 ASN A  15       1.092  -4.859  -5.671  1.00 62.13
ATOM     20  OD1 ASN A  15       2.068  -2.890  -5.207  1.00 62.22
ATOM     21  H   ASN A  15       0.969  -2.272  -1.216  1.00  4.51
ATOM     22  HA  ASN A  15      -0.060  -2.000  -3.964  1.00 62.52
ATOM     23 2HB  ASN A  15       1.576  -4.081  -2.765  1.00 33.53
ATOM     24 3HB  ASN A  15       0.082  -4.735  -3.430  1.00 71.03
ATOM     25 1HD2 ASN A  15       0.528  -5.584  -5.329  1.00  1.33
ATOM     26 2HD2 ASN A  15       1.464  -4.843  -6.578  1.00  0.12
ATOM     27  N   ARG A  16      -2.124  -3.679  -3.353  1.00 53.35
ATOM     28  CA  ARG A  16      -3.476  -4.063  -2.964  1.00 25.42
ATOM     29  C   ARG A  16      -3.453  -4.934  -1.711  1.00  1.01
ATOM     30  O   ARG A  16      -2.438  -5.018  -1.019  1.00 22.22
ATOM     31  CB  ARG A  16      -4.165  -4.812  -4.106  1.00 22.31
ATOM     32  CG  ARG A  16      -4.009  -4.137  -5.459  1.00 22.14
ATOM     33  CD  ARG A  16      -5.327  -4.095  -6.216  1.00 10.15
ATOM     34  NE  ARG A  16      -6.242  -3.098  -5.666  1.00 42.34
ATOM     35  CZ  ARG A  16      -6.066  -1.788  -5.798  1.00 52.34
ATOM     36  NH1 ARG A  16      -5.016  -1.319  -6.458  1.00 62.42
ATOM     37  NH2 ARG A  16      -6.943  -0.943  -5.270  1.00 62.03
ATOM     38  H   ARG A  16      -1.780  -3.962  -4.226  1.00 41.33
ATOM     39  HA  ARG A  16      -4.029  -3.161  -2.751  1.00 31.20
ATOM     40 2HB  ARG A  16      -3.746  -5.806  -4.174  1.00 13.21
ATOM     41 3HB  ARG A  16      -5.219  -4.889  -3.885  1.00 42.34
ATOM     42 2HG  ARG A  16      -3.661  -3.126  -5.308  1.00  4.10
ATOM     43 3HG  ARG A  16      -3.285  -4.686  -6.043  1.00 13.11
ATOM     44 2HD  ARG A  16      -5.126  -3.854  -7.249  1.00 30.52
ATOM     45 3HD  ARG A  16      -5.792  -5.068  -6.156  1.00 43.24
ATOM     46  HE  ARG A  16      -7.025  -3.422  -5.175  1.00 42.10
ATOM     47 1HH1 ARG A  16      -4.354  -1.954  -6.858  1.00 53.50
ATOM     48 2HH1 ARG A  16      -4.887  -0.332  -6.557  1.00 64.42
ATOM     49 1HH2 ARG A  16      -7.736  -1.292  -4.772  1.00 60.35
ATOM     50 2HH2 ARG A  16      -6.810   0.043  -5.370  1.00 62.50
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ATOM     51  N   HIS A  17      -4.579  -5.580  -1.425  1.00 11.33
ATOM     52  CA  HIS A  17      -4.689  -6.444  -0.255  1.00 24.10
ATOM     53  C   HIS A  17      -3.518  -7.421  -0.190  1.00 14.01
ATOM     54  O   HIS A  17      -3.001  -7.714   0.888  1.00 75.24
ATOM     55  CB  HIS A  17      -6.009  -7.214  -0.285  1.00 54.32
ATOM     56  CG  HIS A  17      -7.055  -6.645   0.624  1.00 22.23
ATOM     57  CD2 HIS A  17      -7.165  -5.421   1.190  1.00  2.43
ATOM     58  ND1 HIS A  17      -8.152  -7.363   1.051  1.00 53.22
ATOM     59  CE1 HIS A  17      -8.893  -6.604   1.838  1.00  0.34
ATOM     60  NE2 HIS A  17      -8.315  -5.420   1.940  1.00 75.23
ATOM     61  H   HIS A  17      -5.354  -5.472  -2.014  1.00 72.53
ATOM     62  HA  HIS A  17      -4.667  -5.817   0.624  1.00 73.44
ATOM     63 2HB  HIS A  17      -6.403  -7.201  -1.291  1.00  1.21
ATOM     64 3HB  HIS A  17      -5.830  -8.237   0.013  1.00 43.41
ATOM     65  HD1 HIS A  17      -8.358  -8.290   0.811  1.00 54.15
ATOM     66  HD2 HIS A  17      -6.476  -4.596   1.074  1.00  2.42
ATOM     67  HE1 HIS A  17      -9.814  -6.900   2.318  1.00  3.25
ATOM     68  N   ALA A  18      -3.107  -7.922  -1.350  1.00 43.20
ATOM     69  CA  ALA A  18      -1.997  -8.864  -1.425  1.00 34.34
ATOM     70  C   ALA A  18      -0.766  -8.321  -0.708  1.00 41.42
ATOM     71  O   ALA A  18       0.037  -9.082  -0.169  1.00 52.22
ATOM     72  CB  ALA A  18      -1.669  -9.180  -2.876  1.00 54.35
ATOM     73  H   ALA A  18      -3.559  -7.650  -2.175  1.00 50.35
ATOM     74  HA  ALA A  18      -2.306  -9.781  -0.943  1.00 63.54
ATOM     75 1HB  ALA A  18      -1.830  -8.298  -3.480  1.00 72.45
ATOM     76 2HB  ALA A  18      -0.637  -9.486  -2.954  1.00 20.23
ATOM     77 3HB  ALA A  18      -2.309  -9.977  -3.225  1.00 12.33
ATOM     78  N   ALA A  19      -0.623  -6.999  -0.707  1.00 60.31
ATOM     79  CA  ALA A  19       0.510  -6.354  -0.056  1.00 22.03
ATOM     80  C   ALA A  19       0.621  -6.782   1.404  1.00 50.32
ATOM     81  O   ALA A  19       1.721  -6.894   1.946  1.00 74.43
ATOM     82  CB  ALA A  19       0.385  -4.841  -0.156  1.00 43.03
ATOM     83  H   ALA A  19      -1.296  -6.445  -1.154  1.00 35.43
ATOM     84  HA  ALA A  19       1.409  -6.652  -0.577  1.00 13.11
ATOM     85 1HB  ALA A  19      -0.199  -4.586  -1.029  1.00 23.11
ATOM     86 2HB  ALA A  19      -0.103  -4.461   0.728  1.00 14.32
ATOM     87 3HB  ALA A  19       1.369  -4.404  -0.241  1.00 11.20
ATOM     88  N   ASP A  20      -0.524  -7.018   2.035  1.00 40.24
ATOM     89  CA  ASP A  20      -0.555  -7.434   3.432  1.00 14.41
ATOM     90  C   ASP A  20       0.188  -8.752   3.624  1.00 50.14
ATOM     91  O   ASP A  20       0.840  -8.966   4.646  1.00 14.11
ATOM     92  CB  ASP A  20      -2.001  -7.574   3.912  1.00 23.41
ATOM     93  CG  ASP A  20      -2.297  -6.707   5.120  1.00 42.13
ATOM     94  OD1 ASP A  20      -1.378  -6.496   5.939  1.00 43.33
ATOM     95  OD2 ASP A  20      -3.447  -6.238   5.245  1.00 33.43
ATOM     96  H   ASP A  20      -1.369  -6.911   1.549  1.00 45.45
ATOM     97  HA  ASP A  20      -0.065  -6.670   4.016  1.00 24.04
ATOM     98 2HB  ASP A  20      -2.668  -7.286   3.113  1.00 34.31
ATOM     99 3HB  ASP A  20      -2.186  -8.605   4.177  1.00 54.20
ATOM    100  N   TYR A  21       0.085  -9.632   2.634  1.00 31.33
ATOM    101  CA  TYR A  21       0.744 -10.931   2.695  1.00 23.34
ATOM    102  C   TYR A  21       2.247 -10.770   2.901  1.00 45.03
ATOM    103  O   TYR A  21       2.879 -11.570   3.590  1.00 64.12
ATOM    104  CB  TYR A  21       0.475 -11.724   1.415  1.00  3.11
ATOM    105  CG  TYR A  21       1.733 -12.157   0.695  1.00 13.34
ATOM    106  CD1 TYR A  21       2.340 -11.329  -0.241  1.00 23.10
ATOM    107  CD2 TYR A  21       2.313 -13.393   0.951  1.00 75.12
ATOM    108  CE1 TYR A  21       3.489 -11.720  -0.902  1.00 32.44
ATOM    109  CE2 TYR A  21       3.462 -13.792   0.296  1.00 33.01
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ATOM    110  CZ  TYR A  21       4.046 -12.952  -0.629  1.00 71.43
ATOM    111  OH  TYR A  21       5.190 -13.347  -1.285  1.00 12.24
ATOM    112  H   TYR A  21      -0.449  -9.404   1.845  1.00 63.33
ATOM    113  HA  TYR A  21       0.334 -11.473   3.535  1.00 12.41
ATOM    114 2HB  TYR A  21      -0.087 -12.611   1.661  1.00 74.24
ATOM    115 3HB  TYR A  21      -0.102 -11.113   0.737  1.00 72.35
ATOM    116  HD1 TYR A  21       1.902 -10.365  -0.452  1.00 54.51
ATOM    117  HD2 TYR A  21       1.852 -14.048   1.676  1.00 60.51
ATOM    118  HE1 TYR A  21       3.947 -11.063  -1.626  1.00 72.21
ATOM    119  HE2 TYR A  21       3.898 -14.757   0.509  1.00 52.12
ATOM    120  HH  TYR A  21       5.938 -12.844  -0.953  1.00 73.20
ATOM    121  N   GLN A  22       2.812  -9.729   2.297  1.00  1.15
ATOM    122  CA  GLN A  22       4.241  -9.462   2.414  1.00 52.23
ATOM    123  C   GLN A  22       4.683  -9.490   3.873  1.00 60.20
ATOM    124  O   GLN A  22       5.783  -9.942   4.188  1.00  4.05
ATOM    125  CB  GLN A  22       4.580  -8.106   1.792  1.00 51.01
ATOM    126  CG  GLN A  22       6.022  -7.678   2.014  1.00 34.31
ATOM    127  CD  GLN A  22       7.013  -8.574   1.298  1.00 21.34
ATOM    128  NE2 GLN A  22       6.949  -8.587  -0.028  1.00 25.41
ATOM    129  OE1 GLN A  22       7.828  -9.248   1.930  1.00 15.35
ATOM    130  H   GLN A  22       2.255  -9.127   1.762  1.00 63.01
ATOM    131  HA  GLN A  22       4.767 -10.236   1.876  1.00  3.30
ATOM    132 2HB  GLN A  22       4.402  -8.156   0.728  1.00 35.42
ATOM    133 3HB  GLN A  22       3.934  -7.355   2.222  1.00 42.40
ATOM    134 2HG  GLN A  22       6.145  -6.669   1.650  1.00 14.00
ATOM    135 3HG  GLN A  22       6.232  -7.706   3.073  1.00  3.10
ATOM    136 1HE2 GLN A  22       6.276  -8.024  -0.464  1.00 74.10
ATOM    137 2HE2 GLN A  22       7.579  -9.157  -0.516  1.00 11.21
ATOM    138  N   GLN A  23       3.818  -9.004   4.758  1.00 63.43
ATOM    139  CA  GLN A  23       4.121  -8.973   6.184  1.00 63.53
ATOM    140  C   GLN A  23       3.945 -10.354   6.808  1.00 42.04
ATOM    141  O   GLN A  23       4.701 -10.745   7.698  1.00 60.50
ATOM    142  CB  GLN A  23       3.223  -7.961   6.896  1.00 51.44
ATOM    143  CG  GLN A  23       3.960  -6.714   7.360  1.00 74.55
ATOM    144  CD  GLN A  23       5.187  -7.037   8.189  1.00 41.13
ATOM    145  NE2 GLN A  23       6.296  -6.370   7.890  1.00 14.40
ATOM    146  OE1 GLN A  23       5.140  -7.877   9.088  1.00 11.41
ATOM    147  H   GLN A  23       2.957  -8.659   4.444  1.00  3.54
ATOM    148  HA  GLN A  23       5.151  -8.670   6.297  1.00 12.31
ATOM    149 2HB  GLN A  23       2.437  -7.658   6.221  1.00 55.24
ATOM    150 3HB  GLN A  23       2.782  -8.434   7.760  1.00 33.13
ATOM    151 2HG  GLN A  23       4.269  -6.150   6.492  1.00 73.50
ATOM    152 3HG  GLN A  23       3.287  -6.116   7.956  1.00 40.32
ATOM    153 1HE2 GLN A  23       6.259  -5.714   7.161  1.00 33.35
ATOM    154 2HE2 GLN A  23       7.103  -6.557   8.410  1.00 24.54
ATOM    155  N   LEU A  24       2.943 -11.088   6.336  1.00 43.54
ATOM    156  CA  LEU A  24       2.667 -12.425   6.848  1.00 63.45
ATOM    157  C   LEU A  24       3.926 -13.287   6.827  1.00  1.43
ATOM    158  O   LEU A  24       4.140 -14.112   7.715  1.00 12.15
ATOM    159  CB  LEU A  24       1.566 -13.092   6.021  1.00 42.00
ATOM    160  CG  LEU A  24       1.287 -14.562   6.336  1.00 13.24
ATOM    161  CD1 LEU A  24       0.596 -14.696   7.684  1.00 33.45
ATOM    162  CD2 LEU A  24       0.444 -15.192   5.238  1.00 74.24
ATOM    163  H   LEU A  24       2.375 -10.722   5.626  1.00  3.02
ATOM    164  HA  LEU A  24       2.330 -12.326   7.868  1.00 32.35
ATOM    165 2HB  LEU A  24       0.653 -12.540   6.181  1.00 32.21
ATOM    166 3HB  LEU A  24       1.848 -13.024   4.980  1.00 42.32
ATOM    167  HG  LEU A  24       2.225 -15.097   6.388  1.00 31.11
ATOM    168 1HD1 LEU A  24      -0.471 -14.774   7.536  1.00  3.31
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ATOM    169 2HD1 LEU A  24       0.813 -13.828   8.289  1.00 62.14
ATOM    170 3HD1 LEU A  24       0.955 -15.583   8.186  1.00  4.23
ATOM    171 1HD2 LEU A  24      -0.539 -15.420   5.624  1.00 23.12
ATOM    172 2HD2 LEU A  24       0.917 -16.102   4.898  1.00 32.43
ATOM    173 3HD2 LEU A  24       0.355 -14.502   4.412  1.00 73.44
ATOM    174  N   ARG A  25       4.757 -13.087   5.809  1.00 30.14
ATOM    175  CA  ARG A  25       5.995 -13.845   5.674  1.00  2.32
ATOM    176  C   ARG A  25       6.903 -13.623   6.881  1.00 74.22
ATOM    177  O   ARG A  25       7.453 -14.572   7.437  1.00 24.42
ATOM    178  CB  ARG A  25       6.727 -13.443   4.392  1.00 14.10
ATOM    179  CG  ARG A  25       7.034 -14.614   3.474  1.00 61.33
ATOM    180  CD  ARG A  25       6.282 -14.502   2.157  1.00 45.25
ATOM    181  NE  ARG A  25       6.902 -15.300   1.103  1.00 65.44
ATOM    182  CZ  ARG A  25       7.987 -14.922   0.436  1.00 64.20
ATOM    183  NH1 ARG A  25       8.569 -13.764   0.713  1.00 45.41
ATOM    184  NH2 ARG A  25       8.493 -15.704  -0.510  1.00 13.03
ATOM    185  H   ARG A  25       4.532 -12.415   5.133  1.00 73.04
ATOM    186  HA  ARG A  25       5.739 -14.892   5.619  1.00 61.12
ATOM    187 2HB  ARG A  25       6.115 -12.739   3.848  1.00 54.52
ATOM    188 3HB  ARG A  25       7.659 -12.967   4.658  1.00 74.42
ATOM    189 2HG  ARG A  25       8.095 -14.631   3.270  1.00 74.13
ATOM    190 3HG  ARG A  25       6.746 -15.531   3.966  1.00 15.11
ATOM    191 2HD  ARG A  25       5.269 -14.844   2.305  1.00 22.22
ATOM    192 3HD  ARG A  25       6.271 -13.466   1.852  1.00 61.15
ATOM    193  HE  ARG A  25       6.489 -16.160   0.882  1.00 74.33
ATOM    194 1HH1 ARG A  25       8.192 -13.173   1.426  1.00 55.03
ATOM    195 2HH1 ARG A  25       9.387 -13.482   0.210  1.00  1.33
ATOM    196 1HH2 ARG A  25       8.057 -16.578  -0.721  1.00 72.21
ATOM    197 2HH2 ARG A  25       9.309 -15.418  -1.011  1.00 31.52
ATOM    198  N   GLU A  26       7.053 -12.364   7.278  1.00 10.45
ATOM    199  CA  GLU A  26       7.895 -12.018   8.418  1.00 73.30
ATOM    200  C   GLU A  26       7.345 -12.627   9.705  1.00 62.53
ATOM    201  O   GLU A  26       8.100 -13.123  10.541  1.00  4.23
ATOM    202  CB  GLU A  26       7.997 -10.498   8.563  1.00 35.52
ATOM    203  CG  GLU A  26       9.357  -9.940   8.181  1.00 70.32
ATOM    204  CD  GLU A  26       9.256  -8.689   7.331  1.00 40.33
ATOM    205  OE1 GLU A  26       9.678  -7.614   7.806  1.00 13.44
ATOM    206  OE2 GLU A  26       8.756  -8.784   6.191  1.00 55.23
ATOM    207  H   GLU A  26       6.588 -11.650   6.794  1.00 34.20
ATOM    208  HA  GLU A  26       8.880 -12.420   8.236  1.00  1.12
ATOM    209 2HB  GLU A  26       7.251 -10.038   7.932  1.00 14.25
ATOM    210 3HB  GLU A  26       7.799 -10.234   9.591  1.00 15.44
ATOM    211 2HG  GLU A  26       9.900  -9.701   9.083  1.00 64.24
ATOM    212 3HG  GLU A  26       9.897 -10.693   7.625  1.00  3.41
ATOM    213  N   ARG A  27       6.025 -12.586   9.855  1.00 24.14
ATOM    214  CA  ARG A  27       5.374 -13.132  11.040  1.00  2.11
ATOM    215  C   ARG A  27       5.507 -14.651  11.082  1.00 21.42
ATOM    216  O   ARG A  27       5.597 -15.248  12.156  1.00 22.10
ATOM    217  CB  ARG A  27       3.896 -12.738  11.063  1.00  3.31
ATOM    218  CG  ARG A  27       3.383 -12.379  12.448  1.00  1.11
ATOM    219  CD  ARG A  27       2.731 -11.005  12.462  1.00 75.42
ATOM    220  NE  ARG A  27       2.206 -10.662  13.781  1.00 44.31
ATOM    221  CZ  ARG A  27       1.878  -9.426  14.142  1.00 23.22
ATOM    222  NH1 ARG A  27       2.019  -8.422  13.287  1.00 22.55
ATOM    223  NH2 ARG A  27       1.408  -9.193  15.361  1.00 53.13
ATOM    224  H   ARG A  27       5.476 -12.178   9.154  1.00 63.15
ATOM    225  HA  ARG A  27       5.862 -12.716  11.909  1.00 42.54
ATOM    226 2HB  ARG A  27       3.753 -11.883  10.418  1.00 24.10
ATOM    227 3HB  ARG A  27       3.310 -13.563  10.689  1.00 63.35
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ATOM    228 2HG  ARG A  27       2.654 -13.115  12.753  1.00 12.45
ATOM    229 3HG  ARG A  27       4.212 -12.381  13.140  1.00 33.44
ATOM    230 2HD  ARG A  27       3.466 -10.269  12.174  1.00 22.14
ATOM    231 3HD  ARG A  27       1.919 -11.000  11.749  1.00 21.35
ATOM    232  HE  ARG A  27       2.094 -11.388  14.428  1.00 23.32
ATOM    233 1HH1 ARG A  27       2.373  -8.596  12.368  1.00 14.54
ATOM    234 2HH1 ARG A  27       1.770  -7.493  13.562  1.00 62.33
ATOM    235 1HH2 ARG A  27       1.300  -9.947  16.008  1.00 71.12
ATOM    236 2HH2 ARG A  27       1.161  -8.263  15.632  1.00 43.03
ATOM    237  N   LEU A  28       5.518 -15.272   9.908  1.00 40.34
ATOM    238  CA  LEU A  28       5.639 -16.722   9.809  1.00 24.24
ATOM    239  C   LEU A  28       7.072 -17.168  10.081  1.00 25.41
ATOM    240  O   LEU A  28       7.313 -18.047  10.910  1.00 12.41
ATOM    241  CB  LEU A  28       5.199 -17.198   8.424  1.00 41.01
ATOM    242  CG  LEU A  28       3.690 -17.310   8.201  1.00 45.33
ATOM    243  CD1 LEU A  28       3.376 -17.408   6.716  1.00 64.21
ATOM    244  CD2 LEU A  28       3.128 -18.511   8.947  1.00  4.44
ATOM    245  H   LEU A  28       5.443 -14.743   9.086  1.00 11.04
ATOM    246  HA  LEU A  28       4.992 -17.160  10.554  1.00 15.12
ATOM    247 2HB  LEU A  28       5.590 -16.504   7.696  1.00  2.32
ATOM    248 3HB  LEU A  28       5.633 -18.174   8.257  1.00 15.11
ATOM    249  HG  LEU A  28       3.209 -16.421   8.585  1.00 43.33
ATOM    250 1HD1 LEU A  28       3.652 -16.486   6.228  1.00 54.41
ATOM    251 2HD1 LEU A  28       2.319 -17.585   6.583  1.00 44.14
ATOM    252 3HD1 LEU A  28       3.935 -18.226   6.283  1.00 11.45
ATOM    253 1HD2 LEU A  28       3.074 -18.285  10.002  1.00  3.22
ATOM    254 2HD2 LEU A  28       3.774 -19.364   8.795  1.00 53.44
ATOM    255 3HD2 LEU A  28       2.140 -18.735   8.576  1.00 52.03
ATOM    256  N   ILE A  29       8.020 -16.556   9.379  1.00 23.33
ATOM    257  CA  ILE A  29       9.430 -16.888   9.548  1.00 75.43
ATOM    258  C   ILE A  29       9.856 -16.754  11.006  1.00 53.34
ATOM    259  O   ILE A  29      10.684 -17.522  11.493  1.00 21.22
ATOM    260  CB  ILE A  29      10.328 -15.990   8.677  1.00 54.11
ATOM    261  CG1 ILE A  29      10.332 -16.486   7.229  1.00  1.35
ATOM    262  CG2 ILE A  29      11.742 -15.955   9.235  1.00 24.12
ATOM    263  CD1 ILE A  29      11.039 -15.551   6.273  1.00 54.02
ATOM    264  H   ILE A  29       7.766 -15.865   8.734  1.00 51.32
ATOM    265  HA  ILE A  29       9.570 -17.913   9.236  1.00 74.51
ATOM    266  HB  ILE A  29       9.931 -14.987   8.705  1.00 15.31
ATOM    267 2HG1 ILE A  29      10.828 -17.442   7.185  1.00 64.23
ATOM    268 3HG1 ILE A  29       9.312 -16.598   6.892  1.00 33.03
ATOM    269 1HG2 ILE A  29      11.970 -16.904   9.698  1.00 62.23
ATOM    270 2HG2 ILE A  29      12.441 -15.770   8.433  1.00 11.10
ATOM    271 3HG2 ILE A  29      11.821 -15.168   9.970  1.00 34.42
ATOM    272 1HD1 ILE A  29      10.918 -14.532   6.610  1.00 40.15
ATOM    273 2HD1 ILE A  29      12.089 -15.798   6.237  1.00 12.41
ATOM    274 3HD1 ILE A  29      10.611 -15.656   5.286  1.00 52.32
ATOM    275  N   GLN A  30       9.282 -15.773  11.696  1.00 62.41
ATOM    276  CA  GLN A  30       9.602 -15.539  13.099  1.00 23.20
ATOM    277  C   GLN A  30       8.907 -16.560  13.994  1.00 53.32
ATOM    278  O   GLN A  30       9.558 -17.290  14.740  1.00 72.44
ATOM    279  CB  GLN A  30       9.194 -14.123  13.508  1.00 51.24
ATOM    280  CG  GLN A  30      10.374 -13.203  13.777  1.00 20.32
ATOM    281  CD  GLN A  30      10.467 -12.783  15.231  1.00 74.50
ATOM    282  NE2 GLN A  30       9.680 -11.783  15.610  1.00 40.12
ATOM    283  OE1 GLN A  30      11.237 -13.352  16.005  1.00 32.05
ATOM    284  H   GLN A  30       8.629 -15.194  11.251  1.00 25.24
ATOM    285  HA  GLN A  30      10.670 -15.644  13.217  1.00 21.22
ATOM    286 2HB  GLN A  30       8.601 -13.690  12.716  1.00 13.43
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ATOM    287 3HB  GLN A  30       8.596 -14.178  14.406  1.00 65.24
ATOM    288 2HG  GLN A  30      11.284 -13.719  13.509  1.00  4.32
ATOM    289 3HG  GLN A  30      10.270 -12.318  13.168  1.00 42.24
ATOM    290 1HE2 GLN A  30       9.091 -11.378  14.938  1.00 31.34
ATOM    291 2HE2 GLN A  30       9.719 -11.492  16.544  1.00 52.33
ATOM    292  N   GLU A  31       7.580 -16.603  13.914  1.00 64.14
ATOM    293  CA  GLU A  31       6.797 -17.534  14.718  1.00 43.12
ATOM    294  C   GLU A  31       7.329 -18.957  14.575  1.00 23.03
ATOM    295  O   GLU A  31       7.599 -19.633  15.569  1.00 64.54
ATOM    296  CB  GLU A  31       5.325 -17.485  14.306  1.00 54.54
ATOM    297  CG  GLU A  31       4.371 -17.933  15.400  1.00 32.40
ATOM    298  CD  GLU A  31       4.159 -16.871  16.461  1.00 23.13
ATOM    299  OE1 GLU A  31       3.829 -15.724  16.094  1.00 74.11
ATOM    300  OE2 GLU A  31       4.324 -17.186  17.658  1.00 23.11
ATOM    301  H   GLU A  31       7.118 -15.995  13.300  1.00  1.10
ATOM    302  HA  GLU A  31       6.882 -17.233  15.751  1.00 45.52
ATOM    303 2HB  GLU A  31       5.074 -16.471  14.031  1.00 13.50
ATOM    304 3HB  GLU A  31       5.182 -18.126  13.448  1.00  0.52
ATOM    305 2HG  GLU A  31       3.416 -18.169  14.954  1.00 64.32
ATOM    306 3HG  GLU A  31       4.775 -18.817  15.872  1.00 73.23
ATOM    307  N   LEU A  32       7.477 -19.405  13.334  1.00 73.45
ATOM    308  CA  LEU A  32       7.976 -20.748  13.059  1.00 32.53
ATOM    309  C   LEU A  32       9.476 -20.836  13.322  1.00 72.12
ATOM    310  O   LEU A  32      10.024 -21.925  13.488  1.00  1.35
ATOM    311  CB  LEU A  32       7.676 -21.139  11.611  1.00 23.30
ATOM    312  CG  LEU A  32       6.262 -21.650  11.332  1.00 23.34
ATOM    313  CD1 LEU A  32       5.244 -20.539  11.533  1.00 11.12
ATOM    314  CD2 LEU A  32       6.167 -22.215   9.922  1.00  4.24
ATOM    315  H   LEU A  32       7.245 -18.820  12.583  1.00 71.42
ATOM    316  HA  LEU A  32       7.466 -21.433  13.721  1.00  1.21
ATOM    317 2HB  LEU A  32       7.841 -20.270  10.993  1.00 22.02
ATOM    318 3HB  LEU A  32       8.372 -21.917  11.329  1.00 51.24
ATOM    319  HG  LEU A  32       6.030 -22.445  12.028  1.00 11.11
ATOM    320 1HD1 LEU A  32       4.560 -20.522  10.698  1.00 21.22
ATOM    321 2HD1 LEU A  32       5.755 -19.590  11.599  1.00  1.11
ATOM    322 3HD1 LEU A  32       4.694 -20.715  12.446  1.00 21.33
ATOM    323 1HD2 LEU A  32       7.156 -22.278   9.493  1.00  5.02
ATOM    324 2HD2 LEU A  32       5.553 -21.566   9.316  1.00 54.24
ATOM    325 3HD2 LEU A  32       5.726 -23.200   9.958  1.00  4.20
ATOM    326  N   ASN A  33      10.133 -19.682  13.359  1.00  2.42
ATOM    327  CA  ASN A  33      11.570 -19.628  13.603  1.00  0.24
ATOM    328  C   ASN A  33      12.339 -20.310  12.476  1.00 23.34
ATOM    329  O   ASN A  33      13.376 -20.934  12.707  1.00 60.43
ATOM    330  CB  ASN A  33      11.906 -20.291  14.940  1.00 23.44
ATOM    331  CG  ASN A  33      13.236 -19.824  15.499  1.00 25.33
ATOM    332  ND2 ASN A  33      13.459 -20.076  16.784  1.00  2.41
ATOM    333  OD1 ASN A  33      14.054 -19.245  14.784  1.00 12.31
ATOM    334  H   ASN A  33       9.641 -18.846  13.219  1.00 51.11
ATOM    335  HA  ASN A  33      11.860 -18.589  13.644  1.00  5.13
ATOM    336 2HB  ASN A  33      11.134 -20.054  15.657  1.00 34.53
ATOM    337 3HB  ASN A  33      11.949 -21.361  14.804  1.00 24.50
ATOM    338 1HD2 ASN A  33      12.763 -20.542  17.293  1.00 52.25
ATOM    339 2HD2 ASN A  33      14.311 -19.784  17.171  1.00 12.05
ATOM    340  N   LEU A  34      11.825 -20.187  11.258  1.00 45.13
ATOM    341  CA  LEU A  34      12.464 -20.791  10.093  1.00 10.04
ATOM    342  C   LEU A  34      13.265 -19.754   9.312  1.00 21.24
ATOM    343  O   LEU A  34      13.431 -18.618   9.757  1.00 52.54
ATOM    344  CB  LEU A  34      11.412 -21.430   9.185  1.00 44.03
ATOM    345  CG  LEU A  34      11.473 -22.952   9.055  1.00 32.44
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ATOM    346  CD1 LEU A  34      10.381 -23.453   8.122  1.00  2.42
ATOM    347  CD2 LEU A  34      12.843 -23.392   8.560  1.00  0.32
ATOM    348  H   LEU A  34      10.997 -19.678  11.137  1.00 44.33
ATOM    349  HA  LEU A  34      13.138 -21.558  10.446  1.00 55.03
ATOM    350 2HB  LEU A  34      10.439 -21.170   9.571  1.00  2.43
ATOM    351 3HB  LEU A  34      11.530 -21.008   8.197  1.00 60.04
ATOM    352  HG  LEU A  34      11.309 -23.397  10.028  1.00 43.33
ATOM    353 1HD1 LEU A  34      10.450 -22.935   7.178  1.00 42.15
ATOM    354 2HD1 LEU A  34       9.415 -23.265   8.566  1.00 74.11
ATOM    355 3HD1 LEU A  34      10.503 -24.514   7.962  1.00 43.12
ATOM    356 1HD2 LEU A  34      12.854 -24.465   8.438  1.00  1.34
ATOM    357 2HD2 LEU A  34      13.595 -23.103   9.280  1.00 23.53
ATOM    358 3HD2 LEU A  34      13.052 -22.919   7.612  1.00 35.10
ATOM    359  N   THR A  35      13.759 -20.153   8.144  1.00  3.43
ATOM    360  CA  THR A  35      14.542 -19.258   7.301  1.00 71.45
ATOM    361  C   THR A  35      13.724 -18.770   6.110  1.00  3.13
ATOM    362  O   THR A  35      12.724 -19.374   5.724  1.00 73.23
ATOM    363  CB  THR A  35      15.819 -19.948   6.784  1.00 75.05
ATOM    364  CG2 THR A  35      16.968 -19.764   7.763  1.00 35.24
ATOM    365  OG1 THR A  35      15.574 -21.345   6.584  1.00 42.34
ATOM    366  H   THR A  35      13.593 -21.071   7.845  1.00 42.35
ATOM    367  HA  THR A  35      14.834 -18.407   7.898  1.00 64.11
ATOM    368  HB  THR A  35      16.095 -19.500   5.840  1.00 55.23
ATOM    369  HG1 THR A  35      16.199 -21.690   5.941  1.00 74.20
ATOM    370 1HG2 THR A  35      17.085 -20.661   8.353  1.00 31.22
ATOM    371 2HG2 THR A  35      16.755 -18.930   8.415  1.00 12.20
ATOM    372 3HG2 THR A  35      17.878 -19.571   7.217  1.00 25.41
ATOM    373  N   PRO A  36      14.158 -17.650   5.513  1.00  1.01
ATOM    374  CA  PRO A  36      13.481 -17.056   4.357  1.00 72.25
ATOM    375  C   PRO A  36      13.633 -17.903   3.098  1.00 61.32
ATOM    376  O   PRO A  36      12.771 -17.887   2.220  1.00 14.52
ATOM    377  CB  PRO A  36      14.188 -15.710   4.184  1.00 42.21
ATOM    378  CG  PRO A  36      15.536 -15.910   4.785  1.00 24.33
ATOM    379  CD  PRO A  36      15.344 -16.877   5.921  1.00 74.34
ATOM    380  HA  PRO A  36      12.432 -16.891   4.553  1.00 14.10
ATOM    381 2HB  PRO A  36      14.256 -15.468   3.132  1.00 33.14
ATOM    382 3HB  PRO A  36      13.636 -14.940   4.701  1.00 11.12
ATOM    383 2HG  PRO A  36      16.209 -16.325   4.050  1.00 53.22
ATOM    384 3HG  PRO A  36      15.916 -14.970   5.155  1.00  4.54
ATOM    385 2HD  PRO A  36      16.206 -17.519   6.021  1.00 45.15
ATOM    386 3HD  PRO A  36      15.158 -16.345   6.842  1.00 20.31
ATOM    387  N   GLN A  37      14.735 -18.643   3.017  1.00 13.42
ATOM    388  CA  GLN A  37      14.999 -19.496   1.865  1.00 53.02
ATOM    389  C   GLN A  37      14.262 -20.825   1.992  1.00 72.25
ATOM    390  O   GLN A  37      13.857 -21.418   0.992  1.00 14.10
ATOM    391  CB  GLN A  37      16.501 -19.744   1.721  1.00 63.11
ATOM    392  CG  GLN A  37      17.161 -18.880   0.658  1.00 25.34
ATOM    393  CD  GLN A  37      18.675 -18.956   0.703  1.00 51.35
ATOM    394  NE2 GLN A  37      19.333 -17.866   0.325  1.00 65.34
ATOM    395  OE1 GLN A  37      19.246 -19.982   1.072  1.00  4.11
ATOM    396  H   GLN A  37      15.385 -18.613   3.749  1.00 33.12
ATOM    397  HA  GLN A  37      14.642 -18.983   0.984  1.00 30.54
ATOM    398 2HB  GLN A  37      16.980 -19.542   2.667  1.00 12.24
ATOM    399 3HB  GLN A  37      16.660 -20.780   1.461  1.00 74.33
ATOM    400 2HG  GLN A  37      16.829 -19.211  -0.314  1.00 74.13
ATOM    401 3HG  GLN A  37      16.862 -17.854   0.810  1.00 11.13
ATOM    402 1HE2 GLN A  37      18.812 -17.085   0.044  1.00 51.15
ATOM    403 2HE2 GLN A  37      20.312 -17.887   0.344  1.00  1.11
ATOM    404  N   GLN A  38      14.093 -21.287   3.226  1.00 34.03
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ATOM    405  CA  GLN A  38      13.405 -22.547   3.482  1.00 21.25
ATOM    406  C   GLN A  38      11.898 -22.389   3.313  1.00 73.21
ATOM    407  O   GLN A  38      11.281 -23.063   2.486  1.00  3.12
ATOM    408  CB  GLN A  38      13.722 -23.048   4.893  1.00 40.32
ATOM    409  CG  GLN A  38      12.815 -24.177   5.356  1.00 45.24
ATOM    410  CD  GLN A  38      12.724 -25.303   4.345  1.00 30.21
ATOM    411  NE2 GLN A  38      13.874 -25.782   3.886  1.00 23.34
ATOM    412  OE1 GLN A  38      11.631 -25.738   3.980  1.00 23.34
ATOM    413  H   GLN A  38      14.438 -20.769   3.982  1.00 43.20
ATOM    414  HA  GLN A  38      13.762 -23.271   2.765  1.00 15.22
ATOM    415 2HB  GLN A  38      14.742 -23.401   4.916  1.00 60.01
ATOM    416 3HB  GLN A  38      13.618 -22.225   5.585  1.00 24.54
ATOM    417 2HG  GLN A  38      13.202 -24.576   6.282  1.00 44.34
ATOM    418 3HG  GLN A  38      11.825 -23.780   5.522  1.00 72.31
ATOM    419 1HE2 GLN A  38      14.707 -25.388   4.223  1.00 54.42
ATOM    420 2HE2 GLN A  38      13.845 -26.511   3.233  1.00 13.11
ATOM    421  N   LEU A  39      11.309 -21.496   4.101  1.00 43.14
ATOM    422  CA  LEU A  39       9.873 -21.249   4.038  1.00 32.21
ATOM    423  C   LEU A  39       9.525 -20.355   2.852  1.00 31.31
ATOM    424  O   LEU A  39       9.146 -19.196   3.025  1.00 61.31
ATOM    425  CB  LEU A  39       9.389 -20.603   5.338  1.00 64.04
ATOM    426  CG  LEU A  39       7.917 -20.819   5.687  1.00 15.20
ATOM    427  CD1 LEU A  39       7.731 -20.897   7.194  1.00  4.25
ATOM    428  CD2 LEU A  39       7.060 -19.706   5.100  1.00 65.24
ATOM    429  H   LEU A  39      11.853 -20.990   4.739  1.00 14.44
ATOM    430  HA  LEU A  39       9.378 -22.201   3.913  1.00 25.12
ATOM    431 2HB  LEU A  39       9.983 -21.002   6.146  1.00 74.22
ATOM    432 3HB  LEU A  39       9.560 -19.539   5.260  1.00 53.42
ATOM    433  HG  LEU A  39       7.586 -21.756   5.262  1.00 72.52
ATOM    434 1HD1 LEU A  39       8.028 -21.874   7.543  1.00 33.34
ATOM    435 2HD1 LEU A  39       6.693 -20.727   7.439  1.00 43.51
ATOM    436 3HD1 LEU A  39       8.341 -20.143   7.671  1.00 23.43
ATOM    437 1HD2 LEU A  39       6.235 -19.499   5.764  1.00 10.23
ATOM    438 2HD2 LEU A  39       6.679 -20.016   4.137  1.00 14.14
ATOM    439 3HD2 LEU A  39       7.660 -18.816   4.980  1.00 13.13
ATOM    440  N   HIS A  40       9.654 -20.902   1.647  1.00 30.24
ATOM    441  CA  HIS A  40       9.350 -20.155   0.432  1.00  4.01
ATOM    442  C   HIS A  40       7.843 -20.022   0.238  1.00 32.42
ATOM    443  O   HIS A  40       7.063 -20.749   0.853  1.00 71.24
ATOM    444  CB  HIS A  40       9.974 -20.842  -0.783  1.00 42.42
ATOM    445  CG  HIS A  40      10.010 -19.978  -2.006  1.00 50.13
ATOM    446  CD2 HIS A  40      10.472 -18.719  -2.188  1.00  5.22
ATOM    447  ND1 HIS A  40       9.528 -20.388  -3.231  1.00 41.15
ATOM    448  CE1 HIS A  40       9.694 -19.419  -4.114  1.00 62.11
ATOM    449  NE2 HIS A  40      10.265 -18.395  -3.506  1.00 11.20
ATOM    450  H   HIS A  40       9.960 -21.830   1.574  1.00  1.03
ATOM    451  HA  HIS A  40       9.776 -19.168   0.535  1.00 75.13
ATOM    452 2HB  HIS A  40      10.990 -21.124  -0.547  1.00 53.41
ATOM    453 3HB  HIS A  40       9.405 -21.729  -1.019  1.00 73.02
ATOM    454  HD1 HIS A  40       9.126 -21.260  -3.426  1.00 11.25
ATOM    455  HD2 HIS A  40      10.922 -18.086  -1.436  1.00  2.43
ATOM    456  HE1 HIS A  40       9.411 -19.457  -5.155  1.00 44.14
ATOM    457  N   GLU A  41       7.441 -19.089  -0.619  1.00 70.21
ATOM    458  CA  GLU A  41       6.027 -18.861  -0.892  1.00 33.43
ATOM    459  C   GLU A  41       5.338 -20.156  -1.314  1.00 24.34
ATOM    460  O   GLU A  41       4.177 -20.390  -0.981  1.00 60.12
ATOM    461  CB  GLU A  41       5.859 -17.803  -1.984  1.00  1.45
ATOM    462  CG  GLU A  41       6.376 -18.243  -3.343  1.00  4.23
ATOM    463  CD  GLU A  41       6.262 -17.153  -4.391  1.00 65.11
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ATOM    464  OE1 GLU A  41       5.159 -16.586  -4.539  1.00 65.33
ATOM    465  OE2 GLU A  41       7.275 -16.867  -5.063  1.00 63.31
ATOM    466  H   GLU A  41       8.111 -18.541  -1.078  1.00 70.24
ATOM    467  HA  GLU A  41       5.567 -18.503   0.017  1.00 23.52
ATOM    468 2HB  GLU A  41       4.810 -17.565  -2.080  1.00 11.02
ATOM    469 3HB  GLU A  41       6.395 -16.912  -1.689  1.00 73.13
ATOM    470 2HG  GLU A  41       7.415 -18.520  -3.246  1.00 23.22
ATOM    471 3HG  GLU A  41       5.805 -19.099  -3.671  1.00  5.10
ATOM    472  N   GLU A  42       6.064 -20.993  -2.048  1.00 64.33
ATOM    473  CA  GLU A  42       5.523 -22.264  -2.517  1.00  1.32
ATOM    474  C   GLU A  42       5.917 -23.402  -1.579  1.00 54.43
ATOM    475  O   GLU A  42       6.008 -24.557  -1.993  1.00 32.41
ATOM    476  CB  GLU A  42       6.017 -22.562  -3.934  1.00 74.01
ATOM    477  CG  GLU A  42       5.193 -21.890  -5.020  1.00 34.34
ATOM    478  CD  GLU A  42       5.478 -22.451  -6.399  1.00 53.45
ATOM    479  OE1 GLU A  42       5.848 -21.662  -7.294  1.00 63.13
ATOM    480  OE2 GLU A  42       5.330 -23.677  -6.585  1.00  3.43
ATOM    481  H   GLU A  42       6.985 -20.751  -2.281  1.00 12.31
ATOM    482  HA  GLU A  42       4.447 -22.181  -2.531  1.00 11.34
ATOM    483 2HB  GLU A  42       7.039 -22.224  -4.025  1.00 75.41
ATOM    484 3HB  GLU A  42       5.984 -23.629  -4.096  1.00 23.42
ATOM    485 2HG  GLU A  42       4.145 -22.033  -4.799  1.00 63.54
ATOM    486 3HG  GLU A  42       5.417 -20.834  -5.023  1.00  3.24
ATOM    487  N   SER A  43       6.149 -23.065  -0.315  1.00 21.14
ATOM    488  CA  SER A  43       6.537 -24.057   0.681  1.00  2.14
ATOM    489  C   SER A  43       5.414 -24.283   1.689  1.00 61.31
ATOM    490  O   SER A  43       5.043 -23.378   2.435  1.00 25.43
ATOM    491  CB  SER A  43       7.807 -23.611   1.408  1.00  4.21
ATOM    492  OG  SER A  43       8.784 -24.638   1.406  1.00 54.12
ATOM    493  H   SER A  43       6.060 -22.127  -0.046  1.00 12.41
ATOM    494  HA  SER A  43       6.735 -24.985   0.166  1.00 53.23
ATOM    495 2HB  SER A  43       8.215 -22.742   0.914  1.00 23.14
ATOM    496 3HB  SER A  43       7.565 -23.363   2.431  1.00 11.15
ATOM    497  HG  SER A  43       8.987 -24.885   0.501  1.00 54.04
ATOM    498  N   ASN A  44       4.877 -25.499   1.703  1.00 14.21
ATOM    499  CA  ASN A  44       3.795 -25.846   2.618  1.00 40.50
ATOM    500  C   ASN A  44       4.196 -25.569   4.064  1.00 52.22
ATOM    501  O   ASN A  44       5.285 -25.944   4.501  1.00 52.25
ATOM    502  CB  ASN A  44       3.414 -27.318   2.456  1.00 62.54
ATOM    503  CG  ASN A  44       2.235 -27.511   1.521  1.00 25.21
ATOM    504  ND2 ASN A  44       2.326 -28.512   0.653  1.00 21.44
ATOM    505  OD1 ASN A  44       1.255 -26.769   1.579  1.00  2.22
ATOM    506  H   ASN A  44       5.215 -26.179   1.084  1.00 52.34
ATOM    507  HA  ASN A  44       2.942 -25.233   2.370  1.00 53.25
ATOM    508 2HB  ASN A  44       4.259 -27.860   2.055  1.00 73.23
ATOM    509 3HB  ASN A  44       3.156 -27.726   3.421  1.00 34.31
ATOM    510 1HD2 ASN A  44       3.137 -29.063   0.664  1.00 31.14
ATOM    511 2HD2 ASN A  44       1.579 -28.659   0.037  1.00 35.31
ATOM    512  N   LEU A  45       3.309 -24.911   4.802  1.00 12.11
ATOM    513  CA  LEU A  45       3.569 -24.584   6.200  1.00 72.01
ATOM    514  C   LEU A  45       3.432 -25.820   7.083  1.00 70.32
ATOM    515  O   LEU A  45       4.233 -26.036   7.993  1.00 34.50
ATOM    516  CB  LEU A  45       2.607 -23.494   6.677  1.00 43.15
ATOM    517  CG  LEU A  45       2.623 -22.189   5.879  1.00 62.40
ATOM    518  CD1 LEU A  45       1.632 -21.195   6.463  1.00 53.23
ATOM    519  CD2 LEU A  45       4.024 -21.596   5.854  1.00 24.43
ATOM    520  H   LEU A  45       2.459 -24.638   4.399  1.00 73.31
ATOM    521  HA  LEU A  45       4.581 -24.216   6.271  1.00  4.10
ATOM    522 2HB  LEU A  45       1.606 -23.895   6.635  1.00 43.34
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ATOM    523 3HB  LEU A  45       2.857 -23.259   7.702  1.00 73.33
ATOM    524  HG  LEU A  45       2.328 -22.395   4.859  1.00 11.32
ATOM    525 1HD1 LEU A  45       2.063 -20.727   7.335  1.00 54.34
ATOM    526 2HD1 LEU A  45       0.726 -21.712   6.742  1.00 13.22
ATOM    527 3HD1 LEU A  45       1.402 -20.440   5.724  1.00 30.45
ATOM    528 1HD2 LEU A  45       4.601 -22.002   6.673  1.00 54.41
ATOM    529 2HD2 LEU A  45       3.962 -20.522   5.955  1.00 64.31
ATOM    530 3HD2 LEU A  45       4.504 -21.844   4.919  1.00 74.01
ATOM    531  N   ILE A  46       2.414 -26.629   6.806  1.00  5.33
ATOM    532  CA  ILE A  46       2.175 -27.845   7.573  1.00  5.13
ATOM    533  C   ILE A  46       3.440 -28.692   7.669  1.00 72.02
ATOM    534  O   ILE A  46       3.686 -29.344   8.683  1.00 72.30
ATOM    535  CB  ILE A  46       1.050 -28.691   6.950  1.00 33.43
ATOM    536  CG1 ILE A  46      -0.257 -27.896   6.915  1.00  3.35
ATOM    537  CG2 ILE A  46       0.867 -29.986   7.729  1.00 44.31
ATOM    538  CD1 ILE A  46      -1.285 -28.463   5.962  1.00 23.51
ATOM    539  H   ILE A  46       1.811 -26.402   6.069  1.00 72.54
ATOM    540  HA  ILE A  46       1.872 -27.556   8.569  1.00 23.15
ATOM    541  HB  ILE A  46       1.336 -28.944   5.941  1.00 42.01
ATOM    542 2HG1 ILE A  46      -0.691 -27.885   7.903  1.00 60.14
ATOM    543 3HG1 ILE A  46      -0.044 -26.882   6.609  1.00  4.45
ATOM    544 1HG2 ILE A  46       1.183 -30.820   7.119  1.00  0.35
ATOM    545 2HG2 ILE A  46       1.465 -29.952   8.628  1.00 54.33
ATOM    546 3HG2 ILE A  46      -0.173 -30.105   7.991  1.00  1.24
ATOM    547 1HD1 ILE A  46      -1.636 -29.414   6.335  1.00 21.31
ATOM    548 2HD1 ILE A  46      -2.115 -27.779   5.878  1.00 35.43
ATOM    549 3HD1 ILE A  46      -0.835 -28.604   4.990  1.00 42.35
ATOM    550  N   GLN A  47       4.238 -28.675   6.607  1.00 64.25
ATOM    551  CA  GLN A  47       5.479 -29.441   6.572  1.00 75.34
ATOM    552  C   GLN A  47       6.601 -28.693   7.284  1.00 72.43
ATOM    553  O   GLN A  47       7.463 -29.303   7.915  1.00 63.20
ATOM    554  CB  GLN A  47       5.882 -29.733   5.125  1.00 32.32
ATOM    555  CG  GLN A  47       5.995 -31.217   4.813  1.00 44.42
ATOM    556  CD  GLN A  47       7.421 -31.725   4.904  1.00 12.30
ATOM    557  NE2 GLN A  47       8.180 -31.556   3.828  1.00 52.34
ATOM    558  OE1 GLN A  47       7.836 -32.263   5.931  1.00 74.53
ATOM    559  H   GLN A  47       3.988 -28.136   5.829  1.00 53.34
ATOM    560  HA  GLN A  47       5.305 -30.376   7.083  1.00 60.12
ATOM    561 2HB  GLN A  47       5.144 -29.303   4.464  1.00 32.45
ATOM    562 3HB  GLN A  47       6.839 -29.273   4.931  1.00 41.50
ATOM    563 2HG  GLN A  47       5.388 -31.767   5.516  1.00 61.21
ATOM    564 3HG  GLN A  47       5.630 -31.389   3.811  1.00 23.22
ATOM    565 1HE2 GLN A  47       7.782 -31.117   3.046  1.00 44.11
ATOM    566 2HE2 GLN A  47       9.105 -31.874   3.859  1.00  2.22
ATOM    567  N   ALA A  48       6.583 -27.369   7.177  1.00  0.21
ATOM    568  CA  ALA A  48       7.598 -26.538   7.812  1.00  1.43
ATOM    569  C   ALA A  48       7.534 -26.658   9.331  1.00  3.51
ATOM    570  O   ALA A  48       8.466 -27.153   9.964  1.00 13.21
ATOM    571  CB  ALA A  48       7.433 -25.086   7.388  1.00 14.21
ATOM    572  H   ALA A  48       5.869 -26.940   6.660  1.00 24.42
ATOM    573  HA  ALA A  48       8.567 -26.877   7.475  1.00 72.42
ATOM    574 1HB  ALA A  48       6.382 -24.867   7.260  1.00  4.43
ATOM    575 2HB  ALA A  48       7.846 -24.440   8.148  1.00 11.40
ATOM    576 3HB  ALA A  48       7.951 -24.922   6.455  1.00 33.41
ATOM    577  N   GLY A  49       6.428 -26.200   9.911  1.00 44.15
ATOM    578  CA  GLY A  49       6.265 -26.264  11.351  1.00 35.50
ATOM    579  C   GLY A  49       4.997 -25.579  11.822  1.00 41.14
ATOM    580  O   GLY A  49       4.966 -24.988  12.902  1.00 23.10
ATOM    581  H   GLY A  49       5.718 -25.815   9.355  1.00 22.12
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ATOM    582 2HA  GLY A  49       6.234 -27.301  11.653  1.00 43.32
ATOM    583 3HA  GLY A  49       7.113 -25.788  11.820  1.00 11.10
ATOM    584  N   LEU A  50       3.949 -25.655  11.009  1.00 33.24
ATOM    585  CA  LEU A  50       2.672 -25.035  11.348  1.00 61.53
ATOM    586  C   LEU A  50       1.579 -26.088  11.498  1.00 74.22
ATOM    587  O   LEU A  50       1.087 -26.633  10.509  1.00 42.41
ATOM    588  CB  LEU A  50       2.275 -24.021  10.274  1.00  1.31
ATOM    589  CG  LEU A  50       1.477 -22.809  10.758  1.00 71.51
ATOM    590  CD1 LEU A  50       2.179 -21.518  10.370  1.00 44.33
ATOM    591  CD2 LEU A  50       0.064 -22.841  10.193  1.00 64.33
ATOM    592  H   LEU A  50       4.034 -26.140  10.162  1.00 11.52
ATOM    593  HA  LEU A  50       2.793 -24.522  12.290  1.00 74.00
ATOM    594 2HB  LEU A  50       3.180 -23.657   9.812  1.00 20.03
ATOM    595 3HB  LEU A  50       1.679 -24.538   9.536  1.00 52.12
ATOM    596  HG  LEU A  50       1.407 -22.840  11.837  1.00 43.34
ATOM    597 1HD1 LEU A  50       2.735 -21.142  11.215  1.00 12.15
ATOM    598 2HD1 LEU A  50       1.445 -20.786  10.067  1.00  2.20
ATOM    599 3HD1 LEU A  50       2.856 -21.709   9.550  1.00 41.54
ATOM    600 1HD2 LEU A  50      -0.341 -23.837  10.294  1.00 20.21
ATOM    601 2HD2 LEU A  50       0.089 -22.567   9.148  1.00 73.42
ATOM    602 3HD2 LEU A  50      -0.556 -22.143  10.734  1.00  2.23
ATOM    603  N   ASP A  51       1.201 -26.368  12.740  1.00 30.32
ATOM    604  CA  ASP A  51       0.163 -27.353  13.020  1.00 32.41
ATOM    605  C   ASP A  51      -1.188 -26.886  12.486  1.00 22.14
ATOM    606  O   ASP A  51      -1.305 -25.838  12.416  1.00 54.22
ATOM    607  CB  ASP A  51       0.069 -27.613  14.524  1.00 35.24
ATOM    608  CG  ASP A  51       0.423 -29.041  14.889  1.00 64.43
ATOM    609  OD1 ASP A  51      -0.505 -29.838  15.141  1.00  0.13
ATOM    610  OD2 ASP A  51       1.630 -29.363  14.920  1.00 15.13
ATOM    611  H   ASP A  51       1.630 -25.901  13.487  1.00  4.32
ATOM    612  HA  ASP A  51       0.434 -28.272  12.522  1.00 41.11
ATOM    613 2HB  ASP A  51       0.748 -26.950  15.041  1.00 73.41
ATOM    614 3HB  ASP A  51      -0.941 -27.416  14.854  1.00 22.45
ATOM    615  N   SRP A  52      -2.069 -27.855  12.168  1.00 42.52
ATOM    616  CA  SRP A  52      -3.392 -27.499  11.648  1.00 65.44
ATOM    617  C   SRP A  52      -4.005 -26.434  12.518  1.00  0.14
ATOM    618  O   SRP A  52      -4.571 -25.502  11.945  1.00 31.55
ATOM    619  CB  SRP A  52      -4.289 -28.738  11.648  1.00 20.14
ATOM    620  OG  SRP A  52      -5.035 -28.785  12.866  1.00 14.12
ATOM    621  CJ  SRP A  52      -7.895 -28.111  13.366  1.00 75.50
ATOM    622  CK  SRP A  52      -9.141 -27.274  13.069  1.00 12.53
ATOM    623  CL1 SRP A  52      -9.779 -27.753  11.764  1.00 11.04
ATOM    624  CL2 SRP A  52      -8.745 -25.802  12.933  1.00 32.33
ATOM    625  CL3 SRP A  52     -10.144 -27.428  14.215  1.00 22.51
ATOM    626  CM  SRP A  52     -11.142 -26.300  14.165  1.00 62.01
ATOM    627  OM  SRP A  52      -9.450 -27.397  15.463  1.00  1.42
ATOM    628  NN  SRP A  52     -12.285 -26.442  13.465  1.00  2.42
ATOM    629  ON  SRP A  52     -10.916 -25.265  14.756  1.00 51.34
ATOM    630  P   SRP A  52      -6.278 -29.778  12.613  1.00 23.21
ATOM    631  O1P SRP A  52      -6.567 -30.626  13.951  1.00 52.33
ATOM    632  O2P SRP A  52      -5.952 -30.703  11.504  1.00 23.14
ATOM    633  O3P SRP A  52      -7.582 -28.918  12.228  1.00 34.13
ATOM    634  CO  SRP A  52     -13.212 -25.314  13.343  1.00 32.35
ATOM    635  CP  SRP A  52     -13.623 -25.148  11.878  1.00  1.22
ATOM    636  CQ  SRP A  52     -14.086 -23.787  11.426  1.00 23.22
ATOM    637  CS  SRP A  52     -14.050 -21.932   9.846  1.00 75.33
ATOM    638  CT  SRP A  52     -13.428 -20.858  10.739  1.00 25.23
ATOM    639  NR  SRP A  52     -13.601 -23.255  10.286  1.00 21.13
ATOM    640  OR  SRP A  52     -14.894 -23.170  12.087  1.00 24.43
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ATOM    641  SU  SRP A  52     -14.625 -19.521  11.001  1.00 12.42
ATOM    642  H   SRP A  52      -1.828 -28.787  12.283  1.00 22.35
ATOM    643  HN  SRP A  52     -12.493 -27.288  13.042  1.00 24.41
ATOM    644  HA  SRP A  52      -3.292 -27.123  10.629  1.00 20.30
ATOM    645 2HB  SRP A  52      -4.975 -28.690  10.803  1.00 52.44
ATOM    646 3HB  SRP A  52      -3.673 -29.634  11.565  1.00  5.41
ATOM    647 2HJ  SRP A  52      -8.086 -28.755  14.226  1.00 51.45
ATOM    648 3HJ  SRP A  52      -7.057 -27.451  13.585  1.00 11.21
ATOM    649 1HL1 SRP A  52     -10.622 -27.109  11.514  1.00 62.42
ATOM    650 2HL1 SRP A  52      -9.041 -27.713  10.963  1.00  2.53
ATOM    651 3HL1 SRP A  52     -10.128 -28.778  11.885  1.00 23.02
ATOM    652 1HL2 SRP A  52      -8.435 -25.418  13.905  1.00 42.43
ATOM    653 2HL2 SRP A  52      -7.921 -25.712  12.226  1.00  3.44
ATOM    654 3HL2 SRP A  52      -9.598 -25.228  12.571  1.00 12.21
ATOM    655  HL3 SRP A  52     -10.666 -28.380  14.114  1.00 70.50
ATOM    656  HM  SRP A  52      -9.002 -26.540  15.512  1.00 53.21
ATOM    657 2HO  SRP A  52     -14.098 -25.505  13.949  1.00 43.23
ATOM    658 3HO  SRP A  52     -12.724 -24.403  13.689  1.00 15.44
ATOM    659 2HP  SRP A  52     -12.666 -25.381  11.411  1.00 32.11
ATOM    660 3HP  SRP A  52     -14.360 -25.897  11.589  1.00 32.43
ATOM    661  HR  SRP A  52     -12.954 -23.748   9.757  1.00 31.23
ATOM    662 2HS  SRP A  52     -13.743 -21.769   8.812  1.00 21.33
ATOM    663 3HS  SRP A  52     -15.137 -21.877   9.914  1.00 23.11
ATOM    664 2HT  SRP A  52     -13.161 -21.294  11.707  1.00 11.03
ATOM    665 3HT  SRP A  52     -12.536 -20.458  10.258  1.00  5.43
ATOM    666  HU  SRP A  52     -15.581 -19.890  10.130  1.00  4.51
ATOM    667  N   ILE A  53      -3.920 -26.526  13.841  1.00 34.12
ATOM    668  CA  ILE A  53      -4.500 -25.514  14.716  1.00 72.25
ATOM    669  C   ILE A  53      -4.062 -24.113  14.301  1.00 34.53
ATOM    670  O   ILE A  53      -4.878 -23.195  14.223  1.00 53.14
ATOM    671  CB  ILE A  53      -4.107 -25.749  16.186  1.00 13.21
ATOM    672  CG1 ILE A  53      -4.779 -27.015  16.721  1.00 74.25
ATOM    673  CG2 ILE A  53      -4.486 -24.544  17.034  1.00  4.41
ATOM    674  CD1 ILE A  53      -6.291 -26.947  16.712  1.00  5.33
ATOM    675  H   ILE A  53      -3.456 -27.292  14.238  1.00 35.14
ATOM    676  HA  ILE A  53      -5.576 -25.582  14.636  1.00 43.01
ATOM    677  HB  ILE A  53      -3.036 -25.871  16.234  1.00 11.42
ATOM    678 2HG1 ILE A  53      -4.483 -27.856  16.114  1.00 61.12
ATOM    679 3HG1 ILE A  53      -4.459 -27.181  17.739  1.00 14.22
ATOM    680 1HG2 ILE A  53      -5.507 -24.263  16.825  1.00 34.12
ATOM    681 2HG2 ILE A  53      -4.389 -24.795  18.080  1.00 60.24
ATOM    682 3HG2 ILE A  53      -3.830 -23.718  16.800  1.00 75.22
ATOM    683 1HD1 ILE A  53      -6.685 -27.751  16.109  1.00 25.31
ATOM    684 2HD1 ILE A  53      -6.661 -27.038  17.722  1.00 11.51
ATOM    685 3HD1 ILE A  53      -6.605 -26.000  16.297  1.00 15.24
ATOM    686  N   ARG A  54      -2.770 -23.958  14.036  1.00 45.12
ATOM    687  CA  ARG A  54      -2.223 -22.669  13.629  1.00 61.13
ATOM    688  C   ARG A  54      -2.985 -22.109  12.432  1.00 55.24
ATOM    689  O   ARG A  54      -3.170 -20.897  12.311  1.00 12.15
ATOM    690  CB  ARG A  54      -0.739 -22.807  13.283  1.00 51.14
ATOM    691  CG  ARG A  54       0.156 -22.980  14.498  1.00  4.14
ATOM    692  CD  ARG A  54       1.386 -22.089  14.416  1.00 11.11
ATOM    693  NE  ARG A  54       2.067 -21.976  15.703  1.00 65.32
ATOM    694  CZ  ARG A  54       2.832 -22.934  16.216  1.00 51.12
ATOM    695  NH1 ARG A  54       3.012 -24.069  15.554  1.00 14.05
ATOM    696  NH2 ARG A  54       3.419 -22.757  17.393  1.00 51.14
ATOM    697  H   ARG A  54      -2.169 -24.728  14.116  1.00  5.14
ATOM    698  HA  ARG A  54      -2.328 -21.987  14.459  1.00 41.22
ATOM    699 2HB  ARG A  54      -0.609 -23.667  12.642  1.00  0.20
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ATOM    700 3HB  ARG A  54      -0.422 -21.922  12.752  1.00 11.31
ATOM    701 2HG  ARG A  54      -0.403 -22.721  15.386  1.00 62.54
ATOM    702 3HG  ARG A  54       0.472 -24.011  14.557  1.00  4.31
ATOM    703 2HD  ARG A  54       2.070 -22.508  13.693  1.00 52.31
ATOM    704 3HD  ARG A  54       1.080 -21.105  14.094  1.00 53.02
ATOM    705  HE  ARG A  54       1.948 -21.146  16.208  1.00  4.23
ATOM    706 1HH1 ARG A  54       2.571 -24.205  14.667  1.00  4.31
ATOM    707 2HH1 ARG A  54       3.589 -24.788  15.942  1.00 13.05
ATOM    708 1HH2 ARG A  54       3.286 -21.903  17.894  1.00 50.51
ATOM    709 2HH2 ARG A  54       3.994 -23.478  17.778  1.00 72.12
ATOM    710  N   LEU A  55      -3.426 -22.998  11.548  1.00 24.14
ATOM    711  CA  LEU A  55      -4.168 -22.593  10.360  1.00 51.02
ATOM    712  C   LEU A  55      -5.337 -21.686  10.731  1.00 40.12
ATOM    713  O   LEU A  55      -5.436 -20.557  10.250  1.00 32.34
ATOM    714  CB  LEU A  55      -4.681 -23.824   9.611  1.00 61.05
ATOM    715  CG  LEU A  55      -4.723 -23.713   8.086  1.00  1.31
ATOM    716  CD1 LEU A  55      -5.612 -22.555   7.660  1.00 44.33
ATOM    717  CD2 LEU A  55      -3.318 -23.544   7.525  1.00 75.42
ATOM    718  H   LEU A  55      -3.248 -23.950  11.698  1.00  2.31
ATOM    719  HA  LEU A  55      -3.493 -22.046   9.718  1.00 34.21
ATOM    720 2HB  LEU A  55      -4.041 -24.655   9.864  1.00 71.34
ATOM    721 3HB  LEU A  55      -5.685 -24.026   9.956  1.00 22.24
ATOM    722  HG  LEU A  55      -5.141 -24.622   7.676  1.00  0.04
ATOM    723 1HD1 LEU A  55      -6.288 -22.886   6.886  1.00 44.31
ATOM    724 2HD1 LEU A  55      -4.998 -21.750   7.282  1.00 70.31
ATOM    725 3HD1 LEU A  55      -6.179 -22.205   8.510  1.00 75.05
ATOM    726 1HD2 LEU A  55      -2.688 -24.343   7.888  1.00 73.05
ATOM    727 2HD2 LEU A  55      -2.915 -22.594   7.844  1.00 62.30
ATOM    728 3HD2 LEU A  55      -3.356 -23.576   6.446  1.00 22.41
ATOM    729  N   MET A  56      -6.218 -22.187  11.590  1.00 15.20
ATOM    730  CA  MET A  56      -7.379 -21.420  12.028  1.00  2.22
ATOM    731  C   MET A  56      -6.948 -20.154  12.763  1.00 31.40
ATOM    732  O   MET A  56      -7.430 -19.060  12.469  1.00 32.43
ATOM    733  CB  MET A  56      -8.268 -22.273  12.935  1.00  2.33
ATOM    734  CG  MET A  56      -9.700 -21.771  13.028  1.00 22.31
ATOM    735  SD  MET A  56      -9.879 -20.390  14.173  1.00 52.11
ATOM    736  CE  MET A  56      -9.225 -21.109  15.677  1.00 31.51
ATOM    737  H   MET A  56      -6.086 -23.093  11.939  1.00 63.13
ATOM    738  HA  MET A  56      -7.940 -21.139  11.150  1.00 15.41
ATOM    739 2HB  MET A  56      -8.287 -23.283  12.554  1.00  2.22
ATOM    740 3HB  MET A  56      -7.847 -22.279  13.930  1.00 62.34
ATOM    741 2HG  MET A  56     -10.020 -21.451  12.048  1.00 63.02
ATOM    742 3HG  MET A  56     -10.329 -22.583  13.362  1.00 13.35
ATOM    743 1HE  MET A  56      -8.301 -20.617  15.940  1.00 41.42
ATOM    744 2HE  MET A  56      -9.940 -20.984  16.476  1.00 13.24
ATOM    745 3HE  MET A  56      -9.040 -22.162  15.521  1.00 60.50
ATOM    746  N   ARG A  57      -6.039 -20.311  13.719  1.00 24.23
ATOM    747  CA  ARG A  57      -5.545 -19.181  14.497  1.00 63.13
ATOM    748  C   ARG A  57      -5.069 -18.057  13.581  1.00 72.34
ATOM    749  O   ARG A  57      -5.138 -16.881  13.938  1.00 63.32
ATOM    750  CB  ARG A  57      -4.402 -19.625  15.412  1.00 13.03
ATOM    751  CG  ARG A  57      -4.752 -19.574  16.891  1.00 44.04
ATOM    752  CD  ARG A  57      -3.685 -18.842  17.690  1.00 12.02
ATOM    753  NE  ARG A  57      -4.147 -18.497  19.032  1.00 73.20
ATOM    754  CZ  ARG A  57      -3.340 -18.094  20.006  1.00  4.34
ATOM    755  NH1 ARG A  57      -2.036 -17.985  19.789  1.00 13.41
ATOM    756  NH2 ARG A  57      -3.836 -17.798  21.201  1.00  5.11
ATOM    757  H   ARG A  57      -5.692 -21.209  13.907  1.00  1.52
ATOM    758  HA  ARG A  57      -6.359 -18.815  15.104  1.00 41.33
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ATOM    759 2HB  ARG A  57      -4.131 -20.641  15.164  1.00 11.31
ATOM    760 3HB  ARG A  57      -3.551 -18.982  15.243  1.00 35.33
ATOM    761 2HG  ARG A  57      -5.693 -19.058  17.011  1.00 31.41
ATOM    762 3HG  ARG A  57      -4.841 -20.583  17.265  1.00 41.13
ATOM    763 2HD  ARG A  57      -2.816 -19.477  17.772  1.00 62.24
ATOM    764 3HD  ARG A  57      -3.421 -17.936  17.166  1.00  4.43
ATOM    765  HE  ARG A  57      -5.107 -18.571  19.214  1.00  1.33
ATOM    766 1HH1 ARG A  57      -1.660 -18.206  18.890  1.00 40.24
ATOM    767 2HH1 ARG A  57      -1.430 -17.679  20.524  1.00 34.42
ATOM    768 1HH2 ARG A  57      -4.818 -17.879  21.369  1.00 44.25
ATOM    769 2HH2 ARG A  57      -3.227 -17.495  21.934  1.00 50.44
ATOM    770  N   TRP A  58      -4.588 -18.428  12.400  1.00 44.22
ATOM    771  CA  TRP A  58      -4.100 -17.451  11.433  1.00 51.23
ATOM    772  C   TRP A  58      -5.258 -16.691  10.796  1.00 53.22
ATOM    773  O   TRP A  58      -5.145 -15.500  10.500  1.00 20.42
ATOM    774  CB  TRP A  58      -3.272 -18.144  10.350  1.00 61.13
ATOM    775  CG  TRP A  58      -1.796 -17.937  10.507  1.00 22.22
ATOM    776  CD1 TRP A  58      -0.824 -18.896  10.459  1.00 51.41
ATOM    777  CD2 TRP A  58      -1.125 -16.694  10.740  1.00 21.12
ATOM    778  CE2 TRP A  58       0.253 -16.974  10.822  1.00 44.51
ATOM    779  CE3 TRP A  58      -1.554 -15.372  10.886  1.00 63.13
ATOM    780  NE1 TRP A  58       0.411 -18.323  10.648  1.00 74.10
ATOM    781  CZ2 TRP A  58       1.202 -15.979  11.044  1.00 63.22
ATOM    782  CZ3 TRP A  58      -0.611 -14.386  11.106  1.00 24.42
ATOM    783  CH2 TRP A  58       0.754 -14.694  11.183  1.00 44.43
ATOM    784  H   TRP A  58      -4.559 -19.381  12.172  1.00 22.04
ATOM    785  HA  TRP A  58      -3.471 -16.749  11.960  1.00 30.02
ATOM    786 2HB  TRP A  58      -3.465 -19.206  10.382  1.00  1.10
ATOM    787 3HB  TRP A  58      -3.562 -17.758   9.383  1.00 31.41
ATOM    788  HD1 TRP A  58      -1.014 -19.946  10.297  1.00  5.32
ATOM    789  HE1 TRP A  58       1.265 -18.804  10.655  1.00  2.32
ATOM    790  HE3 TRP A  58      -2.601 -15.115  10.830  1.00 73.42
ATOM    791  HZ2 TRP A  58       2.258 -16.200  11.105  1.00 41.23
ATOM    792  HZ3 TRP A  58      -0.923 -13.359  11.222  1.00 54.14
ATOM    793  HH2 TRP A  58       1.455 -13.892  11.356  1.00  4.04
ATOM    794  N   LEU A  59      -6.372 -17.385  10.587  1.00 43.42
ATOM    795  CA  LEU A  59      -7.552 -16.774   9.985  1.00 61.14
ATOM    796  C   LEU A  59      -7.919 -15.477  10.699  1.00 22.30
ATOM    797  O   LEU A  59      -8.400 -14.529  10.078  1.00 10.13
ATOM    798  CB  LEU A  59      -8.732 -17.746  10.030  1.00 73.15
ATOM    799  CG  LEU A  59     -10.037 -17.246   9.409  1.00 34.13
ATOM    800  CD1 LEU A  59      -9.759 -16.476   8.128  1.00 62.12
ATOM    801  CD2 LEU A  59     -10.980 -18.410   9.140  1.00 12.12
ATOM    802  H   LEU A  59      -6.402 -18.330  10.843  1.00 10.51
ATOM    803  HA  LEU A  59      -7.320 -16.550   8.954  1.00  4.01
ATOM    804 2HB  LEU A  59      -8.441 -18.644   9.507  1.00 20.20
ATOM    805 3HB  LEU A  59      -8.926 -17.982  11.066  1.00 13.44
ATOM    806  HG  LEU A  59     -10.524 -16.574  10.103  1.00 41.12
ATOM    807 1HD1 LEU A  59      -8.843 -16.836   7.683  1.00 34.14
ATOM    808 2HD1 LEU A  59      -9.660 -15.425   8.354  1.00 53.32
ATOM    809 3HD1 LEU A  59     -10.576 -16.620   7.437  1.00 74.15
ATOM    810 1HD2 LEU A  59     -11.279 -18.855  10.078  1.00 44.10
ATOM    811 2HD2 LEU A  59     -10.476 -19.149   8.535  1.00 25.44
ATOM    812 3HD2 LEU A  59     -11.854 -18.052   8.617  1.00 12.51
ATOM    813  N   HIS A  60      -7.686 -15.442  12.007  1.00 33.34
ATOM    814  CA  HIS A  60      -7.990 -14.260  12.806  1.00 22.34
ATOM    815  C   HIS A  60      -7.293 -13.027  12.239  1.00 71.42
ATOM    816  O   HIS A  60      -7.904 -11.968  12.097  1.00  3.13
ATOM    817  CB  HIS A  60      -7.564 -14.478  14.259  1.00 52.42
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ATOM    818  CG  HIS A  60      -8.671 -14.968  15.140  1.00 13.13
ATOM    819  CD2 HIS A  60      -9.824 -15.610  14.839  1.00 32.24
ATOM    820  ND1 HIS A  60      -8.666 -14.815  16.511  1.00 51.23
ATOM    821  CE1 HIS A  60      -9.767 -15.343  17.015  1.00 61.32
ATOM    822  NE2 HIS A  60     -10.487 -15.832  16.021  1.00 30.34
ATOM    823  H   HIS A  60      -7.301 -16.230  12.445  1.00 14.44
ATOM    824  HA  HIS A  60      -9.057 -14.103  12.773  1.00 51.40
ATOM    825 2HB  HIS A  60      -6.769 -15.208  14.289  1.00 51.15
ATOM    826 3HB  HIS A  60      -7.204 -13.543  14.665  1.00 32.43
ATOM    827  HD1 HIS A  60      -7.960 -14.385  17.036  1.00 42.53
ATOM    828  HD2 HIS A  60     -10.161 -15.896  13.853  1.00 40.03
ATOM    829  HE1 HIS A  60     -10.034 -15.371  18.061  1.00 43.34
ATOM    830  N   TRP A  61      -6.013 -13.173  11.917  1.00 71.24
ATOM    831  CA  TRP A  61      -5.234 -12.071  11.365  1.00  5.42
ATOM    832  C   TRP A  61      -5.847 -11.568  10.063  1.00 63.32
ATOM    833  O   TRP A  61      -5.835 -10.370   9.782  1.00 51.34
ATOM    834  CB  TRP A  61      -3.788 -12.510  11.127  1.00 71.35
ATOM    835  CG  TRP A  61      -2.966 -11.484  10.408  1.00 41.40
ATOM    836  CD1 TRP A  61      -2.478 -10.317  10.924  1.00 41.02
ATOM    837  CD2 TRP A  61      -2.538 -11.531   9.043  1.00 42.04
ATOM    838  CE2 TRP A  61      -1.793 -10.360   8.799  1.00 73.35
ATOM    839  CE3 TRP A  61      -2.709 -12.449   8.003  1.00 30.11
ATOM    840  NE1 TRP A  61      -1.772  -9.636   9.961  1.00 32.21
ATOM    841  CZ2 TRP A  61      -1.224 -10.086   7.558  1.00  3.11
ATOM    842  CZ3 TRP A  61      -2.143 -12.175   6.772  1.00 33.15
ATOM    843  CH2 TRP A  61      -1.407 -11.002   6.558  1.00 33.14
ATOM    844  H   TRP A  61      -5.581 -14.043  12.053  1.00 54.24
ATOM    845  HA  TRP A  61      -5.241 -11.267  12.087  1.00 53.02
ATOM    846 2HB  TRP A  61      -3.317 -12.709  12.077  1.00  1.55
ATOM    847 3HB  TRP A  61      -3.788 -13.413  10.533  1.00 22.44
ATOM    848  HD1 TRP A  61      -2.634  -9.990  11.940  1.00  4.43
ATOM    849  HE1 TRP A  61      -1.325  -8.773  10.088  1.00 61.03
ATOM    850  HE3 TRP A  61      -3.273 -13.359   8.149  1.00 42.24
ATOM    851  HZ2 TRP A  61      -0.653  -9.187   7.377  1.00 11.54
ATOM    852  HZ3 TRP A  61      -2.265 -12.873   5.957  1.00 55.20
ATOM    853  HH2 TRP A  61      -0.984 -10.829   5.581  1.00 24.22
ATOM    854  N   PHE A  62      -6.382 -12.492   9.271  1.00 11.40
ATOM    855  CA  PHE A  62      -7.000 -12.141   7.997  1.00 23.43
ATOM    856  C   PHE A  62      -8.302 -11.377   8.216  1.00 32.22
ATOM    857  O   PHE A  62      -8.490 -10.284   7.683  1.00 41.25
ATOM    858  CB  PHE A  62      -7.267 -13.402   7.172  1.00 34.15
ATOM    859  CG  PHE A  62      -6.025 -14.013   6.591  1.00 43.02
ATOM    860  CD1 PHE A  62      -5.420 -15.100   7.201  1.00 75.53
ATOM    861  CD2 PHE A  62      -5.460 -13.499   5.434  1.00 34.22
ATOM    862  CE1 PHE A  62      -4.277 -15.665   6.668  1.00 60.32
ATOM    863  CE2 PHE A  62      -4.317 -14.060   4.897  1.00 74.14
ATOM    864  CZ  PHE A  62      -3.724 -15.144   5.515  1.00 52.43
ATOM    865  H   PHE A  62      -6.361 -13.431   9.550  1.00 23.20
ATOM    866  HA  PHE A  62      -6.311 -11.509   7.459  1.00 52.22
ATOM    867 2HB  PHE A  62      -7.737 -14.143   7.802  1.00  0.32
ATOM    868 3HB  PHE A  62      -7.931 -13.156   6.357  1.00  2.22
ATOM    869  HD1 PHE A  62      -5.852 -15.509   8.104  1.00 73.35
ATOM    870  HD2 PHE A  62      -5.922 -12.651   4.950  1.00 33.32
ATOM    871  HE1 PHE A  62      -3.816 -16.512   7.154  1.00 70.31
ATOM    872  HE2 PHE A  62      -3.887 -13.650   3.995  1.00 21.21
ATOM    873  HZ  PHE A  62      -2.831 -15.584   5.096  1.00 14.43
ATOM    874  N   ARG A  63      -9.199 -11.961   9.004  1.00 23.43
ATOM    875  CA  ARG A  63     -10.484 -11.337   9.293  1.00 73.32
ATOM    876  C   ARG A  63     -10.291  -9.964   9.929  1.00 33.03
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ATOM    877  O   ARG A  63     -11.063  -9.038   9.680  1.00 52.21
ATOM    878  CB  ARG A  63     -11.312 -12.229  10.220  1.00 23.42
ATOM    879  CG  ARG A  63     -12.010 -13.373   9.502  1.00  2.22
ATOM    880  CD  ARG A  63     -13.451 -13.523   9.963  1.00 10.04
ATOM    881  NE  ARG A  63     -14.007 -14.825   9.607  1.00 60.53
ATOM    882  CZ  ARG A  63     -14.432 -15.134   8.387  1.00 54.24
ATOM    883  NH1 ARG A  63     -14.365 -14.238   7.411  1.00 33.05
ATOM    884  NH2 ARG A  63     -14.926 -16.341   8.140  1.00 43.30
ATOM    885  H   ARG A  63      -8.991 -12.833   9.401  1.00 72.43
ATOM    886  HA  ARG A  63     -11.012 -11.217   8.359  1.00 60.04
ATOM    887 2HB  ARG A  63     -10.660 -12.650  10.972  1.00 60.22
ATOM    888 3HB  ARG A  63     -12.063 -11.625  10.705  1.00 54.13
ATOM    889 2HG  ARG A  63     -12.002 -13.177   8.440  1.00 11.10
ATOM    890 3HG  ARG A  63     -11.478 -14.291   9.705  1.00 52.51
ATOM    891 2HD  ARG A  63     -13.485 -13.410  11.037  1.00 53.54
ATOM    892 3HD  ARG A  63     -14.045 -12.749   9.501  1.00 72.13
ATOM    893  HE  ARG A  63     -14.066 -15.502  10.312  1.00 23.52
ATOM    894 1HH1 ARG A  63     -13.993 -13.328   7.594  1.00 31.22
ATOM    895 2HH1 ARG A  63     -14.685 -14.473   6.493  1.00 32.13
ATOM    896 1HH2 ARG A  63     -14.978 -17.019   8.873  1.00 44.35
ATOM    897 2HH2 ARG A  63     -15.246 -16.572   7.222  1.00 43.33
ATOM    898  N   LYS A  64      -9.256  -9.840  10.753  1.00 14.23
ATOM    899  CA  LYS A  64      -8.960  -8.580  11.426  1.00 71.51
ATOM    900  C   LYS A  64      -8.616  -7.492  10.415  1.00 43.52
ATOM    901  O   LYS A  64      -9.111  -6.369  10.505  1.00 75.35
ATOM    902  CB  LYS A  64      -7.801  -8.764  12.409  1.00 54.34
ATOM    903  CG  LYS A  64      -8.217  -8.658  13.866  1.00 71.13
ATOM    904  CD  LYS A  64      -7.674  -9.816  14.686  1.00 42.01
ATOM    905  CE  LYS A  64      -6.153  -9.846  14.669  1.00 12.10
ATOM    906  NZ  LYS A  64      -5.611 -10.953  15.504  1.00 21.12
ATOM    907  H   LYS A  64      -8.677 -10.615  10.912  1.00  4.44
ATOM    908  HA  LYS A  64      -9.841  -8.281  11.973  1.00 32.31
ATOM    909 2HB  LYS A  64      -7.362  -9.738  12.251  1.00 40.41
ATOM    910 3HB  LYS A  64      -7.056  -8.006  12.213  1.00 71.11
ATOM    911 2HG  LYS A  64      -7.837  -7.733  14.273  1.00 30.01
ATOM    912 3HG  LYS A  64      -9.296  -8.663  13.924  1.00 54.32
ATOM    913 2HD  LYS A  64      -8.009  -9.711  15.707  1.00 20.21
ATOM    914 3HD  LYS A  64      -8.048 -10.743  14.276  1.00 71.34
ATOM    915 2HE  LYS A  64      -5.820  -9.978  13.651  1.00 11.01
ATOM    916 3HE  LYS A  64      -5.784  -8.905  15.049  1.00 24.04
ATOM    917 1HZ  LYS A  64      -4.711 -11.292  15.107  1.00  0.23
ATOM    918 2HZ  LYS A  64      -6.285 -11.745  15.530  1.00 42.44
ATOM    919 3HZ  LYS A  64      -5.446 -10.621  16.476  1.00 41.45
ATOM    920  N   ASN A  65      -7.764  -7.832   9.453  1.00 54.35
ATOM    921  CA  ASN A  65      -7.355  -6.883   8.424  1.00 42.53
ATOM    922  C   ASN A  65      -8.510  -6.576   7.475  1.00 30.05
ATOM    923  O   ASN A  65      -8.445  -5.636   6.684  1.00 21.22
ATOM    924  CB  ASN A  65      -6.166  -7.435   7.635  1.00  3.11
ATOM    925  CG  ASN A  65      -4.936  -7.627   8.502  1.00 73.31
ATOM    926  ND2 ASN A  65      -3.825  -8.000   7.878  1.00 40.22
ATOM    927  OD1 ASN A  65      -4.986  -7.443   9.718  1.00  4.31
ATOM    928  H   ASN A  65      -7.403  -8.742   9.434  1.00 64.33
ATOM    929  HA  ASN A  65      -7.056  -5.969   8.916  1.00 71.23
ATOM    930 2HB  ASN A  65      -6.436  -8.391   7.211  1.00 50.14
ATOM    931 3HB  ASN A  65      -5.919  -6.749   6.839  1.00 50.11
ATOM    932 1HD2 ASN A  65      -3.860  -8.128   6.907  1.00 62.04
ATOM    933 2HD2 ASN A  65      -3.016  -8.132   8.414  1.00 25.01
ATOM    934  N   GLY A  66      -9.568  -7.377   7.562  1.00 12.40
ATOM    935  CA  GLY A  66     -10.723  -7.175   6.707  1.00 52.41
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ATOM    936  C   GLY A  66     -10.772  -8.160   5.556  1.00 31.02
ATOM    937  O   GLY A  66     -11.256  -7.835   4.472  1.00 74.32
ATOM    938  H   GLY A  66      -9.564  -8.110   8.212  1.00 74.41
ATOM    939 2HA  GLY A  66     -11.619  -7.284   7.299  1.00 14.31
ATOM    940 3HA  GLY A  66     -10.689  -6.172   6.306  1.00 63.23
ATOM    941  N   TYR A  67     -10.268  -9.366   5.791  1.00 72.40
ATOM    942  CA  TYR A  67     -10.253 -10.401   4.764  1.00 64.30
ATOM    943  C   TYR A  67     -11.282 -11.486   5.068  1.00 43.13
ATOM    944  O   TYR A  67     -11.103 -12.287   5.985  1.00 31.30
ATOM    945  CB  TYR A  67      -8.859 -11.021   4.656  1.00 25.42
ATOM    946  CG  TYR A  67      -7.817 -10.077   4.098  1.00 35.41
ATOM    947  CD1 TYR A  67      -7.425  -8.948   4.806  1.00 23.22
ATOM    948  CD2 TYR A  67      -7.227 -10.314   2.863  1.00 55.13
ATOM    949  CE1 TYR A  67      -6.474  -8.082   4.300  1.00 34.52
ATOM    950  CE2 TYR A  67      -6.275  -9.455   2.350  1.00 54.54
ATOM    951  CZ  TYR A  67      -5.902  -8.340   3.072  1.00 74.22
ATOM    952  OH  TYR A  67      -4.955  -7.481   2.563  1.00 14.15
ATOM    953  H   TYR A  67      -9.896  -9.566   6.675  1.00 13.34
ATOM    954  HA  TYR A  67     -10.503  -9.937   3.821  1.00 32.04
ATOM    955 2HB  TYR A  67      -8.533 -11.331   5.637  1.00  3.22
ATOM    956 3HB  TYR A  67      -8.905 -11.885   4.009  1.00 51.34
ATOM    957  HD1 TYR A  67      -7.874  -8.749   5.768  1.00 35.02
ATOM    958  HD2 TYR A  67      -7.522 -11.188   2.299  1.00 13.54
ATOM    959  HE1 TYR A  67      -6.182  -7.210   4.865  1.00  3.24
ATOM    960  HE2 TYR A  67      -5.828  -9.656   1.388  1.00 42.24
ATOM    961  HH  TYR A  67      -4.262  -7.987   2.134  1.00 60.22
ATOM    962  N   ARG A  68     -12.359 -11.504   4.290  1.00 33.31
ATOM    963  CA  ARG A  68     -13.418 -12.489   4.475  1.00 32.20
ATOM    964  C   ARG A  68     -13.008 -13.843   3.903  1.00 43.24
ATOM    965  O   ARG A  68     -13.667 -14.377   3.010  1.00 71.31
ATOM    966  CB  ARG A  68     -14.710 -12.012   3.808  1.00 22.14
ATOM    967  CG  ARG A  68     -15.242 -10.707   4.377  1.00 53.12
ATOM    968  CD  ARG A  68     -16.762 -10.706   4.442  1.00 64.41
ATOM    969  NE  ARG A  68     -17.340  -9.571   3.728  1.00 63.44
ATOM    970  CZ  ARG A  68     -17.405  -8.343   4.230  1.00 75.33
ATOM    971  NH1 ARG A  68     -16.931  -8.093   5.442  1.00  1.02
ATOM    972  NH2 ARG A  68     -17.946  -7.362   3.518  1.00 33.43
ATOM    973  H   ARG A  68     -12.445 -10.839   3.575  1.00 22.32
ATOM    974  HA  ARG A  68     -13.590 -12.597   5.536  1.00 65.25
ATOM    975 2HB  ARG A  68     -14.526 -11.871   2.753  1.00 31.14
ATOM    976 3HB  ARG A  68     -15.467 -12.771   3.935  1.00 14.44
ATOM    977 2HG  ARG A  68     -14.850 -10.573   5.374  1.00 14.22
ATOM    978 3HG  ARG A  68     -14.917  -9.892   3.747  1.00 31.04
ATOM    979 2HD  ARG A  68     -17.128 -11.621   4.001  1.00 61.33
ATOM    980 3HD  ARG A  68     -17.064 -10.660   5.477  1.00 21.35
ATOM    981  HE  ARG A  68     -17.696  -9.734   2.830  1.00 74.01
ATOM    982 1HH1 ARG A  68     -16.522  -8.830   5.980  1.00  0.10
ATOM    983 2HH1 ARG A  68     -16.981  -7.167   5.817  1.00 24.14
ATOM    984 1HH2 ARG A  68     -18.305  -7.547   2.604  1.00 61.32
ATOM    985 2HH2 ARG A  68     -17.995  -6.439   3.897  1.00 54.20
ATOM    986  N   LEU A  69     -11.915 -14.392   4.421  1.00  1.24
ATOM    987  CA  LEU A  69     -11.415 -15.683   3.962  1.00 35.20
ATOM    988  C   LEU A  69     -11.986 -16.819   4.805  1.00  1.14
ATOM    989  O   LEU A  69     -12.565 -16.588   5.867  1.00 32.45
ATOM    990  CB  LEU A  69      -9.887 -15.710   4.017  1.00 50.11
ATOM    991  CG  LEU A  69      -9.163 -14.882   2.955  1.00 63.25
ATOM    992  CD1 LEU A  69      -7.917 -14.235   3.540  1.00 70.23
ATOM    993  CD2 LEU A  69      -8.803 -15.749   1.757  1.00 71.13
ATOM    994  H   LEU A  69     -11.432 -13.919   5.130  1.00  1.51
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ATOM    995  HA  LEU A  69     -11.733 -15.816   2.939  1.00 73.24
ATOM    996 2HB  LEU A  69      -9.585 -15.342   4.985  1.00 24.02
ATOM    997 3HB  LEU A  69      -9.571 -16.738   3.909  1.00  0.23
ATOM    998  HG  LEU A  69      -9.819 -14.093   2.613  1.00 63.42
ATOM    999 1HD1 LEU A  69      -7.773 -13.263   3.094  1.00 54.41
ATOM   1000 2HD1 LEU A  69      -7.058 -14.856   3.333  1.00 30.32
ATOM   1001 3HD1 LEU A  69      -8.035 -14.128   4.608  1.00 30.52
ATOM   1002 1HD2 LEU A  69      -8.500 -15.118   0.934  1.00 15.02
ATOM   1003 2HD2 LEU A  69      -9.664 -16.333   1.464  1.00 24.51
ATOM   1004 3HD2 LEU A  69      -7.991 -16.410   2.021  1.00 34.15
ATOM   1005  N   THR A  70     -11.816 -18.048   4.327  1.00 54.43
ATOM   1006  CA  THR A  70     -12.313 -19.220   5.036  1.00  0.34
ATOM   1007  C   THR A  70     -11.164 -20.096   5.523  1.00 51.51
ATOM   1008  O   THR A  70     -10.153 -20.249   4.836  1.00 20.02
ATOM   1009  CB  THR A  70     -13.245 -20.063   4.146  1.00 42.23
ATOM   1010  CG2 THR A  70     -14.390 -20.645   4.960  1.00 74.24
ATOM   1011  OG1 THR A  70     -13.768 -19.257   3.084  1.00 74.42
ATOM   1012  H   THR A  70     -11.347 -18.167   3.475  1.00  5.11
ATOM   1013  HA  THR A  70     -12.879 -18.877   5.891  1.00 63.32
ATOM   1014  HB  THR A  70     -12.674 -20.877   3.722  1.00  4.41
ATOM   1015  HG1 THR A  70     -13.382 -19.537   2.250  1.00 55.40
ATOM   1016 1HG2 THR A  70     -15.149 -19.890   5.105  1.00 72.45
ATOM   1017 2HG2 THR A  70     -14.020 -20.973   5.920  1.00 41.44
ATOM   1018 3HG2 THR A  70     -14.815 -21.486   4.432  1.00 55.51
ATOM   1019  N   LEU A  71     -11.325 -20.669   6.710  1.00 13.12
ATOM   1020  CA  LEU A  71     -10.301 -21.531   7.289  1.00 62.42
ATOM   1021  C   LEU A  71     -10.052 -22.750   6.405  1.00  1.52
ATOM   1022  O   LEU A  71      -8.912 -23.183   6.236  1.00 33.50
ATOM   1023  CB  LEU A  71     -10.716 -21.980   8.691  1.00 74.42
ATOM   1024  CG  LEU A  71      -9.981 -23.199   9.251  1.00 54.31
ATOM   1025  CD1 LEU A  71      -8.496 -22.905   9.397  1.00 33.41
ATOM   1026  CD2 LEU A  71     -10.579 -23.614  10.587  1.00 21.32
ATOM   1027  H   LEU A  71     -12.152 -20.509   7.210  1.00 33.35
ATOM   1028  HA  LEU A  71      -9.387 -20.960   7.359  1.00 54.33
ATOM   1029 2HB  LEU A  71     -10.549 -21.155   9.365  1.00 14.24
ATOM   1030 3HB  LEU A  71     -11.772 -22.213   8.663  1.00  4.04
ATOM   1031  HG  LEU A  71     -10.091 -24.025   8.563  1.00 75.54
ATOM   1032 1HD1 LEU A  71      -7.949 -23.424   8.625  1.00 72.41
ATOM   1033 2HD1 LEU A  71      -8.157 -23.240  10.366  1.00 30.41
ATOM   1034 3HD1 LEU A  71      -8.329 -21.842   9.305  1.00 22.14
ATOM   1035 1HD2 LEU A  71      -9.790 -23.719  11.317  1.00 64.21
ATOM   1036 2HD2 LEU A  71     -11.092 -24.558  10.474  1.00 70.40
ATOM   1037 3HD2 LEU A  71     -11.278 -22.861  10.919  1.00 72.24
ATOM   1038  N   ARG A  72     -11.125 -23.295   5.843  1.00 71.24
ATOM   1039  CA  ARG A  72     -11.023 -24.463   4.975  1.00  0.43
ATOM   1040  C   ARG A  72     -10.199 -24.145   3.731  1.00 54.13
ATOM   1041  O   ARG A  72      -9.379 -24.952   3.295  1.00 33.32
ATOM   1042  CB  ARG A  72     -12.416 -24.946   4.568  1.00 13.43
ATOM   1043  CG  ARG A  72     -12.826 -26.250   5.231  1.00 33.52
ATOM   1044  CD  ARG A  72     -14.250 -26.639   4.864  1.00 40.32
ATOM   1045  NE  ARG A  72     -14.296 -27.865   4.072  1.00 21.13
ATOM   1046  CZ  ARG A  72     -14.028 -29.069   4.566  1.00 42.10
ATOM   1047  NH1 ARG A  72     -13.697 -29.207   5.842  1.00  3.14
ATOM   1048  NH2 ARG A  72     -14.091 -30.138   3.782  1.00 10.23
ATOM   1049  H   ARG A  72     -12.007 -22.904   6.015  1.00 20.04
ATOM   1050  HA  ARG A  72     -10.528 -25.246   5.530  1.00 40.32
ATOM   1051 2HB  ARG A  72     -13.139 -24.189   4.836  1.00 74.03
ATOM   1052 3HB  ARG A  72     -12.436 -25.089   3.499  1.00 40.25
ATOM   1053 2HG  ARG A  72     -12.157 -27.034   4.908  1.00 43.22
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ATOM   1054 3HG  ARG A  72     -12.759 -26.136   6.303  1.00 45.33
ATOM   1055 2HD  ARG A  72     -14.814 -26.787   5.772  1.00 14.33
ATOM   1056 3HD  ARG A  72     -14.692 -25.836   4.293  1.00 45.32
ATOM   1057  HE  ARG A  72     -14.538 -27.786   3.127  1.00 74.15
ATOM   1058 1HH1 ARG A  72     -13.649 -28.403   6.435  1.00 33.34
ATOM   1059 2HH1 ARG A  72     -13.496 -30.115   6.212  1.00 55.41
ATOM   1060 1HH2 ARG A  72     -14.340 -30.038   2.820  1.00 55.33
ATOM   1061 2HH2 ARG A  72     -13.889 -31.043   4.155  1.00 61.04
ATOM   1062  N   GLU A  73     -10.425 -22.964   3.164  1.00 41.24
ATOM   1063  CA  GLU A  73      -9.704 -22.541   1.969  1.00 54.15
ATOM   1064  C   GLU A  73      -8.200 -22.725   2.147  1.00 50.33
ATOM   1065  O   GLU A  73      -7.549 -23.411   1.357  1.00 10.35
ATOM   1066  CB  GLU A  73     -10.016 -21.077   1.649  1.00 32.41
ATOM   1067  CG  GLU A  73     -11.164 -20.899   0.670  1.00 72.43
ATOM   1068  CD  GLU A  73     -10.950 -21.659  -0.625  1.00 22.42
ATOM   1069  OE1 GLU A  73     -10.002 -21.317  -1.363  1.00 32.21
ATOM   1070  OE2 GLU A  73     -11.729 -22.595  -0.900  1.00 31.41
ATOM   1071  H   GLU A  73     -11.092 -22.363   3.558  1.00 64.43
ATOM   1072  HA  GLU A  73     -10.035 -23.157   1.146  1.00 32.34
ATOM   1073 2HB  GLU A  73     -10.270 -20.567   2.567  1.00 70.33
ATOM   1074 3HB  GLU A  73      -9.135 -20.619   1.225  1.00 10.12
ATOM   1075 2HG  GLU A  73     -12.073 -21.255   1.132  1.00 70.05
ATOM   1076 3HG  GLU A  73     -11.266 -19.849   0.441  1.00 44.33
ATOM   1077  N   LEU A  74      -7.654 -22.107   3.188  1.00  1.21
ATOM   1078  CA  LEU A  74      -6.226 -22.201   3.471  1.00  1.20
ATOM   1079  C   LEU A  74      -5.820 -23.644   3.751  1.00 71.33
ATOM   1080  O   LEU A  74      -4.709 -24.062   3.423  1.00 31.14
ATOM   1081  CB  LEU A  74      -5.863 -21.317   4.665  1.00 12.53
ATOM   1082  CG  LEU A  74      -5.938 -19.807   4.430  1.00 23.53
ATOM   1083  CD1 LEU A  74      -7.374 -19.321   4.539  1.00 14.42
ATOM   1084  CD2 LEU A  74      -5.046 -19.069   5.418  1.00 32.22
ATOM   1085  H   LEU A  74      -8.223 -21.575   3.781  1.00 14.45
ATOM   1086  HA  LEU A  74      -5.692 -21.852   2.600  1.00 41.23
ATOM   1087 2HB  LEU A  74      -6.537 -21.559   5.473  1.00 41.13
ATOM   1088 3HB  LEU A  74      -4.851 -21.557   4.959  1.00 72.23
ATOM   1089  HG  LEU A  74      -5.586 -19.587   3.432  1.00 71.23
ATOM   1090 1HD1 LEU A  74      -7.382 -18.297   4.880  1.00 15.42
ATOM   1091 2HD1 LEU A  74      -7.912 -19.939   5.243  1.00  5.11
ATOM   1092 3HD1 LEU A  74      -7.850 -19.382   3.571  1.00 65.31
ATOM   1093 1HD2 LEU A  74      -4.281 -18.530   4.879  1.00 73.33
ATOM   1094 2HD2 LEU A  74      -4.582 -19.781   6.086  1.00 51.14
ATOM   1095 3HD2 LEU A  74      -5.642 -18.374   5.990  1.00  2.42
ATOM   1096  N   TYR A  75      -6.728 -24.402   4.356  1.00 51.13
ATOM   1097  CA  TYR A  75      -6.465 -25.799   4.680  1.00 42.14
ATOM   1098  C   TYR A  75      -6.257 -26.622   3.412  1.00 22.10
ATOM   1099  O   TYR A  75      -5.441 -27.543   3.384  1.00 72.14
ATOM   1100  CB  TYR A  75      -7.620 -26.382   5.496  1.00 40.54
ATOM   1101  CG  TYR A  75      -7.307 -26.530   6.967  1.00 32.14
ATOM   1102  CD1 TYR A  75      -6.151 -27.174   7.390  1.00 22.31
ATOM   1103  CD2 TYR A  75      -8.168 -26.027   7.935  1.00 20.51
ATOM   1104  CE1 TYR A  75      -5.861 -27.313   8.734  1.00 70.22
ATOM   1105  CE2 TYR A  75      -7.886 -26.160   9.281  1.00 64.42
ATOM   1106  CZ  TYR A  75      -6.731 -26.804   9.675  1.00 32.11
ATOM   1107  OH  TYR A  75      -6.447 -26.940  11.015  1.00 40.23
ATOM   1108  H   TYR A  75      -7.596 -24.012   4.592  1.00 64.22
ATOM   1109  HA  TYR A  75      -5.563 -25.838   5.273  1.00 42.35
ATOM   1110 2HB  TYR A  75      -8.479 -25.735   5.403  1.00  1.15
ATOM   1111 3HB  TYR A  75      -7.868 -27.359   5.108  1.00 11.05
ATOM   1112  HD1 TYR A  75      -5.471 -27.572   6.650  1.00 11.04
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ATOM   1113  HD2 TYR A  75      -9.072 -25.524   7.623  1.00 64.22
ATOM   1114  HE1 TYR A  75      -4.957 -27.817   9.043  1.00 11.11
ATOM   1115  HE2 TYR A  75      -8.567 -25.762  10.018  1.00 30.31
ATOM   1116  HH  TYR A  75      -6.174 -26.091  11.371  1.00 24.32
ATOM   1117  N   ALA A  76      -7.001 -26.282   2.365  1.00 41.03
ATOM   1118  CA  ALA A  76      -6.897 -26.987   1.093  1.00 54.51
ATOM   1119  C   ALA A  76      -5.579 -26.670   0.396  1.00 44.12
ATOM   1120  O   ALA A  76      -4.879 -27.570  -0.067  1.00 63.01
ATOM   1121  CB  ALA A  76      -8.071 -26.628   0.194  1.00 73.02
ATOM   1122  H   ALA A  76      -7.634 -25.539   2.449  1.00  4.42
ATOM   1123  HA  ALA A  76      -6.941 -28.047   1.294  1.00 22.35
ATOM   1124 1HB  ALA A  76      -7.776 -25.842  -0.486  1.00  1.22
ATOM   1125 2HB  ALA A  76      -8.371 -27.498  -0.370  1.00 73.43
ATOM   1126 3HB  ALA A  76      -8.898 -26.289   0.800  1.00 41.41
ATOM   1127  N   ALA A  77      -5.246 -25.385   0.324  1.00 71.21
ATOM   1128  CA  ALA A  77      -4.011 -24.950  -0.316  1.00 23.52
ATOM   1129  C   ALA A  77      -3.173 -24.097   0.631  1.00 53.14
ATOM   1130  O   ALA A  77      -3.009 -22.892   0.438  1.00 72.13
ATOM   1131  CB  ALA A  77      -4.319 -24.180  -1.591  1.00 73.10
ATOM   1132  H   ALA A  77      -5.845 -24.714   0.712  1.00 74.13
ATOM   1133  HA  ALA A  77      -3.446 -25.832  -0.585  1.00  1.35
ATOM   1134 1HB  ALA A  77      -3.395 -23.912  -2.081  1.00 64.13
ATOM   1135 2HB  ALA A  77      -4.911 -24.798  -2.250  1.00 40.31
ATOM   1136 3HB  ALA A  77      -4.870 -23.284  -1.346  1.00 22.34
ATOM   1137  N   PRO A  78      -2.631 -24.733   1.679  1.00 24.32
ATOM   1138  CA  PRO A  78      -1.801 -24.051   2.677  1.00 51.23
ATOM   1139  C   PRO A  78      -0.451 -23.623   2.113  1.00 44.23
ATOM   1140  O   PRO A  78       0.535 -24.354   2.211  1.00 65.02
ATOM   1141  CB  PRO A  78      -1.614 -25.109   3.767  1.00 72.23
ATOM   1142  CG  PRO A  78      -1.778 -26.412   3.062  1.00 14.52
ATOM   1143  CD  PRO A  78      -2.784 -26.168   1.971  1.00 35.45
ATOM   1144  HA  PRO A  78      -2.306 -23.190   3.091  1.00 70.42
ATOM   1145 2HB  PRO A  78      -0.628 -25.014   4.199  1.00 62.33
ATOM   1146 3HB  PRO A  78      -2.363 -24.978   4.533  1.00 11.01
ATOM   1147 2HG  PRO A  78      -0.835 -26.722   2.640  1.00 60.11
ATOM   1148 3HG  PRO A  78      -2.146 -27.157   3.751  1.00 34.34
ATOM   1149 2HD  PRO A  78      -2.551 -26.766   1.103  1.00 72.02
ATOM   1150 3HD  PRO A  78      -3.782 -26.385   2.324  1.00 54.55
ATOM   1151  N   THR A  79      -0.412 -22.433   1.521  1.00  4.44
ATOM   1152  CA  THR A  79       0.818 -21.907   0.941  1.00 32.41
ATOM   1153  C   THR A  79       0.810 -20.383   0.923  1.00 30.21
ATOM   1154  O   THR A  79      -0.171 -19.762   0.512  1.00 40.10
ATOM   1155  CB  THR A  79       1.027 -22.425  -0.494  1.00 64.44
ATOM   1156  CG2 THR A  79       1.390 -23.903  -0.489  1.00  5.30
ATOM   1157  OG1 THR A  79      -0.162 -22.224  -1.266  1.00 43.04
ATOM   1158  H   THR A  79      -1.230 -21.896   1.475  1.00 74.44
ATOM   1159  HA  THR A  79       1.645 -22.247   1.548  1.00 13.41
ATOM   1160  HB  THR A  79       1.839 -21.872  -0.946  1.00 34.14
ATOM   1161  HG1 THR A  79      -0.055 -22.629  -2.130  1.00 62.25
ATOM   1162 1HG2 THR A  79       1.944 -24.134   0.409  1.00 30.20
ATOM   1163 2HG2 THR A  79       1.997 -24.127  -1.354  1.00 33.41
ATOM   1164 3HG2 THR A  79       0.488 -24.495  -0.518  1.00  2.32
ATOM   1165  N   LEU A  80       1.909 -19.785   1.370  1.00 32.42
ATOM   1166  CA  LEU A  80       2.029 -18.332   1.405  1.00 50.13
ATOM   1167  C   LEU A  80       1.805 -17.734   0.020  1.00 53.04
ATOM   1168  O   LEU A  80       1.275 -16.631  -0.113  1.00 34.31
ATOM   1169  CB  LEU A  80       3.407 -17.927   1.931  1.00 41.23
ATOM   1170  CG  LEU A  80       3.432 -17.268   3.310  1.00 31.35
ATOM   1171  CD1 LEU A  80       4.840 -17.283   3.884  1.00 64.42
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ATOM   1172  CD2 LEU A  80       2.902 -15.844   3.231  1.00 35.25
ATOM   1173  H   LEU A  80       2.657 -20.333   1.685  1.00 65.23
ATOM   1174  HA  LEU A  80       1.271 -17.953   2.074  1.00  3.23
ATOM   1175 2HB  LEU A  80       4.017 -18.816   1.978  1.00 43.54
ATOM   1176 3HB  LEU A  80       3.839 -17.233   1.224  1.00 51.43
ATOM   1177  HG  LEU A  80       2.793 -17.827   3.981  1.00 64.33
ATOM   1178 1HD1 LEU A  80       5.548 -17.038   3.107  1.00 50.53
ATOM   1179 2HD1 LEU A  80       5.060 -18.267   4.273  1.00 41.40
ATOM   1180 3HD1 LEU A  80       4.912 -16.557   4.680  1.00 25.23
ATOM   1181 1HD2 LEU A  80       3.168 -15.311   4.132  1.00 41.10
ATOM   1182 2HD2 LEU A  80       1.826 -15.866   3.131  1.00 11.22
ATOM   1183 3HD2 LEU A  80       3.334 -15.346   2.376  1.00 35.24
ATOM   1184  N   ALA A  81       2.210 -18.470  -1.010  1.00 22.31
ATOM   1185  CA  ALA A  81       2.050 -18.015  -2.385  1.00 53.31
ATOM   1186  C   ALA A  81       0.578 -17.976  -2.782  1.00 70.14
ATOM   1187  O   ALA A  81       0.058 -16.931  -3.172  1.00 33.13
ATOM   1188  CB  ALA A  81       2.831 -18.913  -3.333  1.00 51.41
ATOM   1189  H   ALA A  81       2.626 -19.341  -0.840  1.00 71.12
ATOM   1190  HA  ALA A  81       2.458 -17.017  -2.456  1.00 14.41
ATOM   1191 1HB  ALA A  81       2.277 -19.031  -4.253  1.00 63.23
ATOM   1192 2HB  ALA A  81       3.790 -18.464  -3.545  1.00 21.33
ATOM   1193 3HB  ALA A  81       2.978 -19.879  -2.874  1.00 51.31
ATOM   1194  N   ALA A  82      -0.087 -19.122  -2.682  1.00 75.21
ATOM   1195  CA  ALA A  82      -1.500 -19.218  -3.030  1.00 23.42
ATOM   1196  C   ALA A  82      -2.340 -18.273  -2.178  1.00 75.41
ATOM   1197  O   ALA A  82      -3.229 -17.589  -2.686  1.00 62.44
ATOM   1198  CB  ALA A  82      -1.986 -20.651  -2.869  1.00 74.11
ATOM   1199  H   ALA A  82       0.382 -19.921  -2.365  1.00 63.43
ATOM   1200  HA  ALA A  82      -1.607 -18.942  -4.069  1.00 72.20
ATOM   1201 1HB  ALA A  82      -2.996 -20.732  -3.246  1.00 44.21
ATOM   1202 2HB  ALA A  82      -1.340 -21.315  -3.424  1.00 11.14
ATOM   1203 3HB  ALA A  82      -1.970 -20.921  -1.824  1.00 24.41
ATOM   1204  N   TRP A  83      -2.055 -18.241  -0.882  1.00 21.24
ATOM   1205  CA  TRP A  83      -2.786 -17.380   0.041  1.00 53.23
ATOM   1206  C   TRP A  83      -2.846 -15.949  -0.482  1.00 53.04
ATOM   1207  O   TRP A  83      -3.924 -15.369  -0.608  1.00 30.23
ATOM   1208  CB  TRP A  83      -2.130 -17.404   1.422  1.00 12.12
ATOM   1209  CG  TRP A  83      -2.418 -18.655   2.195  1.00 71.52
ATOM   1210  CD1 TRP A  83      -3.049 -19.776   1.734  1.00  3.05
ATOM   1211  CD2 TRP A  83      -2.088 -18.912   3.564  1.00 64.50
ATOM   1212  CE2 TRP A  83      -2.547 -20.209   3.867  1.00 31.11
ATOM   1213  CE3 TRP A  83      -1.447 -18.175   4.563  1.00 44.43
ATOM   1214  NE1 TRP A  83      -3.130 -20.714   2.735  1.00 32.21
ATOM   1215  CZ2 TRP A  83      -2.386 -20.780   5.127  1.00 70.13
ATOM   1216  CZ3 TRP A  83      -1.288 -18.743   5.812  1.00  2.43
ATOM   1217  CH2 TRP A  83      -1.755 -20.035   6.086  1.00 70.15
ATOM   1218  H   TRP A  83      -1.335 -18.810  -0.536  1.00 33.02
ATOM   1219  HA  TRP A  83      -3.793 -17.763   0.123  1.00 24.14
ATOM   1220 2HB  TRP A  83      -1.060 -17.322   1.307  1.00 22.01
ATOM   1221 3HB  TRP A  83      -2.492 -16.565   1.999  1.00 41.33
ATOM   1222  HD1 TRP A  83      -3.425 -19.893   0.730  1.00 44.54
ATOM   1223  HE1 TRP A  83      -3.538 -21.602   2.651  1.00 53.43
ATOM   1224  HE3 TRP A  83      -1.080 -17.177   4.371  1.00 25.04
ATOM   1225  HZ2 TRP A  83      -2.740 -21.775   5.353  1.00 70.43
ATOM   1226  HZ3 TRP A  83      -0.795 -18.187   6.597  1.00 72.10
ATOM   1227  HH2 TRP A  83      -1.609 -20.439   7.076  1.00 54.44
ATOM   1228  N   ASN A  84      -1.682 -15.385  -0.786  1.00 63.25
ATOM   1229  CA  ASN A  84      -1.603 -14.021  -1.296  1.00 40.01
ATOM   1230  C   ASN A  84      -2.555 -13.824  -2.472  1.00 11.43
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ATOM   1231  O   ASN A  84      -3.077 -12.729  -2.683  1.00 32.45
ATOM   1232  CB  ASN A  84      -0.171 -13.697  -1.725  1.00 44.33
ATOM   1233  CG  ASN A  84      -0.034 -12.285  -2.263  1.00 61.55
ATOM   1234  ND2 ASN A  84       0.323 -12.170  -3.538  1.00 34.35
ATOM   1235  OD1 ASN A  84      -0.246 -11.311  -1.542  1.00 55.21
ATOM   1236  H   ASN A  84      -0.856 -15.898  -0.665  1.00 63.31
ATOM   1237  HA  ASN A  84      -1.890 -13.352  -0.499  1.00 35.42
ATOM   1238 2HB  ASN A  84       0.486 -13.802  -0.874  1.00  2.40
ATOM   1239 3HB  ASN A  84       0.133 -14.388  -2.497  1.00  3.03
ATOM   1240 1HD2 ASN A  84       0.475 -12.991  -4.052  1.00  2.41
ATOM   1241 2HD2 ASN A  84       0.419 -11.270  -3.911  1.00 50.51
ATOM   1242  N   GLN A  85      -2.776 -14.891  -3.233  1.00  2.41
ATOM   1243  CA  GLN A  85      -3.665 -14.834  -4.387  1.00 60.12
ATOM   1244  C   GLN A  85      -5.107 -14.598  -3.952  1.00 55.11
ATOM   1245  O   GLN A  85      -5.791 -13.720  -4.481  1.00  3.12
ATOM   1246  CB  GLN A  85      -3.569 -16.129  -5.195  1.00 71.42
ATOM   1247  CG  GLN A  85      -4.115 -16.007  -6.609  1.00  2.53
ATOM   1248  CD  GLN A  85      -3.547 -17.053  -7.547  1.00 23.23
ATOM   1249  NE2 GLN A  85      -3.054 -16.612  -8.698  1.00  3.31
ATOM   1250  OE1 GLN A  85      -3.551 -18.246  -7.240  1.00 43.23
ATOM   1251  H   GLN A  85      -2.330 -15.735  -3.014  1.00 12.34
ATOM   1252  HA  GLN A  85      -3.350 -14.009  -5.008  1.00 61.31
ATOM   1253 2HB  GLN A  85      -2.533 -16.426  -5.257  1.00  4.53
ATOM   1254 3HB  GLN A  85      -4.126 -16.901  -4.684  1.00  2.33
ATOM   1255 2HG  GLN A  85      -5.188 -16.119  -6.578  1.00 15.35
ATOM   1256 3HG  GLN A  85      -3.867 -15.028  -6.992  1.00 54.32
ATOM   1257 1HE2 GLN A  85      -3.083 -15.647  -8.874  1.00 20.40
ATOM   1258 2HE2 GLN A  85      -2.679 -17.266  -9.323  1.00 34.14
ATOM   1259  N   LEU A  86      -5.565 -15.387  -2.986  1.00 54.42
ATOM   1260  CA  LEU A  86      -6.928 -15.264  -2.480  1.00  1.35
ATOM   1261  C   LEU A  86      -7.138 -13.912  -1.805  1.00 53.22
ATOM   1262  O   LEU A  86      -8.264 -13.425  -1.707  1.00 51.33
ATOM   1263  CB  LEU A  86      -7.229 -16.392  -1.491  1.00 52.23
ATOM   1264  CG  LEU A  86      -7.203 -17.810  -2.063  1.00  2.21
ATOM   1265  CD1 LEU A  86      -6.198 -18.670  -1.311  1.00 55.43
ATOM   1266  CD2 LEU A  86      -8.590 -18.434  -2.006  1.00 44.52
ATOM   1267  H   LEU A  86      -4.974 -16.068  -2.604  1.00 12.21
ATOM   1268  HA  LEU A  86      -7.602 -15.342  -3.319  1.00 61.35
ATOM   1269 2HB  LEU A  86      -6.498 -16.341  -0.699  1.00 72.21
ATOM   1270 3HB  LEU A  86      -8.214 -16.217  -1.082  1.00 30.23
ATOM   1271  HG  LEU A  86      -6.896 -17.768  -3.099  1.00  0.20
ATOM   1272 1HD1 LEU A  86      -5.957 -19.540  -1.902  1.00 32.43
ATOM   1273 2HD1 LEU A  86      -6.625 -18.980  -0.369  1.00 23.31
ATOM   1274 3HD1 LEU A  86      -5.301 -18.098  -1.128  1.00 45.55
ATOM   1275 1HD2 LEU A  86      -9.331 -17.654  -1.913  1.00  1.33
ATOM   1276 2HD2 LEU A  86      -8.653 -19.094  -1.153  1.00 44.04
ATOM   1277 3HD2 LEU A  86      -8.769 -18.995  -2.911  1.00 51.30
ATOM   1278  N   MET A  87      -6.047 -13.310  -1.344  1.00 23.32
ATOM   1279  CA  MET A  87      -6.112 -12.012  -0.682  1.00 22.52
ATOM   1280  C   MET A  87      -6.519 -10.920  -1.666  1.00 23.23
ATOM   1281  O   MET A  87      -7.469 -10.175  -1.423  1.00 51.15
ATOM   1282  CB  MET A  87      -4.761 -11.669  -0.051  1.00 62.50
ATOM   1283  CG  MET A  87      -4.554 -12.293   1.320  1.00 74.22
ATOM   1284  SD  MET A  87      -2.840 -12.205   1.872  1.00 72.01
ATOM   1285  CE  MET A  87      -2.805 -10.572   2.606  1.00 45.40
ATOM   1286  H   MET A  87      -5.177 -13.748  -1.451  1.00 64.44
ATOM   1287  HA  MET A  87      -6.857 -12.075   0.097  1.00 61.11
ATOM   1288 2HB  MET A  87      -3.974 -12.017  -0.703  1.00 63.22
ATOM   1289 3HB  MET A  87      -4.686 -10.597   0.051  1.00 61.13
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ATOM   1290 2HG  MET A  87      -5.174 -11.773   2.035  1.00 75.23
ATOM   1291 3HG  MET A  87      -4.852 -13.330   1.276  1.00 23.51
ATOM   1292 1HE  MET A  87      -2.103 -10.561   3.427  1.00 33.12
ATOM   1293 2HE  MET A  87      -2.500  -9.850   1.863  1.00 44.12
ATOM   1294 3HE  MET A  87      -3.790 -10.320   2.971  1.00 41.44
ATOM   1295  N   LEU A  88      -5.794 -10.830  -2.775  1.00 71.05
ATOM   1296  CA  LEU A  88      -6.080  -9.828  -3.796  1.00 43.15
ATOM   1297  C   LEU A  88      -7.252 -10.260  -4.671  1.00 33.50
ATOM   1298  O   LEU A  88      -7.962  -9.426  -5.232  1.00 11.10
ATOM   1299  CB  LEU A  88      -4.843  -9.588  -4.664  1.00 21.30
ATOM   1300  CG  LEU A  88      -4.962 -10.001  -6.131  1.00 60.44
ATOM   1301  CD1 LEU A  88      -5.679  -8.926  -6.932  1.00 55.12
ATOM   1302  CD2 LEU A  88      -3.587 -10.279  -6.721  1.00 23.25
ATOM   1303  H   LEU A  88      -5.049 -11.451  -2.913  1.00 34.44
ATOM   1304  HA  LEU A  88      -6.341  -8.908  -3.294  1.00 61.41
ATOM   1305 2HB  LEU A  88      -4.618  -8.533  -4.635  1.00 32.20
ATOM   1306 3HB  LEU A  88      -4.023 -10.141  -4.229  1.00 24.41
ATOM   1307  HG  LEU A  88      -5.545 -10.910  -6.197  1.00  4.01
ATOM   1308 1HD1 LEU A  88      -5.698  -8.007  -6.366  1.00 23.33
ATOM   1309 2HD1 LEU A  88      -6.691  -9.244  -7.136  1.00 14.44
ATOM   1310 3HD1 LEU A  88      -5.159  -8.764  -7.865  1.00 30.31
ATOM   1311 1HD2 LEU A  88      -3.359  -9.534  -7.468  1.00 43.03
ATOM   1312 2HD2 LEU A  88      -3.581 -11.259  -7.176  1.00 35.12
ATOM   1313 3HD2 LEU A  88      -2.845 -10.242  -5.937  1.00 11.24
ATOM   1314  N   SER A  89      -7.451 -11.570  -4.781  1.00 25.24
ATOM   1315  CA  SER A  89      -8.536 -12.114  -5.588  1.00 13.01
ATOM   1316  C   SER A  89      -9.892 -11.699  -5.025  1.00 33.31
ATOM   1317  O   SER A  89     -10.851 -11.499  -5.771  1.00 11.45
ATOM   1318  CB  SER A  89      -8.441 -13.640  -5.647  1.00 51.24
ATOM   1319  OG  SER A  89      -7.388 -14.052  -6.501  1.00 71.23
ATOM   1320  H   SER A  89      -6.850 -12.185  -4.309  1.00 74.30
ATOM   1321  HA  SER A  89      -8.438 -11.716  -6.587  1.00 64.41
ATOM   1322 2HB  SER A  89      -8.257 -14.025  -4.656  1.00 64.34
ATOM   1323 3HB  SER A  89      -9.371 -14.041  -6.023  1.00 34.24
ATOM   1324  HG  SER A  89      -7.708 -14.100  -7.405  1.00 55.20
ATOM   1325  N   ARG A  90      -9.964 -11.573  -3.704  1.00  3.11
ATOM   1326  CA  ARG A  90     -11.202 -11.183  -3.040  1.00 23.45
ATOM   1327  C   ARG A  90     -11.342  -9.665  -2.999  1.00 11.45
ATOM   1328  O   ARG A  90     -12.453  -9.134  -3.001  1.00  3.41
ATOM   1329  CB  ARG A  90     -11.242 -11.749  -1.619  1.00 15.45
ATOM   1330  CG  ARG A  90     -10.215 -11.128  -0.686  1.00 42.15
ATOM   1331  CD  ARG A  90     -10.508 -11.462   0.768  1.00 53.42
ATOM   1332  NE  ARG A  90     -11.791 -10.918   1.206  1.00  2.21
ATOM   1333  CZ  ARG A  90     -12.017  -9.621   1.383  1.00 54.15
ATOM   1334  NH1 ARG A  90     -11.053  -8.739   1.159  1.00 64.53
ATOM   1335  NH2 ARG A  90     -13.211  -9.203   1.783  1.00 35.22
ATOM   1336  H   ARG A  90      -9.165 -11.746  -3.163  1.00 32.42
ATOM   1337  HA  ARG A  90     -12.025 -11.594  -3.605  1.00 20.15
ATOM   1338 2HB  ARG A  90     -12.224 -11.575  -1.202  1.00 71.25
ATOM   1339 3HB  ARG A  90     -11.061 -12.812  -1.662  1.00 14.11
ATOM   1340 2HG  ARG A  90      -9.236 -11.507  -0.941  1.00 31.43
ATOM   1341 3HG  ARG A  90     -10.231 -10.055  -0.811  1.00 61.53
ATOM   1342 2HD  ARG A  90     -10.526 -12.535   0.880  1.00 33.44
ATOM   1343 3HD  ARG A  90      -9.723 -11.049   1.383  1.00 11.53
ATOM   1344  HE  ARG A  90     -12.518 -11.552   1.377  1.00  1.42
ATOM   1345 1HH1 ARG A  90     -10.152  -9.051   0.856  1.00 72.22
ATOM   1346 2HH1 ARG A  90     -11.226  -7.763   1.291  1.00 32.32
ATOM   1347 1HH2 ARG A  90     -13.941  -9.865   1.953  1.00 54.34
ATOM   1348 2HH2 ARG A  90     -13.381  -8.227   1.916  1.00 60.22
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ATOM   1349  N   SER A  91     -10.209  -8.971  -2.960  1.00 64.44
ATOM   1350  CA  SER A  91     -10.205  -7.514  -2.914  1.00 51.14
ATOM   1351  C   SER A  91     -11.084  -6.933  -4.018  1.00 63.44
ATOM   1352  O   SER A  91     -11.397  -7.593  -5.009  1.00 60.53
ATOM   1353  CB  SER A  91      -8.777  -6.982  -3.051  1.00 12.24
ATOM   1354  OG  SER A  91      -8.397  -6.242  -1.903  1.00 52.34
ATOM   1355  H   SER A  91      -9.354  -9.452  -2.961  1.00 34.23
ATOM   1356  HA  SER A  91     -10.603  -7.212  -1.957  1.00 51.53
ATOM   1357 2HB  SER A  91      -8.097  -7.811  -3.171  1.00  3.22
ATOM   1358 3HB  SER A  91      -8.717  -6.338  -3.916  1.00 51.02
ATOM   1359  HG  SER A  91      -7.620  -5.716  -2.105  1.00  2.44
ATOM   1360  N   PRO A  92     -11.492  -5.668  -3.844  1.00 43.45
ATOM   1361  CA  PRO A  92     -12.339  -4.969  -4.815  1.00 55.30
ATOM   1362  C   PRO A  92     -11.600  -4.656  -6.111  1.00 42.32
ATOM   1363  O   PRO A  92     -10.541  -4.029  -6.096  1.00 22.42
ATOM   1364  CB  PRO A  92     -12.717  -3.675  -4.089  1.00 74.12
ATOM   1365  CG  PRO A  92     -11.615  -3.453  -3.112  1.00 30.21
ATOM   1366  CD  PRO A  92     -11.156  -4.821  -2.687  1.00 55.13
ATOM   1367  HA  PRO A  92     -13.233  -5.532  -5.039  1.00 74.11
ATOM   1368 2HB  PRO A  92     -12.783  -2.865  -4.802  1.00 73.43
ATOM   1369 3HB  PRO A  92     -13.667  -3.802  -3.591  1.00 43.30
ATOM   1370 2HG  PRO A  92     -10.807  -2.917  -3.585  1.00 41.14
ATOM   1371 3HG  PRO A  92     -11.985  -2.901  -2.261  1.00 34.55
ATOM   1372 2HD  PRO A  92     -10.092  -4.822  -2.504  1.00 72.00
ATOM   1373 3HD  PRO A  92     -11.693  -5.142  -1.807  1.00 32.41
ATOM   1374  N   GLU A  93     -12.165  -5.095  -7.231  1.00 74.51
ATOM   1375  CA  GLU A  93     -11.558  -4.861  -8.536  1.00 21.52
ATOM   1376  C   GLU A  93     -12.206  -3.668  -9.231  1.00 45.44
ATOM   1377  O   GLU A  93     -13.243  -3.802  -9.878  1.00 74.15
ATOM   1378  CB  GLU A  93     -11.686  -6.108  -9.414  1.00 21.23
ATOM   1379  CG  GLU A  93     -10.552  -7.102  -9.228  1.00 63.23
ATOM   1380  CD  GLU A  93      -9.203  -6.528  -9.617  1.00 53.12
ATOM   1381  OE1 GLU A  93      -8.520  -5.969  -8.733  1.00 70.25
ATOM   1382  OE2 GLU A  93      -8.831  -6.637 -10.804  1.00 54.42
ATOM   1383  H   GLU A  93     -13.010  -5.589  -7.178  1.00 54.04
ATOM   1384  HA  GLU A  93     -10.511  -4.648  -8.381  1.00 12.13
ATOM   1385 2HB  GLU A  93     -12.615  -6.605  -9.179  1.00 34.43
ATOM   1386 3HB  GLU A  93     -11.703  -5.803 -10.450  1.00 34.43
ATOM   1387 2HG  GLU A  93     -10.514  -7.397  -8.190  1.00 52.23
ATOM   1388 3HG  GLU A  93     -10.747  -7.970  -9.841  1.00 31.22
TER    1389      GLU A  93
ENDMDL
END
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**LOADED (PDB 2N6Z):**

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HEADER    STRUCTURE FROM CYANA 2.1                03-JUL-15     1PDB
EXPDTA    NMR, 20 STRUCTURES
REMARK  99 B-FACTOR COLUMN STORES ADDITIONAL COORDINATE DIGITS.
MODEL        1
ATOM      1  N   ASP A  14       1.328   0.000   0.000  1.00  4.00
ATOM      2  CA  ASP A  14       2.093  -0.001  -1.242  1.00  0.02
ATOM      3  C   ASP A  14       2.266   1.418  -1.775  1.00 20.14
ATOM      4  O   ASP A  14       1.300   2.171  -1.888  1.00 32.13
ATOM      5  CB  ASP A  14       1.401  -0.872  -2.291  1.00 72.22
ATOM      6  CG  ASP A  14      -0.088  -0.600  -2.379  1.00 41.22
ATOM      7  OD1 ASP A  14      -0.473   0.385  -3.044  1.00  1.33
ATOM      8  OD2 ASP A  14      -0.868  -1.372  -1.784  1.00 72.14
ATOM      9  H   ASP A  14       1.806  -0.000   0.856  1.00 64.11
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ATOM     10  HA  ASP A  14       3.068  -0.414  -1.031  1.00 12.03
ATOM     11 2HB  ASP A  14       1.841  -0.678  -3.258  1.00 41.24
ATOM     12 3HB  ASP A  14       1.544  -1.912  -2.037  1.00 62.24
ATOM     13  N   ASN A  15       3.504   1.776  -2.099  1.00 61.23
ATOM     14  CA  ASN A  15       3.804   3.105  -2.619  1.00  2.24
ATOM     15  C   ASN A  15       3.712   3.128  -4.141  1.00 60.03
ATOM     16  O   ASN A  15       3.429   2.109  -4.771  1.00 63.15
ATOM     17  CB  ASN A  15       5.200   3.546  -2.174  1.00 63.13
ATOM     18  CG  ASN A  15       5.179   4.863  -1.424  1.00  2.44
ATOM     19  ND2 ASN A  15       5.500   4.816  -0.136  1.00 32.32
ATOM     20  OD1 ASN A  15       4.878   5.911  -1.995  1.00 43.51
ATOM     21  H   ASN A  15       4.234   1.131  -1.987  1.00 14.12
ATOM     22  HA  ASN A  15       3.075   3.791  -2.215  1.00 75.10
ATOM     23 2HB  ASN A  15       5.620   2.791  -1.525  1.00 71.13
ATOM     24 3HB  ASN A  15       5.830   3.658  -3.044  1.00 22.21
ATOM     25 1HD2 ASN A  15       5.729   3.945   0.253  1.00 51.44
ATOM     26 2HD2 ASN A  15       5.494   5.653   0.374  1.00 74.24
ATOM     27  N   ARG A  16       3.953   4.297  -4.726  1.00 22.12
ATOM     28  CA  ARG A  16       3.897   4.453  -6.174  1.00 70.23
ATOM     29  C   ARG A  16       5.196   3.984  -6.822  1.00 64.04
ATOM     30  O   ARG A  16       5.184   3.365  -7.887  1.00 55.31
ATOM     31  CB  ARG A  16       3.630   5.914  -6.541  1.00 73.33
ATOM     32  CG  ARG A  16       2.379   6.486  -5.893  1.00 64.51
ATOM     33  CD  ARG A  16       1.249   6.634  -6.899  1.00 35.31
ATOM     34  NE  ARG A  16      -0.008   7.014  -6.258  1.00 64.21
ATOM     35  CZ  ARG A  16      -1.176   7.040  -6.889  1.00 72.22
ATOM     36  NH1 ARG A  16      -1.249   6.709  -8.171  1.00 45.01
ATOM     37  NH2 ARG A  16      -2.276   7.397  -6.238  1.00 24.44
ATOM     38  H   ARG A  16       4.173   5.073  -4.170  1.00  4.42
ATOM     39  HA  ARG A  16       3.085   3.844  -6.542  1.00 51.03
ATOM     40 2HB  ARG A  16       4.474   6.511  -6.231  1.00 44.23
ATOM     41 3HB  ARG A  16       3.520   5.989  -7.613  1.00 31.44
ATOM     42 2HG  ARG A  16       2.059   5.822  -5.103  1.00 40.32
ATOM     43 3HG  ARG A  16       2.611   7.456  -5.480  1.00 25.45
ATOM     44 2HD  ARG A  16       1.520   7.394  -7.616  1.00 72.33
ATOM     45 3HD  ARG A  16       1.112   5.691  -7.408  1.00 12.23
ATOM     46  HE  ARG A  16       0.023   7.262  -5.311  1.00 20.00
ATOM     47 1HH1 ARG A  16      -0.422   6.439  -8.664  1.00 61.32
ATOM     48 2HH1 ARG A  16      -2.130   6.728  -8.644  1.00  0.23
ATOM     49 1HH2 ARG A  16      -2.225   7.646  -5.271  1.00 50.42
ATOM     50 2HH2 ARG A  16      -3.154   7.416  -6.713  1.00 74.04
ATOM     51  N   HIS A  17       6.317   4.283  -6.173  1.00 41.32
ATOM     52  CA  HIS A  17       7.625   3.892  -6.686  1.00 44.42
ATOM     53  C   HIS A  17       7.987   2.481  -6.233  1.00 40.04
ATOM     54  O   HIS A  17       8.656   1.740  -6.953  1.00 52.23
ATOM     55  CB  HIS A  17       8.695   4.880  -6.220  1.00  4.02
ATOM     56  CG  HIS A  17       9.519   5.443  -7.337  1.00 71.21
ATOM     57  CD2 HIS A  17      10.190   4.828  -8.339  1.00 30.11
ATOM     58  ND1 HIS A  17       9.726   6.795  -7.512  1.00 63.21
ATOM     59  CE1 HIS A  17      10.488   6.987  -8.574  1.00 52.23
ATOM     60  NE2 HIS A  17      10.783   5.809  -9.094  1.00  5.50
ATOM     61  H   HIS A  17       6.263   4.778  -5.329  1.00 52.24
ATOM     62  HA  HIS A  17       7.578   3.910  -7.764  1.00 75.24
ATOM     63 2HB  HIS A  17       8.218   5.705  -5.712  1.00 54.14
ATOM     64 3HB  HIS A  17       9.363   4.380  -5.533  1.00 64.25
ATOM     65  HD1 HIS A  17       9.367   7.507  -6.944  1.00  2.05
ATOM     66  HD2 HIS A  17      10.248   3.763  -8.513  1.00 61.43
ATOM     67  HE1 HIS A  17      10.814   7.944  -8.953  1.00 41.14
ATOM     68  N   ALA A  18       7.541   2.116  -5.036  1.00 12.52
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ATOM     69  CA  ALA A  18       7.816   0.794  -4.488  1.00 43.10
ATOM     70  C   ALA A  18       7.492  -0.298  -5.501  1.00 73.41
ATOM     71  O   ALA A  18       8.113  -1.361  -5.503  1.00 12.22
ATOM     72  CB  ALA A  18       7.026   0.579  -3.206  1.00  2.04
ATOM     73  H   ALA A  18       7.013   2.752  -4.509  1.00 35.50
ATOM     74  HA  ALA A  18       8.868   0.746  -4.246  1.00 64.30
ATOM     75 1HB  ALA A  18       6.295   1.367  -3.098  1.00  1.21
ATOM     76 2HB  ALA A  18       6.524  -0.376  -3.249  1.00 14.44
ATOM     77 3HB  ALA A  18       7.699   0.594  -2.362  1.00  4.44
ATOM     78  N   ALA A  19       6.515  -0.030  -6.361  1.00 35.20
ATOM     79  CA  ALA A  19       6.109  -0.990  -7.380  1.00 34.21
ATOM     80  C   ALA A  19       7.316  -1.525  -8.143  1.00  1.25
ATOM     81  O   ALA A  19       7.322  -2.672  -8.589  1.00 22.22
ATOM     82  CB  ALA A  19       5.116  -0.353  -8.340  1.00 55.51
ATOM     83  H   ALA A  19       6.057   0.835  -6.310  1.00 33.54
ATOM     84  HA  ALA A  19       5.615  -1.814  -6.885  1.00 12.14
ATOM     85 1HB  ALA A  19       4.119  -0.432  -7.931  1.00 73.41
ATOM     86 2HB  ALA A  19       5.366   0.689  -8.478  1.00 62.41
ATOM     87 3HB  ALA A  19       5.157  -0.862  -9.291  1.00 34.30
ATOM     88  N   ASP A  20       8.336  -0.686  -8.289  1.00 20.31
ATOM     89  CA  ASP A  20       9.550  -1.075  -8.998  1.00 32.03
ATOM     90  C   ASP A  20      10.089  -2.399  -8.466  1.00 70.30
ATOM     91  O   ASP A  20      10.617  -3.215  -9.223  1.00 15.04
ATOM     92  CB  ASP A  20      10.615   0.014  -8.864  1.00  1.21
ATOM     93  CG  ASP A  20      10.740   0.859 -10.116  1.00 52.15
ATOM     94  OD1 ASP A  20      11.823   0.842 -10.739  1.00 34.12
ATOM     95  OD2 ASP A  20       9.754   1.537 -10.475  1.00 23.20
ATOM     96  H   ASP A  20       8.271   0.216  -7.910  1.00 64.34
ATOM     97  HA  ASP A  20       9.300  -1.195 -10.041  1.00 64.40
ATOM     98 2HB  ASP A  20      10.356   0.663  -8.039  1.00 62.43
ATOM     99 3HB  ASP A  20      11.571  -0.448  -8.666  1.00 72.54
ATOM    100  N   TYR A  21       9.954  -2.606  -7.161  1.00 10.22
ATOM    101  CA  TYR A  21      10.431  -3.829  -6.527  1.00 73.42
ATOM    102  C   TYR A  21       9.676  -5.046  -7.055  1.00  2.21
ATOM    103  O   TYR A  21      10.253  -6.119  -7.230  1.00 51.33
ATOM    104  CB  TYR A  21      10.273  -3.737  -5.009  1.00  3.15
ATOM    105  CG  TYR A  21      11.572  -3.910  -4.253  1.00 72.15
ATOM    106  CD1 TYR A  21      11.633  -4.695  -3.109  1.00 32.24
ATOM    107  CD2 TYR A  21      12.737  -3.288  -4.684  1.00 61.20
ATOM    108  CE1 TYR A  21      12.817  -4.856  -2.415  1.00 13.10
ATOM    109  CE2 TYR A  21      13.926  -3.444  -3.998  1.00 33.54
ATOM    110  CZ  TYR A  21      13.960  -4.229  -2.864  1.00 24.03
ATOM    111  OH  TYR A  21      15.142  -4.386  -2.176  1.00 41.03
ATOM    112  H   TYR A  21       9.525  -1.918  -6.610  1.00 30.54
ATOM    113  HA  TYR A  21      11.479  -3.939  -6.765  1.00 32.25
ATOM    114 2HB  TYR A  21       9.869  -2.770  -4.754  1.00 12.44
ATOM    115 3HB  TYR A  21       9.591  -4.506  -4.677  1.00  1.12
ATOM    116  HD1 TYR A  21      10.735  -5.185  -2.760  1.00 23.14
ATOM    117  HD2 TYR A  21      12.706  -2.674  -5.572  1.00 43.04
ATOM    118  HE1 TYR A  21      12.845  -5.470  -1.527  1.00 75.41
ATOM    119  HE2 TYR A  21      14.821  -2.953  -4.349  1.00 22.25
ATOM    120  HH  TYR A  21      14.963  -4.408  -1.233  1.00 41.13
ATOM    121  N   GLN A  22       8.383  -4.869  -7.306  1.00 41.41
ATOM    122  CA  GLN A  22       7.549  -5.951  -7.814  1.00 33.32
ATOM    123  C   GLN A  22       8.188  -6.605  -9.034  1.00 42.03
ATOM    124  O   GLN A  22       8.126  -7.823  -9.201  1.00 52.42
ATOM    125  CB  GLN A  22       6.157  -5.426  -8.172  1.00 64.20
ATOM    126  CG  GLN A  22       5.454  -4.730  -7.018  1.00 61.01
ATOM    127  CD  GLN A  22       4.014  -4.381  -7.338  1.00 31.15
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ATOM    128  NE2 GLN A  22       3.082  -4.992  -6.615  1.00  2.44
ATOM    129  OE1 GLN A  22       3.741  -3.572  -8.224  1.00 42.35
ATOM    130  H   GLN A  22       7.981  -3.990  -7.146  1.00 61.00
ATOM    131  HA  GLN A  22       7.454  -6.691  -7.033  1.00 43.31
ATOM    132 2HB  GLN A  22       6.250  -4.723  -8.986  1.00 74.23
ATOM    133 3HB  GLN A  22       5.544  -6.256  -8.491  1.00 13.21
ATOM    134 2HG  GLN A  22       5.467  -5.383  -6.158  1.00 64.32
ATOM    135 3HG  GLN A  22       5.987  -3.820  -6.785  1.00 50.25
ATOM    136 1HE2 GLN A  22       3.373  -5.624  -5.924  1.00  4.32
ATOM    137 2HE2 GLN A  22       2.143  -4.784  -6.799  1.00 63.22
ATOM    138  N   GLN A  23       8.802  -5.788  -9.884  1.00 10.42
ATOM    139  CA  GLN A  23       9.452  -6.287 -11.090  1.00 32.44
ATOM    140  C   GLN A  23      10.874  -6.748 -10.790  1.00 64.41
ATOM    141  O   GLN A  23      11.372  -7.697 -11.398  1.00 32.41
ATOM    142  CB  GLN A  23       9.471  -5.205 -12.170  1.00 53.03
ATOM    143  CG  GLN A  23       8.146  -4.476 -12.325  1.00 35.24
ATOM    144  CD  GLN A  23       7.758  -4.271 -13.776  1.00 33.43
ATOM    145  NE2 GLN A  23       6.832  -5.090 -14.263  1.00 25.03
ATOM    146  OE1 GLN A  23       8.284  -3.387 -14.452  1.00 72.11
ATOM    147  H   GLN A  23       8.818  -4.827  -9.696  1.00 13.44
ATOM    148  HA  GLN A  23       8.882  -7.131 -11.448  1.00 15.10
ATOM    149 2HB  GLN A  23      10.230  -4.479 -11.922  1.00 40.53
ATOM    150 3HB  GLN A  23       9.717  -5.663 -13.117  1.00 41.40
ATOM    151 2HG  GLN A  23       7.373  -5.054 -11.840  1.00 73.30
ATOM    152 3HG  GLN A  23       8.223  -3.510 -11.848  1.00 23.21
ATOM    153 1HE2 GLN A  23       6.456  -5.770 -13.665  1.00 63.40
ATOM    154 2HE2 GLN A  23       6.562  -4.980 -15.197  1.00 43.42
ATOM    155  N   LEU A  24      11.525  -6.071  -9.851  1.00 31.14
ATOM    156  CA  LEU A  24      12.892  -6.411  -9.470  1.00 53.11
ATOM    157  C   LEU A  24      12.950  -7.792  -8.825  1.00 50.12
ATOM    158  O   LEU A  24      13.653  -8.682  -9.304  1.00 33.21
ATOM    159  CB  LEU A  24      13.450  -5.362  -8.507  1.00 13.31
ATOM    160  CG  LEU A  24      14.973  -5.236  -8.461  1.00 11.42
ATOM    161  CD1 LEU A  24      15.389  -3.773  -8.502  1.00 31.43
ATOM    162  CD2 LEU A  24      15.527  -5.915  -7.217  1.00 32.01
ATOM    163  H   LEU A  24      11.077  -5.325  -9.401  1.00 54.15
ATOM    164  HA  LEU A  24      13.493  -6.420 -10.367  1.00 74.12
ATOM    165 2HB  LEU A  24      13.047  -4.402  -8.794  1.00 23.42
ATOM    166 3HB  LEU A  24      13.107  -5.611  -7.513  1.00 31.23
ATOM    167  HG  LEU A  24      15.395  -5.726  -9.327  1.00 72.50
ATOM    168 1HD1 LEU A  24      16.322  -3.650  -7.973  1.00 50.22
ATOM    169 2HD1 LEU A  24      14.627  -3.169  -8.033  1.00 34.03
ATOM    170 3HD1 LEU A  24      15.512  -3.463  -9.529  1.00 63.00
ATOM    171 1HD2 LEU A  24      14.884  -6.737  -6.940  1.00 73.40
ATOM    172 2HD2 LEU A  24      15.569  -5.202  -6.406  1.00 34.21
ATOM    173 3HD2 LEU A  24      16.520  -6.287  -7.422  1.00 15.12
ATOM    174  N   ARG A  25      12.206  -7.963  -7.738  1.00 35.43
ATOM    175  CA  ARG A  25      12.172  -9.236  -7.028  1.00 32.32
ATOM    176  C   ARG A  25      11.925 -10.391  -7.994  1.00 33.30
ATOM    177  O   ARG A  25      12.470 -11.481  -7.825  1.00 63.21
ATOM    178  CB  ARG A  25      11.085  -9.216  -5.952  1.00 15.11
ATOM    179  CG  ARG A  25      11.160  -8.008  -5.033  1.00 14.41
ATOM    180  CD  ARG A  25      11.036  -8.410  -3.572  1.00 35.42
ATOM    181  NE  ARG A  25      10.020  -7.627  -2.873  1.00 23.35
ATOM    182  CZ  ARG A  25       8.719  -7.724  -3.119  1.00 34.32
ATOM    183  NH1 ARG A  25       8.276  -8.567  -4.042  1.00  2.20
ATOM    184  NH2 ARG A  25       7.856  -6.978  -2.440  1.00 44.14
ATOM    185  H   ARG A  25      11.667  -7.216  -7.404  1.00 54.22
ATOM    186  HA  ARG A  25      13.132  -9.378  -6.554  1.00 53.23
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ATOM    187 2HB  ARG A  25      10.118  -9.215  -6.433  1.00 54.44
ATOM    188 3HB  ARG A  25      11.176 -10.106  -5.348  1.00 72.33
ATOM    189 2HG  ARG A  25      12.109  -7.514  -5.179  1.00 61.12
ATOM    190 3HG  ARG A  25      10.357  -7.329  -5.280  1.00 51.10
ATOM    191 2HD  ARG A  25      10.768  -9.455  -3.522  1.00 31.33
ATOM    192 3HD  ARG A  25      11.989  -8.260  -3.089  1.00  4.22
ATOM    193  HE  ARG A  25      10.325  -6.998  -2.186  1.00 63.42
ATOM    194 1HH1 ARG A  25       8.924  -9.131  -4.554  1.00 35.21
ATOM    195 2HH1 ARG A  25       7.295  -8.639  -4.225  1.00  4.14
ATOM    196 1HH2 ARG A  25       8.186  -6.342  -1.744  1.00  2.25
ATOM    197 2HH2 ARG A  25       6.877  -7.052  -2.626  1.00 42.45
ATOM    198  N   GLU A  26      11.099 -10.143  -9.006  1.00 33.43
ATOM    199  CA  GLU A  26      10.779 -11.164  -9.997  1.00 51.53
ATOM    200  C   GLU A  26      11.926 -11.337 -10.989  1.00 31.02
ATOM    201  O   GLU A  26      12.366 -12.455 -11.256  1.00 32.43
ATOM    202  CB  GLU A  26       9.496 -10.795 -10.745  1.00 35.33
ATOM    203  CG  GLU A  26       8.239 -10.937  -9.903  1.00 33.13
ATOM    204  CD  GLU A  26       7.008 -10.381 -10.592  1.00 44.55
ATOM    205  OE1 GLU A  26       7.100 -10.052 -11.794  1.00 62.20
ATOM    206  OE2 GLU A  26       5.955 -10.273  -9.932  1.00 15.15
ATOM    207  H   GLU A  26      10.695  -9.254  -9.087  1.00 33.34
ATOM    208  HA  GLU A  26      10.626 -12.096  -9.476  1.00 74.31
ATOM    209 2HB  GLU A  26       9.568  -9.770 -11.077  1.00 61.20
ATOM    210 3HB  GLU A  26       9.399 -11.438 -11.608  1.00  4.43
ATOM    211 2HG  GLU A  26       8.074 -11.984  -9.697  1.00 65.35
ATOM    212 3HG  GLU A  26       8.382 -10.407  -8.972  1.00 65.53
ATOM    213  N   ARG A  27      12.405 -10.222 -11.531  1.00 72.44
ATOM    214  CA  ARG A  27      13.499 -10.250 -12.495  1.00 31.44
ATOM    215  C   ARG A  27      14.659 -11.094 -11.975  1.00 23.03
ATOM    216  O   ARG A  27      15.180 -11.957 -12.683  1.00 51.11
ATOM    217  CB  ARG A  27      13.981  -8.829 -12.793  1.00 31.54
ATOM    218  CG  ARG A  27      13.684  -8.371 -14.211  1.00 12.52
ATOM    219  CD  ARG A  27      12.662  -7.245 -14.229  1.00 52.45
ATOM    220  NE  ARG A  27      12.231  -6.919 -15.586  1.00 72.13
ATOM    221  CZ  ARG A  27      11.559  -5.817 -15.899  1.00 51.24
ATOM    222  NH1 ARG A  27      11.243  -4.939 -14.957  1.00 43.34
ATOM    223  NH2 ARG A  27      11.202  -5.591 -17.157  1.00 54.22
ATOM    224  H   ARG A  27      12.013  -9.360 -11.279  1.00 34.52
ATOM    225  HA  ARG A  27      13.127 -10.694 -13.406  1.00 43.42
ATOM    226 2HB  ARG A  27      13.498  -8.147 -12.109  1.00  1.04
ATOM    227 3HB  ARG A  27      15.049  -8.785 -12.639  1.00 75.02
ATOM    228 2HG  ARG A  27      14.599  -8.019 -14.665  1.00 14.34
ATOM    229 3HG  ARG A  27      13.297  -9.206 -14.776  1.00  3.43
ATOM    230 2HD  ARG A  27      11.801  -7.548 -13.652  1.00  4.21
ATOM    231 3HD  ARG A  27      13.105  -6.367 -13.782  1.00 34.41
ATOM    232  HE  ARG A  27      12.454  -7.554 -16.298  1.00 34.20
ATOM    233 1HH1 ARG A  27      11.512  -5.106 -14.009  1.00 41.10
ATOM    234 2HH1 ARG A  27      10.738  -4.109 -15.196  1.00 43.10
ATOM    235 1HH2 ARG A  27      11.438  -6.250 -17.870  1.00 70.30
ATOM    236 2HH2 ARG A  27      10.696  -4.761 -17.392  1.00 30.23
ATOM    237  N   LEU A  28      15.060 -10.839 -10.734  1.00 42.23
ATOM    238  CA  LEU A  28      16.160 -11.574 -10.119  1.00 34.11
ATOM    239  C   LEU A  28      15.950 -13.079 -10.252  1.00 31.14
ATOM    240  O   LEU A  28      16.833 -13.800 -10.718  1.00 13.13
ATOM    241  CB  LEU A  28      16.290 -11.194  -8.643  1.00 25.10
ATOM    242  CG  LEU A  28      17.190  -9.997  -8.335  1.00 42.44
ATOM    243  CD1 LEU A  28      16.435  -8.693  -8.545  1.00 72.54
ATOM    244  CD2 LEU A  28      17.724 -10.082  -6.913  1.00 65.21
ATOM    245  H   LEU A  28      14.607 -10.140 -10.219  1.00 51.31
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ATOM    246  HA  LEU A  28      17.069 -11.303 -10.634  1.00 50.31
ATOM    247 2HB  LEU A  28      15.303 -10.970  -8.271  1.00 12.54
ATOM    248 3HB  LEU A  28      16.686 -12.051  -8.116  1.00  0.44
ATOM    249  HG  LEU A  28      18.034 -10.005  -9.012  1.00 30.23
ATOM    250 1HD1 LEU A  28      17.128  -7.867  -8.517  1.00  2.25
ATOM    251 2HD1 LEU A  28      15.699  -8.574  -7.764  1.00  2.02
ATOM    252 3HD1 LEU A  28      15.939  -8.715  -9.505  1.00 63.41
ATOM    253 1HD2 LEU A  28      16.917 -10.332  -6.240  1.00 63.24
ATOM    254 2HD2 LEU A  28      18.147  -9.129  -6.629  1.00 61.25
ATOM    255 3HD2 LEU A  28      18.487 -10.845  -6.860  1.00 51.04
ATOM    256  N   ILE A  29      14.776 -13.546  -9.841  1.00 14.00
ATOM    257  CA  ILE A  29      14.449 -14.965  -9.917  1.00 41.53
ATOM    258  C   ILE A  29      14.711 -15.514 -11.315  1.00 73.34
ATOM    259  O   ILE A  29      15.106 -16.669 -11.474  1.00 50.13
ATOM    260  CB  ILE A  29      12.978 -15.225  -9.543  1.00  1.44
ATOM    261  CG1 ILE A  29      12.878 -15.733  -8.103  1.00  1.01
ATOM    262  CG2 ILE A  29      12.354 -16.222 -10.507  1.00 23.31
ATOM    263  CD1 ILE A  29      13.627 -14.876  -7.106  1.00 61.42
ATOM    264  H   ILE A  29      14.113 -12.922  -9.479  1.00 10.30
ATOM    265  HA  ILE A  29      15.078 -15.489  -9.212  1.00 74.32
ATOM    266  HB  ILE A  29      12.438 -14.294  -9.626  1.00 45.35
ATOM    267 2HG1 ILE A  29      11.841 -15.755  -7.807  1.00 23.42
ATOM    268 3HG1 ILE A  29      13.284 -16.733  -8.053  1.00 60.14
ATOM    269 1HG2 ILE A  29      12.993 -17.090 -10.590  1.00 53.54
ATOM    270 2HG2 ILE A  29      11.386 -16.524 -10.136  1.00 42.41
ATOM    271 3HG2 ILE A  29      12.242 -15.763 -11.478  1.00 32.35
ATOM    272 1HD1 ILE A  29      13.462 -15.256  -6.109  1.00 24.42
ATOM    273 2HD1 ILE A  29      14.682 -14.900  -7.332  1.00  5.02
ATOM    274 3HD1 ILE A  29      13.269 -13.858  -7.166  1.00 62.40
ATOM    275  N   GLN A  30      14.489 -14.679 -12.325  1.00 11.10
ATOM    276  CA  GLN A  30      14.702 -15.082 -13.710  1.00 51.41
ATOM    277  C   GLN A  30      16.174 -15.383 -13.969  1.00 44.51
ATOM    278  O   GLN A  30      16.508 -16.333 -14.676  1.00 32.24
ATOM    279  CB  GLN A  30      14.218 -13.986 -14.662  1.00 32.40
ATOM    280  CG  GLN A  30      12.904 -13.350 -14.239  1.00 12.20
ATOM    281  CD  GLN A  30      12.250 -12.563 -15.358  1.00 34.23
ATOM    282  NE2 GLN A  30      11.180 -13.113 -15.921  1.00 40.41
ATOM    283  OE1 GLN A  30      12.701 -11.474 -15.712  1.00 55.40
ATOM    284  H   GLN A  30      14.174 -13.771 -12.134  1.00 63.20
ATOM    285  HA  GLN A  30      14.128 -15.978 -13.886  1.00 72.54
ATOM    286 2HB  GLN A  30      14.969 -13.212 -14.712  1.00 73.15
ATOM    287 3HB  GLN A  30      14.086 -14.413 -15.645  1.00 74.32
ATOM    288 2HG  GLN A  30      12.226 -14.129 -13.924  1.00 73.10
ATOM    289 3HG  GLN A  30      13.092 -12.682 -13.411  1.00 64.23
ATOM    290 1HE2 GLN A  30      10.877 -13.983 -15.586  1.00 54.12
ATOM    291 2HE2 GLN A  30      10.737 -12.626 -16.646  1.00  0.32
ATOM    292  N   GLU A  31      17.051 -14.566 -13.393  1.00 13.32
ATOM    293  CA  GLU A  31      18.488 -14.745 -13.563  1.00 52.12
ATOM    294  C   GLU A  31      19.016 -15.828 -12.627  1.00 12.12
ATOM    295  O   GLU A  31      19.929 -16.577 -12.977  1.00 41.52
ATOM    296  CB  GLU A  31      19.223 -13.428 -13.304  1.00 33.23
ATOM    297  CG  GLU A  31      18.450 -12.201 -13.756  1.00 43.52
ATOM    298  CD  GLU A  31      19.291 -10.939 -13.729  1.00 25.20
ATOM    299  OE1 GLU A  31      19.675 -10.459 -14.816  1.00 52.04
ATOM    300  OE2 GLU A  31      19.567 -10.433 -12.621  1.00 54.44
ATOM    301  H   GLU A  31      16.723 -13.825 -12.841  1.00 22.22
ATOM    302  HA  GLU A  31      18.665 -15.050 -14.583  1.00 62.33
ATOM    303 2HB  GLU A  31      19.413 -13.339 -12.244  1.00 50.33
ATOM    304 3HB  GLU A  31      20.166 -13.447 -13.829  1.00 22.50
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ATOM    305 2HG  GLU A  31      18.103 -12.361 -14.766  1.00 20.22
ATOM    306 3HG  GLU A  31      17.601 -12.064 -13.102  1.00 44.24
ATOM    307  N   LEU A  32      18.435 -15.905 -11.434  1.00 44.14
ATOM    308  CA  LEU A  32      18.847 -16.896 -10.446  1.00 12.32
ATOM    309  C   LEU A  32      18.337 -18.283 -10.821  1.00 34.44
ATOM    310  O   LEU A  32      18.861 -19.295 -10.356  1.00 41.43
ATOM    311  CB  LEU A  32      18.330 -16.507  -9.060  1.00 11.04
ATOM    312  CG  LEU A  32      18.785 -15.147  -8.531  1.00  3.55
ATOM    313  CD1 LEU A  32      18.198 -14.886  -7.152  1.00 53.13
ATOM    314  CD2 LEU A  32      20.305 -15.073  -8.487  1.00 54.53
ATOM    315  H   LEU A  32      17.713 -15.281 -11.212  1.00 62.55
ATOM    316  HA  LEU A  32      19.926 -16.915 -10.426  1.00 63.40
ATOM    317 2HB  LEU A  32      17.251 -16.502  -9.098  1.00 65.33
ATOM    318 3HB  LEU A  32      18.660 -17.262  -8.361  1.00 20.44
ATOM    319  HG  LEU A  32      18.431 -14.371  -9.196  1.00 34.50
ATOM    320 1HD1 LEU A  32      18.921 -14.362  -6.546  1.00 21.53
ATOM    321 2HD1 LEU A  32      17.948 -15.826  -6.684  1.00 31.32
ATOM    322 3HD1 LEU A  32      17.306 -14.284  -7.249  1.00 74.43
ATOM    323 1HD2 LEU A  32      20.624 -14.827  -7.485  1.00 62.13
ATOM    324 2HD2 LEU A  32      20.647 -14.309  -9.171  1.00 63.53
ATOM    325 3HD2 LEU A  32      20.720 -16.027  -8.774  1.00 72.04
ATOM    326  N   ASN A  33      17.311 -18.323 -11.666  1.00  4.05
ATOM    327  CA  ASN A  33      16.731 -19.587 -12.105  1.00  1.15
ATOM    328  C   ASN A  33      16.211 -20.389 -10.915  1.00 53.34
ATOM    329  O   ASN A  33      16.524 -21.570 -10.764  1.00 70.33
ATOM    330  CB  ASN A  33      17.768 -20.408 -12.873  1.00 60.43
ATOM    331  CG  ASN A  33      17.136 -21.297 -13.927  1.00 32.43
ATOM    332  ND2 ASN A  33      17.860 -22.331 -14.340  1.00 74.20
ATOM    333  OD1 ASN A  33      16.010 -21.057 -14.363  1.00 70.42
ATOM    334  H   ASN A  33      16.936 -17.483 -12.002  1.00 13.53
ATOM    335  HA  ASN A  33      15.905 -19.362 -12.761  1.00 55.44
ATOM    336 2HB  ASN A  33      18.458 -19.737 -13.364  1.00 22.33
ATOM    337 3HB  ASN A  33      18.311 -21.033 -12.180  1.00 13.44
ATOM    338 1HD2 ASN A  33      18.748 -22.461 -13.948  1.00  5.22
ATOM    339 2HD2 ASN A  33      17.475 -22.922 -15.021  1.00  3.00
ATOM    340  N   LEU A  34      15.414 -19.739 -10.074  1.00 42.10
ATOM    341  CA  LEU A  34      14.849 -20.391  -8.898  1.00 12.22
ATOM    342  C   LEU A  34      13.508 -19.769  -8.522  1.00 53.32
ATOM    343  O   LEU A  34      13.008 -18.879  -9.212  1.00  2.12
ATOM    344  CB  LEU A  34      15.819 -20.290  -7.719  1.00 75.31
ATOM    345  CG  LEU A  34      16.599 -18.980  -7.602  1.00 33.43
ATOM    346  CD1 LEU A  34      15.647 -17.804  -7.445  1.00 62.53
ATOM    347  CD2 LEU A  34      17.571 -19.042  -6.432  1.00 54.43
ATOM    348  H   LEU A  34      15.200 -18.799 -10.247  1.00  4.31
ATOM    349  HA  LEU A  34      14.694 -21.432  -9.138  1.00 62.15
ATOM    350 2HB  LEU A  34      15.250 -20.418  -6.811  1.00 74.41
ATOM    351 3HB  LEU A  34      16.534 -21.096  -7.811  1.00 14.54
ATOM    352  HG  LEU A  34      17.171 -18.828  -8.506  1.00 45.41
ATOM    353 1HD1 LEU A  34      16.214 -16.887  -7.395  1.00 31.21
ATOM    354 2HD1 LEU A  34      15.074 -17.924  -6.538  1.00 54.21
ATOM    355 3HD1 LEU A  34      14.977 -17.769  -8.292  1.00 43.41
ATOM    356 1HD2 LEU A  34      17.226 -18.389  -5.644  1.00 35.33
ATOM    357 2HD2 LEU A  34      18.549 -18.722  -6.761  1.00 23.53
ATOM    358 3HD2 LEU A  34      17.627 -20.055  -6.063  1.00 55.24
ATOM    359  N   THR A  35      12.929 -20.241  -7.422  1.00 61.35
ATOM    360  CA  THR A  35      11.647 -19.731  -6.954  1.00 73.21
ATOM    361  C   THR A  35      11.816 -18.404  -6.224  1.00  5.12
ATOM    362  O   THR A  35      12.909 -18.046  -5.782  1.00 53.14
ATOM    363  CB  THR A  35      10.952 -20.735  -6.015  1.00 72.43
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ATOM    364  CG2 THR A  35       9.823 -21.457  -6.735  1.00 73.33
ATOM    365  OG1 THR A  35      11.902 -21.690  -5.529  1.00 71.24
ATOM    366  H   THR A  35      13.376 -20.951  -6.915  1.00 44.45
ATOM    367  HA  THR A  35      11.014 -19.579  -7.816  1.00 55.40
ATOM    368  HB  THR A  35      10.536 -20.194  -5.177  1.00 44.35
ATOM    369  HG1 THR A  35      11.482 -22.255  -4.876  1.00 24.30
ATOM    370 1HG2 THR A  35       9.026 -21.667  -6.037  1.00 10.41
ATOM    371 2HG2 THR A  35      10.193 -22.384  -7.148  1.00  2.05
ATOM    372 3HG2 THR A  35       9.448 -20.833  -7.532  1.00 75.11
ATOM    373  N   PRO A  36      10.712 -17.655  -6.091  1.00 53.04
ATOM    374  CA  PRO A  36      10.713 -16.355  -5.413  1.00 60.33
ATOM    375  C   PRO A  36      10.923 -16.487  -3.909  1.00 13.33
ATOM    376  O   PRO A  36      11.284 -15.521  -3.237  1.00 53.32
ATOM    377  CB  PRO A  36       9.319 -15.798  -5.712  1.00 41.12
ATOM    378  CG  PRO A  36       8.474 -17.001  -5.953  1.00 52.33
ATOM    379  CD  PRO A  36       9.376 -18.019  -6.593  1.00 20.40
ATOM    380  HA  PRO A  36      11.462 -15.694  -5.824  1.00 25.53
ATOM    381 2HB  PRO A  36       8.966 -15.230  -4.863  1.00 42.40
ATOM    382 3HB  PRO A  36       9.361 -15.163  -6.585  1.00 34.52
ATOM    383 2HG  PRO A  36       8.091 -17.375  -5.016  1.00  2.51
ATOM    384 3HG  PRO A  36       7.661 -16.750  -6.619  1.00 31.11
ATOM    385 2HD  PRO A  36       9.104 -19.016  -6.277  1.00 41.41
ATOM    386 3HD  PRO A  36       9.334 -17.938  -7.669  1.00 72.12
ATOM    387  N   GLN A  37      10.695 -17.688  -3.387  1.00 15.53
ATOM    388  CA  GLN A  37      10.859 -17.944  -1.961  1.00 13.23
ATOM    389  C   GLN A  37      12.204 -18.603  -1.678  1.00 24.35
ATOM    390  O   GLN A  37      12.773 -18.436  -0.599  1.00 51.30
ATOM    391  CB  GLN A  37       9.724 -18.832  -1.447  1.00  1.44
ATOM    392  CG  GLN A  37       9.117 -18.347  -0.140  1.00 21.33
ATOM    393  CD  GLN A  37       9.591 -19.149   1.056  1.00 31.24
ATOM    394  NE2 GLN A  37      10.691 -18.717   1.661  1.00 64.01
ATOM    395  OE1 GLN A  37       8.975 -20.147   1.433  1.00 12.41
ATOM    396  H   GLN A  37      10.409 -18.418  -3.974  1.00 12.53
ATOM    397  HA  GLN A  37      10.822 -16.995  -1.447  1.00 71.02
ATOM    398 2HB  GLN A  37       8.943 -18.864  -2.191  1.00 60.53
ATOM    399 3HB  GLN A  37      10.106 -19.830  -1.292  1.00 70.05
ATOM    400 2HG  GLN A  37       9.391 -17.313   0.009  1.00 64.34
ATOM    401 3HG  GLN A  37       8.042 -18.427  -0.206  1.00 21.42
ATOM    402 1HE2 GLN A  37      11.129 -17.914   1.306  1.00 31.42
ATOM    403 2HE2 GLN A  37      11.019 -19.216   2.437  1.00 45.30
ATOM    404  N   GLN A  38      12.707 -19.353  -2.653  1.00 22.21
ATOM    405  CA  GLN A  38      13.986 -20.039  -2.507  1.00 51.40
ATOM    406  C   GLN A  38      15.138 -19.040  -2.474  1.00 62.03
ATOM    407  O   GLN A  38      16.142 -19.256  -1.794  1.00 32.14
ATOM    408  CB  GLN A  38      14.189 -21.033  -3.652  1.00  2.33
ATOM    409  CG  GLN A  38      13.658 -22.425  -3.350  1.00 41.22
ATOM    410  CD  GLN A  38      14.513 -23.170  -2.344  1.00 35.02
ATOM    411  NE2 GLN A  38      14.473 -24.496  -2.401  1.00 25.15
ATOM    412  OE1 GLN A  38      15.200 -22.561  -1.524  1.00 43.31
ATOM    413  H   GLN A  38      12.207 -19.448  -3.489  1.00 73.04
ATOM    414  HA  GLN A  38      13.968 -20.579  -1.573  1.00 14.34
ATOM    415 2HB  GLN A  38      13.684 -20.660  -4.530  1.00 72.22
ATOM    416 3HB  GLN A  38      15.246 -21.112  -3.860  1.00 51.24
ATOM    417 2HG  GLN A  38      12.657 -22.336  -2.954  1.00 24.53
ATOM    418 3HG  GLN A  38      13.631 -22.992  -4.269  1.00 24.34
ATOM    419 1HE2 GLN A  38      13.904 -24.913  -3.081  1.00 33.21
ATOM    420 2HE2 GLN A  38      15.016 -25.003  -1.763  1.00  4.14
ATOM    421  N   LEU A  39      14.988 -17.947  -3.214  1.00 41.10
ATOM    422  CA  LEU A  39      16.017 -16.914  -3.270  1.00 52.02
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ATOM    423  C   LEU A  39      16.453 -16.503  -1.868  1.00 21.04
ATOM    424  O   LEU A  39      15.702 -16.653  -0.903  1.00 70.24
ATOM    425  CB  LEU A  39      15.501 -15.693  -4.034  1.00 74.42
ATOM    426  CG  LEU A  39      14.891 -14.578  -3.184  1.00 45.22
ATOM    427  CD1 LEU A  39      15.968 -13.605  -2.729  1.00 62.11
ATOM    428  CD2 LEU A  39      13.805 -13.848  -3.961  1.00 31.42
ATOM    429  H   LEU A  39      14.167 -17.830  -3.735  1.00 33.51
ATOM    430  HA  LEU A  39      16.868 -17.323  -3.794  1.00  2.32
ATOM    431 2HB  LEU A  39      16.328 -15.274  -4.586  1.00 21.34
ATOM    432 3HB  LEU A  39      14.744 -16.034  -4.727  1.00 40.30
ATOM    433  HG  LEU A  39      14.440 -15.011  -2.302  1.00 71.45
ATOM    434 1HD1 LEU A  39      15.884 -13.447  -1.665  1.00 14.23
ATOM    435 2HD1 LEU A  39      15.844 -12.664  -3.244  1.00 40.02
ATOM    436 3HD1 LEU A  39      16.942 -14.014  -2.957  1.00 11.22
ATOM    437 1HD2 LEU A  39      13.063 -14.559  -4.295  1.00 23.02
ATOM    438 2HD2 LEU A  39      14.243 -13.356  -4.817  1.00 62.41
ATOM    439 3HD2 LEU A  39      13.338 -13.113  -3.322  1.00 70.44
ATOM    440  N   HIS A  40      17.671 -15.982  -1.761  1.00 43.32
ATOM    441  CA  HIS A  40      18.207 -15.546  -0.476  1.00 52.14
ATOM    442  C   HIS A  40      17.514 -14.272  -0.003  1.00 12.21
ATOM    443  O   HIS A  40      18.062 -13.176  -0.120  1.00 73.45
ATOM    444  CB  HIS A  40      19.714 -15.312  -0.581  1.00 41.32
ATOM    445  CG  HIS A  40      20.519 -16.575  -0.568  1.00 11.33
ATOM    446  CD2 HIS A  40      21.658 -16.906  -1.220  1.00 10.33
ATOM    447  ND1 HIS A  40      20.174 -17.679   0.182  1.00 33.13
ATOM    448  CE1 HIS A  40      21.066 -18.634  -0.007  1.00 65.15
ATOM    449  NE2 HIS A  40      21.978 -18.190  -0.855  1.00 34.35
ATOM    450  H   HIS A  40      18.223 -15.888  -2.566  1.00 15.43
ATOM    451  HA  HIS A  40      18.022 -16.329   0.243  1.00 63.53
ATOM    452 2HB  HIS A  40      19.928 -14.793  -1.504  1.00 53.21
ATOM    453 3HB  HIS A  40      20.036 -14.703   0.251  1.00 22.04
ATOM    454  HD1 HIS A  40      19.392 -17.751   0.768  1.00 73.41
ATOM    455  HD2 HIS A  40      22.214 -16.276  -1.901  1.00 34.41
ATOM    456  HE1 HIS A  40      21.054 -19.612   0.451  1.00 40.41
ATOM    457  N   GLU A  41      16.306 -14.424   0.532  1.00 61.35
ATOM    458  CA  GLU A  41      15.539 -13.285   1.021  1.00 74.03
ATOM    459  C   GLU A  41      16.337 -12.494   2.053  1.00 60.01
ATOM    460  O   GLU A  41      16.432 -11.270   1.973  1.00 11.23
ATOM    461  CB  GLU A  41      14.218 -13.757   1.633  1.00  1.52
ATOM    462  CG  GLU A  41      14.387 -14.846   2.678  1.00 32.54
ATOM    463  CD  GLU A  41      13.067 -15.470   3.089  1.00 21.22
ATOM    464  OE1 GLU A  41      13.014 -16.711   3.223  1.00 42.20
ATOM    465  OE2 GLU A  41      12.088 -14.719   3.276  1.00 12.55
ATOM    466  H   GLU A  41      15.922 -15.324   0.598  1.00 43.52
ATOM    467  HA  GLU A  41      15.325 -12.643   0.179  1.00 24.05
ATOM    468 2HB  GLU A  41      13.729 -12.913   2.098  1.00 60.02
ATOM    469 3HB  GLU A  41      13.586 -14.138   0.845  1.00 50.00
ATOM    470 2HG  GLU A  41      15.022 -15.620   2.274  1.00 23.01
ATOM    471 3HG  GLU A  41      14.854 -14.419   3.553  1.00 22.24
ATOM    472  N   GLU A  42      16.908 -13.204   3.021  1.00  4.31
ATOM    473  CA  GLU A  42      17.697 -12.568   4.070  1.00 41.33
ATOM    474  C   GLU A  42      19.137 -13.072   4.049  1.00 62.10
ATOM    475  O   GLU A  42      19.843 -13.010   5.056  1.00 54.32
ATOM    476  CB  GLU A  42      17.072 -12.833   5.441  1.00 70.11
ATOM    477  CG  GLU A  42      15.766 -12.090   5.668  1.00 22.15
ATOM    478  CD  GLU A  42      14.959 -12.667   6.816  1.00 44.52
ATOM    479  OE1 GLU A  42      14.508 -11.881   7.676  1.00 70.51
ATOM    480  OE2 GLU A  42      14.780 -13.902   6.854  1.00 53.41
ATOM    481  H   GLU A  42      16.796 -14.177   3.031  1.00 64.14
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ATOM    482  HA  GLU A  42      17.698 -11.504   3.885  1.00 64.21
ATOM    483 2HB  GLU A  42      16.882 -13.892   5.538  1.00 50.22
ATOM    484 3HB  GLU A  42      17.772 -12.531   6.206  1.00 14.21
ATOM    485 2HG  GLU A  42      15.988 -11.057   5.889  1.00 44.34
ATOM    486 3HG  GLU A  42      15.173 -12.146   4.767  1.00  5.53
ATOM    487  N   SER A  43      19.566 -13.572   2.895  1.00 62.43
ATOM    488  CA  SER A  43      20.920 -14.092   2.743  1.00 62.02
ATOM    489  C   SER A  43      21.648 -13.388   1.602  1.00 54.44
ATOM    490  O   SER A  43      21.024 -12.753   0.752  1.00 42.11
ATOM    491  CB  SER A  43      20.885 -15.600   2.487  1.00 52.15
ATOM    492  OG  SER A  43      22.056 -16.031   1.814  1.00 14.54
ATOM    493  H   SER A  43      18.956 -13.595   2.128  1.00 42.14
ATOM    494  HA  SER A  43      21.452 -13.904   3.663  1.00 24.35
ATOM    495 2HB  SER A  43      20.813 -16.121   3.429  1.00 62.00
ATOM    496 3HB  SER A  43      20.025 -15.838   1.877  1.00 63.42
ATOM    497  HG  SER A  43      22.673 -16.398   2.451  1.00 63.45
ATOM    498  N   ASN A  44      22.971 -13.505   1.590  1.00 24.21
ATOM    499  CA  ASN A  44      23.785 -12.880   0.554  1.00  3.42
ATOM    500  C   ASN A  44      23.403 -13.402  -0.827  1.00 40.24
ATOM    501  O   ASN A  44      23.601 -14.578  -1.136  1.00  4.24
ATOM    502  CB  ASN A  44      25.270 -13.139   0.817  1.00 61.11
ATOM    503  CG  ASN A  44      25.909 -12.046   1.652  1.00 61.22
ATOM    504  ND2 ASN A  44      25.426 -11.880   2.878  1.00 43.44
ATOM    505  OD1 ASN A  44      26.826 -11.360   1.200  1.00 61.32
ATOM    506  H   ASN A  44      23.412 -14.024   2.295  1.00 73.50
ATOM    507  HA  ASN A  44      23.604 -11.816   0.587  1.00 15.03
ATOM    508 2HB  ASN A  44      25.378 -14.077   1.343  1.00 11.50
ATOM    509 3HB  ASN A  44      25.792 -13.198  -0.126  1.00 71.24
ATOM    510 1HD2 ASN A  44      24.695 -12.463   3.171  1.00 40.23
ATOM    511 2HD2 ASN A  44      25.821 -11.180   3.439  1.00 54.43
ATOM    512  N   LEU A  45      22.854 -12.520  -1.656  1.00 25.20
ATOM    513  CA  LEU A  45      22.445 -12.891  -3.006  1.00 35.20
ATOM    514  C   LEU A  45      23.648 -13.309  -3.845  1.00 51.41
ATOM    515  O   LEU A  45      23.529 -14.133  -4.752  1.00 34.11
ATOM    516  CB  LEU A  45      21.719 -11.724  -3.679  1.00 23.43
ATOM    517  CG  LEU A  45      20.394 -11.302  -3.044  1.00 32.32
ATOM    518  CD1 LEU A  45      19.683 -10.283  -3.920  1.00 40.40
ATOM    519  CD2 LEU A  45      19.506 -12.515  -2.806  1.00 60.23
ATOM    520  H   LEU A  45      22.722 -11.598  -1.354  1.00 14.11
ATOM    521  HA  LEU A  45      21.767 -13.729  -2.928  1.00 43.31
ATOM    522 2HB  LEU A  45      22.380 -10.871  -3.663  1.00 32.33
ATOM    523 3HB  LEU A  45      21.522 -12.006  -4.703  1.00 52.45
ATOM    524  HG  LEU A  45      20.592 -10.839  -2.087  1.00 33.11
ATOM    525 1HD1 LEU A  45      18.694 -10.642  -4.160  1.00 52.31
ATOM    526 2HD1 LEU A  45      20.244 -10.137  -4.831  1.00 65.51
ATOM    527 3HD1 LEU A  45      19.608  -9.344  -3.391  1.00 14.12
ATOM    528 1HD2 LEU A  45      19.611 -12.842  -1.782  1.00 73.33
ATOM    529 2HD2 LEU A  45      19.802 -13.314  -3.471  1.00 43.32
ATOM    530 3HD2 LEU A  45      18.477 -12.251  -2.997  1.00 14.44
ATOM    531  N   ILE A  46      24.806 -12.736  -3.535  1.00 40.32
ATOM    532  CA  ILE A  46      26.031 -13.051  -4.259  1.00 25.03
ATOM    533  C   ILE A  46      26.280 -14.555  -4.290  1.00 75.35
ATOM    534  O   ILE A  46      26.787 -15.089  -5.276  1.00 62.22
ATOM    535  CB  ILE A  46      27.252 -12.354  -3.629  1.00 61.12
ATOM    536  CG1 ILE A  46      27.015 -10.845  -3.540  1.00 64.02
ATOM    537  CG2 ILE A  46      28.507 -12.652  -4.436  1.00 72.23
ATOM    538  CD1 ILE A  46      26.798 -10.187  -4.885  1.00 23.11
ATOM    539  H   ILE A  46      24.837 -12.086  -2.802  1.00 62.33
ATOM    540  HA  ILE A  46      25.921 -12.694  -5.272  1.00 40.44
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ATOM    541  HB  ILE A  46      27.391 -12.749  -2.634  1.00 53.14
ATOM    542 2HG1 ILE A  46      26.142 -10.659  -2.936  1.00 11.13
ATOM    543 3HG1 ILE A  46      27.874 -10.380  -3.077  1.00 61.43
ATOM    544 1HG2 ILE A  46      29.028 -11.730  -4.646  1.00 12.54
ATOM    545 2HG2 ILE A  46      29.151 -13.308  -3.870  1.00  2.30
ATOM    546 3HG2 ILE A  46      28.233 -13.130  -5.365  1.00 10.21
ATOM    547 1HD1 ILE A  46      26.804 -10.940  -5.660  1.00 13.35
ATOM    548 2HD1 ILE A  46      25.848  -9.674  -4.886  1.00 64.43
ATOM    549 3HD1 ILE A  46      27.591  -9.476  -5.070  1.00 30.22
ATOM    550  N   GLN A  47      25.916 -15.232  -3.206  1.00 61.51
ATOM    551  CA  GLN A  47      26.098 -16.676  -3.111  1.00  4.02
ATOM    552  C   GLN A  47      25.354 -17.394  -4.232  1.00 10.13
ATOM    553  O   GLN A  47      25.731 -18.493  -4.636  1.00 21.45
ATOM    554  CB  GLN A  47      25.612 -17.184  -1.752  1.00 61.14
ATOM    555  CG  GLN A  47      26.731 -17.393  -0.745  1.00 10.43
ATOM    556  CD  GLN A  47      26.220 -17.518   0.677  1.00  0.21
ATOM    557  NE2 GLN A  47      27.124 -17.405   1.643  1.00 30.43
ATOM    558  OE1 GLN A  47      25.026 -17.714   0.905  1.00 51.41
ATOM    559  H   GLN A  47      25.517 -14.750  -2.453  1.00 32.30
ATOM    560  HA  GLN A  47      27.153 -16.884  -3.206  1.00  4.33
ATOM    561 2HB  GLN A  47      24.915 -16.468  -1.342  1.00 65.40
ATOM    562 3HB  GLN A  47      25.105 -18.127  -1.895  1.00 22.13
ATOM    563 2HG  GLN A  47      27.264 -18.296  -1.000  1.00 22.44
ATOM    564 3HG  GLN A  47      27.406 -16.551  -0.797  1.00 31.03
ATOM    565 1HE2 GLN A  47      28.057 -17.249   1.387  1.00  5.42
ATOM    566 2HE2 GLN A  47      26.821 -17.481   2.571  1.00 24.44
ATOM    567  N   ALA A  48      24.295 -16.765  -4.730  1.00 13.53
ATOM    568  CA  ALA A  48      23.498 -17.343  -5.805  1.00 44.40
ATOM    569  C   ALA A  48      23.997 -16.876  -7.169  1.00 32.52
ATOM    570  O   ALA A  48      24.996 -16.165  -7.266  1.00 14.15
ATOM    571  CB  ALA A  48      22.031 -16.984  -5.626  1.00 54.34
ATOM    572  H   ALA A  48      24.044 -15.890  -4.366  1.00 52.01
ATOM    573  HA  ALA A  48      23.590 -18.418  -5.748  1.00  3.34
ATOM    574 1HB  ALA A  48      21.881 -16.565  -4.642  1.00 35.44
ATOM    575 2HB  ALA A  48      21.744 -16.259  -6.373  1.00 40.35
ATOM    576 3HB  ALA A  48      21.427 -17.872  -5.736  1.00 62.31
ATOM    577  N   GLY A  49      23.294 -17.283  -8.222  1.00 31.44
ATOM    578  CA  GLY A  49      23.681 -16.898  -9.566  1.00 63.30
ATOM    579  C   GLY A  49      23.655 -15.396  -9.769  1.00 64.30
ATOM    580  O   GLY A  49      22.639 -14.835 -10.181  1.00 20.31
ATOM    581  H   GLY A  49      22.506 -17.850  -8.084  1.00 52.11
ATOM    582 2HA  GLY A  49      24.680 -17.260  -9.759  1.00 22.04
ATOM    583 3HA  GLY A  49      23.001 -17.357 -10.269  1.00 45.54
ATOM    584  N   LEU A  50      24.775 -14.742  -9.478  1.00 75.43
ATOM    585  CA  LEU A  50      24.876 -13.295  -9.630  1.00  2.03
ATOM    586  C   LEU A  50      26.335 -12.848  -9.624  1.00 74.12
ATOM    587  O   LEU A  50      27.030 -12.977  -8.616  1.00 52.43
ATOM    588  CB  LEU A  50      24.111 -12.590  -8.509  1.00 34.14
ATOM    589  CG  LEU A  50      24.658 -11.230  -8.074  1.00 70.02
ATOM    590  CD1 LEU A  50      24.678 -10.263  -9.248  1.00 25.30
ATOM    591  CD2 LEU A  50      23.832 -10.664  -6.929  1.00 15.32
ATOM    592  H   LEU A  50      25.551 -15.244  -9.154  1.00 43.43
ATOM    593  HA  LEU A  50      24.434 -13.029 -10.579  1.00 25.44
ATOM    594 2HB  LEU A  50      23.094 -12.446  -8.842  1.00 65.11
ATOM    595 3HB  LEU A  50      24.116 -13.241  -7.646  1.00 12.02
ATOM    596  HG  LEU A  50      25.674 -11.353  -7.726  1.00  3.42
ATOM    597 1HD1 LEU A  50      24.011  -9.439  -9.047  1.00 60.11
ATOM    598 2HD1 LEU A  50      24.358 -10.776 -10.143  1.00 20.54
ATOM    599 3HD1 LEU A  50      25.682  -9.889  -9.388  1.00 41.12
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ATOM    600 1HD2 LEU A  50      24.078 -11.185  -6.016  1.00  1.04
ATOM    601 2HD2 LEU A  50      22.781 -10.793  -7.145  1.00 32.43
ATOM    602 3HD2 LEU A  50      24.049  -9.612  -6.814  1.00 31.34
ATOM    603  N   ASP A  51      26.791 -12.321 -10.755  1.00 74.11
ATOM    604  CA  ASP A  51      28.166 -11.852 -10.880  1.00 14.51
ATOM    605  C   ASP A  51      28.303 -10.427 -10.353  1.00  2.41
ATOM    606  O   ASP A  51      28.310  -9.889  -9.336  1.00 22.02
ATOM    607  CB  ASP A  51      28.618 -11.915 -12.340  1.00  1.44
ATOM    608  CG  ASP A  51      28.719 -13.337 -12.853  1.00 65.34
ATOM    609  OD1 ASP A  51      29.095 -13.518 -14.031  1.00  1.02
ATOM    610  OD2 ASP A  51      28.424 -14.270 -12.078  1.00 21.12
ATOM    611  H   ASP A  51      26.188 -12.245 -11.524  1.00 73.34
ATOM    612  HA  ASP A  51      28.793 -12.502 -10.290  1.00 21.21
ATOM    613 2HB  ASP A  51      27.908 -11.380 -12.953  1.00 53.14
ATOM    614 3HB  ASP A  51      29.588 -11.448 -12.429  1.00 61.14
ATOM    615  N   SPS A  52      28.501  -9.275 -11.461  1.00 35.03
ATOM    616  CA  SPS A  52      28.691  -7.873 -11.083  1.00  3.41
ATOM    617  CAA SPS A  52      31.096  -9.682  -8.582  1.00  3.11
ATOM    618  C   SPS A  52      27.820  -6.997 -11.946  1.00 45.25
ATOM    619  O   SPS A  52      27.298  -6.022 -11.405  1.00 51.25
ATOM    620  CB  SPS A  52      30.159  -7.486 -11.282  1.00 13.43
ATOM    621  OG  SPS A  52      30.337  -6.954 -12.595  1.00 62.15
ATOM    622  CZ1 SPS A  52      31.275 -10.707  -7.674  1.00 62.42
ATOM    623  CZ2 SPS A  52      31.567  -8.410  -8.303  1.00 44.43
ATOM    624  OZ  SPS A  52      32.105 -11.475  -5.582  1.00 51.55
ATOM    625  CJ  SPS A  52      31.914  -4.743 -11.372  1.00 41.05
ATOM    626  CK  SPS A  52      32.566  -3.958 -10.233  1.00  5.00
ATOM    627  CL1 SPS A  52      32.858  -4.902  -9.065  1.00 23.52
ATOM    628  CL2 SPS A  52      31.619  -2.850  -9.768  1.00 43.11
ATOM    629  CL3 SPS A  52      33.875  -3.336 -10.725  1.00 72.24
ATOM    630  CM  SPS A  52      34.422  -2.413  -9.668  1.00 42.01
ATOM    631  OM  SPS A  52      33.630  -2.596 -11.923  1.00 75.41
ATOM    632  NN  SPS A  52      35.125  -2.915  -8.633  1.00 73.20
ATOM    633  ON  SPS A  52      34.229  -1.218  -9.747  1.00 63.33
ATOM    634  P   SPS A  52      31.919  -6.729 -12.794  1.00 44.32
ATOM    635  O1P SPS A  52      32.171  -5.783 -14.073  1.00 71.41
ATOM    636  O2P SPS A  52      32.581  -8.035 -13.009  1.00 42.22
ATOM    637  O3P SPS A  52      32.531  -6.027 -11.480  1.00 50.13
ATOM    638  CX  SPS A  52      32.406  -9.182  -6.190  1.00  2.15
ATOM    639  CO  SPS A  52      35.580  -2.029  -7.559  1.00 73.32
ATOM    640  CP  SPS A  52      36.299  -2.854  -6.489  1.00 34.22
ATOM    641  CQ  SPS A  52      35.294  -3.698  -5.746  1.00 13.30
ATOM    642  CS  SPS A  52      34.726  -5.337  -4.036  1.00 65.31
ATOM    643  CT  SPS A  52      34.137  -6.383  -4.985  1.00 20.22
ATOM    644  CV  SPS A  52      33.102  -8.916  -4.916  1.00  4.10
ATOM    645  CY1 SPS A  52      31.928 -10.468  -6.475  1.00 23.12
ATOM    646  CY2 SPS A  52      32.214  -8.153  -7.113  1.00 15.42
ATOM    647  NR  SPS A  52      35.702  -4.518  -4.757  1.00 61.25
ATOM    648  OR  SPS A  52      34.118  -3.638  -6.038  1.00 63.32
ATOM    649  OW  SPS A  52      33.820  -9.766  -4.425  1.00  0.33
ATOM    650  SU  SPS A  52      32.896  -7.364  -4.107  1.00 33.12
ATOM    651  H   SPS A  52      28.522  -9.532 -12.397  1.00 21.24
ATOM    652  HN  SPS A  52      35.328  -3.863  -8.600  1.00 42.31
ATOM    653  HA  SPS A  52      28.418  -7.738 -10.036  1.00 50.33
ATOM    654  HAA SPS A  52      30.586  -9.874  -9.515  1.00 25.22
ATOM    655 2HB  SPS A  52      30.440  -6.735 -10.544  1.00 14.32
ATOM    656 3HB  SPS A  52      30.787  -8.369 -11.158  1.00 32.11
ATOM    657  HZ  SPS A  52      32.722 -12.100  -5.986  1.00  3.14
ATOM    658  HZ1 SPS A  52      30.905 -11.697  -7.900  1.00  3.23
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ATOM    659  HZ2 SPS A  52      31.424  -7.615  -9.019  1.00 52.34
ATOM    660 2HJ  SPS A  52      32.041  -4.198 -12.308  1.00 24.54
ATOM    661 3HJ  SPS A  52      30.851  -4.867 -11.165  1.00 73.02
ATOM    662 1HL1 SPS A  52      32.285  -5.821  -9.189  1.00 33.23
ATOM    663 2HL1 SPS A  52      33.922  -5.139  -9.046  1.00 24.21
ATOM    664 3HL1 SPS A  52      32.576  -4.421  -8.129  1.00 60.43
ATOM    665 1HL2 SPS A  52      32.089  -2.284  -8.964  1.00 64.21
ATOM    666 2HL2 SPS A  52      31.402  -2.183 -10.603  1.00 23.21
ATOM    667 3HL2 SPS A  52      30.692  -3.293  -9.406  1.00 41.15
ATOM    668  HL3 SPS A  52      34.599  -4.125 -10.929  1.00 60.51
ATOM    669  HM  SPS A  52      32.985  -1.909 -11.700  1.00 62.24
ATOM    670 2HO  SPS A  52      36.265  -1.287  -7.966  1.00 31.00
ATOM    671 3HO  SPS A  52      34.721  -1.527  -7.114  1.00 13.44
ATOM    672 2HP  SPS A  52      37.037  -3.501  -6.963  1.00 74.53
ATOM    673 3HP  SPS A  52      36.799  -2.185  -5.789  1.00 54.45
ATOM    674  HR  SPS A  52      36.643  -4.565  -4.524  1.00 42.43
ATOM    675 2HS  SPS A  52      35.219  -5.839  -3.203  1.00 33.34
ATOM    676 3HS  SPS A  52      33.928  -4.701  -3.656  1.00 53.23
ATOM    677 2HT  SPS A  52      33.671  -5.882  -5.833  1.00 22.20
ATOM    678 3HT  SPS A  52      34.932  -7.038  -5.342  1.00 14.12
ATOM    679  HY2 SPS A  52      32.579  -7.159  -6.900  1.00 53.21
ATOM    680  N   ILE A  53      27.646  -7.292 -13.230  1.00 63.31
ATOM    681  CA  ILE A  53      26.811  -6.470 -14.096  1.00 40.33
ATOM    682  C   ILE A  53      25.379  -6.404 -13.578  1.00 35.13
ATOM    683  O   ILE A  53      24.688  -5.401 -13.758  1.00 74.21
ATOM    684  CB  ILE A  53      26.798  -7.006 -15.540  1.00 43.42
ATOM    685  CG1 ILE A  53      26.853  -5.847 -16.538  1.00 11.21
ATOM    686  CG2 ILE A  53      25.561  -7.858 -15.778  1.00 20.43
ATOM    687  CD1 ILE A  53      25.789  -4.798 -16.304  1.00 54.51
ATOM    688  H   ILE A  53      28.089  -8.082 -13.603  1.00 62.52
ATOM    689  HA  ILE A  53      27.225  -5.472 -14.108  1.00 14.44
ATOM    690  HB  ILE A  53      27.668  -7.630 -15.676  1.00 50.15
ATOM    691 2HG1 ILE A  53      27.815  -5.364 -16.467  1.00 73.13
ATOM    692 3HG1 ILE A  53      26.722  -6.236 -17.537  1.00 44.04
ATOM    693 1HG2 ILE A  53      25.644  -8.354 -16.734  1.00 31.44
ATOM    694 2HG2 ILE A  53      25.479  -8.598 -14.996  1.00 34.04
ATOM    695 3HG2 ILE A  53      24.684  -7.230 -15.773  1.00 54.53
ATOM    696 1HD1 ILE A  53      24.857  -5.280 -16.047  1.00  3.14
ATOM    697 2HD1 ILE A  53      26.094  -4.148 -15.498  1.00 12.12
ATOM    698 3HD1 ILE A  53      25.654  -4.215 -17.204  1.00 41.23
ATOM    699  N   ARG A  54      24.939  -7.479 -12.931  1.00 62.03
ATOM    700  CA  ARG A  54      23.589  -7.543 -12.385  1.00 71.55
ATOM    701  C   ARG A  54      23.398  -6.506 -11.283  1.00 21.22
ATOM    702  O   ARG A  54      22.344  -5.877 -11.183  1.00 41.54
ATOM    703  CB  ARG A  54      23.303  -8.943 -11.838  1.00 63.35
ATOM    704  CG  ARG A  54      22.482  -9.809 -12.780  1.00 31.13
ATOM    705  CD  ARG A  54      23.260 -10.156 -14.039  1.00 62.31
ATOM    706  NE  ARG A  54      22.418 -10.802 -15.043  1.00 11.34
ATOM    707  CZ  ARG A  54      22.893 -11.367 -16.147  1.00 34.43
ATOM    708  NH1 ARG A  54      24.196 -11.368 -16.388  1.00  4.34
ATOM    709  NH2 ARG A  54      22.062 -11.935 -17.012  1.00 45.04
ATOM    710  H   ARG A  54      25.537  -8.248 -12.819  1.00 41.54
ATOM    711  HA  ARG A  54      22.897  -7.332 -13.186  1.00 54.54
ATOM    712 2HB  ARG A  54      24.243  -9.443 -11.653  1.00 34.33
ATOM    713 3HB  ARG A  54      22.764  -8.850 -10.908  1.00  4.32
ATOM    714 2HG  ARG A  54      22.215 -10.724 -12.272  1.00 13.05
ATOM    715 3HG  ARG A  54      21.586  -9.274 -13.056  1.00 50.33
ATOM    716 2HD  ARG A  54      23.668  -9.248 -14.456  1.00 41.32
ATOM    717 3HD  ARG A  54      24.066 -10.824 -13.775  1.00 62.51
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ATOM    718  HE  ARG A  54      21.451 -10.813 -14.885  1.00  3.15
ATOM    719 1HH1 ARG A  54      24.824 -10.942 -15.737  1.00  3.25
ATOM    720 2HH1 ARG A  54      24.551 -11.796 -17.219  1.00 44.52
ATOM    721 1HH2 ARG A  54      21.079 -11.937 -16.834  1.00 50.11
ATOM    722 2HH2 ARG A  54      22.421 -12.360 -17.843  1.00 35.30
ATOM    723  N   LEU A  55      24.424  -6.334 -10.456  1.00 53.32
ATOM    724  CA  LEU A  55      24.369  -5.373  -9.360  1.00 25.03
ATOM    725  C   LEU A  55      24.405  -3.942  -9.887  1.00 71.21
ATOM    726  O   LEU A  55      23.816  -3.038  -9.296  1.00  2.32
ATOM    727  CB  LEU A  55      25.535  -5.603  -8.396  1.00 43.43
ATOM    728  CG  LEU A  55      25.332  -6.694  -7.344  1.00 52.45
ATOM    729  CD1 LEU A  55      26.661  -7.334  -6.976  1.00 71.52
ATOM    730  CD2 LEU A  55      24.652  -6.123  -6.108  1.00 43.44
ATOM    731  H   LEU A  55      25.237  -6.864 -10.585  1.00 70.34
ATOM    732  HA  LEU A  55      23.441  -5.526  -8.831  1.00 35.11
ATOM    733 2HB  LEU A  55      26.402  -5.867  -8.983  1.00 13.41
ATOM    734 3HB  LEU A  55      25.723  -4.673  -7.878  1.00 40.22
ATOM    735  HG  LEU A  55      24.692  -7.464  -7.753  1.00 63.00
ATOM    736 1HD1 LEU A  55      26.904  -7.095  -5.952  1.00 63.32
ATOM    737 2HD1 LEU A  55      27.435  -6.957  -7.628  1.00 21.41
ATOM    738 3HD1 LEU A  55      26.587  -8.406  -7.089  1.00 31.34
ATOM    739 1HD2 LEU A  55      25.403  -5.778  -5.413  1.00 11.44
ATOM    740 2HD2 LEU A  55      24.053  -6.890  -5.640  1.00 63.30
ATOM    741 3HD2 LEU A  55      24.019  -5.296  -6.395  1.00 65.10
ATOM    742  N   MET A  56      25.098  -3.746 -11.004  1.00 53.22
ATOM    743  CA  MET A  56      25.207  -2.425 -11.613  1.00 74.22
ATOM    744  C   MET A  56      23.893  -2.022 -12.275  1.00 13.43
ATOM    745  O   MET A  56      23.535  -0.844 -12.299  1.00  4.31
ATOM    746  CB  MET A  56      26.337  -2.407 -12.644  1.00 72.10
ATOM    747  CG  MET A  56      27.662  -1.915 -12.085  1.00 13.43
ATOM    748  SD  MET A  56      28.594  -3.218 -11.258  1.00 41.21
ATOM    749  CE  MET A  56      27.796  -3.240  -9.655  1.00 23.03
ATOM    750  H   MET A  56      25.546  -4.506 -11.430  1.00 33.50
ATOM    751  HA  MET A  56      25.434  -1.717 -10.830  1.00 62.53
ATOM    752 2HB  MET A  56      26.480  -3.409 -13.021  1.00 40.44
ATOM    753 3HB  MET A  56      26.053  -1.760 -13.461  1.00 23.22
ATOM    754 2HG  MET A  56      28.258  -1.525 -12.896  1.00 71.24
ATOM    755 3HG  MET A  56      27.465  -1.125 -11.375  1.00 21.05
ATOM    756 1HE  MET A  56      28.486  -2.883  -8.904  1.00 51.23
ATOM    757 2HE  MET A  56      26.926  -2.601  -9.677  1.00 71.32
ATOM    758 3HE  MET A  56      27.496  -4.250  -9.416  1.00 63.33
ATOM    759  N   ARG A  57      23.178  -3.006 -12.810  1.00 43.25
ATOM    760  CA  ARG A  57      21.905  -2.752 -13.474  1.00 31.24
ATOM    761  C   ARG A  57      20.906  -2.119 -12.509  1.00 22.40
ATOM    762  O   ARG A  57      20.299  -1.093 -12.814  1.00 12.00
ATOM    763  CB  ARG A  57      21.331  -4.053 -14.038  1.00 22.34
ATOM    764  CG  ARG A  57      20.587  -3.872 -15.350  1.00 73.13
ATOM    765  CD  ARG A  57      19.080  -3.913 -15.146  1.00 43.35
ATOM    766  NE  ARG A  57      18.354  -3.521 -16.352  1.00  1.14
ATOM    767  CZ  ARG A  57      18.205  -4.311 -17.409  1.00 41.32
ATOM    768  NH1 ARG A  57      18.729  -5.529 -17.410  1.00 52.21
ATOM    769  NH2 ARG A  57      17.531  -3.883 -18.469  1.00 14.44
ATOM    770  H   ARG A  57      23.516  -3.925 -12.759  1.00 53.44
ATOM    771  HA  ARG A  57      22.085  -2.066 -14.288  1.00 24.15
ATOM    772 2HB  ARG A  57      22.141  -4.749 -14.202  1.00 30.02
ATOM    773 3HB  ARG A  57      20.647  -4.473 -13.316  1.00 22.41
ATOM    774 2HG  ARG A  57      20.855  -2.917 -15.777  1.00 43.10
ATOM    775 3HG  ARG A  57      20.871  -4.664 -16.027  1.00  4.11
ATOM    776 2HD  ARG A  57      18.794  -4.918 -14.876  1.00 71.13
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ATOM    777 3HD  ARG A  57      18.821  -3.237 -14.345  1.00 72.12
ATOM    778  HE  ARG A  57      17.959  -2.625 -16.372  1.00 40.22
ATOM    779 1HH1 ARG A  57      19.237  -5.854 -16.613  1.00 34.42
ATOM    780 2HH1 ARG A  57      18.614  -6.122 -18.207  1.00 41.03
ATOM    781 1HH2 ARG A  57      17.134  -2.965 -18.471  1.00 63.15
ATOM    782 2HH2 ARG A  57      17.419  -4.478 -19.264  1.00  2.50
ATOM    783  N   TRP A  58      20.742  -2.739 -11.346  1.00 14.21
ATOM    784  CA  TRP A  58      19.816  -2.236 -10.337  1.00 30.42
ATOM    785  C   TRP A  58      20.120  -0.782  -9.995  1.00 50.24
ATOM    786  O   TRP A  58      19.222   0.061  -9.971  1.00  2.23
ATOM    787  CB  TRP A  58      19.890  -3.096  -9.074  1.00  3.11
ATOM    788  CG  TRP A  58      19.810  -4.567  -9.351  1.00 14.33
ATOM    789  CD1 TRP A  58      20.669  -5.532  -8.910  1.00 21.12
ATOM    790  CD2 TRP A  58      18.816  -5.238 -10.133  1.00 31.23
ATOM    791  CE2 TRP A  58      19.135  -6.610 -10.122  1.00 73.33
ATOM    792  CE3 TRP A  58      17.687  -4.815 -10.839  1.00 12.43
ATOM    793  NE1 TRP A  58      20.269  -6.763  -9.371  1.00 25.45
ATOM    794  CZ2 TRP A  58      18.365  -7.558 -10.792  1.00 22.13
ATOM    795  CZ3 TRP A  58      16.924  -5.756 -11.503  1.00 23.52
ATOM    796  CH2 TRP A  58      17.265  -7.115 -11.475  1.00 64.30
ATOM    797  H   TRP A  58      21.255  -3.554 -11.161  1.00 15.53
ATOM    798  HA  TRP A  58      18.818  -2.297 -10.745  1.00 34.25
ATOM    799 2HB  TRP A  58      20.825  -2.903  -8.569  1.00 13.33
ATOM    800 3HB  TRP A  58      19.071  -2.834  -8.420  1.00 51.52
ATOM    801  HD1 TRP A  58      21.533  -5.341  -8.292  1.00  0.41
ATOM    802  HE1 TRP A  58      20.723  -7.613  -9.188  1.00 60.34
ATOM    803  HE3 TRP A  58      17.408  -3.772 -10.872  1.00 15.22
ATOM    804  HZ2 TRP A  58      18.615  -8.609 -10.779  1.00 74.13
ATOM    805  HZ3 TRP A  58      16.048  -5.448 -12.054  1.00 43.42
ATOM    806  HH2 TRP A  58      16.641  -7.816 -12.008  1.00 43.42
ATOM    807  N   LEU A  59      21.390  -0.493  -9.733  1.00 32.43
ATOM    808  CA  LEU A  59      21.812   0.861  -9.393  1.00 22.03
ATOM    809  C   LEU A  59      21.212   1.877 -10.359  1.00 13.34
ATOM    810  O   LEU A  59      20.475   2.776  -9.952  1.00  1.44
ATOM    811  CB  LEU A  59      23.338   0.961  -9.413  1.00 65.44
ATOM    812  CG  LEU A  59      24.003   1.363  -8.096  1.00 53.23
ATOM    813  CD1 LEU A  59      23.631   2.791  -7.726  1.00 24.44
ATOM    814  CD2 LEU A  59      23.609   0.402  -6.985  1.00 33.25
ATOM    815  H   LEU A  59      22.060  -1.207  -9.768  1.00 51.00
ATOM    816  HA  LEU A  59      21.459   1.078  -8.396  1.00 32.44
ATOM    817 2HB  LEU A  59      23.729  -0.004  -9.699  1.00 51.00
ATOM    818 3HB  LEU A  59      23.611   1.693 -10.160  1.00 61.11
ATOM    819  HG  LEU A  59      25.077   1.318  -8.214  1.00 12.24
ATOM    820 1HD1 LEU A  59      24.490   3.287  -7.301  1.00 45.41
ATOM    821 2HD1 LEU A  59      22.829   2.778  -7.003  1.00 22.44
ATOM    822 3HD1 LEU A  59      23.309   3.320  -8.610  1.00 62.05
ATOM    823 1HD2 LEU A  59      23.452  -0.583  -7.400  1.00 15.23
ATOM    824 2HD2 LEU A  59      22.697   0.745  -6.518  1.00 53.41
ATOM    825 3HD2 LEU A  59      24.397   0.361  -6.248  1.00 62.30
ATOM    826  N   HIS A  60      21.530   1.727 -11.641  1.00 15.34
ATOM    827  CA  HIS A  60      21.019   2.631 -12.666  1.00 31.43
ATOM    828  C   HIS A  60      19.517   2.440 -12.858  1.00 44.35
ATOM    829  O   HIS A  60      18.842   3.295 -13.432  1.00  5.54
ATOM    830  CB  HIS A  60      21.748   2.398 -13.989  1.00 44.52
ATOM    831  CG  HIS A  60      21.190   3.194 -15.129  1.00 34.14
ATOM    832  CD2 HIS A  60      20.882   2.830 -16.396  1.00 10.05
ATOM    833  ND1 HIS A  60      20.885   4.535 -15.032  1.00 50.31
ATOM    834  CE1 HIS A  60      20.413   4.962 -16.190  1.00 34.33
ATOM    835  NE2 HIS A  60      20.401   3.946 -17.034  1.00 51.34
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ATOM    836  H   HIS A  60      22.121   0.992 -11.903  1.00 71.42
ATOM    837  HA  HIS A  60      21.201   3.642 -12.337  1.00  4.42
ATOM    838 2HB  HIS A  60      22.787   2.671 -13.873  1.00 11.22
ATOM    839 3HB  HIS A  60      21.683   1.352 -14.250  1.00 51.03
ATOM    840  HD1 HIS A  60      20.997   5.091 -14.233  1.00 52.44
ATOM    841  HD2 HIS A  60      20.993   1.844 -16.825  1.00 44.22
ATOM    842  HE1 HIS A  60      20.091   5.969 -16.409  1.00 60.22
ATOM    843  N   TRP A  61      19.002   1.315 -12.377  1.00 64.24
ATOM    844  CA  TRP A  61      17.581   1.012 -12.498  1.00 14.41
ATOM    845  C   TRP A  61      16.737   2.075 -11.802  1.00 22.22
ATOM    846  O   TRP A  61      15.917   2.742 -12.433  1.00 31.22
ATOM    847  CB  TRP A  61      17.279  -0.365 -11.905  1.00  1.10
ATOM    848  CG  TRP A  61      16.163  -1.081 -12.604  1.00 24.22
ATOM    849  CD1 TRP A  61      16.124  -1.454 -13.917  1.00 64.11
ATOM    850  CD2 TRP A  61      14.925  -1.509 -12.026  1.00 51.34
ATOM    851  CE2 TRP A  61      14.183  -2.135 -13.047  1.00 44.34
ATOM    852  CE3 TRP A  61      14.371  -1.426 -10.746  1.00 42.41
ATOM    853  NE1 TRP A  61      14.936  -2.088 -14.191  1.00  2.32
ATOM    854  CZ2 TRP A  61      12.918  -2.672 -12.826  1.00  1.14
ATOM    855  CZ3 TRP A  61      13.115  -1.959 -10.528  1.00  2.13
ATOM    856  CH2 TRP A  61      12.400  -2.576 -11.563  1.00 22.34
ATOM    857  H   TRP A  61      19.592   0.671 -11.930  1.00 53.43
ATOM    858  HA  TRP A  61      17.332   1.004 -13.549  1.00 64.00
ATOM    859 2HB  TRP A  61      18.164  -0.980 -11.972  1.00 33.32
ATOM    860 3HB  TRP A  61      17.003  -0.249 -10.867  1.00  2.03
ATOM    861  HD1 TRP A  61      16.918  -1.270 -14.625  1.00 54.42
ATOM    862  HE1 TRP A  61      14.672  -2.449 -15.063  1.00 41.22
ATOM    863  HE3 TRP A  61      14.907  -0.954  -9.936  1.00 13.35
ATOM    864  HZ2 TRP A  61      12.355  -3.151 -13.613  1.00 33.42
ATOM    865  HZ3 TRP A  61      12.671  -1.904  -9.545  1.00 11.43
ATOM    866  HH2 TRP A  61      11.423  -2.979 -11.347  1.00 13.24
ATOM    867  N   PHE A  62      16.944   2.228 -10.498  1.00 72.20
ATOM    868  CA  PHE A  62      16.201   3.210  -9.716  1.00 62.52
ATOM    869  C   PHE A  62      16.845   4.589  -9.823  1.00 55.01
ATOM    870  O   PHE A  62      16.156   5.610  -9.807  1.00 61.43
ATOM    871  CB  PHE A  62      16.132   2.779  -8.250  1.00 24.43
ATOM    872  CG  PHE A  62      17.020   1.611  -7.926  1.00  1.13
ATOM    873  CD1 PHE A  62      18.316   1.812  -7.479  1.00 11.25
ATOM    874  CD2 PHE A  62      16.559   0.312  -8.069  1.00 13.51
ATOM    875  CE1 PHE A  62      19.135   0.740  -7.179  1.00 43.11
ATOM    876  CE2 PHE A  62      17.373  -0.763  -7.771  1.00 22.54
ATOM    877  CZ  PHE A  62      18.663  -0.550  -7.326  1.00 45.54
ATOM    878  H   PHE A  62      17.612   1.666 -10.051  1.00 15.22
ATOM    879  HA  PHE A  62      15.200   3.261 -10.115  1.00 32.41
ATOM    880 2HB  PHE A  62      16.432   3.606  -7.624  1.00 41.03
ATOM    881 3HB  PHE A  62      15.117   2.501  -8.011  1.00 12.41
ATOM    882  HD1 PHE A  62      18.686   2.821  -7.363  1.00 43.32
ATOM    883  HD2 PHE A  62      15.550   0.143  -8.417  1.00 44.42
ATOM    884  HE1 PHE A  62      20.144   0.911  -6.832  1.00 54.21
ATOM    885  HE2 PHE A  62      17.002  -1.771  -7.887  1.00  1.21
ATOM    886  HZ  PHE A  62      19.302  -1.388  -7.092  1.00 74.54
ATOM    887  N   ARG A  63      18.169   4.611  -9.931  1.00 71.11
ATOM    888  CA  ARG A  63      18.906   5.864 -10.039  1.00  1.13
ATOM    889  C   ARG A  63      18.295   6.764 -11.108  1.00 51.35
ATOM    890  O   ARG A  63      18.282   7.988 -10.973  1.00 23.01
ATOM    891  CB  ARG A  63      20.375   5.590 -10.366  1.00 61.11
ATOM    892  CG  ARG A  63      21.208   6.851 -10.531  1.00 72.45
ATOM    893  CD  ARG A  63      21.149   7.724  -9.288  1.00 40.21
ATOM    894  NE  ARG A  63      21.892   8.970  -9.459  1.00 31.02
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ATOM    895  CZ  ARG A  63      21.406  10.036 -10.085  1.00 74.32
ATOM    896  NH1 ARG A  63      20.183  10.007 -10.597  1.00 51.31
ATOM    897  NH2 ARG A  63      22.143  11.133 -10.200  1.00 73.00
ATOM    898  H   ARG A  63      18.662   3.764  -9.938  1.00  4.21
ATOM    899  HA  ARG A  63      18.847   6.367  -9.085  1.00 72.11
ATOM    900 2HB  ARG A  63      20.806   5.002  -9.569  1.00  2.53
ATOM    901 3HB  ARG A  63      20.427   5.027 -11.286  1.00 22.13
ATOM    902 2HG  ARG A  63      22.235   6.571 -10.713  1.00 41.21
ATOM    903 3HG  ARG A  63      20.831   7.412 -11.374  1.00 31.34
ATOM    904 2HD  ARG A  63      20.116   7.958  -9.077  1.00 42.34
ATOM    905 3HD  ARG A  63      21.570   7.175  -8.459  1.00 51.40
ATOM    906  HE  ARG A  63      22.798   9.013  -9.088  1.00 74.32
ATOM    907 1HH1 ARG A  63      19.625   9.182 -10.511  1.00 52.21
ATOM    908 2HH1 ARG A  63      19.819  10.812 -11.067  1.00 74.42
ATOM    909 1HH2 ARG A  63      23.065  11.158  -9.815  1.00 52.22
ATOM    910 2HH2 ARG A  63      21.776  11.934 -10.672  1.00  0.34
ATOM    911  N   LYS A  64      17.789   6.150 -12.173  1.00  1.33
ATOM    912  CA  LYS A  64      17.175   6.894 -13.266  1.00 44.32
ATOM    913  C   LYS A  64      16.038   7.773 -12.755  1.00 40.14
ATOM    914  O   LYS A  64      15.815   8.872 -13.262  1.00 30.23
ATOM    915  CB  LYS A  64      16.650   5.932 -14.334  1.00 24.22
ATOM    916  CG  LYS A  64      17.346   6.075 -15.676  1.00 60.45
ATOM    917  CD  LYS A  64      16.529   6.919 -16.641  1.00 24.34
ATOM    918  CE  LYS A  64      15.418   6.107 -17.288  1.00 13.11
ATOM    919  NZ  LYS A  64      14.289   6.970 -17.735  1.00 45.03
ATOM    920  H   LYS A  64      17.829   5.172 -12.223  1.00 73.34
ATOM    921  HA  LYS A  64      17.933   7.526 -13.704  1.00 63.23
ATOM    922 2HB  LYS A  64      16.788   4.918 -13.987  1.00 13.44
ATOM    923 3HB  LYS A  64      15.595   6.114 -14.478  1.00 20.12
ATOM    924 2HG  LYS A  64      18.306   6.546 -15.526  1.00 52.23
ATOM    925 3HG  LYS A  64      17.488   5.092 -16.104  1.00 45.20
ATOM    926 2HD  LYS A  64      16.089   7.743 -16.100  1.00  4.40
ATOM    927 3HD  LYS A  64      17.182   7.300 -17.413  1.00 60.34
ATOM    928 2HE  LYS A  64      15.821   5.585 -18.142  1.00 42.40
ATOM    929 3HE  LYS A  64      15.049   5.390 -16.570  1.00 15.14
ATOM    930 1HZ  LYS A  64      14.523   7.421 -18.643  1.00 70.54
ATOM    931 2HZ  LYS A  64      14.106   7.712 -17.030  1.00 51.15
ATOM    932 3HZ  LYS A  64      13.428   6.399 -17.855  1.00  4.42
ATOM    933  N   ASN A  65      15.323   7.282 -11.749  1.00 31.33
ATOM    934  CA  ASN A  65      14.209   8.023 -11.169  1.00  0.41
ATOM    935  C   ASN A  65      14.712   9.101 -10.212  1.00 72.55
ATOM    936  O   ASN A  65      14.031  10.095  -9.968  1.00 14.33
ATOM    937  CB  ASN A  65      13.264   7.072 -10.432  1.00 41.00
ATOM    938  CG  ASN A  65      13.142   5.728 -11.124  1.00 30.14
ATOM    939  ND2 ASN A  65      12.761   5.750 -12.396  1.00 22.44
ATOM    940  OD1 ASN A  65      13.387   4.683 -10.521  1.00 64.20
ATOM    941  H   ASN A  65      15.549   6.399 -11.387  1.00 40.41
ATOM    942  HA  ASN A  65      13.671   8.497 -11.976  1.00 11.52
ATOM    943 2HB  ASN A  65      13.637   6.908  -9.431  1.00 60.54
ATOM    944 3HB  ASN A  65      12.283   7.519 -10.377  1.00 71.02
ATOM    945 1HD2 ASN A  65      12.583   6.619 -12.811  1.00 51.30
ATOM    946 2HD2 ASN A  65      12.674   4.895 -12.867  1.00 35.23
ATOM    947  N   GLY A  66      15.910   8.894  -9.675  1.00  3.43
ATOM    948  CA  GLY A  66      16.485   9.856  -8.752  1.00 34.12
ATOM    949  C   GLY A  66      16.915   9.220  -7.445  1.00 62.42
ATOM    950  O   GLY A  66      16.845   9.847  -6.388  1.00 53.02
ATOM    951  H   GLY A  66      16.409   8.083  -9.907  1.00 35.34
ATOM    952 2HA  GLY A  66      17.344  10.316  -9.217  1.00 32.13
ATOM    953 3HA  GLY A  66      15.750  10.619  -8.542  1.00 13.22
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ATOM    954  N   TYR A  67      17.361   7.970  -7.516  1.00 51.32
ATOM    955  CA  TYR A  67      17.801   7.247  -6.329  1.00 14.01
ATOM    956  C   TYR A  67      19.313   7.044  -6.344  1.00 35.43
ATOM    957  O   TYR A  67      19.826   6.172  -7.046  1.00  0.42
ATOM    958  CB  TYR A  67      17.094   5.894  -6.240  1.00 34.54
ATOM    959  CG  TYR A  67      15.602   6.003  -6.018  1.00 51.04
ATOM    960  CD1 TYR A  67      14.703   5.534  -6.969  1.00 12.15
ATOM    961  CD2 TYR A  67      15.091   6.576  -4.860  1.00 44.13
ATOM    962  CE1 TYR A  67      13.339   5.633  -6.771  1.00 70.43
ATOM    963  CE2 TYR A  67      13.729   6.677  -4.654  1.00  2.41
ATOM    964  CZ  TYR A  67      12.857   6.204  -5.612  1.00 42.53
ATOM    965  OH  TYR A  67      11.500   6.305  -5.411  1.00 74.21
ATOM    966  H   TYR A  67      17.394   7.523  -8.387  1.00 74.23
ATOM    967  HA  TYR A  67      17.537   7.838  -5.464  1.00 34.31
ATOM    968 2HB  TYR A  67      17.253   5.350  -7.158  1.00 51.52
ATOM    969 3HB  TYR A  67      17.511   5.331  -5.417  1.00 72.23
ATOM    970  HD1 TYR A  67      15.083   5.087  -7.875  1.00 62.44
ATOM    971  HD2 TYR A  67      15.777   6.946  -4.112  1.00 23.11
ATOM    972  HE1 TYR A  67      12.656   5.262  -7.521  1.00 53.23
ATOM    973  HE2 TYR A  67      13.352   7.126  -3.747  1.00 33.43
ATOM    974  HH  TYR A  67      11.270   7.219  -5.229  1.00 51.25
ATOM    975  N   ARG A  68      20.020   7.854  -5.563  1.00 14.00
ATOM    976  CA  ARG A  68      21.473   7.765  -5.486  1.00 33.43
ATOM    977  C   ARG A  68      21.902   6.899  -4.305  1.00 21.40
ATOM    978  O   ARG A  68      21.649   7.238  -3.148  1.00 60.41
ATOM    979  CB  ARG A  68      22.085   9.161  -5.357  1.00 73.31
ATOM    980  CG  ARG A  68      22.781   9.639  -6.621  1.00  3.14
ATOM    981  CD  ARG A  68      23.937  10.575  -6.300  1.00 35.53
ATOM    982  NE  ARG A  68      23.803  11.861  -6.978  1.00  5.12
ATOM    983  CZ  ARG A  68      24.737  12.806  -6.951  1.00 31.11
ATOM    984  NH1 ARG A  68      25.865  12.609  -6.284  1.00 24.24
ATOM    985  NH2 ARG A  68      24.542  13.951  -7.593  1.00 64.31
ATOM    986  H   ARG A  68      19.553   8.529  -5.027  1.00 22.24
ATOM    987  HA  ARG A  68      21.826   7.309  -6.398  1.00 62.14
ATOM    988 2HB  ARG A  68      21.301   9.864  -5.116  1.00 41.15
ATOM    989 3HB  ARG A  68      22.807   9.151  -4.555  1.00 44.13
ATOM    990 2HG  ARG A  68      23.164   8.783  -7.156  1.00 23.33
ATOM    991 3HG  ARG A  68      22.067  10.162  -7.238  1.00 55.03
ATOM    992 2HD  ARG A  68      23.961  10.742  -5.233  1.00 65.42
ATOM    993 3HD  ARG A  68      24.858  10.107  -6.612  1.00 61.32
ATOM    994  HE  ARG A  68      22.977  12.028  -7.477  1.00 23.21
ATOM    995 1HH1 ARG A  68      26.015  11.747  -5.800  1.00 20.23
ATOM    996 2HH1 ARG A  68      26.567  13.321  -6.266  1.00  2.41
ATOM    997 1HH2 ARG A  68      23.693  14.103  -8.097  1.00 60.24
ATOM    998 2HH2 ARG A  68      25.245  14.661  -7.572  1.00 42.12
ATOM    999  N   LEU A  69      22.552   5.780  -4.604  1.00 62.55
ATOM   1000  CA  LEU A  69      23.017   4.864  -3.568  1.00 73.11
ATOM   1001  C   LEU A  69      24.368   4.261  -3.940  1.00 34.10
ATOM   1002  O   LEU A  69      24.584   3.849  -5.080  1.00 74.42
ATOM   1003  CB  LEU A  69      21.992   3.750  -3.347  1.00 53.21
ATOM   1004  CG  LEU A  69      20.945   3.573  -4.448  1.00 23.01
ATOM   1005  CD1 LEU A  69      20.525   2.115  -4.555  1.00 52.40
ATOM   1006  CD2 LEU A  69      19.738   4.460  -4.184  1.00 14.35
ATOM   1007  H   LEU A  69      22.724   5.563  -5.544  1.00 64.01
ATOM   1008  HA  LEU A  69      23.127   5.427  -2.654  1.00  0.34
ATOM   1009 2HB  LEU A  69      22.530   2.820  -3.250  1.00 60.02
ATOM   1010 3HB  LEU A  69      21.470   3.960  -2.424  1.00 42.30
ATOM   1011  HG  LEU A  69      21.376   3.866  -5.396  1.00 13.14
ATOM   1012 1HD1 LEU A  69      20.603   1.646  -3.586  1.00 42.12
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ATOM   1013 2HD1 LEU A  69      21.170   1.605  -5.255  1.00 55.44
ATOM   1014 3HD1 LEU A  69      19.503   2.060  -4.901  1.00 50.21
ATOM   1015 1HD2 LEU A  69      19.556   4.513  -3.120  1.00 71.42
ATOM   1016 2HD2 LEU A  69      18.871   4.045  -4.677  1.00 33.54
ATOM   1017 3HD2 LEU A  69      19.929   5.452  -4.566  1.00 30.23
ATOM   1018  N   THR A  70      25.275   4.210  -2.969  1.00 53.23
ATOM   1019  CA  THR A  70      26.604   3.657  -3.194  1.00 21.32
ATOM   1020  C   THR A  70      26.535   2.164  -3.494  1.00 35.33
ATOM   1021  O   THR A  70      25.719   1.442  -2.919  1.00 32.24
ATOM   1022  CB  THR A  70      27.519   3.882  -1.976  1.00 24.15
ATOM   1023  CG2 THR A  70      28.866   4.444  -2.407  1.00 32.32
ATOM   1024  OG1 THR A  70      26.895   4.782  -1.053  1.00 72.51
ATOM   1025  H   THR A  70      25.043   4.555  -2.082  1.00 30.43
ATOM   1026  HA  THR A  70      27.038   4.165  -4.043  1.00 20.13
ATOM   1027  HB  THR A  70      27.682   2.932  -1.486  1.00 42.23
ATOM   1028  HG1 THR A  70      27.498   4.967  -0.329  1.00 15.11
ATOM   1029 1HG2 THR A  70      28.732   5.075  -3.273  1.00 31.30
ATOM   1030 2HG2 THR A  70      29.533   3.631  -2.653  1.00 32.13
ATOM   1031 3HG2 THR A  70      29.288   5.025  -1.601  1.00 33.44
ATOM   1032  N   LEU A  71      27.395   1.706  -4.396  1.00 72.25
ATOM   1033  CA  LEU A  71      27.432   0.297  -4.773  1.00 34.25
ATOM   1034  C   LEU A  71      27.806  -0.576  -3.579  1.00 12.22
ATOM   1035  O   LEU A  71      27.418  -1.742  -3.504  1.00 12.23
ATOM   1036  CB  LEU A  71      28.430   0.078  -5.911  1.00 55.41
ATOM   1037  CG  LEU A  71      27.929   0.416  -7.316  1.00 61.51
ATOM   1038  CD1 LEU A  71      26.814  -0.534  -7.728  1.00  3.53
ATOM   1039  CD2 LEU A  71      27.454   1.860  -7.381  1.00 35.43
ATOM   1040  H   LEU A  71      28.020   2.329  -4.821  1.00 24.14
ATOM   1041  HA  LEU A  71      26.445   0.018  -5.111  1.00 52.52
ATOM   1042 2HB  LEU A  71      29.296   0.691  -5.713  1.00 71.53
ATOM   1043 3HB  LEU A  71      28.717  -0.963  -5.902  1.00 62.43
ATOM   1044  HG  LEU A  71      28.743   0.299  -8.019  1.00 34.31
ATOM   1045 1HD1 LEU A  71      27.206  -1.536  -7.805  1.00 72.52
ATOM   1046 2HD1 LEU A  71      26.416  -0.228  -8.684  1.00 11.42
ATOM   1047 3HD1 LEU A  71      26.029  -0.509  -6.986  1.00 71.15
ATOM   1048 1HD2 LEU A  71      27.133   2.088  -8.386  1.00 73.24
ATOM   1049 2HD2 LEU A  71      28.264   2.518  -7.103  1.00 40.25
ATOM   1050 3HD2 LEU A  71      26.628   1.997  -6.699  1.00 14.41
ATOM   1051  N   ARG A  72      28.560  -0.003  -2.647  1.00  1.43
ATOM   1052  CA  ARG A  72      28.986  -0.728  -1.456  1.00 13.23
ATOM   1053  C   ARG A  72      27.781  -1.222  -0.661  1.00 32.24
ATOM   1054  O   ARG A  72      27.843  -2.260  -0.003  1.00 23.30
ATOM   1055  CB  ARG A  72      29.860   0.165  -0.574  1.00 43.41
ATOM   1056  CG  ARG A  72      30.135  -0.418   0.802  1.00 34.42
ATOM   1057  CD  ARG A  72      30.903  -1.728   0.709  1.00 15.40
ATOM   1058  NE  ARG A  72      32.189  -1.561   0.039  1.00 42.24
ATOM   1059  CZ  ARG A  72      32.989  -2.573  -0.278  1.00 43.35
ATOM   1060  NH1 ARG A  72      32.637  -3.817   0.012  1.00 35.31
ATOM   1061  NH2 ARG A  72      34.145  -2.341  -0.888  1.00 52.40
ATOM   1062  H   ARG A  72      28.838   0.930  -2.763  1.00 12.11
ATOM   1063  HA  ARG A  72      29.565  -1.581  -1.776  1.00  3.41
ATOM   1064 2HB  ARG A  72      30.807   0.323  -1.069  1.00  4.42
ATOM   1065 3HB  ARG A  72      29.367   1.117  -0.446  1.00  2.22
ATOM   1066 2HG  ARG A  72      30.718   0.288   1.373  1.00  3.53
ATOM   1067 3HG  ARG A  72      29.194  -0.597   1.301  1.00 74.42
ATOM   1068 2HD  ARG A  72      31.074  -2.101   1.708  1.00 73.04
ATOM   1069 3HD  ARG A  72      30.308  -2.439   0.156  1.00 61.22
ATOM   1070  HE  ARG A  72      32.470  -0.649  -0.185  1.00 75.44
ATOM   1071 1HH1 ARG A  72      31.766  -3.995   0.470  1.00 31.24
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ATOM   1072 2HH1 ARG A  72      33.240  -4.578  -0.229  1.00  3.42
ATOM   1073 1HH2 ARG A  72      34.414  -1.404  -1.109  1.00  0.31
ATOM   1074 2HH2 ARG A  72      34.746  -3.103  -1.126  1.00 42.40
ATOM   1075  N   GLU A  73      26.686  -0.471  -0.726  1.00 41.23
ATOM   1076  CA  GLU A  73      25.468  -0.833  -0.011  1.00 50.32
ATOM   1077  C   GLU A  73      24.864  -2.114  -0.578  1.00 64.45
ATOM   1078  O   GLU A  73      24.192  -2.864   0.130  1.00 33.24
ATOM   1079  CB  GLU A  73      24.447   0.304  -0.091  1.00 35.21
ATOM   1080  CG  GLU A  73      25.008   1.657   0.313  1.00 64.51
ATOM   1081  CD  GLU A  73      25.226   1.775   1.809  1.00 73.00
ATOM   1082  OE1 GLU A  73      24.985   0.779   2.523  1.00 13.34
ATOM   1083  OE2 GLU A  73      25.636   2.862   2.265  1.00  1.42
ATOM   1084  H   GLU A  73      26.698   0.346  -1.268  1.00 22.13
ATOM   1085  HA  GLU A  73      25.728  -0.999   1.023  1.00 13.33
ATOM   1086 2HB  GLU A  73      24.084   0.376  -1.106  1.00 21.52
ATOM   1087 3HB  GLU A  73      23.618   0.073   0.562  1.00 72.40
ATOM   1088 2HG  GLU A  73      25.955   1.802  -0.185  1.00 42.12
ATOM   1089 3HG  GLU A  73      24.317   2.426   0.002  1.00  4.42
ATOM   1090  N   LEU A  74      25.109  -2.359  -1.861  1.00 60.00
ATOM   1091  CA  LEU A  74      24.590  -3.550  -2.525  1.00 51.43
ATOM   1092  C   LEU A  74      25.592  -4.697  -2.448  1.00 10.01
ATOM   1093  O   LEU A  74      25.210  -5.861  -2.330  1.00 72.52
ATOM   1094  CB  LEU A  74      24.263  -3.240  -3.987  1.00 64.34
ATOM   1095  CG  LEU A  74      23.181  -2.187  -4.225  1.00 52.10
ATOM   1096  CD1 LEU A  74      23.745  -0.788  -4.030  1.00 30.23
ATOM   1097  CD2 LEU A  74      22.589  -2.335  -5.619  1.00 60.41
ATOM   1098  H   LEU A  74      25.651  -1.725  -2.374  1.00 64.02
ATOM   1099  HA  LEU A  74      23.684  -3.844  -2.017  1.00 52.00
ATOM   1100 2HB  LEU A  74      25.169  -2.896  -4.463  1.00 20.42
ATOM   1101 3HB  LEU A  74      23.940  -4.160  -4.455  1.00  2.32
ATOM   1102  HG  LEU A  74      22.385  -2.329  -3.506  1.00 44.32
ATOM   1103 1HD1 LEU A  74      23.084  -0.067  -4.485  1.00 41.34
ATOM   1104 2HD1 LEU A  74      24.720  -0.726  -4.491  1.00 15.42
ATOM   1105 3HD1 LEU A  74      23.833  -0.580  -2.973  1.00 61.13
ATOM   1106 1HD2 LEU A  74      21.882  -1.538  -5.796  1.00 72.51
ATOM   1107 2HD2 LEU A  74      22.085  -3.288  -5.696  1.00 54.24
ATOM   1108 3HD2 LEU A  74      23.380  -2.285  -6.353  1.00 35.21
ATOM   1109  N   TYR A  75      26.875  -4.360  -2.513  1.00 22.03
ATOM   1110  CA  TYR A  75      27.933  -5.362  -2.450  1.00 74.02
ATOM   1111  C   TYR A  75      28.104  -5.885  -1.027  1.00 43.22
ATOM   1112  O   TYR A  75      28.239  -7.088  -0.808  1.00 73.32
ATOM   1113  CB  TYR A  75      29.252  -4.773  -2.952  1.00 22.32
ATOM   1114  CG  TYR A  75      29.474  -4.961  -4.436  1.00 14.43
ATOM   1115  CD1 TYR A  75      29.704  -3.871  -5.267  1.00 14.24
ATOM   1116  CD2 TYR A  75      29.452  -6.227  -5.007  1.00 52.22
ATOM   1117  CE1 TYR A  75      29.906  -4.037  -6.623  1.00 52.11
ATOM   1118  CE2 TYR A  75      29.654  -6.402  -6.362  1.00 64.43
ATOM   1119  CZ  TYR A  75      29.881  -5.305  -7.166  1.00 53.41
ATOM   1120  OH  TYR A  75      30.082  -5.475  -8.517  1.00 35.33
ATOM   1121  H   TYR A  75      27.118  -3.415  -2.606  1.00 74.25
ATOM   1122  HA  TYR A  75      27.649  -6.184  -3.092  1.00  4.42
ATOM   1123 2HB  TYR A  75      29.267  -3.714  -2.746  1.00 63.11
ATOM   1124 3HB  TYR A  75      30.071  -5.248  -2.431  1.00 41.14
ATOM   1125  HD1 TYR A  75      29.723  -2.879  -4.838  1.00 73.03
ATOM   1126  HD2 TYR A  75      29.274  -7.085  -4.375  1.00 12.53
ATOM   1127  HE1 TYR A  75      30.083  -3.178  -7.253  1.00  3.41
ATOM   1128  HE2 TYR A  75      29.634  -7.395  -6.788  1.00  3.12
ATOM   1129  HH  TYR A  75      29.262  -5.304  -8.986  1.00 53.31
ATOM   1130  N   ALA A  76      28.098  -4.970  -0.063  1.00 71.11
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ATOM   1131  CA  ALA A  76      28.250  -5.337   1.339  1.00 20.43
ATOM   1132  C   ALA A  76      27.077  -6.187   1.815  1.00 75.24
ATOM   1133  O   ALA A  76      27.250  -7.344   2.196  1.00 23.15
ATOM   1134  CB  ALA A  76      28.384  -4.090   2.200  1.00 14.10
ATOM   1135  H   ALA A  76      27.987  -4.026  -0.301  1.00 31.14
ATOM   1136  HA  ALA A  76      29.160  -5.912   1.437  1.00  2.41
ATOM   1137 1HB  ALA A  76      28.729  -4.369   3.185  1.00 11.41
ATOM   1138 2HB  ALA A  76      29.094  -3.414   1.747  1.00 73.51
ATOM   1139 3HB  ALA A  76      27.423  -3.603   2.279  1.00 21.24
ATOM   1140  N   ALA A  77      25.882  -5.605   1.789  1.00 31.41
ATOM   1141  CA  ALA A  77      24.680  -6.310   2.216  1.00 33.22
ATOM   1142  C   ALA A  77      23.736  -6.548   1.042  1.00 64.20
ATOM   1143  O   ALA A  77      22.699  -5.899   0.906  1.00 44.41
ATOM   1144  CB  ALA A  77      23.972  -5.530   3.314  1.00  3.31
ATOM   1145  H   ALA A  77      25.807  -4.681   1.474  1.00  4.31
ATOM   1146  HA  ALA A  77      24.980  -7.265   2.623  1.00 35.24
ATOM   1147 1HB  ALA A  77      23.684  -4.559   2.936  1.00 23.33
ATOM   1148 2HB  ALA A  77      23.092  -6.070   3.629  1.00 10.44
ATOM   1149 3HB  ALA A  77      24.639  -5.406   4.154  1.00  3.41
ATOM   1150  N   PRO A  78      24.102  -7.501   0.172  1.00 44.03
ATOM   1151  CA  PRO A  78      23.302  -7.846  -1.007  1.00 30.31
ATOM   1152  C   PRO A  78      21.999  -8.547  -0.638  1.00 12.33
ATOM   1153  O   PRO A  78      21.941  -9.775  -0.564  1.00 15.45
ATOM   1154  CB  PRO A  78      24.215  -8.793  -1.790  1.00 75.15
ATOM   1155  CG  PRO A  78      25.117  -9.385  -0.764  1.00 31.53
ATOM   1156  CD  PRO A  78      25.325  -8.315   0.271  1.00  4.05
ATOM   1157  HA  PRO A  78      23.084  -6.975  -1.607  1.00 74.23
ATOM   1158 2HB  PRO A  78      23.618  -9.551  -2.278  1.00 34.22
ATOM   1159 3HB  PRO A  78      24.770  -8.235  -2.529  1.00 11.42
ATOM   1160 2HG  PRO A  78      24.649 -10.251  -0.319  1.00 45.14
ATOM   1161 3HG  PRO A  78      26.059  -9.657  -1.216  1.00 61.05
ATOM   1162 2HD  PRO A  78      25.418  -8.753   1.254  1.00 31.22
ATOM   1163 3HD  PRO A  78      26.200  -7.726   0.035  1.00 73.51
ATOM   1164  N   THR A  79      20.953  -7.758  -0.407  1.00 62.51
ATOM   1165  CA  THR A  79      19.651  -8.303  -0.045  1.00 52.00
ATOM   1166  C   THR A  79      18.546  -7.274  -0.256  1.00 45.51
ATOM   1167  O   THR A  79      18.703  -6.101   0.086  1.00 43.41
ATOM   1168  CB  THR A  79      19.626  -8.772   1.422  1.00  1.00
ATOM   1169  CG2 THR A  79      19.720 -10.288   1.507  1.00  0.11
ATOM   1170  OG1 THR A  79      20.712  -8.180   2.144  1.00 61.42
ATOM   1171  H   THR A  79      21.062  -6.788  -0.482  1.00 44.50
ATOM   1172  HA  THR A  79      19.459  -9.158  -0.678  1.00 11.54
ATOM   1173  HB  THR A  79      18.693  -8.458   1.869  1.00 64.23
ATOM   1174  HG1 THR A  79      20.647  -7.224   2.093  1.00 41.45
ATOM   1175 1HG2 THR A  79      19.191 -10.729   0.675  1.00 43.20
ATOM   1176 2HG2 THR A  79      19.279 -10.624   2.433  1.00 32.44
ATOM   1177 3HG2 THR A  79      20.757 -10.586   1.473  1.00 71.32
ATOM   1178  N   LEU A  80      17.429  -7.719  -0.821  1.00  4.44
ATOM   1179  CA  LEU A  80      16.297  -6.835  -1.077  1.00 21.22
ATOM   1180  C   LEU A  80      15.737  -6.276   0.227  1.00  2.50
ATOM   1181  O   LEU A  80      15.426  -5.089   0.322  1.00 40.35
ATOM   1182  CB  LEU A  80      15.201  -7.586  -1.835  1.00 51.43
ATOM   1183  CG  LEU A  80      15.612  -8.201  -3.173  1.00 73.43
ATOM   1184  CD1 LEU A  80      14.405  -8.804  -3.876  1.00 64.41
ATOM   1185  CD2 LEU A  80      16.280  -7.159  -4.057  1.00 42.34
ATOM   1186  H   LEU A  80      17.363  -8.663  -1.071  1.00 63.33
ATOM   1187  HA  LEU A  80      16.648  -6.015  -1.685  1.00 71.13
ATOM   1188 2HB  LEU A  80      14.846  -8.382  -1.200  1.00 74.42
ATOM   1189 3HB  LEU A  80      14.395  -6.891  -2.023  1.00 52.42
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ATOM   1190  HG  LEU A  80      16.324  -8.995  -2.994  1.00 32.13
ATOM   1191 1HD1 LEU A  80      14.735  -9.562  -4.571  1.00 20.25
ATOM   1192 2HD1 LEU A  80      13.877  -8.030  -4.412  1.00 71.12
ATOM   1193 3HD1 LEU A  80      13.747  -9.248  -3.144  1.00 31.23
ATOM   1194 1HD2 LEU A  80      15.567  -6.386  -4.304  1.00  2.34
ATOM   1195 2HD2 LEU A  80      16.630  -7.628  -4.966  1.00  0.13
ATOM   1196 3HD2 LEU A  80      17.116  -6.723  -3.531  1.00 64.31
ATOM   1197  N   ALA A  81      15.614  -7.138   1.231  1.00 72.15
ATOM   1198  CA  ALA A  81      15.096  -6.729   2.530  1.00 12.01
ATOM   1199  C   ALA A  81      15.741  -5.427   2.993  1.00 31.12
ATOM   1200  O   ALA A  81      15.086  -4.581   3.601  1.00  2.02
ATOM   1201  CB  ALA A  81      15.323  -7.827   3.558  1.00 35.42
ATOM   1202  H   ALA A  81      15.879  -8.071   1.094  1.00 72.31
ATOM   1203  HA  ALA A  81      14.031  -6.576   2.432  1.00 74.12
ATOM   1204 1HB  ALA A  81      15.880  -8.634   3.105  1.00 60.23
ATOM   1205 2HB  ALA A  81      15.879  -7.429   4.393  1.00 24.32
ATOM   1206 3HB  ALA A  81      14.369  -8.198   3.904  1.00 25.34
ATOM   1207  N   ALA A  82      17.029  -5.274   2.702  1.00 15.10
ATOM   1208  CA  ALA A  82      17.761  -4.074   3.088  1.00 64.44
ATOM   1209  C   ALA A  82      17.690  -3.012   1.996  1.00 72.54
ATOM   1210  O   ALA A  82      17.418  -1.844   2.270  1.00  2.34
ATOM   1211  CB  ALA A  82      19.211  -4.418   3.398  1.00 73.32
ATOM   1212  H   ALA A  82      17.496  -5.984   2.215  1.00  2.11
ATOM   1213  HA  ALA A  82      17.310  -3.682   3.987  1.00 33.05
ATOM   1214 1HB  ALA A  82      19.765  -3.508   3.577  1.00 21.53
ATOM   1215 2HB  ALA A  82      19.252  -5.045   4.276  1.00 12.43
ATOM   1216 3HB  ALA A  82      19.643  -4.944   2.560  1.00 71.03
ATOM   1217  N   TRP A  83      17.936  -3.426   0.758  1.00 74.32
ATOM   1218  CA  TRP A  83      17.899  -2.509  -0.376  1.00 25.22
ATOM   1219  C   TRP A  83      16.594  -1.721  -0.397  1.00 63.53
ATOM   1220  O   TRP A  83      16.575  -0.545  -0.756  1.00 72.04
ATOM   1221  CB  TRP A  83      18.066  -3.279  -1.687  1.00 25.43
ATOM   1222  CG  TRP A  83      19.417  -3.911  -1.836  1.00 63.25
ATOM   1223  CD1 TRP A  83      20.403  -3.970  -0.894  1.00 25.44
ATOM   1224  CD2 TRP A  83      19.930  -4.571  -2.999  1.00 25.33
ATOM   1225  CE2 TRP A  83      21.234  -5.007  -2.689  1.00 32.01
ATOM   1226  CE3 TRP A  83      19.415  -4.839  -4.270  1.00  4.41
ATOM   1227  NE1 TRP A  83      21.499  -4.628  -1.400  1.00 10.42
ATOM   1228  CZ2 TRP A  83      22.026  -5.693  -3.605  1.00 64.12
ATOM   1229  CZ3 TRP A  83      20.203  -5.519  -5.178  1.00 64.33
ATOM   1230  CH2 TRP A  83      21.497  -5.941  -4.842  1.00 72.04
ATOM   1231  H   TRP A  83      18.146  -4.371   0.602  1.00  4.10
ATOM   1232  HA  TRP A  83      18.722  -1.818  -0.268  1.00  1.32
ATOM   1233 2HB  TRP A  83      17.325  -4.063  -1.734  1.00  1.23
ATOM   1234 3HB  TRP A  83      17.921  -2.601  -2.515  1.00  2.00
ATOM   1235  HD1 TRP A  83      20.321  -3.555   0.099  1.00 21.42
ATOM   1236  HE1 TRP A  83      22.334  -4.798  -0.915  1.00 31.20
ATOM   1237  HE3 TRP A  83      18.421  -4.522  -4.547  1.00 52.25
ATOM   1238  HZ2 TRP A  83      23.025  -6.025  -3.361  1.00 70.23
ATOM   1239  HZ3 TRP A  83      19.822  -5.734  -6.166  1.00 24.51
ATOM   1240  HH2 TRP A  83      22.077  -6.469  -5.583  1.00 73.34
ATOM   1241  N   ASN A  84      15.505  -2.378  -0.010  1.00 43.04
ATOM   1242  CA  ASN A  84      14.195  -1.738   0.014  1.00  2.30
ATOM   1243  C   ASN A  84      14.257  -0.401   0.746  1.00 53.40
ATOM   1244  O   ASN A  84      13.522   0.531   0.419  1.00 42.04
ATOM   1245  CB  ASN A  84      13.170  -2.653   0.686  1.00 73.00
ATOM   1246  CG  ASN A  84      11.804  -2.004   0.802  1.00 71.11
ATOM   1247  ND2 ASN A  84      10.841  -2.512   0.041  1.00 44.23
ATOM   1248  OD1 ASN A  84      11.617  -1.058   1.567  1.00 52.11
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ATOM   1249  H   ASN A  84      15.584  -3.315   0.265  1.00 63.21
ATOM   1250  HA  ASN A  84      13.893  -1.562  -1.007  1.00 61.34
ATOM   1251 2HB  ASN A  84      13.068  -3.558   0.105  1.00 65.04
ATOM   1252 3HB  ASN A  84      13.515  -2.904   1.678  1.00 55.22
ATOM   1253 1HD2 ASN A  84      11.063  -3.266  -0.545  1.00 10.12
ATOM   1254 2HD2 ASN A  84       9.949  -2.111   0.095  1.00 12.13
ATOM   1255  N   GLN A  85      15.138  -0.315   1.737  1.00  1.31
ATOM   1256  CA  GLN A  85      15.295   0.908   2.515  1.00  2.43
ATOM   1257  C   GLN A  85      16.024   1.977   1.708  1.00 51.42
ATOM   1258  O   GLN A  85      15.685   3.160   1.775  1.00 25.13
ATOM   1259  CB  GLN A  85      16.059   0.620   3.809  1.00 40.31
ATOM   1260  CG  GLN A  85      15.346   1.111   5.059  1.00 42.45
ATOM   1261  CD  GLN A  85      15.239   0.042   6.127  1.00 35.24
ATOM   1262  NE2 GLN A  85      14.208  -0.790   6.031  1.00 13.24
ATOM   1263  OE1 GLN A  85      16.073  -0.036   7.030  1.00 74.51
ATOM   1264  H   GLN A  85      15.695  -1.092   1.950  1.00 11.32
ATOM   1265  HA  GLN A  85      14.310   1.272   2.763  1.00 34.04
ATOM   1266 2HB  GLN A  85      16.203  -0.446   3.898  1.00 43.00
ATOM   1267 3HB  GLN A  85      17.024   1.103   3.758  1.00 12.12
ATOM   1268 2HG  GLN A  85      15.894   1.949   5.464  1.00 15.41
ATOM   1269 3HG  GLN A  85      14.351   1.431   4.787  1.00 33.52
ATOM   1270 1HE2 GLN A  85      13.584  -0.668   5.285  1.00 74.42
ATOM   1271 2HE2 GLN A  85      14.114  -1.491   6.708  1.00 21.11
ATOM   1272  N   LEU A  86      17.026   1.555   0.945  1.00 72.13
ATOM   1273  CA  LEU A  86      17.803   2.476   0.124  1.00 45.34
ATOM   1274  C   LEU A  86      16.914   3.182  -0.894  1.00 54.43
ATOM   1275  O   LEU A  86      17.280   4.225  -1.435  1.00 55.43
ATOM   1276  CB  LEU A  86      18.926   1.726  -0.596  1.00 55.34
ATOM   1277  CG  LEU A  86      20.200   1.487   0.214  1.00 61.34
ATOM   1278  CD1 LEU A  86      20.431  -0.003   0.417  1.00 10.44
ATOM   1279  CD2 LEU A  86      21.398   2.124  -0.475  1.00 53.54
ATOM   1280  H   LEU A  86      17.249   0.601   0.932  1.00 14.03
ATOM   1281  HA  LEU A  86      18.239   3.217   0.778  1.00 34.32
ATOM   1282 2HB  LEU A  86      18.540   0.765  -0.898  1.00 31.52
ATOM   1283 3HB  LEU A  86      19.193   2.296  -1.475  1.00 13.52
ATOM   1284  HG  LEU A  86      20.091   1.943   1.188  1.00 42.32
ATOM   1285 1HD1 LEU A  86      20.581  -0.478  -0.540  1.00 54.00
ATOM   1286 2HD1 LEU A  86      19.570  -0.437   0.905  1.00 45.24
ATOM   1287 3HD1 LEU A  86      21.306  -0.150   1.034  1.00 34.10
ATOM   1288 1HD2 LEU A  86      21.542   1.667  -1.443  1.00 35.30
ATOM   1289 2HD2 LEU A  86      22.282   1.976   0.128  1.00 35.51
ATOM   1290 3HD2 LEU A  86      21.220   3.182  -0.600  1.00  0.20
ATOM   1291  N   MET A  87      15.743   2.607  -1.148  1.00 53.45
ATOM   1292  CA  MET A  87      14.799   3.184  -2.099  1.00 51.10
ATOM   1293  C   MET A  87      14.255   4.514  -1.586  1.00 62.15
ATOM   1294  O   MET A  87      14.508   5.567  -2.173  1.00  4.12
ATOM   1295  CB  MET A  87      13.645   2.213  -2.357  1.00 51.42
ATOM   1296  CG  MET A  87      14.045   0.998  -3.178  1.00 40.20
ATOM   1297  SD  MET A  87      12.672  -0.138  -3.452  1.00 53.54
ATOM   1298  CE  MET A  87      12.431   0.043  -5.218  1.00 71.21
ATOM   1299  H   MET A  87      15.507   1.776  -0.686  1.00 13.33
ATOM   1300  HA  MET A  87      15.326   3.357  -3.025  1.00 71.02
ATOM   1301 2HB  MET A  87      13.260   1.870  -1.409  1.00 23.43
ATOM   1302 3HB  MET A  87      12.862   2.736  -2.886  1.00 72.23
ATOM   1303 2HG  MET A  87      14.413   1.333  -4.137  1.00 22.45
ATOM   1304 3HG  MET A  87      14.831   0.472  -2.657  1.00  1.34
ATOM   1305 1HE  MET A  87      11.382  -0.064  -5.451  1.00 71.43
ATOM   1306 2HE  MET A  87      12.771   1.019  -5.530  1.00  2.24
ATOM   1307 3HE  MET A  87      12.995  -0.718  -5.737  1.00 72.55
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ATOM   1308  N   LEU A  88      13.507   4.459  -0.490  1.00 61.21
ATOM   1309  CA  LEU A  88      12.927   5.660   0.101  1.00 21.45
ATOM   1310  C   LEU A  88      13.805   6.188   1.232  1.00 55.35
ATOM   1311  O   LEU A  88      14.149   7.370   1.262  1.00 24.54
ATOM   1312  CB  LEU A  88      11.521   5.365   0.627  1.00 21.13
ATOM   1313  CG  LEU A  88      10.908   4.033   0.194  1.00 21.32
ATOM   1314  CD1 LEU A  88      11.285   2.929   1.170  1.00  2.23
ATOM   1315  CD2 LEU A  88       9.395   4.153   0.081  1.00  4.41
ATOM   1316  H   LEU A  88      13.340   3.591  -0.068  1.00 23.04
ATOM   1317  HA  LEU A  88      12.864   6.412  -0.671  1.00 35.32
ATOM   1318 2HB  LEU A  88      11.563   5.374   1.706  1.00 52.45
ATOM   1319 3HB  LEU A  88      10.869   6.157   0.287  1.00 70.31
ATOM   1320  HG  LEU A  88      11.297   3.764  -0.779  1.00 12.14
ATOM   1321 1HD1 LEU A  88      10.429   2.679   1.779  1.00 44.12
ATOM   1322 2HD1 LEU A  88      12.091   3.269   1.804  1.00 12.12
ATOM   1323 3HD1 LEU A  88      11.604   2.056   0.620  1.00 24.14
ATOM   1324 1HD2 LEU A  88       8.944   3.927   1.036  1.00  4.21
ATOM   1325 2HD2 LEU A  88       9.033   3.457  -0.662  1.00  4.23
ATOM   1326 3HD2 LEU A  88       9.135   5.160  -0.211  1.00 25.11
ATOM   1327  N   SER A  89      14.164   5.305   2.158  1.00 70.05
ATOM   1328  CA  SER A  89      15.000   5.683   3.291  1.00 63.13
ATOM   1329  C   SER A  89      16.373   6.154   2.820  1.00 53.44
ATOM   1330  O   SER A  89      17.029   6.954   3.487  1.00 42.12
ATOM   1331  CB  SER A  89      15.156   4.503   4.252  1.00  2.44
ATOM   1332  OG  SER A  89      15.407   4.952   5.573  1.00 34.11
ATOM   1333  H   SER A  89      13.857   4.377   2.078  1.00 50.54
ATOM   1334  HA  SER A  89      14.511   6.495   3.807  1.00  3.42
ATOM   1335 2HB  SER A  89      14.249   3.918   4.250  1.00 65.11
ATOM   1336 3HB  SER A  89      15.984   3.887   3.931  1.00 54.40
ATOM   1337  HG  SER A  89      14.749   5.607   5.819  1.00 44.10
ATOM   1338  N   ARG A  90      16.800   5.653   1.665  1.00 34.22
ATOM   1339  CA  ARG A  90      18.094   6.021   1.104  1.00 30.24
ATOM   1340  C   ARG A  90      19.198   5.885   2.149  1.00 32.51
ATOM   1341  O   ARG A  90      19.946   6.828   2.403  1.00 43.34
ATOM   1342  CB  ARG A  90      18.054   7.455   0.573  1.00 63.21
ATOM   1343  CG  ARG A  90      18.726   7.622  -0.780  1.00 61.43
ATOM   1344  CD  ARG A  90      20.045   8.368  -0.659  1.00  4.10
ATOM   1345  NE  ARG A  90      20.265   9.277  -1.781  1.00 63.30
ATOM   1346  CZ  ARG A  90      19.619  10.427  -1.933  1.00 13.13
ATOM   1347  NH1 ARG A  90      18.717  10.808  -1.038  1.00 70.53
ATOM   1348  NH2 ARG A  90      19.874  11.200  -2.981  1.00 21.13
ATOM   1349  H   ARG A  90      16.231   5.019   1.179  1.00 11.44
ATOM   1350  HA  ARG A  90      18.304   5.349   0.286  1.00 63.30
ATOM   1351 2HB  ARG A  90      17.023   7.763   0.479  1.00 44.24
ATOM   1352 3HB  ARG A  90      18.552   8.101   1.280  1.00 51.53
ATOM   1353 2HG  ARG A  90      18.915   6.645  -1.201  1.00 24.02
ATOM   1354 3HG  ARG A  90      18.068   8.175  -1.433  1.00 15.34
ATOM   1355 2HD  ARG A  90      20.038   8.939   0.258  1.00 71.24
ATOM   1356 3HD  ARG A  90      20.849   7.648  -0.628  1.00 23.13
ATOM   1357  HE  ARG A  90      20.927   9.015  -2.454  1.00  5.12
ATOM   1358 1HH1 ARG A  90      18.523  10.228  -0.247  1.00 63.31
ATOM   1359 2HH1 ARG A  90      18.232  11.675  -1.154  1.00 63.12
ATOM   1360 1HH2 ARG A  90      20.553  10.917  -3.657  1.00 24.41
ATOM   1361 2HH2 ARG A  90      19.387  12.065  -3.094  1.00 40.30
ATOM   1362  N   SER A  91      19.292   4.704   2.752  1.00 20.23
ATOM   1363  CA  SER A  91      20.301   4.445   3.773  1.00 42.23
ATOM   1364  C   SER A  91      20.214   5.474   4.896  1.00 30.21
ATOM   1365  O   SER A  91      20.967   6.446   4.942  1.00 43.54
ATOM   1366  CB  SER A  91      21.700   4.467   3.154  1.00 60.34
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ATOM   1367  OG  SER A  91      22.602   3.670   3.903  1.00 54.42
ATOM   1368  H   SER A  91      18.666   3.991   2.507  1.00 70.42
ATOM   1369  HA  SER A  91      20.114   3.464   4.183  1.00 15.22
ATOM   1370 2HB  SER A  91      21.651   4.082   2.146  1.00  0.42
ATOM   1371 3HB  SER A  91      22.066   5.483   3.134  1.00 63.00
ATOM   1372  HG  SER A  91      22.118   2.971   4.348  1.00 74.02
ATOM   1373  N   PRO A  92      19.272   5.255   5.826  1.00 50.15
ATOM   1374  CA  PRO A  92      19.063   6.151   6.967  1.00 51.12
ATOM   1375  C   PRO A  92      20.208   6.087   7.972  1.00 62.15
ATOM   1376  O   PRO A  92      20.518   7.075   8.637  1.00 75.32
ATOM   1377  CB  PRO A  92      17.769   5.628   7.596  1.00 24.12
ATOM   1378  CG  PRO A  92      17.706   4.194   7.196  1.00  4.22
ATOM   1379  CD  PRO A  92      18.339   4.116   5.834  1.00 13.12
ATOM   1380  HA  PRO A  92      18.922   7.174   6.648  1.00 62.51
ATOM   1381 2HB  PRO A  92      17.819   5.737   8.670  1.00 11.45
ATOM   1382 3HB  PRO A  92      16.927   6.182   7.211  1.00 42.44
ATOM   1383 2HG  PRO A  92      18.259   3.592   7.901  1.00 34.42
ATOM   1384 3HG  PRO A  92      16.677   3.871   7.150  1.00 12.30
ATOM   1385 2HD  PRO A  92      18.869   3.182   5.717  1.00 13.41
ATOM   1386 3HD  PRO A  92      17.590   4.226   5.064  1.00 51.33
ATOM   1387  N   GLU A  93      20.834   4.918   8.075  1.00 15.44
ATOM   1388  CA  GLU A  93      21.945   4.727   9.000  1.00 33.01
ATOM   1389  C   GLU A  93      22.711   3.449   8.672  1.00 23.13
ATOM   1390  O   GLU A  93      23.858   3.278   9.085  1.00 12.31
ATOM   1391  CB  GLU A  93      21.434   4.673  10.442  1.00 42.15
ATOM   1392  CG  GLU A  93      22.059   5.720  11.348  1.00 54.50
ATOM   1393  CD  GLU A  93      23.362   5.254  11.966  1.00  3.35
ATOM   1394  OE1 GLU A  93      24.404   5.890  11.702  1.00 64.33
ATOM   1395  OE2 GLU A  93      23.341   4.255  12.714  1.00 32.25
ATOM   1396  H   GLU A  93      20.541   4.168   7.518  1.00 75.32
ATOM   1397  HA  GLU A  93      22.612   5.569   8.896  1.00 52.23
ATOM   1398 2HB  GLU A  93      20.364   4.821  10.438  1.00 43.13
ATOM   1399 3HB  GLU A  93      21.652   3.698  10.851  1.00 73.41
ATOM   1400 2HG  GLU A  93      22.251   6.611  10.769  1.00 63.15
ATOM   1401 3HG  GLU A  93      21.363   5.952  12.141  1.00  3.23
TER    1402      GLU A  93
ENDMDL
END
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