Supporting Information

Cellular polyamines promote amyloid-beta (Aβ) peptide fibrillation and modulate the aggregation pathways

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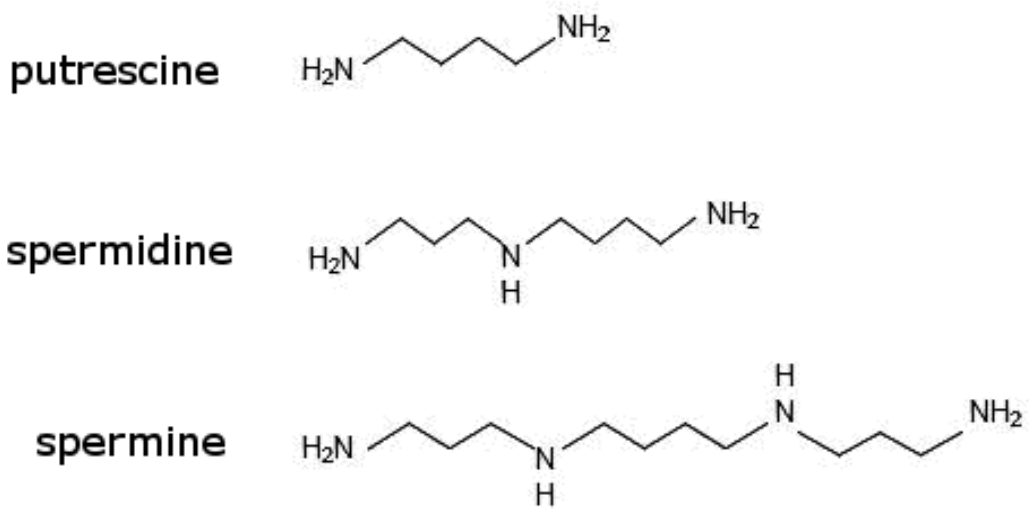
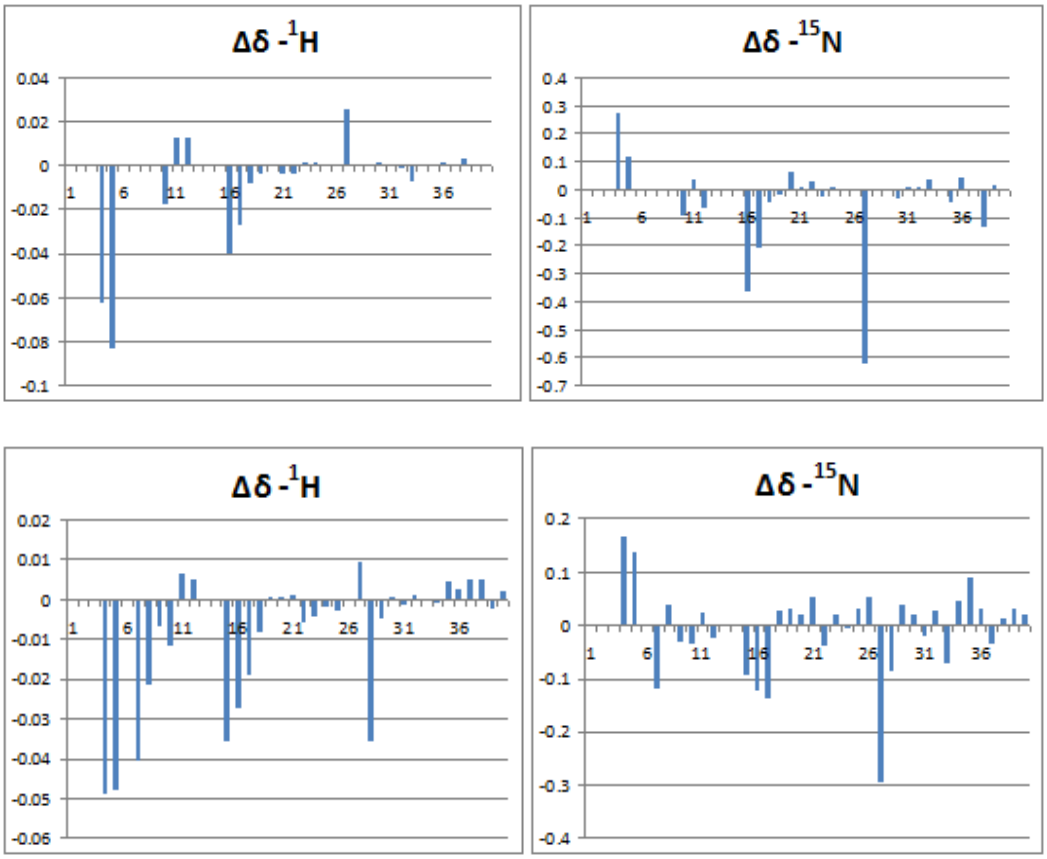
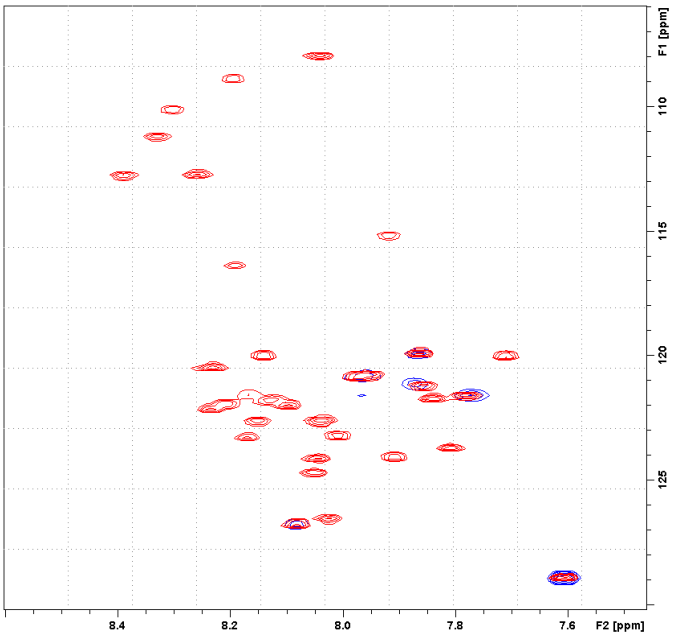


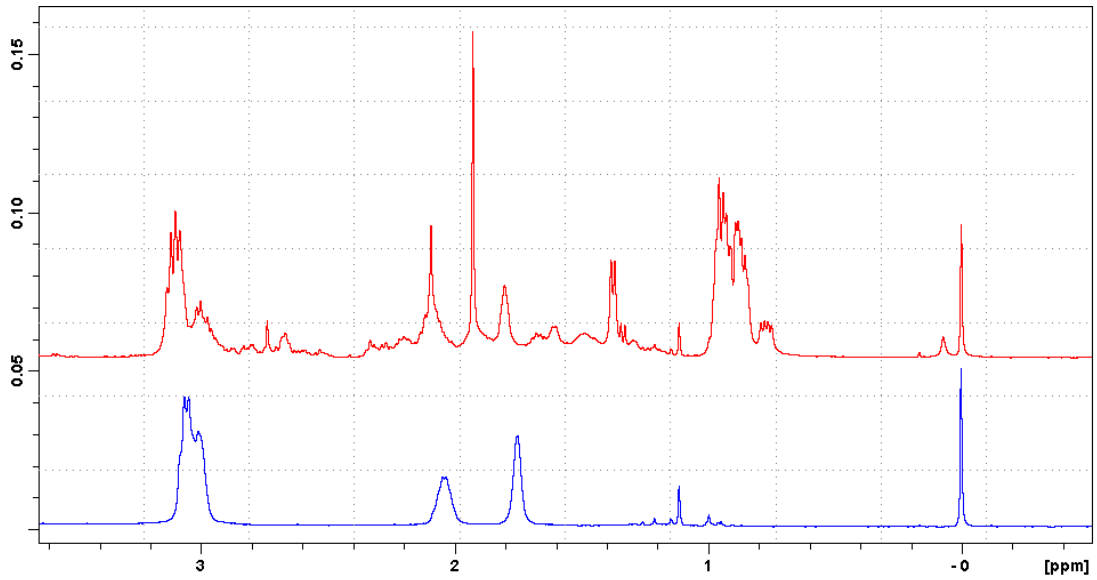
Supporting Information Figure S1. The polycationic alkylamines spermine and spermidine, together with their diamine precursor putrescine.



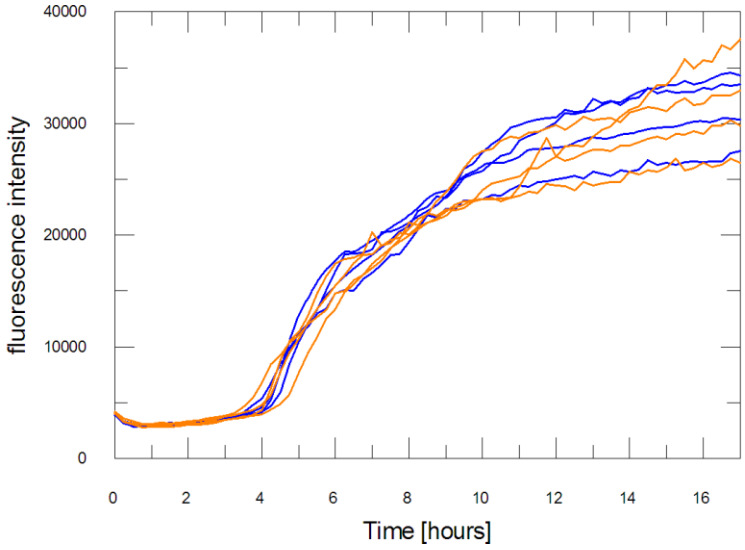
Supporting Information Figure S2. Chemical shift differences in the ^{1}H-^{15}N-HSQC spectra of 100 μM ^{15}N-labeled Aβ(1-40) peptide in 20 mM sodium phosphate buffer at pH 7.3, +5 °C, after addition of 200 μM of spermine (top) or putrescine (bottom).



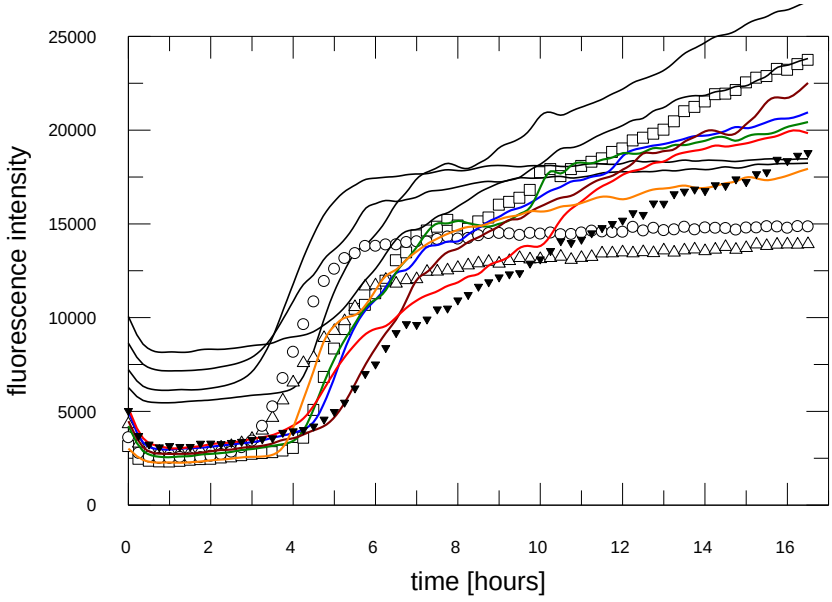
Supporting Figure S3. NMR ^{1}H-^{15}N-HSQC spectra of 100 µM ^{15}N-labeled Aβ (1-40) peptide in 20 mM sodium phosphate buffer at pH 7.3, +5 °C, before (red) and after (blue) addition of 300 µM spermine. Note the unchanged intensity of the V40 cross-peak in the lower right corner.



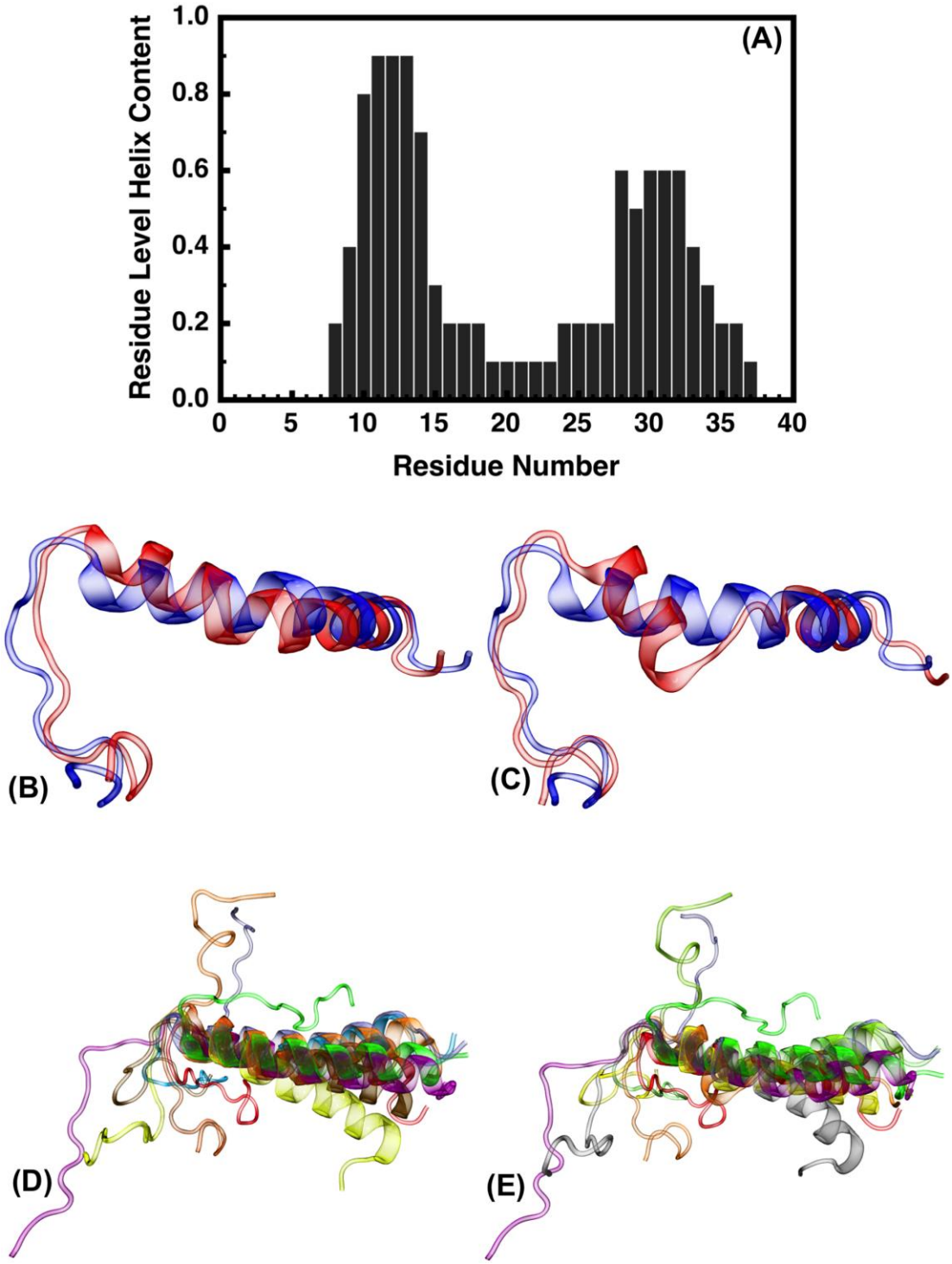
Supporting Information Figure S4. NMR spectra at +5 °C of 150 µM spermine in 10 mM phosphate buffer pH 7.3 (blue, lower), and after addition of 90 µM (red, upper) Aβ(1-40) peptide. Note the chemical shift changes of the spermine signals around 2 ppm. The pH was measured both before and after each measurement, and the spectra were referenced to added TSP (0 ppm).



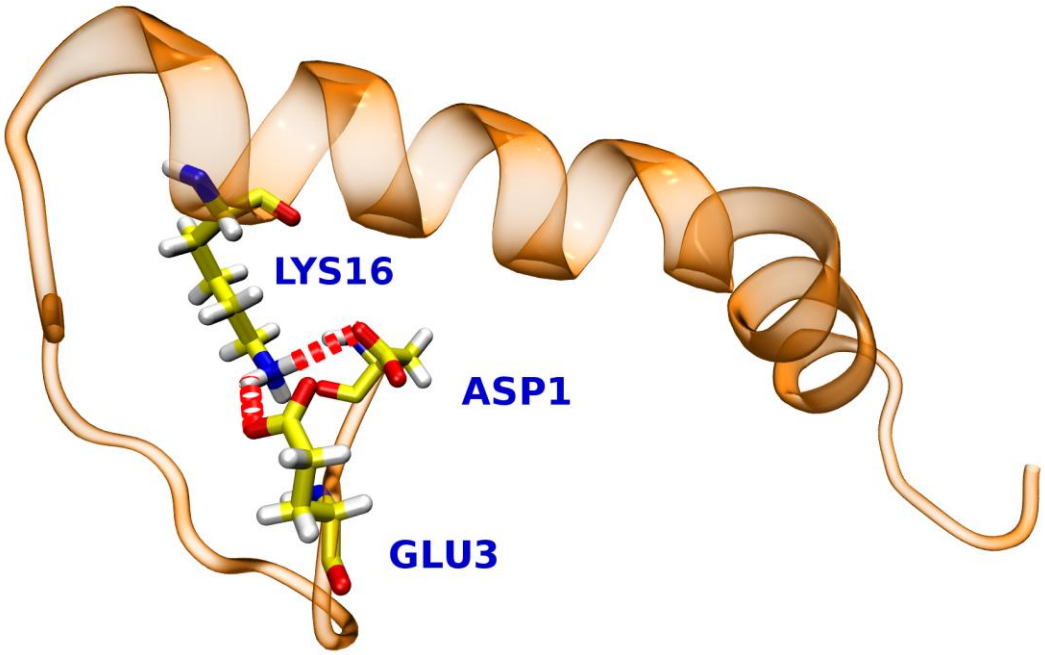
Supporting Information Figure S5. ThT fluorescence curves of 20 µM Aβ(1-40) peptide in 50 mM Tris buffer, pH 7.4, with 500 uM putrescine (blue lines), and with additional 1 mM EDTA present (orange lines).



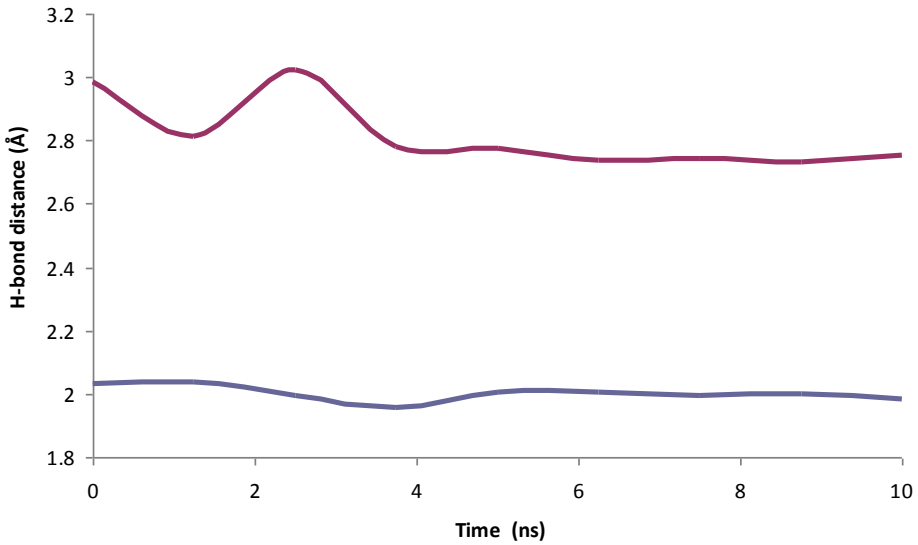
Supporting Information Figure S6. ThT fluorescence curves at +37 °C for Aβ(1-40) aggregation in only 50 mM Tris buffer, pH 7.4 (▼), or in presence also of: 0.5 mM putrescine (□); 0.5 mM spermidine (Δ); 0.5 mM spermine (○); 0.1 mM NaCl (— blue); 0.4 mM NaCl (— green); 2 mM NaCl (— brown); 10 mM NaCl (— red); 100 mM NaCl (— orange).



Supporting Information Figure S7. (A): Helical content for each residue in Aβ(1-40), predicted from the amino acid sequence using the AGADIR algorithm (Muñoz & Serrano, 1997). (B) and (C): Overlays of the initial (blue) and final (red) conformations of a sample isoform of Aβ(1-40), before and after 10ns of MD simulation, in the presence of only neutralizing counterions (B), or 200 mM of NaCl (C). (D) and (E): overlays of 9 different isoforms of Aβ(1-40), after 10ns of MD simulation, again with either only neutralizing counterions (D) or in the presence of 200 mM NaCl (E).



Supporting Information Figure S8. Observed hydrogen bonds between Lys16 and respectively Asp1 and Glu3 after 10ns of MD simulation of the Aβ(1-40) peptide, in the presence of neutralizing counterions only (i.e. no polyamines present).



Supporting Information Figure S9. H-bond distances between Lys16-Asp1(blue line) and Lys16-Glu3 (purple line) during 10ns MD simulation of the Aβ(1-40) peptide, in the presence of neutralizing counterions only (i.e. no polyamines present).

Computational Protocol and Model Validation

The initial atomic coordinates of the uncomplexed form Aβ(1-40) (Coles et al, 1998) as well as the complexes of Aβ(1-40) with putrescine, spermine and spermidine were obtained as outlined in the main text. Partial charges for each ligand were obtained using Gaussian09 (Frisch *et al*, 2009), at the B3LYP/6-31G* level of theory (Becke, 1993), using CHELPG charges (Breneman & Wiberg, 1990) and in conjunction with the COSMO continuum model (Klamt & Schüürmann, 1993). All ligands were kept in their fully protonated states, as would be expected from amines at physiological pH, leading to total charges of +2, +3 and +4 on putrescine, spermidine and spermidine respectively (Supplementary Figure S1). Best-fit conformations of the peptide in complex with the relevant polyamines were obtained using the HEX docking package (Ritchie, 2003), selecting the three most physically reasonable conformations (based on peptide-ligand interactions) from the 15 top-ranked structures in the resulting docking ensemble. In both the native, unliganded form of the peptide, as well as in the peptide-ligand complexes, all ionizable residues were set to their default ionization states at physiological pH (with the exception of histidines, which were kept neutral), and the total system was neutralized by Na^+ or Cl^- ions as relevant, using 3 Na^+ ions for the uncomplexed form of the peptide, and one Na^+, no counterions, and one Cl^- for the peptide complexed with putrescine, spermidine and spermine respectively. For comparison, we also performed simulations on the uncomplexed form of the peptide in the presence of 200 mM NaCl. Ions were added using AmberTools 12 (Case *et al*, 2012), *via* the CHIMERA software package (Pettersen *et al*, 2004).

The entire peptide (or peptide-ligand complex) was solvated using a water sphere of 34Å radius (in order to engulf the entire peptide and capture its flexibility explicitly during the simulation), which was surrounded by first a 2Å grid of Langevin dipoles, and then by bulk solvent, modeled using the surface-constrained all-atom solvent model (SCAAS) (Lee et al, 1993). Each system was equilibrated by gradual heating from 30 to 300K, in 125ps (using temperatures of 30, 50, 80, 100, 150, 200, 250 and 300K), followed by a subsequent 10ns of molecular dynamics (MD) at 300K, monitoring structural and energetic changes along the trajectory. A 1fs timestep was used throughout. Here, it is important to make a note about the size of the peptide: as mentioned above, the ten isoform fits to the NMR data vary in how elongated the peptide is, and, at maximum elongation (i.e. in almost linear form), Aβ(1-40) is approximately 60Å in length, requiring a very large simulation sphere to contain the entire peptide, making it computationally prohibitive to simulate (see also the discussion in the supporting information of (Lin et al, 2012) for the related case of Aβ(1-42). Therefore, we limited our simulations to 9 out of the 10 proposed models, selecting only those structures we could fully accommodate in a water sphere of reasonable size. All 9 isoforms were subjected

to 10ns of MD simulation as outlined above, in order to compare structural diversity after relaxation, and HEX docking was performed on four representative confirmations, to obtain the best three positions, and these were in turn also subjected to 10ns of MD simulation (resulting in 9 simulations of the uncomplexed form of the peptide, and 4x3 simulations of the complexed form of the peptide). All simulations were performed using the MOLARIS simulation package and the ENZYMIX forcefield (Lee et al, 1993), with long-range effects being treated using the local reaction field (LRF) approach (Lee & Warshel, 1992).

As outlined in the main text, the presence of the polyamines appears to trigger structural transitions in the Aβ(1-40) peptides on timescales spanning several hours. Clearly such timescales are beyond the scope of computer simulations, however, our aim in this work has been to perform a preliminary theoretical investigation of the interaction of individual polyamines with the peptide in order to examine how initial contacts may be established between the two, as well as the extent to which secondary structural features are retained or changed on the ns timescale. As our starting point, we used a structure of the Aβ(1-40) peptide solved in the presence of sodium dodecyl sulfate (SDS) micelles, which kept the central residues (15-36) of the peptide in an alpha-helical conformation (Coles et al, 1998). Clearly, objections can be raised against extending this structure to an aqueous solution, where the peptide is believed to adopt a conformation dominated by random coil structure. However, the inherent disorder tendency of the peptide makes it almost impossible to solve a structure in aqueous solution, and, therefore, this model provides one of the best currently available starting points for theoretical exploration of the Aβ(1-40) monomer.

In order to validate our model, we first started by testing the stability of the SDS structure in aqueous solution in the absence of polyamines. Supplementary Figure S7 (A) shows a plot of the predicted helical content of each residue, obtained from the amino acid sequence via the AGADIR algorithm (Muñoz & Serrano, 1997). Supplementary Figure S7 (B) and (C) shows an overlay of the initial and final structures of a sample isoform of Aβ(1-40), before and after 10ns of MD simulation, either in the presence of only neutralizing counterions (B) or in the presence of 200 mM NaCl. The RMSD of the final structure from the initial structure is 0.4 Å and 2.1 Å with and without counterions respectively. Supplementary Figure S7 (D) and (E) shows an overlay of 9 different isoforms of Aβ(1-40) after 10ns of MD simulation, again, with only neutralizing counterions and in the presence of 200 mM NaCl.

It should be noted that AGADIR predicts helical content by evaluating the energy of short-range inter-residue interactions estimated from the local amino acid composition, and does *not* take any information about secondary structure into account when making the prediction. Therefore, it is interesting to see that AGADIR predicts the peptide to display two

alpha helical regions, with a kink in approximately the same location as predicted by the NMR structure (Coles et al, 1998), and with a disordered N-terminus - particularly the first 6-7 residues. This ties in nicely with the SDS model, which resulted in 10 isomers, all of which present a more ordered alpha-helical configuration between residues 15-36, a hinge or kink at residues 25-27, and greater disorder in both termini (although the precise extent of this disorder appears to be pH-dependent). From our simulations on the uncomplexed ligand, in the presence of only neutralizing counterions, it would appear that the central helix is quite stable over the course of 10ns of simulation time even in the absence of SDS micelles (see Supplementary Figure S7 (D)), while in the presence of 200 mM of NaCl (Supplementary Figure S7 (C)) it can be seen that the stability of this helical structure is dependent on the ionic strength used. That is, when comparing 9 different isoforms of the peptide which were taken as starting structures, the final structures do not deviate from each other by more than an RMSD of 0.4 Å (using the final structure shown in Supplementary Figure S7 (B) as a reference point). This suggests that the helical conformation is a valid starting point for examining interactions between the polyamines and the monomeric form of the peptide. Additionally, a tendency towards a helical conformation was recently demonstrated by Pande and coworkers (Lin et al, 2012), who studied the effect of peptide length and pathogenic mutations on structural ensembles of Aβ(1-40) and Aβ(1-42), observing that reducing the peptide length to 40 residues also reduces the tendency towards hairpin formation (note however that the authors used both a very small simulation box of 5x5x5nm, and also did not explore the effect of changing ionic strength on structural stability, which could potentially change their observations, see also Supplementary Figure S7 (C)).

At present, we are only examining initial interactions between the polyamines and the peptide over the course of short simulations, and in the presence of only neutralizing counterions. However, for subsequent work, we plan to explore structural changes upon much longer simulation time, as well as the effects of varying ionic strength.

References

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Appendix A. PDB files

Herein we provide PDB files with atomic coordinates obtained with the MOLARIS simulation package (Lee et al, 1993) for two uncomplexed forms (second and tenth) out of ten NMR isoforms of Aβ(1-40) (Coles et al, 1998) with 3 Na^+ counterions. All ionizable residues were set to their default ionization states at physiological pH (with the exception of histidines, which were kept neutral), and the total system was neutralized using 3 Na^+ ions for the uncomplexed form of the peptide. Ions were added using AmberTools 12 (Case *et al*, 2012), *via* the CHIMERA software package (Pettersen *et al*, 2004). Both isoforms (second and tenth) were subjected to 10ns of MD simulation as outlined in the main text, in order to compare structural diversity after relaxation. We therefore provide both the initial structures at the beginning of the MD simulation, and the final structures obtained after the MD simulation.

Initial MD structure of the second NMR isoform with 3 Na^+ counterions

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ATOM    135  HCB2TYR    10       1.839   8.531  -2.231
ATOM    136  CG  TYR    10       1.996   7.751  -4.137
ATOM    137  CD1 TYR    10       2.880   7.392  -5.139
ATOM    138  HCD1TYR    10       3.842   7.238  -4.918
ATOM    139  CE1 TYR    10       2.445   7.244  -6.439
ATOM    140  HCE1TYR    10       3.093   6.983  -7.153
ATOM    141  CZ  TYR    10       1.118   7.453  -6.762
ATOM    142  OH  TYR    10       0.685   7.302  -8.058
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ATOM    143  HOH TYR    10       0.253   8.072  -8.533
ATOM    144  CE2 TYR    10       0.234   7.812  -5.763
ATOM    145  HCE2TYR    10      -0.728   7.965  -5.985
ATOM    146  CD2 TYR    10       0.668   7.961  -4.461
ATOM    147  HCD2TYR    10       0.019   8.223  -3.748
ATOM    148  C   TYR    10       0.900   6.123  -1.845
ATOM    149  O   TYR    10       0.468   5.174  -2.472
ATOM    150  N   GLU    11       0.178   6.866  -1.041
ATOM    151  HN  GLU    11       0.609   7.630  -0.567
ATOM    152  CA  GLU    11      -1.272   6.597  -0.822
ATOM    153  HA  GLU    11      -1.460   5.615  -0.866
ATOM    154  CB  GLU    11      -1.667   7.127   0.574
ATOM    155  HB1 GLU    11      -1.493   8.112   0.566
ATOM    156  HB2 GLU    11      -1.194   6.549   1.241
ATOM    157  CG  GLU    11      -3.191   6.948   0.831
ATOM    158  HG1 GLU    11      -3.303   6.807   1.816
ATOM    159  HG2 GLU    11      -3.510   6.246   0.194
ATOM    160  CD  GLU    11      -3.947   8.245   0.482
ATOM    161  OE1 GLU    11      -3.833   9.170   1.270
ATOM    162  OE2 GLU    11      -4.600   8.248  -0.551
ATOM    163  C   GLU    11      -2.085   7.301  -1.914
ATOM    164  O   GLU    11      -2.029   8.510  -2.043
ATOM    165  N   VAL    12      -2.817   6.520  -2.668
ATOM    166  HN  VAL    12      -2.803   5.539  -2.491
ATOM    167  CA  VAL    12      -3.665   7.029  -3.766
ATOM    168  HA  VAL    12      -3.548   8.001  -3.975
ATOM    169  CB  VAL    12      -3.280   6.236  -5.080
ATOM    170  HB  VAL    12      -2.660   6.864  -5.551
ATOM    171  CG1 VAL    12      -2.596   4.894  -4.786
ATOM    172  HG11VAL    12      -2.188   4.928  -3.874
ATOM    173  HG12VAL    12      -3.279   4.164  -4.826
ATOM    174  HG13VAL    12      -1.885   4.734  -5.471
ATOM    175  CG2 VAL    12      -4.476   5.900  -5.954
ATOM    176  HG21VAL    12      -5.223   6.529  -5.740
ATOM    177  HG22VAL    12      -4.216   5.995  -6.914
ATOM    178  HG23VAL    12      -4.761   4.959  -5.769
ATOM    179  C   VAL    12      -5.108   6.783  -3.296
ATOM    180  O   VAL    12      -5.357   6.148  -2.287
ATOM    181  N   HIS    13      -6.017   7.300  -4.072
ATOM    182  HN  HIS    13      -5.726   7.799  -4.886
ATOM    183  CA  HIS    13      -7.479   7.171  -3.782
ATOM    184  HA  HIS    13      -7.634   7.180  -2.794
ATOM    185  CB  HIS    13      -8.192   8.366  -4.446
ATOM    186  HB1 HIS    13      -9.175   8.238  -4.304
ATOM    187  HB2 HIS    13      -7.836   8.440  -5.378
ATOM    188  CG  HIS    13      -7.794   9.648  -3.706
ATOM    189  ND1 HIS    13      -8.622  10.464  -3.141
ATOM    190  HD1 HIS    13      -9.613  10.355  -3.121
ATOM    191  CE1 HIS    13      -7.968  11.446  -2.603
ATOM    192  HE1 HIS    13      -8.398  12.200  -2.107
ATOM    193  NE2 HIS    13      -6.676  11.328  -2.787
ATOM    194  CD2 HIS    13      -6.547  10.211  -3.475
ATOM    195  HD2 HIS    13      -5.679   9.825  -3.785
ATOM    196  C   HIS    13      -8.038   5.833  -4.296
ATOM    197  O   HIS    13      -9.204   5.719  -4.628
ATOM    198  N   HIS    14      -7.169   4.853  -4.341
ATOM    199  HN  HIS    14      -6.232   5.034  -4.044
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ATOM    200  CA  HIS    14      -7.518   3.481  -4.810
ATOM    201  HA  HIS    14      -8.480   3.283  -4.619
ATOM    202  CB  HIS    14      -7.293   3.358  -6.328
ATOM    203  HB1 HIS    14      -7.584   2.438  -6.593
ATOM    204  HB2 HIS    14      -6.352   3.646  -6.507
ATOM    205  CG  HIS    14      -8.201   4.334  -7.049
ATOM    206  ND1 HIS    14      -9.473   4.221  -7.242
ATOM    207  HD1 HIS    14     -10.038   3.460  -6.937
ATOM    208  CE1 HIS    14      -9.897   5.259  -7.896
ATOM    209  HE1 HIS    14     -10.848   5.400  -8.166
ATOM    210  NE2 HIS    14      -8.923   6.097  -8.160
ATOM    211  CD2 HIS    14      -7.861   5.522  -7.632
ATOM    212  HD2 HIS    14      -6.937   5.901  -7.653
ATOM    213  C   HIS    14      -6.594   2.507  -4.083
ATOM    214  O   HIS    14      -5.409   2.460  -4.359
ATOM    215  N   GLN    15      -7.141   1.741  -3.170
ATOM    216  HN  GLN    15      -8.117   1.818  -2.980
ATOM    217  CA  GLN    15      -6.304   0.755  -2.413
ATOM    218  HA  GLN    15      -5.607   1.254  -1.897
ATOM    219  CB  GLN    15      -7.219  -0.043  -1.440
ATOM    220  HB1 GLN    15      -7.054  -1.014  -1.618
ATOM    221  HB2 GLN    15      -8.142   0.327  -1.544
ATOM    222  CG  GLN    15      -6.797   0.216   0.027
ATOM    223  HG1 GLN    15      -7.536  -0.132   0.606
ATOM    224  HG2 GLN    15      -6.540   1.181   0.086
ATOM    225  CD  GLN    15      -5.544  -0.599   0.374
ATOM    226  OE1 GLN    15      -4.506  -0.472  -0.244
ATOM    227  NE2 GLN    15      -5.594  -1.453   1.361
ATOM    228  HE21GLN    15      -4.779  -1.984   1.585
ATOM    229  HE22GLN    15      -6.446  -1.559   1.868
ATOM    230  C   GLN    15      -5.580  -0.216  -3.367
ATOM    231  O   GLN    15      -4.654  -0.903  -2.983
ATOM    232  N   LYS    16      -6.019  -0.226  -4.603
ATOM    233  HN  LYS    16      -6.770   0.380  -4.852
ATOM    234  CA  LYS    16      -5.430  -1.108  -5.637
ATOM    235  HA1 LYS    16      -5.282  -2.042  -5.311
ATOM    236  CB  LYS    16      -6.421  -1.160  -6.834
ATOM    237  HB1 LYS    16      -5.995  -0.652  -7.584
ATOM    238  HB2 LYS    16      -7.312  -0.866  -6.485
ATOM    239  CG  LYS    16      -6.596  -2.606  -7.324
ATOM    240  HG1 LYS    16      -7.127  -2.567  -8.171
ATOM    241  HG2 LYS    16      -6.943  -3.140  -6.551
ATOM    242  CD  LYS    16      -5.214  -3.177  -7.682
ATOM    243  HD1 LYS    16      -4.817  -3.527  -6.832
ATOM    244  HD2 LYS    16      -4.730  -2.466  -8.193
ATOM    245  CE  LYS    16      -5.363  -4.377  -8.632
ATOM    246  HE1 LYS    16      -6.085  -4.956  -8.251
ATOM    247  HE2 LYS    16      -4.447  -4.756  -8.765
ATOM    248  NZ  LYS    16      -5.838  -3.919  -9.969
ATOM    249  HZ1 LYS    16      -6.058  -2.947  -9.920
ATOM    250  HZ2 LYS    16      -5.116  -4.072 -10.640
ATOM    251  HZ3 LYS    16      -6.652  -4.439 -10.221
ATOM    252  C   LYS    16      -4.086  -0.510  -6.032
ATOM    253  O   LYS    16      -3.047  -1.137  -5.937
ATOM    254  N   LEU    17      -4.160   0.722  -6.464
ATOM    255  HN  LEU    17      -5.045   1.178  -6.512
ATOM    256  CA  LEU    17      -2.928   1.444  -6.884
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ATOM    257  HA  LEU   17      -2.472   0.983  -7.645
ATOM    258  CB  LEU   17      -3.313   2.867  -7.345
ATOM    259  HB1 LEU   17      -2.455   3.307  -7.613
ATOM    260  HB2 LEU   17      -3.854   3.259  -6.599
ATOM    261  CG  LEU   17      -4.239   2.917  -8.620
ATOM    262  HG  LEU   17      -5.169   3.063  -8.284
ATOM    263  CD1 LEU   17      -3.773   4.065  -9.546
ATOM    264  HD11LEU   17      -3.710   4.909  -9.013
ATOM    265  HD12LEU   17      -2.877   3.834  -9.926
ATOM    266  HD13LEU   17      -4.438   4.178 -10.285
ATOM    267  CD2 LEU   17      -4.253   1.606  -9.434
ATOM    268  HD21LEU   17      -4.262   0.831  -8.803
ATOM    269  HD22LEU   17      -5.072   1.588 -10.008
ATOM    270  HD23LEU   17      -3.434   1.569 -10.007
ATOM    271  C   LEU   17      -1.986   1.493  -5.672
ATOM    272  O   LEU   17      -0.791   1.371  -5.827
ATOM    273  N   VAL   18      -2.542   1.664  -4.496
ATOM    274  HN  VAL   18      -3.534   1.760  -4.439
ATOM    275  CA  VAL   18      -1.733   1.720  -3.240
ATOM    276  HA  VAL   18      -1.139   2.524  -3.220
ATOM    277  CB  VAL   18      -2.722   1.788  -2.035
ATOM    278  HB  VAL   18      -3.468   1.152  -2.232
ATOM    279  CG1 VAL   18      -2.038   1.373  -0.727
ATOM    280  HG11VAL   18      -2.056   2.142  -0.090
ATOM    281  HG12VAL   18      -2.529   0.594  -0.335
ATOM    282  HG13VAL   18      -1.091   1.113  -0.921
ATOM    283  CG2 VAL   18      -3.277   3.215  -1.866
ATOM    284  HG21VAL   18      -2.990   3.573  -0.977
ATOM    285  HG22VAL   18      -2.918   3.793  -2.598
ATOM    286  HG23VAL   18      -4.275   3.184  -1.915
ATOM    287  C   VAL   18      -0.841   0.464  -3.163
ATOM    288  O   VAL   18       0.359   0.566  -3.004
ATOM    289  N   PHE   19      -1.455  -0.688  -3.288
ATOM    290  HN  PHE   19      -2.444  -0.704  -3.422
ATOM    291  CA  PHE   19      -0.695  -1.977  -3.231
ATOM    292  HA  PHE   19      -0.313  -2.081  -2.312
ATOM    293  CB  PHE   19      -1.643  -3.158  -3.537
ATOM    294  HCB1PHE   19      -1.077  -3.984  -3.517
ATOM    295  HCB2PHE   19      -2.129  -2.916  -4.377
ATOM    296  CG  PHE   19      -2.721  -3.349  -2.453
ATOM    297  CD1 PHE   19      -2.443  -3.200  -1.100
ATOM    298  HCD1PHE   19      -1.519  -2.956  -0.808
ATOM    299  CE1 PHE   19      -3.432  -3.385  -0.155
ATOM    300  HCE1PHE   19      -3.221  -3.275   0.815
ATOM    301  CZ  PHE   19      -4.710  -3.722  -0.547
ATOM    302  HCZ PHE   19      -5.424  -3.855   0.137
ATOM    303  CE2 PHE   19      -4.999  -3.872  -1.886
ATOM    304  HCE2PHE   19      -5.924  -4.116  -2.173
ATOM    305  CD2 PHE   19      -4.010  -3.687  -2.832
ATOM    306  HCD2PHE   19      -4.227  -3.796  -3.801
ATOM    307  C   PHE   19       0.443  -1.972  -4.250
ATOM    308  O   PHE   19       1.579  -2.276  -3.931
ATOM    309  N   PHE   20       0.098  -1.613  -5.460
ATOM    310  HN  PHE   20      -0.851  -1.370  -5.651
ATOM    311  CA  PHE   20       1.114  -1.565  -6.550
ATOM    312  HA  PHE   20       1.514  -2.460  -6.746
ATOM    313  CB  PHE   20       0.381  -1.052  -7.831
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ATOM    314  HCB1PHE    20      -0.410  -0.530  -7.511
ATOM    315  HCB2PHE    20       0.240  -1.853  -8.413
ATOM    316  CG  PHE    20       1.237  -0.072  -8.645
ATOM    317  CD1 PHE    20       2.270  -0.536  -9.438
ATOM    318  HCD1PHE    20       2.459  -1.516  -9.484
ATOM    319  CE1 PHE    20       3.042   0.346 -10.165
ATOM    320  HCE1PHE    20       3.786   0.003 -10.736
ATOM    321  CZ  PHE    20       2.789   1.701 -10.105
ATOM    322  HCZ PHE    20       3.349   2.339 -10.630
ATOM    323  CE2 PHE    20       1.759   2.170  -9.315
ATOM    324  HCE2PHE    20       1.572   3.150  -9.269
ATOM    325  CD2 PHE    20       0.990   1.288  -8.591
ATOM    326  HCD2PHE    20       0.247   1.634  -8.019
ATOM    327  C   PHE    20       2.276  -0.649  -6.113
ATOM    328  O   PHE    20       3.421  -1.053  -6.100
ATOM    329  N   ALA    21       1.931   0.560  -5.752
ATOM    330  HN  ALA    21       0.967   0.811  -5.777
ATOM    331  CA  ALA    21       2.934   1.574  -5.305
ATOM    332  HA  ALA    21       3.527   1.820  -6.072
ATOM    333  CB  ALA    21       2.169   2.811  -4.803
ATOM    334  HB1 ALA    21       2.670   3.215  -4.037
ATOM    335  HB2 ALA    21       2.094   3.473  -5.549
ATOM    336  HB3 ALA    21       1.257   2.530  -4.503
ATOM    337  C   ALA    21       3.837   1.021  -4.208
ATOM    338  O   ALA    21       5.033   1.193  -4.263
ATOM    339  N   GLU    22       3.259   0.369  -3.237
ATOM    340  HN  GLU    22       2.266   0.257  -3.240
ATOM    341  CA  GLU    22       4.066  -0.214  -2.121
ATOM    342  HA  GLU    22       4.529   0.518  -1.621
ATOM    343  CB  GLU    22       3.131  -0.970  -1.166
ATOM    344  HB1 GLU    22       3.712  -1.507  -0.553
ATOM    345  HB2 GLU    22       2.453  -1.437  -1.734
ATOM    346  CG  GLU    22       2.365   0.034  -0.288
ATOM    347  HG1 GLU    22       1.953   0.707  -0.903
ATOM    348  HG2 GLU    22       2.996   0.341   0.426
ATOM    349  CD  GLU    22       1.215  -0.704   0.410
ATOM    350  OE1 GLU    22       0.168  -0.784  -0.211
ATOM    351  OE2 GLU    22       1.443  -1.150   1.524
ATOM    352  C   GLU    22       5.121  -1.170  -2.686
ATOM    353  O   GLU    22       6.289  -1.042  -2.379
ATOM    354  N   ASP    23       4.672  -2.097  -3.501
ATOM    355  HN  ASP    23       3.694  -2.136  -3.704
ATOM    356  CA  ASP    23       5.594  -3.096  -4.130
ATOM    357  HA  ASP    23       5.938  -3.725  -3.433
ATOM    358  CB  ASP    23       4.826  -3.884  -5.202
ATOM    359  HB1 ASP    23       4.807  -3.314  -6.024
ATOM    360  HB2 ASP    23       3.964  -4.177  -4.786
ATOM    361  CG  ASP    23       5.607  -5.157  -5.555
ATOM    362  OD1 ASP    23       6.513  -5.029  -6.366
ATOM    363  OD2 ASP    23       5.263  -6.185  -4.997
ATOM    364  C   ASP    23       6.769  -2.364  -4.785
ATOM    365  O   ASP    23       7.931  -2.637  -4.563
ATOM    366  N   VAL    24       6.379  -1.420  -5.592
ATOM    367  HN  VAL    24       5.398  -1.266  -5.707
ATOM    368  CA  VAL    24       7.331  -0.565  -6.347
ATOM    369  HA  VAL    24       7.878  -1.103  -6.989
ATOM    370  CB  VAL    24       6.473   0.458  -7.102
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ATOM    371  HB  VAL    24       5.996   1.028  -6.432
ATOM    372  CG1 VAL    24       7.343   1.340  -7.965
ATOM    373  HG11VAL    24       7.512   2.200  -7.484
ATOM    374  HG12VAL    24       8.209   0.872  -8.140
ATOM    375  HG13VAL    24       6.871   1.519  -8.828
ATOM    376  CG2 VAL    24       5.432  -0.267  -7.982
ATOM    377  HG21VAL    24       4.529   0.130  -7.812
ATOM    378  HG22VAL    24       5.679  -0.151  -8.943
ATOM    379  HG23VAL    24       5.426  -1.239  -7.747
ATOM    380  C   VAL    24       8.335   0.108  -5.404
ATOM    381  O   VAL    24       9.532   0.050  -5.605
ATOM    382  N   GLY    25       7.794   0.724  -4.389
ATOM    383  HN  GLY    25       6.803   0.717  -4.297
ATOM    384  CA  GLY    25       8.607   1.438  -3.365
ATOM    385  HA1 GLY    25       7.978   1.692  -2.629
ATOM    386  HA2 GLY    25       9.112   2.153  -3.849
ATOM    387  C   GLY    25       9.651   0.512  -2.743
ATOM    388  O   GLY    25      10.830   0.800  -2.783
ATOM    389  N   SER    26       9.193  -0.587  -2.193
ATOM    390  HN  SER    26       8.211  -0.773  -2.199
ATOM    391  CA  SER    26      10.138  -1.564  -1.556
ATOM    392  HA  SER    26      10.555  -1.136  -0.754
ATOM    393  CB  SER    26       9.366  -2.839  -1.106
ATOM    394  HB1 SER    26       8.962  -2.648  -0.211
ATOM    395  HB2 SER    26       9.984  -3.619  -1.211
ATOM    396  OG  SER    26       8.299  -3.011  -2.024
ATOM    397  HG  SER    26       8.470  -2.896  -2.979
ATOM    398  C   SER    26      11.239  -1.949  -2.549
ATOM    399  O   SER    26      12.410  -1.937  -2.220
ATOM    400  N   ASN    27      10.831  -2.275  -3.749
ATOM    401  HN  ASN    27       9.853  -2.263  -3.952
ATOM    402  CA  ASN    27      11.797  -2.665  -4.817
ATOM    403  HA  ASN    27      12.251  -3.519  -4.564
ATOM    404  CB  ASN    27      11.023  -2.848  -6.132
ATOM    405  HB1 ASN    27      11.658  -2.626  -6.872
ATOM    406  HB2 ASN    27      10.174  -2.327  -6.039
ATOM    407  CG  ASN    27      10.625  -4.314  -6.321
ATOM    408  OD1 ASN    27      11.457  -5.176  -6.528
ATOM    409  ND2 ASN    27       9.364  -4.643  -6.258
ATOM    410  HD21ASN    27       9.102  -5.598  -6.381
ATOM    411  HD22ASN    27       8.677  -3.937  -6.087
ATOM    412  C   ASN    27      12.869  -1.593  -4.991
ATOM    413  O   ASN    27      14.043  -1.854  -4.828
ATOM    414  N   LYS    28      12.428  -0.407  -5.316
ATOM    415  HN  LYS    28      11.445  -0.273  -5.431
ATOM    416  CA  LYS    28      13.349   0.752  -5.520
ATOM    417  HA1 LYS    28      13.925   0.639  -6.329
ATOM    418  CB  LYS    28      12.472   2.000  -5.693
ATOM    419  HB1 LYS    28      13.087   2.789  -5.697
ATOM    420  HB2 LYS    28      11.751   1.942  -5.001
ATOM    421  CG  LYS    28      11.772   1.970  -7.077
ATOM    422  HG1 LYS    28      10.962   2.553  -7.005
ATOM    423  HG2 LYS    28      11.664   1.007  -7.324
ATOM    424  CD  LYS    28      12.688   2.610  -8.149
ATOM    425  HD1 LYS    28      13.607   2.243  -8.000
ATOM    426  HD2 LYS    28      12.542   3.599  -8.101
ATOM    427  CE  LYS    28      12.255   2.164  -9.559
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ATOM    428  HE1 LYS    28      12.291   1.164  -9.566
ATOM    429  HE2 LYS    28      12.814   2.680 -10.209
ATOM    430  NZ  LYS    28      10.838   2.542  -9.820
ATOM    431  HZ1 LYS    28      10.814   3.250 -10.527
ATOM    432  HZ2 LYS    28      10.337   1.737 -10.132
ATOM    433  HZ3 LYS    28      10.435   2.890  -8.978
ATOM    434  C   LYS    28      14.283   0.873  -4.304
ATOM    435  O   LYS    28      15.471   1.066  -4.457
ATOM    436  N   GLY    29      13.731   0.752  -3.121
ATOM    437  HN  GLY    29      12.747   0.596  -3.051
ATOM    438  CA  GLY    29      14.555   0.843  -1.879
ATOM    439  HA1 GLY    29      13.964   0.575  -1.118
ATOM    440  HA2 GLY    29      14.979   1.750  -1.877
ATOM    441  C   GLY    29      15.694  -0.182  -1.943
ATOM    442  O   GLY    29      16.853   0.164  -1.820
ATOM    443  N   ALA    30      15.332  -1.427  -2.150
ATOM    444  HN  ALA    30      14.363  -1.651  -2.253
ATOM    445  CA  ALA    30      16.365  -2.510  -2.232
ATOM    446  HA  ALA    30      16.849  -2.578  -1.359
ATOM    447  CB  ALA    30      15.662  -3.842  -2.541
ATOM    448  HB1 ALA    30      14.988  -4.028  -1.826
ATOM    449  HB2 ALA    30      15.207  -3.772  -3.429
ATOM    450  HB3 ALA    30      16.344  -4.573  -2.565
ATOM    451  C   ALA    30      17.391  -2.191  -3.325
ATOM    452  O   ALA    30      18.580  -2.293  -3.119
ATOM    453  N   ILE    31      16.888  -1.804  -4.465
ATOM    454  HN  ILE    31      15.896  -1.748  -4.547
ATOM    455  CA  ILE    31      17.718  -1.442  -5.645
ATOM    456  HA  ILE    31      18.241  -2.198  -6.040
ATOM    457  CB  ILE    31      16.689  -0.924  -6.698
ATOM    458  HB  ILE    31      16.002  -0.367  -6.232
ATOM    459  CG2 ILE    31      17.309   0.021  -7.742
ATOM    460  HG21ILE    31      17.450   0.919  -7.326
ATOM    461  HG22ILE    31      18.185  -0.356  -8.043
ATOM    462  HG23ILE    31      16.687   0.100  -8.521
ATOM    463  CG1 ILE    31      16.023  -2.159  -7.359
ATOM    464  HG11ILE    31      15.569  -2.663  -6.623
ATOM    465  HG12ILE    31      16.734  -2.612  -7.899
ATOM    466  CD1 ILE    31      14.920  -1.744  -8.349
ATOM    467  HD11ILE    31      14.526  -0.875  -8.051
ATOM    468  HD12ILE    31      15.321  -1.642  -9.259
ATOM    469  HD13ILE    31      14.213  -2.451  -8.365
ATOM    470  C   ILE    31      18.784  -0.419  -5.226
ATOM    471  O   ILE    31      19.963  -0.625  -5.443
ATOM    472  N   ILE    32      18.345   0.658  -4.629
ATOM    473  HN  ILE    32      17.365   0.773  -4.479
ATOM    474  CA  ILE    32      19.297   1.717  -4.172
ATOM    475  HA  ILE    32      19.777   2.126  -4.948
ATOM    476  CB  ILE    32      18.487   2.821  -3.440
ATOM    477  HB  ILE    32      17.994   2.417  -2.669
ATOM    478  CG2 ILE    32      19.447   3.915  -2.910
ATOM    479  HG21ILE    32      18.981   4.441  -2.198
ATOM    480  HG22ILE    32      20.262   3.477  -2.531
ATOM    481  HG23ILE    32      19.704   4.517  -3.666
ATOM    482  CG1 ILE    32      17.486   3.455  -4.444
ATOM    483  HG11ILE    32      17.077   2.701  -4.959
ATOM    484  HG12ILE    32      17.984   4.171  -4.934
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ATOM 485 CD1 ILE 32 16.336 4.149 -3.690
ATOM 486 HD11ILE 32 16.718 4.851 -3.088
ATOM 487 HD12ILE 32 15.717 4.569 -4.354
ATOM 488 HD13ILE 32 15.844 3.467 -3.149
ATOM 489 C ILE 32 20.336 1.086 -3.238
ATOM 490 O ILE 32 21.523 1.292 -3.401
ATOM 491 N GLY 33 19.855 0.321 -2.288
ATOM 492 HN GLY 33 18.868 0.189 -2.211
ATOM 493 CA GLY 33 20.774 -0.352 -1.322
ATOM 494 HA1 GLY 33 20.223 -1.016 -0.814
ATOM 495 HA2 GLY 33 21.252 0.373 -0.824
ATOM 496 C GLY 33 21.841 -1.149 -2.079
ATOM 497 O GLY 33 23.017 -1.031 -1.801
ATOM 498 N LEU 34 21.402 -1.936 -3.031
ATOM 499 HN LEU 34 20.423 -1.985 -3.215
ATOM 500 CA LEU 34 22.349 -2.758 -3.841
ATOM 501 HA LEU 34 22.835 -3.390 -3.237
ATOM 502 CB LEU 34 21.551 -3.554 -4.897
ATOM 503 HB1 LEU 34 22.221 -3.997 -5.494
ATOM 504 HB2 LEU 34 20.884 -2.921 -5.292
ATOM 505 CG LEU 34 20.744 -4.689 -4.208
ATOM 506 HG LEU 34 20.409 -4.373 -3.320
ATOM 507 CD1 LEU 34 19.549 -5.079 -5.103
ATOM 508 HD11LEU 34 18.780 -4.472 -4.902
ATOM 509 HD12LEU 34 19.816 -4.985 -6.062
ATOM 510 HD13LEU 34 19.294 -6.027 -4.911
ATOM 511 CD2 LEU 34 21.654 -5.922 -4.005
ATOM 512 HD21LEU 34 22.174 -5.808 -3.158
ATOM 513 HD22LEU 34 21.084 -6.742 -3.947
ATOM 514 HD23LEU 34 22.280 -5.997 -4.781
ATOM 515 C LEU 34 23.379 -1.865 -4.532
ATOM 516 O LEU 34 24.557 -2.153 -4.474
ATOM 517 N MET 35 22.918 -0.811 -5.165
ATOM 518 HN MET 35 21.935 -0.633 -5.178
ATOM 519 CA MET 35 23.856 0.121 -5.865
ATOM 520 HA MET 35 24.275 -0.337 -6.648
ATOM 521 CB MET 35 23.069 1.354 -6.362
ATOM 522 HB1 MET 35 23.744 2.023 -6.675
ATOM 523 HB2 MET 35 22.433 1.605 -5.631
ATOM 524 CG MET 35 22.220 0.974 -7.584
ATOM 525 HG1 MET 35 21.676 1.788 -7.790
ATOM 526 HG2 MET 35 21.756 0.125 -7.327
ATOM 527 SD MET 35 23.094 0.589 -9.123
ATOM 528 CE MET 35 23.653 2.262 -9.535
ATOM 529 HE1 MET 35 23.580 2.839 -8.722
ATOM 530 HE2 MET 35 24.604 2.222 -9.840
ATOM 531 HE3 MET 35 23.076 2.627 -10.266
ATOM 532 C MET 35 24.958 0.558 -4.890
ATOM 533 O MET 35 26.134 0.402 -5.163
ATOM 534 N VAL 36 24.507 1.076 -3.775
ATOM 535 HN VAL 36 23.519 1.146 -3.645
ATOM 536 CA VAL 36 25.413 1.563 -2.692
ATOM 537 HA VAL 36 25.947 2.351 -3.001
ATOM 538 CB VAL 36 24.518 1.981 -1.481
ATOM 539 HB VAL 36 23.911 1.219 -1.255
ATOM 540 CG1 VAL 36 25.389 2.315 -0.246
ATOM 541 HG11VAL 36 25.058 3.164 0.166

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ATOM    542 HG12VAL   36      25.320   1.566   0.413
ATOM    543 HG13VAL   36      26.339   2.426  -0.538
ATOM    544 CG2 VAL   36      23.695   3.234  -1.860
ATOM    545 HG21VAL   36      23.768   3.907  -1.124
ATOM    546 HG22VAL   36      24.058   3.618  -2.709
ATOM    547 HG23VAL   36      22.739   2.970  -1.987
ATOM    548 C   VAL   36      26.418   0.467  -2.301
ATOM    549 O   VAL   36      27.614   0.696  -2.307
ATOM    550 N   GLY   37      25.895  -0.691  -1.978
ATOM    551 HN  GLY   37      24.903  -0.800  -2.001
ATOM    552 CA  GLY   37      26.746  -1.851  -1.577
ATOM    553 HA1 GLY   37      26.320  -2.256  -0.768
ATOM    554 HA2 GLY   37      27.687  -1.514  -1.522
ATOM    555 C   GLY   37      26.722  -2.918  -2.671
ATOM    556 O   GLY   37      26.278  -4.028  -2.444
ATOM    557 N   GLY   38      27.200  -2.544  -3.834
ATOM    558 HN  GLY   38      27.544  -1.614  -3.946
ATOM    559 CA  GLY   38      27.234  -3.490  -4.992
ATOM    560 HA1 GLY   38      26.336  -3.437  -5.432
ATOM    561 HA2 GLY   38      27.556  -4.368  -4.636
ATOM    562 C   GLY   38      28.257  -3.034  -6.028
ATOM    563 O   GLY   38      28.973  -3.847  -6.584
ATOM    564 N   VAL   39      28.303  -1.743  -6.259
ATOM    565 HN  VAL   39      27.682  -1.135  -5.765
ATOM    566 CA  VAL   39      29.263  -1.166  -7.249
ATOM    567 HA  VAL   39      29.411  -1.789  -8.017
ATOM    568 CB  VAL   39      28.653   0.172  -7.790
ATOM    569 HB  VAL   39      28.666   0.843  -7.048
ATOM    570 CG1 VAL   39      29.480   0.695  -8.993
ATOM    571 HG11VAL   39      29.803   1.620  -8.789
ATOM    572 HG12VAL   39      30.260   0.087  -9.141
ATOM    573 HG13VAL   39      28.899   0.709  -9.807
ATOM    574 CG2 VAL   39      27.200  -0.071  -8.276
ATOM    575 HG21VAL   39      26.589   0.567  -7.807
ATOM    576 HG22VAL   39      27.157   0.080  -9.264
ATOM    577 HG23VAL   39      26.938  -1.012  -8.064
ATOM    578 C   VAL   39      30.627  -0.939  -6.564
ATOM    579 O   VAL   39      31.386  -0.053  -6.911
ATOM    580 N   VAL   40      30.891  -1.776  -5.593
ATOM    581 HN  VAL   40      30.219  -2.479  -5.368
ATOM    582 CA  VAL   40      32.164  -1.714  -4.814
ATOM    583 HA  VAL   40      32.304  -0.794  -4.449
ATOM    584 CB  VAL   40      32.070  -2.730  -3.641
ATOM    585 HB  VAL   40      31.974  -3.650  -4.021
ATOM    586 CG1 VAL   40      33.350  -2.663  -2.775
ATOM    587 HG11VAL   40      33.271  -1.899  -2.135
ATOM    588 HG12VAL   40      33.448  -3.521  -2.271
ATOM    589 HG13VAL   40      34.141  -2.527  -3.372
ATOM    590 CG2 VAL   40      30.844  -2.395  -2.760
ATOM    591 HG21VAL   40      31.072  -1.626  -2.163
ATOM    592 HG22VAL   40      30.075  -2.151  -3.351
ATOM    593 HG23VAL   40      30.610  -3.196  -2.209
ATOM    594 C   VAL   40      33.355  -2.051  -5.733
ATOM    595 O   VAL   40      34.308  -1.291  -5.691
ATOM    596 NA  NA    41       6.208   8.402 -13.354
ATOM    597 NA  NA    42      -3.792  12.402  -0.354
ATOM    598 NA  NA    43      34.208  -0.598  -9.354
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Final MD structure (after 10 ns relaxation) of the second NMR isoform with 3 Na^+ counterions

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ATOM      1  N   ASP     1      17.508   5.154 -12.330
ATOM      2  HN  ASP     1      17.824   6.036 -11.955
ATOM      3  CA  ASP     1      16.309   5.118 -13.135
ATOM      4  HA  ASP     1      16.507   4.934 -14.103
ATOM      5  CB  ASP     1      15.396   4.110 -12.506
ATOM      6  HB1 ASP     1      15.203   4.468 -11.566
ATOM      7  HB2 ASP     1      15.829   3.210 -12.438
ATOM      8  CG  ASP     1      13.970   4.025 -13.084
ATOM      9  OD1 ASP     1      13.611   4.708 -14.034
ATOM     10  OD2 ASP     1      13.347   3.033 -12.869
ATOM     11  C   ASP     1      15.867   6.530 -12.943
ATOM     12  O   ASP     1      16.240   7.167 -11.969
ATOM     13  N   ALA     2      15.115   7.139 -13.823
ATOM     14  HN  ALA     2      14.818   6.611 -14.652
ATOM     15  CA  ALA     2      14.759   8.506 -13.689
ATOM     16  HA  ALA     2      15.319   8.964 -12.959
ATOM     17  CB  ALA     2      14.831   9.274 -14.993
ATOM     18  HB1 ALA     2      14.525  10.186 -14.753
ATOM     19  HB2 ALA     2      15.735   9.336 -15.457
ATOM     20  HB3 ALA     2      14.213   8.885 -15.662
ATOM     21  C   ALA     2      13.307   8.604 -13.335
ATOM     22  O   ALA     2      12.716   9.602 -13.697
ATOM     23  N   GLU     3      12.867   7.601 -12.622
ATOM     24  HN  GLU     3      13.462   6.813 -12.404
ATOM     25  CA  GLU     3      11.508   7.459 -12.146
ATOM     26  HA  GLU     3      11.545   6.740 -11.529
ATOM     27  CB  GLU     3      10.928   8.741 -11.549
ATOM     28  HB1 GLU     3       9.964   8.557 -11.317
ATOM     29  HB2 GLU     3      10.943   9.417 -12.255
ATOM     30  CG  GLU     3      11.720   9.405 -10.354
ATOM     31  HG1 GLU     3      11.341  10.256 -10.011
ATOM     32  HG2 GLU     3      12.675   9.449 -10.599
ATOM     33  CD  GLU     3      11.679   8.424  -9.146
ATOM     34  OE1 GLU     3      10.704   8.410  -8.381
ATOM     35  OE2 GLU     3      12.676   7.822  -8.740
ATOM     36  C   GLU     3      10.747   7.194 -13.395
ATOM     37  O   GLU     3       9.685   7.791 -13.679
ATOM     38  N   PHE     4      11.249   6.304 -14.228
ATOM     39  HN  PHE     4      12.067   5.819 -14.046
ATOM     40  CA  PHE     4      10.501   6.067 -15.445
ATOM     41  HA  PHE     4       9.713   6.561 -15.561
ATOM     42  CB  PHE     4      11.366   6.106 -16.718
ATOM     43  HCB1PHE     4      10.756   5.748 -17.408
ATOM     44  HCB2PHE     4      12.205   5.543 -16.717
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ATOM     45  CG  PHE     4      11.781   7.475 -17.129
ATOM     46  CD1 PHE     4      10.851   8.564 -16.885
ATOM     47  HCD1PHE     4       9.963   8.362 -16.419
ATOM     48  CE1 PHE     4      11.160   9.890 -17.340
ATOM     49  HCE1PHE     4      10.476  10.603 -17.176
ATOM     50  CZ  PHE     4      12.387  10.242 -18.013
ATOM     51  HCZ PHE     4      12.535  11.132 -18.309
ATOM     52  CE2 PHE     4      13.319   9.174 -18.214
ATOM     53  HCE2PHE     4      14.215   9.304 -18.662
ATOM     54  CD2 PHE     4      13.048   7.795 -17.824
ATOM     55  HCD2PHE     4      13.727   7.126 -18.085
ATOM     56  C   PHE     4      10.108   4.628 -15.476
ATOM     57  O   PHE     4       9.276   4.304 -16.316
ATOM     58  N   ARG     5      10.685   3.693 -14.659
ATOM     59  HN  ARG     5      11.302   3.860 -13.932
ATOM     60  CA  ARG     5      10.307   2.374 -15.018
ATOM     61  HA  ARG     5       9.884   2.516 -15.968
ATOM     62  CB  ARG     5      11.455   1.358 -15.112
ATOM     63  HB1 ARG     5      11.810   1.116 -14.215
ATOM     64  HB2 ARG     5      12.136   1.831 -15.666
ATOM     65  CG  ARG     5      11.158   0.043 -15.927
ATOM     66  HG1 ARG     5      12.011  -0.468 -15.999
ATOM     67  HG2 ARG     5      10.801   0.355 -16.839
ATOM     68  CD  ARG     5      10.112  -0.892 -15.167
ATOM     69  HD1 ARG     5       9.243  -0.319 -15.099
ATOM     70  HD2 ARG     5      10.465  -1.160 -14.254
ATOM     71  NE  ARG     5       9.717  -2.048 -15.984
ATOM     72  HE  ARG     5       8.827  -2.029 -16.387
ATOM     73  CZ  ARG     5      10.596  -3.078 -16.203
ATOM     74  NH1 ARG     5      11.840  -2.979 -15.659
ATOM     75  HH11ARG     5      12.625  -3.579 -15.682
ATOM     76  HH12ARG     5      12.052  -2.204 -15.121
ATOM     77  NH2 ARG     5      10.217  -4.119 -16.949
ATOM     78  HH21ARG     5      10.804  -4.933 -17.152
ATOM     79  HH22ARG     5       9.366  -4.232 -17.313
ATOM     80  C   ARG     5       9.227   2.109 -13.956
ATOM     81  O   ARG     5       9.573   1.475 -12.948
ATOM     82  N   HIS     6       8.003   2.606 -14.169
ATOM     83  HN  HIS     6       7.976   3.035 -15.038
ATOM     84  CA  HIS     6       6.802   2.561 -13.354
ATOM     85  HA  HIS     6       6.245   3.232 -13.758
ATOM     86  CB  HIS     6       5.987   1.238 -13.349
ATOM     87  HB1 HIS     6       5.725   1.103 -14.272
ATOM     88  HB2 HIS     6       5.140   1.394 -12.803
ATOM     89  CG  HIS     6       6.567  -0.024 -12.747
ATOM     90  ND1 HIS     6       7.369  -0.195 -11.704
ATOM     91  HD1 HIS     6       7.726   0.537 -11.149
ATOM     92  CE1 HIS     6       7.631  -1.488 -11.593
ATOM     93  HE1 HIS     6       8.207  -1.844 -10.906
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ATOM 94 NE2 HIS 6 7.038 -2.203 -12.544
ATOM 95 CD2 HIS 6 6.320 -1.292 -13.287
ATOM 96 HD2 HIS 6 5.721 -1.513 -14.035
ATOM 97 C HIS 6 6.931 3.027 -11.949
ATOM 98 O HIS 6 6.020 2.726 -11.148
ATOM 99 N ASP 7 7.950 3.803 -11.572
ATOM 100 HN ASP 7 8.735 4.126 -12.138
ATOM 101 CA ASP 7 8.117 4.358 -10.209
ATOM 102 HA ASP 7 8.418 3.590 -9.547
ATOM 103 CB ASP 7 9.275 5.349 -10.211
ATOM 104 HB1 ASP 7 9.462 5.787 -9.343
ATOM 105 HB2 ASP 7 9.106 6.061 -10.908
ATOM 106 CG ASP 7 10.466 4.529 -10.506
ATOM 107 OD1 ASP 7 11.161 4.145 -9.668
ATOM 108 OD2 ASP 7 10.693 4.062 -11.636
ATOM 109 C ASP 7 6.957 5.139 -9.797
ATOM 110 O ASP 7 6.438 5.987 -10.528
ATOM 111 N SER 8 6.392 4.840 -8.593
ATOM 112 HN SER 8 6.689 4.216 -7.891
ATOM 113 CA SER 8 5.282 5.465 -8.081
ATOM 114 HA SER 8 5.116 6.350 -8.558
ATOM 115 CB SER 8 4.137 4.504 -8.290
ATOM 116 HB1 SER 8 3.306 4.868 -7.988
ATOM 117 HB2 SER 8 4.233 3.588 -7.896
ATOM 118 OG SER 8 3.972 4.316 -9.689
ATOM 119 HG SER 8 4.849 3.968 -10.123
ATOM 120 C SER 8 5.569 5.825 -6.744
ATOM 121 O SER 8 6.317 5.023 -6.116
ATOM 122 N GLY 9 5.116 6.875 -6.095
ATOM 123 HN GLY 9 4.572 7.612 -6.511
ATOM 124 CA GLY 9 5.392 7.057 -4.677
ATOM 125 HA1 GLY 9 6.292 7.449 -4.570
ATOM 126 HA2 GLY 9 5.211 6.138 -4.237
ATOM 127 C GLY 9 4.200 8.034 -4.452
ATOM 128 O GLY 9 4.116 8.989 -5.212
ATOM 129 N TYR 10 3.212 7.681 -3.591
ATOM 130 HN TYR 10 3.206 6.874 -3.047
ATOM 131 CA TYR 10 2.004 8.518 -3.451
ATOM 132 HA TYR 10 2.307 9.439 -3.100
ATOM 133 CB TYR 10 1.055 8.828 -4.652
ATOM 134 HCB1TYR 10 1.405 9.427 -5.349
ATOM 135 HCB2TYR 10 0.282 9.261 -4.209
ATOM 136 CG TYR 10 0.721 7.554 -5.358
ATOM 137 CD1 TYR 10 1.319 7.345 -6.636
ATOM 138 HCD1TYR 10 1.965 8.056 -6.993
ATOM 139 CE1 TYR 10 1.104 6.202 -7.437
ATOM 140 HCE1TYR 10 1.617 6.160 -8.378
ATOM 141 CZ TYR 10 0.246 5.120 -6.902
ATOM 142 OH TYR 10 0.087 4.057 -7.600

ATOM 143 HOH TYR 10 -0.111 3.259 -6.964
ATOM 144 CE2 TYR 10 -0.413 5.328 -5.613
ATOM 145 HCE2TYR 10 -1.027 4.613 -5.306
ATOM 146 CD2 TYR 10 -0.204 6.586 -4.839
ATOM 147 HCD2TYR 10 -0.629 6.839 -3.999
ATOM 148 C TYR 10 1.316 7.795 -2.376
ATOM 149 O TYR 10 1.636 6.644 -2.098
ATOM 150 N GLU 11 0.288 8.339 -1.819
ATOM 151 HN GLU 11 -0.041 9.229 -2.007
ATOM 152 CA GLU 11 -0.479 7.704 -0.809
ATOM 153 HA GLU 11 -0.252 6.741 -0.769
ATOM 154 CB GLU 11 -0.264 8.365 0.560
ATOM 155 HB1 GLU 11 -0.401 9.358 0.432
ATOM 156 HB2 GLU 11 0.696 8.169 0.771
ATOM 157 CG GLU 11 -0.990 7.776 1.736
ATOM 158 HG1 GLU 11 -0.609 8.140 2.563
ATOM 159 HG2 GLU 11 -0.904 6.797 1.696
ATOM 160 CD GLU 11 -2.544 8.052 1.721
ATOM 161 OE1 GLU 11 -3.051 8.994 2.222
ATOM 162 OE2 GLU 11 -3.341 7.214 1.414
ATOM 163 C GLU 11 -1.823 8.095 -1.422
ATOM 164 O GLU 11 -1.916 9.207 -1.881
ATOM 165 N VAL 12 -2.929 7.271 -1.582
ATOM 166 HN VAL 12 -2.973 6.326 -1.179
ATOM 167 CA VAL 12 -4.054 7.728 -2.284
ATOM 168 HA VAL 12 -4.227 8.717 -1.966
ATOM 169 CB VAL 12 -3.947 7.664 -3.832
ATOM 170 HB VAL 12 -3.094 8.210 -4.127
ATOM 171 CG1 VAL 12 -3.679 6.298 -4.354
ATOM 172 HG11VAL 12 -2.883 5.833 -3.880
ATOM 173 HG12VAL 12 -4.417 5.734 -4.188
ATOM 174 HG13VAL 12 -3.527 6.275 -5.335
ATOM 175 CG2 VAL 12 -5.257 8.210 -4.571
ATOM 176 HG21VAL 12 -5.405 9.184 -4.283
ATOM 177 HG22VAL 12 -5.151 8.156 -5.545
ATOM 178 HG23VAL 12 -5.995 7.706 -4.319
ATOM 179 C VAL 12 -5.141 6.947 -1.748
ATOM 180 O VAL 12 -4.853 5.818 -1.261
ATOM 181 N HIS 13 -6.393 7.365 -1.776
ATOM 182 HN HIS 13 -6.560 8.220 -2.212
ATOM 183 CA HIS 13 -7.392 6.522 -1.207
ATOM 184 HA HIS 13 -6.974 6.196 -0.346
ATOM 185 CB HIS 13 -8.647 7.268 -0.927
ATOM 186 HB1 HIS 13 -9.328 6.684 -0.481
ATOM 187 HB2 HIS 13 -9.087 7.488 -1.771
ATOM 188 CG HIS 13 -8.417 8.458 -0.003
ATOM 189 ND1 HIS 13 -7.908 8.406 1.203
ATOM 190 HD1 HIS 13 -7.675 7.493 1.572
ATOM 191 CE1 HIS 13 -7.816 9.635 1.776

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ATOM    192  HE1 HIS    13      -7.455   9.949   2.667
ATOM    193  NE2 HIS    13      -8.292  10.502   0.884
ATOM    194  CD2 HIS    13      -8.681   9.848  -0.223
ATOM    195  HD2 HIS    13      -9.107  10.177  -1.072
ATOM    196  C   HIS    13      -7.853   5.462  -2.063
ATOM    197  O   HIS    13      -9.049   5.346  -2.298
ATOM    198  N   HIS    14      -6.979   4.635  -2.723
ATOM    199  HN  HIS    14      -6.006   4.798  -2.551
ATOM    200  CA  HIS    14      -7.348   3.601  -3.615
ATOM    201  HA  HIS    14      -8.246   3.187  -3.505
ATOM    202  CB  HIS    14      -7.084   3.777  -5.117
ATOM    203  HB1 HIS    14      -7.305   2.894  -5.649
ATOM    204  HB2 HIS    14      -6.146   3.988  -5.197
ATOM    205  CG  HIS    14      -8.035   4.842  -5.577
ATOM    206  ND1 HIS    14      -9.354   4.921  -5.453
ATOM    207  HD1 HIS    14     -10.092   4.389  -5.055
ATOM    208  CE1 HIS    14      -9.698   6.075  -6.007
ATOM    209  HE1 HIS    14     -10.662   6.410  -6.031
ATOM    210  NE2 HIS    14      -8.680   6.751  -6.557
ATOM    211  CD2 HIS    14      -7.579   6.011  -6.243
ATOM    212  HD2 HIS    14      -6.675   6.292  -6.508
ATOM    213  C   HIS    14      -6.316   2.684  -3.087
ATOM    214  O   HIS    14      -5.157   3.075  -3.157
ATOM    215  N   GLN    15      -6.613   1.558  -2.492
ATOM    216  HN  GLN    15      -7.536   1.305  -2.474
ATOM    217  CA  GLN    15      -5.538   0.823  -1.908
ATOM    218  HA  GLN    15      -4.953   1.564  -1.603
ATOM    219  CB  GLN    15      -5.820  -0.014  -0.660
ATOM    220  HB1 GLN    15      -4.961  -0.357  -0.259
ATOM    221  HB2 GLN    15      -6.413  -0.755  -0.893
ATOM    222  CG  GLN    15      -6.570   0.863   0.366
ATOM    223  HG1 GLN    15      -6.812   0.284   1.193
ATOM    224  HG2 GLN    15      -7.472   1.306   0.053
ATOM    225  CD  GLN    15      -5.694   1.997   0.777
ATOM    226  OE1 GLN    15      -6.130   3.116   0.546
ATOM    227  NE2 GLN    15      -4.496   1.763   1.334
ATOM    228  HE21GLN    15      -3.913   2.498   1.571
ATOM    229  HE22GLN    15      -4.185   0.828   1.484
ATOM    230  C   GLN    15      -4.829  -0.074  -2.898
ATOM    231  O   GLN    15      -3.780  -0.476  -2.522
ATOM    232  N   LYS    16      -5.378  -0.470  -4.108
ATOM    233  HN  LYS    16      -6.297  -0.153  -4.371
ATOM    234  CA  LYS    16      -4.611  -1.320  -5.003
ATOM    235  HA1 LYS    16      -4.209  -2.099  -4.592
ATOM    236  CB  LYS    16      -5.590  -1.839  -6.111
ATOM    237  HB1 LYS    16      -5.942  -1.038  -6.626
ATOM    238  HB2 LYS    16      -6.298  -2.271  -5.636
ATOM    239  CG  LYS    16      -4.977  -2.740  -7.215
ATOM    240  HG1 LYS    16      -5.778  -3.058  -7.796
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ATOM 241 HG2 LYS 16 -4.600 -3.572 -6.750
ATOM 242 CD LYS 16 -3.980 -2.091 -8.187
ATOM 243 HD1 LYS 16 -3.205 -1.640 -7.621
ATOM 244 HD2 LYS 16 -4.490 -1.402 -8.743
ATOM 245 CE LYS 16 -3.461 -3.215 -9.129
ATOM 246 HE1 LYS 16 -2.979 -3.970 -8.648
ATOM 247 HE2 LYS 16 -2.795 -2.840 -9.740
ATOM 248 NZ LYS 16 -4.534 -3.744 -9.918
ATOM 249 HZ1 LYS 16 -5.149 -4.240 -9.384
ATOM 250 HZ2 LYS 16 -5.011 -3.058 -10.455
ATOM 251 HZ3 LYS 16 -4.205 -4.436 -10.571
ATOM 252 C LYS 16 -3.492 -0.414 -5.508
ATOM 253 O LYS 16 -2.319 -0.776 -5.699
ATOM 254 N LEU 17 -3.838 0.854 -5.733
ATOM 255 HN LEU 17 -4.736 1.191 -5.645
ATOM 256 CA LEU 17 -2.776 1.786 -6.164
ATOM 257 HA LEU 17 -2.336 1.407 -6.982
ATOM 258 CB LEU 17 -3.091 3.255 -6.437
ATOM 259 HB1 LEU 17 -2.215 3.720 -6.558
ATOM 260 HB2 LEU 17 -3.546 3.671 -5.635
ATOM 261 CG LEU 17 -4.037 3.465 -7.647
ATOM 262 HG LEU 17 -4.875 3.061 -7.443
ATOM 263 CD1 LEU 17 -4.170 5.015 -7.788
ATOM 264 HD11LEU 17 -4.547 5.368 -6.882
ATOM 265 HD12LEU 17 -3.347 5.455 -8.054
ATOM 266 HD13LEU 17 -4.838 5.286 -8.473
ATOM 267 CD2 LEU 17 -3.436 2.904 -8.952
ATOM 268 HD21LEU 17 -3.269 1.936 -8.803
ATOM 269 HD22LEU 17 -4.023 2.971 -9.731
ATOM 270 HD23LEU 17 -2.591 3.394 -9.168
ATOM 271 C LEU 17 -1.796 1.922 -5.064
ATOM 272 O LEU 17 -0.646 2.128 -5.416
ATOM 273 N VAL 18 -2.140 1.912 -3.769
ATOM 274 HN VAL 18 -3.049 1.755 -3.493
ATOM 275 CA VAL 18 -1.156 2.062 -2.732
ATOM 276 HA VAL 18 -0.612 2.874 -2.984
ATOM 277 CB VAL 18 -1.781 2.390 -1.399
ATOM 278 HB VAL 18 -2.318 1.594 -1.150
ATOM 279 CG1 VAL 18 -0.871 2.710 -0.189
ATOM 280 HG11VAL 18 -0.400 3.594 -0.360
ATOM 281 HG12VAL 18 -1.339 2.802 0.658
ATOM 282 HG13VAL 18 -0.150 2.046 -0.099
ATOM 283 CG2 VAL 18 -2.550 3.765 -1.527
ATOM 284 HG21VAL 18 -1.983 4.536 -1.772
ATOM 285 HG22VAL 18 -3.311 3.683 -2.186
ATOM 286 HG23VAL 18 -2.970 3.960 -0.597
ATOM 287 C VAL 18 -0.303 0.810 -2.656
ATOM 288 O VAL 18 0.875 0.965 -2.341
ATOM 289 N PHE 19 -0.788 -0.385 -2.949

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ATOM    290  HN  PHE    19      -1.760  -0.605  -3.178
ATOM    291  CA  PHE    19       0.094  -1.533  -2.911
ATOM    292  HA  PHE    19       0.548  -1.444  -2.003
ATOM    293  CB  PHE    19      -0.537  -2.923  -2.947
ATOM    294 HCB1PHE    19       0.199  -3.647  -2.881
ATOM    295 HCB2PHE    19      -1.074  -3.046  -3.763
ATOM    296  CG  PHE    19      -1.555  -2.909  -1.794
ATOM    297  CD1 PHE    19      -1.249  -2.319  -0.533
ATOM    298 HCD1PHE    19      -0.355  -1.860  -0.376
ATOM    299  CE1 PHE    19      -2.257  -2.444   0.540
ATOM    300 HCE1PHE    19      -2.114  -2.094   1.444
ATOM    301  CZ  PHE    19      -3.563  -3.091   0.332
ATOM    302  HCZ PHE    19      -4.275  -3.183   1.046
ATOM    303  CE2 PHE    19      -3.905  -3.659  -0.979
ATOM    304 HCE2PHE    19      -4.801  -4.082  -1.116
ATOM    305  CD2 PHE    19      -2.881  -3.548  -1.996
ATOM    306 HCD2PHE    19      -3.096  -3.986  -2.916
ATOM    307  C   PHE    19       1.048  -1.496  -4.030
ATOM    308  O   PHE    19       2.159  -1.922  -3.907
ATOM    309  N   PHE    20       0.623  -0.980  -5.207
ATOM    310  HN  PHE    20      -0.312  -0.675  -5.345
ATOM    311  CA  PHE    20       1.603  -0.944  -6.246
ATOM    312  HA  PHE    20       2.204  -1.716  -6.433
ATOM    313  CB  PHE    20       0.680  -0.699  -7.507
ATOM    314 HCB1PHE    20       0.108   0.124  -7.347
ATOM    315 HCB2PHE    20       0.120  -1.464  -7.672
ATOM    316  CG  PHE    20       1.573  -0.527  -8.677
ATOM    317  CD1 PHE    20       2.101  -1.656  -9.279
ATOM    318 HCD1PHE    20       1.900  -2.567  -8.972
ATOM    319  CE1 PHE    20       2.939  -1.553 -10.465
ATOM    320 HCE1PHE    20       3.321  -2.383 -10.897
ATOM    321  CZ  PHE    20       3.282  -0.256 -11.055
ATOM    322  HCZ PHE    20       3.893  -0.176 -11.812
ATOM    323  CE2 PHE    20       2.708   0.952 -10.371
ATOM    324 HCE2PHE    20       2.881   1.900 -10.634
ATOM    325  CD2 PHE    20       1.899   0.811  -9.223
ATOM    326 HCD2PHE    20       1.511   1.591  -8.725
ATOM    327  C   PHE    20       2.544   0.227  -5.942
ATOM    328  O   PHE    20       3.735   0.051  -6.152
ATOM    329  N   ALA    21       2.113   1.400  -5.367
ATOM    330  HN  ALA    21       1.196   1.685  -5.120
ATOM    331  CA  ALA    21       3.131   2.362  -5.136
ATOM    332  HA  ALA    21       3.714   2.314  -5.963
ATOM    333  CB  ALA    21       2.738   3.864  -4.843
ATOM    334  HB1 ALA    21       3.575   4.418  -4.843
ATOM    335  HB2 ALA    21       2.226   4.248  -5.589
ATOM    336  HB3 ALA    21       2.203   4.004  -4.052
ATOM    337  C   ALA    21       3.995   1.886  -3.961
ATOM    338  O   ALA    21       5.165   2.320  -4.024
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ATOM 339 N GLU 22 3.560 1.199 -2.937
ATOM 340 HN GLU 22 2.668 0.834 -2.808
ATOM 341 CA GLU 22 4.617 0.934 -2.004
ATOM 342 HA GLU 22 5.254 1.711 -2.045
ATOM 343 CB GLU 22 4.141 0.806 -0.543
ATOM 344 HB1 GLU 22 4.909 0.689 -0.017
ATOM 345 HB2 GLU 22 3.517 0.030 -0.468
ATOM 346 CG GLU 22 3.457 2.093 -0.276
ATOM 347 HG1 GLU 22 2.702 2.165 -0.939
ATOM 348 HG2 GLU 22 4.114 2.799 -0.431
ATOM 349 CD GLU 22 2.917 2.194 1.115
ATOM 350 OE1 GLU 22 2.447 3.257 1.500
ATOM 351 OE2 GLU 22 3.025 1.293 1.939
ATOM 352 C GLU 22 5.348 -0.329 -2.486
ATOM 353 O GLU 22 6.455 -0.597 -2.006
ATOM 354 N ASP 23 4.907 -1.200 -3.461
ATOM 355 HN ASP 23 3.967 -1.034 -3.957
ATOM 356 CA ASP 23 5.749 -2.281 -3.896
ATOM 357 HA ASP 23 6.118 -2.756 -3.129
ATOM 358 CB ASP 23 4.885 -3.353 -4.633
ATOM 359 HB1 ASP 23 4.450 -2.948 -5.407
ATOM 360 HB2 ASP 23 4.195 -3.799 -4.072
ATOM 361 CG ASP 23 5.884 -4.376 -5.030
ATOM 362 OD1 ASP 23 5.976 -4.749 -6.207
ATOM 363 OD2 ASP 23 6.609 -4.904 -4.231
ATOM 364 C ASP 23 6.790 -1.726 -4.846
ATOM 365 O ASP 23 7.993 -2.083 -4.649
ATOM 366 N VAL 24 6.531 -0.805 -5.780
ATOM 367 HN VAL 24 5.600 -0.403 -5.861
ATOM 368 CA VAL 24 7.651 -0.308 -6.546
ATOM 369 HA VAL 24 8.216 -1.051 -6.921
ATOM 370 CB VAL 24 7.047 0.453 -7.709
ATOM 371 HB VAL 24 6.659 1.303 -7.331
ATOM 372 CG1 VAL 24 8.021 0.831 -8.819
ATOM 373 HG11VAL 24 8.752 1.430 -8.400
ATOM 374 HG12VAL 24 8.308 -0.034 -9.172
ATOM 375 HG13VAL 24 7.599 1.392 -9.537
ATOM 376 CG2 VAL 24 6.002 -0.549 -8.340
ATOM 377 HG21VAL 24 5.447 -0.066 -9.041
ATOM 378 HG22VAL 24 6.410 -1.329 -8.852
ATOM 379 HG23VAL 24 5.386 -0.843 -7.543
ATOM 380 C VAL 24 8.469 0.571 -5.659
ATOM 381 O VAL 24 9.663 0.464 -5.841
ATOM 382 N GLY 25 8.024 1.347 -4.698
ATOM 383 HN GLY 25 7.041 1.419 -4.464
ATOM 384 CA GLY 25 8.908 2.128 -3.907
ATOM 385 HA1 GLY 25 8.348 2.736 -3.340
ATOM 386 HA2 GLY 25 9.465 2.600 -4.469
ATOM 387 C GLY 25 9.720 1.186 -3.063

ATOM 388 O GLY 25 10.888 1.463 -2.958
ATOM 389 N SER 26 9.250 0.065 -2.505
ATOM 390 HN SER 26 8.326 -0.360 -2.526
ATOM 391 CA SER 26 10.156 -0.758 -1.799
ATOM 392 HA SER 26 10.682 -0.200 -1.199
ATOM 393 CB SER 26 9.414 -1.754 -0.946
ATOM 394 HB1 SER 26 8.948 -1.320 -0.193
ATOM 395 HB2 SER 26 10.081 -2.433 -0.626
ATOM 396 OG SER 26 8.539 -2.471 -1.761
ATOM 397 HG SER 26 7.640 -2.058 -1.682
ATOM 398 C SER 26 11.171 -1.447 -2.705
ATOM 399 O SER 26 12.323 -1.556 -2.327
ATOM 400 N ASN 27 10.905 -1.927 -3.938
ATOM 401 HN ASN 27 9.952 -1.835 -4.266
ATOM 402 CA ASN 27 11.993 -2.489 -4.712
ATOM 403 HA ASN 27 12.582 -2.995 -4.052
ATOM 404 CB ASN 27 11.650 -3.449 -5.842
ATOM 405 HB1 ASN 27 12.468 -3.770 -6.306
ATOM 406 HB2 ASN 27 11.134 -2.984 -6.582
ATOM 407 CG ASN 27 10.864 -4.605 -5.309
ATOM 408 OD1 ASN 27 11.487 -5.635 -5.054
ATOM 409 ND2 ASN 27 9.518 -4.542 -5.032
ATOM 410 HD21ASN 27 8.990 -5.314 -4.663
ATOM 411 HD22ASN 27 8.888 -3.807 -5.152
ATOM 412 C ASN 27 12.912 -1.450 -5.326
ATOM 413 O ASN 27 14.065 -1.735 -5.484
ATOM 414 N LYS 28 12.531 -0.149 -5.524
ATOM 415 HN LYS 28 11.599 0.201 -5.385
ATOM 416 CA LYS 28 13.499 0.814 -5.962
ATOM 417 HA1 LYS 28 14.110 0.351 -6.661
ATOM 418 CB LYS 28 12.849 2.085 -6.550
ATOM 419 HB1 LYS 28 13.516 2.729 -6.878
ATOM 420 HB2 LYS 28 12.340 2.536 -5.825
ATOM 421 CG LYS 28 11.949 1.701 -7.850
ATOM 422 HG1 LYS 28 11.564 2.604 -8.212
ATOM 423 HG2 LYS 28 11.158 1.061 -7.583
ATOM 424 CD LYS 28 13.031 1.082 -8.791
ATOM 425 HD1 LYS 28 13.423 0.260 -8.398
ATOM 426 HD2 LYS 28 13.828 1.711 -8.961
ATOM 427 CE LYS 28 12.372 0.728 -10.172
ATOM 428 HE1 LYS 28 11.592 0.113 -9.980
ATOM 429 HE2 LYS 28 13.017 0.257 -10.802
ATOM 430 NZ LYS 28 11.815 1.886 -10.915
ATOM 431 HZ1 LYS 28 12.440 2.576 -11.214
ATOM 432 HZ2 LYS 28 11.364 1.610 -11.757
ATOM 433 HZ3 LYS 28 11.128 2.440 -10.537
ATOM 434 C LYS 28 14.286 1.132 -4.812
ATOM 435 O LYS 28 15.477 1.399 -5.075
ATOM 436 N GLY 29 13.732 1.112 -3.613

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ATOM    437  HN  GLY    29      12.749   0.939  -3.410
ATOM    438  CA  GLY    29      14.560   1.360  -2.443
ATOM    439  HA1 GLY    29      14.081   1.362  -1.535
ATOM    440  HA2 GLY    29      15.058   2.190  -2.578
ATOM    441  C   GLY    29      15.573   0.224  -2.424
ATOM    442  O   GLY    29      16.743   0.536  -2.179
ATOM    443  N   ALA    30      15.186  -1.059  -2.610
ATOM    444  HN  ALA    30      14.242  -1.291  -2.802
ATOM    445  CA  ALA    30      16.083  -2.111  -2.546
ATOM    446  HA  ALA    30      16.467  -2.161  -1.580
ATOM    447  CB  ALA    30      15.259  -3.395  -2.892
ATOM    448  HB1 ALA    30      14.483  -3.475  -2.288
ATOM    449  HB2 ALA    30      14.939  -3.399  -3.828
ATOM    450  HB3 ALA    30      15.822  -4.143  -2.846
ATOM    451  C   ALA    30      17.186  -1.980  -3.576
ATOM    452  O   ALA    30      18.325  -2.145  -3.183
ATOM    453  N   ILE    31      16.900  -1.670  -4.851
ATOM    454  HN  ILE    31      15.971  -1.512  -5.178
ATOM    455  CA  ILE    31      17.974  -1.390  -5.842
ATOM    456  HA  ILE    31      18.559  -2.194  -5.968
ATOM    457  CB  ILE    31      17.225  -1.141  -7.239
ATOM    458  HB  ILE    31      16.622  -0.351  -7.166
ATOM    459  CG2 ILE    31      18.290  -0.821  -8.344
ATOM    460  HG21ILE    31      18.865  -0.079  -8.035
ATOM    461  HG22ILE    31      18.903  -1.576  -8.426
ATOM    462  HG23ILE    31      17.821  -0.564  -9.240
ATOM    463  CG1 ILE    31      16.435  -2.410  -7.638
ATOM    464  HG11ILE    31      15.850  -2.693  -6.952
ATOM    465  HG12ILE    31      17.139  -3.124  -7.781
ATOM    466  CD1 ILE    31      15.733  -2.126  -8.971
ATOM    467  HD11ILE    31      15.085  -1.455  -8.784
ATOM    468  HD12ILE    31      16.368  -1.759  -9.659
ATOM    469  HD13ILE    31      15.201  -2.967  -9.290
ATOM    470  C   ILE    31      18.818  -0.226  -5.371
ATOM    471  O   ILE    31      20.034  -0.351  -5.667
ATOM    472  N   ILE    32      18.345   0.830  -4.653
ATOM    473  HN  ILE    32      17.338   0.855  -4.448
ATOM    474  CA  ILE    32      19.343   1.834  -4.294
ATOM    475  HA  ILE    32      19.893   1.963  -5.068
ATOM    476  CB  ILE    32      18.709   3.199  -3.924
ATOM    477  HB  ILE    32      18.071   3.183  -3.195
ATOM    478  CG2 ILE    32      19.766   4.248  -3.646
ATOM    479  HG21ILE    32      19.327   5.145  -3.544
ATOM    480  HG22ILE    32      20.311   3.933  -2.822
ATOM    481  HG23ILE    32      20.326   4.286  -4.426
ATOM    482  CG1 ILE    32      17.912   3.636  -5.177
ATOM    483  HG11ILE    32      17.133   2.939  -5.310
ATOM    484  HG12ILE    32      18.523   3.669  -5.961
ATOM    485  CD1 ILE    32      17.407   5.026  -4.842
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ATOM 486 HD11ILE 32 18.146 5.653 -4.753
ATOM 487 HD12ILE 32 16.767 5.354 -5.559
ATOM 488 HD13ILE 32 16.869 4.955 -4.040
ATOM 489 C ILE 32 20.117 1.264 -3.154
ATOM 490 O ILE 32 21.353 1.445 -3.137
ATOM 491 N GLY 33 19.632 0.464 -2.244
ATOM 492 HN GLY 33 18.696 0.112 -2.178
ATOM 493 CA GLY 33 20.544 -0.095 -1.256
ATOM 494 HA1 GLY 33 19.942 -0.603 -0.604
ATOM 495 HA2 GLY 33 20.965 0.664 -0.789
ATOM 496 C GLY 33 21.538 -1.128 -1.937
ATOM 497 O GLY 33 22.641 -1.257 -1.451
ATOM 498 N LEU 34 21.153 -1.799 -2.989
ATOM 499 HN LEU 34 20.250 -1.699 -3.384
ATOM 500 CA LEU 34 22.068 -2.673 -3.709
ATOM 501 HA LEU 34 22.402 -3.352 -3.051
ATOM 502 CB LEU 34 21.411 -3.357 -4.934
ATOM 503 HB1 LEU 34 22.105 -3.863 -5.433
ATOM 504 HB2 LEU 34 21.038 -2.649 -5.518
ATOM 505 CG LEU 34 20.333 -4.392 -4.487
ATOM 506 HG LEU 34 19.595 -3.936 -3.972
ATOM 507 CD1 LEU 34 19.675 -4.996 -5.746
ATOM 508 HD11LEU 34 19.232 -4.240 -6.289
ATOM 509 HD12LEU 34 20.340 -5.519 -6.279
ATOM 510 HD13LEU 34 18.954 -5.616 -5.473
ATOM 511 CD2 LEU 34 20.998 -5.521 -3.649
ATOM 512 HD21LEU 34 21.401 -5.134 -2.816
ATOM 513 HD22LEU 34 20.387 -6.293 -3.427
ATOM 514 HD23LEU 34 21.712 -5.893 -4.132
ATOM 515 C LEU 34 23.152 -1.861 -4.363
ATOM 516 O LEU 34 24.001 -2.500 -5.001
ATOM 517 N MET 35 23.171 -0.509 -4.315
ATOM 518 HN MET 35 22.493 0.107 -3.798
ATOM 519 CA MET 35 24.241 0.232 -4.941
ATOM 520 HA MET 35 24.693 -0.266 -5.664
ATOM 521 CB MET 35 23.840 1.572 -5.470
ATOM 522 HB1 MET 35 24.596 2.119 -5.790
ATOM 523 HB2 MET 35 23.374 2.074 -4.706
ATOM 524 CG MET 35 22.778 1.474 -6.637
ATOM 525 HG1 MET 35 22.480 2.391 -6.966
ATOM 526 HG2 MET 35 21.978 0.969 -6.283
ATOM 527 SD MET 35 23.570 0.557 -7.832
ATOM 528 CE MET 35 24.957 1.587 -8.375
ATOM 529 HE1 MET 35 25.667 1.656 -7.619
ATOM 530 HE2 MET 35 25.355 1.112 -9.207
ATOM 531 HE3 MET 35 24.608 2.488 -8.618
ATOM 532 C MET 35 25.175 0.453 -3.785
ATOM 533 O MET 35 26.336 0.808 -3.987
ATOM 534 N VAL 36 24.746 0.413 -2.489

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ATOM    535  HN  VAL   36      23.785   0.167  -2.153
ATOM    536  CA  VAL   36      25.689   0.700  -1.437
ATOM    537  HA  VAL   36      26.279   1.488  -1.751
ATOM    538  CB  VAL   36      24.761   1.044  -0.342
ATOM    539  HB  VAL   36      24.217   0.248  -0.118
ATOM    540  CG1 VAL   36      25.535   1.444   0.933
ATOM    541 HG11VAL   36      24.911   1.624   1.660
ATOM    542 HG12VAL   36      26.142   0.669   1.135
ATOM    543 HG13VAL   36      26.104   2.223   0.767
ATOM    544  CG2 VAL   36      23.863   2.210  -0.760
ATOM    545 HG21VAL   36      23.131   2.349  -0.037
ATOM    546 HG22VAL   36      24.419   3.024  -0.807
ATOM    547 HG23VAL   36      23.442   2.071  -1.657
ATOM    548  C   VAL   36      26.509  -0.575  -1.175
ATOM    549  O   VAL   36      27.634  -0.461  -0.718
ATOM    550  N   GLY   37      26.041  -1.782  -1.420
ATOM    551  HN  GLY   37      25.139  -1.990  -1.778
ATOM    552  CA  GLY   37      26.938  -2.844  -1.122
ATOM    553  HA1 GLY   37      26.709  -3.357  -0.351
ATOM    554  HA2 GLY   37      27.863  -2.556  -1.072
ATOM    555  C   GLY   37      26.488  -3.543  -2.380
ATOM    556  O   GLY   37      25.280  -3.704  -2.581
ATOM    557  N   GLY   38      27.432  -3.825  -3.289
ATOM    558  HN  GLY   38      28.399  -3.648  -3.114
ATOM    559  CA  GLY   38      27.146  -4.374  -4.620
ATOM    560  HA1 GLY   38      26.182  -4.073  -4.862
ATOM    561  HA2 GLY   38      27.213  -5.376  -4.525
ATOM    562  C   GLY   38      28.185  -3.739  -5.482
ATOM    563  O   GLY   38      28.593  -4.304  -6.503
ATOM    564  N   VAL   39      28.531  -2.503  -5.114
ATOM    565  HN  VAL   39      28.156  -2.015  -4.359
ATOM    566  CA  VAL   39      29.463  -1.828  -5.958
ATOM    567  HA  VAL   39      29.762  -2.391  -6.794
ATOM    568  CB  VAL   39      28.935  -0.443  -6.380
ATOM    569  HB  VAL   39      28.707   0.077  -5.591
ATOM    570  CG1 VAL   39      29.880   0.416  -7.201
ATOM    571 HG11VAL   39      29.492   1.251  -7.370
ATOM    572 HG12VAL   39      30.675   0.567  -6.625
ATOM    573 HG13VAL   39      30.127  -0.015  -8.090
ATOM    574  CG2 VAL   39      27.637  -0.682  -7.225
ATOM    575 HG21VAL   39      27.306   0.133  -7.632
ATOM    576 HG22VAL   39      27.897  -1.231  -7.948
ATOM    577 HG23VAL   39      26.961  -1.117  -6.610
ATOM    578  C   VAL   39      30.456  -1.672  -4.898
ATOM    579  O   VAL   39      29.996  -1.591  -3.749
ATOM    580  N   VAL   40      31.759  -1.551  -5.060
ATOM    581  HN  VAL   40      32.171  -1.559  -5.922
ATOM    582  CA  VAL   40      32.644  -1.342  -3.979
ATOM    583  HA  VAL   40      32.096  -1.206  -3.136
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ATOM    584  CB  VAL    40      33.613  -2.545  -3.870
ATOM    585  HB  VAL    40      34.119  -2.580  -4.753
ATOM    586  CG1 VAL    40      34.655  -2.487  -2.744
ATOM    587  HG11VAL    40      34.130  -2.507  -1.874
ATOM    588  HG12VAL    40      35.344  -3.223  -2.819
ATOM    589  HG13VAL    40      35.179  -1.638  -2.770
ATOM    590  CG2 VAL    40      32.793  -3.874  -3.685
ATOM    591  HG21VAL    40      32.295  -3.873  -2.781
ATOM    592  HG22VAL    40      32.126  -3.983  -4.417
ATOM    593  HG23VAL    40      33.365  -4.747  -3.670
ATOM    594  C   VAL    40      33.341  -0.080  -4.518
ATOM    595  O   VAL    40      33.158   0.076  -5.726
ATOM    596  NA  NA     41       1.045  -9.022 -26.455
ATOM    597  NA  NA     42     -10.298   0.872 -22.376
ATOM    598  NA  NA     43      20.230 -10.218 -25.353
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Initial MD structure of the tenth NMR isoform with 3 Na^+ counterions

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ATOM      1  N   ASP     1       3.371  23.286  -9.276
ATOM      2  HN  ASP     1       4.191  23.764  -9.582
ATOM      3  CA  ASP     1       2.601  23.796  -8.105
ATOM      4  HA  ASP     1       3.221  24.247  -7.463
ATOM      5  CB  ASP     1       1.543  24.826  -8.602
ATOM      6  HB1 ASP     1       2.001  25.405  -9.277
ATOM      7  HB2 ASP     1       1.143  25.244  -7.786
ATOM      8  CG  ASP     1       0.393  24.111  -9.340
ATOM      9  OD1 ASP     1       0.642  23.698 -10.461
ATOM     10  OD2 ASP     1      -0.667  24.012  -8.740
ATOM     11  C   ASP     1       1.913  22.625  -7.380
ATOM     12  O   ASP     1       2.302  21.483  -7.539
ATOM     13  N   ALA     2       0.909  22.952  -6.603
ATOM     14  HN  ALA     2       0.649  23.913  -6.526
ATOM     15  CA  ALA     2       0.143  21.931  -5.837
ATOM     16  HA  ALA     2       0.306  21.026  -6.232
ATOM     17  CB  ALA     2       0.595  21.930  -4.373
ATOM     18  HB1 ALA     2       0.464  22.845  -3.992
ATOM     19  HB2 ALA     2       0.047  21.267  -3.863
ATOM     20  HB3 ALA     2       1.562  21.678  -4.330
ATOM     21  C   ALA     2      -1.342  22.272  -5.903
ATOM     22  O   ALA     2      -1.727  23.407  -5.699
ATOM     23  N   GLU     3      -2.133  21.269  -6.189
ATOM     24  HN  GLU     3      -1.740  20.366  -6.349
ATOM     25  CA  GLU     3      -3.603  21.456  -6.281
ATOM     26  HA  GLU     3      -3.871  22.324  -6.701
ATOM     27  CB  GLU     3      -4.155  20.314  -7.163
ATOM     28  HB1 GLU     3      -4.199  19.497  -6.588
ATOM     29  HB2 GLU     3      -3.603  20.297  -7.998
ATOM     30  CG  GLU     3      -5.596  20.644  -7.588
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ATOM 31 HG1 GLU 3 -5.547 21.440 -8.193
ATOM 32 HG2 GLU 3 -6.142 20.695 -6.752
ATOM 33 CD GLU 3 -6.153 19.482 -8.419
ATOM 34 OE1 GLU 3 -5.904 19.490 -9.615
ATOM 35 OE2 GLU 3 -6.800 18.643 -7.814
ATOM 36 C GLU 3 -4.155 21.431 -4.846
ATOM 37 O GLU 3 -3.958 22.396 -4.133
ATOM 38 N PHE 4 -4.805 20.360 -4.445
ATOM 39 HN PHE 4 -4.927 19.594 -5.074
ATOM 40 CA PHE 4 -5.368 20.280 -3.060
ATOM 41 HA PHE 4 -4.719 20.707 -2.430
ATOM 42 CB PHE 4 -6.728 21.027 -3.023
ATOM 43 HCB1PHE 4 -7.175 20.771 -2.165
ATOM 44 HCB2PHE 4 -7.186 20.834 -3.892
ATOM 45 CG PHE 4 -6.501 22.544 -2.966
ATOM 46 CD1 PHE 4 -6.005 23.134 -1.816
ATOM 47 HCD1PHE 4 -5.795 22.570 -1.019
ATOM 48 CE1 PHE 4 -5.798 24.498 -1.764
ATOM 49 HCE1PHE 4 -5.442 24.916 -0.930
ATOM 50 CZ PHE 4 -6.083 25.283 -2.861
ATOM 51 HCZ PHE 4 -5.932 26.270 -2.823
ATOM 52 CE2 PHE 4 -6.576 24.702 -4.011
ATOM 53 HCE2PHE 4 -6.784 25.269 -4.806
ATOM 54 CD2 PHE 4 -6.783 23.339 -4.064
ATOM 55 HCD2PHE 4 -7.138 22.922 -4.900
ATOM 56 C PHE 4 -5.564 18.825 -2.606
ATOM 57 O PHE 4 -6.617 18.241 -2.792
ATOM 58 N ARG 5 -4.519 18.285 -2.022
ATOM 59 HN ARG 5 -3.695 18.838 -1.916
ATOM 60 CA ARG 5 -4.513 16.875 -1.505
ATOM 61 HA ARG 5 -3.562 16.618 -1.332
ATOM 62 CB ARG 5 -5.359 16.838 -0.197
ATOM 63 HB1 ARG 5 -6.237 16.420 -0.435
ATOM 64 HB2 ARG 5 -5.342 17.763 0.185
ATOM 65 CG ARG 5 -4.692 15.917 0.847
ATOM 66 HG1 ARG 5 -4.334 15.126 0.349
ATOM 67 HG2 ARG 5 -5.360 15.776 1.578
ATOM 68 CD ARG 5 -3.483 16.633 1.480
ATOM 69 HD1 ARG 5 -3.807 17.520 1.811
ATOM 70 HD2 ARG 5 -2.738 16.599 0.812
ATOM 71 NE ARG 5 -3.044 15.850 2.674
ATOM 72 HE ARG 5 -3.597 15.079 2.983
ATOM 73 CZ ARG 5 -1.947 16.155 3.324
ATOM 74 NH1 ARG 5 -1.204 17.160 2.936
ATOM 75 HH11ARG 5 -0.368 17.393 3.429
ATOM 76 HH12ARG 5 -1.451 17.715 2.144
ATOM 77 NH2 ARG 5 -1.623 15.430 4.359
ATOM 78 HH21ARG 5 -0.787 15.661 4.854
ATOM 79 HH22ARG 5 -2.189 14.663 4.654

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ATOM     80  C   ARG    5      -5.038  15.840  -2.513
ATOM     81  O   ARG    5      -5.513  14.778  -2.154
ATOM     82  N   HIE    6      -4.922  16.211  -3.759
ATOM     83  HN  HIE    6      -4.518  17.103  -3.951
ATOM     84  CA  HIE    6      -5.362  15.375  -4.901
ATOM     85  HA  HIE    6      -5.856  14.538  -4.668
ATOM     86  CB  HIE    6      -6.331  16.244  -5.743
ATOM     87  HB1 HIE    6      -5.789  17.000  -6.113
ATOM     88  HB2 HIE    6      -7.116  16.446  -5.156
ATOM     89  CG  HIE    6      -6.881  15.469  -6.952
ATOM     90  ND1 HIE    6      -7.733  15.945  -7.803
ATOM     91  HE2 HIE    6      -7.359  13.106  -9.040
ATOM     92  CE1 HIE    6      -7.997  15.054  -8.706
ATOM     93  HE1 HIE    6      -8.627  15.198  -9.467
ATOM     94  NE2 HIE    6      -7.336  13.943  -8.498
ATOM     95  CD2 HIE    6      -6.635  14.182  -7.409
ATOM     96  HD2 HIE    6      -6.014  13.531  -6.974
ATOM     97  C   HIE    6      -4.072  15.000  -5.618
ATOM     98  O   HIE    6      -3.248  14.296  -5.071
ATOM     99  N   ASP    7      -3.931  15.487  -6.813
ATOM    100  HN  ASP    7      -4.662  16.060  -7.187
ATOM    101  CA  ASP    7      -2.729  15.229  -7.654
ATOM    102  HA  ASP    7      -2.453  14.271  -7.585
ATOM    103  CB  ASP    7      -3.099  15.570  -9.112
ATOM    104  HB1 ASP    7      -3.643  14.804  -9.456
ATOM    105  HB2 ASP    7      -2.247  15.814  -9.575
ATOM    106  CG  ASP    7      -4.006  16.812  -9.167
ATOM    107  OD1 ASP    7      -3.454  17.892  -9.037
ATOM    108  OD2 ASP    7      -5.200  16.610  -9.331
ATOM    109  C   ASP    7      -1.529  16.075  -7.171
ATOM    110  O   ASP    7      -0.697  16.508  -7.945
ATOM    111  N   SER    8      -1.490  16.284  -5.878
ATOM    112  HN  SER    8      -2.214  15.895  -5.314
ATOM    113  CA  SER    8      -0.417  17.073  -5.215
ATOM    114  HA  SER    8       0.473  16.812  -5.589
ATOM    115  CB  SER    8      -0.685  18.563  -5.477
ATOM    116  HB1 SER    8      -0.687  18.707  -6.468
ATOM    117  HB2 SER    8      -0.059  19.095  -4.905
ATOM    118  OG  SER    8      -2.007  18.776  -5.000
ATOM    119  HG  SER    8      -2.461  19.656  -5.160
ATOM    120  C   SER    8      -0.382  16.790  -3.701
ATOM    121  O   SER    8       0.050  17.619  -2.921
ATOM    122  N   GLY    9      -0.841  15.621  -3.326
ATOM    123  HN  GLY    9      -1.184  14.982  -4.011
ATOM    124  CA  GLY    9      -0.853  15.240  -1.879
ATOM    125  HA1 GLY    9      -1.493  15.867  -1.432
ATOM    126  HA2 GLY    9       0.104  15.225  -1.588
ATOM    127  C   GLY    9      -1.396  13.829  -1.631
ATOM    128  O   GLY    9      -1.142  13.250  -0.593
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ATOM 129 N TYR 10 -2.129 13.311 -2.587
ATOM 130 HN TYR 10 -2.298 13.845 -3.413
ATOM 131 CA TYR 10 -2.719 11.943 -2.475
ATOM 132 HA TYR 10 -2.995 11.716 -1.541
ATOM 133 CB TYR 10 -3.977 11.922 -3.395
ATOM 134 HCB1TYR 10 -3.644 11.670 -4.304
ATOM 135 HCB2TYR 10 -4.424 12.808 -3.264
ATOM 136 CG TYR 10 -5.036 10.861 -3.024
ATOM 137 CD1 TYR 10 -4.757 9.733 -2.263
ATOM 138 HCD1TYR 10 -3.831 9.586 -1.919
ATOM 139 CE1 TYR 10 -5.745 8.813 -1.978
ATOM 140 HCE1TYR 10 -5.527 8.007 -1.431
ATOM 141 CZ TYR 10 -7.032 8.996 -2.442
ATOM 142 OH TYR 10 -8.014 8.075 -2.161
ATOM 143 HOH TYR 10 -8.605 8.204 -1.358
ATOM 144 CE2 TYR 10 -7.317 10.116 -3.199
ATOM 145 HCE2TYR 10 -8.244 10.260 -3.541
ATOM 146 CD2 TYR 10 -6.329 11.038 -3.486
ATOM 147 HCD2TYR 10 -6.551 11.843 -4.035
ATOM 148 C TYR 10 -1.655 10.906 -2.901
ATOM 149 O TYR 10 -0.486 11.065 -2.602
ATOM 150 N GLU 11 -2.091 9.877 -3.585
ATOM 151 HN GLU 11 -3.065 9.822 -3.791
ATOM 152 CA GLU 11 -1.193 8.786 -4.069
ATOM 153 HA GLU 11 -0.377 9.158 -4.512
ATOM 154 CB GLU 11 -0.730 7.912 -2.870
ATOM 155 HB1 GLU 11 -1.440 7.222 -2.725
ATOM 156 HB2 GLU 11 -0.499 8.544 -2.129
ATOM 157 CG GLU 11 0.572 7.144 -3.219
ATOM 158 HG1 GLU 11 1.081 7.036 -2.365
ATOM 159 HG2 GLU 11 0.995 7.629 -3.986
ATOM 160 CD GLU 11 0.239 5.725 -3.718
ATOM 161 OE1 GLU 11 0.025 4.879 -2.862
ATOM 162 OE2 GLU 11 0.216 5.560 -4.928
ATOM 163 C GLU 11 -2.016 7.945 -5.047
ATOM 164 O GLU 11 -1.535 7.549 -6.092
ATOM 165 N VAL 12 -3.247 7.704 -4.657
ATOM 166 HN VAL 12 -3.558 8.068 -3.783
ATOM 167 CA VAL 12 -4.193 6.900 -5.485
ATOM 168 HA VAL 12 -3.849 6.901 -6.425
ATOM 169 CB VAL 12 -4.270 5.440 -4.931
ATOM 170 HB VAL 12 -4.806 4.910 -5.588
ATOM 171 CG1 VAL 12 -2.892 4.826 -4.801
ATOM 172 HG11VAL 12 -2.380 5.320 -4.098
ATOM 173 HG12VAL 12 -2.986 3.865 -4.541
ATOM 174 HG13VAL 12 -2.419 4.897 -5.679
ATOM 175 CG2 VAL 12 -4.964 5.396 -3.541
ATOM 176 HG21VAL 12 -4.799 6.261 -3.067
ATOM 177 HG22VAL 12 -5.946 5.261 -3.671

ATOM 178 HG23VAL 12 -4.584 4.639 -3.010
ATOM 179 C VAL 12 -5.602 7.500 -5.475
ATOM 180 O VAL 12 -5.829 8.627 -5.088
ATOM 181 N HIS 13 -6.479 6.653 -5.937
ATOM 182 HN HIS 13 -6.130 5.768 -6.235
ATOM 183 CA HIS 13 -7.941 6.876 -6.066
ATOM 184 HA HIS 13 -8.317 7.479 -5.362
ATOM 185 CB HIS 13 -8.234 7.538 -7.424
ATOM 186 HB1 HIS 13 -9.228 7.605 -7.512
ATOM 187 HB2 HIS 13 -7.712 7.036 -8.116
ATOM 188 CG HIS 13 -7.683 8.968 -7.388
ATOM 189 ND1 HIS 13 -6.565 9.347 -7.918
ATOM 190 HD1 HIS 13 -5.935 8.756 -8.414
ATOM 191 CE1 HIS 13 -6.389 10.614 -7.704
ATOM 192 HE1 HIS 13 -5.594 11.129 -8.020
ATOM 193 NE2 HIS 13 -7.381 11.134 -7.025
ATOM 194 CD2 HIS 13 -8.200 10.121 -6.818
ATOM 195 HD2 HIS 13 -9.066 10.176 -6.324
ATOM 196 C HIS 13 -8.558 5.454 -5.980
ATOM 197 O HIS 13 -9.749 5.274 -6.152
ATOM 198 N HIS 14 -7.695 4.493 -5.709
ATOM 199 HN HIS 14 -6.741 4.748 -5.580
ATOM 200 CA HIS 14 -8.045 3.050 -5.578
ATOM 201 HA HIS 14 -8.944 2.941 -5.153
ATOM 202 CB HIS 14 -8.069 2.411 -6.974
ATOM 203 HB1 HIS 14 -8.081 1.420 -6.843
ATOM 204 HB2 HIS 14 -7.327 2.829 -7.500
ATOM 205 CG HIS 14 -9.369 2.784 -7.660
ATOM 206 ND1 HIS 14 -10.559 2.405 -7.327
ATOM 207 HD1 HIS 14 -10.782 1.804 -6.564
ATOM 208 CE1 HIS 14 -11.417 2.932 -8.144
ATOM 209 HE1 HIS 14 -12.404 2.786 -8.090
ATOM 210 NE2 HIS 14 -10.832 3.679 -9.049
ATOM 211 CD2 HIS 14 -9.552 3.592 -8.752
ATOM 212 HD2 HIS 14 -8.817 4.049 -9.251
ATOM 213 C HIS 14 -6.971 2.367 -4.707
ATOM 214 O HIS 14 -5.783 2.487 -4.958
ATOM 215 N GLN 15 -7.409 1.656 -3.695
ATOM 216 HN GLN 15 -8.391 1.587 -3.531
ATOM 217 CA GLN 15 -6.449 0.949 -2.784
ATOM 218 HA GLN 15 -5.835 1.623 -2.373
ATOM 219 CB GLN 15 -7.255 0.223 -1.688
ATOM 220 HB1 GLN 15 -7.487 -0.680 -2.051
ATOM 221 HB2 GLN 15 -7.988 0.843 -1.407
ATOM 222 CG GLN 15 -6.371 -0.009 -0.444
ATOM 223 HG1 GLN 15 -6.367 0.847 0.076
ATOM 224 HG2 GLN 15 -5.504 -0.391 -0.768
ATOM 225 CD GLN 15 -7.024 -1.073 0.444
ATOM 226 OE1 GLN 15 -6.735 -2.249 0.341

ATOM 227 NE2 GLN 15 -7.912 -0.704 1.327
ATOM 228 HE21GLN 15 -8.337 -1.397 1.906
ATOM 229 HE22GLN 15 -8.149 0.261 1.412
ATOM 230 C GLN 15 -5.584 -0.067 -3.560
ATOM 231 O GLN 15 -4.591 -0.570 -3.069
ATOM 232 N LYS 16 -5.985 -0.332 -4.778
ATOM 233 HN LYS 16 -6.799 0.125 -5.127
ATOM 234 CA LYS 16 -5.261 -1.292 -5.651
ATOM 235 HA1 LYS 16 -5.100 -2.175 -5.210
ATOM 236 CB LYS 16 -6.117 -1.544 -6.918
ATOM 237 HB1 LYS 16 -6.271 -0.651 -7.341
ATOM 238 HB2 LYS 16 -6.902 -2.091 -6.625
ATOM 239 CG LYS 16 -5.351 -2.396 -7.958
ATOM 240 HG1 LYS 16 -4.561 -1.856 -8.253
ATOM 241 HG2 LYS 16 -6.022 -2.696 -8.637
ATOM 242 CD LYS 16 -4.797 -3.666 -7.283
ATOM 243 HD1 LYS 16 -5.548 -4.064 -6.754
ATOM 244 HD2 LYS 16 -3.954 -3.398 -6.814
ATOM 245 CE LYS 16 -4.405 -4.707 -8.346
ATOM 246 HE1 LYS 16 -3.962 -5.461 -7.861
ATOM 247 HE2 LYS 16 -3.901 -4.215 -9.057
ATOM 248 NZ LYS 16 -5.624 -5.272 -8.994
ATOM 249 HZ1 LYS 16 -6.428 -4.794 -8.646
ATOM 250 HZ2 LYS 16 -5.555 -5.147 -9.981
ATOM 251 HZ3 LYS 16 -5.686 -6.244 -8.777
ATOM 252 C LYS 16 -3.936 -0.636 -5.995
ATOM 253 O LYS 16 -2.869 -1.198 -5.841
ATOM 254 N LEU 17 -4.073 0.578 -6.452
ATOM 255 HN LEU 17 -4.984 0.971 -6.541
ATOM 256 CA LEU 17 -2.885 1.377 -6.839
ATOM 257 HA LEU 17 -2.361 0.943 -7.572
ATOM 258 CB LEU 17 -3.365 2.746 -7.341
ATOM 259 HB1 LEU 17 -2.582 3.173 -7.794
ATOM 260 HB2 LEU 17 -3.788 3.204 -6.557
ATOM 261 CG LEU 17 -4.474 2.599 -8.416
ATOM 262 HG LEU 17 -5.268 2.157 -7.999
ATOM 263 CD1 LEU 17 -4.839 3.999 -8.935
ATOM 264 HD11LEU 17 -4.798 4.649 -8.176
ATOM 265 HD12LEU 17 -4.186 4.264 -9.645
ATOM 266 HD13LEU 17 -5.764 3.975 -9.314
ATOM 267 CD2 LEU 17 -4.009 1.718 -9.594
ATOM 268 HD21LEU 17 -3.144 2.075 -9.946
ATOM 269 HD22LEU 17 -3.883 0.780 -9.270
ATOM 270 HD23LEU 17 -4.705 1.740 -10.312
ATOM 271 C LEU 17 -1.995 1.510 -5.599
ATOM 272 O LEU 17 -0.791 1.519 -5.725
ATOM 273 N VAL 18 -2.588 1.608 -4.429
ATOM 274 HN VAL 18 -3.583 1.601 -4.371
ATOM 275 CA VAL 18 -1.761 1.731 -3.183

ATOM 276 HA VAL 18 -1.173 2.541 -3.187
ATOM 277 CB VAL 18 -2.746 1.851 -1.956
ATOM 278 HB VAL 18 -3.612 1.454 -2.257
ATOM 279 CG1 VAL 18 -2.271 1.082 -0.705
ATOM 280 HG11VAL 18 -2.216 1.716 0.066
ATOM 281 HG12VAL 18 -2.925 0.354 -0.502
ATOM 282 HG13VAL 18 -1.369 0.689 -0.886
ATOM 283 CG2 VAL 18 -2.881 3.329 -1.551
ATOM 284 HG21VAL 18 -2.735 3.411 -0.565
ATOM 285 HG22VAL 18 -2.195 3.866 -2.043
ATOM 286 HG23VAL 18 -3.798 3.649 -1.788
ATOM 287 C VAL 18 -0.859 0.483 -3.096
ATOM 288 O VAL 18 0.350 0.596 -3.045
ATOM 289 N PHE 19 -1.469 -0.678 -3.095
ATOM 290 HN PHE 19 -2.466 -0.703 -3.148
ATOM 291 CA PHE 19 -0.703 -1.965 -3.015
ATOM 292 HA PHE 19 -0.303 -2.077 -2.105
ATOM 293 CB PHE 19 -1.677 -3.134 -3.295
ATOM 294 HCB1PHE 19 -1.133 -3.877 -3.686
ATOM 295 HCB2PHE 19 -2.441 -2.755 -3.818
ATOM 296 CG PHE 19 -2.255 -3.654 -1.969
ATOM 297 CD1 PHE 19 -3.050 -2.842 -1.178
ATOM 298 HCD1PHE 19 -3.251 -1.909 -1.473
ATOM 299 CE1 PHE 19 -3.568 -3.308 0.013
ATOM 300 HCE1PHE 19 -4.141 -2.714 0.575
ATOM 301 CZ PHE 19 -3.293 -4.594 0.427
ATOM 302 HCZ PHE 19 -3.667 -4.933 1.289
ATOM 303 CE2 PHE 19 -2.502 -5.412 -0.352
ATOM 304 HCE2PHE 19 -2.302 -6.344 -0.053
ATOM 305 CD2 PHE 19 -1.984 -4.945 -1.544
ATOM 306 HCD2PHE 19 -1.411 -5.541 -2.103
ATOM 307 C PHE 19 0.437 -1.956 -4.039
ATOM 308 O PHE 19 1.579 -2.238 -3.728
ATOM 309 N PHE 20 0.071 -1.614 -5.247
ATOM 310 HN PHE 20 -0.888 -1.394 -5.420
ATOM 311 CA PHE 20 1.046 -1.544 -6.366
ATOM 312 HA PHE 20 1.463 -2.424 -6.594
ATOM 313 CB PHE 20 0.247 -1.033 -7.599
ATOM 314 HCB1PHE 20 -0.460 -0.421 -7.243
ATOM 315 HCB2PHE 20 -0.021 -1.845 -8.118
ATOM 316 CG PHE 20 1.114 -0.189 -8.532
ATOM 317 CD1 PHE 20 2.002 -0.799 -9.395
ATOM 318 HCD1PHE 20 2.075 -1.795 -9.412
ATOM 319 CE1 PHE 20 2.789 -0.039 -10.233
ATOM 320 HCE1PHE 20 3.430 -0.484 -10.856
ATOM 321 CZ PHE 20 2.693 1.339 -10.213
ATOM 322 HCZ PHE 20 3.263 1.890 -10.820
ATOM 323 CE2 PHE 20 1.806 1.952 -9.350
ATOM 324 HCE2PHE 20 1.734 2.948 -9.332

ATOM 325 CD2 PHE 20 1.021 1.190 -8.514
ATOM 326 HCD2PHE 20 0.381 1.636 -7.891
ATOM 327 C PHE 20 2.206 -0.613 -5.951
ATOM 328 O PHE 20 3.358 -0.992 -6.004
ATOM 329 N ALA 21 1.865 0.582 -5.535
ATOM 330 HN ALA 21 0.899 0.824 -5.505
ATOM 331 CA ALA 21 2.882 1.590 -5.101
ATOM 332 HA ALA 21 3.422 1.869 -5.895
ATOM 333 CB ALA 21 2.148 2.803 -4.504
ATOM 334 HB1 ALA 21 2.706 3.194 -3.772
ATOM 335 HB2 ALA 21 2.004 3.483 -5.223
ATOM 336 HB3 ALA 21 1.267 2.503 -4.137
ATOM 337 C ALA 21 3.850 1.007 -4.073
ATOM 338 O ALA 21 5.041 1.191 -4.196
ATOM 339 N GLU 22 3.341 0.316 -3.089
ATOM 340 HN GLU 22 2.349 0.192 -3.027
ATOM 341 CA GLU 22 4.242 -0.288 -2.052
ATOM 342 HA GLU 22 4.732 0.442 -1.575
ATOM 343 CB GLU 22 3.407 -1.089 -1.028
ATOM 344 HB1 GLU 22 4.036 -1.724 -0.578
ATOM 345 HB2 GLU 22 2.614 -1.449 -1.520
ATOM 346 CG GLU 22 2.864 -0.151 0.069
ATOM 347 HG1 GLU 22 3.522 0.597 0.164
ATOM 348 HG2 GLU 22 2.652 -0.722 0.863
ATOM 349 CD GLU 22 1.542 0.468 -0.400
ATOM 350 OE1 GLU 22 0.558 -0.251 -0.331
ATOM 351 OE2 GLU 22 1.588 1.620 -0.806
ATOM 352 C GLU 22 5.246 -1.228 -2.735
ATOM 353 O GLU 22 6.441 -1.115 -2.532
ATOM 354 N ASP 23 4.719 -2.125 -3.536
ATOM 355 HN ASP 23 3.726 -2.152 -3.653
ATOM 356 CA ASP 23 5.575 -3.108 -4.277
ATOM 357 HA ASP 23 5.929 -3.784 -3.630
ATOM 358 CB ASP 23 4.743 -3.818 -5.359
ATOM 359 HB1 ASP 23 4.559 -3.143 -6.075
ATOM 360 HB2 ASP 23 3.977 -4.261 -4.893
ATOM 361 CG ASP 23 5.586 -4.933 -5.997
ATOM 362 OD1 ASP 23 5.721 -5.961 -5.354
ATOM 363 OD2 ASP 23 6.056 -4.691 -7.099
ATOM 364 C ASP 23 6.728 -2.371 -4.956
ATOM 365 O ASP 23 7.891 -2.677 -4.788
ATOM 366 N VAL 24 6.309 -1.394 -5.710
ATOM 367 HN VAL 24 5.324 -1.234 -5.765
ATOM 368 CA VAL 24 7.210 -0.508 -6.491
ATOM 369 HA VAL 24 7.722 -1.005 -7.191
ATOM 370 CB VAL 24 6.288 0.541 -7.146
ATOM 371 HB VAL 24 5.824 1.047 -6.419
ATOM 372 CG1 VAL 24 7.074 1.552 -7.974
ATOM 373 HG11VAL 24 7.188 2.391 -7.442

ATOM 374 HG12VAL 24 7.969 1.165 -8.197
ATOM 375 HG13VAL 24 6.569 1.748 -8.814
ATOM 376 CG2 VAL 24 5.248 -0.179 -8.034
ATOM 377 HG21VAL 24 4.346 0.223 -7.871
ATOM 378 HG22VAL 24 5.502 -0.065 -8.994
ATOM 379 HG23VAL 24 5.234 -1.151 -7.799
ATOM 380 C VAL 24 8.273 0.116 -5.585
ATOM 381 O VAL 24 9.455 0.015 -5.843
ATOM 382 N GLY 25 7.804 0.741 -4.540
ATOM 383 HN GLY 25 6.817 0.771 -4.400
ATOM 384 CA GLY 25 8.700 1.409 -3.548
ATOM 385 HA1 GLY 25 8.152 1.568 -2.725
ATOM 386 HA2 GLY 25 9.121 2.186 -4.016
ATOM 387 C GLY 25 9.834 0.469 -3.146
ATOM 388 O GLY 25 10.995 0.827 -3.189
ATOM 389 N SER 26 9.439 -0.719 -2.767
ATOM 390 HN SER 26 8.463 -0.931 -2.760
ATOM 391 CA SER 26 10.420 -1.761 -2.345
ATOM 392 HA SER 26 10.980 -1.394 -1.603
ATOM 393 CB SER 26 9.643 -3.005 -1.867
ATOM 394 HB1 SER 26 10.286 -3.607 -1.392
ATOM 395 HB2 SER 26 9.119 -3.359 -2.642
ATOM 396 OG SER 26 8.722 -2.502 -0.909
ATOM 397 HG SER 26 7.900 -2.013 -1.215
ATOM 398 C SER 26 11.365 -2.147 -3.494
ATOM 399 O SER 26 12.565 -1.981 -3.408
ATOM 400 N ASN 27 10.782 -2.642 -4.553
ATOM 401 HN ASN 27 9.788 -2.735 -4.553
ATOM 402 CA ASN 27 11.546 -3.075 -5.755
ATOM 403 HA ASN 27 12.207 -3.778 -5.493
ATOM 404 CB ASN 27 10.522 -3.623 -6.767
ATOM 405 HB1 ASN 27 11.020 -3.799 -7.617
ATOM 406 HB2 ASN 27 9.750 -2.986 -6.772
ATOM 407 CG ASN 27 9.984 -4.976 -6.278
ATOM 408 OD1 ASN 27 10.717 -5.933 -6.129
ATOM 409 ND2 ASN 27 8.711 -5.096 -6.018
ATOM 410 HD21ASN 27 8.359 -5.975 -5.700
ATOM 411 HD22ASN 27 8.105 -4.311 -6.140
ATOM 412 C ASN 27 12.377 -1.954 -6.371
ATOM 413 O ASN 27 13.589 -1.977 -6.285
ATOM 414 N LYS 28 11.715 -1.000 -6.975
ATOM 415 HN LYS 28 10.718 -1.046 -7.009
ATOM 416 CA LYS 28 12.421 0.154 -7.610
ATOM 417 HA1 LYS 28 12.926 -0.140 -8.422
ATOM 418 CB LYS 28 11.374 1.210 -8.031
ATOM 419 HB1 LYS 28 11.589 2.049 -7.533
ATOM 420 HB2 LYS 28 10.473 0.788 -7.921
ATOM 421 CG LYS 28 11.540 1.522 -9.527
ATOM 422 HG1 LYS 28 11.349 0.672 -10.020

ATOM 423 HG2 LYS 28 12.434 1.959 -9.633
ATOM 424 CD LYS 28 10.483 2.552 -9.988
ATOM 425 HD1 LYS 28 9.624 2.304 -9.539
ATOM 426 HD2 LYS 28 10.524 2.577 -10.988
ATOM 427 CE LYS 28 10.849 3.969 -9.496
ATOM 428 HE1 LYS 28 10.375 4.615 -10.096
ATOM 429 HE2 LYS 28 11.847 4.002 -9.430
ATOM 430 NZ LYS 28 10.318 4.194 -8.122
ATOM 431 HZ1 LYS 28 10.572 5.110 -7.821
ATOM 432 HZ2 LYS 28 9.324 4.105 -8.140
ATOM 433 HZ3 LYS 28 10.710 3.513 -7.507
ATOM 434 C LYS 28 13.405 0.744 -6.592
ATOM 435 O LYS 28 14.478 1.172 -6.955
ATOM 436 N GLY 29 13.017 0.739 -5.339
ATOM 437 HN GLY 29 12.122 0.365 -5.100
ATOM 438 CA GLY 29 13.901 1.283 -4.268
ATOM 439 HA1 GLY 29 13.462 1.073 -3.393
ATOM 440 HA2 GLY 29 14.094 2.235 -4.506
ATOM 441 C GLY 29 15.240 0.539 -4.284
ATOM 442 O GLY 29 16.285 1.135 -4.470
ATOM 443 N ALA 30 15.173 -0.759 -4.100
ATOM 444 HN ALA 30 14.285 -1.197 -3.961
ATOM 445 CA ALA 30 16.424 -1.582 -4.097
ATOM 446 HA ALA 30 17.016 -1.287 -3.347
ATOM 447 CB ALA 30 16.041 -3.057 -3.912
ATOM 448 HB1 ALA 30 15.777 -3.208 -2.959
ATOM 449 HB2 ALA 30 15.275 -3.273 -4.517
ATOM 450 HB3 ALA 30 16.828 -3.629 -4.142
ATOM 451 C ALA 30 17.193 -1.400 -5.408
ATOM 452 O ALA 30 18.393 -1.218 -5.414
ATOM 453 N ILE 31 16.465 -1.448 -6.490
ATOM 454 HN ILE 31 15.482 -1.597 -6.398
ATOM 455 CA ILE 31 17.041 -1.289 -7.853
ATOM 456 HA ILE 31 17.667 -2.021 -8.120
ATOM 457 CB ILE 31 15.812 -1.284 -8.805
ATOM 458 HB ILE 31 15.092 -0.716 -8.408
ATOM 459 CG2 ILE 31 16.121 -0.652 -10.172
ATOM 460 HG21ILE 31 16.254 0.333 -10.053
ATOM 461 HG22ILE 31 16.953 -1.065 -10.542
ATOM 462 HG23ILE 31 15.353 -0.819 -10.790
ATOM 463 CG1 ILE 31 15.327 -2.753 -8.958
ATOM 464 HG11ILE 31 15.085 -3.068 -8.040
ATOM 465 HG12ILE 31 16.037 -3.236 -9.471
ATOM 466 CD1 ILE 31 14.040 -2.845 -9.803
ATOM 467 HD11ILE 31 13.411 -2.122 -9.518
ATOM 468 HD12ILE 31 14.275 -2.731 -10.768
ATOM 469 HD13ILE 31 13.618 -3.740 -9.658
ATOM 470 C ILE 31 17.890 -0.015 -7.910
ATOM 471 O ILE 31 19.056 -0.062 -8.255

ATOM 472 N ILE 32 17.291 1.096 -7.566
ATOM 473 HN ILE 32 16.333 1.073 -7.290
ATOM 474 CA ILE 32 18.024 2.394 -7.580
ATOM 475 HA ILE 32 18.314 2.631 -8.507
ATOM 476 CB ILE 32 17.073 3.500 -7.052
ATOM 477 HB ILE 32 16.752 3.258 -6.136
ATOM 478 CG2 ILE 32 17.823 4.855 -6.981
ATOM 479 HG21ILE 32 17.565 5.326 -6.137
ATOM 480 HG22ILE 32 18.808 4.683 -6.988
ATOM 481 HG23ILE 32 17.569 5.410 -7.773
ATOM 482 CG1 ILE 32 15.877 3.626 -8.033
ATOM 483 HG11ILE 32 15.601 2.695 -8.274
ATOM 484 HG12ILE 32 16.164 4.256 -8.756
ATOM 485 CD1 ILE 32 14.670 4.276 -7.330
ATOM 486 HD11ILE 32 14.999 4.989 -6.711
ATOM 487 HD12ILE 32 14.067 4.676 -8.020
ATOM 488 HD13ILE 32 14.179 3.575 -6.813
ATOM 489 C ILE 32 19.270 2.273 -6.703
ATOM 490 O ILE 32 20.344 2.655 -7.118
ATOM 491 N GLY 33 19.099 1.739 -5.521
ATOM 492 HN GLY 33 18.187 1.440 -5.238
ATOM 493 CA GLY 33 20.260 1.574 -4.594
ATOM 494 HA1 GLY 33 19.952 0.977 -3.851
ATOM 495 HA2 GLY 33 20.591 2.494 -4.380
ATOM 496 C GLY 33 21.409 0.843 -5.298
ATOM 497 O GLY 33 22.540 1.289 -5.286
ATOM 498 N LEU 34 21.086 -0.268 -5.913
ATOM 499 HN LEU 34 20.138 -0.584 -5.896
ATOM 500 CA LEU 34 22.122 -1.064 -6.636
ATOM 501 HA LEU 34 22.837 -1.345 -5.996
ATOM 502 CB LEU 34 21.444 -2.314 -7.247
ATOM 503 HB1 LEU 34 22.166 -2.848 -7.688
ATOM 504 HB2 LEU 34 20.674 -1.984 -7.794
ATOM 505 CG LEU 34 20.846 -3.209 -6.119
ATOM 506 HG LEU 34 20.481 -2.618 -5.399
ATOM 507 CD1 LEU 34 19.716 -4.088 -6.696
ATOM 508 HD11LEU 34 18.849 -3.820 -6.277
ATOM 509 HD12LEU 34 19.672 -3.954 -7.686
ATOM 510 HD13LEU 34 19.912 -5.047 -6.491
ATOM 511 CD2 LEU 34 21.937 -4.122 -5.530
ATOM 512 HD21LEU 34 22.295 -3.705 -4.695
ATOM 513 HD22LEU 34 21.537 -5.014 -5.320
ATOM 514 HD23LEU 34 22.671 -4.227 -6.201
ATOM 515 C LEU 34 22.784 -0.221 -7.734
ATOM 516 O LEU 34 23.997 -0.173 -7.823
ATOM 517 N MET 35 21.968 0.424 -8.535
ATOM 518 HN MET 35 20.981 0.337 -8.399
ATOM 519 CA MET 35 22.487 1.286 -9.647
ATOM 520 HA MET 35 22.961 0.717 -10.319

ATOM 521 CB MET 35 21.297 2.004 -10.316
ATOM 522 HB1 MET 35 21.681 2.620 -11.005
ATOM 523 HB2 MET 35 20.738 2.381 -9.577
ATOM 524 CG MET 35 20.414 0.993 -11.070
ATOM 525 HG1 MET 35 20.340 0.201 -10.462
ATOM 526 HG2 MET 35 20.842 0.885 -11.968
ATOM 527 SD MET 35 18.707 1.494 -11.408
ATOM 528 CE MET 35 18.341 0.316 -12.733
ATOM 529 HE1 MET 35 17.459 0.551 -13.143
ATOM 530 HE2 MET 35 19.062 0.368 -13.423
ATOM 531 HE3 MET 35 18.303 -0.606 -12.348
ATOM 532 C MET 35 23.484 2.319 -9.100
ATOM 533 O MET 35 24.578 2.469 -9.613
ATOM 534 N VAL 36 23.050 2.991 -8.064
ATOM 535 HN VAL 36 22.136 2.793 -7.716
ATOM 536 CA VAL 36 23.866 4.038 -7.382
ATOM 537 HA VAL 36 24.057 4.807 -7.993
ATOM 538 CB VAL 36 23.054 4.555 -6.155
ATOM 539 HB VAL 36 22.724 3.768 -5.634
ATOM 540 CG1 VAL 36 23.941 5.426 -5.232
ATOM 541 HG11VAL 36 23.359 6.066 -4.730
ATOM 542 HG12VAL 36 24.426 4.832 -4.590
ATOM 543 HG13VAL 36 24.598 5.930 -5.793
ATOM 544 CG2 VAL 36 21.869 5.413 -6.658
ATOM 545 HG21VAL 36 21.762 6.205 -6.057
ATOM 546 HG22VAL 36 22.060 5.717 -7.591
ATOM 547 HG23VAL 36 21.037 4.859 -6.644
ATOM 548 C VAL 36 25.214 3.438 -6.957
ATOM 549 O VAL 36 26.249 4.013 -7.236
ATOM 550 N GLY 37 25.158 2.306 -6.294
ATOM 551 HN GLY 37 24.269 1.896 -6.094
ATOM 552 CA GLY 37 26.408 1.629 -5.836
ATOM 553 HA1 GLY 37 26.139 0.722 -5.508
ATOM 554 HA2 GLY 37 26.867 2.262 -5.213
ATOM 555 C GLY 37 27.360 1.405 -7.017
ATOM 556 O GLY 37 28.502 1.823 -6.983
ATOM 557 N GLY 38 26.850 0.747 -8.030
ATOM 558 HN GLY 38 25.902 0.436 -7.980
ATOM 559 CA GLY 38 27.653 0.453 -9.258
ATOM 560 HA1 GLY 38 28.340 1.177 -9.335
ATOM 561 HA2 GLY 38 27.000 0.314 -10.003
ATOM 562 C GLY 38 28.414 -0.862 -9.084
ATOM 563 O GLY 38 28.618 -1.601 -10.028
ATOM 564 N VAL 39 28.808 -1.096 -7.857
ATOM 565 HN VAL 39 28.593 -0.422 -7.152
ATOM 566 CA VAL 39 29.562 -2.320 -7.470
ATOM 567 HA VAL 39 29.676 -2.951 -8.238
ATOM 568 CB VAL 39 30.988 -1.903 -6.978
ATOM 569 HB VAL 39 30.905 -1.547 -6.047

ATOM 570 CG1 VAL 39 31.931 -3.129 -6.999
ATOM 571 HG11VAL 39 32.561 -3.069 -6.225
ATOM 572 HG12VAL 39 31.383 -3.963 -6.929
ATOM 573 HG13VAL 39 32.445 -3.130 -7.857
ATOM 574 CG2 VAL 39 31.582 -0.811 -7.902
ATOM 575 HG21VAL 39 31.670 0.041 -7.385
ATOM 576 HG22VAL 39 32.481 -1.109 -8.223
ATOM 577 HG23VAL 39 30.970 -0.675 -8.681
ATOM 578 C VAL 39 28.759 -3.000 -6.348
ATOM 579 O VAL 39 29.294 -3.697 -5.506
ATOM 580 N VAL 40 27.471 -2.757 -6.390
ATOM 581 HN VAL 40 27.117 -2.175 -7.118
ATOM 582 CA VAL 40 26.517 -3.320 -5.391
ATOM 583 HA VAL 40 26.936 -4.068 -4.875
ATOM 584 CB VAL 40 26.105 -2.201 -4.385
ATOM 585 HB VAL 40 25.559 -1.520 -4.873
ATOM 586 CG1 VAL 40 25.281 -2.813 -3.231
ATOM 587 HG11VAL 40 25.220 -2.149 -2.486
ATOM 588 HG12VAL 40 24.365 -3.034 -3.566
ATOM 589 HG13VAL 40 25.736 -3.644 -2.911
ATOM 590 CG2 VAL 40 27.362 -1.522 -3.792
ATOM 591 HG21VAL 40 27.076 -0.817 -3.143
ATOM 592 HG22VAL 40 27.915 -2.212 -3.325
ATOM 593 HG23VAL 40 27.889 -1.108 -4.534
ATOM 594 C VAL 40 25.286 -3.837 -6.157
ATOM 595 O VAL 40 24.953 -4.988 -5.929
ATOM 596 NA NA 41 -2.351 20.713 -11.483
ATOM 597 NA NA 42 3.649 4.713 -0.483
ATOM 598 NA NA 43 -7.351 17.713 -12.483

Final MD structure (after 10 ns relaxation) of the tenth NMR isoform with 3 Na^+ counterions

ATOM 1 N ASP 1 3.793 23.039 -9.572
ATOM 2 HN ASP 1 3.580 22.096 -9.438
ATOM 3 CA ASP 1 2.637 23.892 -9.165
ATOM 4 HA ASP 1 2.967 24.757 -8.764
ATOM 5 CB ASP 1 1.586 24.010 -10.279
ATOM 6 HB1 ASP 1 2.059 24.449 -11.078
ATOM 7 HB2 ASP 1 0.789 24.502 -9.988
ATOM 8 CG ASP 1 1.082 22.616 -10.743
ATOM 9 OD1 ASP 1 1.766 21.799 -11.320
ATOM 10 OD2 ASP 1 -0.139 22.320 -10.595
ATOM 11 C ASP 1 2.006 23.033 -8.131
ATOM 12 O ASP 1 2.638 22.006 -7.865
ATOM 13 N ALA 2 0.922 23.319 -7.471
ATOM 14 HN ALA 2 0.360 24.081 -7.519
ATOM 15 CA ALA 2 0.460 22.349 -6.429
ATOM 16 HA ALA 2 0.671 21.368 -6.771

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ATOM     17  CB  ALA     2       1.000  22.663  -4.984
ATOM     18  HB1 ALA     2       0.786  23.511  -4.654
ATOM     19  HB2 ALA     2       0.542  22.016  -4.423
ATOM     20  HB3 ALA     2       2.024  22.543  -4.851
ATOM     21  C   ALA     2      -1.025  22.504  -6.505
ATOM     22  O   ALA     2      -1.478  23.515  -7.099
ATOM     23  N   GLU     3      -1.849  21.568  -5.942
ATOM     24  HN  GLU     3      -1.480  20.781  -5.493
ATOM     25  CA  GLU     3      -3.282  21.682  -6.001
ATOM     26  HA  GLU     3      -3.538  22.635  -6.235
ATOM     27  CB  GLU     3      -3.861  20.707  -6.916
ATOM     28  HB1 GLU     3      -3.554  19.753  -6.781
ATOM     29  HB2 GLU     3      -3.564  20.901  -7.811
ATOM     30  CG  GLU     3      -5.382  20.711  -7.143
ATOM     31  HG1 GLU     3      -5.700  21.604  -7.526
ATOM     32  HG2 GLU     3      -5.815  20.482  -6.321
ATOM     33  CD  GLU     3      -5.704  19.677  -8.223
ATOM     34  OE1 GLU     3      -6.759  19.128  -8.261
ATOM     35  OE2 GLU     3      -5.007  19.461  -9.191
ATOM     36  C   GLU     3      -3.493  21.324  -4.553
ATOM     37  O   GLU     3      -2.466  21.288  -3.846
ATOM     38  N   PHE     4      -4.720  21.037  -3.952
ATOM     39  HN  PHE     4      -5.591  21.036  -4.311
ATOM     40  CA  PHE     4      -4.691  20.746  -2.536
ATOM     41  HA  PHE     4      -3.844  21.114  -2.216
ATOM     42  CB  PHE     4      -5.729  21.283  -1.597
ATOM     43  HCB1PHE     4      -5.398  21.043  -0.632
ATOM     44  HCB2PHE     4      -6.604  20.864  -1.828
ATOM     45  CG  PHE     4      -5.860  22.802  -1.619
ATOM     46  CD1 PHE     4      -4.729  23.725  -1.790
ATOM     47  HCD1PHE     4      -3.839  23.310  -1.865
ATOM     48  CE1 PHE     4      -4.935  25.120  -1.738
ATOM     49  HCE1PHE     4      -4.156  25.723  -1.810
ATOM     50  CZ  PHE     4      -6.305  25.670  -1.567
ATOM     51  HCZ PHE     4      -6.448  26.623  -1.513
ATOM     52  CE2 PHE     4      -7.443  24.755  -1.443
ATOM     53  HCE2PHE     4      -8.386  25.157  -1.355
ATOM     54  CD2 PHE     4      -7.215  23.328  -1.449
ATOM     55  HCD2PHE     4      -8.049  22.780  -1.374
ATOM     56  C   PHE     4      -4.804  19.263  -2.378
ATOM     57  O   PHE     4      -3.839  18.659  -2.770
ATOM     58  N   ARG     5      -5.831  18.599  -1.822
ATOM     59  HN  ARG     5      -6.638  19.056  -1.518
ATOM     60  CA  ARG     5      -5.757  17.194  -1.705
ATOM     61  HA  ARG     5      -4.787  16.981  -1.544
ATOM     62  CB  ARG     5      -6.766  16.709  -0.667
ATOM     63  HB1 ARG     5      -7.712  16.978  -1.010
ATOM     64  HB2 ARG     5      -6.547  17.170   0.114
ATOM     65  CG  ARG     5      -6.656  15.201  -0.395
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ATOM     66  HG1 ARG     5      -6.819  14.569  -1.205
ATOM     67  HG2 ARG     5      -7.350  14.924   0.265
ATOM     68  CD  ARG     5      -5.267  15.003   0.239
ATOM     69  HD1 ARG     5      -5.169  15.686   0.964
ATOM     70  HD2 ARG     5      -4.608  15.222  -0.434
ATOM     71  NE  ARG     5      -5.156  13.704   0.808
ATOM     72  HE  ARG     5      -5.705  12.973   0.383
ATOM     73  CZ  ARG     5      -4.291  13.577   1.854
ATOM     74  NH1 ARG     5      -3.689  14.711   2.258
ATOM     75  HH11ARG     5      -3.012  14.706   3.049
ATOM     76  HH12ARG     5      -3.813  15.613   1.883
ATOM     77  NH2 ARG     5      -4.095  12.336   2.501
ATOM     78  HH21ARG     5      -3.511  12.255   3.270
ATOM     79  HH22ARG     5      -4.464  11.475   2.255
ATOM     80  C   ARG     5      -6.387  16.569  -2.909
ATOM     81  O   ARG     5      -7.539  16.934  -3.097
ATOM     82  N   HIE     6      -5.763  15.753  -3.708
ATOM     83  HN  HIE     6      -4.792  15.392  -3.666
ATOM     84  CA  HIE     6      -6.428  15.158  -4.902
ATOM     85  HA  HIE     6      -7.150  14.621  -4.577
ATOM     86  CB  HIE     6      -6.770  16.049  -6.124
ATOM     87  HB1 HIE     6      -5.979  16.522  -6.374
ATOM     88  HB2 HIE     6      -7.438  16.685  -5.845
ATOM     89  CG  HIE     6      -7.382  15.319  -7.341
ATOM     90  ND1 HIE     6      -6.850  15.146  -8.559
ATOM     91  HE2 HIE     6      -9.803  13.875  -8.962
ATOM     92  CE1 HIE     6      -7.784  14.503  -9.311
ATOM     93  HE1 HIE     6      -7.585  14.256 -10.264
ATOM     94  NE2 HIE     6      -8.951  14.289  -8.675
ATOM     95  CD2 HIE     6      -8.746  14.819  -7.457
ATOM     96  HD2 HIE     6      -9.407  14.768  -6.789
ATOM     97  C   HIE     6      -5.165  14.396  -5.273
ATOM     98  O   HIE     6      -4.720  13.631  -4.398
ATOM     99  N   ASP     7      -4.582  14.650  -6.487
ATOM    100  HN  ASP     7      -4.935  15.292  -7.074
ATOM    101  CA  ASP     7      -3.369  14.023  -7.051
ATOM    102  HA  ASP     7      -3.429  13.022  -6.921
ATOM    103  CB  ASP     7      -3.222  14.337  -8.558
ATOM    104  HB1 ASP     7      -4.024  14.005  -9.048
ATOM    105  HB2 ASP     7      -2.364  13.944  -8.896
ATOM    106  CG  ASP     7      -3.206  15.756  -8.805
ATOM    107  OD1 ASP     7      -2.442  16.258  -9.652
ATOM    108  OD2 ASP     7      -4.083  16.525  -8.426
ATOM    109  C   ASP     7      -2.157  14.499  -6.348
ATOM    110  O   ASP     7      -1.088  13.855  -6.447
ATOM    111  N   SER     8      -2.228  15.596  -5.624
ATOM    112  HN  SER     8      -3.016  16.163  -5.521
ATOM    113  CA  SER     8      -1.117  16.031  -4.837
ATOM    114  HA  SER     8      -0.320  15.492  -4.925
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ATOM 115 CB SER 8 -0.826 17.552 -5.065
ATOM 116 HB1 SER 8 -0.405 17.611 -5.995
ATOM 117 HB2 SER 8 -0.142 17.962 -4.444
ATOM 118 OG SER 8 -2.033 18.331 -5.096
ATOM 119 HG SER 8 -2.335 18.520 -4.079
ATOM 120 C SER 8 -1.610 15.725 -3.478
ATOM 121 O SER 8 -2.823 15.700 -3.452
ATOM 122 N GLY 9 -0.870 15.494 -2.408
ATOM 123 HN GLY 9 0.111 15.528 -2.421
ATOM 124 CA GLY 9 -1.547 15.275 -1.136
ATOM 125 HA1 GLY 9 -2.351 15.892 -1.050
ATOM 126 HA2 GLY 9 -0.850 15.524 -0.458
ATOM 127 C GLY 9 -1.850 13.783 -1.071
ATOM 128 O GLY 9 -1.624 13.182 0.011
ATOM 129 N TYR 10 -2.457 13.140 -2.068
ATOM 130 HN TYR 10 -2.684 13.557 -2.916
ATOM 131 CA TYR 10 -2.792 11.723 -1.927
ATOM 132 HA TYR 10 -2.404 11.317 -1.122
ATOM 133 CB TYR 10 -4.355 11.510 -1.968
ATOM 134 HCB1TYR 10 -4.687 11.806 -2.823
ATOM 135 HCB2TYR 10 -4.812 12.174 -1.342
ATOM 136 CG TYR 10 -4.858 10.100 -1.640
ATOM 137 CD1 TYR 10 -4.145 9.227 -0.704
ATOM 138 HCD1TYR 10 -3.257 9.649 -0.278
ATOM 139 CE1 TYR 10 -4.757 7.899 -0.387
ATOM 140 HCE1TYR 10 -4.291 7.284 0.282
ATOM 141 CZ TYR 10 -6.008 7.424 -0.967
ATOM 142 OH TYR 10 -6.564 6.277 -0.696
ATOM 143 HOH TYR 10 -6.178 5.792 0.124
ATOM 144 CE2 TYR 10 -6.677 8.302 -1.896
ATOM 145 HCE2TYR 10 -7.509 7.993 -2.331
ATOM 146 CD2 TYR 10 -6.078 9.605 -2.189
ATOM 147 HCD2TYR 10 -6.567 10.151 -2.859
ATOM 148 C TYR 10 -2.052 11.285 -3.086
ATOM 149 O TYR 10 -1.714 12.154 -3.868
ATOM 150 N GLU 11 -1.719 9.997 -3.273
ATOM 151 HN GLU 11 -1.955 9.254 -2.633
ATOM 152 CA GLU 11 -0.899 9.727 -4.444
ATOM 153 HA GLU 11 -0.584 10.552 -4.853
ATOM 154 CB GLU 11 0.497 9.256 -3.907
ATOM 155 HB1 GLU 11 0.448 8.415 -3.404
ATOM 156 HB2 GLU 11 0.771 9.907 -3.228
ATOM 157 CG GLU 11 1.687 9.141 -4.918
ATOM 158 HG1 GLU 11 2.508 9.013 -4.408
ATOM 159 HG2 GLU 11 1.755 9.930 -5.511
ATOM 160 CD GLU 11 1.620 7.961 -5.851
ATOM 161 OE1 GLU 11 1.832 6.863 -5.427
ATOM 162 OE2 GLU 11 1.474 8.086 -7.053
ATOM 163 C GLU 11 -1.626 8.855 -5.469

ATOM 164 O GLU 11 -1.687 9.115 -6.712
ATOM 165 N VAL 12 -2.286 7.743 -5.067
ATOM 166 HN VAL 12 -2.365 7.371 -4.148
ATOM 167 CA VAL 12 -2.907 6.996 -6.058
ATOM 168 HA VAL 12 -2.921 7.406 -6.982
ATOM 169 CB VAL 12 -2.415 5.526 -6.117
ATOM 170 HB VAL 12 -3.036 5.063 -6.776
ATOM 171 CG1 VAL 12 -0.945 5.388 -6.544
ATOM 172 HG11VAL 12 -0.340 5.739 -5.856
ATOM 173 HG12VAL 12 -0.706 4.459 -6.705
ATOM 174 HG13VAL 12 -0.776 5.943 -7.319
ATOM 175 CG2 VAL 12 -2.391 4.783 -4.812
ATOM 176 HG21VAL 12 -1.796 5.222 -4.133
ATOM 177 HG22VAL 12 -3.296 4.858 -4.366
ATOM 178 HG23VAL 12 -2.233 3.830 -4.952
ATOM 179 C VAL 12 -4.257 7.078 -5.495
ATOM 180 O VAL 12 -4.360 7.366 -4.292
ATOM 181 N HIS 13 -5.306 6.945 -6.289
ATOM 182 HN HIS 13 -5.093 6.722 -7.216
ATOM 183 CA HIS 13 -6.622 7.127 -5.818
ATOM 184 HA HIS 13 -6.540 7.391 -4.818
ATOM 185 CB HIS 13 -7.600 7.962 -6.682
ATOM 186 HB1 HIS 13 -8.541 7.977 -6.160
ATOM 187 HB2 HIS 13 -7.609 7.556 -7.627
ATOM 188 CG HIS 13 -7.160 9.387 -6.785
ATOM 189 ND1 HIS 13 -7.325 10.125 -7.870
ATOM 190 HD1 HIS 13 -7.750 9.851 -8.699
ATOM 191 CE1 HIS 13 -6.786 11.334 -7.608
ATOM 192 HE1 HIS 13 -6.811 12.019 -8.378
ATOM 193 NE2 HIS 13 -6.285 11.403 -6.406
ATOM 194 CD2 HIS 13 -6.486 10.193 -5.818
ATOM 195 HD2 HIS 13 -6.209 9.862 -4.897
ATOM 196 C HIS 13 -7.305 5.802 -5.782
ATOM 197 O HIS 13 -8.533 5.845 -5.889
ATOM 198 N HIS 14 -6.670 4.650 -5.665
ATOM 199 HN HIS 14 -5.677 4.532 -5.547
ATOM 200 CA HIS 14 -7.506 3.450 -5.635
ATOM 201 HA HIS 14 -8.445 3.620 -5.270
ATOM 202 CB HIS 14 -7.532 2.681 -6.985
ATOM 203 HB1 HIS 14 -7.977 1.758 -6.842
ATOM 204 HB2 HIS 14 -6.624 2.578 -7.296
ATOM 205 CG HIS 14 -8.399 3.370 -8.029
ATOM 206 ND1 HIS 14 -8.096 4.329 -8.851
ATOM 207 HD1 HIS 14 -7.213 4.743 -8.850
ATOM 208 CE1 HIS 14 -9.122 4.704 -9.629
ATOM 209 HE1 HIS 14 -9.104 5.438 -10.238
ATOM 210 NE2 HIS 14 -10.224 3.929 -9.334
ATOM 211 CD2 HIS 14 -9.787 3.083 -8.356
ATOM 212 HD2 HIS 14 -10.351 2.361 -7.951

ATOM 213 C HIS 14 -6.819 2.718 -4.550
ATOM 214 O HIS 14 -5.572 2.825 -4.530
ATOM 215 N GLN 15 -7.377 1.906 -3.640
ATOM 216 HN GLN 15 -8.344 1.784 -3.608
ATOM 217 CA GLN 15 -6.502 1.292 -2.671
ATOM 218 HA GLN 15 -5.877 2.051 -2.303
ATOM 219 CB GLN 15 -7.294 0.619 -1.494
ATOM 220 HB1 GLN 15 -7.883 -0.140 -1.899
ATOM 221 HB2 GLN 15 -7.818 1.349 -1.070
ATOM 222 CG GLN 15 -6.470 -0.075 -0.315
ATOM 223 HG1 GLN 15 -5.887 0.577 0.140
ATOM 224 HG2 GLN 15 -5.954 -0.797 -0.764
ATOM 225 CD GLN 15 -7.421 -0.550 0.764
ATOM 226 OE1 GLN 15 -7.003 -0.631 1.944
ATOM 227 NE2 GLN 15 -8.704 -0.906 0.451
ATOM 228 HE21GLN 15 -9.366 -1.247 1.096
ATOM 229 HE22GLN 15 -9.065 -0.843 -0.482
ATOM 230 C GLN 15 -5.730 0.159 -3.328
ATOM 231 O GLN 15 -4.672 -0.143 -2.903
ATOM 232 N LYS 16 -6.111 -0.479 -4.468
ATOM 233 HN LYS 16 -6.937 -0.220 -4.901
ATOM 234 CA LYS 16 -5.326 -1.598 -4.928
ATOM 235 HA1 LYS 16 -4.937 -2.037 -4.066
ATOM 236 CB LYS 16 -6.145 -2.637 -5.747
ATOM 237 HB1 LYS 16 -6.565 -2.166 -6.555
ATOM 238 HB2 LYS 16 -6.938 -2.934 -5.175
ATOM 239 CG LYS 16 -5.499 -3.961 -6.262
ATOM 240 HG1 LYS 16 -4.791 -3.764 -7.017
ATOM 241 HG2 LYS 16 -6.244 -4.418 -6.669
ATOM 242 CD LYS 16 -4.984 -4.809 -5.118
ATOM 243 HD1 LYS 16 -5.661 -5.018 -4.391
ATOM 244 HD2 LYS 16 -4.197 -4.313 -4.655
ATOM 245 CE LYS 16 -4.419 -6.116 -5.787
ATOM 246 HE1 LYS 16 -3.944 -6.687 -5.133
ATOM 247 HE2 LYS 16 -3.770 -5.847 -6.506
ATOM 248 NZ LYS 16 -5.492 -6.854 -6.449
ATOM 249 HZ1 LYS 16 -6.067 -6.312 -7.047
ATOM 250 HZ2 LYS 16 -5.093 -7.607 -6.970
ATOM 251 HZ3 LYS 16 -6.055 -7.274 -5.732
ATOM 252 C LYS 16 -4.160 -0.937 -5.687
ATOM 253 O LYS 16 -3.104 -1.534 -5.981
ATOM 254 N LEU 17 -4.243 0.357 -5.899
ATOM 255 HN LEU 17 -5.058 0.864 -5.665
ATOM 256 CA LEU 17 -3.146 0.961 -6.509
ATOM 257 HA LEU 17 -2.759 0.269 -7.185
ATOM 258 CB LEU 17 -3.352 2.243 -7.290
ATOM 259 HB1 LEU 17 -2.453 2.545 -7.551
ATOM 260 HB2 LEU 17 -3.822 2.918 -6.638
ATOM 261 CG LEU 17 -4.054 2.201 -8.605

ATOM 262 HG LEU 17 -4.980 1.915 -8.361
ATOM 263 CD1 LEU 17 -4.077 3.583 -9.308
ATOM 264 HD11LEU 17 -4.355 4.258 -8.630
ATOM 265 HD12LEU 17 -3.180 3.864 -9.594
ATOM 266 HD13LEU 17 -4.707 3.570 -10.089
ATOM 267 CD2 LEU 17 -3.494 1.055 -9.499
ATOM 268 HD21LEU 17 -2.575 1.287 -9.848
ATOM 269 HD22LEU 17 -3.567 0.174 -9.020
ATOM 270 HD23LEU 17 -4.048 1.002 -10.320
ATOM 271 C LEU 17 -2.238 1.265 -5.387
ATOM 272 O LEU 17 -1.072 1.453 -5.694
ATOM 273 N VAL 18 -2.523 1.317 -4.122
ATOM 274 HN VAL 18 -3.434 1.172 -3.764
ATOM 275 CA VAL 18 -1.443 1.535 -3.140
ATOM 276 HA VAL 18 -0.971 2.435 -3.300
ATOM 277 CB VAL 18 -2.295 1.616 -1.861
ATOM 278 HB VAL 18 -2.815 0.795 -1.869
ATOM 279 CG1 VAL 18 -1.557 1.649 -0.506
ATOM 280 HG11VAL 18 -2.239 1.520 0.201
ATOM 281 HG12VAL 18 -0.920 0.852 -0.497
ATOM 282 HG13VAL 18 -1.050 2.549 -0.329
ATOM 283 CG2 VAL 18 -3.251 2.833 -2.025
ATOM 284 HG21VAL 18 -3.859 2.768 -1.230
ATOM 285 HG22VAL 18 -2.782 3.701 -2.050
ATOM 286 HG23VAL 18 -3.770 2.755 -2.802
ATOM 287 C VAL 18 -0.518 0.307 -3.052
ATOM 288 O VAL 18 0.674 0.421 -2.708
ATOM 289 N PHE 19 -1.044 -0.881 -3.388
ATOM 290 HN PHE 19 -1.995 -1.002 -3.647
ATOM 291 CA PHE 19 -0.143 -2.043 -3.374
ATOM 292 HA PHE 19 0.460 -1.933 -2.599
ATOM 293 CB PHE 19 -0.753 -3.409 -3.238
ATOM 294 HCB1PHE 19 0.001 -4.066 -3.176
ATOM 295 HCB2PHE 19 -1.312 -3.694 -4.033
ATOM 296 CG PHE 19 -1.594 -3.478 -1.973
ATOM 297 CD1 PHE 19 -3.061 -3.198 -1.977
ATOM 298 HCD1PHE 19 -3.583 -2.951 -2.777
ATOM 299 CE1 PHE 19 -3.813 -3.277 -0.744
ATOM 300 HCE1PHE 19 -4.785 -3.105 -0.733
ATOM 301 CZ PHE 19 -3.090 -3.699 0.457
ATOM 302 HCZ PHE 19 -3.552 -3.740 1.375
ATOM 303 CE2 PHE 19 -1.671 -3.976 0.466
ATOM 304 HCE2PHE 19 -1.192 -4.230 1.312
ATOM 305 CD2 PHE 19 -0.912 -3.872 -0.732
ATOM 306 HCD2PHE 19 0.017 -4.068 -0.725
ATOM 307 C PHE 19 0.585 -2.033 -4.675
ATOM 308 O PHE 19 1.467 -2.760 -4.937
ATOM 309 N PHE 20 0.157 -1.216 -5.638
ATOM 310 HN PHE 20 -0.590 -0.554 -5.570

ATOM 311 CA PHE 20 0.819 -1.257 -6.899
ATOM 312 HA PHE 20 1.170 -2.173 -7.159
ATOM 313 CB PHE 20 -0.109 -0.740 -8.054
ATOM 314 HCB1PHE 20 -0.537 0.160 -7.835
ATOM 315 HCB2PHE 20 -0.831 -1.432 -8.168
ATOM 316 CG PHE 20 0.675 -0.780 -9.338
ATOM 317 CD1 PHE 20 1.199 -2.068 -9.848
ATOM 318 HCD1PHE 20 1.022 -2.950 -9.373
ATOM 319 CE1 PHE 20 1.939 -2.123 -11.094
ATOM 320 HCE1PHE 20 2.236 -3.000 -11.419
ATOM 321 CZ PHE 20 2.205 -0.933 -11.862
ATOM 322 HCZ PHE 20 2.688 -0.911 -12.712
ATOM 323 CE2 PHE 20 1.717 0.363 -11.345
ATOM 324 HCE2PHE 20 1.934 1.180 -11.866
ATOM 325 CD2 PHE 20 0.948 0.420 -10.113
ATOM 326 HCD2PHE 20 0.597 1.230 -9.762
ATOM 327 C PHE 20 1.954 -0.278 -6.738
ATOM 328 O PHE 20 3.111 -0.634 -7.011
ATOM 329 N ALA 21 1.713 0.961 -6.304
ATOM 330 HN ALA 21 0.756 1.190 -6.064
ATOM 331 CA ALA 21 2.831 1.955 -6.146
ATOM 332 HA ALA 21 3.264 1.941 -7.035
ATOM 333 CB ALA 21 2.428 3.367 -5.749
ATOM 334 HB1 ALA 21 3.269 3.935 -5.653
ATOM 335 HB2 ALA 21 1.835 3.783 -6.417
ATOM 336 HB3 ALA 21 1.987 3.337 -4.884
ATOM 337 C ALA 21 3.849 1.508 -5.102
ATOM 338 O ALA 21 5.055 1.742 -5.326
ATOM 339 N GLU 22 3.475 0.960 -3.953
ATOM 340 HN GLU 22 2.520 0.734 -3.742
ATOM 341 CA GLU 22 4.535 0.600 -2.969
ATOM 342 HA GLU 22 5.281 1.270 -3.094
ATOM 343 CB GLU 22 4.138 0.628 -1.466
ATOM 344 HB1 GLU 22 4.869 0.196 -0.896
ATOM 345 HB2 GLU 22 3.274 0.122 -1.273
ATOM 346 CG GLU 22 4.047 2.140 -0.938
ATOM 347 HG1 GLU 22 4.932 2.520 -1.059
ATOM 348 HG2 GLU 22 3.787 2.138 0.096
ATOM 349 CD GLU 22 3.154 3.148 -1.661
ATOM 350 OE1 GLU 22 1.935 2.983 -1.775
ATOM 351 OE2 GLU 22 3.618 4.233 -2.062
ATOM 352 C GLU 22 5.078 -0.666 -3.496
ATOM 353 O GLU 22 6.211 -0.908 -3.122
ATOM 354 N ASP 23 4.491 -1.522 -4.351
ATOM 355 HN ASP 23 3.604 -1.387 -4.697
ATOM 356 CA ASP 23 5.279 -2.714 -4.725
ATOM 357 HA ASP 23 5.839 -3.114 -3.927
ATOM 358 CB ASP 23 4.471 -3.846 -5.329
ATOM 359 HB1 ASP 23 3.931 -3.477 -6.043

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ATOM    360  HB2 ASP    23       3.910  -4.234  -4.661
ATOM    361  CG  ASP    23       5.407  -4.902  -5.885
ATOM    362  OD1 ASP    23       6.172  -5.556  -5.211
ATOM    363  OD2 ASP    23       5.504  -5.099  -7.090
ATOM    364  C   ASP    23       6.315  -2.238  -5.673
ATOM    365  O   ASP    23       7.475  -2.609  -5.513
ATOM    366  N   VAL    24       5.977  -1.360  -6.689
ATOM    367  HN  VAL    24       5.050  -1.086  -6.788
ATOM    368  CA  VAL    24       6.893  -0.860  -7.633
ATOM    369  HA  VAL    24       7.318  -1.669  -7.983
ATOM    370  CB  VAL    24       6.251  -0.130  -8.853
ATOM    371  HB  VAL    24       5.826   0.714  -8.542
ATOM    372  CG1 VAL    24       7.234   0.194 -10.021
ATOM    373  HG11VAL    24       7.907   0.865  -9.682
ATOM    374  HG12VAL    24       7.750  -0.620 -10.294
ATOM    375  HG13VAL    24       6.664   0.550 -10.783
ATOM    376  CG2 VAL    24       5.248  -1.061  -9.498
ATOM    377  HG21VAL    24       4.948  -0.565 -10.302
ATOM    378  HG22VAL    24       5.701  -1.959  -9.704
ATOM    379  HG23VAL    24       4.555  -1.179  -8.822
ATOM    380  C   VAL    24       7.935  -0.017  -6.938
ATOM    381  O   VAL    24       9.061  -0.028  -7.355
ATOM    382  N   GLY    25       7.641   0.779  -5.895
ATOM    383  HN  GLY    25       6.722   0.815  -5.460
ATOM    384  CA  GLY    25       8.696   1.593  -5.268
ATOM    385  HA1 GLY    25       8.360   2.293  -4.672
ATOM    386  HA2 GLY    25       9.244   1.983  -6.016
ATOM    387  C   GLY    25       9.607   0.646  -4.505
ATOM    388  O   GLY    25      10.806   0.812  -4.715
ATOM    389  N   SER    26       9.119  -0.359  -3.790
ATOM    390  HN  SER    26       8.135  -0.532  -3.662
ATOM    391  CA  SER    26      10.069  -1.195  -3.081
ATOM    392  HA  SER    26      10.612  -0.561  -2.579
ATOM    393  CB  SER    26       9.290  -2.177  -2.145
ATOM    394  HB1 SER    26       9.984  -2.676  -1.627
ATOM    395  HB2 SER    26       8.698  -2.817  -2.641
ATOM    396  OG  SER    26       8.375  -1.401  -1.352
ATOM    397  HG  SER    26       7.412  -1.327  -1.762
ATOM    398  C   SER    26      10.850  -2.009  -3.971
ATOM    399  O   SER    26      12.017  -2.240  -3.648
ATOM    400  N   ASN    27      10.410  -2.476  -5.156
ATOM    401  HN  ASN    27       9.439  -2.344  -5.405
ATOM    402  CA  ASN    27      11.347  -3.245  -6.044
ATOM    403  HA  ASN    27      12.028  -3.792  -5.415
ATOM    404  CB  ASN    27      10.792  -4.236  -7.099
ATOM    405  HB1 ASN    27      11.565  -4.720  -7.551
ATOM    406  HB2 ASN    27      10.250  -3.714  -7.755
ATOM    407  CG  ASN    27       9.992  -5.312  -6.380
ATOM    408  OD1 ASN    27      10.560  -6.344  -6.049
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ATOM 409 ND2 ASN 27 8.746 -5.109 -6.135
ATOM 410 HD21ASN 27 8.064 -5.661 -5.708
ATOM 411 HD22ASN 27 8.280 -4.270 -6.415
ATOM 412 C ASN 27 12.155 -2.331 -6.834
ATOM 413 O ASN 27 13.240 -2.770 -7.147
ATOM 414 N LYS 28 11.778 -1.062 -7.167
ATOM 415 HN LYS 28 10.877 -0.592 -6.941
ATOM 416 CA LYS 28 12.706 -0.294 -7.947
ATOM 417 HA1 LYS 28 13.148 -0.962 -8.533
ATOM 418 CB LYS 28 11.912 0.798 -8.828
ATOM 419 HB1 LYS 28 11.389 1.385 -8.213
ATOM 420 HB2 LYS 28 11.256 0.367 -9.448
ATOM 421 CG LYS 28 12.818 1.708 -9.725
ATOM 422 HG1 LYS 28 13.252 1.060 -10.288
ATOM 423 HG2 LYS 28 13.460 2.203 -9.130
ATOM 424 CD LYS 28 12.187 2.781 -10.673
ATOM 425 HD1 LYS 28 11.526 2.331 -11.298
ATOM 426 HD2 LYS 28 12.921 3.146 -11.247
ATOM 427 CE LYS 28 11.573 4.020 -10.028
ATOM 428 HE1 LYS 28 11.411 4.653 -10.727
ATOM 429 HE2 LYS 28 12.230 4.379 -9.418
ATOM 430 NZ LYS 28 10.462 3.761 -9.051
ATOM 431 HZ1 LYS 28 10.283 4.632 -8.654
ATOM 432 HZ2 LYS 28 9.638 3.403 -9.528
ATOM 433 HZ3 LYS 28 10.717 3.133 -8.372
ATOM 434 C LYS 28 13.666 0.281 -6.956
ATOM 435 O LYS 28 14.681 0.843 -7.381
ATOM 436 N GLY 29 13.402 0.352 -5.599
ATOM 437 HN GLY 29 12.601 -0.020 -5.195
ATOM 438 CA GLY 29 14.432 0.998 -4.841
ATOM 439 HA1 GLY 29 14.163 1.194 -3.887
ATOM 440 HA2 GLY 29 14.656 1.855 -5.254
ATOM 441 C GLY 29 15.666 0.146 -4.768
ATOM 442 O GLY 29 16.731 0.631 -4.485
ATOM 443 N ALA 30 15.610 -1.157 -5.184
ATOM 444 HN ALA 30 14.783 -1.619 -5.491
ATOM 445 CA ALA 30 16.834 -1.929 -5.209
ATOM 446 HA ALA 30 17.288 -1.722 -4.330
ATOM 447 CB ALA 30 16.705 -3.440 -5.394
ATOM 448 HB1 ALA 30 16.094 -3.874 -4.693
ATOM 449 HB2 ALA 30 16.336 -3.650 -6.308
ATOM 450 HB3 ALA 30 17.566 -3.875 -5.375
ATOM 451 C ALA 30 17.653 -1.510 -6.377
ATOM 452 O ALA 30 18.868 -1.638 -6.430
ATOM 453 N ILE 31 16.991 -0.997 -7.426
ATOM 454 HN ILE 31 16.007 -0.941 -7.355
ATOM 455 CA ILE 31 17.727 -0.566 -8.584
ATOM 456 HA ILE 31 18.439 -1.199 -8.892
ATOM 457 CB ILE 31 16.763 -0.338 -9.814

ATOM 458 HB ILE 31 16.085 0.389 -9.562
ATOM 459 CG2 ILE 31 17.490 0.009 -11.142
ATOM 460 HG21ILE 31 18.055 0.879 -11.074
ATOM 461 HG22ILE 31 18.156 -0.691 -11.362
ATOM 462 HG23ILE 31 16.822 0.065 -11.901
ATOM 463 CG1 ILE 31 16.046 -1.642 -9.985
ATOM 464 HG11ILE 31 15.468 -1.833 -9.237
ATOM 465 HG12ILE 31 16.732 -2.429 -10.052
ATOM 466 CD1 ILE 31 15.175 -1.705 -11.235
ATOM 467 HD11ILE 31 14.549 -0.971 -11.179
ATOM 468 HD12ILE 31 15.770 -1.559 -12.026
ATOM 469 HD13ILE 31 14.743 -2.592 -11.219
ATOM 470 C ILE 31 18.345 0.789 -8.275
ATOM 471 O ILE 31 19.493 1.119 -8.640
ATOM 472 N ILE 32 17.656 1.662 -7.499
ATOM 473 HN ILE 32 16.739 1.525 -7.163
ATOM 474 CA ILE 32 18.218 2.886 -7.148
ATOM 475 HA ILE 32 18.676 3.252 -8.027
ATOM 476 CB ILE 32 17.103 3.894 -6.758
ATOM 477 HB ILE 32 16.610 3.669 -5.909
ATOM 478 CG2 ILE 32 17.690 5.318 -6.656
ATOM 479 HG21ILE 32 16.994 5.930 -6.399
ATOM 480 HG22ILE 32 18.439 5.344 -5.958
ATOM 481 HG23ILE 32 18.107 5.585 -7.537
ATOM 482 CG1 ILE 32 16.142 3.887 -7.994
ATOM 483 HG11ILE 32 15.721 2.946 -8.074
ATOM 484 HG12ILE 32 16.541 4.125 -8.833
ATOM 485 CD1 ILE 32 15.083 4.960 -7.680
ATOM 486 HD11ILE 32 15.553 5.785 -7.535
ATOM 487 HD12ILE 32 14.426 5.014 -8.406
ATOM 488 HD13ILE 32 14.556 4.773 -6.830
ATOM 489 C ILE 32 19.322 2.609 -6.134
ATOM 490 O ILE 32 20.302 3.329 -6.104
ATOM 491 N GLY 33 19.290 1.588 -5.230
ATOM 492 HN GLY 33 18.596 0.912 -5.164
ATOM 493 CA GLY 33 20.342 1.423 -4.300
ATOM 494 HA1 GLY 33 20.129 0.990 -3.423
ATOM 495 HA2 GLY 33 20.662 2.313 -4.074
ATOM 496 C GLY 33 21.477 0.771 -5.094
ATOM 497 O GLY 33 22.640 1.016 -4.787
ATOM 498 N LEU 34 21.300 -0.033 -6.138
ATOM 499 HN LEU 34 20.372 -0.281 -6.440
ATOM 500 CA LEU 34 22.479 -0.530 -6.758
ATOM 501 HA LEU 34 23.163 -0.749 -6.074
ATOM 502 CB LEU 34 22.315 -1.832 -7.559
ATOM 503 HB1 LEU 34 23.177 -2.099 -7.989
ATOM 504 HB2 LEU 34 21.593 -1.712 -8.268
ATOM 505 CG LEU 34 22.040 -2.946 -6.430
ATOM 506 HG LEU 34 21.130 -2.872 -6.038

ATOM 507 CD1 LEU 34 22.133 -4.275 -7.142
ATOM 508 HD11LEU 34 21.493 -4.321 -7.907
ATOM 509 HD12LEU 34 23.069 -4.405 -7.539
ATOM 510 HD13LEU 34 21.945 -5.000 -6.534
ATOM 511 CD2 LEU 34 23.109 -2.900 -5.298
ATOM 512 HD21LEU 34 23.111 -2.051 -4.726
ATOM 513 HD22LEU 34 22.962 -3.650 -4.682
ATOM 514 HD23LEU 34 24.032 -3.001 -5.621
ATOM 515 C LEU 34 23.058 0.506 -7.667
ATOM 516 O LEU 34 24.263 0.454 -7.940
ATOM 517 N MET 35 22.325 1.561 -8.182
ATOM 518 HN MET 35 21.336 1.634 -8.012
ATOM 519 CA MET 35 23.002 2.572 -9.018
ATOM 520 HA MET 35 23.757 2.121 -9.536
ATOM 521 CB MET 35 22.121 3.278 -9.983
ATOM 522 HB1 MET 35 22.696 3.948 -10.340
ATOM 523 HB2 MET 35 21.429 3.752 -9.444
ATOM 524 CG MET 35 21.517 2.318 -11.087
ATOM 525 HG1 MET 35 20.920 1.585 -10.765
ATOM 526 HG2 MET 35 22.291 1.979 -11.620
ATOM 527 SD MET 35 20.313 3.180 -12.167
ATOM 528 CE MET 35 19.196 3.900 -10.873
ATOM 529 HE1 MET 35 18.583 4.542 -11.387
ATOM 530 HE2 MET 35 18.736 3.039 -10.549
ATOM 531 HE3 MET 35 19.608 4.390 -10.098
ATOM 532 C MET 35 23.650 3.605 -8.092
ATOM 533 O MET 35 24.628 4.161 -8.597
ATOM 534 N VAL 36 23.150 3.809 -6.871
ATOM 535 HN VAL 36 22.348 3.351 -6.527
ATOM 536 CA VAL 36 23.810 4.760 -6.014
ATOM 537 HA VAL 36 24.072 5.475 -6.658
ATOM 538 CB VAL 36 22.885 5.329 -4.950
ATOM 539 HB VAL 36 22.428 4.635 -4.381
ATOM 540 CG1 VAL 36 23.534 6.331 -3.956
ATOM 541 HG11VAL 36 22.870 6.602 -3.330
ATOM 542 HG12VAL 36 24.289 5.868 -3.413
ATOM 543 HG13VAL 36 23.869 7.038 -4.479
ATOM 544 CG2 VAL 36 21.887 6.121 -5.757
ATOM 545 HG21VAL 36 21.247 6.488 -5.121
ATOM 546 HG22VAL 36 22.438 6.859 -6.200
ATOM 547 HG23VAL 36 21.363 5.587 -6.447
ATOM 548 C VAL 36 25.020 3.995 -5.423
ATOM 549 O VAL 36 26.043 4.649 -5.145
ATOM 550 N GLY 37 24.984 2.654 -5.235
ATOM 551 HN GLY 37 24.191 2.111 -5.441
ATOM 552 CA GLY 37 26.179 2.011 -4.707
ATOM 553 HA1 GLY 37 25.884 1.159 -4.328
ATOM 554 HA2 GLY 37 26.628 2.542 -4.010
ATOM 555 C GLY 37 27.178 1.676 -5.788

ATOM 556 O GLY 37 28.335 2.119 -5.691
ATOM 557 N GLY 38 26.879 0.906 -6.866
ATOM 558 HN GLY 38 26.045 0.473 -7.131
ATOM 559 CA GLY 38 27.976 0.656 -7.742
ATOM 560 HA1 GLY 38 28.875 0.919 -7.299
ATOM 561 HA2 GLY 38 27.861 1.118 -8.611
ATOM 562 C GLY 38 27.805 -0.807 -7.780
ATOM 563 O GLY 38 26.615 -1.299 -7.764
ATOM 564 N VAL 39 28.804 -1.669 -7.755
ATOM 565 HN VAL 39 29.756 -1.560 -7.693
ATOM 566 CA VAL 39 28.424 -3.070 -7.829
ATOM 567 HA VAL 39 27.411 -3.283 -7.944
ATOM 568 CB VAL 39 29.279 -3.724 -8.932
ATOM 569 HB VAL 39 30.228 -3.449 -8.734
ATOM 570 CG1 VAL 39 29.180 -5.220 -8.863
ATOM 571 HG11VAL 39 29.787 -5.645 -9.612
ATOM 572 HG12VAL 39 29.482 -5.417 -7.918
ATOM 573 HG13VAL 39 28.212 -5.473 -8.991
ATOM 574 CG2 VAL 39 28.873 -3.212 -10.328
ATOM 575 HG21VAL 39 29.019 -2.239 -10.342
ATOM 576 HG22VAL 39 29.533 -3.684 -10.944
ATOM 577 HG23VAL 39 27.959 -3.445 -10.564
ATOM 578 C VAL 39 28.893 -3.386 -6.497
ATOM 579 O VAL 39 29.887 -2.712 -6.061
ATOM 580 N VAL 40 28.255 -4.205 -5.705
ATOM 581 HN VAL 40 27.422 -4.765 -5.904
ATOM 582 CA VAL 40 28.738 -4.383 -4.349
ATOM 583 HA VAL 40 29.582 -3.872 -4.294
ATOM 584 CB VAL 40 27.736 -3.916 -3.343
ATOM 585 HB VAL 40 26.893 -4.466 -3.496
ATOM 586 CG1 VAL 40 28.245 -3.959 -1.873
ATOM 587 HG11VAL 40 27.482 -3.708 -1.291
ATOM 588 HG12VAL 40 28.552 -4.868 -1.686
ATOM 589 HG13VAL 40 29.012 -3.338 -1.768
ATOM 590 CG2 VAL 40 27.320 -2.471 -3.599
ATOM 591 HG21VAL 40 26.706 -2.170 -2.868
ATOM 592 HG22VAL 40 28.127 -1.933 -3.755
ATOM 593 HG23VAL 40 26.841 -2.379 -4.459
ATOM 594 C VAL 40 28.842 -5.847 -4.271
ATOM 595 O VAL 40 28.291 -6.392 -5.218
ATOM 596 NA NA 41 -2.881 18.414 -9.029
ATOM 597 NA NA 42 2.706 5.783 -3.510
ATOM 598 NA NA 43 -5.774 17.466 -9.719