

Supporting Information

Membrane Interaction of the Factor VIIIa Discoidin Domains in Atomistic Detail

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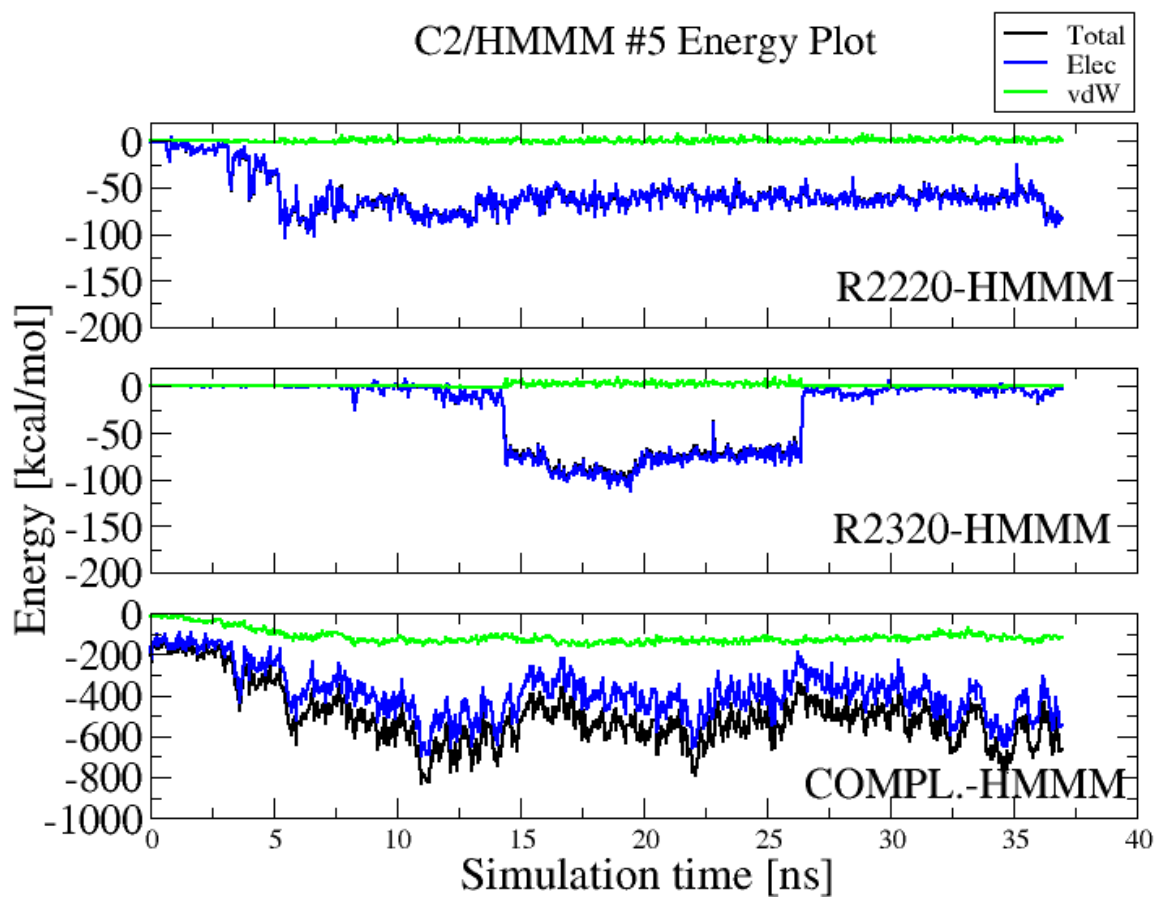


Figure S1: Non-bonded interactions energies between the HMMM membrane and specific portions of FVIII C2 domain: R2220 (*top*), R2320 (*middle*), or the complementary selection (i.e., C2 domain excluding R2220 and R2320; *bottom*) calculated for one of the C2/HMMM trajectory (#5). The energies are decomposed into electrostatic (blue) and van der Waals (green) terms; the total (black) is the sum of the two terms.

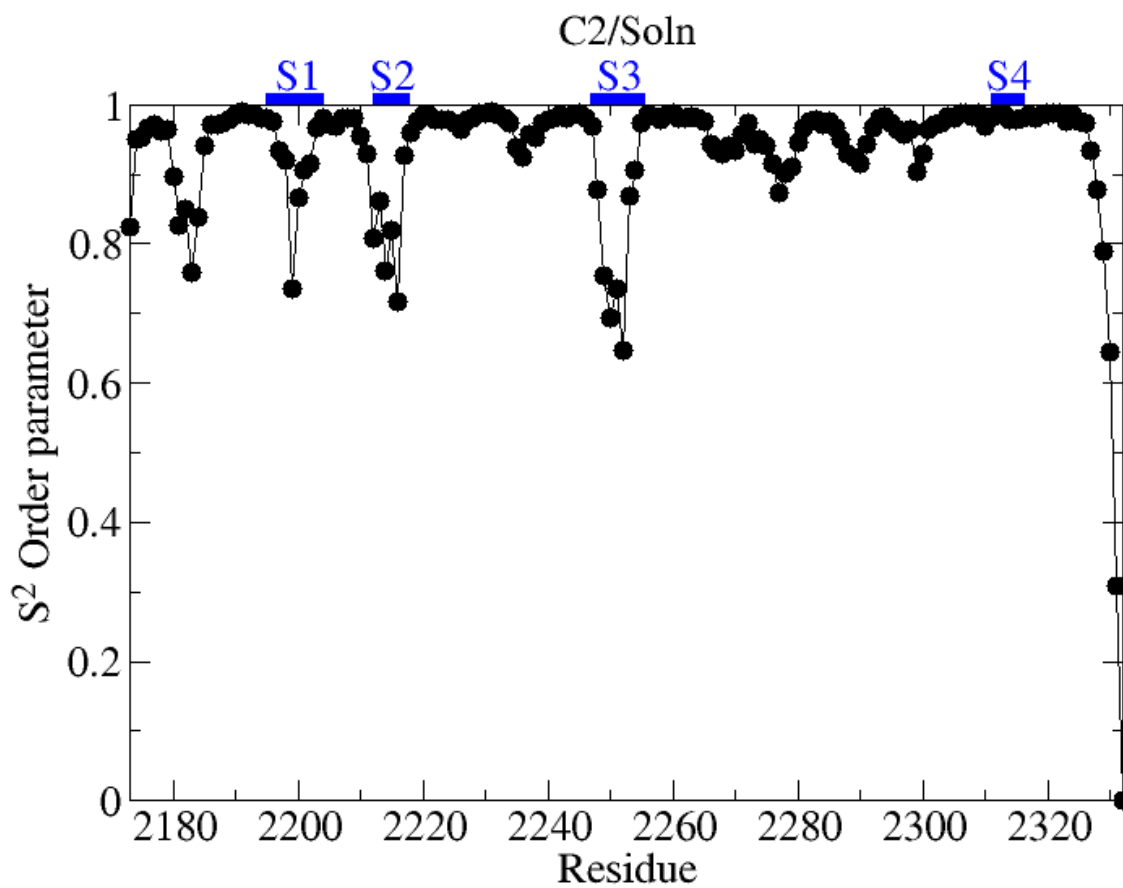


Figure S2: Calculated amide ($C_i - N_i$ vector) S^2 order parameters for human FVIII C2 in bulk water (C2/Soln trajectory).

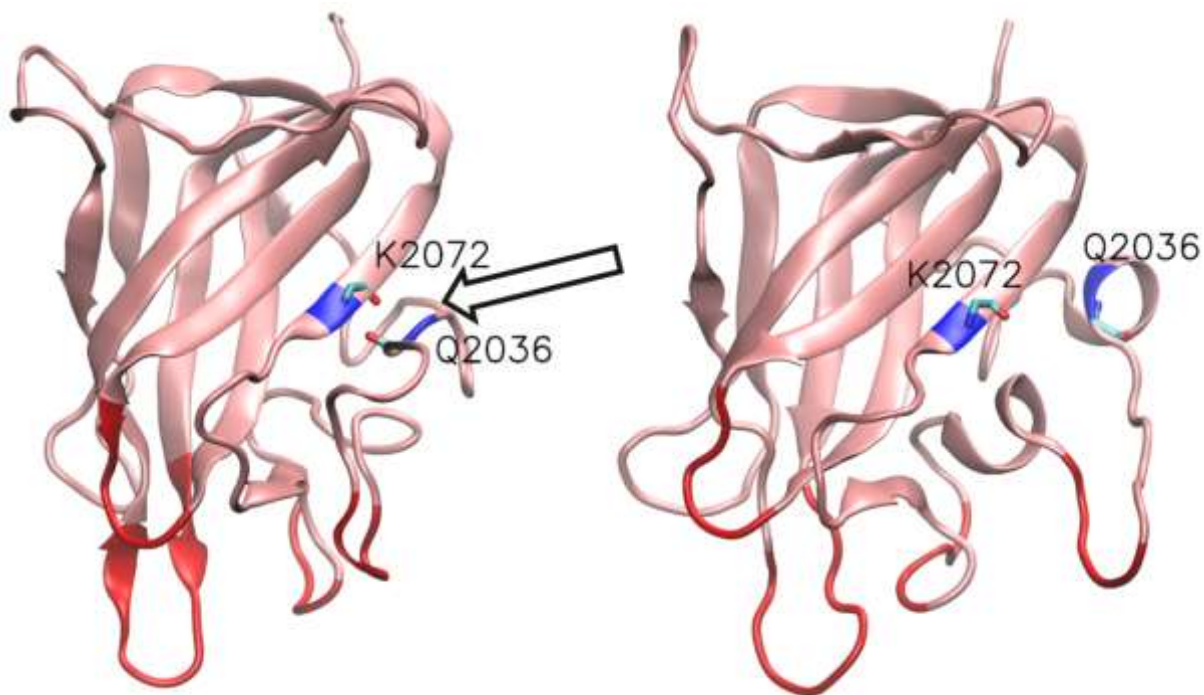


Figure S3: Structural change in FVIII C1 upon the release of the main chain leading to Spike 1 from the body of the β -barrel. The C1 domain is shown in cartoon representation (pink) with the Spikes 1-4 highlighted (red). Positions of residues Q2036 and K2072 which restrain the loopy segment in the X-ray crystallographic structure are indicated in blue and backbone atoms are shown as sticks. (*left*) X-ray crystallographic reference structure. (*right*) Snap-shot taken from C1/HMMM trajectory #2 at $t = \sim 32$ ns.

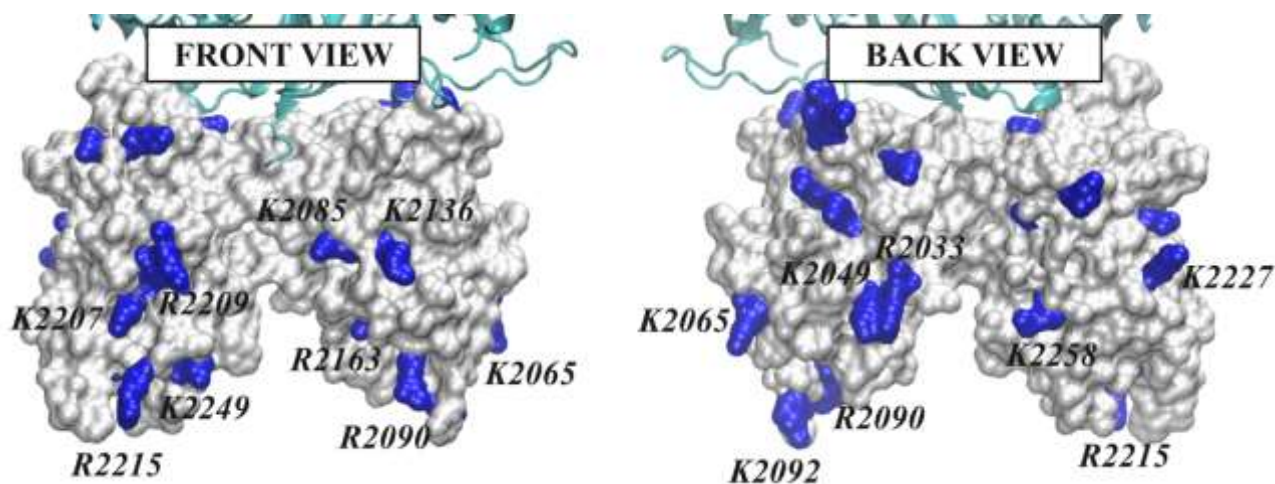
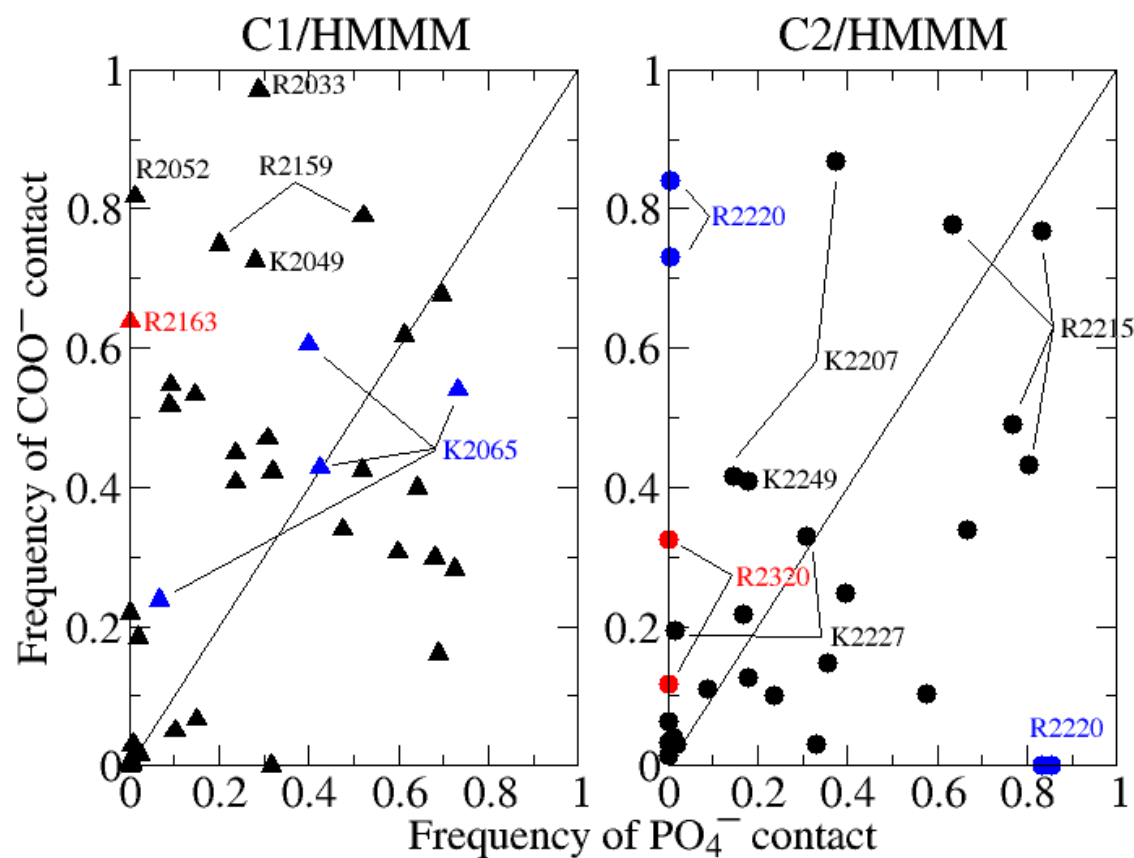


Figure S4: (top) Observed frequency of close interaction (cutoff = 3 Å) between basic residues and negatively charged functional groups (PO_4^- along the x-axis; COO^- along the y-axis) of the PS head groups. Each point in the plot corresponds to the interaction frequency between single residue averaged over a single membrane-binding trajectory of the individual C2-like domains (top left: FVIII C1; top right: FVIII C2.) (bottom) Front and back views of FVIII C1 and C2 shown as surface (PDB ID code 3cdz) with basic residues (K or R) highlighted (blue). Front view corresponds to the orientation of Fig. 6A with FVIII C1 positioned to the right and FVIII C2 to the left.

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Atomic coordinates for the constructed tenase complex model (Fig. 6A, in the manuscript).

C_alpha atom coordinates only.

For complete *.PDB-files, please contact author O.H.O. or J.J.M.

Two containing files are '3cdz_rot_a2_ca.pdb' (below) and 'hum_FIX_ca.pdb' (from p.28)

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File (1 of 2): 3cdz_rot_a2_ca.pdb

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|------|-----|----|-----|---|----|--------|---------|---------|------------|---|---|
| ATOM | 2 | CA | ALA | A | 1 | -0.109 | -50.617 | -13.433 | 1.00204.42 | A | C |
| ATOM | 7 | CA | THR | A | 2 | 3.194 | -51.633 | -11.722 | 1.00203.98 | A | C |
| ATOM | 14 | CA | ARG | A | 3 | 6.520 | -50.614 | -13.422 | 1.00204.23 | A | C |
| ATOM | 25 | CA | ARG | A | 4 | 10.009 | -52.247 | -13.332 | 1.00204.93 | A | C |
| ATOM | 36 | CA | TYR | A | 5 | 13.401 | -50.848 | -14.379 | 1.00205.77 | A | C |
| ATOM | 48 | CA | TYR | A | 6 | 16.078 | -53.579 | -13.954 | 1.00206.04 | A | C |
| ATOM | 60 | CA | LEU | A | 7 | 19.120 | -51.328 | -14.592 | 1.00204.73 | A | C |
| ATOM | 68 | CA | GLY | A | 8 | 22.393 | -51.164 | -12.590 | 1.00202.62 | A | C |
| ATOM | 72 | CA | ALA | A | 9 | 25.297 | -48.663 | -12.610 | 1.00201.79 | A | C |
| ATOM | 77 | CA | VAL | A | 10 | 28.691 | -48.927 | -14.412 | 1.00200.92 | A | C |
| ATOM | 84 | CA | GLU | A | 11 | 32.182 | -47.590 | -15.241 | 1.00200.13 | A | C |
| ATOM | 93 | CA | LEU | A | 12 | 32.562 | -46.111 | -18.749 | 1.00198.09 | A | C |
| ATOM | 101 | CA | SER | A | 13 | 35.137 | -44.184 | -20.817 | 1.00195.94 | A | C |
| ATOM | 107 | CA | TRP | A | 14 | 34.044 | -40.739 | -22.172 | 1.00194.30 | A | C |
| ATOM | 121 | CA | ASP | A | 15 | 34.982 | -37.968 | -24.687 | 1.00193.87 | A | C |
| ATOM | 129 | CA | TYR | A | 16 | 33.597 | -35.013 | -26.745 | 1.00192.63 | A | C |
| ATOM | 141 | CA | VAL | A | 44 | 40.485 | -36.352 | -26.870 | 1.00197.37 | A | C |
| ATOM | 148 | CA | VAL | A | 45 | 40.193 | -35.749 | -23.019 | 1.00197.43 | A | C |
| ATOM | 155 | CA | TYR | A | 46 | 38.632 | -37.451 | -19.832 | 1.00197.01 | A | C |
| ATOM | 167 | CA | LYS | A | 47 | 37.050 | -40.813 | -18.710 | 1.00194.21 | A | C |
| ATOM | 176 | CA | LYS | A | 48 | 34.418 | -41.313 | -15.919 | 1.00193.34 | A | C |
| ATOM | 185 | CA | THR | A | 49 | 31.747 | -43.523 | -14.181 | 1.00194.55 | A | C |
| ATOM | 192 | CA | LEU | A | 50 | 28.242 | -43.436 | -15.709 | 1.00195.23 | A | C |
| ATOM | 200 | CA | PHE | A | 51 | 24.760 | -44.848 | -15.093 | 1.00195.99 | A | C |
| ATOM | 211 | CA | VAL | A | 52 | 23.898 | -47.851 | -17.273 | 1.00197.10 | A | C |
| ATOM | 218 | CA | GLU | A | 53 | 20.798 | -48.889 | -19.074 | 1.00198.63 | A | C |
| ATOM | 227 | CA | PHE | A | 54 | 20.726 | -52.695 | -19.439 | 1.00199.86 | A | C |
| ATOM | 238 | CA | THR | A | 55 | 18.301 | -55.640 | -19.417 | 1.00201.87 | A | C |
| ATOM | 245 | CA | ASP | A | 56 | 20.522 | -57.681 | -17.050 | 1.00205.24 | A | C |
| ATOM | 253 | CA | HIS | A | 57 | 20.349 | -60.559 | -14.824 | 1.00207.70 | A | C |
| ATOM | 263 | CA | LEU | A | 58 | 24.118 | -60.458 | -15.352 | 1.00209.60 | A | C |
| ATOM | 271 | CA | PHE | A | 59 | 26.157 | -57.993 | -17.509 | 1.00211.13 | A | C |
| ATOM | 282 | CA | ASN | A | 60 | 24.717 | -57.852 | -21.099 | 1.00211.61 | A | C |
| ATOM | 290 | CA | ILE | A | 61 | 24.495 | -54.863 | -23.558 | 1.00212.61 | A | C |
| ATOM | 298 | CA | ALA | A | 62 | 21.225 | -52.711 | -23.881 | 1.00213.33 | A | C |
| ATOM | 303 | CA | LYS | A | 63 | 21.061 | -49.213 | -25.352 | 1.00215.58 | A | C |
| ATOM | 312 | CA | PRO | A | 64 | 18.431 | -46.408 | -25.880 | 1.00217.49 | A | C |
| ATOM | 319 | CA | ARG | A | 65 | 21.066 | -43.736 | -25.826 | 1.00218.40 | A | C |
| ATOM | 330 | CA | PRO | A | 66 | 21.868 | -42.709 | -29.441 | 1.00219.19 | A | C |
| ATOM | 337 | CA | PRO | A | 67 | 20.823 | -39.092 | -29.469 | 1.00219.28 | A | C |
| ATOM | 344 | CA | TRP | A | 68 | 20.184 | -36.544 | -26.752 | 1.00219.11 | A | C |
| ATOM | 358 | CA | MET | A | 69 | 20.913 | -39.239 | -24.141 | 1.00218.16 | A | C |
| ATOM | 366 | CA | GLY | A | 70 | 24.423 | -38.333 | -23.011 | 1.00215.30 | A | C |
| ATOM | 370 | CA | LEU | A | 71 | 25.721 | -39.670 | -19.775 | 1.00213.01 | A | C |
| ATOM | 378 | CA | LEU | A | 72 | 22.220 | -40.606 | -18.627 | 1.00211.29 | A | C |

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|------|-----|----|-----|---|-----|--------|---------|---------|------------|---|---|
| ATOM | 386 | CA | GLY | A | 73 | 20.604 | -43.429 | -16.727 | 1.00209.12 | A | C |
| ATOM | 390 | CA | PRO | A | 74 | 17.464 | -44.001 | -18.805 | 1.00207.75 | A | C |
| ATOM | 397 | CA | THR | A | 75 | 14.734 | -41.401 | -18.542 | 1.00206.42 | A | C |
| ATOM | 404 | CA | ILE | A | 76 | 12.363 | -43.327 | -16.242 | 1.00204.58 | A | C |
| ATOM | 412 | CA | GLN | A | 77 | 8.687 | -42.390 | -16.353 | 1.00203.09 | A | C |
| ATOM | 421 | CA | ALA | A | 78 | 5.969 | -43.263 | -13.819 | 1.00201.33 | A | C |
| ATOM | 426 | CA | GLU | A | 79 | 2.377 | -41.990 | -13.556 | 1.00200.28 | A | C |
| ATOM | 435 | CA | VAL | A | 80 | 0.591 | -40.613 | -10.428 | 1.00198.73 | A | C |
| ATOM | 442 | CA | TYR | A | 81 | -0.566 | -43.989 | -9.054 | 1.00197.77 | A | C |
| ATOM | 454 | CA | ASP | A | 82 | 2.330 | -46.294 | -9.935 | 1.00196.72 | A | C |
| ATOM | 462 | CA | THR | A | 83 | 5.148 | -48.192 | -8.252 | 1.00195.15 | A | C |
| ATOM | 469 | CA | VAL | A | 84 | 8.678 | -48.363 | -9.758 | 1.00194.25 | A | C |
| ATOM | 476 | CA | VAL | A | 85 | 11.318 | -51.036 | -9.057 | 1.00194.43 | A | C |
| ATOM | 483 | CA | ILE | A | 86 | 14.900 | -50.173 | -9.943 | 1.00194.90 | A | C |
| ATOM | 491 | CA | THR | A | 87 | 17.347 | -52.937 | -9.012 | 1.00194.64 | A | C |
| ATOM | 498 | CA | LEU | A | 88 | 20.912 | -51.601 | -9.271 | 1.00194.93 | A | C |
| ATOM | 506 | CA | LYS | A | 89 | 23.848 | -53.962 | -10.022 | 1.00194.65 | A | C |
| ATOM | 515 | CA | ASN | A | 90 | 26.979 | -52.038 | -8.988 | 1.00194.09 | A | C |
| ATOM | 523 | CA | MET | A | 91 | 30.220 | -52.344 | -10.912 | 1.00193.81 | A | C |
| ATOM | 531 | CA | ALA | A | 92 | 32.916 | -49.779 | -9.928 | 1.00192.40 | A | C |
| ATOM | 536 | CA | SER | A | 93 | 35.886 | -49.197 | -7.551 | 1.00191.19 | A | C |
| ATOM | 542 | CA | HIS | A | 94 | 33.332 | -46.853 | -6.039 | 1.00190.16 | A | C |
| ATOM | 552 | CA | PRO | A | 95 | 30.862 | -47.356 | -3.190 | 1.00189.59 | A | C |
| ATOM | 559 | CA | VAL | A | 96 | 27.801 | -45.959 | -4.966 | 1.00189.25 | A | C |
| ATOM | 566 | CA | SER | A | 97 | 24.162 | -45.337 | -3.987 | 1.00189.65 | A | C |
| ATOM | 572 | CA | LEU | A | 98 | 20.849 | -44.506 | -5.685 | 1.00190.00 | A | C |
| ATOM | 580 | CA | HIS | A | 99 | 18.571 | -41.782 | -4.325 | 1.00191.00 | A | C |
| ATOM | 590 | CA | ALA | A | 100 | 15.509 | -39.994 | -5.676 | 1.00191.89 | A | C |
| ATOM | 595 | CA | VAL | A | 101 | 13.856 | -36.643 | -5.383 | 1.00191.97 | A | C |
| ATOM | 602 | CA | GLY | A | 102 | 10.206 | -35.525 | -5.920 | 1.00192.29 | A | C |
| ATOM | 606 | CA | VAL | A | 103 | 9.041 | -39.012 | -4.966 | 1.00192.47 | A | C |
| ATOM | 613 | CA | SER | A | 104 | 8.154 | -40.847 | -1.762 | 1.00193.37 | A | C |
| ATOM | 619 | CA | TYR | A | 105 | 9.516 | -44.138 | -0.386 | 1.00193.52 | A | C |
| ATOM | 631 | CA | TRP | A | 106 | 10.227 | -46.120 | 2.746 | 1.00194.08 | A | C |
| ATOM | 645 | CA | LYS | A | 107 | 13.291 | -45.740 | 4.941 | 1.00192.85 | A | C |
| ATOM | 654 | CA | ALA | A | 108 | 14.107 | -49.126 | 3.249 | 1.00191.91 | A | C |
| ATOM | 659 | CA | SER | A | 109 | 15.127 | -47.124 | 0.203 | 1.00190.20 | A | C |
| ATOM | 665 | CA | GLU | A | 110 | 15.989 | -43.420 | 0.285 | 1.00189.67 | A | C |
| ATOM | 674 | CA | GLY | A | 111 | 19.540 | -44.544 | -0.617 | 1.00189.73 | A | C |
| ATOM | 678 | CA | ALA | A | 112 | 21.063 | -41.941 | 1.649 | 1.00189.81 | A | C |
| ATOM | 683 | CA | GLU | A | 113 | 23.530 | -42.795 | 4.400 | 1.00189.89 | A | C |
| ATOM | 692 | CA | TYR | A | 114 | 23.342 | -41.010 | 7.777 | 1.00189.00 | A | C |
| ATOM | 704 | CA | ASP | A | 115 | 21.629 | -42.174 | 10.942 | 1.00190.72 | A | C |
| ATOM | 712 | CA | ASP | A | 116 | 17.925 | -42.205 | 10.118 | 1.00191.79 | A | C |
| ATOM | 720 | CA | GLN | A | 117 | 17.928 | -44.681 | 13.054 | 1.00191.91 | A | C |
| ATOM | 729 | CA | THR | A | 118 | 17.218 | -47.453 | 10.604 | 1.00191.84 | A | C |
| ATOM | 736 | CA | SER | A | 119 | 17.482 | -51.069 | 11.679 | 1.00192.46 | A | C |
| ATOM | 742 | CA | GLN | A | 120 | 19.970 | -53.418 | 10.093 | 1.00192.80 | A | C |
| ATOM | 751 | CA | ARG | A | 121 | 18.252 | -53.990 | 6.736 | 1.00192.93 | A | C |
| ATOM | 762 | CA | GLU | A | 122 | 16.925 | -50.413 | 6.577 | 1.00193.30 | A | C |
| ATOM | 771 | CA | LYS | A | 123 | 20.434 | -48.942 | 6.113 | 1.00192.99 | A | C |
| ATOM | 780 | CA | GLU | A | 124 | 21.666 | -51.299 | 3.334 | 1.00192.48 | A | C |
| ATOM | 789 | CA | ASP | A | 125 | 19.877 | -49.121 | 0.753 | 1.00191.85 | A | C |
| ATOM | 797 | CA | ASP | A | 126 | 21.989 | -46.166 | 1.891 | 1.00192.61 | A | C |
| ATOM | 805 | CA | LYS | A | 127 | 25.311 | -47.426 | 0.403 | 1.00192.13 | A | C |
| ATOM | 814 | CA | VAL | A | 128 | 25.717 | -50.209 | -2.195 | 1.00192.70 | A | C |

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|------|------|----|-----|---|-----|--------|---------|---------|------------|---|---|
| ATOM | 821 | CA | PHE | A | 129 | 29.118 | -51.595 | -1.202 | 1.00193.69 | A | C |
| ATOM | 832 | CA | PRO | A | 130 | 31.487 | -51.686 | -4.284 | 1.00193.82 | A | C |
| ATOM | 839 | CA | GLY | A | 131 | 30.388 | -54.353 | -6.770 | 1.00193.44 | A | C |
| ATOM | 843 | CA | GLY | A | 132 | 27.249 | -55.028 | -4.719 | 1.00193.52 | A | C |
| ATOM | 847 | CA | SER | A | 133 | 23.595 | -55.299 | -5.814 | 1.00193.19 | A | C |
| ATOM | 853 | CA | HIS | A | 134 | 20.340 | -53.934 | -4.298 | 1.00192.56 | A | C |
| ATOM | 863 | CA | THR | A | 135 | 16.583 | -53.626 | -5.109 | 1.00190.26 | A | C |
| ATOM | 870 | CA | TYR | A | 136 | 14.751 | -50.255 | -4.890 | 1.00188.33 | A | C |
| ATOM | 882 | CA | VAL | A | 137 | 11.243 | -49.540 | -3.554 | 1.00187.07 | A | C |
| ATOM | 889 | CA | TRP | A | 138 | 9.762 | -46.410 | -5.207 | 1.00185.84 | A | C |
| ATOM | 903 | CA | GLN | A | 139 | 6.276 | -44.914 | -4.880 | 1.00185.61 | A | C |
| ATOM | 912 | CA | VAL | A | 140 | 4.332 | -42.042 | -6.262 | 1.00185.78 | A | C |
| ATOM | 919 | CA | LEU | A | 141 | 1.365 | -41.234 | -4.020 | 1.00187.88 | A | C |
| ATOM | 927 | CA | LYS | A | 142 | -1.342 | -38.658 | -4.806 | 1.00189.92 | A | C |
| ATOM | 936 | CA | GLU | A | 143 | 0.545 | -36.222 | -2.510 | 1.00192.27 | A | C |
| ATOM | 945 | CA | ASN | A | 144 | 3.598 | -36.201 | -4.864 | 1.00191.57 | A | C |
| ATOM | 953 | CA | GLY | A | 145 | 1.871 | -36.180 | -8.226 | 1.00191.36 | A | C |
| ATOM | 957 | CA | PRO | A | 146 | 1.752 | -32.824 | -10.017 | 1.00191.70 | A | C |
| ATOM | 964 | CA | MET | A | 147 | -0.579 | -30.028 | -8.971 | 1.00194.13 | A | C |
| ATOM | 972 | CA | ALA | A | 148 | -3.949 | -29.306 | -10.509 | 1.00195.06 | A | C |
| ATOM | 977 | CA | SER | A | 149 | -2.563 | -26.675 | -12.906 | 1.00195.21 | A | C |
| ATOM | 983 | CA | ASP | A | 150 | 1.103 | -26.724 | -13.868 | 1.00196.70 | A | C |
| ATOM | 991 | CA | PRO | A | 151 | 3.510 | -28.811 | -16.085 | 1.00197.79 | A | C |
| ATOM | 998 | CA | LEU | A | 152 | 1.620 | -31.825 | -17.479 | 1.00197.47 | A | C |
| ATOM | 1006 | CA | CYS | A | 153 | 4.627 | -33.694 | -16.354 | 1.00198.13 | A | C |
| ATOM | 1012 | CA | LEU | A | 154 | 7.124 | -32.887 | -13.679 | 1.00199.33 | A | C |
| ATOM | 1020 | CA | THR | A | 155 | 10.846 | -32.444 | -14.008 | 1.00199.95 | A | C |
| ATOM | 1027 | CA | TYR | A | 156 | 12.697 | -34.692 | -11.539 | 1.00197.73 | A | C |
| ATOM | 1039 | CA | SER | A | 157 | 16.082 | -36.395 | -11.608 | 1.00196.12 | A | C |
| ATOM | 1045 | CA | TYR | A | 158 | 17.581 | -39.444 | -9.848 | 1.00194.59 | A | C |
| ATOM | 1057 | CA | LEU | A | 159 | 20.807 | -38.883 | -8.064 | 1.00192.98 | A | C |
| ATOM | 1065 | CA | SER | A | 160 | 23.414 | -41.004 | -6.335 | 1.00193.85 | A | C |
| ATOM | 1071 | CA | HIS | A | 161 | 24.767 | -40.009 | -2.894 | 1.00195.43 | A | C |
| ATOM | 1081 | CA | VAL | A | 162 | 27.291 | -41.759 | -0.684 | 1.00196.63 | A | C |
| ATOM | 1088 | CA | ASP | A | 163 | 29.921 | -38.995 | -1.149 | 1.00197.41 | A | C |
| ATOM | 1096 | CA | LEU | A | 164 | 27.645 | -36.453 | -2.803 | 1.00196.96 | A | C |
| ATOM | 1104 | CA | VAL | A | 165 | 30.523 | -34.480 | -4.397 | 1.00196.55 | A | C |
| ATOM | 1111 | CA | LYS | A | 166 | 32.284 | -37.618 | -5.746 | 1.00195.49 | A | C |
| ATOM | 1120 | CA | ASP | A | 167 | 29.238 | -39.638 | -6.872 | 1.00194.30 | A | C |
| ATOM | 1128 | CA | LEU | A | 168 | 28.201 | -36.688 | -8.990 | 1.00192.48 | A | C |
| ATOM | 1136 | CA | ASN | A | 169 | 31.226 | -35.073 | -10.651 | 1.00191.42 | A | C |
| ATOM | 1144 | CA | SER | A | 170 | 32.260 | -38.620 | -11.482 | 1.00190.41 | A | C |
| ATOM | 1150 | CA | GLY | A | 171 | 29.091 | -38.982 | -13.647 | 1.00189.33 | A | C |
| ATOM | 1154 | CA | LEU | A | 172 | 26.069 | -40.532 | -11.866 | 1.00188.72 | A | C |
| ATOM | 1162 | CA | ILE | A | 173 | 22.818 | -38.779 | -12.855 | 1.00188.39 | A | C |
| ATOM | 1170 | CA | GLY | A | 174 | 19.569 | -39.712 | -14.650 | 1.00188.82 | A | C |
| ATOM | 1174 | CA | ALA | A | 175 | 16.175 | -38.217 | -15.444 | 1.00189.01 | A | C |
| ATOM | 1179 | CA | LEU | A | 176 | 13.073 | -39.320 | -13.522 | 1.00189.44 | A | C |
| ATOM | 1187 | CA | LEU | A | 177 | 9.637 | -38.142 | -14.622 | 1.00190.90 | A | C |
| ATOM | 1195 | CA | VAL | A | 178 | 6.262 | -38.252 | -12.859 | 1.00193.12 | A | C |
| ATOM | 1202 | CA | CYS | A | 179 | 2.778 | -37.131 | -14.029 | 1.00197.43 | A | C |
| ATOM | 1208 | CA | ARG | A | 180 | -1.051 | -37.490 | -14.081 | 1.00200.32 | A | C |
| ATOM | 1219 | CA | GLU | A | 181 | -3.170 | -40.610 | -14.806 | 1.00202.90 | A | C |
| ATOM | 1228 | CA | GLY | A | 182 | -2.311 | -41.199 | -18.509 | 1.00204.71 | A | C |
| ATOM | 1232 | CA | SER | A | 183 | 1.090 | -41.792 | -20.117 | 1.00207.01 | A | C |
| ATOM | 1238 | CA | LEU | A | 184 | 0.887 | -45.527 | -20.954 | 1.00210.38 | A | C |

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|------|------|----|-----|---|-----|--------|---------|---------|------------|---|---|
| ATOM | 1246 | CA | ALA | A | 185 | -2.654 | -44.649 | -22.281 | 1.00213.06 | A | C |
| ATOM | 1251 | CA | LYS | A | 186 | -2.638 | -40.973 | -23.399 | 1.00214.65 | A | C |
| ATOM | 1260 | CA | GLU | A | 187 | 0.854 | -41.093 | -24.925 | 1.00215.94 | A | C |
| ATOM | 1269 | CA | LYS | A | 188 | 0.028 | -44.422 | -26.608 | 1.00215.55 | A | C |
| ATOM | 1278 | CA | THR | A | 189 | -2.555 | -42.232 | -28.360 | 1.00214.66 | A | C |
| ATOM | 1285 | CA | GLN | A | 190 | -0.979 | -38.747 | -27.930 | 1.00212.97 | A | C |
| ATOM | 1294 | CA | THR | A | 191 | 1.892 | -37.070 | -29.791 | 1.00210.24 | A | C |
| ATOM | 1301 | CA | LEU | A | 192 | 4.560 | -35.238 | -27.747 | 1.00206.68 | A | C |
| ATOM | 1309 | CA | HIS | A | 193 | 7.993 | -33.865 | -28.681 | 1.00202.85 | A | C |
| ATOM | 1319 | CA | LYS | A | 194 | 10.040 | -34.044 | -25.528 | 1.00198.91 | A | C |
| ATOM | 1328 | CA | PHE | A | 195 | 13.705 | -34.281 | -24.611 | 1.00195.22 | A | C |
| ATOM | 1339 | CA | ILE | A | 196 | 15.763 | -34.158 | -21.497 | 1.00191.13 | A | C |
| ATOM | 1347 | CA | LEU | A | 197 | 18.560 | -31.601 | -21.596 | 1.00188.04 | A | C |
| ATOM | 1355 | CA | LEU | A | 198 | 20.991 | -32.039 | -18.695 | 1.00187.71 | A | C |
| ATOM | 1363 | CA | PHE | A | 199 | 22.621 | -28.619 | -18.109 | 1.00189.15 | A | C |
| ATOM | 1374 | CA | ALA | A | 200 | 25.645 | -29.931 | -16.177 | 1.00192.78 | A | C |
| ATOM | 1379 | CA | VAL | A | 201 | 29.139 | -28.904 | -14.934 | 1.00194.31 | A | C |
| ATOM | 1386 | CA | PHE | A | 202 | 31.294 | -31.959 | -13.997 | 1.00195.62 | A | C |
| ATOM | 1397 | CA | ASP | A | 203 | 34.756 | -30.980 | -12.671 | 1.00196.77 | A | C |
| ATOM | 1405 | CA | GLU | A | 204 | 37.355 | -33.749 | -13.252 | 1.00197.03 | A | C |
| ATOM | 1414 | CA | GLY | A | 205 | 39.401 | -32.504 | -10.262 | 1.00198.66 | A | C |
| ATOM | 1418 | CA | LYS | A | 206 | 36.439 | -33.437 | -8.034 | 1.00200.44 | A | C |
| ATOM | 1427 | CA | SER | A | 207 | 36.052 | -36.781 | -9.861 | 1.00201.80 | A | C |
| ATOM | 1433 | CA | TRP | A | 208 | 36.345 | -40.260 | -8.487 | 1.00202.76 | A | C |
| ATOM | 1447 | CA | HIS | A | 209 | 39.932 | -39.749 | -9.762 | 1.00204.02 | A | C |
| ATOM | 1457 | CA | SER | A | 210 | 43.240 | -38.094 | -8.743 | 1.00203.18 | A | C |
| ATOM | 1463 | CA | SER | A | 224 | 57.686 | -30.887 | -14.569 | 1.00212.76 | A | C |
| ATOM | 1469 | CA | ALA | A | 225 | 53.978 | -31.896 | -14.255 | 1.00212.64 | A | C |
| ATOM | 1474 | CA | ARG | A | 226 | 51.925 | -29.125 | -15.991 | 1.00212.86 | A | C |
| ATOM | 1485 | CA | ALA | A | 227 | 48.187 | -29.719 | -16.913 | 1.00212.05 | A | C |
| ATOM | 1490 | CA | TRP | A | 228 | 45.678 | -30.202 | -14.008 | 1.00211.22 | A | C |
| ATOM | 1504 | CA | PRO | A | 229 | 42.006 | -31.544 | -14.481 | 1.00210.03 | A | C |
| ATOM | 1511 | CA | LYS | A | 230 | 39.003 | -29.798 | -16.226 | 1.00207.97 | A | C |
| ATOM | 1520 | CA | MET | A | 231 | 35.488 | -29.690 | -18.011 | 1.00207.13 | A | C |
| ATOM | 1528 | CA | HIS | A | 232 | 32.219 | -27.497 | -17.643 | 1.00205.95 | A | C |
| ATOM | 1538 | CA | THR | A | 233 | 29.425 | -28.472 | -20.015 | 1.00203.58 | A | C |
| ATOM | 1545 | CA | VAL | A | 234 | 25.929 | -29.429 | -21.319 | 1.00202.35 | A | C |
| ATOM | 1552 | CA | ASN | A | 235 | 24.702 | -33.001 | -21.445 | 1.00202.81 | A | C |
| ATOM | 1560 | CA | GLY | A | 236 | 28.363 | -33.888 | -21.254 | 1.00203.48 | A | C |
| ATOM | 1564 | CA | TYR | A | 237 | 29.002 | -32.322 | -24.643 | 1.00204.42 | A | C |
| ATOM | 1576 | CA | VAL | A | 238 | 32.004 | -30.161 | -24.202 | 1.00205.40 | A | C |
| ATOM | 1583 | CA | ASN | A | 239 | 33.577 | -26.969 | -25.454 | 1.00189.98 | A | C |
| ATOM | 1591 | CA | ARG | A | 240 | 31.475 | -26.713 | -28.626 | 1.00204.03 | A | C |
| ATOM | 1602 | CA | SER | A | 241 | 30.457 | -30.369 | -28.971 | 1.00201.47 | A | C |
| ATOM | 1608 | CA | LEU | A | 242 | 27.084 | -31.194 | -30.433 | 1.00200.00 | A | C |
| ATOM | 1616 | CA | PRO | A | 243 | 24.734 | -34.070 | -29.437 | 1.00198.92 | A | C |
| ATOM | 1623 | CA | GLY | A | 244 | 21.958 | -35.349 | -31.704 | 1.00198.60 | A | C |
| ATOM | 1627 | CA | LEU | A | 245 | 18.342 | -34.680 | -32.660 | 1.00198.22 | A | C |
| ATOM | 1635 | CA | ILE | A | 246 | 15.621 | -32.173 | -33.498 | 1.00197.40 | A | C |
| ATOM | 1643 | CA | GLY | A | 247 | 11.783 | -31.722 | -33.337 | 1.00197.12 | A | C |
| ATOM | 1647 | CA | CYS | A | 248 | 9.182 | -30.933 | -36.066 | 1.00197.01 | A | C |
| ATOM | 1653 | CA | HIS | A | 249 | 8.698 | -27.309 | -37.134 | 1.00194.80 | A | C |
| ATOM | 1663 | CA | ARG | A | 250 | 5.065 | -26.152 | -37.161 | 1.00193.32 | A | C |
| ATOM | 1674 | CA | LYS | A | 251 | 4.427 | -26.911 | -33.476 | 1.00191.32 | A | C |
| ATOM | 1683 | CA | SER | A | 252 | 5.835 | -27.128 | -29.946 | 1.00188.78 | A | C |
| ATOM | 1689 | CA | VAL | A | 253 | 8.732 | -28.928 | -28.284 | 1.00187.98 | A | C |

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|------|------|----|-----|---|-----|--------|---------|---------|------------|---|---|
| ATOM | 1696 | CA | TYR | A | 254 | 9.003 | -29.614 | -24.529 | 1.00188.34 | A | C |
| ATOM | 1708 | CA | TRP | A | 255 | 12.214 | -30.089 | -22.554 | 1.00189.54 | A | C |
| ATOM | 1722 | CA | HIS | A | 256 | 12.675 | -31.324 | -18.988 | 1.00190.66 | A | C |
| ATOM | 1732 | CA | VAL | A | 257 | 15.732 | -29.394 | -18.033 | 1.00191.30 | A | C |
| ATOM | 1739 | CA | ILE | A | 258 | 17.837 | -30.592 | -15.104 | 1.00192.92 | A | C |
| ATOM | 1747 | CA | GLY | A | 259 | 20.304 | -28.140 | -13.438 | 1.00195.25 | A | C |
| ATOM | 1751 | CA | MET | A | 260 | 23.616 | -29.604 | -12.164 | 1.00196.23 | A | C |
| ATOM | 1759 | CA | GLY | A | 261 | 26.926 | -29.164 | -10.354 | 1.00193.75 | A | C |
| ATOM | 1763 | CA | THR | A | 262 | 28.921 | -29.467 | -7.183 | 1.00192.41 | A | C |
| ATOM | 1770 | CA | THR | A | 263 | 29.122 | -25.709 | -6.574 | 1.00192.78 | A | C |
| ATOM | 1777 | CA | PRO | A | 264 | 27.050 | -22.461 | -6.644 | 1.00193.92 | A | C |
| ATOM | 1784 | CA | GLU | A | 265 | 27.691 | -21.962 | -10.401 | 1.00194.35 | A | C |
| ATOM | 1793 | CA | VAL | A | 266 | 24.896 | -20.056 | -12.200 | 1.00191.97 | A | C |
| ATOM | 1800 | CA | HIS | A | 267 | 24.159 | -20.105 | -15.957 | 1.00190.49 | A | C |
| ATOM | 1810 | CA | SER | A | 268 | 21.683 | -18.370 | -18.343 | 1.00187.81 | A | C |
| ATOM | 1816 | CA | ILE | A | 269 | 20.541 | -20.309 | -21.405 | 1.00186.30 | A | C |
| ATOM | 1824 | CA | PHE | A | 270 | 19.100 | -19.208 | -24.773 | 1.00186.06 | A | C |
| ATOM | 1835 | CA | LEU | A | 271 | 18.006 | -19.936 | -28.308 | 1.00187.27 | A | C |
| ATOM | 1843 | CA | GLU | A | 272 | 15.673 | -18.362 | -30.951 | 1.00188.44 | A | C |
| ATOM | 1852 | CA | GLY | A | 273 | 12.059 | -18.345 | -30.088 | 1.00189.24 | A | C |
| ATOM | 1856 | CA | HIS | A | 274 | 11.111 | -17.341 | -26.615 | 1.00190.98 | A | C |
| ATOM | 1866 | CA | THR | A | 275 | 11.094 | -20.454 | -24.279 | 1.00191.93 | A | C |
| ATOM | 1873 | CA | PHE | A | 276 | 7.701 | -19.450 | -22.839 | 1.00194.33 | A | C |
| ATOM | 1884 | CA | LEU | A | 277 | 6.981 | -22.283 | -20.374 | 1.00196.79 | A | C |
| ATOM | 1892 | CA | VAL | A | 278 | 8.225 | -21.781 | -16.825 | 1.00199.42 | A | C |
| ATOM | 1899 | CA | ARG | A | 279 | 4.776 | -21.962 | -15.462 | 1.00200.11 | A | C |
| ATOM | 1910 | CA | ASN | A | 280 | 2.838 | -20.491 | -18.286 | 1.00200.81 | A | C |
| ATOM | 1918 | CA | HIS | A | 281 | 4.839 | -17.680 | -16.693 | 1.00201.63 | A | C |
| ATOM | 1928 | CA | ARG | A | 282 | 6.612 | -16.570 | -19.785 | 1.00200.74 | A | C |
| ATOM | 1939 | CA | GLN | A | 283 | 10.346 | -16.210 | -19.893 | 1.00198.31 | A | C |
| ATOM | 1948 | CA | ALA | A | 284 | 13.147 | -14.529 | -21.787 | 1.00196.62 | A | C |
| ATOM | 1953 | CA | SER | A | 285 | 15.807 | -17.175 | -21.196 | 1.00194.55 | A | C |
| ATOM | 1959 | CA | LEU | A | 286 | 16.018 | -20.277 | -18.976 | 1.00194.07 | A | C |
| ATOM | 1967 | CA | GLU | A | 287 | 18.082 | -19.385 | -15.979 | 1.00194.10 | A | C |
| ATOM | 1976 | CA | ILE | A | 288 | 19.822 | -22.218 | -14.164 | 1.00193.91 | A | C |
| ATOM | 1984 | CA | SER | A | 289 | 21.481 | -22.407 | -10.745 | 1.00195.00 | A | C |
| ATOM | 1990 | CA | PRO | A | 290 | 23.184 | -25.000 | -8.398 | 1.00195.09 | A | C |
| ATOM | 1997 | CA | ILE | A | 291 | 20.547 | -27.756 | -8.529 | 1.00193.60 | A | C |
| ATOM | 2005 | CA | THR | A | 292 | 17.440 | -26.763 | -10.462 | 1.00192.66 | A | C |
| ATOM | 2012 | CA | PHE | A | 293 | 14.597 | -28.357 | -12.348 | 1.00191.21 | A | C |
| ATOM | 2023 | CA | LEU | A | 294 | 11.423 | -27.044 | -13.700 | 1.00189.04 | A | C |
| ATOM | 2031 | CA | THR | A | 295 | 10.246 | -27.818 | -17.196 | 1.00187.10 | A | C |
| ATOM | 2038 | CA | ALA | A | 296 | 9.685 | -25.602 | -20.234 | 1.00185.48 | A | C |
| ATOM | 2043 | CA | GLN | A | 297 | 8.529 | -25.396 | -23.843 | 1.00184.20 | A | C |
| ATOM | 2052 | CA | THR | A | 298 | 8.974 | -23.458 | -27.129 | 1.00182.95 | A | C |
| ATOM | 2059 | CA | LEU | A | 299 | 7.655 | -23.083 | -30.650 | 1.00183.53 | A | C |
| ATOM | 2067 | CA | LEU | A | 300 | 9.599 | -22.980 | -33.957 | 1.00184.72 | A | C |
| ATOM | 2075 | CA | MET | A | 301 | 10.195 | -21.182 | -37.301 | 1.00187.69 | A | C |
| ATOM | 2083 | CA | ASP | A | 302 | 12.366 | -23.381 | -39.676 | 1.00189.36 | A | C |
| ATOM | 2091 | CA | LEU | A | 303 | 15.552 | -25.564 | -40.479 | 1.00190.28 | A | C |
| ATOM | 2099 | CA | GLY | A | 304 | 17.892 | -22.982 | -38.932 | 1.00191.49 | A | C |
| ATOM | 2103 | CA | GLN | A | 305 | 19.646 | -25.084 | -36.412 | 1.00192.11 | A | C |
| ATOM | 2112 | CA | PHE | A | 306 | 19.382 | -22.563 | -33.650 | 1.00192.48 | A | C |
| ATOM | 2123 | CA | LEU | A | 307 | 22.344 | -21.442 | -31.627 | 1.00193.10 | A | C |
| ATOM | 2131 | CA | LEU | A | 308 | 22.506 | -22.626 | -27.913 | 1.00193.43 | A | C |
| ATOM | 2139 | CA | PHE | A | 309 | 24.257 | -20.339 | -25.402 | 1.00195.02 | A | C |

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|------|------|----|-----|---|-----|--------|---------|---------|------------|---|---|
| ATOM | 2150 | CA | CYS | A | 310 | 25.419 | -20.331 | -21.843 | 1.00195.05 | A | C |
| ATOM | 2156 | CA | HIS | A | 311 | 25.932 | -16.649 | -22.677 | 1.00195.59 | A | C |
| ATOM | 2166 | CA | ILE | A | 312 | 28.139 | -15.443 | -19.819 | 1.00195.44 | A | C |
| ATOM | 2174 | CA | SER | A | 313 | 31.701 | -14.104 | -20.129 | 1.00195.98 | A | C |
| ATOM | 2180 | CA | SER | A | 314 | 33.352 | -16.606 | -17.752 | 1.00196.85 | A | C |
| ATOM | 2186 | CA | HIS | A | 315 | 31.495 | -19.809 | -18.681 | 1.00197.39 | A | C |
| ATOM | 2196 | CA | GLN | A | 316 | 31.771 | -18.921 | -22.384 | 1.00198.41 | A | C |
| ATOM | 2205 | CA | HIS | A | 317 | 35.258 | -20.019 | -23.611 | 1.00199.28 | A | C |
| ATOM | 2215 | CA | ASP | A | 318 | 34.788 | -23.440 | -21.883 | 1.00198.03 | A | C |
| ATOM | 2223 | CA | GLY | A | 319 | 31.028 | -23.342 | -22.498 | 1.00196.41 | A | C |
| ATOM | 2227 | CA | MET | A | 320 | 27.867 | -25.125 | -23.521 | 1.00193.89 | A | C |
| ATOM | 2235 | CA | GLU | A | 321 | 26.385 | -25.499 | -27.002 | 1.00191.97 | A | C |
| ATOM | 2244 | CA | ALA | A | 322 | 23.993 | -27.546 | -29.167 | 1.00190.57 | A | C |
| ATOM | 2249 | CA | TYR | A | 323 | 21.908 | -27.356 | -32.317 | 1.00191.22 | A | C |
| ATOM | 2261 | CA | VAL | A | 324 | 18.224 | -27.756 | -33.362 | 1.00191.96 | A | C |
| ATOM | 2268 | CA | LYS | A | 325 | 17.387 | -28.770 | -36.994 | 1.00195.17 | A | C |
| ATOM | 2277 | CA | VAL | A | 326 | 13.644 | -27.666 | -36.974 | 1.00196.24 | A | C |
| ATOM | 2284 | CA | ASP | A | 327 | 12.576 | -29.729 | -40.046 | 1.00199.70 | A | C |
| ATOM | 2292 | CA | SER | A | 328 | 9.489 | -30.420 | -42.263 | 1.00202.24 | A | C |
| ATOM | 2298 | CA | CYS | A | 329 | 7.101 | -33.150 | -41.126 | 1.00205.02 | A | C |
| ATOM | 2304 | CA | PRO | A | 330 | 6.382 | -36.925 | -40.865 | 1.00207.35 | A | C |
| ATOM | 2311 | CA | GLU | A | 331 | 2.693 | -36.749 | -39.659 | 1.00209.54 | A | C |
| ATOM | 2320 | CA | GLU | A | 332 | 1.505 | -35.752 | -43.156 | 1.00210.96 | A | C |
| ATOM | 2329 | CA | PRO | A | 333 | 2.096 | -38.805 | -45.483 | 1.00211.46 | A | C |
| ATOM | 2336 | CA | LYS | A | 377 | -8.368 | 2.126 | -31.565 | 1.00194.11 | A | C |
| ATOM | 2345 | CA | HIS | A | 378 | -6.152 | -0.121 | -33.734 | 1.00193.78 | A | C |
| ATOM | 2355 | CA | PRO | A | 379 | -2.440 | -1.188 | -33.744 | 1.00194.05 | A | C |
| ATOM | 2362 | CA | LYS | A | 380 | 0.205 | 1.541 | -33.510 | 1.00194.74 | A | C |
| ATOM | 2371 | CA | THR | A | 381 | 3.119 | 2.381 | -35.816 | 1.00195.50 | A | C |
| ATOM | 2378 | CA | TRP | A | 382 | 6.096 | 3.842 | -33.806 | 1.00196.40 | A | C |
| ATOM | 2392 | CA | VAL | A | 383 | 9.027 | 5.969 | -34.990 | 1.00196.17 | A | C |
| ATOM | 2399 | CA | HIS | A | 384 | 12.566 | 6.473 | -33.794 | 1.00197.10 | A | C |
| ATOM | 2409 | CA | TYR | A | 385 | 15.394 | 8.464 | -35.264 | 1.00195.11 | A | C |
| ATOM | 2421 | CA | ILE | A | 386 | 18.362 | 7.332 | -33.133 | 1.00192.60 | A | C |
| ATOM | 2429 | CA | ALA | A | 387 | 22.040 | 8.014 | -33.658 | 1.00191.24 | A | C |
| ATOM | 2434 | CA | ALA | A | 388 | 24.968 | 6.303 | -32.015 | 1.00191.23 | A | C |
| ATOM | 2439 | CA | GLU | A | 389 | 27.147 | 9.146 | -30.849 | 1.00191.88 | A | C |
| ATOM | 2448 | CA | GLU | A | 390 | 30.348 | 9.885 | -28.930 | 1.00191.88 | A | C |
| ATOM | 2457 | CA | GLU | A | 391 | 30.241 | 12.133 | -25.852 | 1.00193.77 | A | C |
| ATOM | 2466 | CA | ASP | A | 392 | 31.997 | 12.336 | -22.435 | 1.00194.82 | A | C |
| ATOM | 2474 | CA | TRP | A | 393 | 30.863 | 10.617 | -19.230 | 1.00196.22 | A | C |
| ATOM | 2488 | CA | ASP | A | 394 | 31.278 | 11.841 | -15.639 | 1.00197.30 | A | C |
| ATOM | 2496 | CA | TYR | A | 395 | 30.066 | 8.861 | -13.596 | 1.00198.34 | A | C |
| ATOM | 2508 | CA | ALA | A | 396 | 30.077 | 10.866 | -10.310 | 1.00200.91 | A | C |
| ATOM | 2513 | CA | PRO | A | 397 | 29.439 | 14.573 | -10.944 | 1.00202.72 | A | C |
| ATOM | 2520 | CA | LEU | A | 398 | 27.113 | 15.843 | -8.171 | 1.00204.81 | A | C |
| ATOM | 2528 | CA | VAL | A | 399 | 29.194 | 14.168 | -5.410 | 1.00205.03 | A | C |
| ATOM | 2535 | CA | LEU | A | 400 | 33.015 | 13.923 | -5.251 | 1.00204.90 | A | C |
| ATOM | 2543 | CA | ALA | A | 401 | 35.460 | 13.627 | -2.290 | 1.00204.88 | A | C |
| ATOM | 2548 | CA | PRO | A | 402 | 38.536 | 11.492 | -3.262 | 1.00205.00 | A | C |
| ATOM | 2555 | CA | ASP | A | 403 | 42.300 | 11.241 | -2.586 | 1.00204.31 | A | C |
| ATOM | 2563 | CA | ASP | A | 404 | 43.853 | 7.887 | -1.630 | 1.00202.88 | A | C |
| ATOM | 2571 | CA | ARG | A | 405 | 41.236 | 8.290 | 1.070 | 1.00201.82 | A | C |
| ATOM | 2582 | CA | SER | A | 406 | 39.133 | 5.271 | -0.011 | 1.00201.92 | A | C |
| ATOM | 2588 | CA | TYR | A | 407 | 38.391 | 2.382 | -2.386 | 1.00201.51 | A | C |
| ATOM | 2600 | CA | LYS | A | 408 | 36.304 | 5.017 | -4.153 | 1.00201.19 | A | C |

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|------|------|----|-----|---|-----|--------|--------|---------|------------|---|---|
| ATOM | 2609 | CA | SER | A | 409 | 39.334 | 7.349 | -4.033 | 1.00201.13 | A | C |
| ATOM | 2615 | CA | GLN | A | 410 | 41.164 | 4.821 | -6.209 | 1.00201.21 | A | C |
| ATOM | 2624 | CA | TYR | A | 411 | 38.598 | 4.813 | -9.079 | 1.00200.50 | A | C |
| ATOM | 2636 | CA | LEU | A | 412 | 39.426 | 6.341 | -12.546 | 1.00199.93 | A | C |
| ATOM | 2644 | CA | ASN | A | 413 | 42.858 | 6.396 | -14.281 | 1.00198.33 | A | C |
| ATOM | 2652 | CA | ASN | A | 414 | 45.326 | 4.769 | -11.832 | 1.00197.64 | A | C |
| ATOM | 2660 | CA | GLY | A | 415 | 48.358 | 6.992 | -12.533 | 1.00197.55 | A | C |
| ATOM | 2664 | CA | PRO | A | 416 | 47.967 | 10.625 | -11.490 | 1.00197.77 | A | C |
| ATOM | 2671 | CA | GLN | A | 417 | 44.298 | 11.594 | -12.344 | 1.00198.28 | A | C |
| ATOM | 2680 | CA | ARG | A | 418 | 41.713 | 10.216 | -9.884 | 1.00198.05 | A | C |
| ATOM | 2691 | CA | ILE | A | 419 | 38.987 | 12.745 | -8.766 | 1.00197.17 | A | C |
| ATOM | 2699 | CA | GLY | A | 420 | 35.287 | 12.531 | -9.832 | 1.00196.19 | A | C |
| ATOM | 2703 | CA | ARG | A | 421 | 35.653 | 10.184 | -12.811 | 1.00195.06 | A | C |
| ATOM | 2714 | CA | LYS | A | 422 | 35.474 | 11.269 | -16.488 | 1.00193.73 | A | C |
| ATOM | 2723 | CA | TYR | A | 423 | 35.704 | 8.970 | -19.542 | 1.00193.06 | A | C |
| ATOM | 2735 | CA | LYS | A | 424 | 34.858 | 9.259 | -23.274 | 1.00193.54 | A | C |
| ATOM | 2744 | CA | LYS | A | 425 | 31.886 | 7.049 | -24.143 | 1.00194.92 | A | C |
| ATOM | 2753 | CA | VAL | A | 426 | 29.558 | 6.303 | -27.074 | 1.00196.15 | A | C |
| ATOM | 2760 | CA | ARG | A | 427 | 25.890 | 6.163 | -26.054 | 1.00196.47 | A | C |
| ATOM | 2771 | CA | PHE | A | 428 | 22.821 | 5.851 | -28.246 | 1.00195.53 | A | C |
| ATOM | 2782 | CA | MET | A | 429 | 20.992 | 9.130 | -28.641 | 1.00197.64 | A | C |
| ATOM | 2790 | CA | ALA | A | 430 | 17.842 | 9.912 | -30.647 | 1.00198.82 | A | C |
| ATOM | 2795 | CA | TYR | A | 431 | 17.188 | 12.911 | -32.923 | 1.00200.83 | A | C |
| ATOM | 2807 | CA | THR | A | 432 | 14.053 | 14.696 | -34.099 | 1.00201.26 | A | C |
| ATOM | 2814 | CA | ASP | A | 433 | 14.000 | 13.832 | -37.788 | 1.00202.68 | A | C |
| ATOM | 2822 | CA | GLU | A | 434 | 15.990 | 12.637 | -40.819 | 1.00204.76 | A | C |
| ATOM | 2831 | CA | THR | A | 435 | 17.910 | 15.903 | -40.705 | 1.00205.42 | A | C |
| ATOM | 2838 | CA | PHE | A | 436 | 19.893 | 14.527 | -37.778 | 1.00206.15 | A | C |
| ATOM | 2849 | CA | LYS | A | 437 | 20.367 | 17.985 | -36.302 | 1.00208.06 | A | C |
| ATOM | 2858 | CA | THR | A | 438 | 17.914 | 18.859 | -33.505 | 1.00209.92 | A | C |
| ATOM | 2865 | CA | ARG | A | 439 | 19.310 | 17.575 | -30.189 | 1.00211.87 | A | C |
| ATOM | 2876 | CA | GLU | A | 440 | 16.672 | 15.472 | -28.408 | 1.00214.09 | A | C |
| ATOM | 2885 | CA | ALA | A | 441 | 16.088 | 16.920 | -24.921 | 1.00215.61 | A | C |
| ATOM | 2890 | CA | ILE | A | 442 | 17.737 | 14.418 | -22.587 | 1.00217.41 | A | C |
| ATOM | 2898 | CA | GLN | A | 443 | 16.572 | 12.406 | -19.533 | 1.00218.13 | A | C |
| ATOM | 2907 | CA | HIS | A | 444 | 19.318 | 13.238 | -16.972 | 1.00216.79 | A | C |
| ATOM | 2917 | CA | GLU | A | 445 | 17.979 | 10.356 | -14.827 | 1.00214.25 | A | C |
| ATOM | 2926 | CA | SER | A | 446 | 18.595 | 7.665 | -17.480 | 1.00210.95 | A | C |
| ATOM | 2932 | CA | GLY | A | 447 | 22.197 | 8.894 | -17.702 | 1.00207.74 | A | C |
| ATOM | 2936 | CA | ILE | A | 448 | 23.975 | 6.709 | -20.222 | 1.00204.65 | A | C |
| ATOM | 2944 | CA | LEU | A | 449 | 20.759 | 4.875 | -21.259 | 1.00202.31 | A | C |
| ATOM | 2952 | CA | GLY | A | 450 | 19.331 | 4.991 | -24.791 | 1.00199.38 | A | C |
| ATOM | 2956 | CA | PRO | A | 451 | 15.919 | 6.532 | -25.602 | 1.00197.00 | A | C |
| ATOM | 2963 | CA | LEU | A | 452 | 12.998 | 4.575 | -24.038 | 1.00195.01 | A | C |
| ATOM | 2971 | CA | LEU | A | 453 | 11.741 | 2.217 | -26.714 | 1.00192.42 | A | C |
| ATOM | 2979 | CA | TYR | A | 454 | 8.161 | 0.969 | -26.578 | 1.00191.57 | A | C |
| ATOM | 2991 | CA | GLY | A | 455 | 5.758 | -1.078 | -28.690 | 1.00189.43 | A | C |
| ATOM | 2995 | CA | GLU | A | 456 | 2.652 | -3.122 | -27.782 | 1.00187.63 | A | C |
| ATOM | 3004 | CA | VAL | A | 457 | 1.806 | -6.431 | -29.334 | 1.00184.71 | A | C |
| ATOM | 3011 | CA | GLY | A | 458 | 0.673 | -5.797 | -32.928 | 1.00184.93 | A | C |
| ATOM | 3015 | CA | ASP | A | 459 | 2.733 | -2.668 | -33.556 | 1.00184.91 | A | C |
| ATOM | 3023 | CA | THR | A | 460 | 5.606 | -1.944 | -35.848 | 1.00184.18 | A | C |
| ATOM | 3030 | CA | LEU | A | 461 | 8.750 | 0.034 | -34.898 | 1.00182.65 | A | C |
| ATOM | 3038 | CA | LEU | A | 462 | 10.280 | 2.010 | -37.807 | 1.00182.41 | A | C |
| ATOM | 3046 | CA | ILE | A | 463 | 13.686 | 2.655 | -36.265 | 1.00181.74 | A | C |
| ATOM | 3054 | CA | ILE | A | 464 | 15.819 | 4.922 | -38.451 | 1.00181.55 | A | C |

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|------|------|----|-----|---|-----|--------|---------|---------|------------|---|---|
| ATOM | 3062 | CA | PHE | A | 465 | 19.401 | 4.796 | -37.302 | 1.00182.70 | A | C |
| ATOM | 3073 | CA | LYS | A | 466 | 22.473 | 7.022 | -37.963 | 1.00184.44 | A | C |
| ATOM | 3082 | CA | ASN | A | 467 | 26.026 | 6.395 | -36.926 | 1.00184.85 | A | C |
| ATOM | 3090 | CA | GLN | A | 468 | 27.765 | 9.577 | -35.907 | 1.00186.25 | A | C |
| ATOM | 3099 | CA | ALA | A | 469 | 30.656 | 7.848 | -34.232 | 1.00188.48 | A | C |
| ATOM | 3104 | CA | SER | A | 470 | 33.801 | 6.916 | -36.196 | 1.00191.05 | A | C |
| ATOM | 3110 | CA | ARG | A | 471 | 34.341 | 3.261 | -35.153 | 1.00192.53 | A | C |
| ATOM | 3121 | CA | PRO | A | 472 | 31.184 | 1.660 | -36.764 | 1.00192.78 | A | C |
| ATOM | 3128 | CA | TYR | A | 473 | 28.212 | -0.009 | -34.928 | 1.00192.50 | A | C |
| ATOM | 3140 | CA | ASN | A | 474 | 24.455 | -1.061 | -35.344 | 1.00192.53 | A | C |
| ATOM | 3148 | CA | ILE | A | 475 | 21.103 | -1.785 | -33.473 | 1.00193.10 | A | C |
| ATOM | 3156 | CA | TYR | A | 476 | 19.327 | -4.930 | -32.446 | 1.00194.56 | A | C |
| ATOM | 3168 | CA | PRO | A | 477 | 16.517 | -5.520 | -29.959 | 1.00195.30 | A | C |
| ATOM | 3175 | CA | HIS | A | 478 | 16.778 | -8.513 | -27.631 | 1.00196.70 | A | C |
| ATOM | 3185 | CA | GLY | A | 479 | 13.005 | -9.149 | -27.539 | 1.00196.68 | A | C |
| ATOM | 3189 | CA | ILE | A | 480 | 11.323 | -9.127 | -30.959 | 1.00195.91 | A | C |
| ATOM | 3197 | CA | THR | A | 481 | 11.974 | -11.782 | -33.580 | 1.00195.79 | A | C |
| ATOM | 3204 | CA | ASP | A | 482 | 10.569 | -10.073 | -36.704 | 1.00196.32 | A | C |
| ATOM | 3212 | CA | VAL | A | 483 | 13.409 | -7.589 | -37.321 | 1.00195.66 | A | C |
| ATOM | 3219 | CA | ARG | A | 484 | 13.945 | -6.851 | -41.004 | 1.00194.56 | A | C |
| ATOM | 3230 | CA | PRO | A | 485 | 15.305 | -3.808 | -42.898 | 1.00193.89 | A | C |
| ATOM | 3237 | CA | LEU | A | 486 | 12.463 | -1.387 | -43.624 | 1.00194.47 | A | C |
| ATOM | 3245 | CA | TYR | A | 487 | 11.604 | -1.820 | -47.258 | 1.00196.05 | A | C |
| ATOM | 3257 | CA | SER | A | 488 | 12.953 | -5.205 | -48.337 | 1.00198.78 | A | C |
| ATOM | 3263 | CA | ARG | A | 489 | 13.512 | -8.668 | -46.974 | 1.00202.08 | A | C |
| ATOM | 3274 | CA | ARG | A | 490 | 17.157 | -8.408 | -48.226 | 1.00205.92 | A | C |
| ATOM | 3285 | CA | LEU | A | 491 | 20.332 | -9.142 | -46.331 | 1.00207.58 | A | C |
| ATOM | 3293 | CA | PRO | A | 492 | 22.885 | -6.298 | -46.627 | 1.00208.60 | A | C |
| ATOM | 3300 | CA | LYS | A | 493 | 24.310 | -7.589 | -49.915 | 1.00208.73 | A | C |
| ATOM | 3309 | CA | GLY | A | 494 | 26.429 | -10.169 | -48.011 | 1.00208.22 | A | C |
| ATOM | 3313 | CA | VAL | A | 495 | 25.843 | -10.961 | -44.307 | 1.00208.12 | A | C |
| ATOM | 3320 | CA | LYS | A | 496 | 23.885 | -13.813 | -42.605 | 1.00208.10 | A | C |
| ATOM | 3329 | CA | HIS | A | 497 | 21.663 | -11.479 | -40.459 | 1.00207.29 | A | C |
| ATOM | 3339 | CA | LEU | A | 498 | 21.491 | -7.779 | -39.390 | 1.00206.07 | A | C |
| ATOM | 3347 | CA | LYS | A | 499 | 23.072 | -8.087 | -35.958 | 1.00206.21 | A | C |
| ATOM | 3356 | CA | ASP | A | 500 | 26.071 | -8.976 | -38.097 | 1.00207.27 | A | C |
| ATOM | 3364 | CA | PHE | A | 501 | 28.263 | -6.240 | -39.624 | 1.00205.82 | A | C |
| ATOM | 3375 | CA | PRO | A | 502 | 26.229 | -3.356 | -41.109 | 1.00202.16 | A | C |
| ATOM | 3382 | CA | ILE | A | 503 | 26.436 | 0.522 | -40.643 | 1.00200.11 | A | C |
| ATOM | 3390 | CA | LEU | A | 504 | 29.709 | 2.455 | -41.067 | 1.00196.68 | A | C |
| ATOM | 3398 | CA | PRO | A | 505 | 30.445 | 5.993 | -39.888 | 1.00195.09 | A | C |
| ATOM | 3405 | CA | GLY | A | 506 | 28.053 | 8.420 | -41.535 | 1.00194.28 | A | C |
| ATOM | 3409 | CA | GLU | A | 507 | 25.573 | 6.063 | -43.255 | 1.00193.96 | A | C |
| ATOM | 3418 | CA | ILE | A | 508 | 21.959 | 5.621 | -41.999 | 1.00192.39 | A | C |
| ATOM | 3426 | CA | PHE | A | 509 | 19.788 | 2.449 | -42.034 | 1.00190.90 | A | C |
| ATOM | 3437 | CA | LYS | A | 510 | 16.006 | 2.158 | -41.830 | 1.00189.17 | A | C |
| ATOM | 3446 | CA | TYR | A | 511 | 15.115 | -0.888 | -39.680 | 1.00187.47 | A | C |
| ATOM | 3458 | CA | LYS | A | 512 | 11.654 | -2.477 | -39.138 | 1.00187.85 | A | C |
| ATOM | 3467 | CA | TRP | A | 513 | 10.733 | -4.084 | -35.821 | 1.00188.92 | A | C |
| ATOM | 3481 | CA | THR | A | 514 | 7.306 | -5.815 | -35.949 | 1.00188.91 | A | C |
| ATOM | 3488 | CA | VAL | A | 515 | 6.004 | -7.117 | -32.624 | 1.00188.85 | A | C |
| ATOM | 3495 | CA | THR | A | 516 | 3.728 | -10.102 | -32.338 | 1.00189.64 | A | C |
| ATOM | 3502 | CA | VAL | A | 517 | 1.929 | -11.910 | -29.525 | 1.00190.58 | A | C |
| ATOM | 3509 | CA | GLU | A | 518 | 4.699 | -14.443 | -29.102 | 1.00191.26 | A | C |
| ATOM | 3518 | CA | ASP | A | 519 | 7.336 | -11.934 | -27.901 | 1.00190.28 | A | C |
| ATOM | 3526 | CA | GLY | A | 520 | 4.997 | -10.030 | -25.628 | 1.00188.66 | A | C |

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|------|------|----|-----|---|-----|---------|---------|---------|------------|---|---|
| ATOM | 3530 | CA | PRO | A | 521 | 3.481 | -10.822 | -22.253 | 1.00187.72 | A | C |
| ATOM | 3537 | CA | THR | A | 522 | 0.478 | -12.972 | -21.605 | 1.00187.29 | A | C |
| ATOM | 3544 | CA | LYS | A | 523 | -2.537 | -13.675 | -19.473 | 1.00188.11 | A | C |
| ATOM | 3553 | CA | SER | A | 524 | -0.042 | -14.471 | -16.734 | 1.00189.36 | A | C |
| ATOM | 3559 | CA | ASP | A | 525 | 3.006 | -12.172 | -16.807 | 1.00190.65 | A | C |
| ATOM | 3567 | CA | PRO | A | 526 | 3.022 | -8.520 | -16.083 | 1.00191.65 | A | C |
| ATOM | 3574 | CA | ARG | A | 527 | 1.576 | -6.525 | -18.922 | 1.00193.84 | A | C |
| ATOM | 3585 | CA | CYS | A | 528 | 4.949 | -5.140 | -19.903 | 1.00194.46 | A | C |
| ATOM | 3591 | CA | LEU | A | 529 | 7.969 | -7.435 | -20.035 | 1.00192.87 | A | C |
| ATOM | 3599 | CA | THR | A | 530 | 11.417 | -5.879 | -19.776 | 1.00193.07 | A | C |
| ATOM | 3606 | CA | ARG | A | 531 | 13.959 | -6.048 | -22.534 | 1.00193.84 | A | C |
| ATOM | 3617 | CA | TYR | A | 532 | 16.655 | -3.898 | -24.171 | 1.00195.11 | A | C |
| ATOM | 3629 | CA | TYR | A | 533 | 18.707 | -3.034 | -27.250 | 1.00196.42 | A | C |
| ATOM | 3641 | CA | SER | A | 534 | 22.501 | -3.308 | -27.450 | 1.00199.52 | A | C |
| ATOM | 3647 | CA | SER | A | 535 | 24.573 | -2.842 | -30.567 | 1.00202.35 | A | C |
| ATOM | 3653 | CA | PHE | A | 536 | 26.088 | -5.960 | -32.103 | 1.00205.38 | A | C |
| ATOM | 3664 | CA | VAL | A | 537 | 29.102 | -5.146 | -34.340 | 1.00206.75 | A | C |
| ATOM | 3671 | CA | ASN | A | 538 | 31.153 | -6.261 | -31.292 | 1.00207.75 | A | C |
| ATOM | 3679 | CA | MET | A | 539 | 29.531 | -7.730 | -28.188 | 1.00207.21 | A | C |
| ATOM | 3687 | CA | GLU | A | 540 | 30.717 | -5.692 | -25.185 | 1.00206.60 | A | C |
| ATOM | 3696 | CA | ARG | A | 541 | 33.846 | -4.447 | -26.875 | 1.00204.75 | A | C |
| ATOM | 3707 | CA | ASP | A | 542 | 30.794 | -2.507 | -28.078 | 1.00202.39 | A | C |
| ATOM | 3715 | CA | LEU | A | 543 | 28.212 | -2.372 | -25.256 | 1.00201.33 | A | C |
| ATOM | 3723 | CA | ALA | A | 544 | 30.777 | -1.623 | -22.518 | 1.00200.07 | A | C |
| ATOM | 3728 | CA | SER | A | 545 | 31.592 | 1.597 | -24.370 | 1.00197.60 | A | C |
| ATOM | 3734 | CA | GLY | A | 546 | 27.985 | 2.864 | -24.079 | 1.00196.22 | A | C |
| ATOM | 3738 | CA | LEU | A | 547 | 25.641 | 1.069 | -26.489 | 1.00195.32 | A | C |
| ATOM | 3746 | CA | ILE | A | 548 | 22.614 | 0.515 | -24.244 | 1.00193.09 | A | C |
| ATOM | 3754 | CA | GLY | A | 549 | 18.886 | 1.414 | -24.366 | 1.00192.27 | A | C |
| ATOM | 3758 | CA | PRO | A | 550 | 15.631 | 0.017 | -22.866 | 1.00191.25 | A | C |
| ATOM | 3765 | CA | LEU | A | 551 | 13.094 | -1.822 | -25.033 | 1.00190.41 | A | C |
| ATOM | 3773 | CA | LEU | A | 552 | 9.627 | -2.335 | -23.672 | 1.00192.70 | A | C |
| ATOM | 3781 | CA | ILE | A | 553 | 7.241 | -4.942 | -25.087 | 1.00196.99 | A | C |
| ATOM | 3789 | CA | CYS | A | 554 | 3.605 | -4.744 | -23.882 | 1.00202.37 | A | C |
| ATOM | 3795 | CA | TYR | A | 555 | 0.001 | -5.995 | -23.791 | 1.00210.07 | A | C |
| ATOM | 3807 | CA | LYS | A | 556 | -2.678 | -4.432 | -26.028 | 1.00216.86 | A | C |
| ATOM | 3816 | CA | GLU | A | 557 | -4.547 | -1.168 | -24.942 | 1.00221.09 | A | C |
| ATOM | 3825 | CA | SER | A | 558 | -5.828 | 2.378 | -26.041 | 1.00224.53 | A | C |
| ATOM | 3831 | CA | VAL | A | 559 | -8.883 | 4.114 | -24.380 | 1.00230.02 | A | C |
| ATOM | 3838 | CA | ASP | A | 560 | -10.031 | 0.447 | -23.814 | 1.00234.25 | A | C |
| ATOM | 3846 | CA | GLN | A | 561 | -8.691 | -2.909 | -22.305 | 1.00235.58 | A | C |
| ATOM | 3855 | CA | ARG | A | 562 | -7.562 | -2.099 | -18.692 | 1.00237.26 | A | C |
| ATOM | 3866 | CA | GLY | A | 563 | -6.620 | 1.061 | -16.752 | 1.00238.31 | A | C |
| ATOM | 3870 | CA | ASN | A | 564 | -7.174 | 3.848 | -19.323 | 1.00238.81 | A | C |
| ATOM | 3878 | CA | GLN | A | 565 | -9.830 | 6.221 | -17.858 | 1.00238.98 | A | C |
| ATOM | 3887 | CA | ILE | A | 566 | -7.962 | 9.246 | -16.259 | 1.00238.97 | A | C |
| ATOM | 3895 | CA | MET | A | 567 | -4.157 | 8.551 | -16.916 | 1.00238.69 | A | C |
| ATOM | 3903 | CA | SER | A | 568 | -1.507 | 5.804 | -17.205 | 1.00236.99 | A | C |
| ATOM | 3909 | CA | ASP | A | 569 | 1.291 | 7.289 | -14.957 | 1.00234.46 | A | C |
| ATOM | 3917 | CA | LYS | A | 570 | 4.735 | 7.448 | -16.758 | 1.00229.88 | A | C |
| ATOM | 3926 | CA | ARG | A | 571 | 7.489 | 4.895 | -17.497 | 1.00224.85 | A | C |
| ATOM | 3937 | CA | ASN | A | 572 | 10.835 | 4.808 | -15.608 | 1.00217.53 | A | C |
| ATOM | 3945 | CA | VAL | A | 573 | 13.958 | 2.565 | -15.979 | 1.00210.38 | A | C |
| ATOM | 3952 | CA | ILE | A | 574 | 16.809 | 1.460 | -13.759 | 1.00204.79 | A | C |
| ATOM | 3960 | CA | LEU | A | 575 | 19.777 | -0.338 | -15.362 | 1.00201.81 | A | C |
| ATOM | 3968 | CA | PHE | A | 576 | 22.242 | -2.242 | -13.200 | 1.00201.35 | A | C |

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|------|------|----|-----|---|-----|--------|--------|---------|------------|---|---|
| ATOM | 3979 | CA | SER | A | 577 | 25.504 | -2.106 | -15.142 | 1.00201.04 | A | C |
| ATOM | 3985 | CA | VAL | A | 578 | 29.196 | -2.709 | -14.669 | 1.00199.63 | A | C |
| ATOM | 3992 | CA | PHE | A | 579 | 31.004 | -0.991 | -17.513 | 1.00198.67 | A | C |
| ATOM | 4003 | CA | ASP | A | 580 | 34.456 | -2.505 | -18.037 | 1.00198.78 | A | C |
| ATOM | 4011 | CA | GLU | A | 581 | 36.377 | 0.389 | -19.556 | 1.00198.53 | A | C |
| ATOM | 4020 | CA | ASN | A | 582 | 39.225 | -2.111 | -19.861 | 1.00199.78 | A | C |
| ATOM | 4028 | CA | ARG | A | 583 | 37.517 | -3.456 | -22.963 | 1.00200.20 | A | C |
| ATOM | 4039 | CA | SER | A | 584 | 35.923 | -0.267 | -24.332 | 1.00199.55 | A | C |
| ATOM | 4045 | CA | TRP | A | 585 | 36.401 | 0.654 | -27.998 | 1.00198.21 | A | C |
| ATOM | 4059 | CA | TYR | A | 586 | 37.904 | 3.905 | -26.641 | 1.00197.86 | A | C |
| ATOM | 4071 | CA | LEU | A | 587 | 40.510 | 2.019 | -24.603 | 1.00198.48 | A | C |
| ATOM | 4079 | CA | THR | A | 588 | 43.824 | 3.915 | -24.644 | 1.00199.25 | A | C |
| ATOM | 4086 | CA | GLU | A | 589 | 42.127 | 6.718 | -26.462 | 1.00198.95 | A | C |
| ATOM | 4095 | CA | ASN | A | 590 | 40.974 | 7.616 | -22.924 | 1.00198.55 | A | C |
| ATOM | 4103 | CA | ILE | A | 591 | 44.542 | 7.416 | -21.456 | 1.00199.21 | A | C |
| ATOM | 4111 | CA | GLN | A | 592 | 46.042 | 10.159 | -23.631 | 1.00199.91 | A | C |
| ATOM | 4120 | CA | ARG | A | 593 | 42.945 | 12.094 | -22.579 | 1.00200.47 | A | C |
| ATOM | 4131 | CA | PHE | A | 594 | 42.085 | 12.353 | -18.873 | 1.00200.10 | A | C |
| ATOM | 4142 | CA | LEU | A | 595 | 45.210 | 10.571 | -17.554 | 1.00197.95 | A | C |
| ATOM | 4150 | CA | PRO | A | 596 | 47.966 | 13.227 | -17.600 | 1.00197.00 | A | C |
| ATOM | 4157 | CA | ASN | A | 597 | 51.221 | 11.634 | -18.736 | 1.00195.81 | A | C |
| ATOM | 4165 | CA | PRO | A | 598 | 51.702 | 8.375 | -20.608 | 1.00194.81 | A | C |
| ATOM | 4172 | CA | ALA | A | 599 | 55.421 | 9.406 | -20.218 | 1.00194.26 | A | C |
| ATOM | 4177 | CA | GLY | A | 600 | 55.219 | 6.069 | -18.476 | 1.00193.61 | A | C |
| ATOM | 4181 | CA | VAL | A | 601 | 52.690 | 4.454 | -20.844 | 1.00193.09 | A | C |
| ATOM | 4188 | CA | GLN | A | 602 | 51.903 | 1.585 | -18.344 | 1.00193.25 | A | C |
| ATOM | 4197 | CA | LEU | A | 603 | 48.982 | -0.843 | -19.079 | 1.00193.48 | A | C |
| ATOM | 4205 | CA | GLU | A | 604 | 47.740 | -4.381 | -18.068 | 1.00193.64 | A | C |
| ATOM | 4214 | CA | ASP | A | 605 | 47.900 | -4.250 | -14.248 | 1.00193.60 | A | C |
| ATOM | 4222 | CA | PRO | A | 606 | 46.572 | -5.628 | -10.917 | 1.00194.23 | A | C |
| ATOM | 4229 | CA | GLU | A | 607 | 44.965 | -2.400 | -9.552 | 1.00194.96 | A | C |
| ATOM | 4238 | CA | PHE | A | 608 | 44.573 | -0.331 | -12.749 | 1.00195.37 | A | C |
| ATOM | 4249 | CA | GLN | A | 609 | 42.442 | -3.018 | -14.407 | 1.00196.24 | A | C |
| ATOM | 4258 | CA | ALA | A | 610 | 40.328 | -2.928 | -11.224 | 1.00197.71 | A | C |
| ATOM | 4263 | CA | SER | A | 611 | 40.447 | 0.891 | -11.440 | 1.00198.75 | A | C |
| ATOM | 4269 | CA | ASN | A | 612 | 38.026 | 1.038 | -14.372 | 1.00200.82 | A | C |
| ATOM | 4277 | CA | ILE | A | 613 | 35.549 | -1.765 | -13.645 | 1.00202.64 | A | C |
| ATOM | 4285 | CA | MET | A | 614 | 32.699 | 0.713 | -13.174 | 1.00203.54 | A | C |
| ATOM | 4293 | CA | HIS | A | 615 | 29.853 | -0.748 | -11.120 | 1.00203.80 | A | C |
| ATOM | 4303 | CA | SER | A | 616 | 26.968 | 1.727 | -11.704 | 1.00204.15 | A | C |
| ATOM | 4309 | CA | ILE | A | 617 | 23.217 | 2.289 | -12.197 | 1.00204.57 | A | C |
| ATOM | 4317 | CA | ASN | A | 618 | 22.689 | 4.277 | -15.413 | 1.00204.69 | A | C |
| ATOM | 4325 | CA | GLY | A | 619 | 26.331 | 5.423 | -15.525 | 1.00204.60 | A | C |
| ATOM | 4329 | CA | TYR | A | 620 | 25.725 | 7.275 | -12.279 | 1.00204.01 | A | C |
| ATOM | 4341 | CA | VAL | A | 621 | 27.688 | 5.757 | -9.370 | 1.00203.92 | A | C |
| ATOM | 4348 | CA | PHE | A | 622 | 28.529 | 6.264 | -5.656 | 1.00203.98 | A | C |
| ATOM | 4359 | CA | ASP | A | 623 | 25.209 | 7.922 | -4.797 | 1.00204.59 | A | C |
| ATOM | 4367 | CA | SER | A | 624 | 25.593 | 10.010 | -7.938 | 1.00204.91 | A | C |
| ATOM | 4373 | CA | LEU | A | 625 | 22.383 | 11.467 | -9.211 | 1.00205.31 | A | C |
| ATOM | 4381 | CA | GLN | A | 626 | 19.703 | 9.509 | -7.335 | 1.00206.15 | A | C |
| ATOM | 4390 | CA | LEU | A | 627 | 16.006 | 9.906 | -8.356 | 1.00205.77 | A | C |
| ATOM | 4398 | CA | SER | A | 628 | 13.192 | 12.320 | -7.550 | 1.00204.40 | A | C |
| ATOM | 4404 | CA | VAL | A | 629 | 9.767 | 10.844 | -6.690 | 1.00202.47 | A | C |
| ATOM | 4411 | CA | CYS | A | 630 | 6.968 | 11.557 | -4.160 | 1.00200.30 | A | C |
| ATOM | 4417 | CA | LEU | A | 631 | 4.600 | 9.749 | -1.773 | 1.00197.39 | A | C |
| ATOM | 4425 | CA | HIS | A | 632 | 1.207 | 8.344 | -2.804 | 1.00196.12 | A | C |

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|------|------|----|-----|---|-----|--------|---------|---------|------------|---|---|
| ATOM | 4435 | CA | GLU | A | 633 | 2.724 | 8.401 | -6.307 | 1.00194.99 | A | C |
| ATOM | 4444 | CA | VAL | A | 634 | 2.427 | 4.987 | -7.905 | 1.00192.98 | A | C |
| ATOM | 4451 | CA | ALA | A | 635 | 3.951 | 3.418 | -11.062 | 1.00191.01 | A | C |
| ATOM | 4456 | CA | TYR | A | 636 | 5.953 | 0.521 | -12.511 | 1.00189.95 | A | C |
| ATOM | 4468 | CA | TRP | A | 637 | 9.724 | 0.150 | -12.382 | 1.00190.39 | A | C |
| ATOM | 4482 | CA | TYR | A | 638 | 11.500 | -1.682 | -15.217 | 1.00188.49 | A | C |
| ATOM | 4494 | CA | ILE | A | 639 | 14.929 | -3.036 | -14.292 | 1.00188.04 | A | C |
| ATOM | 4502 | CA | LEU | A | 640 | 17.705 | -5.165 | -15.823 | 1.00188.19 | A | C |
| ATOM | 4510 | CA | SER | A | 641 | 21.231 | -6.454 | -15.389 | 1.00188.34 | A | C |
| ATOM | 4516 | CA | ILE | A | 642 | 23.579 | -5.792 | -18.266 | 1.00190.23 | A | C |
| ATOM | 4524 | CA | GLY | A | 643 | 27.429 | -5.866 | -18.657 | 1.00193.60 | A | C |
| ATOM | 4528 | CA | ALA | A | 644 | 27.950 | -6.704 | -14.974 | 1.00196.31 | A | C |
| ATOM | 4533 | CA | GLN | A | 645 | 28.182 | -10.397 | -15.638 | 1.00199.11 | A | C |
| ATOM | 4542 | CA | THR | A | 646 | 29.931 | -13.540 | -14.340 | 1.00199.76 | A | C |
| ATOM | 4549 | CA | ASP | A | 647 | 27.487 | -13.050 | -11.386 | 1.00199.67 | A | C |
| ATOM | 4557 | CA | PHE | A | 648 | 23.904 | -12.254 | -10.364 | 1.00197.00 | A | C |
| ATOM | 4568 | CA | LEU | A | 649 | 22.272 | -9.378 | -8.530 | 1.00195.40 | A | C |
| ATOM | 4576 | CA | SER | A | 650 | 19.859 | -9.538 | -5.633 | 1.00193.46 | A | C |
| ATOM | 4582 | CA | VAL | A | 651 | 18.545 | -5.930 | -5.714 | 1.00192.28 | A | C |
| ATOM | 4589 | CA | PHE | A | 652 | 17.717 | -3.580 | -2.879 | 1.00192.25 | A | C |
| ATOM | 4600 | CA | PHE | A | 653 | 15.327 | -0.613 | -2.242 | 1.00191.98 | A | C |
| ATOM | 4611 | CA | SER | A | 654 | 15.413 | 0.506 | 1.383 | 1.00191.86 | A | C |
| ATOM | 4617 | CA | GLY | A | 655 | 12.111 | 0.011 | 3.280 | 1.00191.66 | A | C |
| ATOM | 4621 | CA | TYR | A | 656 | 10.240 | -0.398 | 0.033 | 1.00190.60 | A | C |
| ATOM | 4633 | CA | THR | A | 657 | 8.495 | -3.450 | -1.259 | 1.00189.76 | A | C |
| ATOM | 4640 | CA | PHE | A | 658 | 7.254 | -4.471 | -4.683 | 1.00189.69 | A | C |
| ATOM | 4651 | CA | LYS | A | 659 | 4.695 | -6.640 | -6.507 | 1.00190.12 | A | C |
| ATOM | 4660 | CA | HIS | A | 660 | 6.737 | -8.554 | -9.047 | 1.00190.97 | A | C |
| ATOM | 4670 | CA | LYS | A | 661 | 5.053 | -11.685 | -10.497 | 1.00192.68 | A | C |
| ATOM | 4679 | CA | MET | A | 662 | 1.854 | -10.693 | -8.598 | 1.00193.57 | A | C |
| ATOM | 4687 | CA | VAL | A | 663 | 3.324 | -11.770 | -5.253 | 1.00192.63 | A | C |
| ATOM | 4694 | CA | TYR | A | 664 | 4.953 | -9.270 | -2.870 | 1.00192.61 | A | C |
| ATOM | 4706 | CA | GLU | A | 665 | 8.729 | -9.697 | -2.349 | 1.00190.51 | A | C |
| ATOM | 4715 | CA | ASP | A | 666 | 11.297 | -7.201 | -1.060 | 1.00190.19 | A | C |
| ATOM | 4723 | CA | THR | A | 667 | 14.295 | -8.286 | -3.166 | 1.00189.69 | A | C |
| ATOM | 4730 | CA | LEU | A | 668 | 14.647 | -9.042 | -6.809 | 1.00190.97 | A | C |
| ATOM | 4738 | CA | THR | A | 669 | 17.157 | -11.671 | -7.913 | 1.00192.84 | A | C |
| ATOM | 4745 | CA | LEU | A | 670 | 18.629 | -10.753 | -11.311 | 1.00194.67 | A | C |
| ATOM | 4753 | CA | PHE | A | 671 | 20.910 | -12.704 | -13.677 | 1.00195.92 | A | C |
| ATOM | 4764 | CA | PRO | A | 672 | 22.751 | -11.107 | -16.729 | 1.00197.00 | A | C |
| ATOM | 4771 | CA | PHE | A | 673 | 19.892 | -11.483 | -19.242 | 1.00199.11 | A | C |
| ATOM | 4782 | CA | SER | A | 674 | 17.894 | -10.134 | -16.529 | 1.00198.17 | A | C |
| ATOM | 4788 | CA | GLY | A | 675 | 14.753 | -8.429 | -17.690 | 1.00196.49 | A | C |
| ATOM | 4792 | CA | GLU | A | 676 | 12.211 | -8.109 | -14.918 | 1.00194.69 | A | C |
| ATOM | 4801 | CA | THR | A | 677 | 9.282 | -5.759 | -14.263 | 1.00191.40 | A | C |
| ATOM | 4808 | CA | VAL | A | 678 | 8.152 | -4.660 | -10.762 | 1.00189.13 | A | C |
| ATOM | 4815 | CA | PHE | A | 679 | 5.347 | -2.506 | -9.372 | 1.00187.44 | A | C |
| ATOM | 4826 | CA | MET | A | 680 | 5.408 | -0.223 | -6.357 | 1.00186.63 | A | C |
| ATOM | 4834 | CA | SER | A | 681 | 3.161 | 1.827 | -4.063 | 1.00187.64 | A | C |
| ATOM | 4840 | CA | MET | A | 682 | 5.374 | 4.826 | -3.175 | 1.00188.54 | A | C |
| ATOM | 4848 | CA | GLU | A | 683 | 4.310 | 5.856 | 0.351 | 1.00189.84 | A | C |
| ATOM | 4857 | CA | ASN | A | 684 | 7.350 | 5.606 | 2.658 | 1.00189.80 | A | C |
| ATOM | 4865 | CA | PRO | A | 685 | 8.707 | 9.191 | 3.090 | 1.00190.48 | A | C |
| ATOM | 4872 | CA | GLY | A | 686 | 12.496 | 9.609 | 3.359 | 1.00192.51 | A | C |
| ATOM | 4876 | CA | LEU | A | 687 | 16.001 | 8.870 | 2.076 | 1.00193.93 | A | C |
| ATOM | 4884 | CA | TRP | A | 688 | 16.209 | 5.277 | 0.937 | 1.00193.97 | A | C |

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|------|------|----|-----|---|------|---------|--------|--------|------------|---|---|
| ATOM | 4898 | CA | ILE | A | 689 | 19.494 | 3.670 | -0.059 | 1.00195.02 | A | C |
| ATOM | 4906 | CA | LEU | A | 690 | 18.634 | 1.825 | -3.257 | 1.00195.92 | A | C |
| ATOM | 4914 | CA | GLY | A | 691 | 21.455 | -0.492 | -4.143 | 1.00197.86 | A | C |
| ATOM | 4918 | CA | CYS | A | 692 | 21.689 | -4.222 | -4.202 | 1.00200.20 | A | C |
| ATOM | 4924 | CA | HIS | A | 693 | 21.337 | -6.958 | -1.578 | 1.00204.22 | A | C |
| ATOM | 4934 | CA | ASN | A | 694 | 24.955 | -7.880 | -2.329 | 1.00206.08 | A | C |
| ATOM | 4942 | CA | SER | A | 695 | 27.322 | -5.910 | -0.095 | 1.00206.22 | A | C |
| ATOM | 4948 | CA | ASP | A | 696 | 30.489 | -6.263 | -2.214 | 1.00206.28 | A | C |
| ATOM | 4956 | CA | PHE | A | 697 | 29.547 | -3.960 | -5.098 | 1.00205.07 | A | C |
| ATOM | 4967 | CA | ARG | A | 698 | 27.450 | -1.441 | -3.168 | 1.00204.33 | A | C |
| ATOM | 4978 | CA | ASN | A | 699 | 30.859 | -0.426 | -1.767 | 1.00203.55 | A | C |
| ATOM | 4986 | CA | ARG | A | 700 | 32.605 | -0.620 | -5.167 | 1.00202.08 | A | C |
| ATOM | 4997 | CA | GLY | A | 701 | 30.013 | 2.064 | -6.068 | 1.00200.93 | A | C |
| ATOM | 5001 | CA | MET | A | 702 | 26.797 | 0.469 | -7.317 | 1.00199.18 | A | C |
| ATOM | 5009 | CA | THR | A | 703 | 24.369 | 2.541 | -5.184 | 1.00197.90 | A | C |
| ATOM | 5016 | CA | ALA | A | 704 | 22.036 | 5.402 | -5.754 | 1.00197.23 | A | C |
| ATOM | 5021 | CA | LEU | A | 705 | 19.506 | 7.199 | -3.506 | 1.00197.42 | A | C |
| ATOM | 5029 | CA | LEU | A | 706 | 15.772 | 7.830 | -3.683 | 1.00197.53 | A | C |
| ATOM | 5037 | CA | LYS | A | 707 | 13.734 | 10.685 | -2.235 | 1.00198.18 | A | C |
| ATOM | 5046 | CA | VAL | A | 708 | 10.060 | 10.849 | -1.308 | 1.00197.70 | A | C |
| ATOM | 5053 | CA | SER | A | 709 | 7.833 | 13.702 | -0.030 | 1.00197.96 | A | C |
| ATOM | 5059 | CA | SER | A | 710 | 4.289 | 15.005 | -0.729 | 1.00198.08 | A | C |
| ATOM | 5065 | CA | CYS | A | 711 | 3.500 | 16.702 | -4.111 | 1.00198.91 | A | C |
| ATOM | 5071 | CA | ASP | A | 712 | 1.020 | 19.134 | -4.802 | 1.00143.15 | A | C |
| ATOM | 5079 | CA | LYS | A | 713 | -2.260 | 20.852 | -3.924 | 1.00153.03 | A | C |
| ATOM | 5088 | CA | ASN | A | 714 | -2.841 | 24.603 | -3.681 | 1.00213.32 | A | C |
| ATOM | 5096 | CA | THR | A | 715 | -2.888 | 24.714 | 0.106 | 0.00248.66 | A | C |
| ATOM | 5103 | CA | GLY | A | 716 | -3.495 | 26.261 | 3.290 | 0.00232.37 | A | C |
| ATOM | 5107 | CA | ASP | A | 717 | -5.378 | 28.467 | 3.033 | 0.00 30.00 | A | C |
| ATOM | 5115 | CA | TYR | A | 718 | -3.726 | 31.834 | 3.161 | 0.00 30.00 | A | C |
| ATOM | 5127 | CA | TYR | A | 719 | -7.222 | 33.156 | 3.695 | 0.00 30.00 | A | C |
| ATOM | 5139 | CA | GLU | A | 720 | -8.584 | 31.271 | 6.721 | 0.00 30.00 | A | C |
| ATOM | 5148 | CA | ASP | A | 721 | -5.422 | 31.556 | 8.740 | 0.00 30.00 | A | C |
| ATOM | 5156 | CA | SER | A | 722 | -5.138 | 35.079 | 7.504 | 0.00 30.00 | A | C |
| ATOM | 5162 | CA | TYR | A | 723 | -8.543 | 36.057 | 8.810 | 0.00 30.00 | A | C |
| ATOM | 5174 | CA | GLU | A | 724 | -7.901 | 34.327 | 12.085 | 0.00 30.00 | A | C |
| ATOM | 5183 | CA | ASP | A | 725 | -4.613 | 36.101 | 12.775 | 0.00 30.00 | A | C |
| ATOM | 5191 | CA | ILE | A | 726 | -4.946 | 38.848 | 10.269 | 0.00200.98 | A | C |
| ATOM | 5199 | CA | SER | A | 727 | -6.308 | 40.487 | 7.214 | 0.00224.84 | A | C |
| ATOM | 5205 | CA | ALA | A | 728 | -9.416 | 38.960 | 5.415 | 1.00250.85 | A | C |
| ATOM | 5210 | CA | TYR | A | 729 | -10.114 | 39.453 | 1.711 | 1.00215.05 | A | C |
| ATOM | 5222 | CA | LEU | A | 730 | -12.863 | 39.230 | -0.895 | 1.00177.10 | A | C |
| ATOM | 5230 | CA | LEU | A | 731 | -15.629 | 36.646 | -0.529 | 1.00155.50 | A | C |
| ATOM | 5238 | CA | SER | A | 732 | -16.049 | 35.715 | -4.198 | 1.00130.05 | A | C |
| ATOM | 5244 | CA | LYS | A | 733 | -19.837 | 35.414 | -4.103 | 1.00140.11 | A | C |
| ATOM | 5253 | CA | ASN | A | 734 | -22.929 | 37.128 | -5.506 | 1.00143.81 | A | C |
| ATOM | 5261 | CA | ASN | A | 735 | -25.537 | 37.989 | -2.871 | 1.00136.85 | A | C |
| ATOM | 5269 | CA | ALA | A | 736 | -29.286 | 37.388 | -3.226 | 1.00162.36 | A | C |
| ATOM | 5274 | CA | ILE | A | 737 | -32.353 | 36.570 | -1.112 | 1.00190.71 | A | C |
| ATOM | 5282 | CA | GLU | A | 738 | -35.503 | 38.186 | -2.612 | 1.00186.38 | A | C |
| ATOM | 5291 | CA | PRO | A | 739 | -38.729 | 36.164 | -2.411 | 1.00224.34 | A | C |
| ATOM | 5298 | CA | ARG | A | 740 | -42.054 | 36.927 | -0.721 | 1.00173.98 | A | C |
| ATOM | 5310 | CA | PHE | B | 1691 | -13.831 | -8.651 | 15.338 | 1.00219.65 | B | C |
| ATOM | 5321 | CA | GLN | B | 1692 | -10.918 | -6.472 | 16.515 | 1.00219.14 | B | C |
| ATOM | 5330 | CA | LYS | B | 1693 | -7.429 | -5.053 | 15.648 | 1.00218.33 | B | C |
| ATOM | 5339 | CA | LYS | B | 1694 | -4.408 | -5.631 | 17.953 | 1.00216.45 | B | C |

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|------|------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 5348 | CA | THR | B1695 | -1.347 | -3.597 | 18.907 | 1.00214.61 | B | C |
| ATOM | 5355 | CA | ARG | B1696 | 1.137 | -6.429 | 19.597 | 1.00213.69 | B | C |
| ATOM | 5366 | CA | HIS | B1697 | 4.437 | -5.306 | 21.107 | 1.00213.73 | B | C |
| ATOM | 5376 | CA | TYR | B1698 | 7.532 | -7.505 | 21.280 | 1.00213.42 | B | C |
| ATOM | 5388 | CA | PHE | B1699 | 10.053 | -6.633 | 23.990 | 1.00213.28 | B | C |
| ATOM | 5399 | CA | ILE | B1700 | 13.281 | -7.672 | 22.299 | 1.00213.21 | B | C |
| ATOM | 5407 | CA | ALA | B1701 | 17.065 | -7.117 | 22.545 | 1.00214.28 | B | C |
| ATOM | 5412 | CA | ALA | B1702 | 20.497 | -8.154 | 21.247 | 1.00215.38 | B | C |
| ATOM | 5417 | CA | VAL | B1703 | 23.015 | -10.236 | 23.275 | 1.00217.42 | B | C |
| ATOM | 5424 | CA | GLU | B1704 | 25.798 | -12.944 | 22.903 | 1.00218.38 | B | C |
| ATOM | 5433 | CA | ARG | B1705 | 27.134 | -16.409 | 23.993 | 1.00220.47 | B | C |
| ATOM | 5444 | CA | LEU | B1706 | 27.287 | -18.385 | 20.785 | 1.00222.53 | B | C |
| ATOM | 5452 | CA | TRP | B1707 | 28.281 | -21.568 | 19.104 | 1.00224.36 | B | C |
| ATOM | 5466 | CA | ASP | B1708 | 28.378 | -25.054 | 20.499 | 1.00226.97 | B | C |
| ATOM | 5474 | CA | TYR | B1709 | 29.208 | -28.282 | 18.681 | 1.00229.27 | B | C |
| ATOM | 5486 | CA | GLY | B1710 | 29.498 | -31.199 | 21.190 | 1.00230.00 | B | C |
| ATOM | 5490 | CA | MET | B1711 | 27.350 | -34.060 | 19.780 | 1.00230.68 | B | C |
| ATOM | 5498 | CA | SER | B1712 | 29.515 | -37.127 | 18.943 | 1.00230.55 | B | C |
| ATOM | 5504 | CA | SER | B1713 | 31.413 | -36.269 | 15.729 | 1.00229.76 | B | C |
| ATOM | 5510 | CA | GLY | B1725 | 37.806 | -32.358 | 23.456 | 1.00193.22 | B | C |
| ATOM | 5514 | CA | SER | B1726 | 39.318 | -29.424 | 21.523 | 1.00192.82 | B | C |
| ATOM | 5520 | CA | VAL | B1727 | 36.030 | -27.577 | 20.597 | 1.00192.21 | B | C |
| ATOM | 5527 | CA | PRO | B1728 | 36.299 | -23.738 | 20.117 | 1.00191.48 | B | C |
| ATOM | 5534 | CA | GLN | B1729 | 34.440 | -20.938 | 21.889 | 1.00190.65 | B | C |
| ATOM | 5543 | CA | PHE | B1730 | 32.835 | -18.350 | 19.623 | 1.00189.11 | B | C |
| ATOM | 5554 | CA | LYS | B1731 | 31.380 | -14.967 | 20.676 | 1.00188.06 | B | C |
| ATOM | 5563 | CA | LYS | B1732 | 28.981 | -13.693 | 17.943 | 1.00188.11 | B | C |
| ATOM | 5572 | CA | VAL | B1733 | 25.845 | -11.558 | 18.578 | 1.00189.80 | B | C |
| ATOM | 5579 | CA | VAL | B1734 | 22.176 | -12.680 | 18.605 | 1.00191.46 | B | C |
| ATOM | 5586 | CA | PHE | B1735 | 18.687 | -11.247 | 18.994 | 1.00193.25 | B | C |
| ATOM | 5597 | CA | GLN | B1736 | 16.801 | -12.292 | 22.157 | 1.00195.12 | B | C |
| ATOM | 5606 | CA | GLU | B1737 | 13.192 | -11.939 | 23.280 | 1.00197.55 | B | C |
| ATOM | 5615 | CA | PHE | B1738 | 12.660 | -10.538 | 26.797 | 1.00198.49 | B | C |
| ATOM | 5626 | CA | THR | B1739 | 9.632 | -10.290 | 29.116 | 1.00198.06 | B | C |
| ATOM | 5633 | CA | ASP | B1740 | 8.905 | -6.549 | 29.526 | 1.00198.24 | B | C |
| ATOM | 5641 | CA | GLY | B1741 | 10.466 | -3.040 | 29.642 | 1.00197.55 | B | C |
| ATOM | 5645 | CA | SER | B1742 | 12.576 | -3.989 | 32.690 | 1.00196.67 | B | C |
| ATOM | 5651 | CA | PHE | B1743 | 14.551 | -6.249 | 30.299 | 1.00195.88 | B | C |
| ATOM | 5662 | CA | THR | B1744 | 14.953 | -9.013 | 32.894 | 1.00195.58 | B | C |
| ATOM | 5669 | CA | GLN | B1745 | 13.215 | -12.389 | 32.179 | 1.00196.11 | B | C |
| ATOM | 5678 | CA | PRO | B1746 | 15.232 | -14.115 | 29.473 | 1.00195.84 | B | C |
| ATOM | 5685 | CA | LEU | B1747 | 11.932 | -15.632 | 28.266 | 1.00195.84 | B | C |
| ATOM | 5693 | CA | TYR | B1748 | 13.056 | -19.332 | 28.094 | 1.00196.07 | B | C |
| ATOM | 5705 | CA | ARG | B1749 | 12.864 | -20.631 | 24.493 | 1.00194.66 | B | C |
| ATOM | 5716 | CA | GLY | B1750 | 10.008 | -23.142 | 24.512 | 1.00194.29 | B | C |
| ATOM | 5720 | CA | GLU | B1751 | 10.164 | -26.720 | 23.153 | 1.00194.40 | B | C |
| ATOM | 5729 | CA | LEU | B1752 | 7.824 | -25.522 | 20.428 | 1.00194.56 | B | C |
| ATOM | 5737 | CA | ASN | B1753 | 10.350 | -23.005 | 19.048 | 1.00194.34 | B | C |
| ATOM | 5745 | CA | GLU | B1754 | 13.894 | -24.088 | 19.854 | 1.00193.50 | B | C |
| ATOM | 5754 | CA | HIS | B1755 | 14.598 | -24.878 | 16.231 | 1.00191.30 | B | C |
| ATOM | 5764 | CA | LEU | B1756 | 14.895 | -21.095 | 16.032 | 1.00189.20 | B | C |
| ATOM | 5772 | CA | GLY | B1757 | 17.984 | -21.603 | 18.222 | 1.00188.08 | B | C |
| ATOM | 5776 | CA | LEU | B1758 | 20.883 | -19.313 | 17.019 | 1.00185.76 | B | C |
| ATOM | 5784 | CA | LEU | B1759 | 18.680 | -16.560 | 15.565 | 1.00182.36 | B | C |
| ATOM | 5792 | CA | GLY | B1760 | 15.887 | -14.278 | 16.837 | 1.00182.29 | B | C |
| ATOM | 5796 | CA | PRO | B1761 | 12.316 | -14.803 | 18.020 | 1.00182.59 | B | C |

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|------|------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 5803 | CA | TYR | B1762 | 9.198 | -14.864 | 15.874 | 1.00183.32 | B | C |
| ATOM | 5815 | CA | ILE | B1763 | 7.485 | -11.486 | 15.354 | 1.00184.33 | B | C |
| ATOM | 5823 | CA | ARG | B1764 | 3.909 | -11.952 | 14.106 | 1.00185.43 | B | C |
| ATOM | 5834 | CA | ALA | B1765 | 0.958 | -9.907 | 12.821 | 1.00184.45 | B | C |
| ATOM | 5839 | CA | GLU | B1766 | -2.367 | -9.973 | 10.982 | 1.00184.82 | B | C |
| ATOM | 5848 | CA | VAL | B1767 | -3.406 | -7.679 | 8.067 | 1.00184.58 | B | C |
| ATOM | 5855 | CA | GLU | B1768 | -4.988 | -4.571 | 9.579 | 1.00184.59 | B | C |
| ATOM | 5864 | CA | ASP | B1769 | -2.614 | -4.727 | 12.570 | 1.00184.61 | B | C |
| ATOM | 5872 | CA | ASN | B1770 | -0.070 | -3.013 | 14.822 | 1.00185.01 | B | C |
| ATOM | 5880 | CA | ILE | B1771 | 3.532 | -4.037 | 15.242 | 1.00185.74 | B | C |
| ATOM | 5888 | CA | MET | B1772 | 5.736 | -2.571 | 17.977 | 1.00186.89 | B | C |
| ATOM | 5896 | CA | VAL | B1773 | 9.346 | -3.095 | 19.030 | 1.00187.75 | B | C |
| ATOM | 5903 | CA | THR | B1774 | 10.778 | -1.673 | 22.194 | 1.00188.12 | B | C |
| ATOM | 5910 | CA | PHE | B1775 | 14.481 | -2.441 | 21.688 | 1.00188.62 | B | C |
| ATOM | 5921 | CA | ARG | B1776 | 17.623 | -2.375 | 23.826 | 1.00189.37 | B | C |
| ATOM | 5932 | CA | ASN | B1777 | 21.172 | -2.947 | 22.616 | 1.00190.53 | B | C |
| ATOM | 5940 | CA | GLN | B1778 | 23.632 | -4.677 | 24.925 | 1.00191.60 | B | C |
| ATOM | 5949 | CA | ALA | B1779 | 26.974 | -4.970 | 23.059 | 1.00191.77 | B | C |
| ATOM | 5954 | CA | SER | B1780 | 30.091 | -3.229 | 21.641 | 1.00191.65 | B | C |
| ATOM | 5960 | CA | ARG | B1781 | 29.419 | -2.031 | 18.068 | 1.00191.41 | B | C |
| ATOM | 5971 | CA | PRO | B1782 | 25.945 | -0.374 | 18.230 | 1.00192.36 | B | C |
| ATOM | 5978 | CA | TYR | B1783 | 23.316 | -2.231 | 16.126 | 1.00192.61 | B | C |
| ATOM | 5990 | CA | SER | B1784 | 19.646 | -1.794 | 15.038 | 1.00193.19 | B | C |
| ATOM | 5996 | CA | PHE | B1785 | 16.239 | -3.260 | 14.062 | 1.00193.56 | B | C |
| ATOM | 6007 | CA | TYR | B1786 | 15.316 | -3.111 | 10.372 | 1.00192.98 | B | C |
| ATOM | 6019 | CA | SER | B1787 | 13.056 | -4.825 | 7.898 | 1.00193.69 | B | C |
| ATOM | 6025 | CA | SER | B1788 | 11.066 | -3.833 | 4.838 | 1.00195.07 | B | C |
| ATOM | 6031 | CA | LEU | B1789 | 7.738 | -2.399 | 6.146 | 1.00196.02 | B | C |
| ATOM | 6039 | CA | ILE | B1790 | 9.391 | -0.159 | 8.626 | 1.00197.24 | B | C |
| ATOM | 6047 | CA | SER | B1791 | 6.921 | 2.534 | 7.566 | 1.00198.54 | B | C |
| ATOM | 6053 | CA | TYR | B1792 | 8.489 | 5.660 | 9.069 | 1.00200.02 | B | C |
| ATOM | 6065 | CA | GLU | B1793 | 6.485 | 8.873 | 9.074 | 1.00201.76 | B | C |
| ATOM | 6074 | CA | GLU | B1794 | 6.024 | 12.413 | 7.738 | 1.00203.95 | B | C |
| ATOM | 6083 | CA | ASP | B1795 | 8.945 | 14.891 | 7.786 | 1.00206.08 | B | C |
| ATOM | 6091 | CA | GLN | B1796 | 10.893 | 17.314 | 10.078 | 1.00208.04 | B | C |
| ATOM | 6100 | CA | ARG | B1797 | 12.842 | 20.603 | 10.444 | 1.00208.74 | B | C |
| ATOM | 6111 | CA | GLN | B1798 | 15.925 | 18.720 | 9.253 | 1.00209.22 | B | C |
| ATOM | 6120 | CA | GLY | B1799 | 19.179 | 18.878 | 7.216 | 1.00210.35 | B | C |
| ATOM | 6124 | CA | ALA | B1800 | 18.437 | 16.775 | 4.092 | 1.00211.35 | B | C |
| ATOM | 6129 | CA | GLU | B1801 | 16.415 | 14.152 | 6.119 | 1.00212.14 | B | C |
| ATOM | 6138 | CA | PRO | B1802 | 18.540 | 12.140 | 8.614 | 1.00212.12 | B | C |
| ATOM | 6145 | CA | ARG | B1803 | 16.333 | 9.037 | 8.471 | 1.00211.81 | B | C |
| ATOM | 6156 | CA | LYS | B1804 | 19.241 | 7.078 | 9.977 | 1.00211.14 | B | C |
| ATOM | 6165 | CA | ASN | B1805 | 18.391 | 4.248 | 12.374 | 1.00210.80 | B | C |
| ATOM | 6173 | CA | PHE | B1806 | 21.182 | 3.922 | 14.947 | 1.00210.10 | B | C |
| ATOM | 6184 | CA | VAL | B1807 | 20.752 | 2.148 | 18.325 | 1.00208.86 | B | C |
| ATOM | 6191 | CA | LYS | B1808 | 23.634 | 2.837 | 20.733 | 1.00208.29 | B | C |
| ATOM | 6200 | CA | PRO | B1809 | 24.406 | 0.346 | 23.548 | 1.00208.38 | B | C |
| ATOM | 6207 | CA | ASN | B1810 | 22.108 | 0.547 | 26.615 | 1.00209.21 | B | C |
| ATOM | 6215 | CA | GLU | B1811 | 19.939 | 3.175 | 24.852 | 1.00206.72 | B | C |
| ATOM | 6224 | CA | THR | B1812 | 16.352 | 2.306 | 23.926 | 1.00204.60 | B | C |
| ATOM | 6231 | CA | LYS | B1813 | 15.092 | 2.875 | 20.373 | 1.00202.80 | B | C |
| ATOM | 6240 | CA | THR | B1814 | 11.418 | 2.067 | 20.194 | 1.00201.31 | B | C |
| ATOM | 6247 | CA | TYR | B1815 | 9.609 | 1.780 | 16.829 | 1.00200.44 | B | C |
| ATOM | 6259 | CA | PHE | B1816 | 6.050 | 0.896 | 15.803 | 1.00198.17 | B | C |
| ATOM | 6270 | CA | TRP | B1817 | 3.935 | 1.191 | 12.634 | 1.00198.05 | B | C |

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|------|------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 6284 | CA | LYS | B1818 | 0.732 | 0.107 | 10.889 | 1.00196.94 | B | C |
| ATOM | 6293 | CA | VAL | B1819 | 1.400 | -3.055 | 8.908 | 1.00196.52 | B | C |
| ATOM | 6300 | CA | GLN | B1820 | -0.449 | -2.230 | 5.699 | 1.00196.52 | B | C |
| ATOM | 6309 | CA | HIS | B1821 | -1.557 | -4.727 | 3.012 | 1.00196.11 | B | C |
| ATOM | 6319 | CA | HIS | B1822 | 1.887 | -3.766 | 1.615 | 1.00193.93 | B | C |
| ATOM | 6329 | CA | MET | B1823 | 3.374 | -6.596 | 3.819 | 1.00191.43 | B | C |
| ATOM | 6337 | CA | ALA | B1824 | 0.327 | -8.899 | 3.550 | 1.00189.63 | B | C |
| ATOM | 6342 | CA | PRO | B1825 | -0.036 | -12.218 | 1.678 | 1.00188.61 | B | C |
| ATOM | 6349 | CA | THR | B1826 | -2.943 | -12.533 | -0.808 | 1.00189.53 | B | C |
| ATOM | 6356 | CA | LYS | B1827 | -6.001 | -14.635 | -1.849 | 1.00192.08 | B | C |
| ATOM | 6365 | CA | ASP | B1828 | -3.747 | -16.390 | -4.346 | 1.00194.60 | B | C |
| ATOM | 6373 | CA | GLU | B1829 | -1.114 | -16.966 | -1.618 | 1.00195.36 | B | C |
| ATOM | 6382 | CA | PHE | B1830 | -0.742 | -18.853 | 1.730 | 1.00195.28 | B | C |
| ATOM | 6393 | CA | ASP | B1831 | -2.197 | -18.341 | 5.198 | 1.00196.23 | B | C |
| ATOM | 6401 | CA | CYS | B1832 | 1.012 | -16.427 | 5.986 | 1.00195.42 | B | C |
| ATOM | 6407 | CA | LYS | B1833 | 3.989 | -14.841 | 4.140 | 1.00193.76 | B | C |
| ATOM | 6416 | CA | ALA | B1834 | 7.590 | -14.641 | 5.469 | 1.00193.07 | B | C |
| ATOM | 6421 | CA | TRP | B1835 | 9.853 | -11.618 | 5.942 | 1.00192.27 | B | C |
| ATOM | 6435 | CA | ALA | B1836 | 13.260 | -10.843 | 7.363 | 1.00192.99 | B | C |
| ATOM | 6440 | CA | TYR | B1837 | 14.460 | -8.423 | 10.014 | 1.00194.27 | B | C |
| ATOM | 6452 | CA | PHE | B1838 | 18.149 | -7.719 | 10.769 | 1.00196.54 | B | C |
| ATOM | 6463 | CA | SER | B1839 | 20.672 | -5.083 | 11.846 | 1.00197.14 | B | C |
| ATOM | 6469 | CA | ASP | B1840 | 21.157 | -2.437 | 9.167 | 1.00198.84 | B | C |
| ATOM | 6477 | CA | VAL | B1841 | 24.058 | -0.725 | 10.958 | 1.00199.56 | B | C |
| ATOM | 6484 | CA | ASP | B1842 | 26.176 | -3.003 | 8.792 | 1.00200.07 | B | C |
| ATOM | 6492 | CA | LEU | B1843 | 23.841 | -5.284 | 6.792 | 1.00199.82 | B | C |
| ATOM | 6500 | CA | GLU | B1844 | 27.072 | -6.841 | 5.429 | 1.00198.38 | B | C |
| ATOM | 6509 | CA | LYS | B1845 | 28.769 | -7.765 | 8.726 | 1.00196.80 | B | C |
| ATOM | 6518 | CA | ASP | B1846 | 25.733 | -7.733 | 11.106 | 1.00196.50 | B | C |
| ATOM | 6526 | CA | VAL | B1847 | 24.422 | -10.829 | 9.251 | 1.00195.41 | B | C |
| ATOM | 6533 | CA | HIS | B1848 | 27.548 | -13.022 | 9.692 | 1.00193.57 | B | C |
| ATOM | 6543 | CA | SER | B1849 | 27.672 | -11.429 | 13.143 | 1.00192.56 | B | C |
| ATOM | 6549 | CA | GLY | B1850 | 24.323 | -12.890 | 14.076 | 1.00192.15 | B | C |
| ATOM | 6553 | CA | LEU | B1851 | 21.278 | -10.698 | 13.839 | 1.00192.00 | B | C |
| ATOM | 6561 | CA | ILE | B1852 | 19.077 | -12.802 | 11.520 | 1.00191.35 | B | C |
| ATOM | 6569 | CA | GLY | B1853 | 15.375 | -12.546 | 12.434 | 1.00191.81 | B | C |
| ATOM | 6573 | CA | PRO | B1854 | 11.969 | -13.929 | 11.231 | 1.00191.63 | B | C |
| ATOM | 6580 | CA | LEU | B1855 | 8.765 | -11.974 | 10.742 | 1.00190.41 | B | C |
| ATOM | 6588 | CA | LEU | B1856 | 5.331 | -13.372 | 9.908 | 1.00190.53 | B | C |
| ATOM | 6596 | CA | VAL | B1857 | 2.425 | -11.503 | 8.363 | 1.00191.47 | B | C |
| ATOM | 6603 | CA | CYS | B1858 | -0.981 | -13.208 | 8.406 | 1.00194.08 | B | C |
| ATOM | 6609 | CA | HIS | B1859 | -4.548 | -13.035 | 7.000 | 1.00196.03 | B | C |
| ATOM | 6619 | CA | THR | B1860 | -7.152 | -11.732 | 9.432 | 1.00196.65 | B | C |
| ATOM | 6626 | CA | ASN | B1861 | -8.583 | -14.361 | 11.790 | 1.00198.53 | B | C |
| ATOM | 6634 | CA | THR | B1862 | -5.575 | -16.723 | 11.593 | 1.00200.21 | B | C |
| ATOM | 6641 | CA | LEU | B1863 | -3.857 | -16.213 | 14.964 | 1.00202.65 | B | C |
| ATOM | 6649 | CA | ASN | B1864 | -5.225 | -16.990 | 18.446 | 1.00205.82 | B | C |
| ATOM | 6657 | CA | PRO | B1865 | -5.502 | -16.278 | 22.104 | 1.00208.25 | B | C |
| ATOM | 6664 | CA | ALA | B1866 | -2.913 | -19.121 | 22.403 | 1.00211.23 | B | C |
| ATOM | 6669 | CA | HIS | B1867 | -0.224 | -16.839 | 20.721 | 1.00212.88 | B | C |
| ATOM | 6679 | CA | GLY | B1868 | 0.886 | -17.402 | 17.115 | 1.00213.58 | B | C |
| ATOM | 6683 | CA | ARG | B1869 | -1.304 | -19.657 | 14.992 | 1.00214.47 | B | C |
| ATOM | 6694 | CA | GLN | B1870 | -1.993 | -23.395 | 14.862 | 1.00213.82 | B | C |
| ATOM | 6703 | CA | VAL | B1871 | -5.195 | -24.099 | 12.832 | 1.00213.41 | B | C |
| ATOM | 6710 | CA | THR | B1872 | -3.629 | -27.343 | 11.527 | 1.00213.07 | B | C |
| ATOM | 6717 | CA | VAL | B1873 | -0.348 | -25.370 | 11.361 | 1.00209.56 | B | C |

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|------|------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 6724 | CA | GLN | B1874 | 2.973 | -26.102 | 13.121 | 1.00205.63 | B | C |
| ATOM | 6733 | CA | GLU | B1875 | 5.491 | -23.744 | 11.600 | 1.00202.20 | B | C |
| ATOM | 6742 | CA | PHE | B1876 | 9.298 | -23.794 | 11.328 | 1.00199.21 | B | C |
| ATOM | 6753 | CA | ALA | B1877 | 11.826 | -21.260 | 10.020 | 1.00196.53 | B | C |
| ATOM | 6758 | CA | LEU | B1878 | 15.107 | -22.208 | 8.236 | 1.00195.03 | B | C |
| ATOM | 6766 | CA | PHE | B1879 | 17.978 | -19.686 | 7.960 | 1.00195.32 | B | C |
| ATOM | 6777 | CA | LEU | B1880 | 20.559 | -20.925 | 5.475 | 1.00194.17 | B | C |
| ATOM | 6785 | CA | THR | B1881 | 23.782 | -18.796 | 5.422 | 1.00194.91 | B | C |
| ATOM | 6792 | CA | ILE | B1882 | 27.501 | -19.655 | 5.406 | 1.00194.68 | B | C |
| ATOM | 6800 | CA | PHE | B1883 | 28.742 | -17.589 | 8.351 | 1.00195.50 | B | C |
| ATOM | 6811 | CA | ASP | B1884 | 32.247 | -16.033 | 8.272 | 1.00196.61 | B | C |
| ATOM | 6819 | CA | GLU | B1885 | 34.452 | -14.131 | 10.728 | 1.00197.66 | B | C |
| ATOM | 6828 | CA | THR | B1886 | 36.310 | -11.498 | 8.848 | 1.00199.53 | B | C |
| ATOM | 6835 | CA | LYS | B1887 | 33.092 | -9.864 | 10.040 | 1.00200.51 | B | C |
| ATOM | 6844 | CA | SER | B1888 | 31.916 | -8.379 | 13.407 | 1.00202.28 | B | C |
| ATOM | 6850 | CA | TRP | B1889 | 34.454 | -7.799 | 16.220 | 1.00204.36 | B | C |
| ATOM | 6864 | CA | TYR | B1890 | 36.040 | -11.279 | 15.629 | 1.00205.11 | B | C |
| ATOM | 6876 | CA | PHE | B1891 | 39.386 | -9.821 | 16.789 | 1.00204.93 | B | C |
| ATOM | 6887 | CA | THR | B1892 | 38.000 | -10.423 | 20.318 | 1.00205.34 | B | C |
| ATOM | 6894 | CA | GLU | B1893 | 38.085 | -14.143 | 19.447 | 1.00205.86 | B | C |
| ATOM | 6903 | CA | ASN | B1894 | 41.336 | -14.827 | 17.599 | 1.00206.79 | B | C |
| ATOM | 6911 | CA | MET | B1895 | 43.532 | -13.682 | 20.470 | 1.00208.19 | B | C |
| ATOM | 6919 | CA | GLU | B1896 | 40.780 | -14.015 | 23.092 | 1.00209.37 | B | C |
| ATOM | 6928 | CA | ARG | B1897 | 40.702 | -17.789 | 22.759 | 1.00209.70 | B | C |
| ATOM | 6939 | CA | ASN | B1898 | 42.930 | -20.240 | 20.798 | 1.00210.77 | B | C |
| ATOM | 6947 | CA | CYS | B1899 | 46.051 | -18.265 | 21.724 | 1.00212.77 | B | C |
| ATOM | 6953 | CA | ARG | B1900 | 48.377 | -17.575 | 24.675 | 1.00213.61 | B | C |
| ATOM | 6964 | CA | ALA | B1901 | 52.137 | -18.381 | 24.651 | 1.00214.63 | B | C |
| ATOM | 6969 | CA | PRO | B1902 | 51.428 | -21.078 | 21.962 | 1.00215.26 | B | C |
| ATOM | 6976 | CA | CYS | B1903 | 50.328 | -18.639 | 19.223 | 1.00215.51 | B | C |
| ATOM | 6982 | CA | ASN | B1904 | 51.564 | -17.015 | 15.948 | 1.00215.51 | B | C |
| ATOM | 6990 | CA | ILE | B1905 | 50.184 | -19.839 | 13.761 | 1.00215.19 | B | C |
| ATOM | 6998 | CA | GLN | B1906 | 48.293 | -19.021 | 10.490 | 1.00214.99 | B | C |
| ATOM | 7007 | CA | MET | B1907 | 47.464 | -15.298 | 9.987 | 1.00214.06 | B | C |
| ATOM | 7015 | CA | GLU | B1908 | 44.974 | -15.529 | 7.055 | 1.00213.38 | B | C |
| ATOM | 7024 | CA | ASP | B1909 | 46.692 | -18.365 | 5.068 | 1.00212.21 | B | C |
| ATOM | 7032 | CA | PRO | B1910 | 44.665 | -21.648 | 4.699 | 1.00210.66 | B | C |
| ATOM | 7039 | CA | THR | B1911 | 43.074 | -20.830 | 8.108 | 1.00208.83 | B | C |
| ATOM | 7046 | CA | PHE | B1912 | 39.527 | -19.882 | 6.968 | 1.00206.96 | B | C |
| ATOM | 7057 | CA | LYS | B1913 | 37.813 | -20.420 | 10.365 | 1.00204.66 | B | C |
| ATOM | 7066 | CA | GLU | B1914 | 34.182 | -20.442 | 9.081 | 1.00203.66 | B | C |
| ATOM | 7075 | CA | ASN | B1915 | 35.131 | -21.825 | 5.701 | 1.00202.96 | B | C |
| ATOM | 7083 | CA | TYR | B1916 | 36.728 | -24.226 | 8.234 | 1.00203.80 | B | C |
| ATOM | 7095 | CA | ARG | B1917 | 33.184 | -24.775 | 9.523 | 1.00204.10 | B | C |
| ATOM | 7106 | CA | PHE | B1918 | 30.134 | -22.546 | 9.299 | 1.00203.37 | B | C |
| ATOM | 7117 | CA | HIS | B1919 | 27.418 | -23.714 | 6.869 | 1.00203.18 | B | C |
| ATOM | 7127 | CA | ALA | B1920 | 24.368 | -22.525 | 8.805 | 1.00204.07 | B | C |
| ATOM | 7132 | CA | ILE | B1921 | 20.791 | -23.823 | 8.990 | 1.00203.62 | B | C |
| ATOM | 7140 | CA | ASN | B1922 | 20.707 | -21.501 | 12.021 | 1.00203.78 | B | C |
| ATOM | 7148 | CA | GLY | B1923 | 24.026 | -21.870 | 13.742 | 1.00204.40 | B | C |
| ATOM | 7152 | CA | TYR | B1924 | 23.185 | -25.188 | 15.424 | 1.00204.61 | B | C |
| ATOM | 7164 | CA | ILE | B1925 | 24.585 | -26.295 | 12.118 | 1.00203.18 | B | C |
| ATOM | 7172 | CA | MET | B1926 | 27.066 | -28.840 | 12.633 | 1.00202.48 | B | C |
| ATOM | 7180 | CA | ASP | B1927 | 25.412 | -31.671 | 10.783 | 1.00200.56 | B | C |
| ATOM | 7188 | CA | THR | B1928 | 22.599 | -31.561 | 13.392 | 1.00199.27 | B | C |
| ATOM | 7195 | CA | LEU | B1929 | 20.273 | -28.838 | 14.864 | 1.00197.96 | B | C |

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|------|------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 7203 | CA | PRO | B1930 | 17.547 | -29.601 | 17.443 | 1.00197.99 | B | C |
| ATOM | 7210 | CA | GLY | B1931 | 13.839 | -28.772 | 17.357 | 1.00197.97 | B | C |
| ATOM | 7214 | CA | LEU | B1932 | 12.272 | -30.390 | 14.323 | 1.00198.06 | B | C |
| ATOM | 7222 | CA | VAL | B1933 | 9.332 | -32.082 | 16.042 | 1.00199.16 | B | C |
| ATOM | 7229 | CA | MET | B1934 | 6.153 | -32.750 | 14.024 | 1.00199.70 | B | C |
| ATOM | 7237 | CA | ALA | B1935 | 2.990 | -34.882 | 13.798 | 1.00199.95 | B | C |
| ATOM | 7242 | CA | GLN | B1936 | 2.996 | -37.021 | 10.671 | 1.00200.42 | B | C |
| ATOM | 7251 | CA | ASP | B1937 | -0.248 | -35.293 | 9.656 | 1.00201.09 | B | C |
| ATOM | 7259 | CA | GLN | B1938 | -0.819 | -31.790 | 11.120 | 1.00200.53 | B | C |
| ATOM | 7268 | CA | ARG | B1939 | 0.520 | -30.397 | 7.827 | 1.00200.07 | B | C |
| ATOM | 7279 | CA | ILE | B1940 | 3.608 | -28.333 | 8.362 | 1.00197.45 | B | C |
| ATOM | 7287 | CA | ARG | B1941 | 4.497 | -24.952 | 6.912 | 1.00195.76 | B | C |
| ATOM | 7298 | CA | TRP | B1942 | 8.195 | -24.233 | 6.285 | 1.00194.39 | B | C |
| ATOM | 7312 | CA | TYR | B1943 | 9.652 | -20.709 | 6.270 | 1.00193.88 | B | C |
| ATOM | 7324 | CA | LEU | B1944 | 12.813 | -20.835 | 4.132 | 1.00194.01 | B | C |
| ATOM | 7332 | CA | LEU | B1945 | 14.925 | -17.591 | 4.011 | 1.00195.09 | B | C |
| ATOM | 7340 | CA | SER | B1946 | 18.512 | -17.716 | 2.602 | 1.00197.01 | B | C |
| ATOM | 7346 | CA | MET | B1947 | 20.835 | -14.803 | 3.383 | 1.00198.89 | B | C |
| ATOM | 7354 | CA | GLY | B1948 | 24.606 | -14.096 | 3.425 | 1.00199.34 | B | C |
| ATOM | 7358 | CA | SER | B1949 | 26.802 | -13.204 | 0.419 | 1.00198.91 | B | C |
| ATOM | 7364 | CA | ASN | B1950 | 26.817 | -13.751 | -3.341 | 1.00197.58 | B | C |
| ATOM | 7372 | CA | GLU | B1951 | 27.644 | -17.442 | -3.372 | 1.00196.64 | B | C |
| ATOM | 7381 | CA | ASN | B1952 | 24.895 | -18.005 | -0.840 | 1.00194.74 | B | C |
| ATOM | 7389 | CA | ILE | B1953 | 22.506 | -19.760 | -3.210 | 1.00192.83 | B | C |
| ATOM | 7397 | CA | HIS | B1954 | 21.305 | -22.822 | -1.385 | 1.00191.19 | B | C |
| ATOM | 7407 | CA | SER | B1955 | 19.204 | -25.515 | -2.955 | 1.00190.05 | B | C |
| ATOM | 7413 | CA | ILE | B1956 | 17.406 | -27.380 | -0.124 | 1.00189.36 | B | C |
| ATOM | 7421 | CA | HIS | B1957 | 15.144 | -30.403 | -0.065 | 1.00189.69 | B | C |
| ATOM | 7431 | CA | PHE | B1958 | 13.600 | -32.852 | 2.368 | 1.00189.09 | B | C |
| ATOM | 7442 | CA | SER | B1959 | 14.328 | -36.461 | 1.506 | 1.00189.81 | B | C |
| ATOM | 7448 | CA | GLY | B1960 | 11.324 | -38.632 | 0.623 | 1.00191.81 | B | C |
| ATOM | 7452 | CA | HIS | B1961 | 8.959 | -35.721 | 1.022 | 1.00192.23 | B | C |
| ATOM | 7462 | CA | VAL | B1962 | 7.405 | -33.224 | -1.402 | 1.00191.90 | B | C |
| ATOM | 7469 | CA | PHE | B1963 | 5.965 | -29.781 | -0.845 | 1.00192.40 | B | C |
| ATOM | 7480 | CA | THR | B1964 | 3.674 | -27.346 | -2.590 | 1.00192.82 | B | C |
| ATOM | 7487 | CA | VAL | B1965 | 4.427 | -23.654 | -3.326 | 1.00193.70 | B | C |
| ATOM | 7494 | CA | ARG | B1966 | 1.998 | -20.860 | -4.098 | 1.00196.73 | B | C |
| ATOM | 7505 | CA | LYS | B1967 | 2.626 | -17.867 | -6.333 | 1.00197.67 | B | C |
| ATOM | 7514 | CA | LYS | B1968 | 0.262 | -17.303 | -9.202 | 1.00198.72 | B | C |
| ATOM | 7523 | CA | GLU | B1969 | -1.219 | -20.704 | -8.234 | 1.00198.67 | B | C |
| ATOM | 7532 | CA | GLU | B1970 | 0.130 | -23.640 | -6.305 | 1.00198.85 | B | C |
| ATOM | 7541 | CA | TYR | B1971 | 2.531 | -25.948 | -8.090 | 1.00198.88 | B | C |
| ATOM | 7553 | CA | LYS | B1972 | 4.321 | -28.989 | -6.701 | 1.00198.08 | B | C |
| ATOM | 7562 | CA | MET | B1973 | 8.072 | -29.077 | -6.135 | 1.00197.37 | B | C |
| ATOM | 7570 | CA | ALA | B1974 | 10.807 | -31.323 | -4.654 | 1.00196.30 | B | C |
| ATOM | 7575 | CA | LEU | B1975 | 13.562 | -28.778 | -3.818 | 1.00196.49 | B | C |
| ATOM | 7583 | CA | TYR | B1976 | 13.982 | -24.999 | -3.821 | 1.00197.76 | B | C |
| ATOM | 7595 | CA | ASN | B1977 | 16.952 | -22.873 | -4.861 | 1.00198.41 | B | C |
| ATOM | 7603 | CA | LEU | B1978 | 16.740 | -20.438 | -2.036 | 1.00198.80 | B | C |
| ATOM | 7611 | CA | TYR | B1979 | 18.225 | -17.154 | -3.111 | 1.00198.77 | B | C |
| ATOM | 7623 | CA | PRO | B1980 | 19.710 | -14.455 | -0.939 | 1.00199.76 | B | C |
| ATOM | 7630 | CA | GLY | B1981 | 16.763 | -12.107 | -0.217 | 1.00201.18 | B | C |
| ATOM | 7634 | CA | VAL | B1982 | 13.948 | -14.458 | -1.290 | 1.00202.71 | B | C |
| ATOM | 7641 | CA | PHE | B1983 | 11.824 | -15.354 | 1.681 | 1.00204.55 | B | C |
| ATOM | 7652 | CA | GLU | B1984 | 10.041 | -18.567 | 0.909 | 1.00202.23 | B | C |
| ATOM | 7661 | CA | THR | B1985 | 6.903 | -20.018 | 2.397 | 1.00200.00 | B | C |

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|------|------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 7668 | CA | VAL | B1986 | 6.117 | -23.603 | 1.455 | 1.00197.84 | B | C |
| ATOM | 7675 | CA | GLU | B1987 | 3.809 | -26.293 | 2.977 | 1.00196.84 | B | C |
| ATOM | 7684 | CA | MET | B1988 | 3.811 | -30.135 | 3.016 | 1.00195.63 | B | C |
| ATOM | 7692 | CA | LEU | B1989 | 1.916 | -33.140 | 4.395 | 1.00195.44 | B | C |
| ATOM | 7700 | CA | PRO | B1990 | 4.690 | -35.470 | 5.701 | 1.00195.69 | B | C |
| ATOM | 7707 | CA | SER | B1991 | 2.593 | -38.670 | 5.433 | 1.00197.36 | B | C |
| ATOM | 7713 | CA | LYS | B1992 | 5.697 | -40.909 | 5.748 | 1.00197.87 | B | C |
| ATOM | 7722 | CA | ALA | B1993 | 6.396 | -41.735 | 9.386 | 1.00197.21 | B | C |
| ATOM | 7727 | CA | GLY | B1994 | 9.858 | -42.190 | 10.862 | 1.00196.99 | B | C |
| ATOM | 7731 | CA | ILE | B1995 | 12.993 | -40.023 | 11.017 | 1.00196.25 | B | C |
| ATOM | 7739 | CA | TRP | B1996 | 14.409 | -37.861 | 8.198 | 1.00195.36 | B | C |
| ATOM | 7753 | CA | ARG | B1997 | 16.571 | -34.709 | 7.381 | 1.00195.26 | B | C |
| ATOM | 7764 | CA | VAL | B1998 | 17.050 | -31.412 | 5.425 | 1.00194.54 | B | C |
| ATOM | 7771 | CA | GLU | B1999 | 20.173 | -30.898 | 3.246 | 1.00194.07 | B | C |
| ATOM | 7780 | CA | CYS | B2000 | 21.373 | -28.215 | 0.853 | 1.00192.81 | B | C |
| ATOM | 7786 | CA | LEU | B2001 | 21.838 | -30.509 | -2.079 | 1.00190.99 | B | C |
| ATOM | 7794 | CA | ILE | B2002 | 24.791 | -28.448 | -3.349 | 1.00191.25 | B | C |
| ATOM | 7802 | CA | GLY | B2003 | 27.588 | -31.043 | -3.247 | 1.00191.41 | B | C |
| ATOM | 7806 | CA | GLU | B2004 | 30.294 | -29.088 | -1.426 | 1.00192.75 | B | C |
| ATOM | 7815 | CA | HIS | B2005 | 27.793 | -27.501 | 0.958 | 1.00192.65 | B | C |
| ATOM | 7825 | CA | LEU | B2006 | 26.375 | -30.830 | 2.161 | 1.00191.37 | B | C |
| ATOM | 7833 | CA | HIS | B2007 | 29.884 | -32.125 | 2.827 | 1.00190.64 | B | C |
| ATOM | 7843 | CA | ALA | B2008 | 30.570 | -29.457 | 5.422 | 1.00189.53 | B | C |
| ATOM | 7848 | CA | GLY | B2009 | 27.323 | -29.124 | 7.325 | 1.00188.66 | B | C |
| ATOM | 7852 | CA | MET | B2010 | 23.734 | -29.374 | 6.096 | 1.00188.20 | B | C |
| ATOM | 7860 | CA | SER | B2011 | 22.745 | -33.078 | 6.914 | 1.00188.56 | B | C |
| ATOM | 7866 | CA | THR | B2012 | 20.497 | -31.827 | 9.729 | 1.00188.84 | B | C |
| ATOM | 7873 | CA | LEU | B2013 | 17.755 | -34.216 | 10.958 | 1.00188.43 | B | C |
| ATOM | 7881 | CA | PHE | B2014 | 13.975 | -33.847 | 11.388 | 1.00186.43 | B | C |
| ATOM | 7892 | CA | LEU | B2015 | 11.573 | -36.365 | 12.927 | 1.00186.32 | B | C |
| ATOM | 7900 | CA | VAL | B2016 | 7.961 | -37.382 | 12.181 | 1.00187.23 | B | C |
| ATOM | 7907 | CA | TYR | B2017 | 5.992 | -39.467 | 14.670 | 1.00189.61 | B | C |
| ATOM | 7919 | CA | SER | B2018 | 2.539 | -40.959 | 14.453 | 1.00192.51 | B | C |
| ATOM | 7925 | CA | ASN | B2019 | 0.324 | -39.991 | 17.352 | 1.00195.15 | B | C |
| ATOM | 7933 | CA | LYS | B2020 | -1.681 | -43.122 | 16.660 | 1.00197.65 | B | C |
| ATOM | 7942 | CA | CYS | B2021 | 1.299 | -44.623 | 18.502 | 1.00199.69 | B | C |
| ATOM | 7948 | CA | GLN | B2022 | 0.803 | -44.441 | 22.228 | 1.00199.56 | B | C |
| ATOM | 7957 | CA | THR | B2023 | 1.283 | -47.402 | 24.555 | 1.00198.43 | B | C |
| ATOM | 7964 | CA | PRO | B2024 | 2.013 | -47.448 | 28.258 | 1.00197.81 | B | C |
| ATOM | 7971 | CA | LEU | B2025 | 5.810 | -47.193 | 28.398 | 1.00198.39 | B | C |
| ATOM | 7979 | CA | GLY | B2026 | 5.893 | -50.066 | 30.942 | 1.00199.47 | B | C |
| ATOM | 7983 | CA | MET | B2027 | 5.235 | -49.423 | 34.637 | 1.00199.75 | B | C |
| ATOM | 7991 | CA | ALA | B2028 | 3.313 | -52.587 | 35.101 | 1.00201.46 | B | C |
| ATOM | 7996 | CA | SER | B2029 | 5.080 | -54.120 | 32.110 | 1.00205.11 | B | C |
| ATOM | 8002 | CA | GLY | B2030 | 8.455 | -52.460 | 32.586 | 1.00207.06 | B | C |
| ATOM | 8006 | CA | HIS | B2031 | 11.340 | -53.036 | 34.872 | 1.00208.59 | B | C |
| ATOM | 8016 | CA | ILE | B2032 | 11.178 | -54.685 | 38.356 | 1.00210.81 | B | C |
| ATOM | 8024 | CA | ARG | B2033 | 13.083 | -51.927 | 40.224 | 1.00212.03 | B | C |
| ATOM | 8035 | CA | ASP | B2034 | 14.342 | -49.724 | 37.405 | 1.00213.01 | B | C |
| ATOM | 8043 | CA | PHE | B2035 | 15.442 | -46.216 | 38.501 | 1.00213.85 | B | C |
| ATOM | 8054 | CA | GLN | B2036 | 14.319 | -43.844 | 41.284 | 1.00212.86 | B | C |
| ATOM | 8063 | CA | ILE | B2037 | 16.361 | -40.890 | 42.719 | 1.00212.16 | B | C |
| ATOM | 8071 | CA | THR | B2038 | 19.661 | -40.354 | 44.722 | 1.00212.45 | B | C |
| ATOM | 8078 | CA | ALA | B2039 | 18.468 | -38.545 | 47.948 | 1.00211.80 | B | C |
| ATOM | 8083 | CA | SER | B2040 | 15.116 | -36.981 | 47.020 | 1.00210.11 | B | C |
| ATOM | 8089 | CA | GLY | B2041 | 12.820 | -39.686 | 48.330 | 1.00209.48 | B | C |

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|------|------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 8093 | CA | GLN | B2042 | 12.545 | -41.600 | 51.577 | 1.00208.53 | B | C |
| ATOM | 8102 | CA | TYR | B2043 | 9.982 | -42.927 | 54.019 | 1.00207.68 | B | C |
| ATOM | 8114 | CA | GLY | B2044 | 10.699 | -46.557 | 55.069 | 1.00207.81 | B | C |
| ATOM | 8118 | CA | GLN | B2045 | 8.032 | -47.667 | 52.583 | 1.00208.19 | B | C |
| ATOM | 8127 | CA | TRP | B2046 | 10.374 | -46.236 | 50.041 | 1.00209.18 | B | C |
| ATOM | 8141 | CA | ALA | B2047 | 10.459 | -44.341 | 46.783 | 1.00208.02 | B | C |
| ATOM | 8146 | CA | PRO | B2048 | 9.971 | -45.975 | 43.474 | 1.00206.67 | B | C |
| ATOM | 8153 | CA | LYS | B2049 | 11.163 | -49.471 | 43.806 | 1.00205.53 | B | C |
| ATOM | 8162 | CA | LEU | B2050 | 7.373 | -49.619 | 43.873 | 1.00203.24 | B | C |
| ATOM | 8170 | CA | ALA | B2051 | 5.844 | -46.282 | 42.741 | 1.00200.41 | B | C |
| ATOM | 8175 | CA | ARG | B2052 | 3.838 | -47.589 | 39.785 | 1.00198.91 | B | C |
| ATOM | 8186 | CA | LEU | B2053 | 0.244 | -47.043 | 38.779 | 1.00199.31 | B | C |
| ATOM | 8194 | CA | HIS | B2054 | -2.415 | -49.317 | 40.340 | 1.00199.99 | B | C |
| ATOM | 8204 | CA | TYR | B2055 | 0.088 | -51.025 | 42.663 | 1.00199.93 | B | C |
| ATOM | 8216 | CA | SER | B2056 | -2.104 | -52.680 | 45.346 | 1.00199.66 | B | C |
| ATOM | 8222 | CA | GLY | B2057 | -1.181 | -53.139 | 49.014 | 1.00198.75 | B | C |
| ATOM | 8226 | CA | SER | B2058 | -0.416 | -51.089 | 52.102 | 1.00197.47 | B | C |
| ATOM | 8232 | CA | ILE | B2059 | 3.355 | -50.657 | 51.341 | 1.00196.19 | B | C |
| ATOM | 8240 | CA | ASN | B2060 | 2.511 | -49.027 | 47.974 | 1.00195.10 | B | C |
| ATOM | 8248 | CA | ALA | B2061 | 4.033 | -46.076 | 45.990 | 1.00194.88 | B | C |
| ATOM | 8253 | CA | TRP | B2062 | 6.376 | -43.069 | 46.508 | 1.00194.72 | B | C |
| ATOM | 8267 | CA | SER | B2063 | 6.480 | -41.226 | 49.796 | 1.00196.26 | B | C |
| ATOM | 8273 | CA | THR | B2064 | 8.531 | -38.196 | 50.987 | 1.00197.28 | B | C |
| ATOM | 8280 | CA | LYS | B2065 | 7.760 | -35.321 | 53.313 | 1.00197.70 | B | C |
| ATOM | 8289 | CA | GLU | B2066 | 10.277 | -33.210 | 51.461 | 1.00198.77 | B | C |
| ATOM | 8298 | CA | PRO | B2067 | 9.782 | -29.549 | 50.341 | 1.00198.81 | B | C |
| ATOM | 8305 | CA | PHE | B2068 | 12.523 | -30.223 | 47.779 | 1.00198.93 | B | C |
| ATOM | 8316 | CA | SER | B2069 | 11.741 | -33.526 | 46.044 | 1.00198.06 | B | C |
| ATOM | 8322 | CA | TRP | B2070 | 11.862 | -35.505 | 42.764 | 1.00197.24 | B | C |
| ATOM | 8336 | CA | ILE | B2071 | 11.833 | -38.928 | 41.014 | 1.00196.44 | B | C |
| ATOM | 8344 | CA | LYS | B2072 | 13.700 | -40.154 | 37.959 | 1.00195.59 | B | C |
| ATOM | 8353 | CA | VAL | B2073 | 13.076 | -42.839 | 35.357 | 1.00194.46 | B | C |
| ATOM | 8360 | CA | ASP | B2074 | 15.857 | -44.131 | 33.126 | 1.00193.35 | B | C |
| ATOM | 8368 | CA | LEU | B2075 | 13.976 | -45.112 | 29.980 | 1.00191.23 | B | C |
| ATOM | 8376 | CA | LEU | B2076 | 17.310 | -46.726 | 28.937 | 1.00190.47 | B | C |
| ATOM | 8384 | CA | ALA | B2077 | 17.021 | -45.178 | 25.434 | 1.00189.97 | B | C |
| ATOM | 8389 | CA | PRO | B2078 | 15.951 | -41.927 | 23.721 | 1.00189.67 | B | C |
| ATOM | 8396 | CA | MET | B2079 | 12.126 | -42.264 | 23.679 | 1.00189.89 | B | C |
| ATOM | 8404 | CA | ILE | B2080 | 9.012 | -40.277 | 22.694 | 1.00190.73 | B | C |
| ATOM | 8412 | CA | ILE | B2081 | 6.918 | -39.430 | 25.760 | 1.00191.47 | B | C |
| ATOM | 8420 | CA | HIS | B2082 | 3.351 | -38.213 | 24.875 | 1.00191.35 | B | C |
| ATOM | 8430 | CA | GLY | B2083 | 2.040 | -38.071 | 28.452 | 1.00190.37 | B | C |
| ATOM | 8434 | CA | ILE | B2084 | 1.980 | -39.347 | 32.051 | 1.00189.35 | B | C |
| ATOM | 8442 | CA | LYS | B2085 | -0.868 | -40.923 | 34.018 | 1.00188.42 | B | C |
| ATOM | 8451 | CA | THR | B2086 | -0.399 | -39.778 | 37.553 | 1.00188.99 | B | C |
| ATOM | 8458 | CA | GLN | B2087 | -2.207 | -41.032 | 40.662 | 1.00189.70 | B | C |
| ATOM | 8467 | CA | GLY | B2088 | -2.063 | -40.896 | 44.505 | 1.00190.72 | B | C |
| ATOM | 8471 | CA | ALA | B2089 | -1.943 | -43.209 | 47.505 | 1.00191.22 | B | C |
| ATOM | 8476 | CA | ARG | B2090 | -4.103 | -43.825 | 50.664 | 1.00191.52 | B | C |
| ATOM | 8487 | CA | GLN | B2091 | -2.868 | -43.895 | 54.314 | 1.00190.79 | B | C |
| ATOM | 8496 | CA | LYS | B2092 | -4.186 | -44.613 | 57.810 | 1.00190.97 | B | C |
| ATOM | 8505 | CA | PHE | B2093 | -7.380 | -42.641 | 57.108 | 1.00191.17 | B | C |
| ATOM | 8516 | CA | SER | B2094 | -5.511 | -39.932 | 55.226 | 1.00191.02 | B | C |
| ATOM | 8522 | CA | SER | B2095 | -6.001 | -38.850 | 51.614 | 1.00191.28 | B | C |
| ATOM | 8528 | CA | LEU | B2096 | -2.472 | -38.035 | 50.295 | 1.00191.32 | B | C |
| ATOM | 8536 | CA | TYR | B2097 | -1.264 | -37.200 | 46.783 | 1.00192.58 | B | C |

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|------|------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 8548 | CA | ILE | B2098 | 0.652 | -34.503 | 44.787 | 1.00192.42 | B | C |
| ATOM | 8556 | CA | SER | B2099 | -1.466 | -31.600 | 43.611 | 1.00193.13 | B | C |
| ATOM | 8562 | CA | GLN | B2100 | 0.932 | -29.826 | 41.287 | 1.00193.21 | B | C |
| ATOM | 8571 | CA | PHE | B2101 | 4.114 | -30.630 | 39.376 | 1.00192.27 | B | C |
| ATOM | 8582 | CA | ILE | B2102 | 6.647 | -29.512 | 36.762 | 1.00190.96 | B | C |
| ATOM | 8590 | CA | ILE | B2103 | 8.393 | -31.837 | 34.378 | 1.00191.79 | B | C |
| ATOM | 8598 | CA | MET | B2104 | 12.088 | -31.685 | 33.452 | 1.00192.85 | B | C |
| ATOM | 8606 | CA | TYR | B2105 | 13.897 | -34.061 | 31.093 | 1.00194.39 | B | C |
| ATOM | 8618 | CA | SER | B2106 | 17.310 | -35.104 | 29.873 | 1.00196.00 | B | C |
| ATOM | 8624 | CA | LEU | B2107 | 18.148 | -36.785 | 26.576 | 1.00196.85 | B | C |
| ATOM | 8632 | CA | ASP | B2108 | 21.662 | -37.425 | 27.821 | 1.00198.22 | B | C |
| ATOM | 8640 | CA | GLY | B2109 | 22.083 | -37.290 | 31.604 | 1.00198.84 | B | C |
| ATOM | 8644 | CA | LYS | B2110 | 24.369 | -34.233 | 31.738 | 1.00199.61 | B | C |
| ATOM | 8653 | CA | LYS | B2111 | 22.567 | -30.891 | 30.973 | 1.00199.89 | B | C |
| ATOM | 8662 | CA | TRP | B2112 | 18.868 | -30.846 | 31.841 | 1.00200.34 | B | C |
| ATOM | 8676 | CA | GLN | B2113 | 16.138 | -28.226 | 31.614 | 1.00201.29 | B | C |
| ATOM | 8685 | CA | THR | B2114 | 12.470 | -27.475 | 32.474 | 1.00200.76 | B | C |
| ATOM | 8692 | CA | TYR | B2115 | 9.423 | -27.829 | 30.183 | 1.00199.96 | B | C |
| ATOM | 8704 | CA | ARG | B2116 | 7.057 | -25.499 | 28.359 | 1.00200.91 | B | C |
| ATOM | 8715 | CA | GLY | B2117 | 4.065 | -27.346 | 26.926 | 1.00202.08 | B | C |
| ATOM | 8719 | CA | ASN | B2118 | 2.581 | -25.328 | 24.103 | 1.00203.37 | B | C |
| ATOM | 8727 | CA | SER | B2119 | 2.747 | -21.521 | 24.527 | 1.00203.88 | B | C |
| ATOM | 8733 | CA | THR | B2120 | 2.087 | -21.684 | 28.301 | 1.00203.60 | B | C |
| ATOM | 8740 | CA | GLY | B2121 | 4.162 | -18.985 | 30.091 | 1.00203.13 | B | C |
| ATOM | 8744 | CA | THR | B2122 | 7.646 | -19.488 | 31.558 | 1.00202.63 | B | C |
| ATOM | 8751 | CA | LEU | B2123 | 7.301 | -22.939 | 32.969 | 1.00202.70 | B | C |
| ATOM | 8759 | CA | MET | B2124 | 4.786 | -25.741 | 32.426 | 1.00202.51 | B | C |
| ATOM | 8767 | CA | VAL | B2125 | 2.748 | -26.242 | 35.578 | 1.00202.00 | B | C |
| ATOM | 8774 | CA | PHE | B2126 | 0.932 | -29.589 | 35.720 | 1.00201.65 | B | C |
| ATOM | 8785 | CA | PHE | B2127 | -2.211 | -30.423 | 37.713 | 1.00202.21 | B | C |
| ATOM | 8796 | CA | GLY | B2128 | -1.868 | -33.456 | 40.013 | 1.00202.20 | B | C |
| ATOM | 8800 | CA | ASN | B2129 | -4.542 | -35.708 | 41.522 | 1.00201.50 | B | C |
| ATOM | 8808 | CA | VAL | B2130 | -7.367 | -34.963 | 43.911 | 1.00200.64 | B | C |
| ATOM | 8815 | CA | ASP | B2131 | -7.517 | -38.217 | 45.861 | 1.00199.46 | B | C |
| ATOM | 8823 | CA | SER | B2132 | -6.162 | -41.724 | 46.359 | 1.00197.78 | B | C |
| ATOM | 8829 | CA | SER | B2133 | -7.362 | -42.905 | 42.918 | 1.00197.98 | B | C |
| ATOM | 8835 | CA | GLY | B2134 | -7.151 | -39.722 | 40.839 | 1.00198.90 | B | C |
| ATOM | 8839 | CA | ILE | B2135 | -5.695 | -41.144 | 37.609 | 1.00198.51 | B | C |
| ATOM | 8847 | CA | LYS | B2136 | -5.135 | -37.724 | 35.944 | 1.00197.68 | B | C |
| ATOM | 8856 | CA | HIS | B2137 | -3.721 | -38.729 | 32.585 | 1.00196.77 | B | C |
| ATOM | 8866 | CA | ASN | B2138 | -1.682 | -35.665 | 31.645 | 1.00194.17 | B | C |
| ATOM | 8874 | CA | ILE | B2139 | -0.632 | -35.288 | 27.972 | 1.00193.12 | B | C |
| ATOM | 8882 | CA | PHE | B2140 | 2.430 | -33.465 | 26.690 | 1.00191.90 | B | C |
| ATOM | 8893 | CA | ASN | B2141 | 0.953 | -30.886 | 24.256 | 1.00190.38 | B | C |
| ATOM | 8901 | CA | PRO | B2142 | 4.032 | -30.864 | 22.161 | 1.00188.21 | B | C |
| ATOM | 8908 | CA | PRO | B2143 | 5.618 | -34.252 | 22.864 | 1.00187.10 | B | C |
| ATOM | 8915 | CA | ILE | B2144 | 8.904 | -34.919 | 24.666 | 1.00186.89 | B | C |
| ATOM | 8923 | CA | ILE | B2145 | 11.953 | -36.810 | 23.450 | 1.00187.29 | B | C |
| ATOM | 8931 | CA | ALA | B2146 | 14.059 | -37.893 | 26.454 | 1.00188.12 | B | C |
| ATOM | 8936 | CA | ARG | B2147 | 15.807 | -40.773 | 28.214 | 1.00189.30 | B | C |
| ATOM | 8947 | CA | TYR | B2148 | 15.281 | -39.375 | 31.703 | 1.00189.64 | B | C |
| ATOM | 8959 | CA | ILE | B2149 | 12.239 | -37.696 | 33.259 | 1.00189.28 | B | C |
| ATOM | 8967 | CA | ARG | B2150 | 12.125 | -35.945 | 36.608 | 1.00190.73 | B | C |
| ATOM | 8978 | CA | LEU | B2151 | 8.911 | -35.196 | 38.369 | 1.00191.73 | B | C |
| ATOM | 8986 | CA | HIS | B2152 | 9.037 | -32.381 | 40.922 | 1.00191.99 | B | C |
| ATOM | 8996 | CA | PRO | B2153 | 6.128 | -31.650 | 43.342 | 1.00192.33 | B | C |

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|------|------|----|-----|-------|---------|---------|--------|------------|---|---|
| ATOM | 9003 | CA | THR | B2154 | 4.657 | -28.046 | 43.515 | 1.00193.41 | B | C |
| ATOM | 9010 | CA | HIS | B2155 | 2.148 | -29.002 | 46.185 | 1.00194.33 | B | C |
| ATOM | 9020 | CA | TYR | B2156 | 1.286 | -32.095 | 48.204 | 1.00194.57 | B | C |
| ATOM | 9032 | CA | SER | B2157 | -1.322 | -33.429 | 50.634 | 1.00194.64 | B | C |
| ATOM | 9038 | CA | ILE | B2158 | 0.299 | -34.971 | 53.651 | 1.00195.43 | B | C |
| ATOM | 9046 | CA | ARG | B2159 | 3.402 | -36.113 | 51.804 | 1.00195.70 | B | C |
| ATOM | 9057 | CA | SER | B2160 | 4.627 | -35.613 | 48.259 | 1.00196.44 | B | C |
| ATOM | 9063 | CA | THR | B2161 | 3.065 | -38.991 | 47.262 | 1.00195.72 | B | C |
| ATOM | 9070 | CA | LEU | B2162 | 2.904 | -40.621 | 43.851 | 1.00194.60 | B | C |
| ATOM | 9078 | CA | ARG | B2163 | 2.305 | -43.619 | 41.667 | 1.00196.12 | B | C |
| ATOM | 9089 | CA | MET | B2164 | 2.422 | -43.183 | 37.851 | 1.00196.84 | B | C |
| ATOM | 9097 | CA | GLU | B2165 | 2.622 | -44.600 | 34.327 | 1.00196.90 | B | C |
| ATOM | 9106 | CA | LEU | B2166 | 4.190 | -43.083 | 31.180 | 1.00197.98 | B | C |
| ATOM | 9114 | CA | MET | B2167 | 2.715 | -42.605 | 27.716 | 1.00200.00 | B | C |
| ATOM | 9122 | CA | GLY | B2168 | 4.595 | -42.936 | 24.453 | 1.00201.05 | B | C |
| ATOM | 9126 | CA | CYS | B2169 | 6.771 | -45.158 | 22.276 | 1.00202.86 | B | C |
| ATOM | 9132 | CA | ASP | B2170 | 9.938 | -45.288 | 20.200 | 1.00204.22 | B | C |
| ATOM | 9140 | CA | LEU | B2171 | 10.888 | -42.733 | 17.538 | 1.00204.36 | B | C |
| ATOM | 9148 | CA | ASN | B2172 | 8.915 | -45.099 | 15.478 | 1.00205.48 | B | C |
| ATOM | 9156 | CA | SER | B2173 | 9.834 | -48.674 | 16.231 | 1.00207.25 | B | C |
| ATOM | 9162 | CA | CYS | B2174 | 6.025 | -48.691 | 16.217 | 1.00207.17 | B | C |
| ATOM | 9168 | CA | SER | B2175 | 5.527 | -49.942 | 19.763 | 1.00205.50 | B | C |
| ATOM | 9174 | CA | MET | B2176 | 1.856 | -50.523 | 18.899 | 1.00203.77 | B | C |
| ATOM | 9182 | CA | PRO | B2177 | -0.042 | -53.914 | 18.929 | 1.00203.61 | B | C |
| ATOM | 9189 | CA | LEU | B2178 | 0.043 | -55.411 | 15.445 | 1.00203.51 | B | C |
| ATOM | 9197 | CA | GLY | B2179 | -3.479 | -56.905 | 15.471 | 1.00203.74 | B | C |
| ATOM | 9201 | CA | MET | B2180 | -3.573 | -60.008 | 17.688 | 1.00203.43 | B | C |
| ATOM | 9209 | CA | GLU | B2181 | -5.695 | -58.197 | 20.252 | 1.00203.68 | B | C |
| ATOM | 9218 | CA | SER | B2182 | -7.973 | -56.117 | 18.059 | 1.00203.75 | B | C |
| ATOM | 9224 | CA | LYS | B2183 | -8.129 | -59.295 | 15.882 | 1.00203.40 | B | C |
| ATOM | 9233 | CA | ALA | B2184 | -7.132 | -57.393 | 12.749 | 1.00202.50 | B | C |
| ATOM | 9238 | CA | ILE | B2185 | -5.436 | -60.721 | 12.069 | 1.00200.89 | B | C |
| ATOM | 9246 | CA | SER | B2186 | -8.210 | -63.180 | 11.179 | 1.00200.32 | B | C |
| ATOM | 9252 | CA | ASP | B2187 | -8.723 | -66.549 | 12.899 | 1.00200.33 | B | C |
| ATOM | 9260 | CA | ALA | B2188 | -7.867 | -67.991 | 9.453 | 1.00199.19 | B | C |
| ATOM | 9265 | CA | GLN | B2189 | -4.565 | -66.074 | 9.428 | 1.00197.77 | B | C |
| ATOM | 9274 | CA | ILE | B2190 | -2.786 | -68.228 | 12.056 | 1.00196.38 | B | C |
| ATOM | 9282 | CA | THR | B2191 | -1.978 | -71.917 | 12.064 | 1.00196.72 | B | C |
| ATOM | 9289 | CA | ALA | B2192 | 0.111 | -73.921 | 14.487 | 1.00197.45 | B | C |
| ATOM | 9294 | CA | SER | B2193 | 2.198 | -77.074 | 14.445 | 1.00197.93 | B | C |
| ATOM | 9300 | CA | SER | B2194 | -0.848 | -78.890 | 15.853 | 1.00198.54 | B | C |
| ATOM | 9306 | CA | TYR | B2195 | -3.837 | -78.217 | 18.097 | 1.00199.22 | B | C |
| ATOM | 9318 | CA | PHE | B2196 | -5.288 | -80.104 | 21.052 | 1.00200.36 | B | C |
| ATOM | 9329 | CA | THR | B2197 | -8.919 | -81.084 | 20.385 | 1.00202.05 | B | C |
| ATOM | 9336 | CA | ASN | B2198 | -11.640 | -83.431 | 21.838 | 1.00203.35 | B | C |
| ATOM | 9344 | CA | MET | B2199 | -15.246 | -82.422 | 22.713 | 1.00204.33 | B | C |
| ATOM | 9352 | CA | PHE | B2200 | -15.065 | -80.249 | 25.867 | 1.00205.41 | B | C |
| ATOM | 9363 | CA | ALA | B2201 | -12.220 | -78.233 | 24.179 | 1.00205.44 | B | C |
| ATOM | 9368 | CA | THR | B2202 | -10.600 | -76.968 | 20.949 | 1.00205.09 | B | C |
| ATOM | 9375 | CA | TRP | B2203 | -7.398 | -75.161 | 21.891 | 1.00205.08 | B | C |
| ATOM | 9389 | CA | SER | B2204 | -6.840 | -74.094 | 18.273 | 1.00204.22 | B | C |
| ATOM | 9395 | CA | PRO | B2205 | -3.958 | -71.722 | 17.294 | 1.00203.44 | B | C |
| ATOM | 9402 | CA | SER | B2206 | -6.587 | -69.192 | 16.363 | 1.00202.94 | B | C |
| ATOM | 9408 | CA | LYS | B2207 | -6.988 | -68.553 | 20.090 | 1.00202.31 | B | C |
| ATOM | 9417 | CA | ALA | B2208 | -3.491 | -67.285 | 21.053 | 1.00202.24 | B | C |
| ATOM | 9422 | CA | ARG | B2209 | -4.663 | -63.811 | 22.046 | 1.00202.87 | B | C |

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|------|------|----|-----|-------|---------|---------|--------|------------|---|---|
| ATOM | 9433 | CA | LEU | B2210 | -3.116 | -61.622 | 24.750 | 1.00205.06 | B | C |
| ATOM | 9441 | CA | HIS | B2211 | -6.319 | -61.619 | 26.787 | 1.00205.98 | B | C |
| ATOM | 9451 | CA | LEU | B2212 | -8.927 | -64.135 | 25.745 | 1.00207.23 | B | C |
| ATOM | 9459 | CA | GLN | B2213 | -11.638 | -65.673 | 27.910 | 1.00209.49 | B | C |
| ATOM | 9468 | CA | GLY | B2214 | -13.562 | -68.935 | 27.275 | 1.00209.49 | B | C |
| ATOM | 9472 | CA | ARG | B2215 | -13.556 | -72.676 | 27.909 | 1.00208.82 | B | C |
| ATOM | 9483 | CA | SER | B2216 | -10.751 | -73.131 | 25.343 | 1.00206.05 | B | C |
| ATOM | 9489 | CA | ASN | B2217 | -9.170 | -69.718 | 25.658 | 1.00203.33 | B | C |
| ATOM | 9497 | CA | ALA | B2218 | -5.692 | -70.209 | 24.222 | 1.00201.74 | B | C |
| ATOM | 9502 | CA | TRP | B2219 | -3.554 | -72.233 | 21.833 | 1.00200.79 | B | C |
| ATOM | 9516 | CA | ARG | B2220 | -2.242 | -75.632 | 22.843 | 1.00201.16 | B | C |
| ATOM | 9527 | CA | PRO | B2221 | -0.189 | -78.189 | 20.814 | 1.00201.86 | B | C |
| ATOM | 9534 | CA | GLN | B2222 | -1.520 | -81.749 | 20.489 | 1.00202.20 | B | C |
| ATOM | 9543 | CA | VAL | B2223 | 1.359 | -83.010 | 22.672 | 1.00202.37 | B | C |
| ATOM | 9550 | CA | ASN | B2224 | 4.381 | -81.492 | 24.335 | 1.00202.87 | B | C |
| ATOM | 9558 | CA | ASN | B2225 | 7.554 | -81.059 | 22.196 | 1.00203.30 | B | C |
| ATOM | 9566 | CA | PRO | B2226 | 10.243 | -78.298 | 22.064 | 1.00202.58 | B | C |
| ATOM | 9573 | CA | LYS | B2227 | 10.411 | -78.640 | 18.275 | 1.00201.86 | B | C |
| ATOM | 9582 | CA | GLU | B2228 | 6.760 | -77.540 | 18.469 | 1.00201.86 | B | C |
| ATOM | 9591 | CA | TRP | B2229 | 5.675 | -74.153 | 17.131 | 1.00201.26 | B | C |
| ATOM | 9605 | CA | LEU | B2230 | 3.055 | -71.483 | 16.442 | 1.00200.58 | B | C |
| ATOM | 9613 | CA | GLN | B2231 | 2.878 | -69.455 | 13.206 | 1.00199.89 | B | C |
| ATOM | 9622 | CA | VAL | B2232 | 1.425 | -66.053 | 12.424 | 1.00199.27 | B | C |
| ATOM | 9629 | CA | ASP | B2233 | 0.996 | -65.215 | 8.747 | 1.00197.93 | B | C |
| ATOM | 9637 | CA | PHE | B2234 | 0.812 | -61.543 | 7.857 | 1.00196.73 | B | C |
| ATOM | 9648 | CA | GLN | B2235 | -0.929 | -61.202 | 4.532 | 1.00196.92 | B | C |
| ATOM | 9657 | CA | LYS | B2236 | 1.773 | -58.512 | 3.893 | 1.00196.46 | B | C |
| ATOM | 9666 | CA | THR | B2237 | 5.393 | -57.561 | 4.757 | 1.00195.71 | B | C |
| ATOM | 9673 | CA | MET | B2238 | 5.851 | -56.339 | 8.337 | 1.00194.24 | B | C |
| ATOM | 9681 | CA | LYS | B2239 | 8.413 | -54.871 | 10.755 | 1.00191.08 | B | C |
| ATOM | 9690 | CA | VAL | B2240 | 8.493 | -56.273 | 14.338 | 1.00189.95 | B | C |
| ATOM | 9697 | CA | THR | B2241 | 9.510 | -54.804 | 17.733 | 1.00190.11 | B | C |
| ATOM | 9704 | CA | GLY | B2242 | 8.726 | -57.870 | 19.835 | 1.00190.40 | B | C |
| ATOM | 9708 | CA | VAL | B2243 | 6.222 | -60.532 | 20.878 | 1.00191.24 | B | C |
| ATOM | 9715 | CA | THR | B2244 | 4.108 | -60.150 | 24.068 | 1.00192.63 | B | C |
| ATOM | 9722 | CA | THR | B2245 | 3.626 | -63.567 | 25.652 | 1.00193.81 | B | C |
| ATOM | 9729 | CA | GLN | B2246 | 1.262 | -64.930 | 28.268 | 1.00195.54 | B | C |
| ATOM | 9738 | CA | GLY | B2247 | -0.224 | -68.202 | 29.582 | 1.00197.51 | B | C |
| ATOM | 9742 | CA | VAL | B2248 | -3.697 | -69.592 | 30.213 | 1.00198.59 | B | C |
| ATOM | 9749 | CA | LYS | B2249 | -5.956 | -69.853 | 33.223 | 1.00200.34 | B | C |
| ATOM | 9758 | CA | SER | B2250 | -7.447 | -73.314 | 32.531 | 1.00199.57 | B | C |
| ATOM | 9764 | CA | LEU | B2251 | -9.669 | -73.443 | 35.696 | 1.00198.56 | B | C |
| ATOM | 9772 | CA | LEU | B2252 | -7.896 | -76.844 | 35.924 | 1.00196.77 | B | C |
| ATOM | 9780 | CA | THR | B2253 | -4.321 | -75.638 | 36.707 | 1.00195.58 | B | C |
| ATOM | 9787 | CA | SER | B2254 | -1.878 | -72.917 | 35.652 | 1.00195.03 | B | C |
| ATOM | 9793 | CA | MET | B2255 | -0.358 | -73.072 | 32.131 | 1.00194.00 | B | C |
| ATOM | 9801 | CA | TYR | B2256 | 2.354 | -70.851 | 30.537 | 1.00193.66 | B | C |
| ATOM | 9813 | CA | VAL | B2257 | 5.642 | -70.902 | 28.563 | 1.00193.13 | B | C |
| ATOM | 9820 | CA | LYS | B2258 | 8.894 | -70.157 | 30.429 | 1.00194.65 | B | C |
| ATOM | 9829 | CA | GLU | B2259 | 11.455 | -69.830 | 27.563 | 1.00195.23 | B | C |
| ATOM | 9838 | CA | PHE | B2260 | 11.188 | -69.667 | 23.779 | 1.00195.79 | B | C |
| ATOM | 9849 | CA | LEU | B2261 | 12.803 | -69.070 | 20.375 | 1.00196.73 | B | C |
| ATOM | 9857 | CA | ILE | B2262 | 11.611 | -67.256 | 17.259 | 1.00198.66 | B | C |
| ATOM | 9865 | CA | SER | B2263 | 11.948 | -67.847 | 13.512 | 1.00201.48 | B | C |
| ATOM | 9871 | CA | SER | B2264 | 11.475 | -65.538 | 10.489 | 1.00203.30 | B | C |
| ATOM | 9877 | CA | SER | B2265 | 10.651 | -66.059 | 6.809 | 1.00204.28 | B | C |

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|------|-------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 9883 | CA | GLN | B2266 | 9.941 | -64.168 | 3.589 | 1.00204.49 | B | C |
| ATOM | 9892 | CA | ASP | B2267 | 8.832 | -67.220 | 1.604 | 1.00205.11 | B | C |
| ATOM | 9900 | CA | GLY | B2268 | 6.702 | -68.720 | 4.412 | 1.00205.35 | B | C |
| ATOM | 9904 | CA | HIS | B2269 | 7.916 | -72.286 | 3.770 | 1.00205.19 | B | C |
| ATOM | 9914 | CA | GLN | B2270 | 11.631 | -72.091 | 4.737 | 1.00203.80 | B | C |
| ATOM | 9923 | CA | TRP | B2271 | 12.915 | -70.403 | 7.870 | 1.00202.14 | B | C |
| ATOM | 9937 | CA | THR | B2272 | 15.841 | -68.212 | 8.952 | 0.50201.78 | B | C |
| ATOM | 9944 | CA | LEU | B2273 | 15.529 | -68.108 | 12.753 | 1.00202.29 | B | C |
| ATOM | 9952 | CA | PHE | B2274 | 16.448 | -65.422 | 15.347 | 1.00203.50 | B | C |
| ATOM | 9963 | CA | PHE | B2275 | 19.944 | -64.839 | 16.781 | 1.00204.77 | B | C |
| ATOM | 9974 | CA | GLN | B2276 | 21.785 | -62.892 | 19.470 | 1.00204.98 | B | C |
| ATOM | 9983 | CA | ASN | B2277 | 25.302 | -61.616 | 18.893 | 1.00204.12 | B | C |
| ATOM | 9991 | CA | GLY | B2278 | 26.266 | -65.300 | 19.089 | 1.00202.51 | B | C |
| ATOM | 9995 | CA | LYS | B2279 | 23.957 | -68.361 | 19.216 | 1.00200.38 | B | C |
| ATOM | 10004 | CA | VAL | B2280 | 20.137 | -68.397 | 19.225 | 1.00198.75 | B | C |
| ATOM | 10011 | CA | LYS | B2281 | 18.099 | -66.146 | 21.478 | 1.00198.21 | B | C |
| ATOM | 10020 | CA | VAL | B2282 | 16.996 | -67.876 | 24.672 | 1.00199.38 | B | C |
| ATOM | 10027 | CA | PHE | B2283 | 13.904 | -65.770 | 25.326 | 1.00200.49 | B | C |
| ATOM | 10038 | CA | GLN | B2284 | 12.877 | -64.686 | 28.821 | 1.00201.27 | B | C |
| ATOM | 10047 | CA | GLY | B2285 | 9.233 | -65.750 | 28.991 | 1.00201.80 | B | C |
| ATOM | 10051 | CA | ASN | B2286 | 6.246 | -66.026 | 31.323 | 1.00200.93 | B | C |
| ATOM | 10059 | CA | GLN | B2287 | 5.705 | -67.217 | 34.880 | 1.00199.79 | B | C |
| ATOM | 10068 | CA | ASP | B2288 | 1.868 | -67.194 | 35.296 | 1.00198.35 | B | C |
| ATOM | 10076 | CA | SER | B2289 | -1.632 | -67.908 | 33.951 | 1.00197.47 | B | C |
| ATOM | 10082 | CA | PHE | B2290 | -1.895 | -64.139 | 33.457 | 1.00196.39 | B | C |
| ATOM | 10093 | CA | THR | B2291 | 0.711 | -61.289 | 33.160 | 1.00194.75 | B | C |
| ATOM | 10100 | CA | PRO | B2292 | 2.168 | -60.432 | 29.773 | 1.00193.88 | B | C |
| ATOM | 10107 | CA | VAL | B2293 | 5.840 | -60.025 | 28.667 | 1.00194.34 | B | C |
| ATOM | 10114 | CA | VAL | B2294 | 7.613 | -56.870 | 27.208 | 1.00194.33 | B | C |
| ATOM | 10121 | CA | ASN | B2295 | 9.839 | -59.207 | 25.184 | 1.00194.09 | B | C |
| ATOM | 10129 | CA | SER | B2296 | 11.367 | -57.274 | 22.228 | 1.00193.84 | B | C |
| ATOM | 10135 | CA | LEU | B2297 | 14.050 | -57.754 | 19.569 | 1.00193.51 | B | C |
| ATOM | 10143 | CA | ASP | B2298 | 17.599 | -56.304 | 19.254 | 1.00193.37 | B | C |
| ATOM | 10151 | CA | PRO | B2299 | 17.620 | -56.136 | 15.490 | 1.00192.98 | B | C |
| ATOM | 10158 | CA | PRO | B2300 | 14.058 | -55.132 | 14.625 | 1.00191.99 | B | C |
| ATOM | 10165 | CA | LEU | B2301 | 13.034 | -58.140 | 12.521 | 1.00190.91 | B | C |
| ATOM | 10173 | CA | LEU | B2302 | 11.692 | -57.365 | 9.034 | 1.00190.03 | B | C |
| ATOM | 10181 | CA | THR | B2303 | 9.485 | -60.322 | 8.044 | 1.00189.60 | B | C |
| ATOM | 10188 | CA | ARG | B2304 | 6.020 | -61.641 | 7.049 | 1.00189.44 | B | C |
| ATOM | 10199 | CA | TYR | B2305 | 6.110 | -65.086 | 8.553 | 1.00188.82 | B | C |
| ATOM | 10211 | CA | LEU | B2306 | 6.657 | -65.151 | 12.295 | 1.00189.19 | B | C |
| ATOM | 10219 | CA | ARG | B2307 | 6.917 | -68.439 | 14.213 | 1.00190.30 | B | C |
| ATOM | 10230 | CA | ILE | B2308 | 6.983 | -68.918 | 17.983 | 1.00192.07 | B | C |
| ATOM | 10238 | CA | HIS | B2309 | 9.292 | -71.661 | 19.251 | 1.00194.02 | B | C |
| ATOM | 10248 | CA | PRO | B2310 | 8.533 | -72.780 | 22.844 | 1.00194.00 | B | C |
| ATOM | 10255 | CA | GLN | B2311 | 11.488 | -74.234 | 24.698 | 1.00194.68 | B | C |
| ATOM | 10264 | CA | SER | B2312 | 10.684 | -74.540 | 28.380 | 1.00195.72 | B | C |
| ATOM | 10270 | CA | TRP | B2313 | 7.304 | -74.322 | 30.003 | 1.00196.64 | B | C |
| ATOM | 10284 | CA | VAL | B2314 | 5.314 | -74.891 | 33.223 | 1.00196.07 | B | C |
| ATOM | 10291 | CA | HIS | B2315 | 2.658 | -77.663 | 33.172 | 1.00195.25 | B | C |
| ATOM | 10301 | CA | GLN | B2316 | 1.710 | -77.810 | 29.500 | 1.00195.26 | B | C |
| ATOM | 10310 | CA | ILE | B2317 | 2.660 | -75.583 | 26.595 | 1.00194.25 | B | C |
| ATOM | 10318 | CA | ALA | B2318 | 0.018 | -72.817 | 26.585 | 1.00193.92 | B | C |
| ATOM | 10323 | CA | LEU | B2319 | -0.035 | -69.571 | 24.653 | 1.00194.14 | B | C |
| ATOM | 10331 | CA | ARG | B2320 | -2.035 | -66.379 | 24.567 | 1.00195.06 | B | C |
| ATOM | 10342 | CA | MET | B2321 | 0.098 | -63.779 | 22.773 | 1.00196.84 | B | C |

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|------|-------|----|-----|-------|--------|---------|--------|------------|---|---|
| ATOM | 10350 | CA | GLU | B2322 | 0.543 | -60.604 | 20.691 | 1.00197.25 | B | C |
| ATOM | 10359 | CA | VAL | B2323 | 3.076 | -59.011 | 18.253 | 1.00198.10 | B | C |
| ATOM | 10366 | CA | LEU | B2324 | 4.210 | -55.371 | 18.304 | 1.00199.76 | B | C |
| ATOM | 10374 | CA | GLY | B2325 | 4.918 | -53.408 | 15.120 | 1.00202.52 | B | C |
| ATOM | 10378 | CA | CYS | B2326 | 3.997 | -51.965 | 11.713 | 1.00205.82 | B | C |
| ATOM | 10384 | CA | GLU | B2327 | 5.488 | -52.341 | 8.154 | 1.00208.34 | B | C |
| ATOM | 10393 | CA | ALA | B2328 | 8.222 | -51.160 | 5.792 | 1.00210.38 | B | C |
| ATOM | 10398 | CA | GLN | B2329 | 7.872 | -51.667 | 1.994 | 1.00212.52 | B | C |
| ATOM | 10407 | CA | ASP | B2330 | 5.527 | -54.410 | 0.757 | 1.00214.46 | B | C |
| ATOM | 10415 | CA | LEU | B2331 | 7.427 | -57.663 | 0.059 | 1.00214.86 | B | C |
| ATOM | 10423 | CA | TYR | B2332 | 10.012 | -56.216 | -2.399 | 1.00215.21 | B | C |

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File (2 of 2): hum_FIX_ca.pdb

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|------|-----|----|-----|---|----|---------|---------|--------|------|-------|---|---|
| ATOM | 2 | CA | TYR | L | 1 | -11.903 | -22.407 | 62.876 | 0.00 | 20.00 | L | C |
| ATOM | 14 | CA | ASN | L | 2 | -14.733 | -24.931 | 63.207 | 0.00 | 20.00 | L | C |
| ATOM | 22 | CA | SER | L | 3 | -13.923 | -26.175 | 66.702 | 0.00 | 20.00 | L | C |
| ATOM | 28 | CA | GLY | L | 4 | -16.352 | -24.663 | 69.209 | 0.00 | 20.00 | L | C |
| ATOM | 32 | CA | LYS | L | 5 | -19.741 | -26.355 | 69.378 | 0.00 | 20.00 | L | C |
| ATOM | 41 | CA | LEU | L | 6 | -22.128 | -26.324 | 66.416 | 0.00 | 20.00 | L | C |
| ATOM | 49 | CA | CGU | L | 7 | -20.646 | -23.372 | 64.562 | 0.00 | 20.00 | L | C |
| ATOM | 61 | CA | CGU | L | 8 | -21.401 | -24.669 | 61.107 | 0.00 | 20.00 | L | C |
| ATOM | 73 | CA | PHE | L | 9 | -25.088 | -24.347 | 61.958 | 0.00 | 20.00 | L | C |
| ATOM | 84 | CA | VAL | L | 10 | -24.708 | -20.564 | 61.971 | 0.00 | 20.00 | L | C |
| ATOM | 91 | CA | GLN | L | 11 | -24.564 | -18.360 | 58.877 | 0.00 | 20.00 | L | C |
| ATOM | 100 | CA | GLY | L | 12 | -20.920 | -17.835 | 57.999 | 0.00 | 20.00 | L | C |
| ATOM | 104 | CA | ASN | L | 13 | -19.433 | -14.580 | 59.227 | 0.00 | 20.00 | L | C |
| ATOM | 112 | CA | LEU | L | 14 | -16.028 | -14.296 | 57.636 | 0.00 | 20.00 | L | C |
| ATOM | 120 | CA | CGU | L | 15 | -15.026 | -11.502 | 59.994 | 0.00 | 20.00 | L | C |
| ATOM | 132 | CA | ARG | L | 16 | -15.074 | -14.375 | 62.436 | 0.00 | 20.00 | L | C |
| ATOM | 143 | CA | CGU | L | 17 | -13.861 | -17.493 | 60.654 | 0.00 | 20.00 | L | C |
| ATOM | 155 | CA | CYS | L | 18 | -11.198 | -16.217 | 58.262 | 0.00 | 20.00 | L | C |
| ATOM | 161 | CA | MET | L | 19 | -8.670 | -13.957 | 59.980 | 0.00 | 20.00 | L | C |
| ATOM | 169 | CA | CGU | L | 20 | -8.995 | -15.066 | 63.450 | 0.00 | 20.00 | L | C |

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|------|-----|----|-----|---|----|---------|---------|--------|------|-------|---|---|
| ATOM | 181 | CA | CGU | L | 21 | -6.688 | -17.937 | 63.266 | 0.00 | 20.00 | L | C |
| ATOM | 193 | CA | LYS | L | 22 | -6.985 | -18.434 | 59.495 | 0.00 | 20.00 | L | C |
| ATOM | 202 | CA | CYS | L | 23 | -9.934 | -19.774 | 57.467 | 0.00 | 20.00 | L | C |
| ATOM | 208 | CA | SER | L | 24 | -10.323 | -22.282 | 54.685 | 0.00 | 20.00 | L | C |
| ATOM | 214 | CA | PHE | L | 25 | -11.401 | -21.249 | 51.211 | 0.00 | 20.00 | L | C |
| ATOM | 225 | CA | CGU | L | 26 | -14.798 | -22.889 | 51.571 | 0.00 | 20.00 | L | C |
| ATOM | 237 | CA | CGU | L | 27 | -15.547 | -21.171 | 54.800 | 0.00 | 20.00 | L | C |
| ATOM | 249 | CA | ALA | L | 28 | -14.613 | -18.008 | 52.931 | 0.00 | 20.00 | L | C |
| ATOM | 254 | CA | ARG | L | 29 | -16.656 | -18.912 | 49.882 | 0.00 | 20.00 | L | C |
| ATOM | 265 | CA | CGU | L | 30 | -20.127 | -19.681 | 51.278 | 0.00 | 20.00 | L | C |
| ATOM | 277 | CA | VAL | L | 31 | -19.777 | -16.421 | 53.188 | 0.00 | 20.00 | L | C |
| ATOM | 284 | CA | PHE | L | 32 | -18.686 | -14.378 | 50.212 | 0.00 | 20.00 | L | C |
| ATOM | 295 | CA | CGU | L | 33 | -21.246 | -15.728 | 47.690 | 0.00 | 20.00 | L | C |
| ATOM | 307 | CA | ASN | L | 34 | -19.780 | -13.991 | 44.623 | 0.00 | 20.00 | L | C |
| ATOM | 315 | CA | THR | L | 35 | -16.799 | -16.043 | 43.909 | 0.00 | 20.00 | L | C |
| ATOM | 322 | CA | CGU | L | 36 | -15.098 | -13.829 | 41.589 | 0.00 | 20.00 | L | C |
| ATOM | 334 | CA | ARG | L | 37 | -14.697 | -11.708 | 44.749 | 0.00 | 20.00 | L | C |
| ATOM | 345 | CA | THR | L | 38 | -13.397 | -14.750 | 46.646 | 0.00 | 20.00 | L | C |
| ATOM | 352 | CA | THR | L | 39 | -10.651 | -15.559 | 44.140 | 0.00 | 20.00 | L | C |
| ATOM | 359 | CA | CGU | L | 40 | -8.942 | -12.249 | 44.871 | 0.00 | 20.00 | L | C |
| ATOM | 371 | CA | PHE | L | 41 | -9.745 | -11.782 | 48.582 | 0.00 | 20.00 | L | C |
| ATOM | 382 | CA | TRP | L | 42 | -7.683 | -14.780 | 48.101 | 0.00 | 20.00 | L | C |
| ATOM | 396 | CA | LYS | L | 43 | -4.440 | -14.238 | 46.180 | 0.00 | 20.00 | L | C |
| ATOM | 405 | CA | GLN | L | 44 | -2.758 | -12.029 | 49.129 | 1.00 | 77.52 | L | C |
| ATOM | 414 | CA | TYR | L | 45 | -3.002 | -14.792 | 51.646 | 1.00 | 71.96 | L | C |
| ATOM | 426 | CA | VAL | L | 46 | -0.738 | -17.621 | 50.562 | 1.00 | 65.51 | L | C |
| ATOM | 433 | CA | ASP | L | 47 | 1.260 | -17.829 | 47.433 | 1.00 | 61.31 | L | C |
| ATOM | 441 | CA | GLY | L | 48 | 4.291 | -15.591 | 47.638 | 1.00 | 60.76 | L | C |
| ATOM | 445 | CA | ASP | L | 49 | 2.514 | -12.592 | 46.340 | 1.00 | 64.96 | L | C |
| ATOM | 453 | CA | GLN | L | 50 | 3.910 | -12.193 | 42.933 | 1.00 | 68.13 | L | C |
| ATOM | 462 | CA | CYS | L | 51 | 3.558 | -8.528 | 43.453 | 1.00 | 70.91 | L | C |
| ATOM | 468 | CA | GLU | L | 52 | 6.238 | -8.630 | 46.176 | 1.00 | 67.41 | L | C |
| ATOM | 477 | CA | SER | L | 53 | 8.193 | -5.401 | 46.378 | 1.00 | 63.27 | L | C |
| ATOM | 483 | CA | ASN | L | 54 | 6.096 | -3.611 | 43.770 | 1.00 | 60.24 | L | C |
| ATOM | 491 | CA | PRO | L | 55 | 7.732 | -4.276 | 40.473 | 1.00 | 57.26 | L | C |
| ATOM | 498 | CA | CYS | L | 56 | 5.953 | -1.705 | 38.417 | 1.00 | 55.33 | L | C |
| ATOM | 504 | CA | LEU | L | 57 | 7.373 | 1.699 | 39.004 | 1.00 | 48.99 | L | C |
| ATOM | 512 | CA | ASN | L | 58 | 6.409 | 5.053 | 37.634 | 1.00 | 41.04 | L | C |
| ATOM | 520 | CA | GLY | L | 59 | 3.403 | 5.012 | 39.903 | 1.00 | 35.19 | L | C |
| ATOM | 524 | CA | GLY | L | 60 | 2.311 | 1.773 | 38.359 | 1.00 | 34.69 | L | C |
| ATOM | 528 | CA | SER | L | 61 | -0.230 | -0.151 | 40.319 | 1.00 | 40.14 | L | C |
| ATOM | 534 | CA | CYS | L | 62 | 0.741 | -3.775 | 40.722 | 1.00 | 49.20 | L | C |
| ATOM | 540 | CA | LYS | L | 63 | -2.113 | -6.210 | 40.764 | 1.00 | 55.02 | L | C |
| ATOM | 549 | CA | ASP | L | 64 | -1.162 | -9.721 | 41.844 | 1.00 | 56.11 | L | C |
| ATOM | 557 | CA | ASP | L | 65 | -3.043 | -12.833 | 40.770 | 1.00 | 53.75 | L | C |
| ATOM | 565 | CA | ILE | L | 66 | -2.945 | -16.409 | 41.780 | 1.00 | 50.15 | L | C |
| ATOM | 573 | CA | ASN | L | 67 | -0.473 | -17.330 | 39.069 | 1.00 | 49.73 | L | C |
| ATOM | 581 | CA | SER | L | 68 | 0.850 | -14.054 | 37.775 | 1.00 | 53.17 | L | C |
| ATOM | 587 | CA | TYR | L | 69 | 0.418 | -10.354 | 38.203 | 1.00 | 58.65 | L | C |
| ATOM | 599 | CA | GLU | L | 70 | -0.094 | -7.370 | 35.926 | 1.00 | 65.74 | L | C |
| ATOM | 608 | CA | CYS | L | 71 | 0.639 | -3.718 | 35.978 | 1.00 | 72.65 | L | C |
| ATOM | 614 | CA | TRP | L | 72 | -1.651 | -0.758 | 35.555 | 1.00 | 75.88 | L | C |
| ATOM | 628 | CA | CYS | L | 73 | 0.471 | 2.132 | 34.287 | 1.00 | 76.13 | L | C |
| ATOM | 634 | CA | PRO | L | 74 | -2.296 | 4.674 | 33.803 | 1.00 | 70.38 | L | C |
| ATOM | 641 | CA | PHE | L | 75 | -0.551 | 7.319 | 31.703 | 1.00 | 60.33 | L | C |
| ATOM | 652 | CA | GLY | L | 76 | 2.736 | 8.060 | 29.957 | 1.00 | 49.94 | L | C |

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|------|------|----|-----|---|-----|---------|--------|--------|------|-------|---|---|
| ATOM | 656 | CA | PHE | L | 77 | 4.337 | 4.715 | 30.691 | 1.00 | 42.59 | L | C |
| ATOM | 667 | CA | GLU | L | 78 | 4.483 | 1.481 | 28.728 | 1.00 | 39.90 | L | C |
| ATOM | 676 | CA | GLY | L | 79 | 5.984 | -1.932 | 29.330 | 1.00 | 42.50 | L | C |
| ATOM | 680 | CA | LYS | L | 80 | 5.148 | -4.752 | 31.684 | 1.00 | 49.57 | L | C |
| ATOM | 689 | CA | ASN | L | 81 | 6.727 | -2.826 | 34.514 | 1.00 | 54.54 | L | C |
| ATOM | 697 | CA | CYS | L | 82 | 5.918 | 0.661 | 33.259 | 1.00 | 56.77 | L | C |
| ATOM | 703 | CA | GLU | L | 83 | 9.628 | 1.098 | 32.599 | 1.00 | 53.34 | L | C |
| ATOM | 712 | CA | LEU | L | 84 | 9.300 | 2.485 | 29.135 | 1.00 | 46.85 | L | C |
| ATOM | 720 | CA | ASP | L | 85 | 7.777 | 5.830 | 28.413 | 1.00 | 44.25 | L | C |
| ATOM | 728 | CA | VAL | L | 86 | 4.729 | 5.989 | 26.236 | 1.00 | 44.53 | L | C |
| ATOM | 735 | CA | THR | L | 87 | 5.442 | 7.185 | 22.743 | 1.00 | 50.39 | L | C |
| ATOM | 742 | CA | CYS | L | 88 | 2.581 | 8.199 | 20.499 | 1.00 | 55.43 | L | C |
| ATOM | 748 | CA | ASN | L | 89 | 3.450 | 5.500 | 17.961 | 1.00 | 55.55 | L | C |
| ATOM | 756 | CA | ILE | L | 90 | 2.942 | 2.475 | 20.200 | 1.00 | 54.30 | L | C |
| ATOM | 764 | CA | LYS | L | 91 | -0.731 | 1.661 | 20.745 | 1.00 | 49.92 | L | C |
| ATOM | 773 | CA | ASN | L | 92 | -1.861 | 5.234 | 20.128 | 1.00 | 47.76 | L | C |
| ATOM | 781 | CA | GLY | L | 93 | 0.036 | 6.310 | 23.212 | 1.00 | 48.66 | L | C |
| ATOM | 785 | CA | ARG | L | 94 | -2.821 | 4.778 | 25.189 | 1.00 | 52.01 | L | C |
| ATOM | 796 | CA | CYS | L | 95 | -4.893 | 7.862 | 24.407 | 1.00 | 56.98 | L | C |
| ATOM | 802 | CA | GLU | L | 96 | -8.445 | 7.258 | 23.348 | 1.00 | 62.68 | L | C |
| ATOM | 811 | CA | GLN | L | 97 | -8.471 | 10.020 | 20.823 | 1.00 | 66.16 | L | C |
| ATOM | 820 | CA | PHE | L | 98 | -5.394 | 12.014 | 19.952 | 1.00 | 65.53 | L | C |
| ATOM | 831 | CA | CYS | L | 99 | -1.814 | 11.821 | 21.141 | 1.00 | 62.50 | L | C |
| ATOM | 837 | CA | LYS | L | 100 | 1.114 | 14.081 | 20.433 | 1.00 | 54.39 | L | C |
| ATOM | 846 | CA | ASN | L | 101 | 4.541 | 14.228 | 21.963 | 1.00 | 49.45 | L | C |
| ATOM | 854 | CA | SER | L | 102 | 5.760 | 17.612 | 23.035 | 1.00 | 47.64 | L | C |
| ATOM | 860 | CA | ALA | L | 103 | 7.804 | 19.736 | 25.429 | 1.00 | 48.96 | L | C |
| ATOM | 865 | CA | ASP | L | 104 | 9.513 | 16.493 | 26.313 | 1.00 | 55.89 | L | C |
| ATOM | 873 | CA | ASN | L | 105 | 9.468 | 12.819 | 25.297 | 1.00 | 58.75 | L | C |
| ATOM | 881 | CA | LYS | L | 106 | 6.211 | 11.792 | 27.001 | 1.00 | 61.24 | L | C |
| ATOM | 890 | CA | VAL | L | 107 | 2.766 | 11.530 | 25.439 | 1.00 | 59.90 | L | C |
| ATOM | 897 | CA | VAL | L | 108 | 0.019 | 14.093 | 25.817 | 1.00 | 55.63 | L | C |
| ATOM | 904 | CA | CYS | L | 109 | -3.553 | 13.120 | 25.040 | 1.00 | 53.26 | L | C |
| ATOM | 910 | CA | SER | L | 110 | -6.363 | 15.241 | 23.675 | 1.00 | 48.30 | L | C |
| ATOM | 916 | CA | CYS | L | 111 | -9.876 | 15.003 | 22.299 | 1.00 | 45.61 | L | C |
| ATOM | 922 | CA | THR | L | 112 | -11.903 | 16.504 | 19.463 | 1.00 | 43.15 | L | C |
| ATOM | 929 | CA | GLU | L | 113 | -13.962 | 19.608 | 19.976 | 1.00 | 42.73 | L | C |
| ATOM | 938 | CA | GLY | L | 114 | -16.918 | 18.724 | 22.114 | 1.00 | 44.12 | L | C |
| ATOM | 942 | CA | TYR | L | 115 | -15.046 | 16.205 | 24.216 | 1.00 | 45.45 | L | C |
| ATOM | 954 | CA | ARG | L | 116 | -12.942 | 16.686 | 27.313 | 1.00 | 46.29 | L | C |
| ATOM | 965 | CA | LEU | L | 117 | -10.060 | 14.661 | 28.682 | 1.00 | 43.61 | L | C |
| ATOM | 973 | CA | ALA | L | 118 | -11.015 | 12.340 | 31.510 | 1.00 | 42.30 | L | C |
| ATOM | 978 | CA | GLU | L | 119 | -9.224 | 12.151 | 34.845 | 1.00 | 43.55 | L | C |
| ATOM | 987 | CA | ASN | L | 120 | -7.110 | 9.231 | 33.631 | 1.00 | 45.00 | L | C |
| ATOM | 995 | CA | GLN | L | 121 | -5.886 | 11.617 | 30.939 | 1.00 | 49.29 | L | C |
| ATOM | 1004 | CA | LYS | L | 122 | -6.461 | 8.887 | 28.365 | 1.00 | 51.17 | L | C |
| ATOM | 1013 | CA | SER | L | 123 | -10.192 | 9.009 | 27.731 | 1.00 | 50.00 | L | C |
| ATOM | 1019 | CA | CYS | L | 124 | -12.680 | 11.457 | 26.328 | 1.00 | 51.80 | L | C |
| ATOM | 1025 | CA | GLU | L | 125 | -15.970 | 12.462 | 27.912 | 1.00 | 53.44 | L | C |
| ATOM | 1034 | CA | PRO | L | 126 | -18.439 | 14.762 | 26.298 | 1.00 | 59.94 | L | C |
| ATOM | 1041 | CA | ALA | L | 127 | -18.471 | 18.519 | 26.853 | 1.00 | 69.67 | L | C |
| ATOM | 1046 | CA | VAL | L | 128 | -21.919 | 19.051 | 25.405 | 1.00 | 77.69 | L | C |
| ATOM | 1053 | CA | PRO | L | 129 | -25.135 | 17.220 | 25.247 | 1.00 | 83.75 | L | C |
| ATOM | 1060 | CA | PHE | L | 130 | -24.625 | 16.007 | 21.675 | 1.00 | 81.95 | L | C |
| ATOM | 1071 | CA | PRO | L | 131 | -20.958 | 15.649 | 20.968 | 1.00 | 75.59 | L | C |
| ATOM | 1078 | CA | CYS | L | 132 | -19.705 | 15.053 | 17.453 | 1.00 | 67.59 | L | C |

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|------|------|----|-----|---|-----|---------|--------|--------|------|-------|------|---|
| ATOM | 1084 | CA | GLY | L | 133 | -20.125 | 11.752 | 15.664 | 1.00 | 59.21 | L | C |
| ATOM | 1088 | CA | ARG | L | 134 | -22.274 | 9.683 | 17.948 | 1.00 | 54.78 | L | C |
| ATOM | 1099 | CA | VAL | L | 135 | -25.397 | 7.839 | 16.955 | 1.00 | 49.62 | L | C |
| ATOM | 1106 | CA | SER | L | 136 | -27.832 | 9.118 | 19.563 | 1.00 | 44.09 | L | C |
| ATOM | 1112 | CA | VAL | L | 137 | -30.892 | 6.980 | 18.992 | 1.00 | 41.34 | L | C |
| ATOM | 1119 | CA | SER | L | 138 | -29.209 | 3.730 | 19.876 | 1.00 | 41.02 | L | C |
| ATOM | 1125 | CA | GLN | L | 139 | -27.401 | 5.037 | 22.938 | 1.00 | 45.18 | L | C |
| ATOM | 1134 | CA | THR | L | 140 | -30.320 | 6.907 | 24.416 | 1.00 | 51.68 | L | C |
| ATOM | 1141 | CA | SER | L | 141 | -31.577 | 4.118 | 26.563 | 1.00 | 55.54 | L | C |
| ATOM | 1147 | CA | LYS | L | 142 | -29.936 | 0.805 | 25.799 | 1.00 | 55.44 | L | C |
| ATOM | 1156 | CA | LEU | L | 143 | -27.852 | -0.129 | 22.765 | 1.00 | 52.82 | L | C |
| ATOM | 1164 | CA | THR | L | 144 | -29.253 | -1.816 | 19.695 | 1.00 | 49.76 | L | C |
| ATOM | 1171 | CA | ARG | L | 145 | -29.117 | -5.558 | 19.378 | 1.00 | 45.81 | L | C |
| ATOM | 1184 | CA | VAL | B | 146 | -26.580 | 4.816 | -3.602 | 1.00 | 41.72 | BHUM | C |
| ATOM | 1191 | CA | VAL | B | 147 | -26.513 | 1.774 | -5.788 | 1.00 | 37.81 | BHUM | C |
| ATOM | 1198 | CA | GLY | B | 148 | -26.601 | -1.646 | -4.189 | 1.00 | 32.34 | BHUM | C |
| ATOM | 1202 | CA | GLY | B | 149 | -26.741 | -0.227 | -0.694 | 1.00 | 29.32 | BHUM | C |
| ATOM | 1206 | CA | GLU | B | 150 | -29.290 | -0.738 | 2.041 | 1.00 | 29.21 | BHUM | C |
| ATOM | 1215 | CA | ASP | B | 151 | -31.797 | 1.409 | 3.893 | 1.00 | 29.55 | BHUM | C |
| ATOM | 1223 | CA | ALA | B | 152 | -30.570 | 3.278 | 6.944 | 1.00 | 30.32 | BHUM | C |
| ATOM | 1228 | CA | LYS | B | 153 | -32.405 | 3.410 | 10.242 | 1.00 | 32.09 | BHUM | C |
| ATOM | 1237 | CA | PRO | B | 154 | -33.740 | 6.753 | 11.258 | 1.00 | 33.90 | BHUM | C |
| ATOM | 1244 | CA | GLY | B | 155 | -31.364 | 8.530 | 13.589 | 1.00 | 38.62 | BHUM | C |
| ATOM | 1248 | CA | GLN | B | 156 | -28.492 | 6.386 | 12.370 | 1.00 | 47.92 | BHUM | C |
| ATOM | 1257 | CA | PHE | B | 157 | -26.840 | 9.326 | 10.653 | 1.00 | 55.55 | BHUM | C |
| ATOM | 1268 | CA | PRO | B | 158 | -27.187 | 12.516 | 12.647 | 1.00 | 62.02 | BHUM | C |
| ATOM | 1275 | CA | TRP | B | 159 | -24.859 | 14.397 | 10.283 | 1.00 | 62.57 | BHUM | C |
| ATOM | 1289 | CA | GLN | B | 160 | -26.429 | 13.307 | 7.024 | 1.00 | 57.03 | BHUM | C |
| ATOM | 1298 | CA | VAL | B | 161 | -28.120 | 16.285 | 5.522 | 1.00 | 51.22 | BHUM | C |
| ATOM | 1305 | CA | VAL | B | 162 | -30.275 | 16.559 | 2.418 | 1.00 | 43.03 | BHUM | C |
| ATOM | 1312 | CA | LEU | B | 163 | -29.572 | 19.465 | 0.163 | 1.00 | 37.99 | BHUM | C |
| ATOM | 1320 | CA | ASN | B | 164 | -32.562 | 20.872 | -1.657 | 1.00 | 34.59 | BHUM | C |
| ATOM | 1328 | CA | GLY | B | 165 | -32.136 | 23.460 | -4.332 | 1.00 | 32.49 | BHUM | C |
| ATOM | 1332 | CA | LYS | B | 166 | -33.052 | 23.773 | -7.924 | 1.00 | 34.33 | BHUM | C |
| ATOM | 1341 | CA | VAL | B | 167 | -34.903 | 20.512 | -8.507 | 1.00 | 37.11 | BHUM | C |
| ATOM | 1348 | CA | ASP | B | 168 | -34.104 | 19.438 | -4.914 | 1.00 | 42.34 | BHUM | C |
| ATOM | 1356 | CA | ALA | B | 169 | -32.277 | 16.326 | -3.681 | 1.00 | 45.55 | BHUM | C |
| ATOM | 1361 | CA | PHE | B | 170 | -29.354 | 17.295 | -5.876 | 1.00 | 46.19 | BHUM | C |
| ATOM | 1372 | CA | CYS | B | 171 | -26.745 | 16.851 | -3.184 | 1.00 | 45.03 | BHUM | C |
| ATOM | 1378 | CA | GLY | B | 172 | -26.122 | 15.797 | 0.375 | 1.00 | 42.18 | BHUM | C |
| ATOM | 1382 | CA | GLY | B | 173 | -23.973 | 17.318 | 3.069 | 1.00 | 42.62 | BHUM | C |
| ATOM | 1386 | CA | SER | B | 174 | -22.616 | 16.766 | 6.550 | 1.00 | 48.57 | BHUM | C |
| ATOM | 1392 | CA | ILE | B | 175 | -23.060 | 19.003 | 9.528 | 1.00 | 56.97 | BHUM | C |
| ATOM | 1400 | CA | VAL | B | 176 | -19.804 | 20.377 | 10.821 | 1.00 | 66.04 | BHUM | C |
| ATOM | 1407 | CA | ASN | B | 177 | -21.623 | 22.359 | 13.450 | 1.00 | 74.73 | BHUM | C |
| ATOM | 1415 | CA | GLU | B | 178 | -24.969 | 23.945 | 14.301 | 1.00 | 76.40 | BHUM | C |
| ATOM | 1424 | CA | LYS | B | 179 | -24.320 | 26.882 | 11.923 | 1.00 | 75.56 | BHUM | C |
| ATOM | 1433 | CA | TRP | B | 180 | -22.317 | 25.408 | 9.031 | 1.00 | 72.88 | BHUM | C |
| ATOM | 1447 | CA | ILE | B | 181 | -22.740 | 22.276 | 6.975 | 1.00 | 65.94 | BHUM | C |
| ATOM | 1455 | CA | VAL | B | 182 | -20.292 | 20.801 | 4.476 | 1.00 | 60.24 | BHUM | C |
| ATOM | 1462 | CA | THR | B | 183 | -20.792 | 19.596 | 0.905 | 1.00 | 55.63 | BHUM | C |
| ATOM | 1469 | CA | ALA | B | 184 | -18.954 | 19.337 | -2.389 | 1.00 | 52.59 | BHUM | C |
| ATOM | 1474 | CA | ALA | B | 185 | -18.229 | 22.499 | -4.364 | 1.00 | 52.60 | BHUM | C |
| ATOM | 1479 | CA | HIS | B | 186 | -19.751 | 21.090 | -7.534 | 1.00 | 53.30 | BHUM | C |
| ATOM | 1489 | CA | CYS | B | 187 | -23.123 | 21.338 | -5.780 | 1.00 | 52.43 | BHUM | C |
| ATOM | 1495 | CA | VAL | B | 188 | -23.103 | 25.114 | -5.760 | 1.00 | 47.33 | BHUM | C |

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|------|------|----|-----|---|-----|---------|--------|---------|------|-------|------|---|
| ATOM | 1502 | CA | GLU | B | 189 | -24.952 | 26.220 | -8.835 | 1.00 | 42.16 | BHUM | C |
| ATOM | 1511 | CA | THR | B | 190 | -24.751 | 29.929 | -9.336 | 1.00 | 37.86 | BHUM | C |
| ATOM | 1518 | CA | GLY | B | 191 | -27.946 | 31.808 | -8.680 | 1.00 | 34.83 | BHUM | C |
| ATOM | 1522 | CA | VAL | B | 192 | -29.764 | 29.053 | -6.877 | 1.00 | 37.64 | BHUM | C |
| ATOM | 1529 | CA | LYS | B | 193 | -31.046 | 29.083 | -3.324 | 1.00 | 41.47 | BHUM | C |
| ATOM | 1538 | CA | ILE | B | 194 | -30.239 | 26.044 | -1.257 | 1.00 | 45.70 | BHUM | C |
| ATOM | 1546 | CA | THR | B | 195 | -32.051 | 24.763 | 1.770 | 1.00 | 50.20 | BHUM | C |
| ATOM | 1553 | CA | VAL | B | 196 | -30.447 | 22.213 | 4.051 | 1.00 | 50.86 | BHUM | C |
| ATOM | 1560 | CA | VAL | B | 197 | -32.825 | 19.554 | 5.236 | 1.00 | 50.38 | BHUM | C |
| ATOM | 1567 | CA | ALA | B | 198 | -31.363 | 18.272 | 8.464 | 1.00 | 50.98 | BHUM | C |
| ATOM | 1572 | CA | GLY | B | 199 | -33.086 | 15.359 | 10.159 | 1.00 | 51.77 | BHUM | C |
| ATOM | 1576 | CA | GLU | B | 200 | -34.783 | 14.232 | 6.944 | 1.00 | 55.95 | BHUM | C |
| ATOM | 1585 | CA | HIS | B | 201 | -35.412 | 10.469 | 6.540 | 1.00 | 56.75 | BHUM | C |
| ATOM | 1595 | CA | ASN | B | 202 | -38.076 | 9.690 | 3.942 | 1.00 | 53.42 | BHUM | C |
| ATOM | 1603 | CA | ILE | B | 203 | -38.746 | 12.193 | 1.223 | 1.00 | 48.18 | BHUM | C |
| ATOM | 1611 | CA | GLU | B | 204 | -42.309 | 11.002 | 0.782 | 1.00 | 40.46 | BHUM | C |
| ATOM | 1620 | CA | GLU | B | 205 | -43.268 | 11.709 | 4.358 | 1.00 | 36.46 | BHUM | C |
| ATOM | 1629 | CA | THR | B | 206 | -42.679 | 14.693 | 6.573 | 1.00 | 34.92 | BHUM | C |
| ATOM | 1636 | CA | GLU | B | 207 | -40.553 | 13.628 | 9.491 | 1.00 | 35.77 | BHUM | C |
| ATOM | 1645 | CA | HIS | B | 208 | -40.970 | 15.747 | 12.605 | 1.00 | 36.65 | BHUM | C |
| ATOM | 1655 | CA | THR | B | 209 | -37.200 | 15.700 | 12.997 | 1.00 | 36.47 | BHUM | C |
| ATOM | 1662 | CA | GLU | B | 210 | -36.624 | 17.688 | 9.803 | 1.00 | 36.36 | BHUM | C |
| ATOM | 1671 | CA | GLN | B | 211 | -35.042 | 21.094 | 10.281 | 1.00 | 34.90 | BHUM | C |
| ATOM | 1680 | CA | LYS | B | 212 | -34.745 | 23.221 | 7.178 | 1.00 | 36.49 | BHUM | C |
| ATOM | 1689 | CA | ARG | B | 213 | -32.411 | 26.155 | 6.873 | 1.00 | 39.33 | BHUM | C |
| ATOM | 1700 | CA | ASN | B | 214 | -31.317 | 28.513 | 4.153 | 1.00 | 44.05 | BHUM | C |
| ATOM | 1708 | CA | VAL | B | 215 | -27.762 | 29.046 | 3.046 | 1.00 | 49.17 | BHUM | C |
| ATOM | 1715 | CA | ILE | B | 216 | -26.669 | 32.626 | 3.336 | 1.00 | 49.75 | BHUM | C |
| ATOM | 1723 | CA | ARG | B | 217 | -23.151 | 31.969 | 2.151 | 1.00 | 48.97 | BHUM | C |
| ATOM | 1734 | CA | ILE | B | 218 | -21.418 | 29.253 | 0.196 | 1.00 | 44.61 | BHUM | C |
| ATOM | 1742 | CA | ILE | B | 219 | -17.663 | 29.292 | 0.405 | 1.00 | 40.54 | BHUM | C |
| ATOM | 1750 | CA | PRO | B | 220 | -16.108 | 26.834 | -1.932 | 1.00 | 39.16 | BHUM | C |
| ATOM | 1757 | CA | HIS | B | 221 | -12.487 | 25.961 | -1.367 | 1.00 | 40.05 | BHUM | C |
| ATOM | 1767 | CA | HIS | B | 222 | -10.409 | 28.876 | -2.529 | 1.00 | 43.01 | BHUM | C |
| ATOM | 1777 | CA | ASN | B | 223 | -8.591 | 26.985 | -5.206 | 1.00 | 45.75 | BHUM | C |
| ATOM | 1785 | CA | TYR | B | 224 | -11.574 | 24.938 | -6.235 | 1.00 | 47.29 | BHUM | C |
| ATOM | 1797 | CA | ASN | B | 225 | -11.768 | 25.382 | -9.968 | 1.00 | 46.58 | BHUM | C |
| ATOM | 1805 | CA | ALA | B | 226 | -10.962 | 28.458 | -11.993 | 1.00 | 47.24 | BHUM | C |
| ATOM | 1810 | CA | ALA | B | 227 | -11.380 | 26.418 | -15.145 | 1.00 | 51.24 | BHUM | C |
| ATOM | 1815 | CA | ILE | B | 228 | -9.777 | 23.050 | -14.632 | 1.00 | 62.90 | BHUM | C |
| ATOM | 1823 | CA | ASN | B | 229 | -10.485 | 19.661 | -13.118 | 1.00 | 76.57 | BHUM | C |
| ATOM | 1831 | CA | LYS | B | 230 | -13.855 | 20.381 | -11.500 | 1.00 | 87.60 | BHUM | C |
| ATOM | 1840 | CA | TYR | B | 231 | -13.233 | 17.572 | -9.015 | 1.00 | 93.56 | BHUM | C |
| ATOM | 1852 | CA | ASN | B | 232 | -10.041 | 18.658 | -7.336 | 1.00 | 86.51 | BHUM | C |
| ATOM | 1860 | CA | HIS | B | 233 | -10.746 | 20.845 | -4.307 | 1.00 | 75.45 | BHUM | C |
| ATOM | 1870 | CA | ASP | B | 234 | -14.384 | 19.771 | -4.713 | 1.00 | 62.48 | BHUM | C |
| ATOM | 1878 | CA | ILE | B | 235 | -15.490 | 20.864 | -1.229 | 1.00 | 50.02 | BHUM | C |
| ATOM | 1886 | CA | ALA | B | 236 | -17.497 | 23.776 | 0.114 | 1.00 | 43.88 | BHUM | C |
| ATOM | 1891 | CA | LEU | B | 237 | -18.964 | 25.137 | 3.331 | 1.00 | 41.85 | BHUM | C |
| ATOM | 1899 | CA | LEU | B | 238 | -22.574 | 26.245 | 3.620 | 1.00 | 42.10 | BHUM | C |
| ATOM | 1907 | CA | GLU | B | 239 | -23.398 | 28.753 | 6.320 | 1.00 | 42.92 | BHUM | C |
| ATOM | 1916 | CA | LEU | B | 240 | -26.940 | 28.359 | 7.537 | 1.00 | 42.04 | BHUM | C |
| ATOM | 1924 | CA | ASP | B | 241 | -28.701 | 31.541 | 8.563 | 1.00 | 38.87 | BHUM | C |
| ATOM | 1932 | CA | GLU | B | 242 | -30.251 | 30.231 | 11.743 | 1.00 | 36.71 | BHUM | C |
| ATOM | 1941 | CA | PRO | B | 243 | -28.591 | 27.687 | 13.880 | 1.00 | 35.38 | BHUM | C |
| ATOM | 1948 | CA | LEU | B | 244 | -29.961 | 24.172 | 13.873 | 1.00 | 36.27 | BHUM | C |

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|------|------|----|-----|---|-----|---------|--------|---------|------|-------|------|---|
| ATOM | 1956 | CA | VAL | B | 245 | -31.268 | 22.661 | 17.045 | 1.00 | 37.91 | BHUM | C |
| ATOM | 1963 | CA | LEU | B | 246 | -28.809 | 19.980 | 18.003 | 1.00 | 41.84 | BHUM | C |
| ATOM | 1971 | CA | ASN | B | 247 | -30.426 | 16.733 | 19.014 | 1.00 | 45.97 | BHUM | C |
| ATOM | 1979 | CA | SER | B | 248 | -30.253 | 12.982 | 18.566 | 1.00 | 49.72 | BHUM | C |
| ATOM | 1985 | CA | TYR | B | 249 | -31.374 | 13.656 | 15.005 | 1.00 | 54.15 | BHUM | C |
| ATOM | 1997 | CA | VAL | B | 250 | -29.100 | 16.615 | 14.424 | 1.00 | 54.23 | BHUM | C |
| ATOM | 2004 | CA | THR | B | 251 | -25.525 | 16.035 | 15.514 | 1.00 | 56.48 | BHUM | C |
| ATOM | 2011 | CA | PRO | B | 252 | -22.299 | 17.108 | 13.881 | 1.00 | 59.31 | BHUM | C |
| ATOM | 2018 | CA | ILE | B | 253 | -19.527 | 14.831 | 12.676 | 1.00 | 59.89 | BHUM | C |
| ATOM | 2026 | CA | CYS | B | 254 | -16.098 | 14.942 | 14.141 | 1.00 | 60.02 | BHUM | C |
| ATOM | 2032 | CA | ILE | B | 255 | -13.321 | 16.481 | 12.218 | 1.00 | 55.88 | BHUM | C |
| ATOM | 2040 | CA | ALA | B | 256 | -9.954 | 15.053 | 13.015 | 1.00 | 48.92 | BHUM | C |
| ATOM | 2045 | CA | ASP | B | 257 | -6.680 | 16.826 | 12.553 | 1.00 | 47.51 | BHUM | C |
| ATOM | 2053 | CA | LYS | B | 258 | -4.720 | 16.304 | 9.385 | 1.00 | 47.30 | BHUM | C |
| ATOM | 2062 | CA | GLU | B | 259 | -2.833 | 13.292 | 10.663 | 1.00 | 47.11 | BHUM | C |
| ATOM | 2071 | CA | TYR | B | 260 | -5.659 | 11.351 | 12.257 | 1.00 | 48.48 | BHUM | C |
| ATOM | 2083 | CA | THR | B | 261 | -8.047 | 11.821 | 9.384 | 1.00 | 43.89 | BHUM | C |
| ATOM | 2090 | CA | ASN | B | 262 | -5.675 | 10.034 | 7.060 | 1.00 | 43.06 | BHUM | C |
| ATOM | 2098 | CA | ILE | B | 263 | -5.057 | 7.444 | 9.726 | 1.00 | 45.73 | BHUM | C |
| ATOM | 2106 | CA | PHE | B | 264 | -8.781 | 6.750 | 9.940 | 1.00 | 50.06 | BHUM | C |
| ATOM | 2117 | CA | LEU | B | 265 | -9.024 | 6.559 | 6.158 | 1.00 | 54.79 | BHUM | C |
| ATOM | 2125 | CA | LYS | B | 266 | -6.400 | 3.817 | 5.971 | 1.00 | 53.81 | BHUM | C |
| ATOM | 2134 | CA | PHE | B | 267 | -8.391 | 1.672 | 8.380 | 1.00 | 48.53 | BHUM | C |
| ATOM | 2145 | CA | GLY | B | 268 | -9.892 | 0.201 | 5.265 | 1.00 | 41.55 | BHUM | C |
| ATOM | 2149 | CA | SER | B | 269 | -13.613 | 0.712 | 5.418 | 1.00 | 38.72 | BHUM | C |
| ATOM | 2155 | CA | GLY | B | 270 | -15.973 | 3.634 | 5.715 | 1.00 | 38.37 | BHUM | C |
| ATOM | 2159 | CA | TYR | B | 271 | -19.649 | 4.378 | 5.517 | 1.00 | 41.09 | BHUM | C |
| ATOM | 2171 | CA | VAL | B | 272 | -21.132 | 6.514 | 2.818 | 1.00 | 44.41 | BHUM | C |
| ATOM | 2178 | CA | SER | B | 273 | -24.701 | 7.596 | 3.175 | 1.00 | 42.37 | BHUM | C |
| ATOM | 2184 | CA | GLY | B | 274 | -26.791 | 9.609 | 0.788 | 1.00 | 41.41 | BHUM | C |
| ATOM | 2188 | CA | TRP | B | 275 | -30.108 | 10.113 | -0.938 | 1.00 | 40.25 | BHUM | C |
| ATOM | 2202 | CA | GLY | B | 276 | -29.541 | 9.437 | -4.595 | 1.00 | 37.87 | BHUM | C |
| ATOM | 2206 | CA | ARG | B | 277 | -29.815 | 7.067 | -7.506 | 1.00 | 39.50 | BHUM | C |
| ATOM | 2217 | CA | VAL | B | 278 | -30.554 | 3.567 | -6.295 | 1.00 | 41.32 | BHUM | C |
| ATOM | 2224 | CA | PHE | B | 279 | -29.754 | 2.179 | -9.703 | 1.00 | 42.27 | BHUM | C |
| ATOM | 2235 | CA | HIS | B | 280 | -27.218 | 3.629 | -12.037 | 1.00 | 44.48 | BHUM | C |
| ATOM | 2245 | CA | LYS | B | 281 | -29.468 | 6.355 | -13.415 | 1.00 | 45.48 | BHUM | C |
| ATOM | 2254 | CA | GLY | B | 282 | -32.521 | 4.269 | -12.437 | 1.00 | 42.95 | BHUM | C |
| ATOM | 2258 | CA | ARG | B | 283 | -34.196 | 6.373 | -9.742 | 1.00 | 42.00 | BHUM | C |
| ATOM | 2269 | CA | SER | B | 284 | -33.459 | 8.472 | -6.652 | 1.00 | 40.80 | BHUM | C |
| ATOM | 2275 | CA | ALA | B | 285 | -33.330 | 7.499 | -2.999 | 1.00 | 39.52 | BHUM | C |
| ATOM | 2280 | CA | LEU | B | 286 | -36.591 | 8.096 | -1.211 | 1.00 | 40.89 | BHUM | C |
| ATOM | 2288 | CA | VAL | B | 287 | -35.298 | 6.858 | 2.112 | 1.00 | 41.45 | BHUM | C |
| ATOM | 2295 | CA | LEU | B | 288 | -31.749 | 7.482 | 3.257 | 1.00 | 42.81 | BHUM | C |
| ATOM | 2303 | CA | GLN | B | 289 | -29.436 | 4.694 | 2.122 | 1.00 | 46.02 | BHUM | C |
| ATOM | 2312 | CA | TYR | B | 290 | -25.966 | 3.732 | 3.296 | 1.00 | 48.90 | BHUM | C |
| ATOM | 2324 | CA | LEU | B | 291 | -23.217 | 1.393 | 2.136 | 1.00 | 50.88 | BHUM | C |
| ATOM | 2332 | CA | ARG | B | 292 | -19.789 | 0.436 | 3.449 | 1.00 | 51.46 | BHUM | C |
| ATOM | 2343 | CA | VAL | B | 293 | -17.017 | 0.885 | 0.934 | 1.00 | 48.70 | BHUM | C |
| ATOM | 2350 | CA | PRO | B | 294 | -13.491 | -0.356 | 1.120 | 1.00 | 47.73 | BHUM | C |
| ATOM | 2357 | CA | LEU | B | 295 | -10.673 | 2.078 | 0.468 | 1.00 | 47.83 | BHUM | C |
| ATOM | 2365 | CA | VAL | B | 296 | -9.089 | 1.248 | -2.866 | 1.00 | 46.97 | BHUM | C |
| ATOM | 2372 | CA | ASP | B | 297 | -5.349 | 1.531 | -3.393 | 1.00 | 48.95 | BHUM | C |
| ATOM | 2380 | CA | ARG | B | 298 | -3.881 | 4.185 | -5.656 | 1.00 | 49.22 | BHUM | C |
| ATOM | 2391 | CA | ALA | B | 299 | -2.118 | 1.781 | -7.957 | 1.00 | 48.23 | BHUM | C |
| ATOM | 2396 | CA | THR | B | 300 | -5.403 | 0.130 | -8.742 | 1.00 | 49.24 | BHUM | C |

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| ATOM | 2403 | CA | CYS | B | 301 | -7.401 | 3.288 | -8.946 | 1.00 | 48.06 | BHUM | C |
| ATOM | 2409 | CA | LEU | B | 302 | -5.048 | 5.150 | -11.195 | 1.00 | 47.19 | BHUM | C |
| ATOM | 2417 | CA | ARG | B | 303 | -5.220 | 2.278 | -13.635 | 1.00 | 47.96 | BHUM | C |
| ATOM | 2428 | CA | SER | B | 304 | -9.006 | 2.119 | -13.638 | 1.00 | 49.12 | BHUM | C |
| ATOM | 2434 | CA | THR | B | 305 | -9.491 | 5.710 | -14.560 | 1.00 | 51.63 | BHUM | C |
| ATOM | 2441 | CA | LYS | B | 306 | -8.225 | 7.761 | -17.471 | 1.00 | 53.15 | BHUM | C |
| ATOM | 2450 | CA | PHE | B | 307 | -8.632 | 10.809 | -15.289 | 1.00 | 54.23 | BHUM | C |
| ATOM | 2461 | CA | THR | B | 308 | -5.589 | 11.893 | -13.394 | 1.00 | 54.12 | BHUM | C |
| ATOM | 2468 | CA | ILE | B | 309 | -6.345 | 10.880 | -9.878 | 1.00 | 56.13 | BHUM | C |
| ATOM | 2476 | CA | TYR | B | 310 | -5.081 | 13.817 | -7.883 | 1.00 | 60.19 | BHUM | C |
| ATOM | 2488 | CA | ASN | B | 311 | -3.628 | 13.519 | -4.409 | 1.00 | 63.99 | BHUM | C |
| ATOM | 2496 | CA | ASN | B | 312 | -6.653 | 15.540 | -3.377 | 1.00 | 69.95 | BHUM | C |
| ATOM | 2504 | CA | MET | B | 313 | -8.761 | 12.484 | -3.872 | 1.00 | 69.62 | BHUM | C |
| ATOM | 2512 | CA | PHE | B | 314 | -8.822 | 8.746 | -3.269 | 1.00 | 63.57 | BHUM | C |
| ATOM | 2523 | CA | CYS | B | 315 | -10.781 | 5.806 | -4.528 | 1.00 | 55.59 | BHUM | C |
| ATOM | 2529 | CA | ALA | B | 316 | -13.087 | 3.403 | -2.788 | 1.00 | 43.02 | BHUM | C |
| ATOM | 2534 | CA | GLY | B | 317 | -15.576 | 0.825 | -3.955 | 1.00 | 34.17 | BHUM | C |
| ATOM | 2538 | CA | PHE | B | 318 | -16.122 | -2.826 | -4.738 | 1.00 | 30.12 | BHUM | C |
| ATOM | 2549 | CA | HIS | B | 319 | -13.846 | -4.291 | -7.376 | 1.00 | 27.89 | BHUM | C |
| ATOM | 2559 | CA | GLU | B | 320 | -16.713 | -6.106 | -9.030 | 1.00 | 29.07 | BHUM | C |
| ATOM | 2568 | CA | GLY | B | 321 | -19.649 | -4.205 | -10.394 | 1.00 | 30.79 | BHUM | C |
| ATOM | 2572 | CA | GLY | B | 322 | -22.670 | -3.761 | -8.196 | 1.00 | 33.62 | BHUM | C |
| ATOM | 2576 | CA | ARG | B | 323 | -22.336 | -1.321 | -5.290 | 1.00 | 37.40 | BHUM | C |
| ATOM | 2587 | CA | ASP | B | 324 | -21.302 | 2.328 | -5.205 | 1.00 | 40.22 | BHUM | C |
| ATOM | 2595 | CA | SER | B | 325 | -22.472 | 5.909 | -4.723 | 1.00 | 43.43 | BHUM | C |
| ATOM | 2601 | CA | CYS | B | 326 | -24.244 | 7.396 | -7.692 | 1.00 | 46.59 | BHUM | C |
| ATOM | 2607 | CA | GLN | B | 327 | -25.597 | 10.694 | -8.929 | 1.00 | 49.06 | BHUM | C |
| ATOM | 2616 | CA | GLY | B | 328 | -27.323 | 12.588 | -6.182 | 1.00 | 51.10 | BHUM | C |
| ATOM | 2620 | CA | ASP | B | 329 | -24.839 | 11.612 | -3.493 | 1.00 | 51.16 | BHUM | C |
| ATOM | 2628 | CA | SER | B | 330 | -22.261 | 14.305 | -3.883 | 1.00 | 47.94 | BHUM | C |
| ATOM | 2634 | CA | GLY | B | 331 | -21.342 | 16.319 | -0.861 | 1.00 | 44.92 | BHUM | C |
| ATOM | 2638 | CA | GLY | B | 332 | -22.644 | 13.441 | 1.219 | 1.00 | 43.10 | BHUM | C |
| ATOM | 2642 | CA | PRO | B | 333 | -20.491 | 11.999 | 3.911 | 1.00 | 43.94 | BHUM | C |
| ATOM | 2649 | CA | HIS | B | 334 | -17.811 | 9.363 | 3.949 | 1.00 | 46.38 | BHUM | C |
| ATOM | 2659 | CA | VAL | B | 335 | -17.311 | 8.525 | 7.572 | 1.00 | 48.70 | BHUM | C |
| ATOM | 2666 | CA | THR | B | 336 | -15.110 | 6.069 | 9.380 | 1.00 | 51.02 | BHUM | C |
| ATOM | 2673 | CA | GLU | B | 337 | -16.158 | 5.192 | 12.898 | 1.00 | 49.91 | BHUM | C |
| ATOM | 2682 | CA | VAL | B | 338 | -13.464 | 4.430 | 15.387 | 1.00 | 47.76 | BHUM | C |
| ATOM | 2689 | CA | GLU | B | 339 | -14.993 | 2.658 | 18.343 | 1.00 | 43.74 | BHUM | C |
| ATOM | 2698 | CA | GLY | B | 340 | -18.336 | 4.435 | 18.449 | 1.00 | 39.58 | BHUM | C |
| ATOM | 2702 | CA | THR | B | 341 | -17.258 | 7.943 | 17.670 | 1.00 | 40.13 | BHUM | C |
| ATOM | 2709 | CA | SER | B | 342 | -17.491 | 8.643 | 13.975 | 1.00 | 42.72 | BHUM | C |
| ATOM | 2715 | CA | PHE | B | 343 | -15.201 | 10.915 | 11.971 | 1.00 | 47.11 | BHUM | C |
| ATOM | 2726 | CA | LEU | B | 344 | -15.286 | 12.403 | 8.474 | 1.00 | 51.50 | BHUM | C |
| ATOM | 2734 | CA | THR | B | 345 | -12.786 | 10.973 | 6.001 | 1.00 | 53.50 | BHUM | C |
| ATOM | 2741 | CA | GLY | B | 346 | -13.488 | 12.509 | 2.623 | 1.00 | 55.88 | BHUM | C |
| ATOM | 2745 | CA | ILE | B | 347 | -16.509 | 14.071 | 0.941 | 1.00 | 60.34 | BHUM | C |
| ATOM | 2753 | CA | ILE | B | 348 | -18.189 | 11.981 | -1.731 | 1.00 | 62.46 | BHUM | C |
| ATOM | 2761 | CA | SER | B | 349 | -17.370 | 13.662 | -5.043 | 1.00 | 62.56 | BHUM | C |
| ATOM | 2767 | CA | TRP | B | 350 | -17.756 | 11.751 | -8.312 | 1.00 | 60.27 | BHUM | C |
| ATOM | 2781 | CA | GLY | B | 351 | -17.393 | 8.614 | -10.399 | 1.00 | 54.44 | BHUM | C |
| ATOM | 2785 | CA | GLU | B | 352 | -17.695 | 7.468 | -13.977 | 1.00 | 50.80 | BHUM | C |
| ATOM | 2794 | CA | GLU | B | 353 | -21.109 | 5.840 | -14.104 | 1.00 | 48.18 | BHUM | C |
| ATOM | 2803 | CA | CYS | B | 354 | -22.264 | 3.778 | -11.163 | 1.00 | 46.21 | BHUM | C |
| ATOM | 2809 | CA | ALA | B | 355 | -22.202 | 0.129 | -10.049 | 1.00 | 42.88 | BHUM | C |
| ATOM | 2814 | CA | MET | B | 356 | -20.111 | -1.083 | -12.952 | 1.00 | 39.65 | BHUM | C |

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|------|------|----|-----|---|-----|---------|--------|---------|------|-------|------|---|
| ATOM | 2822 | CA | LYS | B | 357 | -17.080 | -3.312 | -12.551 | 1.00 | 37.04 | BHUM | C |
| ATOM | 2831 | CA | GLY | B | 358 | -13.670 | -1.882 | -13.249 | 1.00 | 33.41 | BHUM | C |
| ATOM | 2835 | CA | LYS | B | 359 | -14.816 | 1.395 | -11.795 | 1.00 | 34.77 | BHUM | C |
| ATOM | 2844 | CA | TYR | B | 360 | -14.592 | 2.743 | -8.275 | 1.00 | 36.78 | BHUM | C |
| ATOM | 2856 | CA | GLY | B | 361 | -16.165 | 5.749 | -6.631 | 1.00 | 39.36 | BHUM | C |
| ATOM | 2860 | CA | ILE | B | 362 | -13.702 | 8.546 | -6.074 | 1.00 | 46.77 | BHUM | C |
| ATOM | 2868 | CA | TYR | B | 363 | -13.953 | 10.800 | -3.045 | 1.00 | 52.64 | BHUM | C |
| ATOM | 2880 | CA | THR | B | 364 | -12.270 | 13.993 | -1.882 | 1.00 | 56.73 | BHUM | C |
| ATOM | 2887 | CA | LYS | B | 365 | -9.572 | 13.554 | 0.697 | 1.00 | 60.72 | BHUM | C |
| ATOM | 2896 | CA | VAL | B | 366 | -10.779 | 15.659 | 3.560 | 1.00 | 63.31 | BHUM | C |
| ATOM | 2903 | CA | SER | B | 367 | -7.390 | 15.285 | 5.167 | 1.00 | 64.87 | BHUM | C |
| ATOM | 2909 | CA | ARG | B | 368 | -6.113 | 18.033 | 2.900 | 1.00 | 66.42 | BHUM | C |
| ATOM | 2920 | CA | TYR | B | 369 | -8.950 | 20.472 | 3.718 | 1.00 | 66.26 | BHUM | C |
| ATOM | 2932 | CA | VAL | B | 370 | -9.692 | 19.615 | 7.329 | 1.00 | 58.86 | BHUM | C |
| ATOM | 2939 | CA | ASN | B | 371 | -7.606 | 22.449 | 8.719 | 1.00 | 50.92 | BHUM | C |
| ATOM | 2947 | CA | TRP | B | 372 | -9.400 | 24.838 | 6.389 | 1.00 | 45.00 | BHUM | C |
| ATOM | 2961 | CA | ILE | B | 373 | -12.689 | 23.609 | 7.724 | 1.00 | 41.63 | BHUM | C |
| ATOM | 2969 | CA | LYS | B | 374 | -11.439 | 24.090 | 11.244 | 1.00 | 45.38 | BHUM | C |
| ATOM | 2978 | CA | GLU | B | 375 | -10.643 | 27.734 | 10.705 | 1.00 | 49.27 | BHUM | C |
| ATOM | 2987 | CA | LYS | B | 376 | -13.651 | 28.384 | 8.516 | 1.00 | 51.26 | BHUM | C |
| ATOM | 2996 | CA | THR | B | 377 | -16.257 | 27.126 | 11.004 | 1.00 | 48.85 | BHUM | C |
| ATOM | 3003 | CA | LYS | B | 378 | -14.809 | 28.823 | 14.108 | 1.00 | 43.68 | BHUM | C |
| ATOM | 3012 | CA | LEU | B | 379 | -17.536 | 30.384 | 16.200 | 1.00 | 37.80 | BHUM | C |
| ATOM | 3020 | CA | THR | B | 380 | -15.131 | 32.854 | 17.690 | 1.00 | 30.35 | BHUM | C |

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