Untitled

```
db<-read.csv("Data Export Summary.csv", row.names=1)
View(db)
```

Q1: What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy.

```
#X-Ray
round(sum(db$X.ray)/sum(db$Total)*100, 2)
```

```
## [1] 87.53
```

```
#EM
round(sum(db$EM)/sum(db$Total)*100, 2)
```

```
## [1] 4.95
```

```
#All
colSums(db)/sum(db$Total)
```

```
##            X.ray              NMR               EM Multiple.methods
##     0.8752836071     0.0735991033     0.0494686958     0.0010555353
##          Neutron            Other            Total
##     0.0003917451     0.0002013134     1.0000000000
```

Q2: What proportion of structures in the PDB are protein?

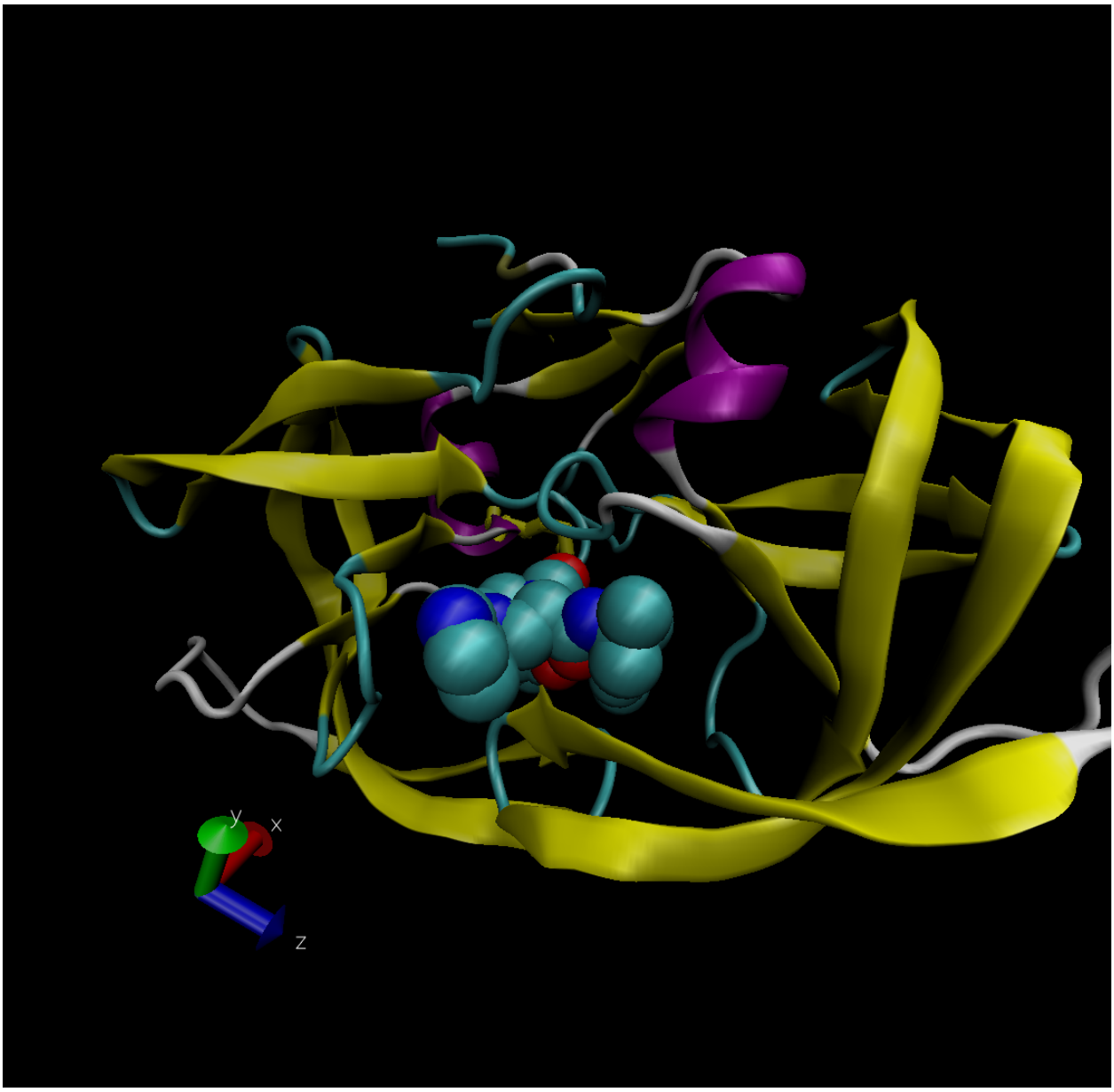
```
db$Total[1]/sum(db$Total)
```

```
## [1] 0.873499
```

Q3: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB?

Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure? Too small for the resolution of the structure.

Q5: There is a conserved water molecule in the binding site. Can you identify this water molecule? What residue number does this water molecule have (see note below)? ASP 25




```
library(bio3d)
pdb <- read.pdb("1hsg")
```

```
##   Note: Accessing on-line PDB file
```

```
pdb
```

```
##
##  Call:  read.pdb(file = "1hsg")
##
##    Total Models#: 1
##      Total Atoms#: 1686,  XYZs#: 5058  Chains#: 2  (values: A B)
##
```

```
##      Protein Atoms#: 1514  (residues/Calpha atoms#: 198)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 172  (residues: 128)
##      Non-protein/nucleic resid values: [ HOH (127), MK1 (1) ]
##
##    Protein sequence:
##       PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYD
##       QILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE
##       ALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTP
##       VNIIGRNLLTQIGCTLNF
##
## + attr: atom, xyz, seqres, helix, sheet,
##         calpha, remark, call
```

Q7: How many amino acid residues are there in this pdb object? 128

Q8: Name one of the two non-protein residues?

Q9: How many protein chains are in this structure? 2

```
pdb$atom
```

```
##        type eleno elety  alt resid chain resno insert      x       y       z o
## 1      ATOM     1     N <NA>   PRO     A     1   <NA> 29.361  39.686   5.862 1
## 2      ATOM     2    CA <NA>   PRO     A     1   <NA> 30.307  38.663   5.319 1
## 3      ATOM     3     C <NA>   PRO     A     1   <NA> 29.760  38.071   4.022 1
## 4      ATOM     4     O <NA>   PRO     A     1   <NA> 28.600  38.302   3.676 1
## 5      ATOM     5    CB <NA>   PRO     A     1   <NA> 30.508  37.541   6.342 1
## 6      ATOM     6    CG <NA>   PRO     A     1   <NA> 29.296  37.591   7.162 1
## 7      ATOM     7    CD <NA>   PRO     A     1   <NA> 28.778  39.015   7.019 1
## 8      ATOM     8     N <NA>   GLN     A     2   <NA> 30.607  37.334   3.305 1
## 9      ATOM     9    CA <NA>   GLN     A     2   <NA> 30.158  36.492   2.199 1
## 10     ATOM    10     C <NA>   GLN     A     2   <NA> 30.298  35.041   2.643 1
## 11     ATOM    11     O <NA>   GLN     A     2   <NA> 31.401  34.494   2.763 1
## 12     ATOM    12    CB <NA>   GLN     A     2   <NA> 30.970  36.738   0.926 1
## 13     ATOM    13    CG <NA>   GLN     A     2   <NA> 30.625  35.783  -0.201 1
## 14     ATOM    14    CD <NA>   GLN     A     2   <NA> 31.184  36.217  -1.549 1
## 15     ATOM    15   OE1 <NA>   GLN     A     2   <NA> 32.006  35.518  -2.156 1
## 16     ATOM    16   NE2 <NA>   GLN     A     2   <NA> 30.684  37.339  -2.061 1
## 17     ATOM    17     N <NA>   ILE     A     3   <NA> 29.160  34.436   2.919 1
## 18     ATOM    18    CA <NA>   ILE     A     3   <NA> 29.123  33.098   3.397 1
## 19     ATOM    19     C <NA>   ILE     A     3   <NA> 28.968  32.155   2.198 1
## 20     ATOM    20     O <NA>   ILE     A     3   <NA> 28.088  32.330   1.368 1
## 21     ATOM    21    CB <NA>   ILE     A     3   <NA> 27.977  32.995   4.409 1
## 22     ATOM    22   CG1 <NA>   ILE     A     3   <NA> 28.341  33.820   5.652 1
## 23     ATOM    23   CG2 <NA>   ILE     A     3   <NA> 27.692  31.548   4.745 1
## 24     ATOM    24   CD1 <NA>   ILE     A     3   <NA> 27.264  33.884   6.696 1
## 25     ATOM    25     N <NA>   THR     A     4   <NA> 29.891  31.210   2.066 1
## 26     ATOM    26    CA <NA>   THR     A     4   <NA> 29.774  30.143   1.062 1
## 27     ATOM    27     C <NA>   THR     A     4   <NA> 28.986  28.975   1.658 1
## 28     ATOM    28     O <NA>   THR     A     4   <NA> 28.690  28.948   2.875 1
## 29     ATOM    29    CB <NA>   THR     A     4   <NA> 31.165  29.618   0.634 1
## 30     ATOM    30   OG1 <NA>   THR     A     4   <NA> 31.866  29.209   1.815 1
```

```
## 31     ATOM    31   CG2 <NA>   THR     A     4   <NA> 31.980  30.688  -0.085 1
## 32     ATOM    32     N <NA>   LEU     A     5   <NA> 28.641  28.019   0.803 1
## 33     ATOM    33    CA <NA>   LEU     A     5   <NA> 27.644  27.003   1.144 1
## 34     ATOM    34     C <NA>   LEU     A     5   <NA> 28.204  25.559   1.071 1
## 35     ATOM    35     O <NA>   LEU     A     5   <NA> 27.446  24.583   0.969 1
## 36     ATOM    36    CB <NA>   LEU     A     5   <NA> 26.411  27.139   0.226 1
## 37     ATOM    37    CG <NA>   LEU     A     5   <NA> 25.676  28.479   0.352 1
## 38     ATOM    38   CD1 <NA>   LEU     A     5   <NA> 24.624  28.624  -0.753 1
## 39     ATOM    39   CD2 <NA>   LEU     A     5   <NA> 25.088  28.590   1.745 1
## 40     ATOM    40     N <NA>   TRP     A     6   <NA> 29.528  25.436   1.146 1
## 41     ATOM    41    CA <NA>   TRP     A     6   <NA> 30.177  24.150   1.279 1
## 42     ATOM    42     C <NA>   TRP     A     6   <NA> 29.837  23.488   2.611 1
## 43     ATOM    43     O <NA>   TRP     A     6   <NA> 29.706  22.271   2.673 1
## 44     ATOM    44    CB <NA>   TRP     A     6   <NA> 31.685  24.301   1.109 1
## 45     ATOM    45    CG <NA>   TRP     A     6   <NA> 32.152  24.955  -0.189 1
## 46     ATOM    46   CD1 <NA>   TRP     A     6   <NA> 32.681  26.216  -0.345 1
## 47     ATOM    47   CD2 <NA>   TRP     A     6   <NA> 32.274  24.314  -1.478 1
## 48     ATOM    48   NE1 <NA>   TRP     A     6   <NA> 33.102  26.385  -1.655 1
## 49     ATOM    49   CE2 <NA>   TRP     A     6   <NA> 32.864  25.258  -2.369 1
## 50     ATOM    50   CE3 <NA>   TRP     A     6   <NA> 31.949  23.035  -1.986 1
## 51     ATOM    51   CZ2 <NA>   TRP     A     6   <NA> 33.093  24.968  -3.717 1
## 52     ATOM    52   CZ3 <NA>   TRP     A     6   <NA> 32.195  22.755  -3.294 1
## 53     ATOM    53   CH2 <NA>   TRP     A     6   <NA> 32.754  23.722  -4.169 1
## 54     ATOM    54     N <NA>   GLN     A     7   <NA> 29.667  24.280   3.667 1
## 55     ATOM    55    CA <NA>   GLN     A     7   <NA> 29.141  23.799   4.960 1
## 56     ATOM    56     C <NA>   GLN     A     7   <NA> 27.747  24.395   5.208 1
## 57     ATOM    57     O <NA>   GLN     A     7   <NA> 27.349  25.330   4.547 1
## 58     ATOM    58    CB <NA>   GLN     A     7   <NA> 30.072  24.227   6.100 1
## 59     ATOM    59    CG <NA>   GLN     A     7   <NA> 31.512  23.694   5.995 1
## 60     ATOM    60    CD <NA>   GLN     A     7   <NA> 32.521  24.750   5.469 1
## 61     ATOM    61   OE1 <NA>   GLN     A     7   <NA> 32.666  25.860   6.038 1
## 62     ATOM    62   NE2 <NA>   GLN     A     7   <NA> 33.268  24.374   4.419 1
## 63     ATOM    63     N <NA>   ARG     A     8   <NA> 26.992  23.877   6.169 1
## 64     ATOM    64    CA <NA>   ARG     A     8   <NA> 25.757  24.566   6.593 1
## 65     ATOM    65     C <NA>   ARG     A     8   <NA> 26.029  26.025   6.996 1
## 66     ATOM    66     O <NA>   ARG     A     8   <NA> 26.947  26.291   7.775 1
## 67     ATOM    67    CB <NA>   ARG     A     8   <NA> 25.087  23.849   7.776 1
## 68     ATOM    68    CG <NA>   ARG     A     8   <NA> 24.646  22.409   7.505 1
## 69     ATOM    69    CD <NA>   ARG     A     8   <NA> 23.728  21.896   8.637 1
## 70     ATOM    70    NE <NA>   ARG     A     8   <NA> 22.952  20.730   8.230 1
## 71     ATOM    71    CZ <NA>   ARG     A     8   <NA> 22.367  19.871   9.064 1
## 72     ATOM    72   NH1 <NA>   ARG     A     8   <NA> 22.376  20.074  10.370 1
## 73     ATOM    73   NH2 <NA>   ARG     A     8   <NA> 21.776  18.789   8.589 1
## 74     ATOM    74     N <NA>   PRO     A     9   <NA> 25.123  26.955   6.645 1
## 75     ATOM    75    CA <NA>   PRO     A     9   <NA> 25.491  28.352   6.938 1
## 76     ATOM    76     C <NA>   PRO     A     9   <NA> 25.127  28.763   8.364 1
## 77     ATOM    77     O <NA>   PRO     A     9   <NA> 24.136  29.472   8.578 1
## 78     ATOM    78    CB <NA>   PRO     A     9   <NA> 24.719  29.176   5.916 1
## 79     ATOM    79    CG <NA>   PRO     A     9   <NA> 23.625  28.254   5.407 1
## 80     ATOM    80    CD <NA>   PRO     A     9   <NA> 24.096  26.855   5.591 1
## 81     ATOM    81     N <NA>   LEU     A    10   <NA> 25.905  28.285   9.330 1
## 82     ATOM    82    CA <NA>   LEU     A    10   <NA> 25.653  28.510  10.750 1
## 83     ATOM    83     C <NA>   LEU     A    10   <NA> 26.383  29.770  11.208 1
## 84     ATOM    84     O <NA>   LEU     A    10   <NA> 27.567  29.927  10.938 1
```

```
## 85     ATOM    85    CB <NA>   LEU     A    10   <NA> 26.120  27.284  11.573 1
## 86     ATOM    86    CG <NA>   LEU     A    10   <NA> 25.161  26.082  11.544 1
## 87     ATOM    87   CD1 <NA>   LEU     A    10   <NA> 25.895  24.743  11.662 1
## 88     ATOM    88   CD2 <NA>   LEU     A    10   <NA> 24.206  26.196  12.696 1
## 89     ATOM    89     N <NA>   VAL     A    11   <NA> 25.667  30.672  11.872 1
## 90     ATOM    90    CA <NA>   VAL     A    11   <NA> 26.267  31.854  12.497 1
## 91     ATOM    91     C <NA>   VAL     A    11   <NA> 25.818  31.957  13.955 1
## 92     ATOM    92     O <NA>   VAL     A    11   <NA> 24.929  31.184  14.402 1
## 93     ATOM    93    CB <NA>   VAL     A    11   <NA> 25.824  33.131  11.791 1
## 94     ATOM    94   CG1 <NA>   VAL     A    11   <NA> 26.270  33.089  10.323 1
## 95     ATOM    95   CG2 <NA>   VAL     A    11   <NA> 24.333  33.275  11.879 1
## 96     ATOM    96     N <NA>   THR     A    12   <NA> 26.397  32.913  14.700 1
## 97     ATOM    97    CA <NA>   THR     A    12   <NA> 26.001  33.143  16.102 1
## 98     ATOM    98     C <NA>   THR     A    12   <NA> 24.915  34.200  16.204 1
## 99     ATOM    99     O <NA>   THR     A    12   <NA> 25.010  35.279  15.610 1
## 100    ATOM   100    CB <NA>   THR     A    12   <NA> 27.201  33.565  16.998 1
## 101    ATOM   101   OG1 <NA>   THR     A    12   <NA> 28.330  32.709  16.751 1
## 102    ATOM   102   CG2 <NA>   THR     A    12   <NA> 26.827  33.430  18.450 1
## 103    ATOM   103     N <NA>   ILE     A    13   <NA> 23.848  33.868  16.909 1
## 104    ATOM   104    CA <NA>   ILE     A    13   <NA> 22.842  34.875  17.206 1
## 105    ATOM   105     C <NA>   ILE     A    13   <NA> 22.770  35.114  18.707 1
## 106    ATOM   106     O <NA>   ILE     A    13   <NA> 23.328  34.363  19.500 1
## 107    ATOM   107    CB <NA>   ILE     A    13   <NA> 21.413  34.460  16.661 1
## 108    ATOM   108   CG1 <NA>   ILE     A    13   <NA> 20.878  33.229  17.431 1
## 109    ATOM   109   CG2 <NA>   ILE     A    13   <NA> 21.510  34.194  15.162 1
## 110    ATOM   110   CD1 <NA>   ILE     A    13   <NA> 19.353  33.201  17.603 1
## 111    ATOM   111     N <NA>   LYS     A    14   <NA> 22.106  36.199  19.087 1
## 112    ATOM   112    CA <NA>   LYS     A    14   <NA> 21.894  36.545  20.492 1
## 113    ATOM   113     C <NA>   LYS     A    14   <NA> 20.442  36.943  20.615 1
## 114    ATOM   114     O <NA>   LYS     A    14   <NA> 19.960  37.808  19.873 1
## 115    ATOM   115    CB <NA>   LYS     A    14   <NA> 22.777  37.724  20.896 1
## 116    ATOM   116    CG <NA>   LYS     A    14   <NA> 22.727  38.056  22.383 1
## 117    ATOM   117    CD <NA>   LYS     A    14   <NA> 23.270  39.450  22.678 1
## 118    ATOM   118    CE <NA>   LYS     A    14   <NA> 24.814  39.490  22.755 1
## 119    ATOM   119    NZ <NA>   LYS     A    14   <NA> 25.394  40.891  22.572 1
## 120    ATOM   120     N <NA>   ILE     A    15   <NA> 19.739  36.267  21.512 1
## 121    ATOM   121    CA <NA>   ILE     A    15   <NA> 18.345  36.563  21.813 1
## 122    ATOM   122     C <NA>   ILE     A    15   <NA> 18.224  36.327  23.316 1
## 123    ATOM   123     O <NA>   ILE     A    15   <NA> 18.886  35.449  23.864 1
## 124    ATOM   124    CB <NA>   ILE     A    15   <NA> 17.380  35.592  21.022 1
## 125    ATOM   125   CG1 <NA>   ILE     A    15   <NA> 15.935  35.812  21.435 1
## 126    ATOM   126   CG2 <NA>   ILE     A    15   <NA> 17.745  34.137  21.266 1
## 127    ATOM   127   CD1 <NA>   ILE     A    15   <NA> 14.929  35.116  20.526 1
## 128    ATOM   128     N <NA>   GLY     A    16   <NA> 17.446  37.139  24.012 1
## 129    ATOM   129    CA <NA>   GLY     A    16   <NA> 17.356  36.968  25.459 1
## 130    ATOM   130     C <NA>   GLY     A    16   <NA> 18.711  36.871  26.160 1
## 131    ATOM   131     O <NA>   GLY     A    16   <NA> 18.866  36.162  27.153 1
## 132    ATOM   132     N <NA>   GLY     A    17   <NA> 19.671  37.659  25.697 1
## 133    ATOM   133    CA <NA>   GLY     A    17   <NA> 20.970  37.660  26.340 1
## 134    ATOM   134     C <NA>   GLY     A    17   <NA> 21.680  36.316  26.278 1
## 135    ATOM   135     O <NA>   GLY     A    17   <NA> 22.785  36.163  26.794 1
## 136    ATOM   136     N <NA>   GLN     A    18   <NA> 21.093  35.361  25.572 1
## 137    ATOM   137    CA <NA>   GLN     A    18   <NA> 21.780  34.106  25.263 1
## 138    ATOM   138     C <NA>   GLN     A    18   <NA> 22.500  34.159  23.907 1
```

```
## 139    ATOM   139     O <NA>   GLN     A    18   <NA> 21.937  34.624  22.915 1
## 140    ATOM   140    CB <NA>   GLN     A    18   <NA> 20.776  32.957  25.228 1
## 141    ATOM   141    CG <NA>   GLN     A    18   <NA> 19.599  33.116  26.176 1
## 142    ATOM   142    CD <NA>   GLN     A    18   <NA> 19.556  31.997  27.179 1
## 143    ATOM   143   OE1 <NA>   GLN     A    18   <NA> 20.393  31.944  28.082 1
## 144    ATOM   144   NE2 <NA>   GLN     A    18   <NA> 18.647  31.035  26.975 1
## 145    ATOM   145     N <NA>   LEU     A    19   <NA> 23.733  33.672  23.848 1
## 146    ATOM   146    CA <NA>   LEU     A    19   <NA> 24.334  33.365  22.552 1
## 147    ATOM   147     C <NA>   LEU     A    19   <NA> 23.896  31.963  22.106 1
## 148    ATOM   148     O <NA>   LEU     A    19   <NA> 23.975  31.020  22.863 1
## 149    ATOM   149    CB <NA>   LEU     A    19   <NA> 25.869  33.432  22.625 1
## 150    ATOM   150    CG <NA>   LEU     A    19   <NA> 26.561  34.761  22.968 1
## 151    ATOM   151   CD1 <NA>   LEU     A    19   <NA> 28.007  34.629  22.620 1
## 152    ATOM   152   CD2 <NA>   LEU     A    19   <NA> 25.983  35.913  22.194 1
## 153    ATOM   153     N <NA>   LYS     A    20   <NA> 23.416  31.855  20.876 1
## 154    ATOM   154    CA <NA>   LYS     A    20   <NA> 23.006  30.584  20.266 1
## 155    ATOM   155     C <NA>   LYS     A    20   <NA> 23.626  30.463  18.874 1
## 156    ATOM   156     O <NA>   LYS     A    20   <NA> 24.024  31.460  18.283 1
## 157    ATOM   157    CB <NA>   LYS     A    20   <NA> 21.494  30.523  20.107 1
## 158    ATOM   158    CG <NA>   LYS     A    20   <NA> 20.778  29.875  21.264 1
## 159    ATOM   159    CD <NA>   LYS     A    20   <NA> 19.868  30.857  21.939 1
## 160    ATOM   160    CE <NA>   LYS     A    20   <NA> 19.112  30.168  23.043 1
## 161    ATOM   161    NZ <NA>   LYS     A    20   <NA> 18.467  28.892  22.571 1
## 162    ATOM   162     N <NA>   GLU     A    21   <NA> 23.725  29.250  18.342 1
## 163    ATOM   163    CA <NA>   GLU     A    21   <NA> 24.053  29.117  16.931 1
## 164    ATOM   164     C <NA>   GLU     A    21   <NA> 22.822  28.761  16.150 1
## 165    ATOM   165     O <NA>   GLU     A    21   <NA> 21.879  28.136  16.672 1
## 166    ATOM   166    CB <NA>   GLU     A    21   <NA> 25.197  28.130  16.679 1
## 167    ATOM   167    CG <NA>   GLU     A    21   <NA> 25.035  26.716  17.168 1
## 168    ATOM   168    CD <NA>   GLU     A    21   <NA> 25.878  25.743  16.334 1
## 169    ATOM   169   OE1 <NA>   GLU     A    21   <NA> 27.022  26.130  15.972 1
## 170    ATOM   170   OE2 <NA>   GLU     A    21   <NA> 25.379  24.639  15.983 1
## 171    ATOM   171     N <NA>   ALA     A    22   <NA> 22.778  29.268  14.927 1
## 172    ATOM   172    CA <NA>   ALA     A    22   <NA> 21.553  29.189  14.165 1
## 173    ATOM   173     C <NA>   ALA     A    22   <NA> 21.870  29.183  12.682 1
## 174    ATOM   174     O <NA>   ALA     A    22   <NA> 22.975  29.578  12.252 1
## 175    ATOM   175    CB <NA>   ALA     A    22   <NA> 20.625  30.359  14.524 1
## 176    ATOM   176     N <NA>   LEU     A    23   <NA> 20.893  28.726  11.903 1
## 177    ATOM   177    CA <NA>   LEU     A    23   <NA> 21.047  28.473  10.476 1
## 178    ATOM   178     C <NA>   LEU     A    23   <NA> 20.381  29.596   9.664 1
## 179    ATOM   179     O <NA>   LEU     A    23   <NA> 19.231  29.943   9.912 1
## 180    ATOM   180    CB <NA>   LEU     A    23   <NA> 20.382  27.135  10.174 1
## 181    ATOM   181    CG <NA>   LEU     A    23   <NA> 20.532  26.573   8.786 1
## 182    ATOM   182   CD1 <NA>   LEU     A    23   <NA> 21.939  26.039   8.621 1
## 183    ATOM   183   CD2 <NA>   LEU     A    23   <NA> 19.490  25.490   8.627 1
## 184    ATOM   184     N <NA>   LEU     A    24   <NA> 21.122  30.163   8.715 1
## 185    ATOM   185    CA <NA>   LEU     A    24   <NA> 20.617  31.144   7.775 1
## 186    ATOM   186     C <NA>   LEU     A    24   <NA> 19.940  30.412   6.617 1
## 187    ATOM   187     O <NA>   LEU     A    24   <NA> 20.567  29.833   5.740 1
## 188    ATOM   188    CB <NA>   LEU     A    24   <NA> 21.767  32.023   7.262 1
## 189    ATOM   189    CG <NA>   LEU     A    24   <NA> 22.647  32.673   8.359 1
## 190    ATOM   190   CD1 <NA>   LEU     A    24   <NA> 23.698  33.581   7.738 1
## 191    ATOM   191   CD2 <NA>   LEU     A    24   <NA> 21.797  33.496   9.368 1
## 192    ATOM   192     N <NA>   ASP     A    25   <NA> 18.626  30.444   6.627 1
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## 193    ATOM   193    CA <NA>   ASP     A    25   <NA> 17.853  29.516   5.837 1
## 194    ATOM   194     C <NA>   ASP     A    25   <NA> 16.945  30.292   4.886 1
## 195    ATOM   195     O <NA>   ASP     A    25   <NA> 15.843  30.678   5.237 1
## 196    ATOM   196    CB <NA>   ASP     A    25   <NA> 17.047  28.642   6.811 1
## 197    ATOM   197    CG <NA>   ASP     A    25   <NA> 16.316  27.513   6.146 1
## 198    ATOM   198   OD1 <NA>   ASP     A    25   <NA> 16.236  27.458   4.905 1
## 199    ATOM   199   OD2 <NA>   ASP     A    25   <NA> 15.762  26.696   6.882 1
## 200    ATOM   200     N <NA>   THR     A    26   <NA> 17.364  30.439   3.645 1
## 201    ATOM   201    CA <NA>   THR     A    26   <NA> 16.548  31.148   2.684 1
## 202    ATOM   202     C <NA>   THR     A    26   <NA> 15.302  30.382   2.289 1
## 203    ATOM   203     O <NA>   THR     A    26   <NA> 14.412  30.939   1.615 1
## 204    ATOM   204    CB <NA>   THR     A    26   <NA> 17.328  31.419   1.447 1
## 205    ATOM   205   OG1 <NA>   THR     A    26   <NA> 17.693  30.177   0.863 1
## 206    ATOM   206   CG2 <NA>   THR     A    26   <NA> 18.601  32.197   1.773 1
## 207    ATOM   207     N <NA>   GLY     A    27   <NA> 15.213  29.111   2.702 1
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## 209    ATOM   209     C <NA>   GLY     A    27   <NA> 12.958  28.456   3.394 1
## 210    ATOM   210     O <NA>   GLY     A    27   <NA> 11.832  28.015   3.171 1
## 211    ATOM   211     N <NA>   ALA     A    28   <NA> 13.301  28.967   4.569 1
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## 216    ATOM   216     N <NA>   ASP     A    29   <NA> 10.296  30.560   5.587 1
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## 237    ATOM   237   OG1 <NA>   THR     A    31   <NA> 13.451  34.082  11.707 1
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## 243    ATOM   243    CB <NA>   VAL     A    32   <NA> 11.528  27.683  13.690 1
## 244    ATOM   244   CG1 <NA>   VAL     A    32   <NA> 10.656  26.825  14.592 1
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## 246    ATOM   246     N <NA>   LEU     A    33   <NA> 12.899  28.904  16.576 1
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## 247    ATOM   247    CA <NA>   LEU     A    33   <NA> 13.996  28.594  17.500 1
## 248    ATOM   248     C <NA>   LEU     A    33   <NA> 13.571  27.454  18.396 1
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## 252    ATOM   252   CD1 <NA>   LEU     A    33   <NA> 15.091  32.156  18.733 1
## 253    ATOM   253   CD2 <NA>   LEU     A    33   <NA> 16.139  30.718  16.927 1
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## 261    ATOM   261   OE1 <NA>   GLU     A    34   <NA> 18.134  23.657  20.375 1
## 262    ATOM   262   OE2 <NA>   GLU     A    34   <NA> 18.443  23.614  18.182 1
## 263    ATOM   263     N <NA>   GLU     A    35   <NA> 12.865  25.288  21.703 1
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## 271    ATOM   271   OE2 <NA>   GLU     A    35   <NA>  8.758  25.047  24.035 1
## 272    ATOM   272     N <NA>   MET     A    36   <NA> 12.495  27.556  24.269 1
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## 285    ATOM   285    OG <NA>   SER     A    37   <NA>  9.948  31.148  29.559 1
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## 289    ATOM   289     O <NA>   LEU     A    38   <NA>  8.616  34.906  27.343 1
## 290    ATOM   290    CB <NA>   LEU     A    38   <NA> 10.409  34.626  24.500 1
## 291    ATOM   291    CG <NA>   LEU     A    38   <NA> 11.559  34.187  23.577 1
## 292    ATOM   292   CD1 <NA>   LEU     A    38   <NA> 11.171  34.399  22.132 1
## 293    ATOM   293   CD2 <NA>   LEU     A    38   <NA> 12.807  34.964  23.875 1
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## 305    ATOM   305     N <NA>   ARG     A    41   <NA>  3.289  37.341  25.729 1
## 306    ATOM   306    CA <NA>   ARG     A    41   <NA>  2.382  36.252  25.509 1
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## 310    ATOM   310    CG <NA>   ARG     A    41   <NA>  0.288  36.021  26.959 1
## 311    ATOM   311    CD <NA>   ARG     A    41   <NA>  0.118  36.953  28.169 1
## 312    ATOM   312    NE <NA>   ARG     A    41   <NA>  1.356  37.143  28.933 1
## 313    ATOM   313    CZ <NA>   ARG     A    41   <NA>  1.830  38.332  29.318 1
## 314    ATOM   314   NH1 <NA>   ARG     A    41   <NA>  1.161  39.450  29.040 1
## 315    ATOM   315   NH2 <NA>   ARG     A    41   <NA>  2.973  38.402  29.994 1
## 316    ATOM   316     N <NA>   TRP     A    42   <NA>  2.145  34.493  23.834 1
## 317    ATOM   317    CA <NA>   TRP     A    42   <NA>  2.295  33.862  22.533 1
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## 319    ATOM   319     O <NA>   TRP     A    42   <NA>  0.031  33.049  22.694 1
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## 322    ATOM   322   CD1 <NA>   TRP     A    42   <NA>  3.473  31.896  25.041 1
## 323    ATOM   323   CD2 <NA>   TRP     A    42   <NA>  1.989  30.710  23.857 1
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## 325    ATOM   325   CE2 <NA>   TRP     A    42   <NA>  1.966  30.246  25.193 1
## 326    ATOM   326   CE3 <NA>   TRP     A    42   <NA>  1.129  30.108  22.909 1
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## 329    ATOM   329   CH2 <NA>   TRP     A    42   <NA>  0.305  28.651  24.686 1
## 330    ATOM   330     N <NA>   LYS     A    43   <NA>  0.781  33.465  20.639 1
## 331    ATOM   331    CA <NA>   LYS     A    43   <NA> -0.305  32.776  19.928 1
## 332    ATOM   332     C <NA>   LYS     A    43   <NA>  0.220  31.412  19.477 1
## 333    ATOM   333     O <NA>   LYS     A    43   <NA>  1.400  31.270  19.145 1
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## 335    ATOM   335    CG <NA>   LYS     A    43   <NA> -1.311  34.967  19.027 1
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## 339    ATOM   339     N <NA>   PRO     A    44   <NA> -0.601  30.363  19.541 1
## 340    ATOM   340    CA <NA>   PRO     A    44   <NA> -0.088  29.114  18.966 1
## 341    ATOM   341     C <NA>   PRO     A    44   <NA> -0.275  29.085  17.454 1
## 342    ATOM   342     O <NA>   PRO     A    44   <NA> -1.185  29.721  16.929 1
## 343    ATOM   343    CB <NA>   PRO     A    44   <NA> -0.893  28.021  19.667 1
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## 359    ATOM   359    CB <NA>   MET     A    46   <NA> -0.047  24.319  12.624 1
## 360    ATOM   360    CG <NA>   MET     A    46   <NA> -0.970  23.867  13.745 1
## 361    ATOM   361    SD <NA>   MET     A    46   <NA> -0.348  22.459  14.681 1
## 362    ATOM   362    CE <NA>   MET     A    46   <NA> -0.585  21.081  13.426 1
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## 365    ATOM   365     C <NA>   ILE     A    47   <NA>  4.420  24.140  10.114 1
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## 368    ATOM   368   CG1 <NA>   ILE     A    47   <NA>  5.959  25.628  12.127 1
## 369    ATOM   369   CG2 <NA>   ILE     A    47   <NA>  4.898  27.703  11.148 1
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## 374    ATOM   374     O <NA>   GLY     A    48   <NA>  6.723  23.689   6.900 1
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## 377    ATOM   377     C <NA>   GLY     A    49   <NA>  8.221  20.379   6.232 1
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## 379    ATOM   379     N <NA>   ILE     A    50   <NA>  9.309  19.619   6.155 1
## 380    ATOM   380    CA <NA>   ILE     A    50   <NA>  9.537  18.544   5.194 1
## 381    ATOM   381     C <NA>   ILE     A    50   <NA>  8.802  17.261   5.658 1
## 382    ATOM   382     O <NA>   ILE     A    50   <NA>  8.143  16.589   4.863 1
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## 384    ATOM   384   CG1 <NA>   ILE     A    50   <NA> 11.553  18.874   3.682 1
## 385    ATOM   385   CG2 <NA>   ILE     A    50   <NA> 11.521  16.945   5.317 1
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## 388    ATOM   388    CA <NA>   GLY     A    51   <NA>  8.174  15.771   7.405 1
## 389    ATOM   389     C <NA>   GLY     A    51   <NA>  6.812  16.062   7.983 1
## 390    ATOM   390     O <NA>   GLY     A    51   <NA>  6.408  15.342   8.870 1
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## 394    ATOM   394     O <NA>   GLY     A    52   <NA>  5.873  19.342   9.280 1
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## 396    ATOM   396    CA <NA>   PHE     A    53   <NA>  3.593  19.996  10.731 1
## 397    ATOM   397     C <NA>   PHE     A    53   <NA>  4.015  19.881  12.194 1
## 398    ATOM   398     O <NA>   PHE     A    53   <NA>  3.930  18.810  12.781 1
## 399    ATOM   399    CB <NA>   PHE     A    53   <NA>  2.121  20.351  10.670 1
## 400    ATOM   400    CG <NA>   PHE     A    53   <NA>  1.760  21.152   9.484 1
## 401    ATOM   401   CD1 <NA>   PHE     A    53   <NA>  1.725  20.567   8.216 1
## 402    ATOM   402   CD2 <NA>   PHE     A    53   <NA>  1.556  22.518   9.607 1
## 403    ATOM   403   CE1 <NA>   PHE     A    53   <NA>  1.500  21.332   7.075 1
## 404    ATOM   404   CE2 <NA>   PHE     A    53   <NA>  1.327  23.302   8.496 1
## 405    ATOM   405    CZ <NA>   PHE     A    53   <NA>  1.290  22.718   7.212 1
## 406    ATOM   406     N <NA>   ILE     A    54   <NA>  4.483  20.969  12.792 1
## 407    ATOM   407    CA <NA>   ILE     A    54   <NA>  4.689  21.005  14.248 1
## 408    ATOM   408     C <NA>   ILE     A    54   <NA>  3.921  22.179  14.858 1
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## 409    ATOM   409     O <NA>   ILE     A    54   <NA>  3.575  23.139  14.182 1
## 410    ATOM   410    CB <NA>   ILE     A    54   <NA>  6.199  21.155  14.625 1
## 411    ATOM   411   CG1 <NA>   ILE     A    54   <NA>  6.796  22.408  13.939 1
## 412    ATOM   412   CG2 <NA>   ILE     A    54   <NA>  6.967  19.888  14.203 1
## 413    ATOM   413   CD1 <NA>   ILE     A    54   <NA>  8.110  22.821  14.465 1
## 414    ATOM   414     N <NA>   LYS     A    55   <NA>  3.632  22.095  16.145 1
## 415    ATOM   415    CA <NA>   LYS     A    55   <NA>  2.968  23.196  16.823 1
## 416    ATOM   416     C <NA>   LYS     A    55   <NA>  4.038  24.093  17.449 1
## 417    ATOM   417     O <NA>   LYS     A    55   <NA>  4.949  23.610  18.157 1
## 418    ATOM   418    CB <NA>   LYS     A    55   <NA>  2.021  22.661  17.895 1
## 419    ATOM   419    CG <NA>   LYS     A    55   <NA>  0.974  23.665  18.300 1
## 420    ATOM   420    CD <NA>   LYS     A    55   <NA>  0.006  23.101  19.304 1
## 421    ATOM   421    CE <NA>   LYS     A    55   <NA> -0.580  24.217  20.149 1
## 422    ATOM   422    NZ <NA>   LYS     A    55   <NA>  0.439  24.751  21.104 1
## 423    ATOM   423     N <NA>   VAL     A    56   <NA>  3.953  25.391  17.185 1
## 424    ATOM   424    CA <NA>   VAL     A    56   <NA>  4.927  26.319  17.754 1
## 425    ATOM   425     C <NA>   VAL     A    56   <NA>  4.225  27.378  18.556 1
## 426    ATOM   426     O <NA>   VAL     A    56   <NA>  3.023  27.557  18.455 1
## 427    ATOM   427    CB <NA>   VAL     A    56   <NA>  5.769  27.009  16.663 1
## 428    ATOM   428   CG1 <NA>   VAL     A    56   <NA>  6.791  26.027  16.120 1
## 429    ATOM   429   CG2 <NA>   VAL     A    56   <NA>  4.881  27.551  15.567 1
## 430    ATOM   430     N <NA>   ARG     A    57   <NA>  4.978  28.079  19.377 1
## 431    ATOM   431    CA <NA>   ARG     A    57   <NA>  4.459  29.271  20.026 1
## 432    ATOM   432     C <NA>   ARG     A    57   <NA>  5.038  30.502  19.335 1
## 433    ATOM   433     O <NA>   ARG     A    57   <NA>  6.242  30.596  19.138 1
## 434    ATOM   434    CB <NA>   ARG     A    57   <NA>  4.824  29.245  21.505 1
## 435    ATOM   435    CG <NA>   ARG     A    57   <NA>  4.168  28.102  22.260 1
## 436    ATOM   436    CD <NA>   ARG     A    57   <NA>  4.656  28.068  23.693 1
## 437    ATOM   437    NE <NA>   ARG     A    57   <NA>  6.032  27.573  23.790 1
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## 439    ATOM   439   NH1 <NA>   ARG     A    57   <NA>  6.825  29.532  24.678 1
## 440    ATOM   440   NH2 <NA>   ARG     A    57   <NA>  8.223  27.723  24.467 1
## 441    ATOM   441     N <NA>   GLN     A    58   <NA>  4.171  31.431  18.958 1
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## 447    ATOM   447    CD <NA>   GLN     A    58   <NA>  2.500  34.473  15.541 1
## 448    ATOM   448   OE1 <NA>   GLN     A    58   <NA>  1.530  33.703  15.489 1
## 449    ATOM   449   NE2 <NA>   GLN     A    58   <NA>  2.508  35.651  14.940 1
## 450    ATOM   450     N <NA>   TYR     A    59   <NA>  5.883  34.378  19.196 1
## 451    ATOM   451    CA <NA>   TYR     A    59   <NA>  6.097  35.658  19.896 1
## 452    ATOM   452     C <NA>   TYR     A    59   <NA>  6.304  36.752  18.835 1
## 453    ATOM   453     O <NA>   TYR     A    59   <NA>  6.923  36.513  17.800 1
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## 455    ATOM   455    CG <NA>   TYR     A    59   <NA>  7.213  34.624  21.955 1
## 456    ATOM   456   CD1 <NA>   TYR     A    59   <NA>  7.479  33.237  21.805 1
## 457    ATOM   457   CD2 <NA>   TYR     A    59   <NA>  6.795  35.087  23.223 1
## 458    ATOM   458   CE1 <NA>   TYR     A    59   <NA>  7.345  32.365  22.871 1
## 459    ATOM   459   CE2 <NA>   TYR     A    59   <NA>  6.638  34.224  24.268 1
## 460    ATOM   460    CZ <NA>   TYR     A    59   <NA>  6.926  32.869  24.102 1
## 461    ATOM   461    OH <NA>   TYR     A    59   <NA>  6.967  32.076  25.200 1
## 462    ATOM   462     N <NA>   ASP     A    60   <NA>  5.767  37.940  19.049 1
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## 463    ATOM   463    CA <NA>   ASP     A    60   <NA>  6.022  39.045  18.125 1
## 464    ATOM   464     C <NA>   ASP     A    60   <NA>  7.025  40.015  18.725 1
## 465    ATOM   465     O <NA>   ASP     A    60   <NA>  7.340  39.951  19.900 1
## 466    ATOM   466    CB <NA>   ASP     A    60   <NA>  4.719  39.777  17.832 1
## 467    ATOM   467    CG <NA>   ASP     A    60   <NA>  3.699  38.899  17.148 1
## 468    ATOM   468   OD1 <NA>   ASP     A    60   <NA>  3.989  38.368  16.050 1
## 469    ATOM   469   OD2 <NA>   ASP     A    60   <NA>  2.570  38.799  17.672 1
## 470    ATOM   470     N <NA>   GLN     A    61   <NA>  7.529  40.913  17.896 1
## 471    ATOM   471    CA <NA>   GLN     A    61   <NA>  8.337  42.060  18.331 1
## 472    ATOM   472     C <NA>   GLN     A    61   <NA>  9.535  41.630  19.179 1
## 473    ATOM   473     O <NA>   GLN     A    61   <NA>  9.777  42.191  20.264 1
## 474    ATOM   474    CB <NA>   GLN     A    61   <NA>  7.471  43.051  19.131 1
## 475    ATOM   475    CG <NA>   GLN     A    61   <NA>  7.718  44.555  18.814 1
## 476    ATOM   476    CD <NA>   GLN     A    61   <NA>  7.182  45.552  19.907 1
## 477    ATOM   477   OE1 <NA>   GLN     A    61   <NA>  7.936  46.461  20.398 1
## 478    ATOM   478   NE2 <NA>   GLN     A    61   <NA>  5.892  45.377  20.306 1
## 479    ATOM   479     N <NA>   ILE     A    62   <NA> 10.283  40.645  18.676 1
## 480    ATOM   480    CA <NA>   ILE     A    62   <NA> 11.484  40.115  19.328 1
## 481    ATOM   481     C <NA>   ILE     A    62   <NA> 12.745  40.584  18.614 1
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## 483    ATOM   483    CB <NA>   ILE     A    62   <NA> 11.465  38.545  19.309 1
## 484    ATOM   484   CG1 <NA>   ILE     A    62   <NA> 10.152  38.035  19.930 1
## 485    ATOM   485   CG2 <NA>   ILE     A    62   <NA> 12.688  37.973  20.027 1
## 486    ATOM   486   CD1 <NA>   ILE     A    62   <NA>  9.966  38.380  21.363 1
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## 488    ATOM   488    CA <NA>   LEU     A    63   <NA> 15.038  41.476  18.822 1
## 489    ATOM   489     C <NA>   LEU     A    63   <NA> 16.033  40.304  18.862 1
## 490    ATOM   490     O <NA>   LEU     A    63   <NA> 16.195  39.661  19.897 1
## 491    ATOM   491    CB <NA>   LEU     A    63   <NA> 15.631  42.666  19.619 1
## 492    ATOM   492    CG <NA>   LEU     A    63   <NA> 16.776  43.426  18.914 1
## 493    ATOM   493   CD1 <NA>   LEU     A    63   <NA> 16.560  44.922  18.993 1
## 494    ATOM   494   CD2 <NA>   LEU     A    63   <NA> 18.103  43.062  19.558 1
## 495    ATOM   495     N <NA>   ILE     A    64   <NA> 16.686  40.036  17.738 1
## 496    ATOM   496    CA <NA>   ILE     A    64   <NA> 17.760  39.039  17.653 1
## 497    ATOM   497     C <NA>   ILE     A    64   <NA> 18.991  39.753  17.116 1
## 498    ATOM   498     O <NA>   ILE     A    64   <NA> 18.862  40.632  16.288 1
## 499    ATOM   499    CB <NA>   ILE     A    64   <NA> 17.390  37.875  16.634 1
## 500    ATOM   500   CG1 <NA>   ILE     A    64   <NA> 16.127  37.137  17.110 1
## 501    ATOM   501   CG2 <NA>   ILE     A    64   <NA> 18.551  36.857  16.518 1
## 502    ATOM   502   CD1 <NA>   ILE     A    64   <NA> 16.194  35.643  16.885 1
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## 506    ATOM   506     O <NA>   GLU     A    65   <NA> 22.866  38.128  16.631 1
## 507    ATOM   507    CB <NA>   GLU     A    65   <NA> 22.307  40.439  18.180 1
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## 510    ATOM   510   OE1 <NA>   GLU     A    65   <NA> 24.094  42.925  18.348 1
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## 513    ATOM   513    CA <NA>   ILE     A    66   <NA> 22.818  38.327  13.863 1
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## 516    ATOM   516    CB <NA>   ILE     A    66   <NA> 21.831  37.964  12.694 1
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## 519    ATOM   519   CD1 <NA>   ILE     A    66   <NA> 19.263  38.072  12.560 1
## 520    ATOM   520     N <NA>   CYS     A    67   <NA> 25.251  38.396  13.731 1
## 521    ATOM   521    CA <NA>   CYS     A    67   <NA> 26.590  38.871  13.351 1
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## 523    ATOM   523     O <NA>   CYS     A    67   <NA> 27.461  41.045  12.763 1
## 524    ATOM   524    CB <NA>   CYS     A    67   <NA> 26.907  38.497  11.905 1
## 525    ATOM   525    SG <NA>   CYS     A    67   <NA> 27.274  36.734  11.705 1
## 526    ATOM   526     N <NA>   GLY     A    68   <NA> 26.239  40.887  14.650 1
## 527    ATOM   527    CA <NA>   GLY     A    68   <NA> 26.319  42.307  14.938 1
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## 531    ATOM   531    CA <NA>   HIS     A    69   <NA> 23.251  43.368  13.013 1
## 532    ATOM   532     C <NA>   HIS     A    69   <NA> 22.009  43.025  13.836 1
## 533    ATOM   533     O <NA>   HIS     A    69   <NA> 21.626  41.865  13.958 1
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## 535    ATOM   535    CG <NA>   HIS     A    69   <NA> 24.157  43.172  10.639 1
## 536    ATOM   536   ND1 <NA>   HIS     A    69   <NA> 25.294  42.398  10.762 1
## 537    ATOM   537   CD2 <NA>   HIS     A    69   <NA> 24.283  43.886   9.518 1
## 538    ATOM   538   CE1 <NA>   HIS     A    69   <NA> 26.075  42.630   9.723 1
## 539    ATOM   539   NE2 <NA>   HIS     A    69   <NA> 25.505  43.532   8.946 1
## 540    ATOM   540     N <NA>   LYS     A    70   <NA> 21.364  44.050  14.376 1
## 541    ATOM   541    CA <NA>   LYS     A    70   <NA> 20.030  43.883  14.945 1
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## 544    ATOM   544    CB <NA>   LYS     A    70   <NA> 19.667  45.075  15.840 1
## 545    ATOM   545    CG <NA>   LYS     A    70   <NA> 20.422  45.141  17.154 1
## 546    ATOM   546    CD <NA>   LYS     A    70   <NA> 19.885  46.281  18.036 1
## 547    ATOM   547    CE <NA>   LYS     A    70   <NA> 20.905  46.699  19.095 1
## 548    ATOM   548    NZ <NA>   LYS     A    70   <NA> 20.376  47.817  19.946 1
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## 550    ATOM   550    CA <NA>   ALA     A    71   <NA> 16.703  42.737  13.499 1
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## 557    ATOM   557     O <NA>   ILE     A    72   <NA> 12.083  42.266  13.025 1
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## 560    ATOM   560   CG2 <NA>   ILE     A    72   <NA> 11.353  43.782  16.409 1
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## 571    ATOM   571   OG1 <NA>   THR     A    74   <NA>  6.030  38.013  14.001 1
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## 593    ATOM   593   CG1 <NA>   VAL     A    77   <NA> 10.306  28.419  21.773 1
## 594    ATOM   594   CG2 <NA>   VAL     A    77   <NA> 10.426  30.686  20.648 1
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## 596    ATOM   596    CA <NA>   GLY     A    78   <NA>  9.027  24.918  19.185 1
## 597    ATOM   597     C <NA>   GLY     A    78   <NA> 10.005  23.782  18.984 1
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## 599    ATOM   599     N <NA>   PRO     A    79   <NA>  9.538  22.542  18.758 1
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## 605    ATOM   605    CD <NA>   PRO     A    79   <NA>  8.170  22.144  18.383 1
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## 609    ATOM   609     O <NA>   THR     A    80   <NA> 14.692  21.666  17.473 1
## 610    ATOM   610    CB <NA>   THR     A    80   <NA> 13.031  23.467  15.319 1
## 611    ATOM   611   OG1 <NA>   THR     A    80   <NA> 13.971  23.419  14.244 1
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## 615    ATOM   615     C <NA>   PRO     A    81   <NA> 17.352  21.205  15.795 1
## 616    ATOM   616     O <NA>   PRO     A    81   <NA> 18.306  21.085  16.567 1
## 617    ATOM   617    CB <NA>   PRO     A    81   <NA> 16.467  19.139  14.669 1
## 618    ATOM   618    CG <NA>   PRO     A    81   <NA> 15.477  19.489  13.607 1
## 619    ATOM   619    CD <NA>   PRO     A    81   <NA> 14.331  20.114  14.238 1
## 620    ATOM   620     N <NA>   VAL     A    82   <NA> 17.220  22.219  14.948 1
## 621    ATOM   621    CA <NA>   VAL     A    82   <NA> 18.236  23.243  14.762 1
## 622    ATOM   622     C <NA>   VAL     A    82   <NA> 17.549  24.626  14.801 1
## 623    ATOM   623     O <NA>   VAL     A    82   <NA> 16.328  24.735  14.569 1
## 624    ATOM   624    CB <NA>   VAL     A    82   <NA> 18.969  23.017  13.388 1
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## 625    ATOM   625   CG1 <NA>   VAL     A    82   <NA> 18.009  22.769  12.263 1
## 626    ATOM   626   CG2 <NA>   VAL     A    82   <NA> 19.843  24.144  13.080 1
## 627    ATOM   627     N <NA>   ASN     A    83   <NA> 18.292  25.671  15.167 1
## 628    ATOM   628    CA <NA>   ASN     A    83   <NA> 17.731  27.051  15.193 1
## 629    ATOM   629     C <NA>   ASN     A    83   <NA> 17.799  27.628  13.799 1
## 630    ATOM   630     O <NA>   ASN     A    83   <NA> 18.794  27.456  13.113 1
## 631    ATOM   631    CB <NA>   ASN     A    83   <NA> 18.508  27.950  16.161 1
## 632    ATOM   632    CG <NA>   ASN     A    83   <NA> 18.236  27.600  17.636 1
## 633    ATOM   633   OD1 <NA>   ASN     A    83   <NA> 17.102  27.381  18.051 1
## 634    ATOM   634   ND2 <NA>   ASN     A    83   <NA> 19.287  27.475  18.398 1
## 635    ATOM   635     N <NA>   ILE     A    84   <NA> 16.729  28.283  13.370 1
## 636    ATOM   636    CA <NA>   ILE     A    84   <NA> 16.588  28.651  11.955 1
## 637    ATOM   637     C <NA>   ILE     A    84   <NA> 16.190  30.132  11.811 1
## 638    ATOM   638     O <NA>   ILE     A    84   <NA> 15.178  30.600  12.384 1
## 639    ATOM   639    CB <NA>   ILE     A    84   <NA> 15.504  27.755  11.242 1
## 640    ATOM   640   CG1 <NA>   ILE     A    84   <NA> 16.049  26.365  11.040 1
## 641    ATOM   641   CG2 <NA>   ILE     A    84   <NA> 15.081  28.324   9.932 1
## 642    ATOM   642   CD1 <NA>   ILE     A    84   <NA> 14.957  25.345  11.321 1
## 643    ATOM   643     N <NA>   ILE     A    85   <NA> 16.991  30.863  11.053 1
## 644    ATOM   644    CA <NA>   ILE     A    85   <NA> 16.710  32.257  10.821 1
## 645    ATOM   645     C <NA>   ILE     A    85   <NA> 16.155  32.252   9.420 1
## 646    ATOM   646     O <NA>   ILE     A    85   <NA> 16.857  31.950   8.464 1
## 647    ATOM   647    CB <NA>   ILE     A    85   <NA> 17.999  33.119  10.844 1
## 648    ATOM   648   CG1 <NA>   ILE     A    85   <NA> 18.724  32.983  12.207 1
## 649    ATOM   649   CG2 <NA>   ILE     A    85   <NA> 17.653  34.600  10.517 1
## 650    ATOM   650   CD1 <NA>   ILE     A    85   <NA> 17.830  33.204  13.418 1
## 651    ATOM   651     N <NA>   GLY     A    86   <NA> 14.888  32.608   9.302 1
## 652    ATOM   652    CA <NA>   GLY     A    86   <NA> 14.238  32.655   8.011 1
## 653    ATOM   653     C <NA>   GLY     A    86   <NA> 14.181  34.034   7.393 1
## 654    ATOM   654     O <NA>   GLY     A    86   <NA> 14.714  34.991   7.894 1
## 655    ATOM   655     N <NA>   ARG     A    87   <NA> 13.398  34.131   6.334 1
## 656    ATOM   656    CA <NA>   ARG     A    87   <NA> 13.370  35.302   5.456 1
## 657    ATOM   657     C <NA>   ARG     A    87   <NA> 12.931  36.548   6.216 1
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## 664    ATOM   664   NH1 <NA>   ARG     A    87   <NA> 10.126  35.860   1.922 1
## 665    ATOM   665   NH2 <NA>   ARG     A    87   <NA>  8.657  34.143   2.300 1
## 666    ATOM   666     N <NA>   ASN     A    88   <NA> 12.063  36.352   7.198 1
## 667    ATOM   667    CA <NA>   ASN     A    88   <NA> 11.458  37.455   7.919 1
## 668    ATOM   668     C <NA>   ASN     A    88   <NA> 12.511  38.266   8.653 1
## 669    ATOM   669     O <NA>   ASN     A    88   <NA> 12.419  39.481   8.723 1
## 670    ATOM   670    CB <NA>   ASN     A    88   <NA> 10.359  36.959   8.863 1
## 671    ATOM   671    CG <NA>   ASN     A    88   <NA> 10.892  36.309  10.125 1
## 672    ATOM   672   OD1 <NA>   ASN     A    88   <NA> 11.577  35.273  10.065 1
## 673    ATOM   673   ND2 <NA>   ASN     A    88   <NA> 10.446  36.809  11.283 1
## 674    ATOM   674     N <NA>   LEU     A    89   <NA> 13.551  37.601   9.136 1
## 675    ATOM   675    CA <NA>   LEU     A    89   <NA> 14.633  38.337   9.729 1
## 676    ATOM   676     C <NA>   LEU     A    89   <NA> 15.802  38.487   8.783 1
## 677    ATOM   677     O <NA>   LEU     A    89   <NA> 16.580  39.394   8.941 1
## 678    ATOM   678    CB <NA>   LEU     A    89   <NA> 15.096  37.687  11.029 1
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## 679    ATOM   679    CG <NA>   LEU     A    89   <NA> 14.146  37.555  12.221 1
## 680    ATOM   680   CD1 <NA>   LEU     A    89   <NA> 14.939  37.022  13.434 1
## 681    ATOM   681   CD2 <NA>   LEU     A    89   <NA> 13.508  38.913  12.527 1
## 682    ATOM   682     N <NA>   LEU     A    90   <NA> 15.910  37.651   7.761 1
## 683    ATOM   683    CA <NA>   LEU     A    90   <NA> 17.078  37.773   6.865 1
## 684    ATOM   684     C <NA>   LEU     A    90   <NA> 17.048  39.068   6.049 1
## 685    ATOM   685     O <NA>   LEU     A    90   <NA> 18.098  39.613   5.652 1
## 686    ATOM   686    CB <NA>   LEU     A    90   <NA> 17.200  36.561   5.913 1
## 687    ATOM   687    CG <NA>   LEU     A    90   <NA> 17.754  35.226   6.440 1
## 688    ATOM   688   CD1 <NA>   LEU     A    90   <NA> 17.798  34.207   5.340 1
## 689    ATOM   689   CD2 <NA>   LEU     A    90   <NA> 19.138  35.441   7.022 1
## 690    ATOM   690     N <NA>   THR     A    91   <NA> 15.835  39.547   5.808 1
## 691    ATOM   691    CA <NA>   THR     A    91   <NA> 15.653  40.738   4.985 1
## 692    ATOM   692     C <NA>   THR     A    91   <NA> 16.137  41.999   5.772 1
## 693    ATOM   693     O <NA>   THR     A    91   <NA> 16.848  42.870   5.252 1
## 694    ATOM   694    CB <NA>   THR     A    91   <NA> 14.157  40.860   4.594 1
## 695    ATOM   695   OG1 <NA>   THR     A    91   <NA> 13.342  40.810   5.786 1
## 696    ATOM   696   CG2 <NA>   THR     A    91   <NA> 13.740  39.709   3.681 1
## 697    ATOM   697     N <NA>   GLN     A    92   <NA> 15.842  42.001   7.064 1
## 698    ATOM   698    CA <NA>   GLN     A    92   <NA> 16.170  43.099   7.967 1
## 699    ATOM   699     C <NA>   GLN     A    92   <NA> 17.650  43.315   8.126 1
## 700    ATOM   700     O <NA>   GLN     A    92   <NA> 18.071  44.440   8.459 1
## 701    ATOM   701    CB <NA>   GLN     A    92   <NA> 15.580  42.837   9.347 1
## 702    ATOM   702    CG <NA>   GLN     A    92   <NA> 14.081  42.603   9.325 1
## 703    ATOM   703    CD <NA>   GLN     A    92   <NA> 13.318  43.811   8.800 1
## 704    ATOM   704   OE1 <NA>   GLN     A    92   <NA> 12.836  43.807   7.683 1
## 705    ATOM   705   NE2 <NA>   GLN     A    92   <NA> 13.349  44.892   9.543 1
## 706    ATOM   706     N <NA>   ILE     A    93   <NA> 18.444  42.266   7.913 1
## 707    ATOM   707    CA <NA>   ILE     A    93   <NA> 19.887  42.417   8.035 1
## 708    ATOM   708     C <NA>   ILE     A    93   <NA> 20.530  42.555   6.677 1
## 709    ATOM   709     O <NA>   ILE     A    93   <NA> 21.744  42.639   6.577 1
## 710    ATOM   710    CB <NA>   ILE     A    93   <NA> 20.557  41.231   8.872 1
## 711    ATOM   711   CG1 <NA>   ILE     A    93   <NA> 20.472  39.878   8.113 1
## 712    ATOM   712   CG2 <NA>   ILE     A    93   <NA> 19.926  41.182  10.272 1
## 713    ATOM   713   CD1 <NA>   ILE     A    93   <NA> 21.520  38.796   8.533 1
## 714    ATOM   714     N <NA>   GLY     A    94   <NA> 19.713  42.563   5.636 1
## 715    ATOM   715    CA <NA>   GLY     A    94   <NA> 20.226  42.870   4.327 1
## 716    ATOM   716     C <NA>   GLY     A    94   <NA> 20.843  41.689   3.611 1
## 717    ATOM   717     O <NA>   GLY     A    94   <NA> 21.680  41.866   2.723 1
## 718    ATOM   718     N <NA>   CYS     A    95   <NA> 20.294  40.507   3.844 1
## 719    ATOM   719    CA <NA>   CYS     A    95   <NA> 20.890  39.296   3.297 1
## 720    ATOM   720     C <NA>   CYS     A    95   <NA> 20.407  39.005   1.897 1
## 721    ATOM   721     O <NA>   CYS     A    95   <NA> 19.217  39.101   1.606 1
## 722    ATOM   722    CB <NA>   CYS     A    95   <NA> 20.585  38.134   4.215 1
## 723    ATOM   723    SG <NA>   CYS     A    95   <NA> 21.505  36.663   3.848 1
## 724    ATOM   724     N <NA>   THR     A    96   <NA> 21.339  38.698   1.005 1
## 725    ATOM   725    CA <NA>   THR     A    96   <NA> 20.969  38.276  -0.346 1
## 726    ATOM   726     C <NA>   THR     A    96   <NA> 21.721  37.024  -0.758 1
## 727    ATOM   727     O <NA>   THR     A    96   <NA> 22.753  36.645  -0.178 1
## 728    ATOM   728    CB <NA>   THR     A    96   <NA> 21.298  39.331  -1.459 1
## 729    ATOM   729   OG1 <NA>   THR     A    96   <NA> 22.688  39.698  -1.364 1
## 730    ATOM   730   CG2 <NA>   THR     A    96   <NA> 20.405  40.560  -1.303 1
## 731    ATOM   731     N <NA>   LEU     A    97   <NA> 21.183  36.413  -1.805 1
## 732    ATOM   732    CA <NA>   LEU     A    97   <NA> 21.718  35.228  -2.473 1
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## 733    ATOM   733     C <NA>   LEU     A    97   <NA> 22.314  35.753  -3.779 1
## 734    ATOM   734     O <NA>   LEU     A    97   <NA> 21.616  36.396  -4.577 1
## 735    ATOM   735    CB <NA>   LEU     A    97   <NA> 20.518  34.349  -2.810 1
## 736    ATOM   736    CG <NA>   LEU     A    97   <NA> 20.318  32.897  -2.464 1
## 737    ATOM   737   CD1 <NA>   LEU     A    97   <NA> 21.285  32.388  -1.422 1
## 738    ATOM   738   CD2 <NA>   LEU     A    97   <NA> 18.896  32.782  -2.010 1
## 739    ATOM   739     N <NA>   ASN     A    98   <NA> 23.577  35.469  -4.026 1
## 740    ATOM   740    CA <NA>   ASN     A    98   <NA> 24.207  35.904  -5.257 1
## 741    ATOM   741     C <NA>   ASN     A    98   <NA> 24.863  34.748  -5.999 1
## 742    ATOM   742     O <NA>   ASN     A    98   <NA> 25.635  33.982  -5.396 1
## 743    ATOM   743    CB <NA>   ASN     A    98   <NA> 25.229  36.991  -4.938 1
## 744    ATOM   744    CG <NA>   ASN     A    98   <NA> 24.609  38.190  -4.212 1
## 745    ATOM   745   OD1 <NA>   ASN     A    98   <NA> 24.263  38.112  -3.019 1
## 746    ATOM   746   ND2 <NA>   ASN     A    98   <NA> 24.354  39.252  -4.955 1
## 747    ATOM   747     N <NA>   PHE     A    99   <NA> 24.539  34.602  -7.287 1
## 748    ATOM   748    CA <NA>   PHE     A    99   <NA> 25.376  33.754  -8.172 1
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## 750    ATOM   750     O <NA>   PHE     A    99   <NA> 24.797  34.890 -10.226 1
## 751    ATOM   751    CB <NA>   PHE     A    99   <NA> 24.743  32.354  -8.375 1
## 752    ATOM   752    CG <NA>   PHE     A    99   <NA> 23.328  32.389  -8.856 1
## 753    ATOM   753   CD1 <NA>   PHE     A    99   <NA> 22.303  32.588  -7.961 1
## 754    ATOM   754   CD2 <NA>   PHE     A    99   <NA> 23.029  32.118 -10.181 1
## 755    ATOM   755   CE1 <NA>   PHE     A    99   <NA> 21.000  32.515  -8.357 1
## 756    ATOM   756   CE2 <NA>   PHE     A    99   <NA> 21.730  32.028 -10.613 1
## 757    ATOM   757    CZ <NA>   PHE     A    99   <NA> 20.700  32.221  -9.700 1
## 758    ATOM   759     N <NA>   PRO     B     1   <NA> 22.659  36.727 -10.823 1
## 759    ATOM   760    CA <NA>   PRO     B     1   <NA> 21.708  37.741 -10.269 1
## 760    ATOM   761     C <NA>   PRO     B     1   <NA> 21.931  37.939  -8.779 1
## 761    ATOM   762     O <NA>   PRO     B     1   <NA> 22.755  37.283  -8.190 1
## 762    ATOM   763    CB <NA>   PRO     B     1   <NA> 20.263  37.289 -10.512 1
## 763    ATOM   764    CG <NA>   PRO     B     1   <NA> 20.385  35.811 -10.891 1
## 764    ATOM   765    CD <NA>   PRO     B     1   <NA> 21.753  35.755 -11.555 1
## 765    ATOM   766     N <NA>   GLN     B     2   <NA> 21.203  38.873  -8.191 1
## 766    ATOM   767    CA <NA>   GLN     B     2   <NA> 21.156  39.043  -6.744 1
## 767    ATOM   768     C <NA>   GLN     B     2   <NA> 19.698  38.882  -6.389 1
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## 769    ATOM   770    CB <NA>   GLN     B     2   <NA> 21.625  40.447  -6.329 1
## 770    ATOM   771    CG <NA>   GLN     B     2   <NA> 21.353  40.777  -4.865 1
## 771    ATOM   772    CD <NA>   GLN     B     2   <NA> 22.139  41.975  -4.358 1
## 772    ATOM   773   OE1 <NA>   GLN     B     2   <NA> 21.577  42.881  -3.752 1
## 773    ATOM   774   NE2 <NA>   GLN     B     2   <NA> 23.450  41.976  -4.586 1
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## 779    ATOM   780   CG1 <NA>   ILE     B     3   <NA> 17.788  35.772  -6.692 1
## 780    ATOM   781   CG2 <NA>   ILE     B     3   <NA> 16.284  35.967  -4.750 1
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## 783    ATOM   784    CA <NA>   THR     B     4   <NA> 16.635  39.571  -2.117 1
## 784    ATOM   785     C <NA>   THR     B     4   <NA> 15.555  38.634  -1.627 1
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## 787    ATOM   788   OG1 <NA>   THR     B     4   <NA> 15.093  41.256  -3.079 1
## 788    ATOM   789   CG2 <NA>   THR     B     4   <NA> 17.283  42.019  -2.472 1
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## 790    ATOM   791    CA <NA>   LEU     B     5   <NA> 14.466  37.636   0.259 1
## 791    ATOM   792     C <NA>   LEU     B     5   <NA> 13.125  38.065   0.821 1
## 792    ATOM   793     O <NA>   LEU     B     5   <NA> 12.585  37.446   1.733 1
## 793    ATOM   794    CB <NA>   LEU     B     5   <NA> 15.340  37.047   1.374 1
## 794    ATOM   795    CG <NA>   LEU     B     5   <NA> 16.622  36.365   0.892 1
## 795    ATOM   796   CD1 <NA>   LEU     B     5   <NA> 17.455  35.953   2.080 1
## 796    ATOM   797   CD2 <NA>   LEU     B     5   <NA> 16.248  35.136  -0.006 1
## 797    ATOM   798     N <NA>   TRP     B     6   <NA> 12.567  39.127   0.262 1
## 798    ATOM   799    CA <NA>   TRP     B     6   <NA> 11.260  39.582   0.682 1
## 799    ATOM   800     C <NA>   TRP     B     6   <NA> 10.196  38.601   0.218 1
## 800    ATOM   801     O <NA>   TRP     B     6   <NA>  9.192  38.404   0.903 1
## 801    ATOM   802    CB <NA>   TRP     B     6   <NA> 11.004  40.992   0.135 1
## 802    ATOM   803    CG <NA>   TRP     B     6   <NA> 12.065  42.014   0.478 1
## 803    ATOM   804   CD1 <NA>   TRP     B     6   <NA> 13.157  42.366  -0.279 1
## 804    ATOM   805   CD2 <NA>   TRP     B     6   <NA> 12.209  42.716   1.739 1
## 805    ATOM   806   NE1 <NA>   TRP     B     6   <NA> 13.979  43.196   0.470 1
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## 807    ATOM   808   CE3 <NA>   TRP     B     6   <NA> 11.443  42.805   2.913 1
## 808    ATOM   809   CZ2 <NA>   TRP     B     6   <NA> 13.914  44.211   2.785 1
## 809    ATOM   810   CZ3 <NA>   TRP     B     6   <NA> 11.903  43.585   3.953 1
## 810    ATOM   811   CH2 <NA>   TRP     B     6   <NA> 13.148  44.273   3.896 1
## 811    ATOM   812     N <NA>   GLN     B     7   <NA> 10.396  38.008  -0.958 1
## 812    ATOM   813    CA <NA>   GLN     B     7   <NA>  9.518  36.960  -1.516 1
## 813    ATOM   814     C <NA>   GLN     B     7   <NA> 10.321  35.670  -1.433 1
## 814    ATOM   815     O <NA>   GLN     B     7   <NA> 11.546  35.694  -1.298 1
## 815    ATOM   816    CB <NA>   GLN     B     7   <NA>  9.215  37.238  -3.000 1
## 816    ATOM   817    CG <NA>   GLN     B     7   <NA>  8.278  38.433  -3.326 1
## 817    ATOM   818    CD <NA>   GLN     B     7   <NA>  7.629  38.332  -4.744 1
## 818    ATOM   819   OE1 <NA>   GLN     B     7   <NA>  8.319  38.100  -5.754 1
## 819    ATOM   820   NE2 <NA>   GLN     B     7   <NA>  6.307  38.532  -4.814 1
## 820    ATOM   821     N <NA>   ARG     B     8   <NA>  9.661  34.528  -1.525 1
## 821    ATOM   822    CA <NA>   ARG     B     8   <NA> 10.385  33.251  -1.642 1
## 822    ATOM   823     C <NA>   ARG     B     8   <NA> 11.348  33.305  -2.780 1
## 823    ATOM   824     O <NA>   ARG     B     8   <NA> 10.964  33.682  -3.906 1
## 824    ATOM   825    CB <NA>   ARG     B     8   <NA>  9.435  32.061  -1.862 1
## 825    ATOM   826    CG <NA>   ARG     B     8   <NA>  8.623  31.716  -0.644 1
## 826    ATOM   827    CD <NA>   ARG     B     8   <NA>  7.828  30.471  -0.844 1
## 827    ATOM   828    NE <NA>   ARG     B     8   <NA>  7.143  30.102   0.378 1
## 828    ATOM   829    CZ <NA>   ARG     B     8   <NA>  6.523  28.938   0.561 1
## 829    ATOM   830   NH1 <NA>   ARG     B     8   <NA>  6.476  28.028  -0.411 1
## 830    ATOM   831   NH2 <NA>   ARG     B     8   <NA>  5.925  28.688   1.719 1
## 831    ATOM   832     N <NA>   PRO     B     9   <NA> 12.533  32.711  -2.598 1
## 832    ATOM   833    CA <NA>   PRO     B     9   <NA> 13.443  32.743  -3.746 1
## 833    ATOM   834     C <NA>   PRO     B     9   <NA> 13.174  31.592  -4.703 1
## 834    ATOM   835     O <NA>   PRO     B     9   <NA> 13.897  30.587  -4.698 1
## 835    ATOM   836    CB <NA>   PRO     B     9   <NA> 14.813  32.658  -3.125 1
## 836    ATOM   837    CG <NA>   PRO     B     9   <NA> 14.564  31.823  -1.917 1
## 837    ATOM   838    CD <NA>   PRO     B     9   <NA> 13.238  32.289  -1.373 1
## 838    ATOM   839     N <NA>   LEU     B    10   <NA> 12.134  31.727  -5.504 1
## 839    ATOM   840    CA <NA>   LEU     B    10   <NA> 11.816  30.740  -6.534 1
## 840    ATOM   841     C <NA>   LEU     B    10   <NA> 12.459  31.075  -7.877 1
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## 841    ATOM   842     O <NA>   LEU     B    10   <NA> 12.274  32.150  -8.406 1
## 842    ATOM   843    CB <NA>   LEU     B    10   <NA> 10.303  30.637  -6.738 1
## 843    ATOM   844    CG <NA>   LEU     B    10   <NA>  9.483  30.307  -5.497 1
## 844    ATOM   845   CD1 <NA>   LEU     B    10   <NA>  8.028  30.334  -5.876 1
## 845    ATOM   846   CD2 <NA>   LEU     B    10   <NA>  9.845  28.975  -4.951 1
## 846    ATOM   847     N <NA>   VAL     B    11   <NA> 13.225  30.141  -8.420 1
## 847    ATOM   848    CA <NA>   VAL     B    11   <NA> 13.759  30.227  -9.768 1
## 848    ATOM   849     C <NA>   VAL     B    11   <NA> 13.103  29.153 -10.641 1
## 849    ATOM   850     O <NA>   VAL     B    11   <NA> 12.381  28.285 -10.135 1
## 850    ATOM   851    CB <NA>   VAL     B    11   <NA> 15.253  29.988  -9.735 1
## 851    ATOM   852   CG1 <NA>   VAL     B    11   <NA> 15.898  31.108  -8.939 1
## 852    ATOM   853   CG2 <NA>   VAL     B    11   <NA> 15.573  28.635  -9.104 1
## 853    ATOM   854     N <NA>   THR     B    12   <NA> 13.346  29.214 -11.949 1
## 854    ATOM   855    CA <NA>   THR     B    12   <NA> 12.809  28.220 -12.873 1
## 855    ATOM   856     C <NA>   THR     B    12   <NA> 13.951  27.253 -13.210 1
## 856    ATOM   857     O <NA>   THR     B    12   <NA> 15.089  27.656 -13.442 1
## 857    ATOM   858    CB <NA>   THR     B    12   <NA> 12.259  28.907 -14.158 1
## 858    ATOM   859   OG1 <NA>   THR     B    12   <NA> 11.693  27.933 -15.028 1
## 859    ATOM   860   CG2 <NA>   THR     B    12   <NA> 13.341  29.639 -14.925 1
## 860    ATOM   861     N <NA>   ILE     B    13   <NA> 13.684  25.961 -13.124 1
## 861    ATOM   862    CA <NA>   ILE     B    13   <NA> 14.708  24.966 -13.446 1
## 862    ATOM   863     C <NA>   ILE     B    13   <NA> 14.230  24.165 -14.639 1
## 863    ATOM   864     O <NA>   ILE     B    13   <NA> 13.014  24.057 -14.918 1
## 864    ATOM   865    CB <NA>   ILE     B    13   <NA> 14.993  23.953 -12.269 1
## 865    ATOM   866   CG1 <NA>   ILE     B    13   <NA> 13.699  23.190 -11.870 1
## 866    ATOM   867   CG2 <NA>   ILE     B    13   <NA> 15.564  24.705 -11.094 1
## 867    ATOM   868   CD1 <NA>   ILE     B    13   <NA> 13.900  22.077 -10.834 1
## 868    ATOM   869     N <NA>   LYS     B    14   <NA> 15.186  23.630 -15.378 1
## 869    ATOM   870    CA <NA>   LYS     B    14   <NA> 14.828  22.733 -16.464 1
## 870    ATOM   871     C <NA>   LYS     B    14   <NA> 15.482  21.387 -16.141 1
## 871    ATOM   872     O <NA>   LYS     B    14   <NA> 16.690  21.305 -15.886 1
## 872    ATOM   873    CB <NA>   LYS     B    14   <NA> 15.340  23.256 -17.814 1
## 873    ATOM   874    CG <NA>   LYS     B    14   <NA> 14.868  22.447 -18.992 1
## 874    ATOM   875    CD <NA>   LYS     B    14   <NA> 14.687  23.295 -20.194 1
## 875    ATOM   876    CE <NA>   LYS     B    14   <NA> 15.979  23.453 -20.922 1
## 876    ATOM   877    NZ <NA>   LYS     B    14   <NA> 15.739  23.451 -22.389 1
## 877    ATOM   878     N <NA>   ILE     B    15   <NA> 14.660  20.354 -16.136 1
## 878    ATOM   879    CA <NA>   ILE     B    15   <NA> 15.108  18.999 -15.906 1
## 879    ATOM   880     C <NA>   ILE     B    15   <NA> 14.188  18.067 -16.702 1
## 880    ATOM   881     O <NA>   ILE     B    15   <NA> 12.968  18.199 -16.719 1
## 881    ATOM   882    CB <NA>   ILE     B    15   <NA> 15.090  18.663 -14.360 1
## 882    ATOM   883   CG1 <NA>   ILE     B    15   <NA> 15.694  17.283 -14.101 1
## 883    ATOM   884   CG2 <NA>   ILE     B    15   <NA> 13.682  18.760 -13.780 1
## 884    ATOM   885   CD1 <NA>   ILE     B    15   <NA> 16.011  17.036 -12.625 1
## 885    ATOM   886     N <NA>   GLY     B    16   <NA> 14.799  17.159 -17.438 1
## 886    ATOM   887    CA <NA>   GLY     B    16   <NA> 14.024  16.279 -18.286 1
## 887    ATOM   888     C <NA>   GLY     B    16   <NA> 13.311  17.029 -19.391 1
## 888    ATOM   889     O <NA>   GLY     B    16   <NA> 12.318  16.549 -19.924 1
## 889    ATOM   890     N <NA>   GLY     B    17   <NA> 13.887  18.145 -19.823 1
## 890    ATOM   891    CA <NA>   GLY     B    17   <NA> 13.243  18.938 -20.850 1
## 891    ATOM   892     C <NA>   GLY     B    17   <NA> 12.009  19.638 -20.345 1
## 892    ATOM   893     O <NA>   GLY     B    17   <NA> 11.392  20.369 -21.084 1
## 893    ATOM   894     N <NA>   GLN     B    18   <NA> 11.676  19.486 -19.073 1
## 894    ATOM   895    CA <NA>   GLN     B    18   <NA> 10.572  20.249 -18.515 1
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## 895    ATOM   896     C <NA>   GLN     B    18   <NA> 11.056  21.466 -17.699 1
## 896    ATOM   897     O <NA>   GLN     B    18   <NA> 12.196  21.494 -17.175 1
## 897    ATOM   898    CB <NA>   GLN     B    18   <NA>  9.708  19.388 -17.619 1
## 898    ATOM   899    CG <NA>   GLN     B    18   <NA>  8.936  18.297 -18.309 1
## 899    ATOM   900    CD <NA>   GLN     B    18   <NA>  9.088  16.973 -17.566 1
## 900    ATOM   901   OE1 <NA>   GLN     B    18   <NA>  9.813  16.078 -18.014 1
## 901    ATOM   902   NE2 <NA>   GLN     B    18   <NA>  8.488  16.884 -16.371 1
## 902    ATOM   903     N <NA>   LEU     B    19   <NA> 10.186  22.475 -17.590 1
## 903    ATOM   904    CA <NA>   LEU     B    19   <NA> 10.450  23.647 -16.749 1
## 904    ATOM   905     C <NA>   LEU     B    19   <NA>  9.631  23.511 -15.483 1
## 905    ATOM   906     O <NA>   LEU     B    19   <NA>  8.432  23.277 -15.551 1
## 906    ATOM   907    CB <NA>   LEU     B    19   <NA> 10.010  24.932 -17.474 1
## 907    ATOM   908    CG <NA>   LEU     B    19   <NA> 10.775  25.419 -18.723 1
## 908    ATOM   909   CD1 <NA>   LEU     B    19   <NA> 10.226  26.727 -19.190 1
## 909    ATOM   910   CD2 <NA>   LEU     B    19   <NA> 12.241  25.543 -18.395 1
## 910    ATOM   911     N <NA>   LYS     B    20   <NA> 10.273  23.619 -14.329 1
## 911    ATOM   912    CA <NA>   LYS     B    20   <NA>  9.576  23.583 -13.044 1
## 912    ATOM   913     C <NA>   LYS     B    20   <NA> 10.018  24.784 -12.260 1
## 913    ATOM   914     O <NA>   LYS     B    20   <NA> 10.998  25.429 -12.605 1
## 914    ATOM   915    CB <NA>   LYS     B    20   <NA>  9.970  22.364 -12.236 1
## 915    ATOM   916    CG <NA>   LYS     B    20   <NA> 10.281  21.123 -13.051 1
## 916    ATOM   917    CD <NA>   LYS     B    20   <NA>  9.037  20.289 -13.305 1
## 917    ATOM   918    CE <NA>   LYS     B    20   <NA>  9.400  18.836 -13.595 1
## 918    ATOM   919    NZ <NA>   LYS     B    20   <NA>  9.672  18.102 -12.328 1
## 919    ATOM   920     N <NA>   GLU     B    21   <NA>  9.324  25.048 -11.162 1
## 920    ATOM   921    CA <NA>   GLU     B    21   <NA>  9.705  26.075 -10.199 1
## 921    ATOM   922     C <NA>   GLU     B    21   <NA> 10.311  25.408  -8.990 1
## 922    ATOM   923     O <NA>   GLU     B    21   <NA>  9.847  24.351  -8.547 1
## 923    ATOM   924    CB <NA>   GLU     B    21   <NA>  8.468  26.848  -9.767 1
## 924    ATOM   925    CG <NA>   GLU     B    21   <NA>  8.676  28.343  -9.687 1
## 925    ATOM   926    CD <NA>   GLU     B    21   <NA>  7.419  29.111 -10.041 1
## 926    ATOM   927   OE1 <NA>   GLU     B    21   <NA>  6.374  28.877  -9.383 1
## 927    ATOM   928   OE2 <NA>   GLU     B    21   <NA>  7.461  29.911 -11.004 1
## 928    ATOM   929     N <NA>   ALA     B    22   <NA> 11.348  26.008  -8.443 1
## 929    ATOM   930    CA <NA>   ALA     B    22   <NA> 12.025  25.431  -7.271 1
## 930    ATOM   931     C <NA>   ALA     B    22   <NA> 12.472  26.569  -6.331 1
## 931    ATOM   932     O <NA>   ALA     B    22   <NA> 12.709  27.701  -6.765 1
## 932    ATOM   933    CB <NA>   ALA     B    22   <NA> 13.248  24.643  -7.708 1
## 933    ATOM   934     N <NA>   LEU     B    23   <NA> 12.560  26.257  -5.054 1
## 934    ATOM   935    CA <NA>   LEU     B    23   <NA> 13.017  27.151  -4.001 1
## 935    ATOM   936     C <NA>   LEU     B    23   <NA> 14.518  27.005  -3.822 1
## 936    ATOM   937     O <NA>   LEU     B    23   <NA> 15.008  25.915  -3.588 1
## 937    ATOM   938    CB <NA>   LEU     B    23   <NA> 12.330  26.721  -2.741 1
## 938    ATOM   939    CG <NA>   LEU     B    23   <NA> 12.592  27.472  -1.469 1
## 939    ATOM   940   CD1 <NA>   LEU     B    23   <NA> 12.006  28.877  -1.562 1
## 940    ATOM   941   CD2 <NA>   LEU     B    23   <NA> 11.917  26.658  -0.379 1
## 941    ATOM   942     N <NA>   LEU     B    24   <NA> 15.266  28.090  -3.963 1
## 942    ATOM   943    CA <NA>   LEU     B    24   <NA> 16.672  28.114  -3.511 1
## 943    ATOM   944     C <NA>   LEU     B    24   <NA> 16.809  28.098  -1.992 1
## 944    ATOM   945     O <NA>   LEU     B    24   <NA> 16.417  29.019  -1.338 1
## 945    ATOM   946    CB <NA>   LEU     B    24   <NA> 17.416  29.342  -4.065 1
## 946    ATOM   947    CG <NA>   LEU     B    24   <NA> 17.444  29.528  -5.585 1
## 947    ATOM   948   CD1 <NA>   LEU     B    24   <NA> 18.151  30.843  -5.884 1
## 948    ATOM   949   CD2 <NA>   LEU     B    24   <NA> 18.170  28.385  -6.270 1
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## 949    ATOM   950     N <NA>   ASP     B    25   <NA> 17.407  27.054  -1.437 1
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## 951    ATOM   952     C <NA>   ASP     B    25   <NA> 18.555  26.446   0.653 1
## 952    ATOM   953     O <NA>   ASP     B    25   <NA> 19.003  25.309   0.692 1
## 953    ATOM   954    CB <NA>   ASP     B    25   <NA> 16.258  25.572   0.084 1
## 954    ATOM   955    CG <NA>   ASP     B    25   <NA> 15.759  25.336   1.493 1
## 955    ATOM   956   OD1 <NA>   ASP     B    25   <NA> 16.399  25.780   2.453 1
## 956    ATOM   957   OD2 <NA>   ASP     B    25   <NA> 14.731  24.675   1.645 1
## 957    ATOM   958     N <NA>   THR     B    26   <NA> 19.163  27.455   1.257 1
## 958    ATOM   959    CA <NA>   THR     B    26   <NA> 20.441  27.290   1.920 1
## 959    ATOM   960     C <NA>   THR     B    26   <NA> 20.319  26.393   3.168 1
## 960    ATOM   961     O <NA>   THR     B    26   <NA> 21.316  25.867   3.637 1
## 961    ATOM   962    CB <NA>   THR     B    26   <NA> 21.063  28.678   2.282 1
## 962    ATOM   963   OG1 <NA>   THR     B    26   <NA> 20.188  29.407   3.146 1
## 963    ATOM   964   CG2 <NA>   THR     B    26   <NA> 21.279  29.499   1.024 1
## 964    ATOM   965     N <NA>   GLY     B    27   <NA> 19.106  26.199   3.688 1
## 965    ATOM   966    CA <NA>   GLY     B    27   <NA> 18.957  25.372   4.876 1
## 966    ATOM   967     C <NA>   GLY     B    27   <NA> 18.845  23.903   4.520 1
## 967    ATOM   968     O <NA>   GLY     B    27   <NA> 18.660  23.054   5.417 1
## 968    ATOM   969     N <NA>   ALA     B    28   <NA> 18.819  23.600   3.217 1
## 969    ATOM   970    CA <NA>   ALA     B    28   <NA> 18.721  22.211   2.738 1
## 970    ATOM   971     C <NA>   ALA     B    28   <NA> 20.089  21.661   2.292 1
## 971    ATOM   972     O <NA>   ALA     B    28   <NA> 20.749  22.243   1.403 1
## 972    ATOM   973    CB <NA>   ALA     B    28   <NA> 17.682  22.117   1.578 1
## 973    ATOM   974     N <NA>   ASP     B    29   <NA> 20.536  20.559   2.918 1
## 974    ATOM   975    CA <NA>   ASP     B    29   <NA> 21.779  19.912   2.496 1
## 975    ATOM   976     C <NA>   ASP     B    29   <NA> 21.693  19.374   1.107 1
## 976    ATOM   977     O <NA>   ASP     B    29   <NA> 22.642  19.502   0.361 1
## 977    ATOM   978    CB <NA>   ASP     B    29   <NA> 22.169  18.827   3.447 1
## 978    ATOM   979    CG <NA>   ASP     B    29   <NA> 22.272  19.337   4.844 1
## 979    ATOM   980   OD1 <NA>   ASP     B    29   <NA> 22.714  20.482   5.029 1
## 980    ATOM   981   OD2 <NA>   ASP     B    29   <NA> 21.836  18.647   5.778 1
## 981    ATOM   982     N <NA>   ASP     B    30   <NA> 20.524  18.868   0.719 1
## 982    ATOM   983    CA <NA>   ASP     B    30   <NA> 20.355  18.227  -0.584 1
## 983    ATOM   984     C <NA>   ASP     B    30   <NA> 19.212  18.807  -1.371 1
## 984    ATOM   985     O <NA>   ASP     B    30   <NA> 18.383  19.523  -0.846 1
## 985    ATOM   986    CB <NA>   ASP     B    30   <NA> 20.084  16.745  -0.413 1
## 986    ATOM   987    CG <NA>   ASP     B    30   <NA> 21.023  16.088   0.586 1
## 987    ATOM   988   OD1 <NA>   ASP     B    30   <NA> 22.233  15.970   0.265 1
## 988    ATOM   989   OD2 <NA>   ASP     B    30   <NA> 20.531  15.682   1.672 1
## 989    ATOM   990     N <NA>   THR     B    31   <NA> 19.152  18.428  -2.643 1
## 990    ATOM   991    CA <NA>   THR     B    31   <NA> 18.113  18.843  -3.603 1
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## 993    ATOM   994    CB <NA>   THR     B    31   <NA> 18.810  19.051  -4.967 1
## 994    ATOM   995   OG1 <NA>   THR     B    31   <NA> 19.740  20.123  -4.831 1
## 995    ATOM   996   CG2 <NA>   THR     B    31   <NA> 17.844  19.330  -6.078 1
## 996    ATOM   997     N <NA>   VAL     B    32   <NA> 15.750  18.102  -3.440 1
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## 999    ATOM  1000     O <NA>   VAL     B    32   <NA> 13.169  18.861  -4.263 1
## 1000   ATOM  1001    CB <NA>   VAL     B    32   <NA> 13.781  17.005  -2.245 1
## 1001   ATOM  1002   CG1 <NA>   VAL     B    32   <NA> 13.297  15.592  -2.184 1
## 1002   ATOM  1003   CG2 <NA>   VAL     B    32   <NA> 14.518  17.455  -1.007 1
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## 1003   ATOM  1004     N <NA>   LEU     B    33   <NA> 13.199  16.926  -5.401 1
## 1004   ATOM  1005    CA <NA>   LEU     B    33   <NA> 12.141  17.335  -6.327 1
## 1005   ATOM  1006     C <NA>   LEU     B    33   <NA> 10.876  16.500  -6.065 1
## 1006   ATOM  1007     O <NA>   LEU     B    33   <NA> 10.948  15.389  -5.534 1
## 1007   ATOM  1008    CB <NA>   LEU     B    33   <NA> 12.618  17.139  -7.766 1
## 1008   ATOM  1009    CG <NA>   LEU     B    33   <NA> 13.889  17.846  -8.247 1
## 1009   ATOM  1010   CD1 <NA>   LEU     B    33   <NA> 13.942  17.794  -9.731 1
## 1010   ATOM  1011   CD2 <NA>   LEU     B    33   <NA> 13.897  19.266  -7.782 1
## 1011   ATOM  1012     N <NA>   GLU     B    34   <NA>  9.719  17.083  -6.361 1
## 1012   ATOM  1013    CA <NA>   GLU     B    34   <NA>  8.442  16.392  -6.346 1
## 1013   ATOM  1014     C <NA>   GLU     B    34   <NA>  8.514  15.172  -7.224 1
## 1014   ATOM  1015     O <NA>   GLU     B    34   <NA>  9.413  15.013  -8.040 1
## 1015   ATOM  1016    CB <NA>   GLU     B    34   <NA>  7.316  17.305  -6.819 1
## 1016   ATOM  1017    CG <NA>   GLU     B    34   <NA>  6.914  18.362  -5.808 1
## 1017   ATOM  1018    CD <NA>   GLU     B    34   <NA>  6.205  19.552  -6.439 1
## 1018   ATOM  1019   OE1 <NA>   GLU     B    34   <NA>  6.323  19.742  -7.666 1
## 1019   ATOM  1020   OE2 <NA>   GLU     B    34   <NA>  5.613  20.369  -5.715 1
## 1020   ATOM  1021     N <NA>   GLU     B    35   <NA>  7.526  14.309  -7.044 1
## 1021   ATOM  1022    CA <NA>   GLU     B    35   <NA>  7.425  13.006  -7.682 1
## 1022   ATOM  1023     C <NA>   GLU     B    35   <NA>  7.528  13.141  -9.172 1
## 1023   ATOM  1024     O <NA>   GLU     B    35   <NA>  6.660  13.711  -9.819 1
## 1024   ATOM  1025    CB <NA>   GLU     B    35   <NA>  6.100  12.361  -7.297 1
## 1025   ATOM  1026    CG <NA>   GLU     B    35   <NA>  5.907  10.953  -7.838 1
## 1026   ATOM  1027    CD <NA>   GLU     B    35   <NA>  7.182  10.093  -7.854 1
## 1027   ATOM  1028   OE1 <NA>   GLU     B    35   <NA>  7.743   9.853  -6.766 1
## 1028   ATOM  1029   OE2 <NA>   GLU     B    35   <NA>  7.521   9.561  -8.946 1
## 1029   ATOM  1030     N <NA>   MET     B    36   <NA>  8.627  12.651  -9.705 1
## 1030   ATOM  1031    CA <NA>   MET     B    36   <NA>  8.791  12.578 -11.145 1
## 1031   ATOM  1032     C <NA>   MET     B    36   <NA>  9.583  11.322 -11.483 1
## 1032   ATOM  1033     O <NA>   MET     B    36   <NA> 10.100  10.637 -10.616 1
## 1033   ATOM  1034    CB <NA>   MET     B    36   <NA>  9.546  13.808 -11.654 1
## 1034   ATOM  1035    CG <NA>   MET     B    36   <NA> 10.867  14.095 -11.014 1
## 1035   ATOM  1036    SD <NA>   MET     B    36   <NA> 11.575  15.547 -11.778 1
## 1036   ATOM  1037    CE <NA>   MET     B    36   <NA> 11.710  15.108 -13.551 1
## 1037   ATOM  1038     N <NA>   SER     B    37   <NA>  9.657  11.016 -12.763 1
## 1038   ATOM  1039    CA <NA>   SER     B    37   <NA> 10.411   9.858 -13.218 1
## 1039   ATOM  1040     C <NA>   SER     B    37   <NA> 11.673  10.374 -13.825 1
## 1040   ATOM  1041     O <NA>   SER     B    37   <NA> 11.636  11.272 -14.685 1
## 1041   ATOM  1042    CB <NA>   SER     B    37   <NA>  9.573   9.049 -14.221 1
## 1042   ATOM  1043    OG <NA>   SER     B    37   <NA>  8.330   8.594 -13.579 1
## 1043   ATOM  1044     N <NA>   LEU     B    38   <NA> 12.793   9.884 -13.330 1
## 1044   ATOM  1045    CA <NA>   LEU     B    38   <NA> 14.091  10.261 -13.857 1
## 1045   ATOM  1046     C <NA>   LEU     B    38   <NA> 14.818   9.018 -14.330 1
## 1046   ATOM  1047     O <NA>   LEU     B    38   <NA> 14.416   7.898 -13.995 1
## 1047   ATOM  1048    CB <NA>   LEU     B    38   <NA> 14.866  10.942 -12.759 1
## 1048   ATOM  1049    CG <NA>   LEU     B    38   <NA> 14.480  12.376 -12.556 1
## 1049   ATOM  1050   CD1 <NA>   LEU     B    38   <NA> 15.159  12.900 -11.300 1
## 1050   ATOM  1051   CD2 <NA>   LEU     B    38   <NA> 14.955  13.131 -13.766 1
## 1051   ATOM  1052     N <NA>   PRO     B    39   <NA> 15.767   9.161 -15.261 1
## 1052   ATOM  1053    CA <NA>   PRO     B    39   <NA> 16.525   8.031 -15.798 1
## 1053   ATOM  1054     C <NA>   PRO     B    39   <NA> 17.366   7.241 -14.777 1
## 1054   ATOM  1055     O <NA>   PRO     B    39   <NA> 17.943   7.817 -13.847 1
## 1055   ATOM  1056    CB <NA>   PRO     B    39   <NA> 17.407   8.673 -16.857 1
## 1056   ATOM  1057    CG <NA>   PRO     B    39   <NA> 17.532  10.100 -16.423 1
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## 1057   ATOM  1058    CD <NA>   PRO     B    39   <NA> 16.150  10.405 -15.968 1
## 1058   ATOM  1059     N <NA>   GLY     B    40   <NA> 17.477   5.932 -14.999 1
## 1059   ATOM  1060    CA <NA>   GLY     B    40   <NA> 18.494   5.171 -14.302 1
## 1060   ATOM  1061     C <NA>   GLY     B    40   <NA> 18.048   4.556 -12.995 1
## 1061   ATOM  1062     O <NA>   GLY     B    40   <NA> 16.865   4.438 -12.729 1
## 1062   ATOM  1063     N <NA>   ARG     B    41   <NA> 19.000   3.939 -12.313 1
## 1063   ATOM  1064    CA <NA>   ARG     B    41   <NA> 18.722   3.282 -11.042 1
## 1064   ATOM  1065     C <NA>   ARG     B    41   <NA> 18.615   4.306  -9.916 1
## 1065   ATOM  1066     O <NA>   ARG     B    41   <NA> 19.168   5.390 -10.018 1
## 1066   ATOM  1067    CB <NA>   ARG     B    41   <NA> 19.852   2.333 -10.662 1
## 1067   ATOM  1068    CG <NA>   ARG     B    41   <NA> 20.359   1.417 -11.726 1
## 1068   ATOM  1069    CD <NA>   ARG     B    41   <NA> 20.905   0.188 -11.023 1
## 1069   ATOM  1070    NE <NA>   ARG     B    41   <NA> 19.927  -0.864 -11.169 1
## 1070   ATOM  1071    CZ <NA>   ARG     B    41   <NA> 19.354  -1.538 -10.177 1
## 1071   ATOM  1072   NH1 <NA>   ARG     B    41   <NA> 19.839  -1.513  -8.939 1
## 1072   ATOM  1073   NH2 <NA>   ARG     B    41   <NA> 18.333  -2.314 -10.472 1
## 1073   ATOM  1074     N <NA>   TRP     B    42   <NA> 17.989   3.918  -8.810 1
## 1074   ATOM  1075    CA <NA>   TRP     B    42   <NA> 17.920   4.766  -7.634 1
## 1075   ATOM  1076     C <NA>   TRP     B    42   <NA> 18.295   3.969  -6.380 1
## 1076   ATOM  1077     O <NA>   TRP     B    42   <NA> 18.163   2.742  -6.361 1
## 1077   ATOM  1078    CB <NA>   TRP     B    42   <NA> 16.525   5.338  -7.459 1
## 1078   ATOM  1079    CG <NA>   TRP     B    42   <NA> 15.444   4.372  -7.312 1
## 1079   ATOM  1080   CD1 <NA>   TRP     B    42   <NA> 14.681   3.834  -8.299 1
## 1080   ATOM  1081   CD2 <NA>   TRP     B    42   <NA> 14.840   3.957  -6.079 1
## 1081   ATOM  1082   NE1 <NA>   TRP     B    42   <NA> 13.640   3.121  -7.756 1
## 1082   ATOM  1083   CE2 <NA>   TRP     B    42   <NA> 13.719   3.166  -6.402 1
## 1083   ATOM  1084   CE3 <NA>   TRP     B    42   <NA> 15.154   4.180  -4.715 1
## 1084   ATOM  1085   CZ2 <NA>   TRP     B    42   <NA> 12.881   2.589  -5.411 1
## 1085   ATOM  1086   CZ3 <NA>   TRP     B    42   <NA> 14.300   3.625  -3.745 1
## 1086   ATOM  1087   CH2 <NA>   TRP     B    42   <NA> 13.168   2.842  -4.106 1
## 1087   ATOM  1088     N <NA>   LYS     B    43   <NA> 18.801   4.689  -5.365 1
## 1088   ATOM  1089    CA <NA>   LYS     B    43   <NA> 19.180   4.182  -4.032 1
## 1089   ATOM  1090     C <NA>   LYS     B    43   <NA> 18.127   4.736  -3.089 1
## 1090   ATOM  1091     O <NA>   LYS     B    43   <NA> 17.442   5.729  -3.400 1
## 1091   ATOM  1092    CB <NA>   LYS     B    43   <NA> 20.561   4.731  -3.581 1
## 1092   ATOM  1093    CG <NA>   LYS     B    43   <NA> 21.777   4.400  -4.445 1
## 1093   ATOM  1094    CD <NA>   LYS     B    43   <NA> 22.996   5.295  -4.048 1
## 1094   ATOM  1095    CE <NA>   LYS     B    43   <NA> 24.193   5.280  -5.063 1
## 1095   ATOM  1096    NZ <NA>   LYS     B    43   <NA> 25.251   6.324  -4.725 1
## 1096   ATOM  1097     N <NA>   PRO     B    44   <NA> 18.053   4.208  -1.878 1
## 1097   ATOM  1098    CA <NA>   PRO     B    44   <NA> 17.102   4.804  -0.946 1
## 1098   ATOM  1099     C <NA>   PRO     B    44   <NA> 17.754   5.853  -0.023 1
## 1099   ATOM  1100     O <NA>   PRO     B    44   <NA> 18.929   5.769   0.330 1
## 1100   ATOM  1101    CB <NA>   PRO     B    44   <NA> 16.596   3.610  -0.171 1
## 1101   ATOM  1102    CG <NA>   PRO     B    44   <NA> 17.803   2.676  -0.117 1
## 1102   ATOM  1103    CD <NA>   PRO     B    44   <NA> 18.649   2.962  -1.335 1
## 1103   ATOM  1104     N <NA>   LYS     B    45   <NA> 16.974   6.847   0.381 1
## 1104   ATOM  1105    CA <NA>   LYS     B    45   <NA> 17.443   7.812   1.371 1
## 1105   ATOM  1106     C <NA>   LYS     B    45   <NA> 16.334   8.328   2.257 1
## 1106   ATOM  1107     O <NA>   LYS     B    45   <NA> 15.192   8.470   1.828 1
## 1107   ATOM  1108    CB <NA>   LYS     B    45   <NA> 18.177   8.988   0.701 1
## 1108   ATOM  1109    CG <NA>   LYS     B    45   <NA> 19.183   9.659   1.670 1
## 1109   ATOM  1110    CD <NA>   LYS     B    45   <NA> 20.095  10.640   1.011 1
## 1110   ATOM  1111    CE <NA>   LYS     B    45   <NA> 20.751  11.491   2.069 1
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## 1111   ATOM  1112    NZ <NA>   LYS     B    45   <NA> 21.413  12.705   1.509 1
## 1112   ATOM  1113     N <NA>   MET     B    46   <NA> 16.672   8.585   3.514 1
## 1113   ATOM  1114    CA <NA>   MET     B    46   <NA> 15.755   9.281   4.404 1
## 1114   ATOM  1115     C <NA>   MET     B    46   <NA> 16.373  10.584   4.732 1
## 1115   ATOM  1116     O <NA>   MET     B    46   <NA> 17.542  10.636   5.104 1
## 1116   ATOM  1117    CB <NA>   MET     B    46   <NA> 15.562   8.530   5.708 1
## 1117   ATOM  1118    CG <NA>   MET     B    46   <NA> 14.763   7.266   5.540 1
## 1118   ATOM  1119    SD <NA>   MET     B    46   <NA> 13.357   7.367   6.566 1
## 1119   ATOM  1120    CE <NA>   MET     B    46   <NA> 14.146   6.922   8.167 1
## 1120   ATOM  1121     N <NA>   ILE     B    47   <NA> 15.582  11.636   4.604 1
## 1121   ATOM  1122    CA <NA>   ILE     B    47   <NA> 16.003  12.986   4.955 1
## 1122   ATOM  1123     C <NA>   ILE     B    47   <NA> 15.018  13.507   5.961 1
## 1123   ATOM  1124     O <NA>   ILE     B    47   <NA> 13.822  13.222   5.884 1
## 1124   ATOM  1125    CB <NA>   ILE     B    47   <NA> 16.040  13.915   3.699 1
## 1125   ATOM  1126   CG1 <NA>   ILE     B    47   <NA> 14.745  13.761   2.918 1
## 1126   ATOM  1127   CG2 <NA>   ILE     B    47   <NA> 17.229  13.534   2.782 1
## 1127   ATOM  1128   CD1 <NA>   ILE     B    47   <NA> 14.742  14.561   1.698 1
## 1128   ATOM  1129     N <NA>   GLY     B    48   <NA> 15.542  14.239   6.941 1
## 1129   ATOM  1130    CA <NA>   GLY     B    48   <NA> 14.714  14.799   8.014 1
## 1130   ATOM  1131     C <NA>   GLY     B    48   <NA> 14.762  16.314   8.114 1
## 1131   ATOM  1132     O <NA>   GLY     B    48   <NA> 15.803  16.952   7.888 1
## 1132   ATOM  1133     N <NA>   GLY     B    49   <NA> 13.583  16.896   8.239 1
## 1133   ATOM  1134    CA <NA>   GLY     B    49   <NA> 13.484  18.319   8.459 1
## 1134   ATOM  1135     C <NA>   GLY     B    49   <NA> 12.647  18.565   9.672 1
## 1135   ATOM  1136     O <NA>   GLY     B    49   <NA> 12.880  17.976  10.721 1
## 1136   ATOM  1137     N <NA>   ILE     B    50   <NA> 11.850  19.611   9.584 1
## 1137   ATOM  1138    CA <NA>   ILE     B    50   <NA> 10.858  19.974  10.594 1
## 1138   ATOM  1139     C <NA>   ILE     B    50   <NA>  9.707  18.988  10.393 1
## 1139   ATOM  1140     O <NA>   ILE     B    50   <NA>  9.341  18.670   9.251 1
## 1140   ATOM  1141    CB <NA>   ILE     B    50   <NA> 10.365  21.453  10.316 1
## 1141   ATOM  1142   CG1 <NA>   ILE     B    50   <NA> 11.556  22.421  10.394 1
## 1142   ATOM  1143   CG2 <NA>   ILE     B    50   <NA>  9.299  21.862  11.270 1
## 1143   ATOM  1144   CD1 <NA>   ILE     B    50   <NA> 11.936  22.850  11.773 1
## 1144   ATOM  1145     N <NA>   GLY     B    51   <NA>  9.164  18.455  11.474 1
## 1145   ATOM  1146    CA <NA>   GLY     B    51   <NA>  8.011  17.583  11.313 1
## 1146   ATOM  1147     C <NA>   GLY     B    51   <NA>  8.360  16.130  11.054 1
## 1147   ATOM  1148     O <NA>   GLY     B    51   <NA>  7.494  15.283  11.167 1
## 1148   ATOM  1149     N <NA>   GLY     B    52   <NA>  9.638  15.842  10.818 1
## 1149   ATOM  1150    CA <NA>   GLY     B    52   <NA> 10.123  14.474  10.792 1
## 1150   ATOM  1151     C <NA>   GLY     B    52   <NA> 10.860  14.080   9.524 1
## 1151   ATOM  1152     O <NA>   GLY     B    52   <NA> 11.419  14.930   8.826 1
## 1152   ATOM  1153     N <NA>   PHE     B    53   <NA> 10.878  12.788   9.221 1
## 1153   ATOM  1154    CA <NA>   PHE     B    53   <NA> 11.638  12.302   8.079 1
## 1154   ATOM  1155     C <NA>   PHE     B    53   <NA> 10.739  11.914   6.924 1
## 1155   ATOM  1156     O <NA>   PHE     B    53   <NA>  9.601  11.543   7.137 1
## 1156   ATOM  1157    CB <NA>   PHE     B    53   <NA> 12.458  11.126   8.531 1
## 1157   ATOM  1158    CG <NA>   PHE     B    53   <NA> 13.464  11.471   9.564 1
## 1158   ATOM  1159   CD1 <NA>   PHE     B    53   <NA> 13.092  11.697  10.886 1
## 1159   ATOM  1160   CD2 <NA>   PHE     B    53   <NA> 14.789  11.625   9.189 1
## 1160   ATOM  1161   CE1 <NA>   PHE     B    53   <NA> 14.036  12.076  11.825 1
## 1161   ATOM  1162   CE2 <NA>   PHE     B    53   <NA> 15.753  12.001  10.078 1
## 1162   ATOM  1163    CZ <NA>   PHE     B    53   <NA> 15.392  12.225  11.421 1
## 1163   ATOM  1164     N <NA>   ILE     B    54   <NA> 11.204  12.078   5.695 1
## 1164   ATOM  1165    CA <NA>   ILE     B    54   <NA> 10.538  11.431   4.563 1
```

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## 1165   ATOM  1166     C <NA>   ILE     B    54   <NA> 11.513  10.453   3.866 1
## 1166   ATOM  1167     O <NA>   ILE     B    54   <NA> 12.727  10.529   4.052 1
## 1167   ATOM  1168    CB <NA>   ILE     B    54   <NA>  9.923  12.446   3.500 1
## 1168   ATOM  1169   CG1 <NA>   ILE     B    54   <NA> 10.968  13.414   2.964 1
## 1169   ATOM  1170   CG2 <NA>   ILE     B    54   <NA>  8.754  13.195   4.090 1
## 1170   ATOM  1171   CD1 <NA>   ILE     B    54   <NA> 10.571  14.020   1.616 1
## 1171   ATOM  1172     N <NA>   LYS     B    55   <NA> 10.983   9.503   3.111 1
## 1172   ATOM  1173    CA <NA>   LYS     B    55   <NA> 11.816   8.478   2.482 1
## 1173   ATOM  1174     C <NA>   LYS     B    55   <NA> 11.862   8.988   1.074 1
## 1174   ATOM  1175     O <NA>   LYS     B    55   <NA> 10.827   9.256   0.525 1
## 1175   ATOM  1176    CB <NA>   LYS     B    55   <NA> 11.062   7.136   2.489 1
## 1176   ATOM  1177    CG <NA>   LYS     B    55   <NA> 11.699   5.963   3.273 1
## 1177   ATOM  1178    CD <NA>   LYS     B    55   <NA> 13.070   5.502   2.689 1
## 1178   ATOM  1179    CE <NA>   LYS     B    55   <NA> 12.949   4.923   1.253 1
## 1179   ATOM  1180    NZ <NA>   LYS     B    55   <NA> 13.964   5.445   0.291 1
## 1180   ATOM  1181     N <NA>   VAL     B    56   <NA> 13.024   9.137   0.474 1
## 1181   ATOM  1182    CA <NA>   VAL     B    56   <NA> 13.072   9.652  -0.897 1
## 1182   ATOM  1183     C <NA>   VAL     B    56   <NA> 13.885   8.719  -1.786 1
## 1183   ATOM  1184     O <NA>   VAL     B    56   <NA> 14.547   7.817  -1.279 1
## 1184   ATOM  1185    CB <NA>   VAL     B    56   <NA> 13.757  11.033  -0.959 1
## 1185   ATOM  1186   CG1 <NA>   VAL     B    56   <NA> 12.766  12.134  -0.523 1
## 1186   ATOM  1187   CG2 <NA>   VAL     B    56   <NA> 15.032  11.016  -0.119 1
## 1187   ATOM  1188     N <NA>   ARG     B    57   <NA> 13.889   8.977  -3.102 1
## 1188   ATOM  1189    CA <NA>   ARG     B    57   <NA> 14.697   8.220  -4.083 1
## 1189   ATOM  1190     C <NA>   ARG     B    57   <NA> 15.894   9.023  -4.591 1
## 1190   ATOM  1191     O <NA>   ARG     B    57   <NA> 15.735  10.066  -5.210 1
## 1191   ATOM  1192    CB <NA>   ARG     B    57   <NA> 13.862   7.854  -5.298 1
## 1192   ATOM  1193    CG <NA>   ARG     B    57   <NA> 12.767   6.845  -5.041 1
## 1193   ATOM  1194    CD <NA>   ARG     B    57   <NA> 12.224   6.316  -6.354 1
## 1194   ATOM  1195    NE <NA>   ARG     B    57   <NA> 10.944   6.937  -6.617 1
## 1195   ATOM  1196    CZ <NA>   ARG     B    57   <NA> 10.717   7.776  -7.614 1
## 1196   ATOM  1197   NH1 <NA>   ARG     B    57   <NA> 11.534   7.792  -8.658 1
## 1197   ATOM  1198   NH2 <NA>   ARG     B    57   <NA>  9.555   8.403  -7.678 1
## 1198   ATOM  1199     N <NA>   GLN     B    58   <NA> 17.095   8.516  -4.388 1
## 1199   ATOM  1200    CA <NA>   GLN     B    58   <NA> 18.306   9.218  -4.819 1
## 1200   ATOM  1201     C <NA>   GLN     B    58   <NA> 18.742   8.833  -6.226 1
## 1201   ATOM  1202     O <NA>   GLN     B    58   <NA> 19.157   7.694  -6.438 1
## 1202   ATOM  1203    CB <NA>   GLN     B    58   <NA> 19.465   8.920  -3.861 1
## 1203   ATOM  1204    CG <NA>   GLN     B    58   <NA> 20.738   9.622  -4.271 1
## 1204   ATOM  1205    CD <NA>   GLN     B    58   <NA> 21.825   9.463  -3.248 1
## 1205   ATOM  1206   OE1 <NA>   GLN     B    58   <NA> 21.554   9.424  -2.048 1
## 1206   ATOM  1207   NE2 <NA>   GLN     B    58   <NA> 23.045   9.365  -3.692 1
## 1207   ATOM  1208     N <NA>   TYR     B    59   <NA> 18.705   9.773  -7.167 1
## 1208   ATOM  1209    CA <NA>   TYR     B    59   <NA> 19.361   9.587  -8.464 1
## 1209   ATOM  1210     C <NA>   TYR     B    59   <NA> 20.689  10.330  -8.544 1
## 1210   ATOM  1211     O <NA>   TYR     B    59   <NA> 20.860  11.368  -7.943 1
## 1211   ATOM  1212    CB <NA>   TYR     B    59   <NA> 18.472  10.082  -9.563 1
## 1212   ATOM  1213    CG <NA>   TYR     B    59   <NA> 17.116   9.383  -9.609 1
## 1213   ATOM  1214   CD1 <NA>   TYR     B    59   <NA> 16.157   9.612  -8.615 1
## 1214   ATOM  1215   CD2 <NA>   TYR     B    59   <NA> 16.814   8.484 -10.637 1
## 1215   ATOM  1216   CE1 <NA>   TYR     B    59   <NA> 14.959   8.977  -8.640 1
## 1216   ATOM  1217   CE2 <NA>   TYR     B    59   <NA> 15.647   7.851 -10.673 1
## 1217   ATOM  1218    CZ <NA>   TYR     B    59   <NA> 14.704   8.066  -9.679 1
## 1218   ATOM  1219    OH <NA>   TYR     B    59   <NA> 13.561   7.307  -9.711 1
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## 1219   ATOM  1220     N <NA>   ASP     B    60   <NA> 21.665   9.797  -9.258 1
## 1220   ATOM  1221    CA <NA>   ASP     B    60   <NA> 22.959  10.470  -9.336 1
## 1221   ATOM  1222     C <NA>   ASP     B    60   <NA> 23.303  10.921 -10.737 1
## 1222   ATOM  1223     O <NA>   ASP     B    60   <NA> 22.793  10.396 -11.707 1
## 1223   ATOM  1224    CB <NA>   ASP     B    60   <NA> 24.042   9.554  -8.834 1
## 1224   ATOM  1225    CG <NA>   ASP     B    60   <NA> 23.843   9.184  -7.407 1
## 1225   ATOM  1226   OD1 <NA>   ASP     B    60   <NA> 23.463  10.074  -6.620 1
## 1226   ATOM  1227   OD2 <NA>   ASP     B    60   <NA> 24.107   8.012  -7.044 1
## 1227   ATOM  1228     N <NA>   GLN     B    61   <NA> 24.189  11.897 -10.837 1
## 1228   ATOM  1229    CA <NA>   GLN     B    61   <NA> 24.622  12.478 -12.111 1
## 1229   ATOM  1230     C <NA>   GLN     B    61   <NA> 23.474  12.903 -13.022 1
## 1230   ATOM  1231     O <NA>   GLN     B    61   <NA> 23.492  12.665 -14.229 1
## 1231   ATOM  1232    CB <NA>   GLN     B    61   <NA> 25.596  11.549 -12.869 1
## 1232   ATOM  1233    CG <NA>   GLN     B    61   <NA> 26.892  12.283 -13.369 1
## 1233   ATOM  1234    CD <NA>   GLN     B    61   <NA> 28.007  11.392 -13.985 1
## 1234   ATOM  1235   OE1 <NA>   GLN     B    61   <NA> 28.747  11.845 -14.875 1
## 1235   ATOM  1236   NE2 <NA>   GLN     B    61   <NA> 28.197  10.173 -13.442 1
## 1236   ATOM  1237     N <NA>   ILE     B    62   <NA> 22.493  13.589 -12.452 1
## 1237   ATOM  1238    CA <NA>   ILE     B    62   <NA> 21.380  14.141 -13.224 1
## 1238   ATOM  1239     C <NA>   ILE     B    62   <NA> 21.710  15.575 -13.686 1
## 1239   ATOM  1240     O <NA>   ILE     B    62   <NA> 22.247  16.373 -12.924 1
## 1240   ATOM  1241    CB <NA>   ILE     B    62   <NA> 20.090  14.147 -12.331 1
## 1241   ATOM  1242   CG1 <NA>   ILE     B    62   <NA> 19.709  12.702 -11.952 1
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## 1243   ATOM  1244   CD1 <NA>   ILE     B    62   <NA> 19.068  11.933 -13.057 1
## 1244   ATOM  1245     N <NA>   LEU     B    63   <NA> 21.400  15.900 -14.931 1
## 1245   ATOM  1246    CA <NA>   LEU     B    63   <NA> 21.600  17.263 -15.431 1
## 1246   ATOM  1247     C <NA>   LEU     B    63   <NA> 20.386  18.085 -15.052 1
## 1247   ATOM  1248     O <NA>   LEU     B    63   <NA> 19.260  17.703 -15.355 1
## 1248   ATOM  1249    CB <NA>   LEU     B    63   <NA> 21.769  17.265 -16.962 1
## 1249   ATOM  1250    CG <NA>   LEU     B    63   <NA> 21.792  18.587 -17.759 1
## 1250   ATOM  1251   CD1 <NA>   LEU     B    63   <NA> 22.903  19.529 -17.300 1
## 1251   ATOM  1252   CD2 <NA>   LEU     B    63   <NA> 21.997  18.246 -19.205 1
## 1252   ATOM  1253     N <NA>   ILE     B    64   <NA> 20.626  19.203 -14.381 1
## 1253   ATOM  1254    CA <NA>   ILE     B    64   <NA> 19.548  20.111 -14.029 1
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## 1258   ATOM  1259   CG2 <NA>   ILE     B    64   <NA> 20.311  19.766 -11.655 1
## 1259   ATOM  1260   CD1 <NA>   ILE     B    64   <NA> 17.324  20.544 -10.930 1
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## 1266   ATOM  1267    CD <NA>   GLU     B    65   <NA> 19.960  25.126 -18.805 1
## 1267   ATOM  1268   OE1 <NA>   GLU     B    65   <NA> 19.601  24.094 -19.445 1
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## 1269   ATOM  1270     N <NA>   ILE     B    66   <NA> 19.709  25.427 -13.547 1
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## 1272   ATOM  1273     O <NA>   ILE     B    66   <NA> 20.684  28.254 -13.167 1
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## 1273   ATOM  1274   CB <NA>   ILE     B    66   <NA> 19.663  26.199 -11.203 1
## 1274   ATOM  1275  CG1 <NA>   ILE     B    66   <NA> 19.566  24.717 -10.848 1
## 1275   ATOM  1276  CG2 <NA>   ILE     B    66   <NA> 18.824  27.018 -10.232 1
## 1276   ATOM  1277  CD1 <NA>   ILE     B    66   <NA> 20.510  24.280  -9.745 1
## 1277   ATOM  1278    N <NA>   CYS     B    67   <NA> 18.504  28.630 -13.516 1
## 1278   ATOM  1279   CA <NA>   CYS     B    67   <NA> 18.684  29.971 -14.104 1
## 1279   ATOM  1280    C <NA>   CYS     B    67   <NA> 19.685  29.990 -15.245 1
## 1280   ATOM  1281    O <NA>   CYS     B    67   <NA> 20.565  30.852 -15.294 1
## 1281   ATOM  1282   CB <NA>   CYS     B    67   <NA> 19.124  30.970 -13.037 1
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## 1283   ATOM  1284    N <NA>   GLY     B    68   <NA> 19.562  29.010 -16.143 1
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## 1285   ATOM  1286    C <NA>   GLY     B    68   <NA> 21.899  28.603 -16.811 1
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## 1287   ATOM  1288    N <NA>   HIS     B    69   <NA> 22.059  28.002 -15.633 1
## 1288   ATOM  1289   CA <NA>   HIS     B    69   <NA> 23.354  27.479 -15.197 1
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## 1291   ATOM  1292   CB <NA>   HIS     B    69   <NA> 23.711  27.993 -13.810 1
## 1292   ATOM  1293   CG <NA>   HIS     B    69   <NA> 23.976  29.473 -13.740 1
## 1293   ATOM  1294  ND1 <NA>   HIS     B    69   <NA> 25.177  29.994 -13.361 1
## 1294   ATOM  1295  CD2 <NA>   HIS     B    69   <NA> 23.114  30.512 -13.920 1
## 1295   ATOM  1296  CE1 <NA>   HIS     B    69   <NA> 25.058  31.325 -13.286 1
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## 1297   ATOM  1298    N <NA>   LYS     B    70   <NA> 23.995  25.240 -15.820 1
## 1298   ATOM  1299   CA <NA>   LYS     B    70   <NA> 23.935  23.791 -15.800 1
## 1299   ATOM  1300    C <NA>   LYS     B    70   <NA> 24.749  23.243 -14.652 1
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## 1303   ATOM  1304   CD <NA>   LYS     B    70   <NA> 24.261  23.524 -19.576 1
## 1304   ATOM  1305   CE <NA>   LYS     B    70   <NA> 23.377  23.737 -20.816 1
## 1305   ATOM  1306   NZ <NA>   LYS     B    70   <NA> 22.863  22.443 -21.404 1
## 1306   ATOM  1307    N <NA>   ALA     B    71   <NA> 24.104  22.353 -13.909 1
## 1307   ATOM  1308   CA <NA>   ALA     B    71   <NA> 24.689  21.612 -12.802 1
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## 1311   ATOM  1312    N <NA>   ILE     B    72   <NA> 25.330  19.253 -12.902 1
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## 1313   ATOM  1314    C <NA>   ILE     B    72   <NA> 25.312  17.246 -11.637 1
## 1314   ATOM  1315    O <NA>   ILE     B    72   <NA> 26.442  17.315 -11.167 1
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## 1317   ATOM  1318  CG2 <NA>   ILE     B    72   <NA> 25.615  15.649 -14.171 1
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## 1319   ATOM  1320    N <NA>   GLY     B    73   <NA> 24.303  16.690 -10.975 1
## 1320   ATOM  1321   CA <NA>   GLY     B    73   <NA> 24.545  16.248  -9.616 1
## 1321   ATOM  1322    C <NA>   GLY     B    73   <NA> 23.470  15.337  -9.095 1
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## 1323   ATOM  1324    N <NA>   THR     B    74   <NA> 23.517  15.041  -7.794 1
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## 1327   ATOM  1328    CB <NA>   THR     B    74   <NA> 23.128  13.638  -5.748 1
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## 1329   ATOM  1330   CG2 <NA>   THR     B    74   <NA> 22.071  12.763  -5.030 1
## 1330   ATOM  1331     N <NA>   VAL     B    75   <NA> 20.177  14.227  -7.192 1
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## 1333   ATOM  1334     O <NA>   VAL     B    75   <NA> 17.993  12.504  -6.743 1
## 1334   ATOM  1335    CB <NA>   VAL     B    75   <NA> 18.229  15.113  -8.501 1
## 1335   ATOM  1336   CG1 <NA>   VAL     B    75   <NA> 16.760  15.421  -8.434 1
## 1336   ATOM  1337   CG2 <NA>   VAL     B    75   <NA> 18.967  16.317  -9.099 1
## 1337   ATOM  1338     N <NA>   LEU     B    76   <NA> 17.295  14.086  -5.303 1
## 1338   ATOM  1339    CA <NA>   LEU     B    76   <NA> 16.390  13.196  -4.575 1
## 1339   ATOM  1340     C <NA>   LEU     B    76   <NA> 14.972  13.423  -5.073 1
## 1340   ATOM  1341     O <NA>   LEU     B    76   <NA> 14.652  14.514  -5.518 1
## 1341   ATOM  1342    CB <NA>   LEU     B    76   <NA> 16.450  13.476  -3.067 1
## 1342   ATOM  1343    CG <NA>   LEU     B    76   <NA> 17.787  13.595  -2.330 1
## 1343   ATOM  1344   CD1 <NA>   LEU     B    76   <NA> 17.591  13.640  -0.845 1
## 1344   ATOM  1345   CD2 <NA>   LEU     B    76   <NA> 18.678  12.463  -2.705 1
## 1345   ATOM  1346     N <NA>   VAL     B    77   <NA> 14.135  12.391  -5.049 1
## 1346   ATOM  1347    CA <NA>   VAL     B    77   <NA> 12.749  12.509  -5.485 1
## 1347   ATOM  1348     C <NA>   VAL     B    77   <NA> 11.826  11.894  -4.472 1
## 1348   ATOM  1349     O <NA>   VAL     B    77   <NA> 12.052  10.766  -3.999 1
## 1349   ATOM  1350    CB <NA>   VAL     B    77   <NA> 12.502  11.835  -6.868 1
## 1350   ATOM  1351   CG1 <NA>   VAL     B    77   <NA> 11.065  12.148  -7.398 1
## 1351   ATOM  1352   CG2 <NA>   VAL     B    77   <NA> 13.593  12.322  -7.843 1
## 1352   ATOM  1353     N <NA>   GLY     B    78   <NA> 10.778  12.616  -4.125 1
## 1353   ATOM  1354    CA <NA>   GLY     B    78   <NA> 10.004  12.229  -2.965 1
## 1354   ATOM  1355     C <NA>   GLY     B    78   <NA>  8.832  13.128  -2.672 1
## 1355   ATOM  1356     O <NA>   GLY     B    78   <NA>  8.614  14.117  -3.393 1
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## 1357   ATOM  1358    CA <NA>   PRO     B    79   <NA>  6.887  13.664  -1.350 1
## 1358   ATOM  1359     C <NA>   PRO     B    79   <NA>  7.292  14.915  -0.550 1
## 1359   ATOM  1360     O <NA>   PRO     B    79   <NA>  7.007  15.036   0.638 1
## 1360   ATOM  1361    CB <NA>   PRO     B    79   <NA>  5.951  12.742  -0.594 1
## 1361   ATOM  1362    CG <NA>   PRO     B    79   <NA>  6.838  11.781   0.040 1
## 1362   ATOM  1363    CD <NA>   PRO     B    79   <NA>  8.096  11.665  -0.739 1
## 1363   ATOM  1364     N <NA>   THR     B    80   <NA>  7.997  15.816  -1.220 1
## 1364   ATOM  1365    CA <NA>   THR     B    80   <NA>  8.324  17.137  -0.702 1
## 1365   ATOM  1366     C <NA>   THR     B    80   <NA>  7.227  18.114  -1.090 1
## 1366   ATOM  1367     O <NA>   THR     B    80   <NA>  6.528  17.896  -2.080 1
## 1367   ATOM  1368    CB <NA>   THR     B    80   <NA>  9.677  17.594  -1.299 1
## 1368   ATOM  1369   OG1 <NA>   THR     B    80   <NA>  9.952  18.951  -0.924 1
## 1369   ATOM  1370   CG2 <NA>   THR     B    80   <NA>  9.688  17.449  -2.825 1
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## 1372   ATOM  1373     C <NA>   PRO     B    81   <NA>  6.244  20.969  -1.727 1
## 1373   ATOM  1374     O <NA>   PRO     B    81   <NA>  5.343  21.294  -2.509 1
## 1374   ATOM  1375    CB <NA>   PRO     B    81   <NA>  5.694  20.874   0.729 1
## 1375   ATOM  1376    CG <NA>   PRO     B    81   <NA>  6.274  19.954   1.831 1
## 1376   ATOM  1377    CD <NA>   PRO     B    81   <NA>  7.387  19.243   1.190 1
## 1377   ATOM  1378     N <NA>   VAL     B    82   <NA>  7.520  21.355  -1.868 1
## 1378   ATOM  1379    CA <NA>   VAL     B    82   <NA>  7.990  22.207  -2.983 1
## 1379   ATOM  1380     C <NA>   VAL     B    82   <NA>  9.255  21.636  -3.581 1
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## 1382   ATOM  1383   CG1 <NA>   VAL     B    82   <NA>  7.122  24.513  -2.361 1
## 1383   ATOM  1384   CG2 <NA>   VAL     B    82   <NA>  9.101  23.485  -1.163 1
## 1384   ATOM  1385     N <NA>   ASN     B    83   <NA>  9.588  21.960  -4.812 1
## 1385   ATOM  1386    CA <NA>   ASN     B    83   <NA> 10.914  21.521  -5.319 1
## 1386   ATOM  1387     C <NA>   ASN     B    83   <NA> 11.922  22.373  -4.576 1
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## 1388   ATOM  1389    CB <NA>   ASN     B    83   <NA> 11.068  21.763  -6.823 1
## 1389   ATOM  1390    CG <NA>   ASN     B    83   <NA> 10.096  20.950  -7.647 1
## 1390   ATOM  1391   OD1 <NA>   ASN     B    83   <NA> 10.013  19.733  -7.494 1
## 1391   ATOM  1392   ND2 <NA>   ASN     B    83   <NA>  9.305  21.627  -8.498 1
## 1392   ATOM  1393     N <NA>   ILE     B    84   <NA> 12.983  21.755  -4.066 1
## 1393   ATOM  1394    CA <NA>   ILE     B    84   <NA> 13.979  22.449  -3.233 1
## 1394   ATOM  1395     C <NA>   ILE     B    84   <NA> 15.345  22.255  -3.870 1
## 1395   ATOM  1396     O <NA>   ILE     B    84   <NA> 15.779  21.111  -4.072 1
## 1396   ATOM  1397    CB <NA>   ILE     B    84   <NA> 14.041  21.833  -1.837 1
## 1397   ATOM  1398   CG1 <NA>   ILE     B    84   <NA> 12.754  22.151  -1.088 1
## 1398   ATOM  1399   CG2 <NA>   ILE     B    84   <NA> 15.323  22.264  -1.122 1
## 1399   ATOM  1400   CD1 <NA>   ILE     B    84   <NA> 12.438  21.217   0.060 1
## 1400   ATOM  1401     N <NA>   ILE     B    85   <NA> 16.044  23.346  -4.167 1
## 1401   ATOM  1402    CA <NA>   ILE     B    85   <NA> 17.441  23.243  -4.575 1
## 1402   ATOM  1403     C <NA>   ILE     B    85   <NA> 18.305  23.504  -3.345 1
## 1403   ATOM  1404     O <NA>   ILE     B    85   <NA> 18.262  24.613  -2.802 1
## 1404   ATOM  1405    CB <NA>   ILE     B    85   <NA> 17.805  24.332  -5.644 1
## 1405   ATOM  1406   CG1 <NA>   ILE     B    85   <NA> 16.809  24.299  -6.827 1
## 1406   ATOM  1407   CG2 <NA>   ILE     B    85   <NA> 19.271  24.191  -6.067 1
## 1407   ATOM  1408   CD1 <NA>   ILE     B    85   <NA> 16.672  22.956  -7.581 1
## 1408   ATOM  1409     N <NA>   GLY     B    86   <NA> 19.121  22.530  -2.936 1
## 1409   ATOM  1410    CA <NA>   GLY     B    86   <NA> 19.857  22.642  -1.690 1
## 1410   ATOM  1411     C <NA>   GLY     B    86   <NA> 21.324  22.800  -1.940 1
## 1411   ATOM  1412     O <NA>   GLY     B    86   <NA> 21.750  22.958  -3.056 1
## 1412   ATOM  1413     N <NA>   ARG     B    87   <NA> 22.117  22.755  -0.887 1
## 1413   ATOM  1414    CA <NA>   ARG     B    87   <NA> 23.533  23.126  -0.985 1
## 1414   ATOM  1415     C <NA>   ARG     B    87   <NA> 24.413  22.356  -1.973 1
## 1415   ATOM  1416     O <NA>   ARG     B    87   <NA> 25.398  22.903  -2.461 1
## 1416   ATOM  1417    CB <NA>   ARG     B    87   <NA> 24.171  23.147   0.403 1
## 1417   ATOM  1418    CG <NA>   ARG     B    87   <NA> 23.646  24.256   1.283 1
## 1418   ATOM  1419    CD <NA>   ARG     B    87   <NA> 24.429  24.306   2.576 1
## 1419   ATOM  1420    NE <NA>   ARG     B    87   <NA> 24.362  23.068   3.371 1
## 1420   ATOM  1421    CZ <NA>   ARG     B    87   <NA> 25.357  22.185   3.495 1
## 1421   ATOM  1422   NH1 <NA>   ARG     B    87   <NA> 26.467  22.303   2.795 1
## 1422   ATOM  1423   NH2 <NA>   ARG     B    87   <NA> 25.255  21.190   4.368 1
## 1423   ATOM  1424     N <NA>   ASN     B    88   <NA> 24.074  21.101  -2.275 1
## 1424   ATOM  1425    CA <NA>   ASN     B    88   <NA> 24.950  20.312  -3.132 1
## 1425   ATOM  1426     C <NA>   ASN     B    88   <NA> 24.980  20.893  -4.527 1
## 1426   ATOM  1427     O <NA>   ASN     B    88   <NA> 26.015  20.853  -5.202 1
## 1427   ATOM  1428    CB <NA>   ASN     B    88   <NA> 24.512  18.849  -3.197 1
## 1428   ATOM  1429    CG <NA>   ASN     B    88   <NA> 23.126  18.649  -3.777 1
## 1429   ATOM  1430   OD1 <NA>   ASN     B    88   <NA> 22.167  19.280  -3.351 1
## 1430   ATOM  1431   ND2 <NA>   ASN     B    88   <NA> 23.020  17.775  -4.767 1
## 1431   ATOM  1432     N <NA>   LEU     B    89   <NA> 23.863  21.490  -4.949 1
## 1432   ATOM  1433    CA <NA>   LEU     B    89   <NA> 23.811  22.125  -6.273 1
## 1433   ATOM  1434     C <NA>   LEU     B    89   <NA> 24.018  23.645  -6.231 1
## 1434   ATOM  1435     O <NA>   LEU     B    89   <NA> 24.321  24.242  -7.236 1
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## 1435   ATOM  1436    CB <NA>   LEU     B    89   <NA> 22.457  21.815  -6.962 1
## 1436   ATOM  1437    CG <NA>   LEU     B    89   <NA> 22.219  20.372  -7.436 1
## 1437   ATOM  1438   CD1 <NA>   LEU     B    89   <NA> 20.937  20.300  -8.243 1
## 1438   ATOM  1439   CD2 <NA>   LEU     B    89   <NA> 23.408  19.901  -8.273 1
## 1439   ATOM  1440     N <NA>   LEU     B    90   <NA> 23.819  24.255  -5.075 1
## 1440   ATOM  1441    CA <NA>   LEU     B    90   <NA> 24.020  25.701  -4.954 1
## 1441   ATOM  1442     C <NA>   LEU     B    90   <NA> 25.511  26.005  -5.072 1
## 1442   ATOM  1443     O <NA>   LEU     B    90   <NA> 25.907  26.959  -5.732 1
## 1443   ATOM  1444    CB <NA>   LEU     B    90   <NA> 23.430  26.234  -3.624 1
## 1444   ATOM  1445    CG <NA>   LEU     B    90   <NA> 21.900  26.309  -3.475 1
## 1445   ATOM  1446   CD1 <NA>   LEU     B    90   <NA> 21.487  26.779  -2.081 1
## 1446   ATOM  1447   CD2 <NA>   LEU     B    90   <NA> 21.358  27.241  -4.506 1
## 1447   ATOM  1448     N <NA>   THR     B    91   <NA> 26.336  25.143  -4.491 1
## 1448   ATOM  1449    CA <NA>   THR     B    91   <NA> 27.785  25.304  -4.546 1
## 1449   ATOM  1450     C <NA>   THR     B    91   <NA> 28.270  25.184  -5.969 1
## 1450   ATOM  1451     O <NA>   THR     B    91   <NA> 29.168  25.903  -6.378 1
## 1451   ATOM  1452    CB <NA>   THR     B    91   <NA> 28.501  24.261  -3.669 1
## 1452   ATOM  1453   OG1 <NA>   THR     B    91   <NA> 27.898  22.990  -3.894 1
## 1453   ATOM  1454   CG2 <NA>   THR     B    91   <NA> 28.366  24.579  -2.208 1
## 1454   ATOM  1455     N <NA>   GLN     B    92   <NA> 27.619  24.323  -6.741 1
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## 1456   ATOM  1457     C <NA>   GLN     B    92   <NA> 27.823  25.361  -8.999 1
## 1457   ATOM  1458     O <NA>   GLN     B    92   <NA> 28.719  25.701  -9.794 1
## 1458   ATOM  1459    CB <NA>   GLN     B    92   <NA> 27.226  22.956  -8.793 1
## 1459   ATOM  1460    CG <NA>   GLN     B    92   <NA> 27.720  21.588  -8.406 1
## 1460   ATOM  1461    CD <NA>   GLN     B    92   <NA> 27.313  20.496  -9.421 1
## 1461   ATOM  1462   OE1 <NA>   GLN     B    92   <NA> 27.138  20.746 -10.620 1
## 1462   ATOM  1463   NE2 <NA>   GLN     B    92   <NA> 27.230  19.281  -8.941 1
## 1463   ATOM  1464     N <NA>   ILE     B    93   <NA> 26.683  26.043  -8.820 1
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## 1468   ATOM  1469   CG1 <NA>   ILE     B    93   <NA> 24.103  27.648  -8.559 1
## 1469   ATOM  1470   CG2 <NA>   ILE     B    93   <NA> 24.300  26.092 -10.460 1
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## 1471   ATOM  1472     N <NA>   GLY     B    94   <NA> 27.741  28.369  -7.949 1
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## 1473   ATOM  1474     C <NA>   GLY     B    94   <NA> 27.749  30.439  -6.488 1
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## 1475   ATOM  1476     N <NA>   CYS     B    95   <NA> 26.808  29.899  -5.748 1
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## 1479   ATOM  1480    CB <NA>   CYS     B    95   <NA> 24.578  29.989  -4.978 1
## 1480   ATOM  1481    SG <NA>   CYS     B    95   <NA> 23.221  30.929  -4.410 1
## 1481   ATOM  1482     N <NA>   THR     B    96   <NA> 26.473  32.277  -3.244 1
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## 1483   ATOM  1484     C <NA>   THR     B    96   <NA> 25.672  33.544  -1.205 1
## 1484   ATOM  1485     O <NA>   THR     B    96   <NA> 24.760  34.079  -1.852 1
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## 1486   ATOM  1487   OG1 <NA>   THR     B    96   <NA> 27.888  34.689  -2.857 1
## 1487   ATOM  1488   CG2 <NA>   THR     B    96   <NA> 29.316  32.870  -2.141 1
## 1488   ATOM  1489     N <NA>   LEU     B    97   <NA> 25.759  33.617   0.119 1
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## 1489   ATOM  1490    CA <NA>   LEU     B    97   <NA> 24.902  34.468   0.963 1
## 1490   ATOM  1491     C <NA>   LEU     B    97   <NA> 25.714  35.689   1.398 1
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## 1492   ATOM  1493    CB <NA>   LEU     B    97   <NA> 24.489  33.718   2.236 1
## 1493   ATOM  1494    CG <NA>   LEU     B    97   <NA> 23.211  32.901   2.344 1
## 1494   ATOM  1495   CD1 <NA>   LEU     B    97   <NA> 23.114  32.358   3.719 1
## 1495   ATOM  1496   CD2 <NA>   LEU     B    97   <NA> 22.037  33.773   2.076 1
## 1496   ATOM  1497     N <NA>   ASN     B    98   <NA> 25.121  36.868   1.264 1
## 1497   ATOM  1498    CA <NA>   ASN     B    98   <NA> 25.870  38.101   1.449 1
## 1498   ATOM  1499     C <NA>   ASN     B    98   <NA> 25.102  39.038   2.370 1
## 1499   ATOM  1500     O <NA>   ASN     B    98   <NA> 23.889  39.124   2.261 1
## 1500   ATOM  1501    CB <NA>   ASN     B    98   <NA> 26.140  38.756   0.086 1
## 1501   ATOM  1502    CG <NA>   ASN     B    98   <NA> 27.048  37.921  -0.814 1
## 1502   ATOM  1503   OD1 <NA>   ASN     B    98   <NA> 28.268  37.895  -0.630 1
## 1503   ATOM  1504   ND2 <NA>   ASN     B    98   <NA> 26.455  37.192  -1.754 1
## 1504   ATOM  1505     N <NA>   PHE     B    99   <NA> 25.809  39.706   3.283 1
## 1505   ATOM  1506    CA <NA>   PHE     B    99   <NA> 25.267  40.855   4.034 1
## 1506   ATOM  1507     C <NA>   PHE     B    99   <NA> 26.351  41.742   4.659 1
## 1507   ATOM  1508     O <NA>   PHE     B    99   <NA> 27.448  41.208   5.013 1
## 1508   ATOM  1509    CB <NA>   PHE     B    99   <NA> 24.284  40.418   5.127 1
## 1509   ATOM  1510    CG <NA>   PHE     B    99   <NA> 24.859  39.479   6.130 1
## 1510   ATOM  1511   CD1 <NA>   PHE     B    99   <NA> 25.061  38.150   5.808 1
## 1511   ATOM  1512   CD2 <NA>   PHE     B    99   <NA> 25.071  39.890   7.436 1
## 1512   ATOM  1513   CE1 <NA>   PHE     B    99   <NA> 25.450  37.240   6.756 1
## 1513   ATOM  1514   CE2 <NA>   PHE     B    99   <NA> 25.473  38.988   8.409 1
## 1514   ATOM  1515    CZ <NA>   PHE     B    99   <NA> 25.658  37.663   8.073 1
## 1515 HETATM  1517    N1 <NA>   MK1     B   902   <NA>  9.280  23.763   3.004 1
## 1516 HETATM  1518    C1 <NA>   MK1     B   902   <NA>  9.498  23.983   4.459 1
## 1517 HETATM  1519    C2 <NA>   MK1     B   902   <NA> 10.591  24.905   4.962 1
## 1518 HETATM  1520    C3 <NA>   MK1     B   902   <NA> 10.591  24.864   6.466 1
## 1519 HETATM  1521    O1 <NA>   MK1     B   902   <NA> 10.937  23.849   7.057 1
## 1520 HETATM  1522    N2 <NA>   MK1     B   902   <NA> 10.193  25.953   7.094 1
## 1521 HETATM  1523    C4 <NA>   MK1     B   902   <NA> 10.145  26.250   8.490 1
## 1522 HETATM  1524    C5 <NA>   MK1     B   902   <NA>  9.379  27.577   8.641 1
## 1523 HETATM  1525    C6 <NA>   MK1     B   902   <NA> 11.398  26.347   9.074 1
## 1524 HETATM  1526    C7 <NA>   MK1     B   902   <NA>  9.364  25.283   9.268 1
## 1525 HETATM  1527    N3 <NA>   MK1     B   902   <NA> 11.819  24.282   4.355 1
## 1526 HETATM  1528    C8 <NA>   MK1     B   902   <NA> 11.753  23.776   2.961 1
## 1527 HETATM  1529    C9 <NA>   MK1     B   902   <NA> 10.440  23.182   2.493 1
## 1528 HETATM  1530   C10 <NA>   MK1     B   902   <NA> 13.083  24.963   4.552 1
## 1529 HETATM  1531   C11 <NA>   MK1     B   902   <NA> 14.203  24.064   5.078 1
## 1530 HETATM  1532    O2 <NA>   MK1     B   902   <NA> 15.242  24.884   4.634 1
## 1531 HETATM  1533   C12 <NA>   MK1     B   902   <NA> 14.440  23.761   6.569 1
## 1532 HETATM  1534   C13 <NA>   MK1     B   902   <NA> 15.573  22.821   7.005 1
## 1533 HETATM  1535   C14 <NA>   MK1     B   902   <NA> 15.644  22.664   8.534 1
## 1534 HETATM  1536   C15 <NA>   MK1     B   902   <NA> 16.733  21.750   8.961 1
## 1535 HETATM  1537   C16 <NA>   MK1     B   902   <NA> 18.058  21.916   8.553 1
## 1536 HETATM  1538   C17 <NA>   MK1     B   902   <NA> 19.037  21.016   8.947 1
## 1537 HETATM  1539   C18 <NA>   MK1     B   902   <NA> 18.673  19.939   9.758 1
## 1538 HETATM  1540   C19 <NA>   MK1     B   902   <NA> 17.347  19.773  10.176 1
## 1539 HETATM  1541   C20 <NA>   MK1     B   902   <NA> 16.374  20.687   9.772 1
## 1540 HETATM  1542   C21 <NA>   MK1     B   902   <NA> 15.447  21.440   6.373 1
## 1541 HETATM  1543    O3 <NA>   MK1     B   902   <NA> 14.367  20.831   6.397 1
## 1542 HETATM  1544    N4 <NA>   MK1     B   902   <NA> 16.583  20.913   5.924 1
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## 1543 HETATM  1545   C22 <NA>   MK1     B   902   <NA> 16.692  19.500   5.604 1
## 1544 HETATM  1546   C23 <NA>   MK1     B   902   <NA> 18.067  18.945   5.936 1
## 1545 HETATM  1547    O4 <NA>   MK1     B   902   <NA> 19.061  19.938   5.729 1
## 1546 HETATM  1548   C24 <NA>   MK1     B   902   <NA> 18.226  17.726   5.057 1
## 1547 HETATM  1549   C25 <NA>   MK1     B   902   <NA> 17.476  17.904   3.760 1
## 1548 HETATM  1550   C26 <NA>   MK1     B   902   <NA> 17.500  17.363   2.496 1
## 1549 HETATM  1551   C27 <NA>   MK1     B   902   <NA> 16.613  17.872   1.541 1
## 1550 HETATM  1552   C28 <NA>   MK1     B   902   <NA> 15.722  18.906   1.865 1
## 1551 HETATM  1553   C29 <NA>   MK1     B   902   <NA> 15.683  19.479   3.129 1
## 1552 HETATM  1554   C30 <NA>   MK1     B   902   <NA> 16.504  19.061   4.128 1
## 1553 HETATM  1555   C31 <NA>   MK1     B   902   <NA>  8.033  23.100   2.604 1
## 1554 HETATM  1556   C32 <NA>   MK1     B   902   <NA>  6.666  23.739   2.876 1
## 1555 HETATM  1557   C33 <NA>   MK1     B   902   <NA>  6.158  24.808   2.124 1
## 1556 HETATM  1558    N5 <NA>   MK1     B   902   <NA>  4.911  25.430   2.300 1
## 1557 HETATM  1559   C34 <NA>   MK1     B   902   <NA>  4.207  24.839   3.348 1
## 1558 HETATM  1560   C35 <NA>   MK1     B   902   <NA>  4.654  23.774   4.136 1
## 1559 HETATM  1561   C36 <NA>   MK1     B   902   <NA>  5.905  23.211   3.897 1
## 1560 HETATM  1562     O <NA>   HOH     A   305   <NA> 20.857  43.192  21.450 1
## 1561 HETATM  1563     O <NA>   HOH     A   307   <NA> 14.076  19.789  19.440 1
## 1562 HETATM  1564     O <NA>   HOH     A   309   <NA> 28.075  21.177   7.222 1
## 1563 HETATM  1565     O <NA>   HOH     A   314   <NA> 16.759  40.274   1.287 1
## 1564 HETATM  1566     O <NA>   HOH     A   315   <NA> 13.997  22.233  21.468 1
## 1565 HETATM  1567     O <NA>   HOH     A   324   <NA> 11.282  30.738   1.625 1
## 1566 HETATM  1568     O <NA>   HOH     A   325   <NA> 16.774  42.740   2.296 1
## 1567 HETATM  1569     O <NA>   HOH     A   327   <NA> 14.623  29.552  28.235 1
## 1568 HETATM  1570     O <NA>   HOH     A   328   <NA>  1.651  36.463  19.459 1
## 1569 HETATM  1571     O <NA>   HOH     A   329   <NA> 14.435  44.966  11.913 1
## 1570 HETATM  1572     O <NA>   HOH     A   330   <NA> 19.877  40.160  21.917 1
## 1571 HETATM  1573     O <NA>   HOH     A   331   <NA> 17.126  45.934  10.801 1
## 1572 HETATM  1574     O <NA>   HOH     A   332   <NA>  8.840  28.026   4.860 1
## 1573 HETATM  1575     O <NA>   HOH     A   335   <NA> 10.341  18.480  14.477 1
## 1574 HETATM  1576     O <NA>   HOH     A   341   <NA> 19.233  16.711   9.027 1
## 1575 HETATM  1577     O <NA>   HOH     A   342   <NA> 23.799  21.928  12.391 1
## 1576 HETATM  1578     O <NA>   HOH     A   344   <NA>  9.953  37.934   4.548 1
## 1577 HETATM  1579     O <NA>   HOH     A   345   <NA>  8.478  35.995   5.789 1
## 1578 HETATM  1580     O <NA>   HOH     A   357   <NA>  3.960  19.389  17.384 1
## 1579 HETATM  1581     O <NA>   HOH     A   373   <NA> 27.561  43.155  19.015 1
## 1580 HETATM  1582     O <NA>   HOH     A   384   <NA>  1.245  19.292  18.124 1
## 1581 HETATM  1583     O <NA>   HOH     A   386   <NA> 31.402  27.051   3.335 1
## 1582 HETATM  1584     O <NA>   HOH     A   389   <NA> 32.446  31.200   4.417 1
## 1583 HETATM  1585     O <NA>   HOH     A   391   <NA> 25.480  38.468  17.938 1
## 1584 HETATM  1586     O <NA>   HOH     A   394   <NA> 23.940  41.721   0.346 1
## 1585 HETATM  1587     O <NA>   HOH     A   401   <NA>  5.912  15.727   3.369 1
## 1586 HETATM  1588     O <NA>   HOH     A   406   <NA>  9.272  33.891  12.681 1
## 1587 HETATM  1589     O <NA>   HOH     A   408   <NA> 21.185  25.233  16.048 1
## 1588 HETATM  1590     O <NA>   HOH     A   416   <NA> 18.474  26.012  21.664 1
## 1589 HETATM  1591     O <NA>   HOH     A   420   <NA>  9.469  16.910  17.371 1
## 1590 HETATM  1592     O <NA>   HOH     A   422   <NA> 13.074  17.786  16.615 1
## 1591 HETATM  1593     O <NA>   HOH     A   439   <NA> 28.821  29.338   7.342 1
## 1592 HETATM  1594     O <NA>   HOH     A   457   <NA> 23.284  23.107  15.132 1
## 1593 HETATM  1595     O <NA>   HOH     A   468   <NA>  3.114  26.260   6.773 1
## 1594 HETATM  1596     O <NA>   HOH     A   501   <NA>  6.382  26.424   5.893 1
## 1595 HETATM  1597     O <NA>   HOH     A   503   <NA> 35.293  43.006   5.212 1
## 1596 HETATM  1598     O <NA>   HOH     A   510   <NA> 21.891  49.715   7.192 1
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## 1597 HETATM  1599     O <NA>   HOH     A   524   <NA> 34.085  32.735   2.849 1
## 1598 HETATM  1600     O <NA>   HOH     A   529   <NA> 31.491  41.524   6.678 1
## 1599 HETATM  1601     O <NA>   HOH     A   553   <NA>  5.943  34.223   6.748 1
## 1600 HETATM  1602     O <NA>   HOH     A   561   <NA>  0.934  40.259  19.405 1
## 1601 HETATM  1603     O <NA>   HOH     A   567   <NA> 29.539  25.486  13.281 1
## 1602 HETATM  1604     O <NA>   HOH     A   572   <NA> 24.552  17.352  10.295 1
## 1603 HETATM  1605     O <NA>   HOH     A   575   <NA> 23.112  15.510   8.776 1
## 1604 HETATM  1606     O <NA>   HOH     B   301   <NA> 20.445   8.036 -12.631 1
## 1605 HETATM  1607     O <NA>   HOH     B   303   <NA> 20.044  14.822   4.638 1
## 1606 HETATM  1608     O <NA>   HOH     B   304   <NA> 21.538   6.875 -10.099 1
## 1607 HETATM  1609     O <NA>   HOH     B   306   <NA> 22.449  23.958   5.252 1
## 1608 HETATM  1610     O <NA>   HOH     B   308   <NA> 11.720  21.289   7.190 1
## 1609 HETATM  1611     O <NA>   HOH     B   312   <NA> 14.097   5.111 -11.638 1
## 1610 HETATM  1612     O <NA>   HOH     B   313   <NA> 20.998  21.834   6.561 1
## 1611 HETATM  1613     O <NA>   HOH     B   316   <NA> 22.659  14.583  -2.196 1
## 1612 HETATM  1614     O <NA>   HOH     B   317   <NA> 28.724  15.629 -11.660 1
## 1613 HETATM  1615     O <NA>   HOH     B   318   <NA> 16.539  45.207   0.079 1
## 1614 HETATM  1616     O <NA>   HOH     B   319   <NA> 23.678  14.931   2.680 1
## 1615 HETATM  1617     O <NA>   HOH     B   321   <NA> 20.718  15.976  -3.657 1
## 1616 HETATM  1618     O <NA>   HOH     B   323   <NA> 31.249  26.796  -9.595 1
## 1617 HETATM  1619     O <NA>   HOH     B   326   <NA> 28.813  28.445  -2.106 1
## 1618 HETATM  1620     O <NA>   HOH     B   333   <NA> 12.251  39.551  -2.672 1
## 1619 HETATM  1621     O <NA>   HOH     B   334   <NA> 25.465  12.592  -8.670 1
## 1620 HETATM  1622     O <NA>   HOH     B   338   <NA> 12.998  36.205  -3.972 1
## 1621 HETATM  1623     O <NA>   HOH     B   339   <NA> 17.541  17.060 -17.194 1
## 1622 HETATM  1624     O <NA>   HOH     B   340   <NA>  5.321  14.325  -4.866 1
## 1623 HETATM  1625     O <NA>   HOH     B   346   <NA>  9.314  17.330  -9.801 1
## 1624 HETATM  1626     O <NA>   HOH     B   347   <NA>  7.435  26.652 -14.854 1
## 1625 HETATM  1627     O <NA>   HOH     B   348   <NA>  4.405  16.704  -3.635 1
## 1626 HETATM  1628     O <NA>   HOH     B   349   <NA> 19.414   7.026   4.428 1
## 1627 HETATM  1629     O <NA>   HOH     B   350   <NA>  6.718  34.538  -1.322 1
## 1628 HETATM  1630     O <NA>   HOH     B   354   <NA> 15.041  31.743 -13.235 1
## 1629 HETATM  1631     O <NA>   HOH     B   355   <NA> 27.404  32.078 -10.860 1
## 1630 HETATM  1632     O <NA>   HOH     B   356   <NA> 27.673  18.789  -6.155 1
## 1631 HETATM  1633     O <NA>   HOH     B   358   <NA> 21.289  -1.161  -5.102 1
## 1632 HETATM  1634     O <NA>   HOH     B   359   <NA>  6.973  36.523   1.489 1
## 1633 HETATM  1635     O <NA>   HOH     B   360   <NA> 27.602  21.234  -0.635 1
## 1634 HETATM  1636     O <NA>   HOH     B   362   <NA>  3.902   9.376  -0.027 1
## 1635 HETATM  1637     O <NA>   HOH     B   364   <NA> 28.498  36.632  -7.529 1
## 1636 HETATM  1638     O <NA>   HOH     B   366   <NA> 18.572  40.567 -10.042 1
## 1637 HETATM  1639     O <NA>   HOH     B   367   <NA> 25.658  18.970   0.428 1
## 1638 HETATM  1640     O <NA>   HOH     B   369   <NA> 20.843   1.263  -7.014 1
## 1639 HETATM  1641     O <NA>   HOH     B   370   <NA> 13.975  15.741  12.070 1
## 1640 HETATM  1642     O <NA>   HOH     B   374   <NA>  7.661  23.876  -6.324 1
## 1641 HETATM  1643     O <NA>   HOH     B   375   <NA> 10.125   5.706  -1.458 1
## 1642 HETATM  1644     O <NA>   HOH     B   376   <NA> 18.450  20.497 -18.728 1
## 1643 HETATM  1645     O <NA>   HOH     B   377   <NA> 29.267  20.487  -3.497 1
## 1644 HETATM  1646     O <NA>   HOH     B   379   <NA>  6.685  26.541  -5.608 1
## 1645 HETATM  1647     O <NA>   HOH     B   381   <NA> 25.810  26.789 -19.106 1
## 1646 HETATM  1648     O <NA>   HOH     B   383   <NA> 21.144  -4.428 -11.331 1
## 1647 HETATM  1649     O <NA>   HOH     B   387   <NA> 16.904  27.594 -15.938 1
## 1648 HETATM  1650     O <NA>   HOH     B   388   <NA> 23.926  45.612  -4.998 1
## 1649 HETATM  1651     O <NA>   HOH     B   390   <NA> 25.300  17.493   3.076 1
## 1650 HETATM  1652     O <NA>   HOH     B   392   <NA>  6.618  28.079  -3.427 1
```

```
## 1651 HETATM  1653     O <NA>   HOH     B   393   <NA> 19.795  13.651 -16.606 1
## 1652 HETATM  1654     O <NA>   HOH     B   395   <NA>  7.202   9.982  -4.103 1
## 1653 HETATM  1655     O <NA>   HOH     B   400   <NA>  8.474  34.203  -4.893 1
## 1654 HETATM  1656     O <NA>   HOH     B   405   <NA> 16.659  15.866  11.446 1
## 1655 HETATM  1657     O <NA>   HOH     B   410   <NA> 26.400  10.057  -3.287 1
## 1656 HETATM  1658     O <NA>   HOH     B   414   <NA>  9.503   3.489  -4.419 1
## 1657 HETATM  1659     O <NA>   HOH     B   419   <NA> 15.438  12.973 -18.484 1
## 1658 HETATM  1660     O <NA>   HOH     B   425   <NA> 11.428  19.956 -24.551 1
## 1659 HETATM  1661     O <NA>   HOH     B   430   <NA> 18.725  43.171  -5.575 1
## 1660 HETATM  1662     O <NA>   HOH     B   436   <NA> 32.141  29.620  -8.580 1
## 1661 HETATM  1663     O <NA>   HOH     B   443   <NA>  8.811  13.667 -20.256 1
## 1662 HETATM  1664     O <NA>   HOH     B   444   <NA>  4.071  26.169  -0.230 1
## 1663 HETATM  1665     O <NA>   HOH     B   461   <NA> 11.425  44.636  -3.033 1
## 1664 HETATM  1666     O <NA>   HOH     B   469   <NA>  6.902  23.686 -10.066 1
## 1665 HETATM  1667     O <NA>   HOH     B   471   <NA>  5.749  25.785 -19.792 1
## 1666 HETATM  1668     O <NA>   HOH     B   500   <NA> 25.592  16.404  -5.805 1
## 1667 HETATM  1669     O <NA>   HOH     B   502   <NA>  4.040  15.516  -7.200 1
## 1668 HETATM  1670     O <NA>   HOH     B   505   <NA> 28.640  34.232  -5.637 1
## 1669 HETATM  1671     O <NA>   HOH     B   506   <NA>  8.979  11.173  11.112 1
## 1670 HETATM  1672     O <NA>   HOH     B   509   <NA> 19.882   3.986 -18.136 1
## 1671 HETATM  1673     O <NA>   HOH     B   514   <NA> 27.409  15.355   2.200 1
## 1672 HETATM  1674     O <NA>   HOH     B   515   <NA> 17.222  39.766 -23.774 1
## 1673 HETATM  1675     O <NA>   HOH     B   517   <NA> 28.742  24.158 -16.641 1
## 1674 HETATM  1676     O <NA>   HOH     B   525   <NA> 22.694  -2.192 -12.589 1
## 1675 HETATM  1677     O <NA>   HOH     B   526   <NA> 17.901  43.157 -14.082 1
## 1676 HETATM  1678     O <NA>   HOH     B   531   <NA> 18.192   8.914  11.344 1
## 1677 HETATM  1679     O <NA>   HOH     B   532   <NA> 19.507  45.215   1.709 1
## 1678 HETATM  1680     O <NA>   HOH     B   548   <NA>  1.442  14.700  -6.128 1
## 1679 HETATM  1681     O <NA>   HOH     B   549   <NA> 19.908   8.718 -19.215 1
## 1680 HETATM  1682     O <NA>   HOH     B   556   <NA> 21.499  44.884  -1.280 1
## 1681 HETATM  1683     O <NA>   HOH     B   564   <NA> 10.031   8.593 -22.052 1
## 1682 HETATM  1684     O <NA>   HOH     B   568   <NA>  2.817  28.133   2.191 1
## 1683 HETATM  1685     O <NA>   HOH     B   591   <NA> 15.835  40.105  -5.971 1
## 1684 HETATM  1686     O <NA>   HOH     B   595   <NA>  4.515  36.451  -4.499 1
## 1685 HETATM  1687     O <NA>   HOH     B   613   <NA> 24.127 -10.994  -0.982 1
## 1686 HETATM  1688     O <NA>   HOH     B   617   <NA> 30.112  17.912  -4.791 1
##          b segid elesy charge
## 1    38.10  <NA>     N   <NA>
## 2    40.62  <NA>     C   <NA>
## 3    42.64  <NA>     C   <NA>
## 4    43.40  <NA>     O   <NA>
## 5    37.87  <NA>     C   <NA>
## 6    38.40  <NA>     C   <NA>
## 7    38.74  <NA>     C   <NA>
## 8    41.76  <NA>     N   <NA>
## 9    41.30  <NA>     C   <NA>
## 10   41.38  <NA>     C   <NA>
## 11   43.09  <NA>     O   <NA>
## 12   40.81  <NA>     C   <NA>
## 13   46.61  <NA>     C   <NA>
## 14   50.36  <NA>     C   <NA>
## 15   53.89  <NA>     O   <NA>
## 16   51.46  <NA>     N   <NA>
## 17   37.80  <NA>     N   <NA>
```

```
## 18   34.13  <NA>     C   <NA>
## 19   33.19  <NA>     C   <NA>
## 20   32.74  <NA>     O   <NA>
## 21   34.34  <NA>     C   <NA>
## 22   33.95  <NA>     C   <NA>
## 23   33.06  <NA>     C   <NA>
## 24   32.50  <NA>     C   <NA>
## 25   31.65  <NA>     N   <NA>
## 26   30.14  <NA>     C   <NA>
## 27   29.74  <NA>     C   <NA>
## 28   27.88  <NA>     O   <NA>
## 29   29.24  <NA>     C   <NA>
## 30   27.60  <NA>     O   <NA>
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## 32   29.27  <NA>     N   <NA>
## 33   30.12  <NA>     C   <NA>
## 34   32.98  <NA>     C   <NA>
## 35   32.32  <NA>     O   <NA>
## 36   26.21  <NA>     C   <NA>
## 37   24.56  <NA>     C   <NA>
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## 39   21.87  <NA>     C   <NA>
## 40   31.52  <NA>     N   <NA>
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## 44   28.66  <NA>     C   <NA>
## 45   26.42  <NA>     C   <NA>
## 46   28.49  <NA>     C   <NA>
## 47   28.47  <NA>     C   <NA>
## 48   29.88  <NA>     N   <NA>
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## 50   25.06  <NA>     C   <NA>
## 51   32.14  <NA>     C   <NA>
## 52   27.41  <NA>     C   <NA>
## 53   30.03  <NA>     C   <NA>
## 54   33.01  <NA>     N   <NA>
## 55   32.37  <NA>     C   <NA>
## 56   29.95  <NA>     C   <NA>
## 57   26.55  <NA>     O   <NA>
## 58   38.12  <NA>     C   <NA>
## 59   48.91  <NA>     C   <NA>
## 60   59.75  <NA>     C   <NA>
## 61   61.83  <NA>     O   <NA>
## 62   59.99  <NA>     N   <NA>
## 63   27.34  <NA>     N   <NA>
## 64   29.87  <NA>     C   <NA>
## 65   31.94  <NA>     C   <NA>
## 66   33.83  <NA>     O   <NA>
## 67   28.16  <NA>     C   <NA>
## 68   27.47  <NA>     C   <NA>
## 69   25.45  <NA>     C   <NA>
## 70   23.06  <NA>     N   <NA>
## 71   28.80  <NA>     C   <NA>
```

```
## 72   30.95  <NA>     N   <NA>
## 73   26.02  <NA>     N   <NA>
## 74   30.21  <NA>     N   <NA>
## 75   29.48  <NA>     C   <NA>
## 76   29.45  <NA>     C   <NA>
## 77   28.45  <NA>     O   <NA>
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## 79   28.12  <NA>     C   <NA>
## 80   31.64  <NA>     C   <NA>
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## 86   35.91  <NA>     C   <NA>
## 87   40.15  <NA>     C   <NA>
## 88   40.51  <NA>     C   <NA>
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## 90   30.14  <NA>     C   <NA>
## 91   33.13  <NA>     C   <NA>
## 92   34.48  <NA>     O   <NA>
## 93   27.12  <NA>     C   <NA>
## 94   28.48  <NA>     C   <NA>
## 95   26.29  <NA>     C   <NA>
## 96   32.34  <NA>     N   <NA>
## 97   32.56  <NA>     C   <NA>
## 98   33.07  <NA>     C   <NA>
## 99   33.62  <NA>     O   <NA>
## 100  33.81  <NA>     C   <NA>
## 101  40.47  <NA>     O   <NA>
## 102  34.22  <NA>     C   <NA>
## 103  31.84  <NA>     N   <NA>
## 104  32.26  <NA>     C   <NA>
## 105  33.69  <NA>     C   <NA>
## 106  30.43  <NA>     O   <NA>
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## 110  32.46  <NA>     C   <NA>
## 111  36.78  <NA>     N   <NA>
## 112  38.20  <NA>     C   <NA>
## 113  37.51  <NA>     C   <NA>
## 114  33.78  <NA>     O   <NA>
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## 116  50.67  <NA>     C   <NA>
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## 118  62.89  <NA>     C   <NA>
## 119  69.50  <NA>     N   <NA>
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## 121  46.34  <NA>     C   <NA>
## 122  49.77  <NA>     C   <NA>
## 123  52.38  <NA>     O   <NA>
## 124  45.04  <NA>     C   <NA>
## 125  46.91  <NA>     C   <NA>
```

```
## 126  47.78  <NA>     C   <NA>
## 127  50.24  <NA>     C   <NA>
## 128  53.37  <NA>     N   <NA>
## 129  56.32  <NA>     C   <NA>
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## 132  57.90  <NA>     N   <NA>
## 133  59.71  <NA>     C   <NA>
## 134  60.57  <NA>     C   <NA>
## 135  63.20  <NA>     O   <NA>
## 136  59.37  <NA>     N   <NA>
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## 140  63.37  <NA>     C   <NA>
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## 142  72.39  <NA>     C   <NA>
## 143  76.16  <NA>     O   <NA>
## 144  74.55  <NA>     N   <NA>
## 145  53.88  <NA>     N   <NA>
## 146  49.32  <NA>     C   <NA>
## 147  46.38  <NA>     C   <NA>
## 148  43.18  <NA>     O   <NA>
## 149  47.14  <NA>     C   <NA>
## 150  46.02  <NA>     C   <NA>
## 151  46.45  <NA>     C   <NA>
## 152  46.45  <NA>     C   <NA>
## 153  44.76  <NA>     N   <NA>
## 154  44.52  <NA>     C   <NA>
## 155  42.87  <NA>     C   <NA>
## 156  41.39  <NA>     O   <NA>
## 157  43.50  <NA>     C   <NA>
## 158  46.90  <NA>     C   <NA>
## 159  49.38  <NA>     C   <NA>
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## 164  35.18  <NA>     C   <NA>
## 165  30.96  <NA>     O   <NA>
## 166  45.21  <NA>     C   <NA>
## 167  55.20  <NA>     C   <NA>
## 168  63.88  <NA>     C   <NA>
## 169  67.73  <NA>     O   <NA>
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## 172  26.79  <NA>     C   <NA>
## 173  26.36  <NA>     C   <NA>
## 174  24.88  <NA>     O   <NA>
## 175  22.80  <NA>     C   <NA>
## 176  25.58  <NA>     N   <NA>
## 177  25.08  <NA>     C   <NA>
## 178  23.67  <NA>     C   <NA>
## 179  25.94  <NA>     O   <NA>
```

```
## 180  27.31  <NA>     C   <NA>
## 181  27.99  <NA>     C   <NA>
## 182  29.29  <NA>     C   <NA>
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## 185  18.03  <NA>     C   <NA>
## 186  19.77  <NA>     C   <NA>
## 187  20.40  <NA>     O   <NA>
## 188  15.36  <NA>     C   <NA>
## 189  18.86  <NA>     C   <NA>
## 190  16.70  <NA>     C   <NA>
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## 195  17.64  <NA>     O   <NA>
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## 198  22.87  <NA>     O   <NA>
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## 200  15.44  <NA>     N   <NA>
## 201  15.16  <NA>     C   <NA>
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## 209  13.84  <NA>     C   <NA>
## 210  14.08  <NA>     O   <NA>
## 211  12.94  <NA>     N   <NA>
## 212  13.20  <NA>     C   <NA>
## 213  17.23  <NA>     C   <NA>
## 214  15.43  <NA>     O   <NA>
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## 221  23.38  <NA>     C   <NA>
## 222  23.84  <NA>     O   <NA>
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## 229  25.77  <NA>     C   <NA>
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## 231  33.64  <NA>     O   <NA>
## 232  21.65  <NA>     N   <NA>
## 233  19.28  <NA>     C   <NA>
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## 235  21.27  <NA>     O   <NA>
## 236  21.21  <NA>     C   <NA>
## 237  17.85  <NA>     O   <NA>
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## 242  21.86  <NA>     O   <NA>
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## 263  32.88  <NA>     N   <NA>
## 264  33.85  <NA>     C   <NA>
## 265  34.72  <NA>     C   <NA>
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## 269  45.60  <NA>     C   <NA>
## 270  50.36  <NA>     O   <NA>
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## 272  33.77  <NA>     N   <NA>
## 273  32.08  <NA>     C   <NA>
## 274  33.50  <NA>     C   <NA>
## 275  33.82  <NA>     O   <NA>
## 276  31.77  <NA>     C   <NA>
## 277  33.78  <NA>     C   <NA>
## 278  38.76  <NA>     S   <NA>
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## 282  32.96  <NA>     C   <NA>
## 283  32.62  <NA>     O   <NA>
## 284  34.02  <NA>     C   <NA>
## 285  38.20  <NA>     O   <NA>
## 286  35.12  <NA>     N   <NA>
## 287  38.10  <NA>     C   <NA>
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## 290  35.60  <NA>     C   <NA>
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## 294  45.17  <NA>     N   <NA>
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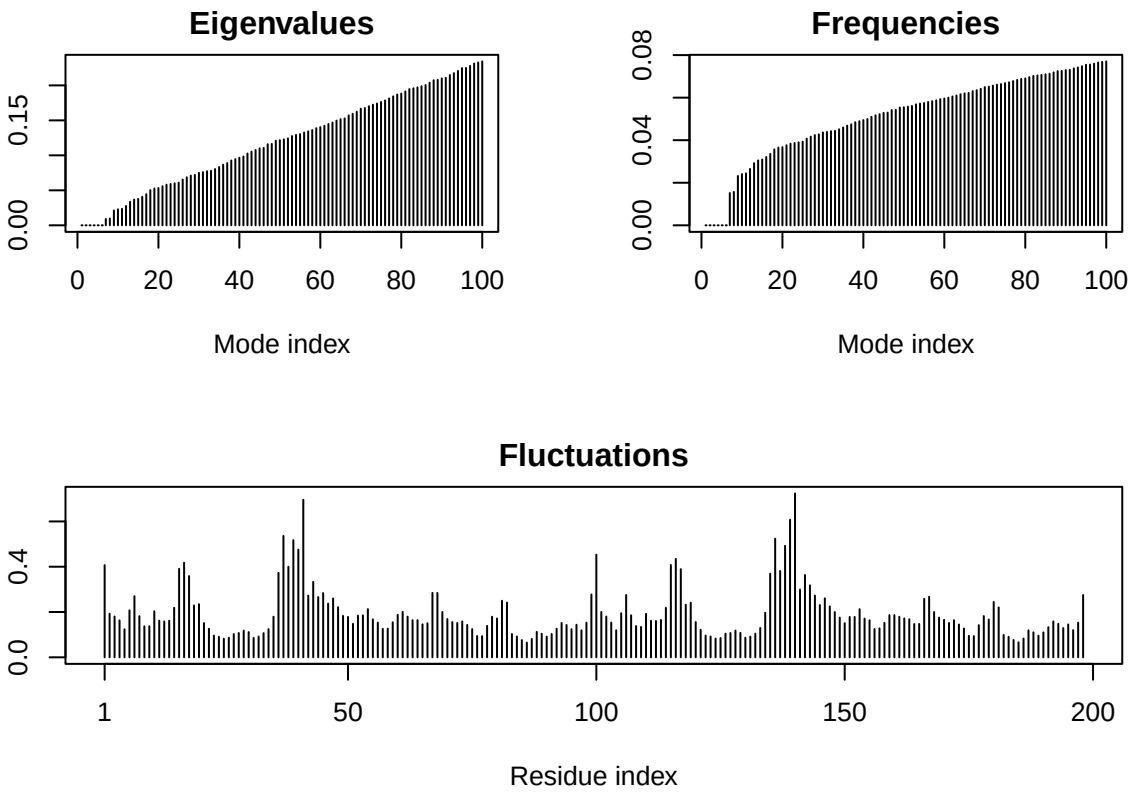
## 1659 52.97  <NA>     0   <NA>
## 1660 72.75  <NA>     0   <NA>
## 1661 75.75  <NA>     0   <NA>
## 1662 38.25  <NA>     0   <NA>
## 1663 68.43  <NA>     0   <NA>
## 1664 54.20  <NA>     0   <NA>
## 1665 63.96  <NA>     0   <NA>
## 1666 23.98  <NA>     0   <NA>
## 1667 52.93  <NA>     0   <NA>
## 1668 58.06  <NA>     0   <NA>
## 1669 64.79  <NA>     0   <NA>
## 1670 55.54  <NA>     0   <NA>
## 1671 61.69  <NA>     0   <NA>
## 1672 69.12  <NA>     0   <NA>
## 1673 78.93  <NA>     0   <NA>
## 1674 71.37  <NA>     0   <NA>
## 1675 78.14  <NA>     0   <NA>
## 1676 54.05  <NA>     0   <NA>
## 1677 72.78  <NA>     0   <NA>
## 1678 58.40  <NA>     0   <NA>
## 1679 58.78  <NA>     0   <NA>
## 1680 68.40  <NA>     0   <NA>
## 1681 64.90  <NA>     0   <NA>
## 1682 67.95  <NA>     0   <NA>
## 1683 53.68  <NA>     0   <NA>
## 1684 49.41  <NA>     0   <NA>
## 1685 64.49  <NA>     0   <NA>
## 1686 54.09  <NA>     0   <NA>
```

```
m <- nma(pdb)
```

```
## Warning in nma.pdb(pdb): Possible multi-chain structure or missing in-structure residue(s) present
##   Fluctuations at neighboring positions may be affected.
```

```
##  Building Hessian...     Done in 0.106 seconds.
##  Diagonalizing Hessian...    Done in 0.491 seconds.
```

```
plot(m)
```




```
mktrj(m,file='nma.pdb')
```