# SUPPLEMENTARY MATERIAL
# for
# Protein topology from predicted residue contacts

William R. Taylor, David T. Jones and Michael I. Sadowski

November 8, 2011

# 1 Protein Data

For each protein, following a summary taken from the main paper, the following data sets are included:

1. RASMOL images are shown of the $\alpha$-carbon trace of the best (reranked) model: [*top left*] coloured by secondary structure type as: red = $\alpha$-helix and green = $\beta$-strand and [*top right*] coloured by chain position (blue = amino to red = carboxy terminus). [*lower left*] The native structure coloured by chain position. [*lower right*] The top ranked model superposed on the native structure (using the SAP program) and coloured by chain position.

   All structures are viewed along the first $\beta$-strand in the sheet with it approaching the viewer and with the first $\alpha$-helix following this strand lying above the sheet. This corresponds to the orientation of the topology diagram taken from the topology string when 'A' is the top layer and 'a' is the bottom layer with negative numbers to the left and positive to the right. (See Figure of the main text for exmples).

2. Multiple sequence alignment and predicted secondary structures. [*panel 1*] Amino acids are coloured individually using the colour wheel defined by Taylor, Prot.Eng. (1997) 10:743-746. [*panel 2*] Secondary structure predicted by PSIPRED and coloured red = $\alpha$ and green = $\beta$. [*panel 3*] The average colour values in panel 2. [*panel 4*] The average colour values in panel 1.

3. Dot plot of predicted (red) and observed (green) residue contacts. The latter are plotted first with a slightly larger dot size to allow coincident points to be distinguished. (Plots were made with GNUPLOT). An observed contacts is plotted if two virtual centroids positions come within 8Å. The virtual centroid is a point 2Å distant from the $\alpha$-carbon along the line bisecting the virtual $\alpha$-carbon bond angle. It generally lies between the

$\beta$-carbon and $\gamma$-carbon positions of the side-chain. No allowance is made for glycine as the model represents a multiple sequence alignment and not a single sequence.

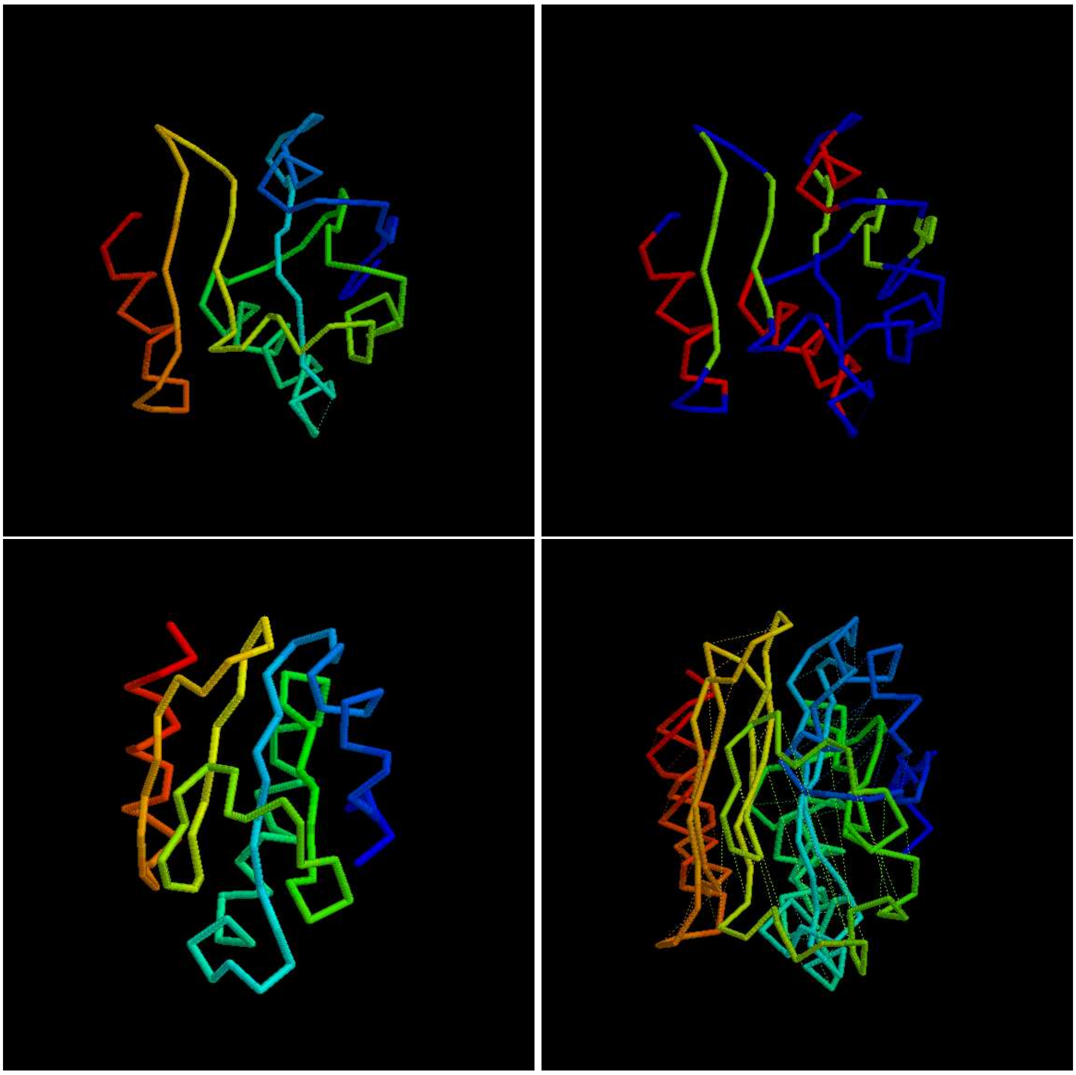
4. Ranked topology lists: (only the top part of the file is shown here. The full lists can be obtained from the data archive given below.) [*upper*] The full list of models ranked on field 7 which is the product of the PLATO score (field 8) and the the contact score (field 9). The topology string is field 12. [*middle*] the best list (top 500 models from the full list). [*lower*] the best list reranked on contact score (field 9).

All the above data are included in the zipped tar archive at `http:mathbio.nimr.mrc.ac.uk/wiki/Software#Supplementary_info`

## 1.1 ‘Training’ test set

`2trxA (108) = +B+0.-A+0.+B-2.-a+0.+B-1.[-A-1.]-B-3.+B-4.-a-1.`

**Thioredoxin** has a typical glutaredoxin fold. The protein contains the unusual topological feature of a helix located in a loop between two antiparallel $\beta$-strands. This helix (bracketed in the topology string) is usually poorly predicted by the secondary structure prediction methods and often is modelled as a loop giving a larger RMS value when compared to the PDB structure for a protein of this size.



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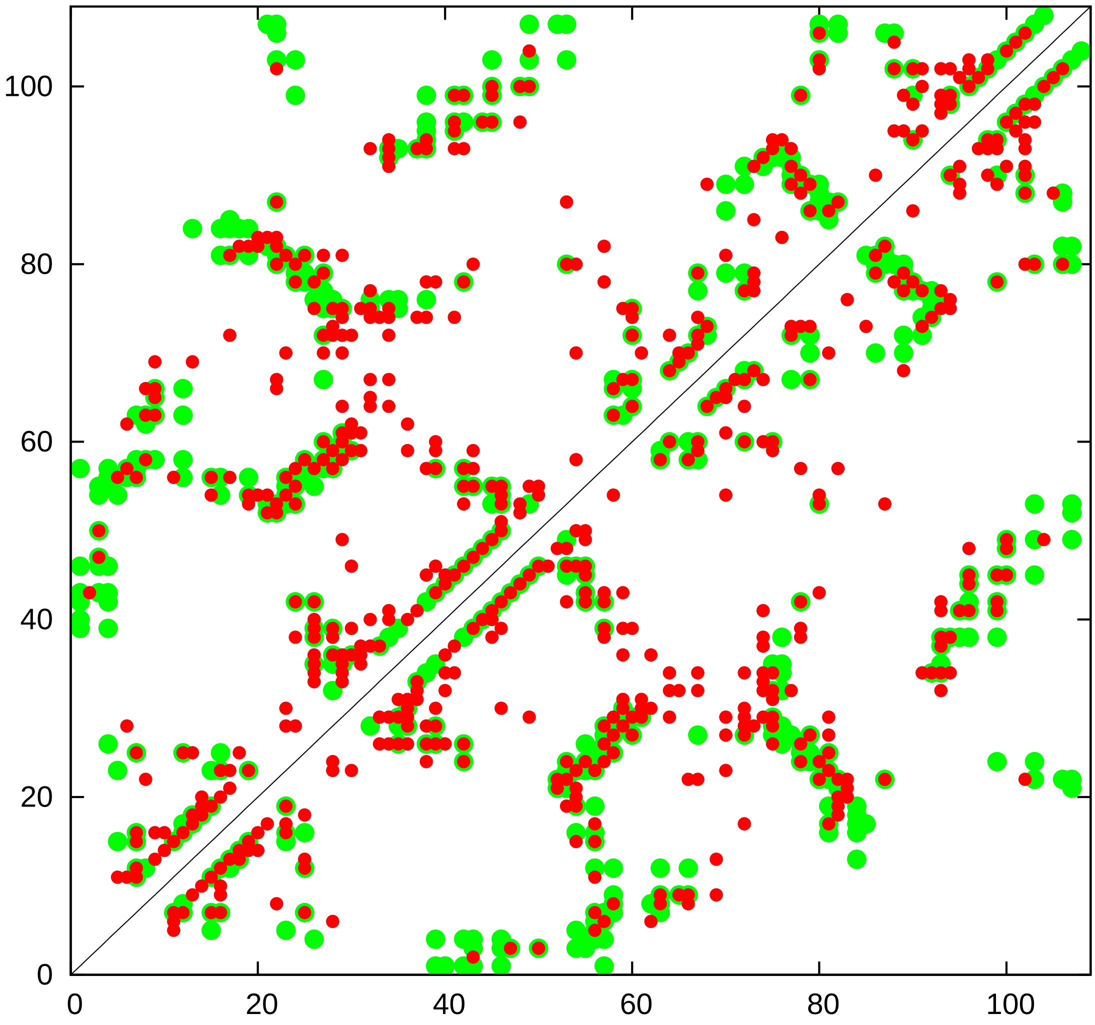
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full.list

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best.list

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reranked best.list

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fold-13-3-1 Build Rank 1 Fold 241 1942.635 43.94 44.22 aACcdDEebBFfgGHh aCdEbFgH +B+0.-A+0.+B-2.-a+0.+B-1.-B-3.+B-4.-a-1. 2640.01
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fold-12-16-3 Build Rank 3 Fold 441 1426.004 32.34 44.10 aAeEFfgGHhdDBbcC aeFgHdBc +B+0.+A+0.-B-3.+a+0.-B-4.+B-2.-B-1.+a+1. 1611.72
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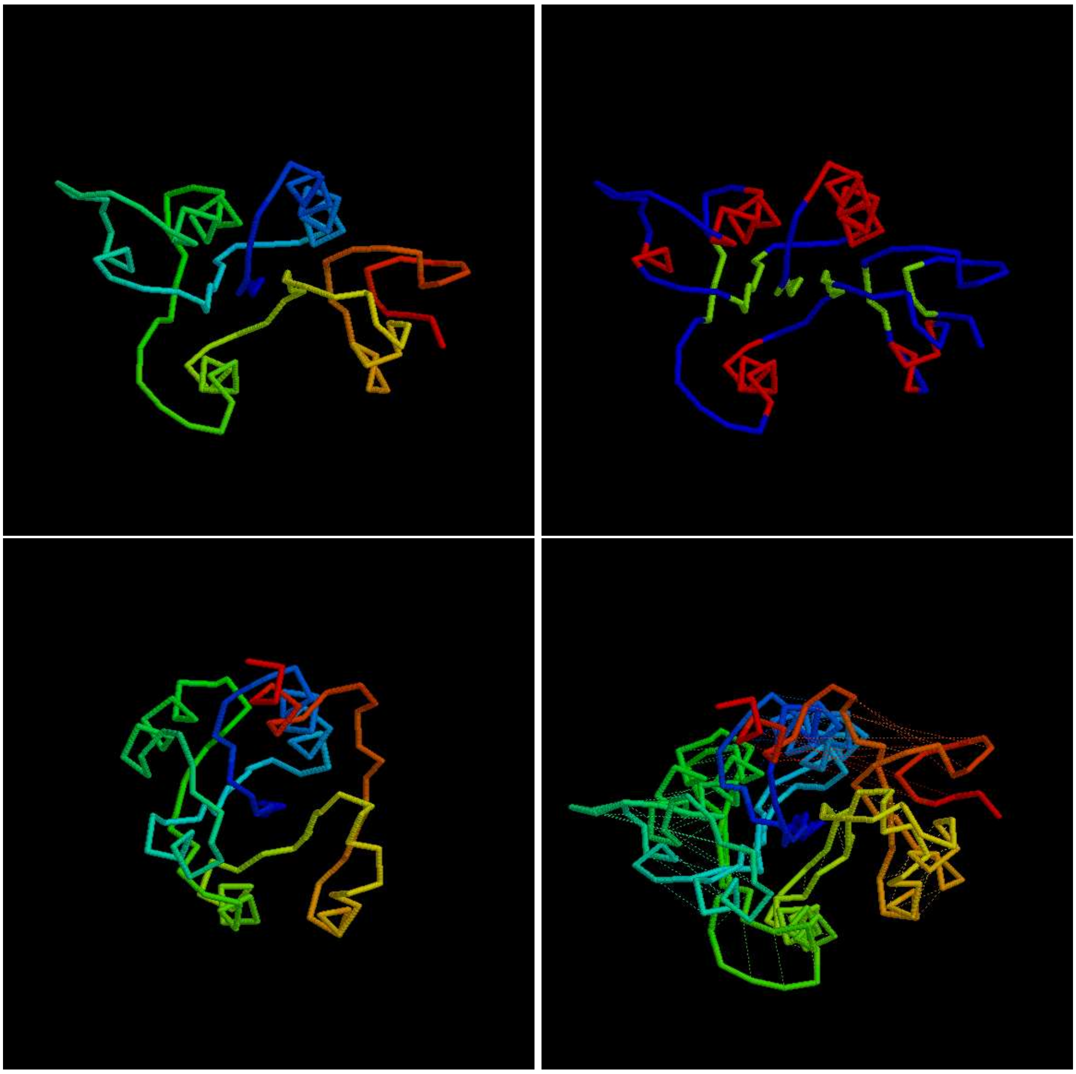
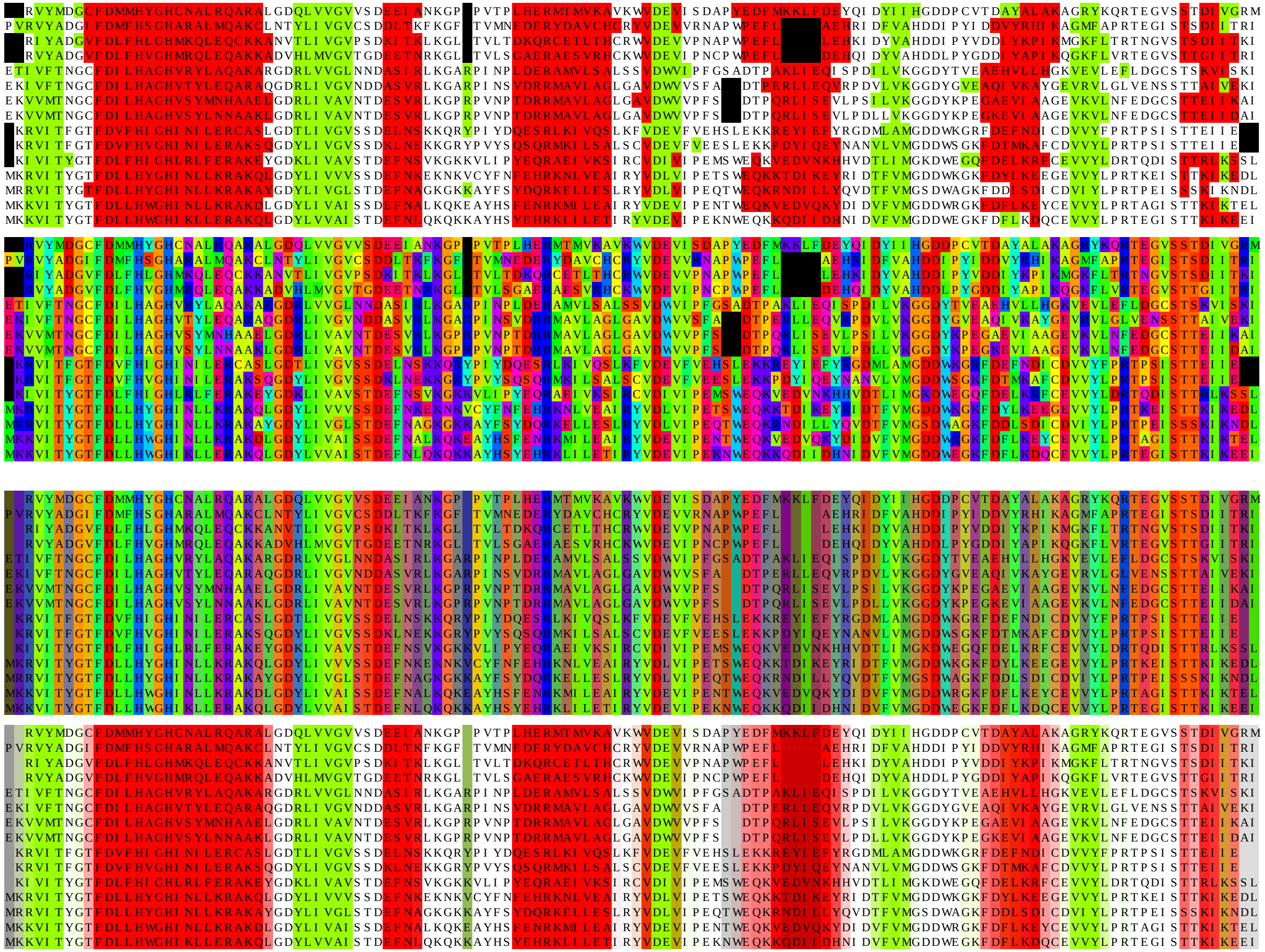
`1cozA (126) = +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.[+-]A+1.`

**Chorismate mutase** has a mini-Rossman type fold plus a carboxy-terminal helix that packs across to the opposing monomer in this dimeric structure. In the definition of the correct fold, this terminal helix was considered correct if it packed back onto the domain either in an antiparallel or parallel connection, with the latter being a better approximation to the native structure. This protein has quite variable secondary structure predictions making it a difficult target.





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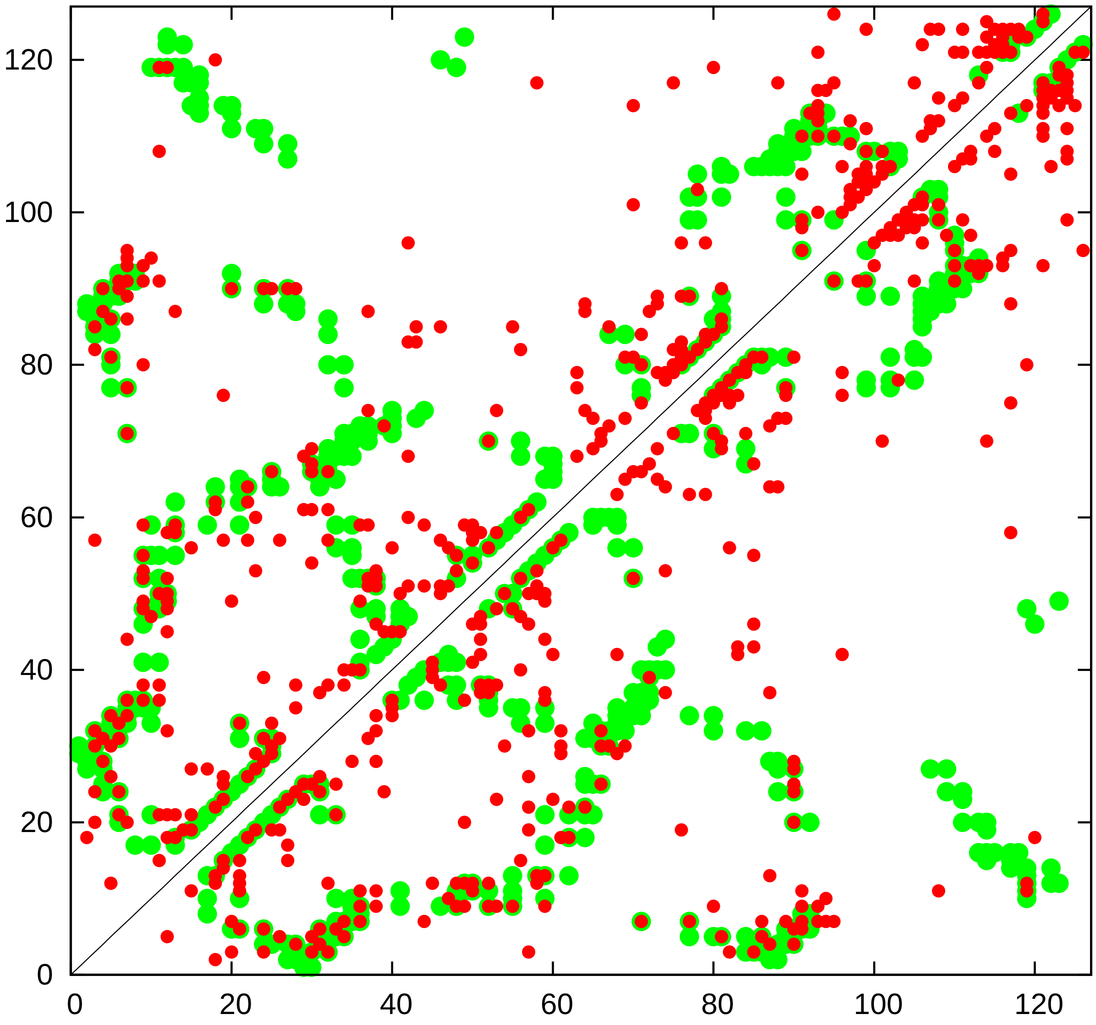
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120
0
20
40
60
80
100
120

```
full.list

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build1cozA/folds/fold-1-0-40:REMARK Build  Rank  58 Fold     55   171.304 13.27 12.91  GghHIiFfbBeEDdaACc GhIFbeDaC +B+0.-A+0.+B-1.+a+0.-a+1.-B+1.+A+1.-B+3.+B+2. 163.967
build1cozA/folds/fold-1-0-60:REMARK Build  Rank  87 Fold     31   144.405 13.61 10.61  eEDdaABbfFCchHIiGg eDaBfChIG +B+0.-A+0.+B-2.-a+0.+a+1.-B-1.+A+1.-B+2.-B+1. 135.696
build1cozA/folds/fold-1-10-20:REMARK Build  Rank  20 Fold    263   315.317 17.64 17.88  AacCDdiIEeBbgGFfHh AcDiEBgFH +B+0.-A+0.+B-2.-a+0.+a+1.+B-1.-A-1.+B-3.+B-4. 311.742
build1cozA/folds/fold-1-10-50:REMARK Build  Rank  50 Fold     70   246.843 15.09 16.36  fFIihHGgcCDdeEBbaA fIhGcDeBa +B+0.-A+0.+B-1.-a+0.+a+1.-B+1.+A+1.-B+2.+B+3. 240.084
build1cozA/folds/fold-1-1-10:REMARK Build  Rank  17 Fold    115   240.544 14.93 16.11  cCDdaABbfFEeHhiIGg cDaBfEHiG +B+0.-A+0.+B-1.-a+0.+a+1.-B+1.-A+1.+B+3.-B+2. 237.067
build1cozA/folds/fold-1-11-20:REMARK Build  Rank  20 Fold    263   315.317 17.64 17.88  AacCDdiIEeBbgGFfHh AcDiEBgFH +B+0.-A+0.+B-2.-a+0.+a+1.+B-1.-A-1.+B-3.+B-4. 311.506
build1cozA/folds/fold-1-11-30:REMARK Build  Rank  30 Fold     49   286.511 15.95 17.96  DdGghHIieEfFCcaABb DGhIefCaB +B+0.+A+0.-B-2.+a+0.-a+1.-B-1.+A+1.-B+2.+B+1. 282.013
build1cozA/folds/fold-1-1-60:REMARK Build  Rank  87 Fold     31   144.405 13.61 10.61  eEDdaABbfFCchHIiGg eDaBfChIG +B+0.-A+0.+B-2.-a+0.+a+1.-B-1.+A+1.-B+2.-B+1. 135.519
build1cozA/folds/fold-1-2-10:REMARK Build  Rank  16 Fold     15   236.609 14.48 16.34  CcdDAabBFfeEHhIigG CdAbFeHIg +B+0.-A+0.+B-1.-a+0.+a+1.-B+1.+A+1.+B+3.-B+2. 233.115
```

```
best.list

fold-17-29-1 Build Rank 1 Fold 4 943.272 32.18 29.32 EefFGgjJIihHDdbBCcaA EfGjIhDbCa +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+3. 1852.64
fold-17-28-1 Build Rank 1 Fold 4 943.272 32.18 29.32 EefFGgjJIihHDdbBCcaA EfGjIhDbCa +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+3. 1892.1
fold-17-28-2 Build Rank 2 Fold 1 941.757 29.93 31.46 EefFGgjJIihHDdbBAacC EfGjIhDbAc +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+3.-B+2. 2922.51
fold-17-29-2 Build Rank 2 Fold 1 941.757 29.93 31.46 EefFGgjJIihHDdbBAacC EfGjIhDbAc +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+3.-B+2. 2761.17
fold-25-14-1 Build Rank 1 Fold 37 911.103 26.48 34.41 fFDdhHKkGgjJIieEBbcCAa fDhKGjIeBcA +B+0.-A+0.+B-1.-A-2.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+3. 2226.68
fold-25-15-1 Build Rank 1 Fold 37 911.103 26.48 34.41 fFDdhHKkGgjJIieEBbcCAa fDhKGjIeBcA +B+0.-A+0.+B-1.-A-2.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+3. 2802.87
fold-17-14-1 Build Rank 1 Fold 14 902.860 31.46 28.70 eEFfgGJjiIHhdDBbaACc eFgJiHdBaC +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+3.-B+2. 2483.21
fold-17-15-1 Build Rank 1 Fold 14 902.860 31.46 28.70 eEFfgGJjiIHhdDBbaACc eFgJiHdBaC +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+3.-B+2. 2747.42
fold-17-29-3 Build Rank 3 Fold 7 874.379 25.70 34.02 EefFGgjJiIHhDdbBAacC EfGjiHDbAc +B+0.-A+0.+B-1.-A-1.-B-2.+a+0.+B+1.-a+1.+B+3.-B+2. 2205.77
fold-17-28-3 Build Rank 3 Fold 7 874.379 25.70 34.02 EefFGgjJiIHhDdbBAacC EfGjiHDbAc +B+0.-A+0.+B-1.-A-1.-B-2.+a+0.+B+1.-a+1.+B+3.-B+2. 1886.78
```

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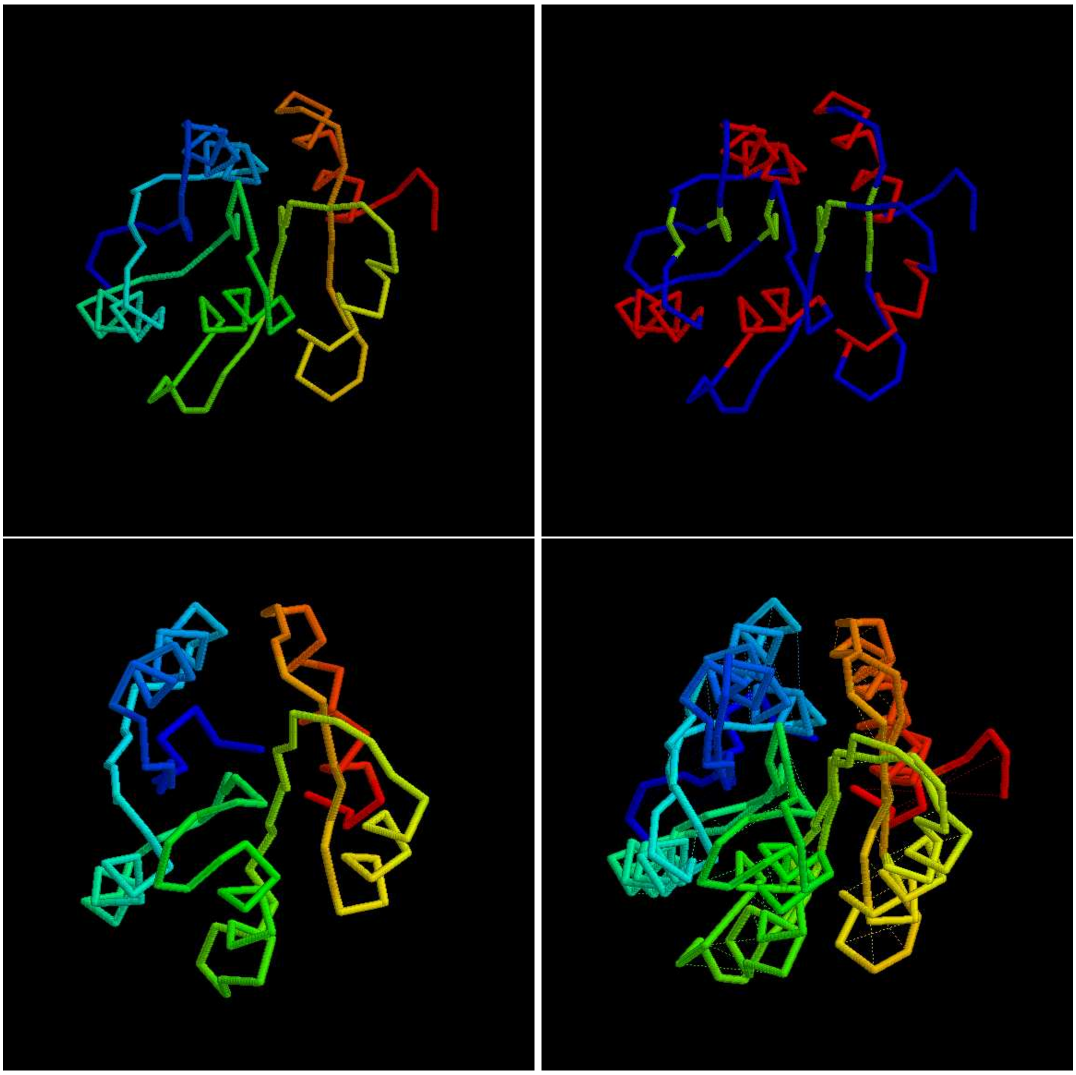
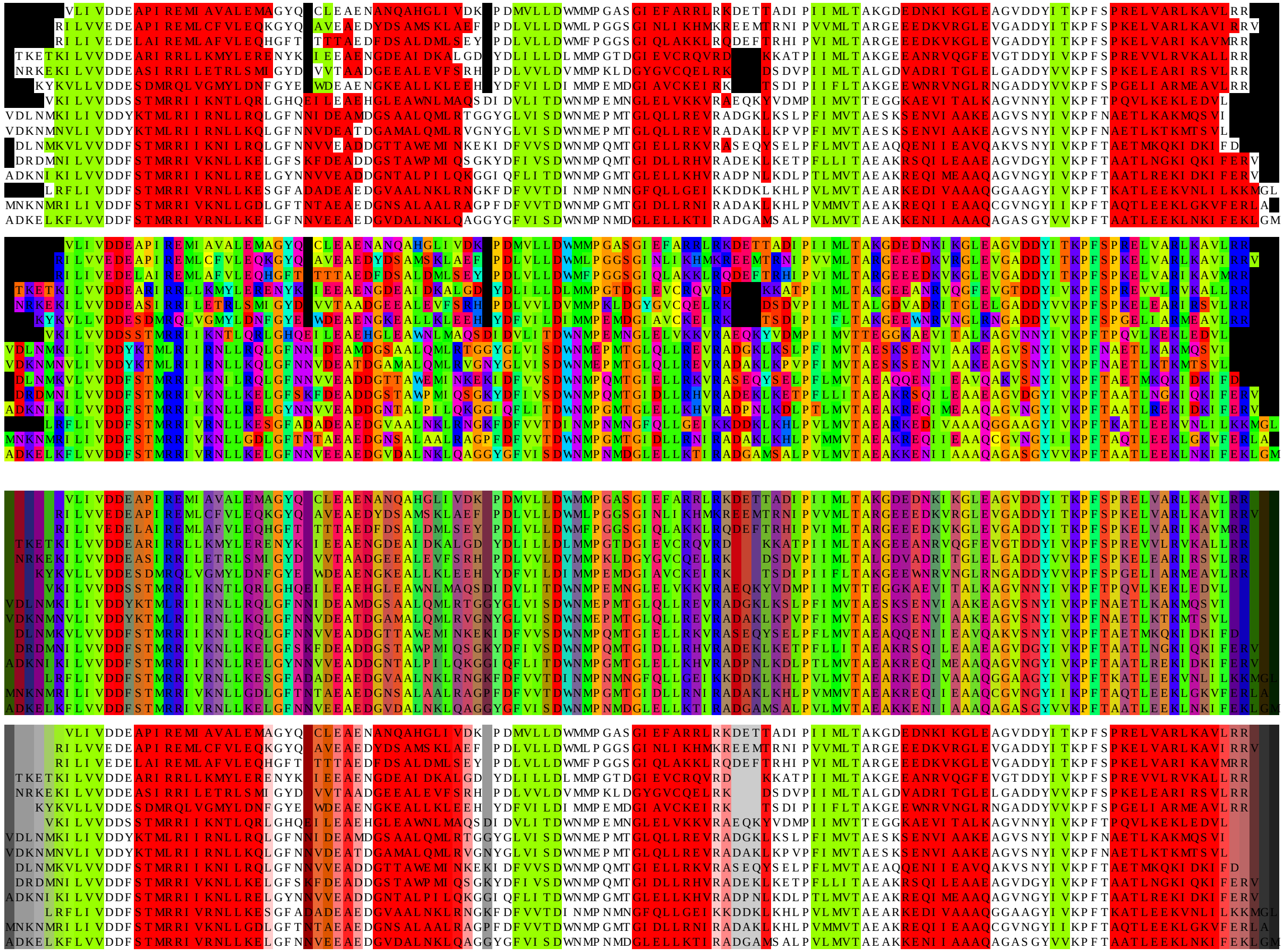
reranked best.list

fold-25-15-1 Build Rank 1 Fold 37 911.103 26.48 34.41 fFDdhHKkGgjJIieEBbcCAa fDhKGjIeBcA +B+0.-A+0.+B-1.-A-2.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+3. 2802.87
fold-25-14-1 Build Rank 1 Fold 37 911.103 26.48 34.41 fFDdhHKkGgjJIieEBbcCAa fDhKGjIeBcA +B+0.-A+0.+B-1.-A-2.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+3. 2226.68
fold-6-1-6 Build Rank 6 Fold 125 634.089 18.44 34.39 eEFfcCBbAadDgGHhIijJ eFcBAdgHIj +B+0.-A+0.+B-1.-A-1.-B-2.+a+0.+B+1.-a+1.-B+2.+A+1. 1793.28
fold-6-0-6 Build Rank 6 Fold 125 634.089 18.44 34.39 eEFfcCBbAadDgGHhIijJ eFcBAdgHIj +B+0.-A+0.+B-1.-A-1.-B-2.+a+0.+B+1.-a+1.-B+2.+A+1. 1780.15
fold-17-29-3 Build Rank 3 Fold 7 874.379 25.70 34.02 EefFGgjJiIHhDdbBAacC EfGjiHDbAc +B+0.-A+0.+B-1.-A-1.-B-2.+a+0.+B+1.-a+1.+B+3.-B+2. 2205.77
fold-17-28-3 Build Rank 3 Fold 7 874.379 25.70 34.02 EefFGgjJiIHhDdbBAacC EfGjiHDbAc +B+0.-A+0.+B-1.-A-1.-B-2.+a+0.+B+1.-a+1.+B+3.-B+2. 1886.78
fold-6-1-2 Build Rank 2 Fold 123 766.177 22.76 33.66 eEFfcCBbAadDgGHhiIJj eFcBAdgHiJ +B+0.-A+0.+B-1.-A-1.-B-2.+a+0.+B+1.-a+1.+B+2.-A+1. 1497.53
fold-25-21-1 Build Rank 1 Fold 73 774.002 23.07 33.55 fFEehHKkIijJGgdDCcbBAa fEhKIjGdCbA +B+0.-A+0.+B-1.-A-2.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+3. 3096.44
fold-25-20-1 Build Rank 1 Fold 73 774.002 23.07 33.55 fFEehHKkIijJGgdDCcbBAa fEhKIjGdCbA +B+0.-A+0.+B-1.-A-2.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+3. 2696.88
fold-6-5-3 Build Rank 3 Fold 13 782.472 23.75 32.95 EefFCcbBaADdGghHIijJ EfCbaDGhIj +B+0.-A+0.+B-1.-A-1.-B-2.+a+0.+B+1.-a+1.+B+2.-A+1. 2224.05
```

`3chyA (128) = +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1.`

**The chemotaxis Y protein (CheY)** has a compact flavodoxin-like fold that generally predicts well using just secondary structure prediction methods, or 3D prediction both with and without correlated mutation data.

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RILIVEDELAIREMLAFVLEQHGFT TTTAEDFDSALDMLSEY PDLVLLDWMFPGGSGIQLAKKLRQDEFTRHIPVIMLTARGEEEDKVKGLEVGADDYITKPFSPKELVARIKAVMRR
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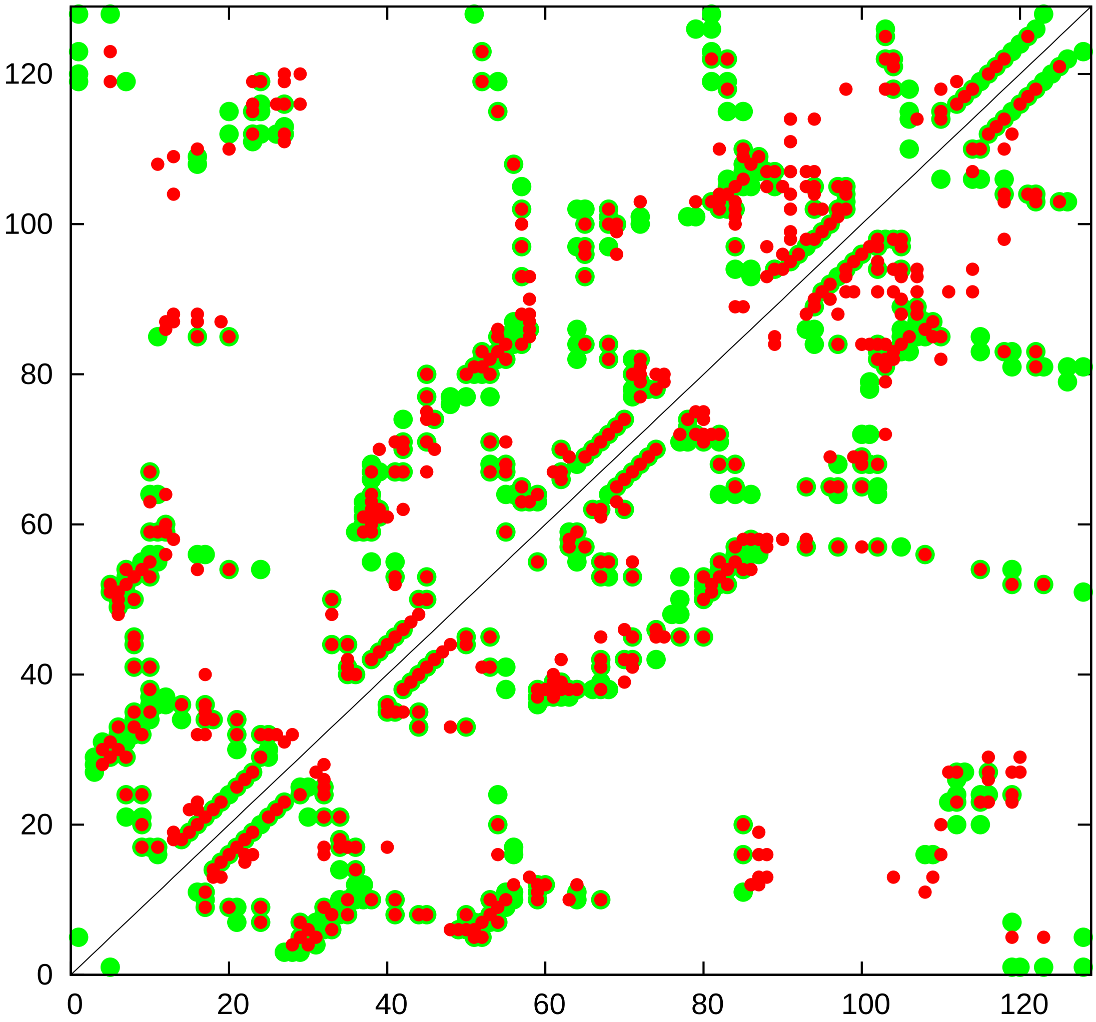
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100
120

full.list

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build3chyA/folds/fold-0-0-20:REMARK Build  Rank  20 Fold    577   975.228 24.56 39.71  CcdDAabBEefFIihHGgJj CdAbEfIhGJ +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+3.-A+1.+B+2.+a+2. 970.952
build3chyA/folds/fold-0-1-10:REMARK Build  Rank  10 Fold    581  1095.312 26.91 40.71  CcdDAabBEefFGgjJiIHh CdAbEfGjiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.-B+3.+A+1. 1092.49
build3chyA/folds/fold-0-1-20:REMARK Build  Rank  20 Fold    577   975.228 24.56 39.71  CcdDAabBEefFIihHGgJj CdAbEfIhGJ +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+3.-A+1.+B+2.+a+2. 971.398
build3chyA/folds/fold-0-1-30:REMARK Build  Rank  30 Fold   1154   911.670 22.04 41.37  cCbBAaFfeEDdgGHhiIjJ cbAFeDgHij +B+0.+A+0.-B-1.-A+1.+B+1.-a+0.+B+2.-a+1.+B+3.+A+2. 906.575
build3chyA/folds/fold-0-2-10:REMARK Build  Rank  10 Fold    125  1055.070 25.43 41.49  cCDdaABbeEFfgGHhIijJ cDaBeFgHIj +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1.-B+3.+A+2. 1052.73
build3chyA/folds/fold-0-2-20:REMARK Build  Rank  20 Fold    165   879.030 25.56 34.39  cCDdaAbBEehHGgjJIifF cDabEhGjIf +B+0.-A+0.+B-1.+a+0.-B+1.+A+1.-B+2.+A+2.-B+3.+a+1. 875.247
build3chyA/folds/fold-0-2-30:REMARK Build  Rank  30 Fold    139   773.146 21.36 36.19  cCDdaABbeEfFGghHIijJ cDaBefGhIj +B+0.-A+0.+B-1.-a+0.+B+1.+a+1.-B+2.+A+1.-B+3.+A+2. 768.566
build3chyA/folds/fold-0-3-10:REMARK Build  Rank  10 Fold    125  1055.070 25.43 41.49  cCDdaABbeEFfgGHhIijJ cDaBeFgHIj +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1.-B+3.+A+2. 1052.64
build3chyA/folds/fold-0-3-20:REMARK Build  Rank  20 Fold    165   879.030 25.56 34.39  cCDdaAbBEehHGgjJIifF cDabEhGjIf +B+0.-A+0.+B-1.+a+0.-B+1.+A+1.-B+2.+A+2.-B+3.+a+1. 875.359
```

best.list

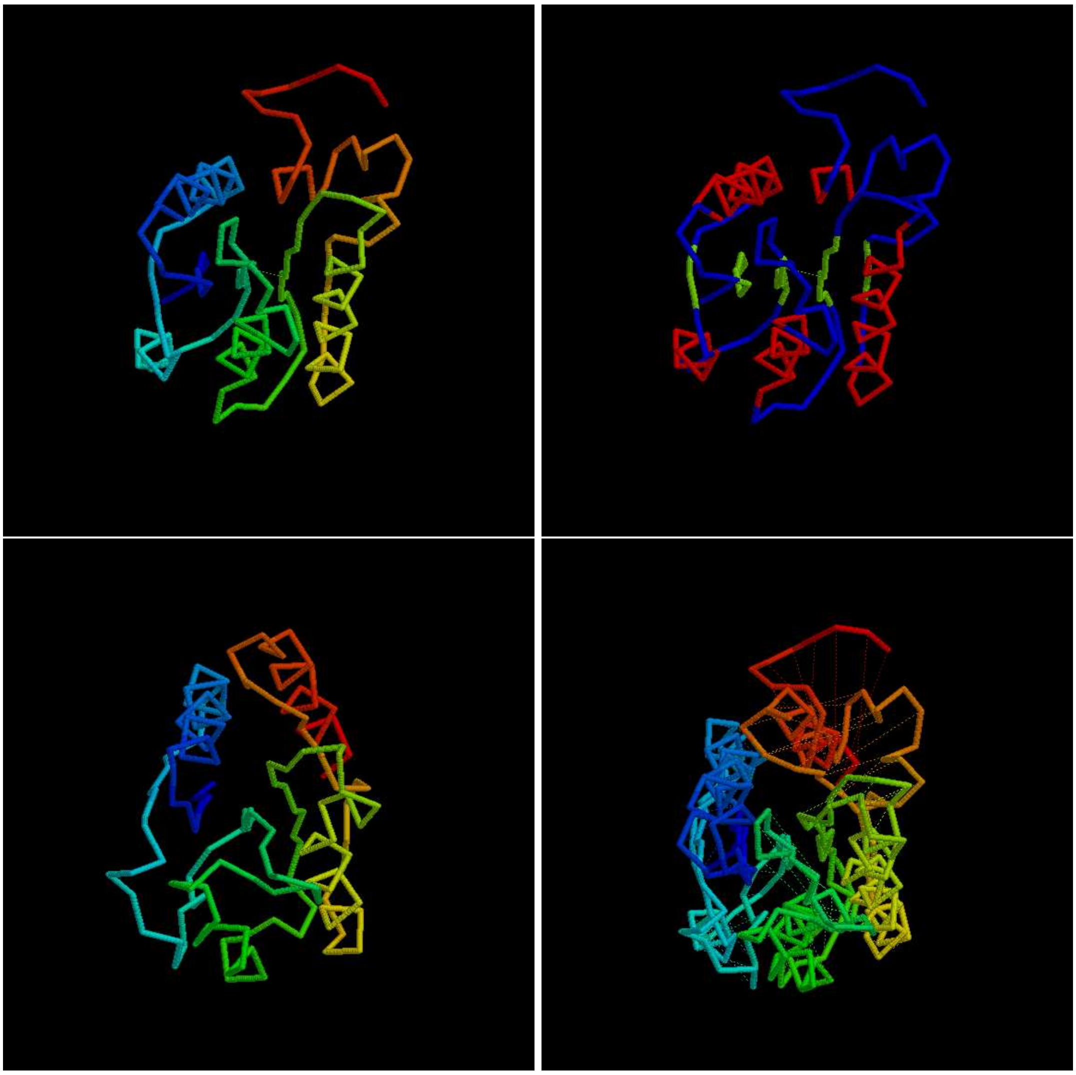
```
fold-0-2-1 Build Rank 1 Fold 87 1898.612 35.55 53.41 CcbBAadDEehHGgjJIifF CbAdEhGjIf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6171.8
fold-0-3-1 Build Rank 1 Fold 87 1898.612 35.55 53.41 CcbBAadDEehHGgjJIifF CbAdEhGjIf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6709.77
fold-0-4-1 Build Rank 1 Fold 791 1791.719 33.75 53.09 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 7400.66
fold-0-5-1 Build Rank 1 Fold 791 1791.719 33.75 53.09 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 8785.25
fold-0-4-2 Build Rank 2 Fold 1355 1791.443 33.75 53.07 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6464.43
fold-0-5-2 Build Rank 2 Fold 1355 1791.443 33.75 53.07 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 7208.71
fold-0-1-1 Build Rank 1 Fold 579 1736.851 33.38 52.03 CcdDAabBEefFGgjJIihH CdAbEfGjIh +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5966.08
fold-0-0-1 Build Rank 1 Fold 579 1736.851 33.38 52.03 CcdDAabBEefFGgjJIihH CdAbEfGjIh +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6243.38
fold-0-7-1 Build Rank 1 Fold 1222 1719.575 34.62 49.67 CcbBAadDEehHGgjJIifF CbAdEhGjIf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5499.18
fold-0-6-1 Build Rank 1 Fold 1222 1719.575 34.62 49.67 CcbBAadDEehHGgjJIifF CbAdEhGjIf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 4496.97
```

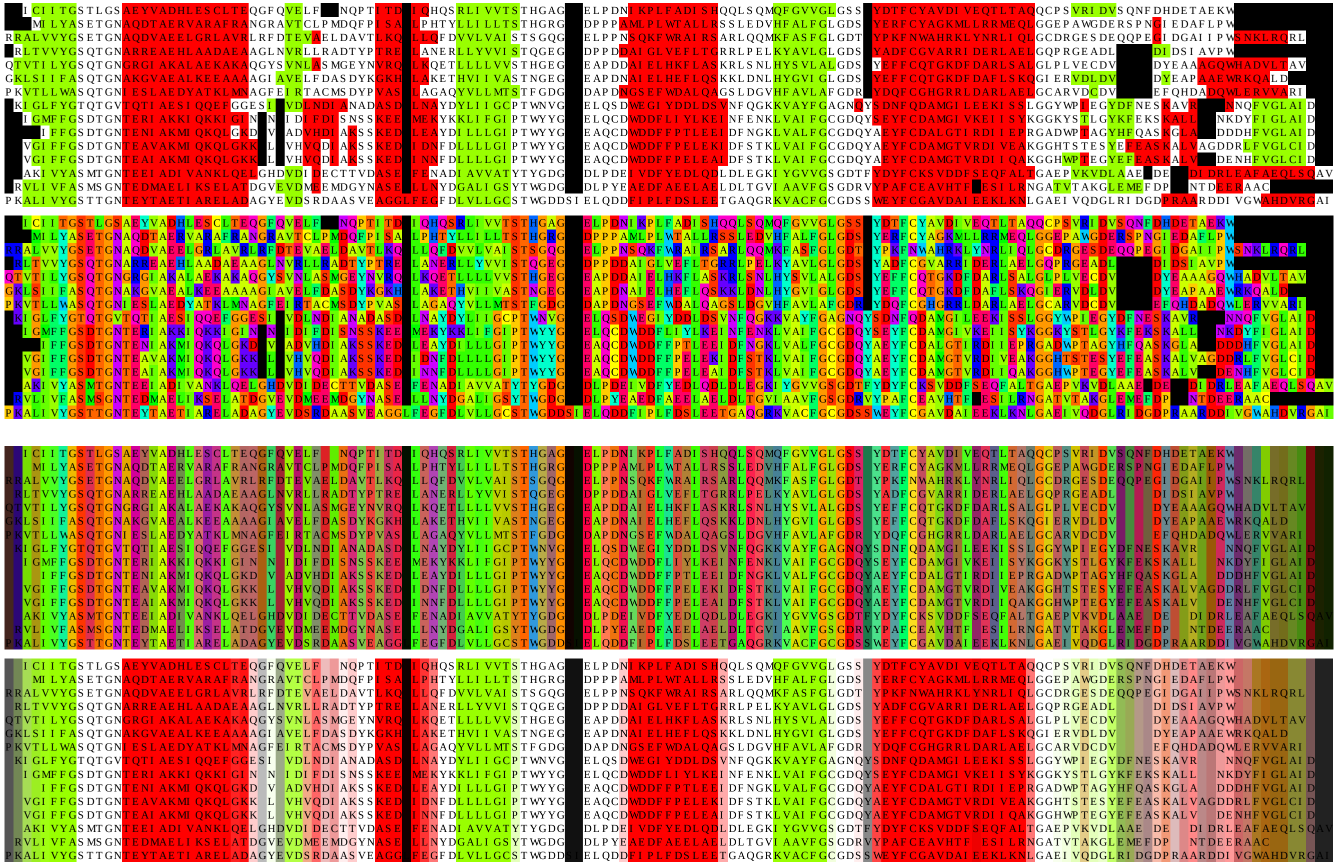
reranked best.list

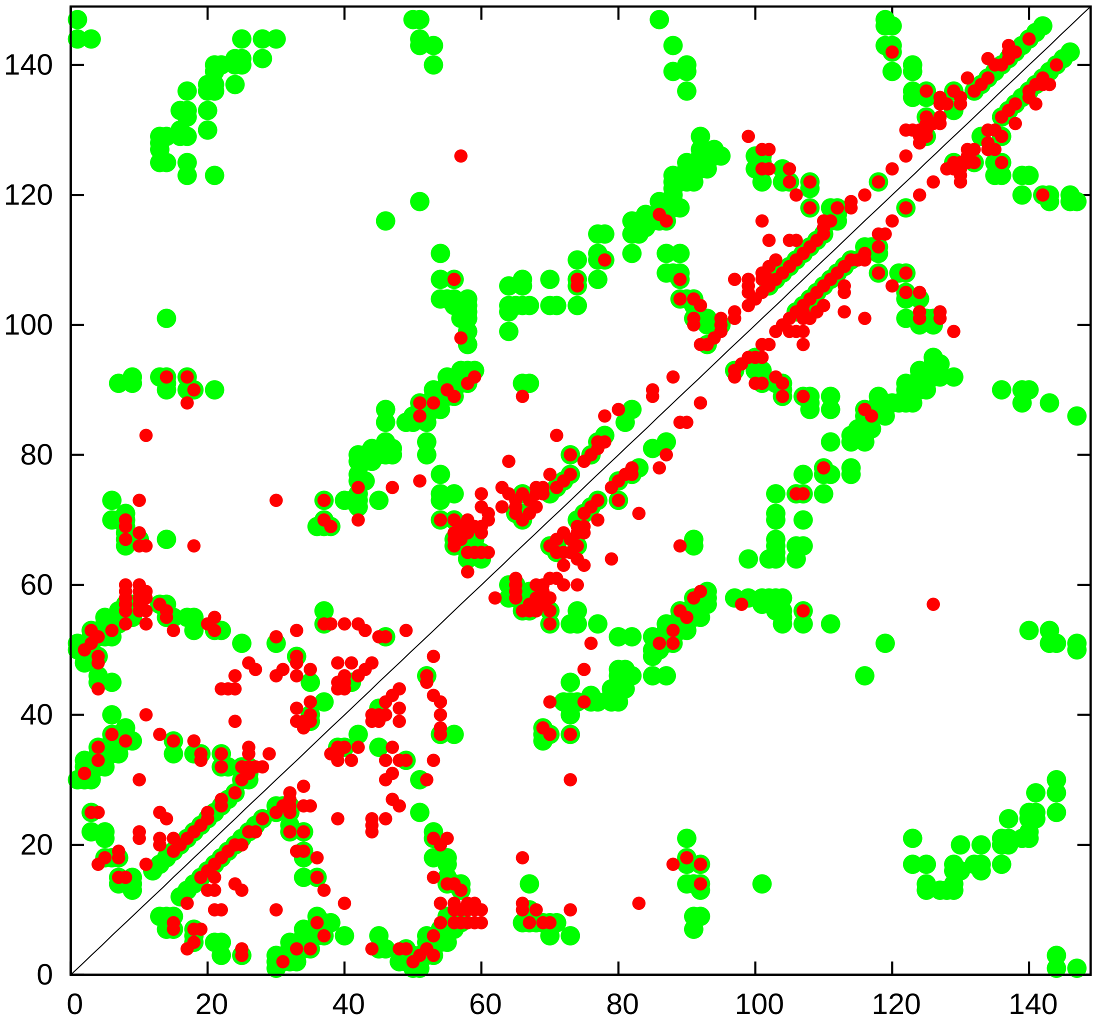
```
fold-1-1-1 Build Rank 1 Fold 1 1685.107 31.24 53.94 CcdDAabBEefFGgjJIihH CdAbEfGjIh +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6766.11
fold-1-0-1 Build Rank 1 Fold 1 1685.107 31.24 53.94 CcdDAabBEefFGgjJIihH CdAbEfGjIh +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5950.19
fold-1-5-1 Build Rank 1 Fold 762 1665.887 31.00 53.74 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5762.78
fold-1-4-1 Build Rank 1 Fold 762 1665.887 31.00 53.74 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6430.24
fold-1-5-2 Build Rank 2 Fold 1578 1665.129 31.00 53.71 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5486.65
fold-1-4-2 Build Rank 2 Fold 1578 1665.129 31.00 53.71 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6198.43
fold-0-3-1 Build Rank 1 Fold 87 1898.612 35.55 53.41 CcbBAadDEehHGgjJIifF CbAdEhGjIf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6709.77
fold-0-2-1 Build Rank 1 Fold 87 1898.612 35.55 53.41 CcbBAadDEehHGgjJIifF CbAdEhGjIf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6171.8
fold-2-1-1 Build Rank 1 Fold 1 1613.286 30.29 53.26 CcdDAabBEefFGgjJIihH CdAbEfGjIh +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5077.46
fold-2-0-1 Build Rank 1 Fold 1 1613.286 30.29 53.26 CcdDAabBEefFGgjJIihH CdAbEfGjIh +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6251.59
```

`1f4pA (148) +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1.`

**A classic (short-chain) flavodoxin**. Although this protein has the same basic fold as `3chyA`, the secondary structure elements are quite distinct both in size and packing and the two proteins are not even remotely homologous.






0
20
40
60
80
100
120
140
0
20
40
60
80
100
120
140

full.list

```
build1f4pA/folds/fold-0-0-10:REMARK Build  Rank  10 Fold     14   712.671 29.17 24.43  EegGfFCcbBAaDd EgfCbAD +B+0.-A+0.-B-1.+B+1.-a+0.+B+2.+A+1. 710.475
build1f4pA/folds/fold-0-0-20:REMARK Build  Rank  20 Fold    288   563.175 24.98 22.55  fFBbAaeEGgcCDd fBAeGcD +B+0.-A+0.-B+3.+B+1.-a+0.+B+2.-a+1. 558.715
build1f4pA/folds/fold-0-0-30:REMARK Build  Rank  30 Fold    395   487.963 33.13 14.73  AabBfFCcgGeEDd AbfCgeD +B+0.-A+0.-B+3.+B+1.-a+0.-B+2.+a-1. 483.098
build1f4pA/folds/fold-0-10-10:REMARK Build  Rank  10 Fold     32   600.118 26.41 22.73  CcgGFfDdeEAaBb CgFDeAB +B+0.-A+0.+B-2.+B-1.-a+0.+B+1.+a+1. 597.065
build1f4pA/folds/fold-0-10-20:REMARK Build  Rank  20 Fold    161   493.677 22.52 21.92  aABbcCDdgGFfEe aBcDgFE +B+0.-A+0.+B-1.-B-2.+a+0.-B-3.-A-1. 489.586
build1f4pA/folds/fold-0-10-30:REMARK Build  Rank  30 Fold     86   426.342 18.89 22.56  DdbBAaCcgGFfeE DbACgFe +B+0.-A+0.+B-2.+B-1.-a+0.+B+1.-A+1. 421.166
build1f4pA/folds/fold-0-1-10:REMARK Build  Rank  10 Fold     14   712.671 29.17 24.43  EegGfFCcbBAaDd EgfCbAD +B+0.-A+0.-B-1.+B+1.-a+0.+B+2.+A+1. 710.16
build1f4pA/folds/fold-0-11-10:REMARK Build  Rank  10 Fold     32   600.118 26.41 22.73  CcgGFfDdeEAaBb CgFDeAB +B+0.-A+0.+B-2.+B-1.-a+0.+B+1.+a+1. 596.998
build1f4pA/folds/fold-0-11-30:REMARK Build  Rank  30 Fold     86   426.342 18.89 22.56  DdbBAaCcgGFfeE DbACgFe +B+0.-A+0.+B-2.+B-1.-a+0.+B+1.-A+1. 421.295
build1f4pA/folds/fold-0-11-40:REMARK Build  Rank  40 Fold     46   389.974 30.82 12.65  cCBbAadDGgFfeE cBAdGFe +B+0.-A+0.-B+1.+B-1.-a+0.-B-2.+A-1. 384.323
```

best.list

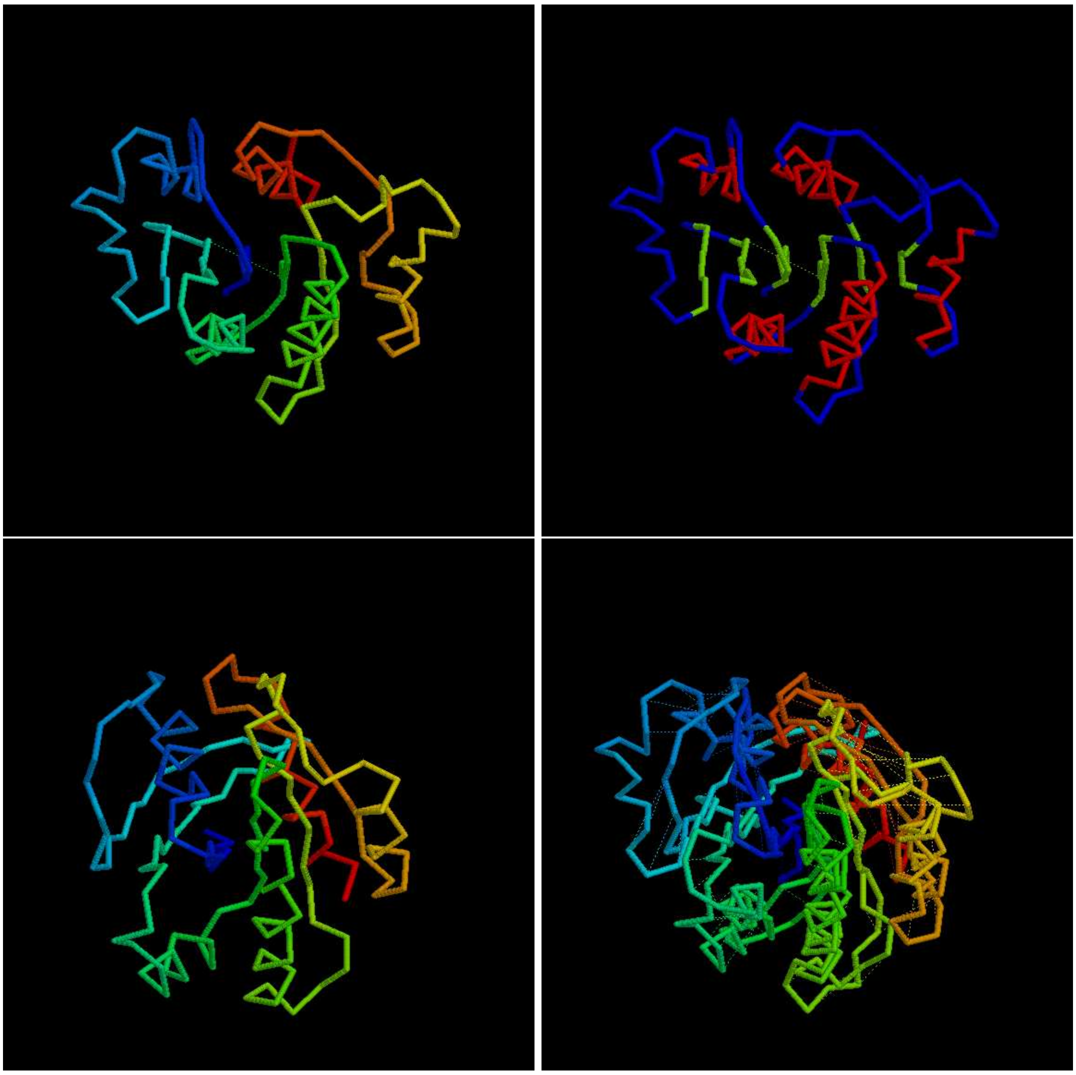
```
fold-18-4-1 Build Rank 1 Fold 1267 1548.307 34.86 44.42 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6617.08
fold-18-5-1 Build Rank 1 Fold 1267 1548.307 34.86 44.42 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5673.46
fold-18-5-2 Build Rank 2 Fold 728 1548.043 34.85 44.42 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5782.47
fold-18-4-2 Build Rank 2 Fold 728 1548.043 34.85 44.42 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6634.26
fold-31-2-1 Build Rank 1 Fold 3 1534.279 47.93 32.01 AadDCcfFEeBb AdCfEB +B+0.-A+0.+B-1.-A-1.+B-2.+a+0. 5613.95
fold-18-0-1 Build Rank 1 Fold 918 1505.223 36.04 41.77 CcdDAabBEefFGgjJIihH CdAbEfGjIh +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5442.44
fold-18-1-1 Build Rank 1 Fold 918 1505.223 36.04 41.77 CcdDAabBEefFGgjJIihH CdAbEfGjIh +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6637.49
fold-17-4-1 Build Rank 1 Fold 2168 1436.239 35.61 40.34 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5062.74
fold-17-5-1 Build Rank 1 Fold 2168 1436.239 35.61 40.34 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 8742.33
fold-18-3-1 Build Rank 1 Fold 5 1433.421 35.53 40.35 CcbBAadDEehHGgfFiIJj CbAdEhGfiJ +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1.-B+3.+a+2. 4040.74
```

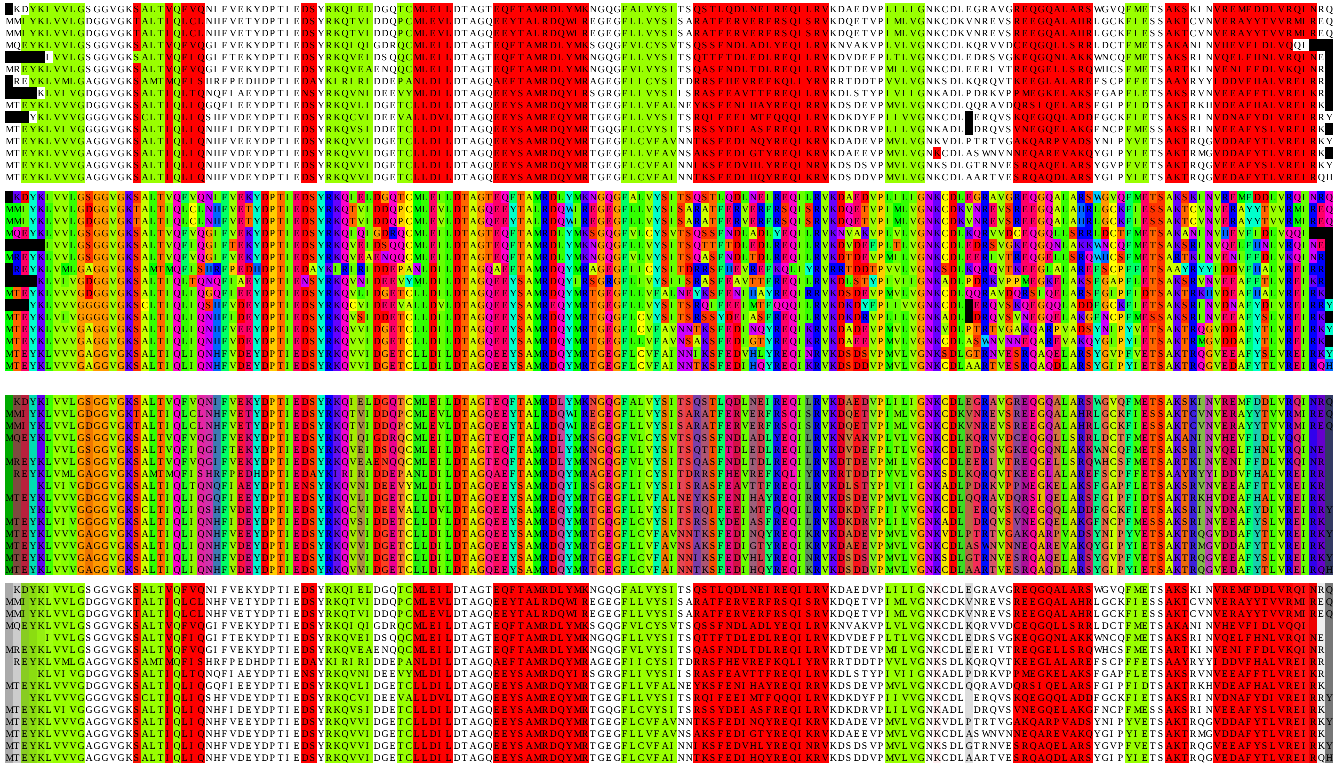
reranked best.list

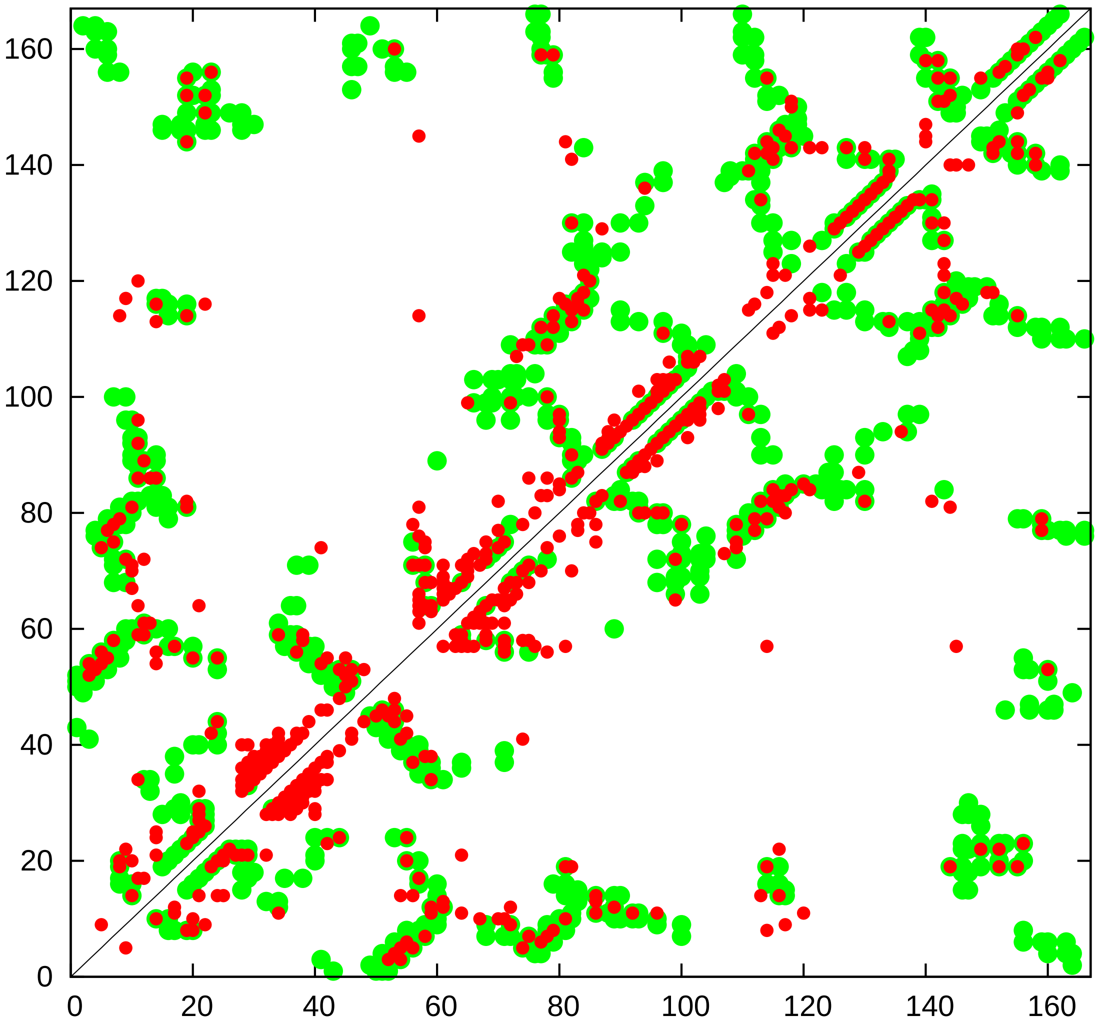
```
fold-18-5-4 Build Rank 4 Fold 729 1410.655 31.76 44.42 cCDdaABbeEFfgGJjiIhH cDaBeFgJih +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 7690.11
fold-18-5-3 Build Rank 3 Fold 1268 1410.884 31.76 44.42 GghHIijJEefFCcbBAaDd GhIjEfCbAD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 7416.02
fold-18-5-2 Build Rank 2 Fold 728 1548.043 34.85 44.42 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5782.47
fold-18-5-1 Build Rank 1 Fold 1267 1548.307 34.86 44.42 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 5673.46
fold-18-4-4 Build Rank 4 Fold 729 1410.655 31.76 44.42 cCDdaABbeEFfgGJjiIhH cDaBeFgJih +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 7590.84
fold-18-4-3 Build Rank 3 Fold 1268 1410.884 31.76 44.42 GghHIijJEefFCcbBAaDd GhIjEfCbAD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 8050.22
fold-18-4-2 Build Rank 2 Fold 728 1548.043 34.85 44.42 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6634.26
fold-18-4-1 Build Rank 1 Fold 1267 1548.307 34.86 44.42 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 6617.08
fold-18-5-5 Build Rank 5 Fold 725 1399.178 33.07 42.31 cCDdaABbeEFfgGHhIijJ cDaBeFgHIj +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1.-B+3.+a+2. 3951.84
fold-18-4-5 Build Rank 5 Fold 725 1399.178 33.07 42.31 cCDdaABbeEFfgGHhIijJ cDaBeFgHIj +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1.-B+3.+a+2. 3272.52
```

`5p21A (166) +B+0.-A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1.`

**The Ras p21 G-protein** which, although Rossmann-like, has a unusual embellishment of the edge of the domain comprising a parallel $\alpha\beta$ connection leading into a long $\beta$-hairpin.






0
20
40
60
80
100
120
140
160
0
20
40
60
80
100
120
140
160

full.list

```
build5p21A/folds/fold-0-0-10:REMARK Build  Rank  10 Fold   1654  1155.908 27.48 42.06  GgiIjJKkhHEefFCcDdaAbB GijKhEfCDab +B+0.-B-1.-B-2.+A+0.-A+1.+B+1.-a+0.+B+2.+A+2.-B+3.-a+1. 1152.89
build5p21A/folds/fold-0-0-20:REMARK Build  Rank  20 Fold   1451   986.253 27.59 35.75  GgeEAaDdhHIikKJjfFCcbB GeADhIkJfCb +B+0.-B+1.+B+3.+A+0.-A-1.+B-1.-A-2.+B-2.-a+0.+B+2.-a+1. 982.181
build5p21A/folds/fold-0-0-30:REMARK Build  Rank  30 Fold     74   920.888 26.32 34.99  EegGJjFfbBAadDCchHIikK EgJFbAdChIk +B+0.-B+1.+B+3.+A+0.-A-1.+B-2.-a+0.+B-1.-a+1.+B+2.-a+2. 915.411
build5p21A/folds/fold-0-10-10:REMARK Build  Rank  10 Fold     78   841.459 25.56 32.92  EeaAcCDdgGHhkKJjiIFfbB EacDgHkJiFb +B+0.-B+2.-B+1.+A+0.-A-1.+B-2.-A-2.+B-3.-a+0.+B-1.-a+1. 839.062
build5p21A/folds/fold-0-10-50:REMARK Build  Rank  50 Fold    482   610.515 18.57 32.88  cCaAEedDGgJjiIHhkKfFBb caEdGJiHkfB +B+0.+B-1.-B+1.+A+0.-A+1.-B+4.+a+0.-B+3.+A+2.+B+2.-a-1. 603.613
build5p21A/folds/fold-0-1-10:REMARK Build  Rank  10 Fold   1654  1155.908 27.48 42.06  GgiIjJKkhHEefFCcDdaAbB GijKhEfCDab +B+0.-B-1.-B-2.+A+0.-A+1.+B+1.-a+0.+B+2.+A+2.-B+3.-a+1. 1152.91
build5p21A/folds/fold-0-11-10:REMARK Build  Rank  10 Fold     78   841.459 25.56 32.92  EeaAcCDdgGHhkKJjiIFfbB EacDgHkJiFb +B+0.-B+2.-B+1.+A+0.-A-1.+B-2.-A-2.+B-3.-a+0.+B-1.-a+1. 839.089
build5p21A/folds/fold-0-1-20:REMARK Build  Rank  20 Fold   1451   986.253 27.59 35.75  GgeEAaDdhHIikKJjfFCcbB GeADhIkJfCb +B+0.-B+1.+B+3.+A+0.-A-1.+B-1.-A-2.+B-2.-a+0.+B+2.-a+1. 981.822
build5p21A/folds/fold-0-1-30:REMARK Build  Rank  30 Fold     74   920.888 26.32 34.99  EegGJjFfbBAadDCchHIikK EgJFbAdChIk +B+0.-B+1.+B+3.+A+0.-A-1.+B-2.-a+0.+B-1.-a+1.+B+2.-a+2. 915.553
build5p21A/folds/fold-0-16-10:REMARK Build  Rank  10 Fold    697  1024.487 30.85 33.21  DdbBAaCcgGHheEFfkKJjIi DbACgHeFkJI +B+0.-B+1.+B+2.+A+0.-A-1.+B-2.-a+0.+B-1.-A-2.+B-3.+a-1. 1022.28
```

best.list

```
fold-7-21-1 Build Rank 1 Fold 458 2263.359 36.63 61.80 dDcCAabBEefFIihHKkjJGg dcAbEfIhKjG +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 12685.7
fold-7-20-1 Build Rank 1 Fold 458 2263.359 36.63 61.80 dDcCAabBEefFIihHKkjJGg dcAbEfIhKjG +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 11983.8
fold-6-20-1 Build Rank 1 Fold 383 2263.174 37.32 60.64 dDcCAabBEefFIihHKkjJGg dcAbEfIhKjG +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 12968.8
fold-6-21-1 Build Rank 1 Fold 383 2263.174 37.32 60.64 dDcCAabBEefFIihHKkjJGg dcAbEfIhKjG +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 14091.6
fold-0-21-1 Build Rank 1 Fold 27 2082.695 38.44 54.19 dDBbAacCGgfFEehHIijJKk dBAcGfEhIjK +B+0.-B-1.-B-2.+A+0.-A+1.+B+1.-a+0.+B+2.-a+1.+B+3.-a+2. 4054.46
fold-6-4-1 Build Rank 1 Fold 120 2073.412 33.83 61.29 dDeEAabBCcfFGghHKkjJIi deAbCfGhKjI +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 11628
fold-6-5-1 Build Rank 1 Fold 120 2073.412 33.83 61.29 dDeEAabBCcfFGghHKkjJIi deAbCfGhKjI +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 11140.5
fold-7-21-2 Build Rank 2 Fold 457 2060.518 33.57 61.38 dDcCAabBEefFIihHKkjJgG dcAbEfIhKjg +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 6825.96
fold-7-20-2 Build Rank 2 Fold 457 2060.518 33.57 61.38 dDcCAabBEefFIihHKkjJgG dcAbEfIhKjg +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 7224.33
fold-6-20-2 Build Rank 2 Fold 382 2058.172 34.18 60.22 dDcCAabBEefFIihHKkjJgG dcAbEfIhKjg +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 9163.06
```

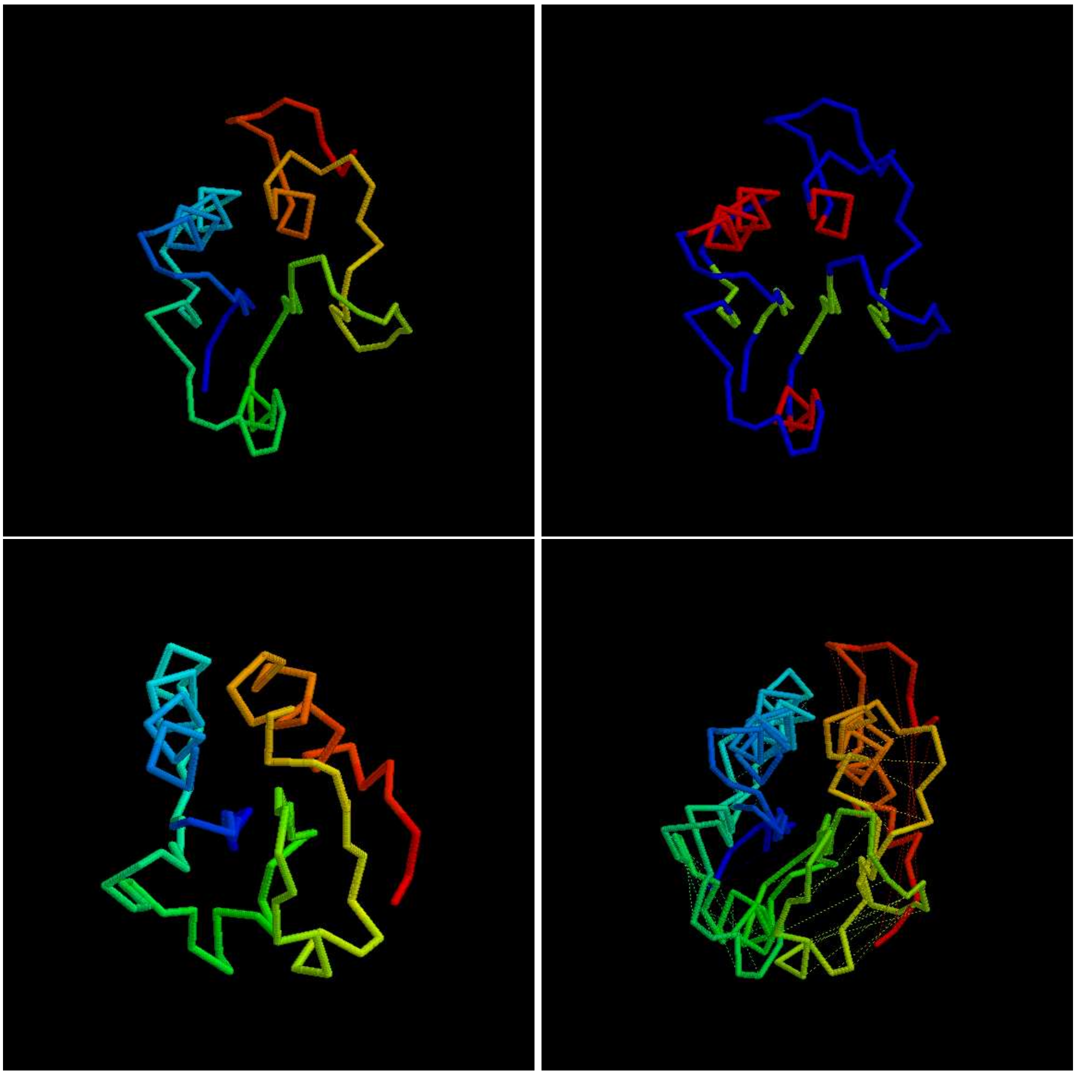
reranked best.list

```
fold-7-21-1 Build Rank 1 Fold 458 2263.359 36.63 61.80 dDcCAabBEefFIihHKkjJGg dcAbEfIhKjG +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 12685.7
fold-7-20-1 Build Rank 1 Fold 458 2263.359 36.63 61.80 dDcCAabBEefFIihHKkjJGg dcAbEfIhKjG +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 11983.8
fold-7-5-1 Build Rank 1 Fold 120 2042.016 33.26 61.40 dDeEAabBCcfFGghHKkjJIi deAbCfGhKjI +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 8534.68
fold-7-4-1 Build Rank 1 Fold 120 2042.016 33.26 61.40 dDeEAabBCcfFGghHKkjJIi deAbCfGhKjI +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 8963.33
fold-7-21-2 Build Rank 2 Fold 457 2060.518 33.57 61.38 dDcCAabBEefFIihHKkjJgG dcAbEfIhKjg +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 6825.96
fold-7-20-2 Build Rank 2 Fold 457 2060.518 33.57 61.38 dDcCAabBEefFIihHKkjJgG dcAbEfIhKjg +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 7224.33
fold-6-5-1 Build Rank 1 Fold 120 2073.412 33.83 61.29 dDeEAabBCcfFGghHKkjJIi deAbCfGhKjI +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 11140.5
fold-6-4-1 Build Rank 1 Fold 120 2073.412 33.83 61.29 dDeEAabBCcfFGghHKkjJIi deAbCfGhKjI +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 11628
fold-8-21-1 Build Rank 1 Fold 383 1965.641 32.19 61.06 dDcCAabBEefFIihHKkjJGg dcAbEfIhKjG +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 8938.13
fold-8-20-1 Build Rank 1 Fold 383 1965.641 32.19 61.06 dDcCAabBEefFIihHKkjJGg dcAbEfIhKjG +B+0.+A+0.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 9524.64
```

## 1.2 Target test set

`2r4qA (102) = +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1`

**A domain of fruA from Bacillus subtilis**. The top scoring folds under all ranking schemes had the correct $\beta$-sheet topology for this protein but under the combined packing/contact score, the terminal helix was flipped. Re-ranking the best list by just the contact score brought the correct fold at the top.



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 KIVAITSCIAGHTPMAAKALEQAASKMGHEIKVEQQGAMGRVNTITKEEAQDADFILIASDQTIGMERFDGKKVIKVKIGIALKKPEAVLTKCIE
  IVCVAACTAGHTYIAREKLIKGAKALGHTIKVETQGTIGTENELQAADISAADVVILAVDVKIGEERFTNKRIVRVKTEIVIKSPVQFLEKV
 KIVGVAACTVGHTYIAQEKLENASKAAGHDVKIETQGTIGIENQLTSEEIAAADIVLLAVDVKIGEERFEGKKVVKVPTEVAIKSPNKLIAKLVE
  IIGIAACTSGHTYIAKEKLTKAGTALGHNVHIETQGTIGIEDELSAEQVKNADVVIIAADIKIGKDRFKGKRVVEIPTDLAIKAPKQIINKIDKE
 KIIAVTACPSGHTYMAAEALESAAKAKGWDVKVETQGSIGLENELTAEDVASADMVILTKDIGIFEERFAGKTIVRVNISDAVKRADAIMNKI
 KVVAITACPTGHTYMAAEKLESTGRRLGHDVKVETQGAIGIENELSSRDIQAADVVLLAVDIAIGEERFEDKRVVRVPIQNVLKDANAVFA
 KLVAVTACVSGHTYMVAERLDKLCLQLKWQLKVETQGALGVEYSLTEDDILQADAVILINDVAIEQERFQNCRCVQADIQTFLCHPEKILA
  LVAVTACVSGHTYMAAERLEKLCQQEKWSIKIETQGALGTENRLTEEDIRRADVVLLITDIELGVERFTRSRYVQSGISAFLREPQRVMS
 KIVAVTACPTGHTYMAADVLKKAAAKLGVSIKVETQGAMGVENVLTPVDIVSADLVIIASDIEIDKNRFLGINSKQFPIETILTDVEGILKKHL
 RIVAVTACPTGHTYMAADALNKTAPKFNVSIKVETQGAMGIENLLTAQDITLADKVLIVSDIDIQPSRFDPAKTVFIPMEEVLLSVDKVFIKH
 KIVAVTACPTGHTYMAADALMKAAPKHNVQIKVETQGAMGIENQLTPHDIAQADRVLIVSDIEIQPGRFEGTRQIQIPIEEVLLNVDKVF
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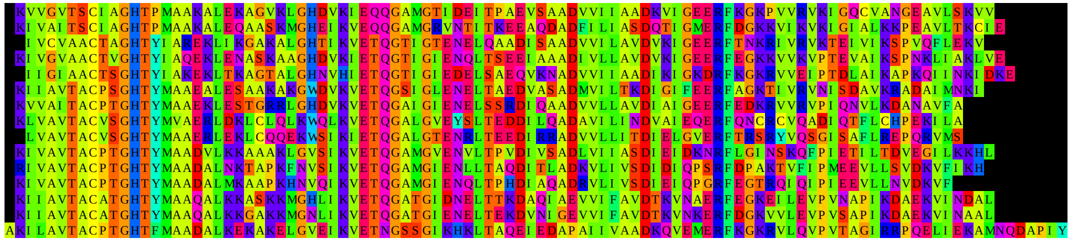
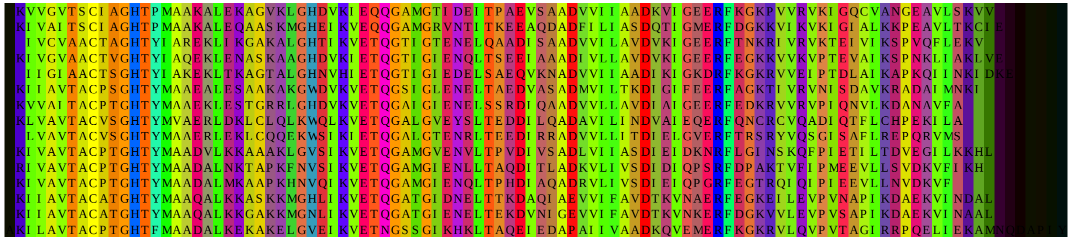
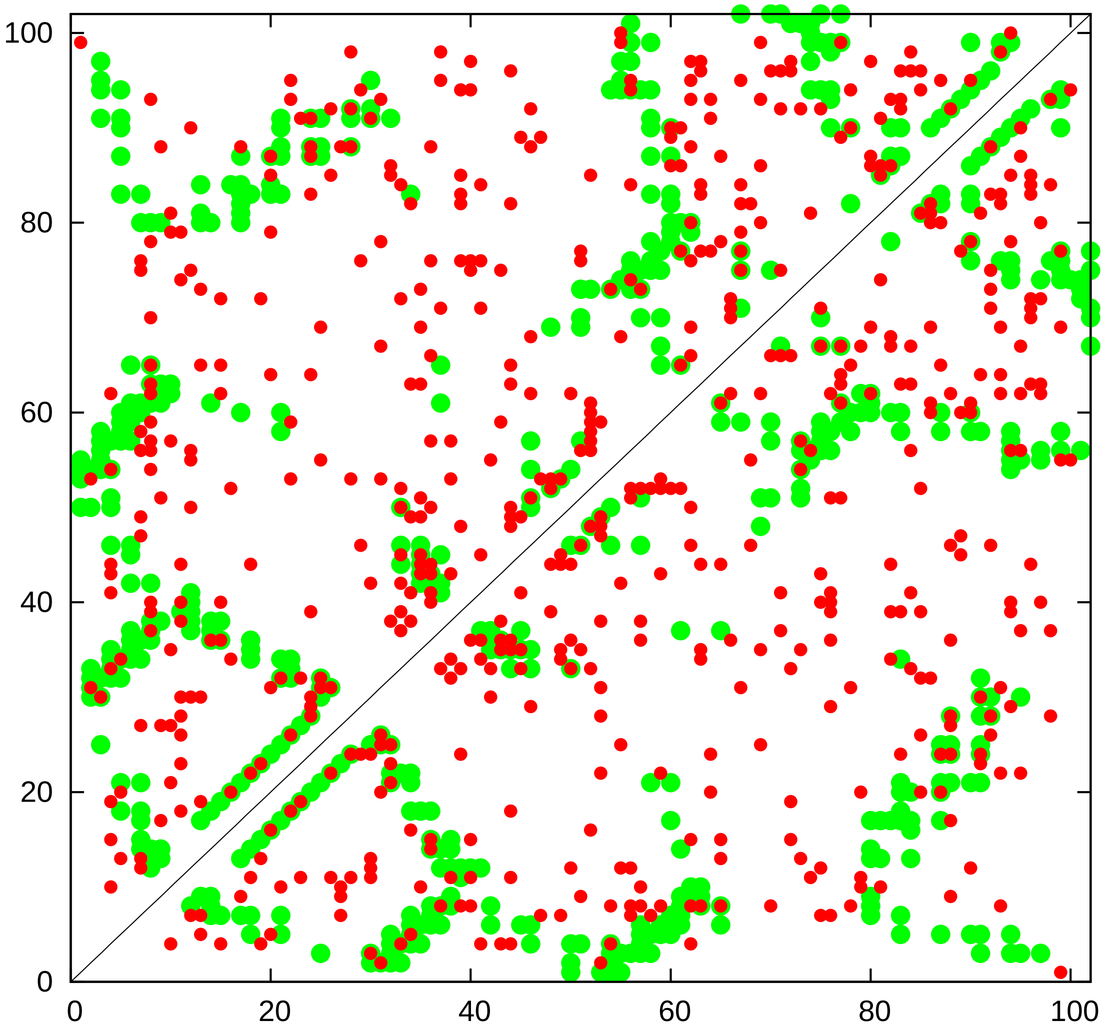





0
20
40
60
80
100
0
20
40
60
80
100

```
wtaylor@mull1:~/fewpred/pred2r4qA$ head folds.sort

build2r4qA/folds/fold-4-0-1:REMARK Build  Rank   1 Fold    181  1217.459 55.23 22.05  cCDdaABbeEFfgG cDaBeFg +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 1216.68
build2r4qA/folds/fold-4-1-1:REMARK Build  Rank   1 Fold    181  1217.459 55.23 22.05  cCDdaABbeEFfgG cDaBeFg +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 1216.57
build2r4qA/folds/fold-3-1-1:REMARK Build  Rank   1 Fold    181  1157.376 54.60 21.20  cCDdaABbeEFfgG cDaBeFg +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 1157.3
build2r4qA/folds/fold-3-0-1:REMARK Build  Rank   1 Fold    181  1157.376 54.60 21.20  cCDdaABbeEFfgG cDaBeFg +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 1156.42
build2r4qA/folds/fold-2-1-1:REMARK Build  Rank   1 Fold    114  1157.226 46.40 24.94  cCDdaABbeEfFGg cDaBefG +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 1156.28
build2r4qA/folds/fold-2-0-1:REMARK Build  Rank   1 Fold    114  1157.226 46.40 24.94  cCDdaABbeEfFGg cDaBefG +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 1156.27
build2r4qA/folds/fold-3-1-2:REMARK Build  Rank   2 Fold    183  1146.891 47.02 24.39  cCDdaABbeEfFGg cDaBefG +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 1146.2
build2r4qA/folds/fold-3-0-2:REMARK Build  Rank   2 Fold    183  1146.891 47.02 24.39  cCDdaABbeEfFGg cDaBefG +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 1145.83
build2r4qA/folds/fold-9-1-1:REMARK Build  Rank   1 Fold    183  1144.679 52.66 21.74  EegGFfbBCcaADd EgFbCaD +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 1144.55
build2r4qA/folds/fold-9-0-1:REMARK Build  Rank   1 Fold    183  1144.679 52.66 21.74  EegGFfbBCcaADd EgFbCaD +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 1143.95
```

```
wtaylor@mull1:~/fewpred/pred2r4qA$ head folds.best

fold-4-0-1 Build Rank 1 Fold 181 1217.459 55.23 22.05 cCDdaABbeEFfgG cDaBeFg +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 4205.81
fold-4-1-1 Build Rank 1 Fold 181 1217.459 55.23 22.05 cCDdaABbeEFfgG cDaBeFg +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 4375.06
fold-3-1-1 Build Rank 1 Fold 181 1157.376 54.60 21.20 cCDdaABbeEFfgG cDaBeFg +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 4007.3
fold-3-0-1 Build Rank 1 Fold 181 1157.376 54.60 21.20 cCDdaABbeEFfgG cDaBeFg +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 3439.09
fold-2-1-1 Build Rank 1 Fold 114 1157.226 46.40 24.94 cCDdaABbeEfFGg cDaBefG +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 2478.88
fold-2-0-1 Build Rank 1 Fold 114 1157.226 46.40 24.94 cCDdaABbeEfFGg cDaBefG +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 4751.84
fold-3-1-2 Build Rank 2 Fold 183 1146.891 47.02 24.39 cCDdaABbeEfFGg cDaBefG +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 2318.53
fold-3-0-2 Build Rank 2 Fold 183 1146.891 47.02 24.39 cCDdaABbeEfFGg cDaBefG +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 3824.3
fold-9-1-1 Build Rank 1 Fold 183 1144.679 52.66 21.74 EegGFfbBCcaADd EgFbCaD +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 4754.6
fold-9-0-1 Build Rank 1 Fold 183 1144.679 52.66 21.74 EegGFfbBCcaADd EgFbCaD +B+0.-A+0.+B-1.-a+0.+B+1.-B+2.+A+1. 2955.84
```

```
wtaylor@mull1:~/fewpred/pred2r4qA$ sort -nr -k9 folds.best | head

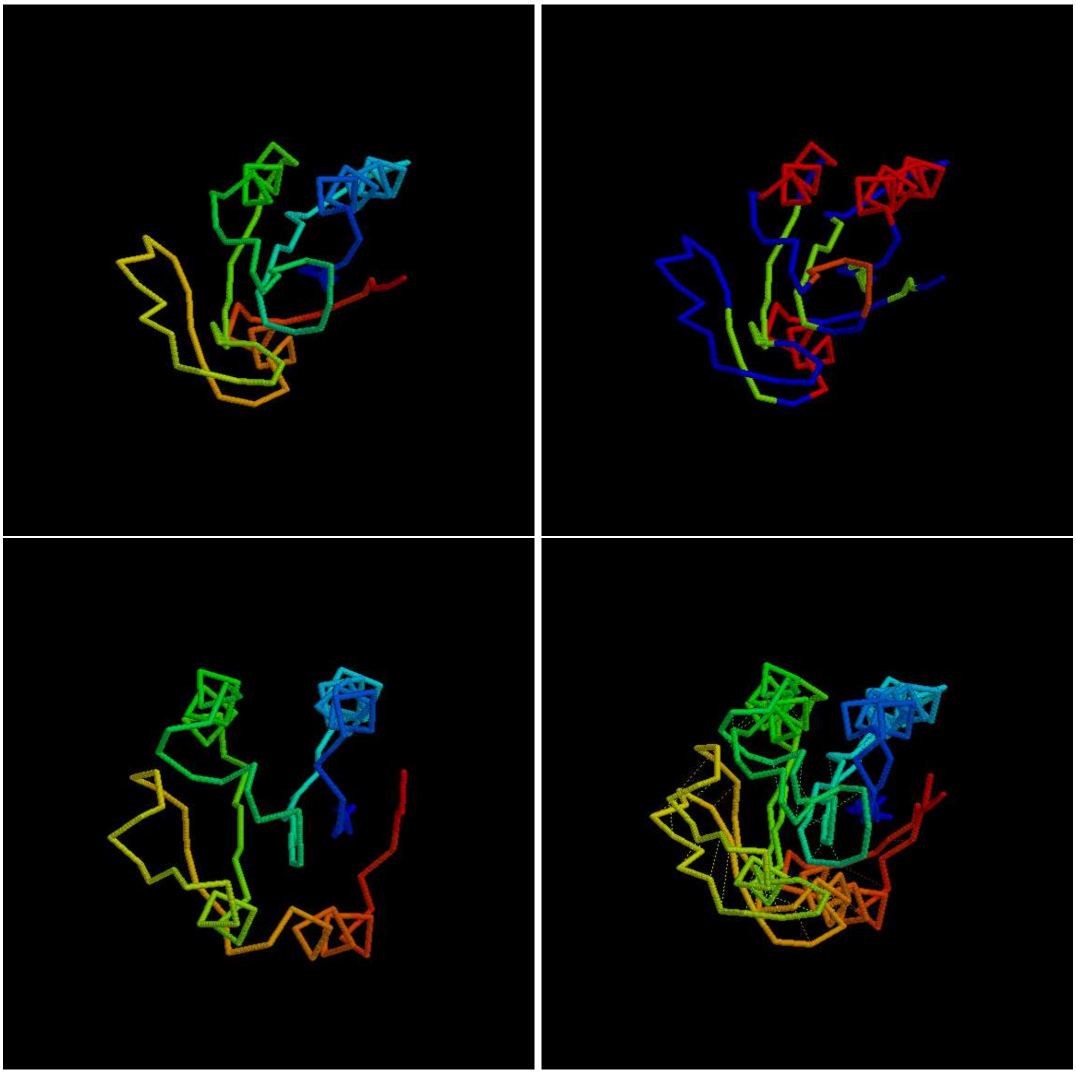
fold-2-9-1 Build Rank 1 Fold 177 1047.627 39.16 26.76 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 4423.34
fold-2-8-1 Build Rank 1 Fold 177 1047.627 39.16 26.76 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 4831.22
fold-3-9-1 Build Rank 1 Fold 44 1046.772 39.65 26.40 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 4811.99
fold-3-8-1 Build Rank 1 Fold 44 1046.772 39.65 26.40 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 4505.79
fold-8-9-4 Build Rank 4 Fold 177 932.545 35.42 26.33 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 4304.11
fold-8-8-4 Build Rank 4 Fold 177 932.545 35.42 26.33 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 3622.81
fold-1-9-1 Build Rank 1 Fold 44 1010.522 38.50 26.25 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 4537.93
fold-1-8-1 Build Rank 1 Fold 44 1010.522 38.50 26.25 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 3638.6
fold-4-9-3 Build Rank 3 Fold 44 1006.216 40.02 25.14 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 5014.47
fold-4-8-3 Build Rank 3 Fold 44 1006.216 40.02 25.14 DdgGFfeEBbAacC DgFeBAc +B+0.-A+0.+B-1.-a+0.+B+1.+B+2.-A+1. 4397.92
```

`3a2eA (108) = +B+0.-A+0.+B+4.-B+3.+A-1.-B+1.+B+2`

**Ginkbilobin-2, an antifungal protein from Ginkgo biloba.** The PLATO server made many models with the correct 0-4-2 architecture for this protein but the native protein contains a left-handed $\beta\alpha\beta$ connection combined with a pair of crossing loops, both of which are filtered-out by PLATO.

`1l1sA (111) = +B+0.-A+0.+B-1.-A-1.+B-2.+B-3.-a+0.+B+1`

**A protein of Unknown Function MTH1491 from Methanobacterium thermoautotrophicum**. Ranked on the combined score, the top models were based on a small Form with 1-3-2 architecture and despite having the correct overall fold, the edge strands and some helices were poorly constrained. The reranked best list however had a model with the more complete 1-5-2 Form in top position with the correct fold.



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  KVVVQIKDFDKVPQAL  RSVINLYNDIKDAEIEVVLHQSAIKAL KDSDTRSIIEDLIKKNILIVGCENSIRSQNLSHDQLIPGIKIVTSGVGEIVRKQSEGWIYL
  KIIVHIDEMAKWPMVLNNLNHLAQAYPAPNNQIELLVNGDAVMGV   KEAEKIRHALTSQIVIAV CQNSLTQRKITTEDLLNNSTIVASGVVELVEKQALGYHYLRP
  KLVFHINEPDKWQRVIMNINNFLNDVGQGNADIEVVANGEAVSAFQTNKMLIEQMQKLAEIGVNFVACQNALKAQSIAKESLPEFVTVVPAGITEIARKQTEGFAYIKP
QDKVAYHVNEAQTQALATL RNIRNHLDTDPSAQITVVTHANGVDFLPNGGEYAATVSALVSRGVKFEICEITLKNRNLKKEQFIQEATFTPSGVVRLTKMQLQGYAYIKP
    MYHLTEGIEEAVRAM RNVRNHLDADPTAKIVVVANGAGIDFLKNGNPFDAIVQDLVTRHVEFRACRNTLTTRNIDPSKLLPEATLVQSGVAEAARLQAEGFAYLRP
 YKVVYQISEGTEQAVRAI GNLRNHLNGAPGTRIVVVALGRGIDFLDKGRSFDAPVAALASMGVEFRVCHNSLAAFKVPEDKLLLEAKVVPAGVVEITRLQQEGFAYLKP
  KVVYQLSEGIDQAVRAM GNLRNHLNGAPGTKIVVVAFGYGVDFLSRGNTFEGPVGALASAGVEFRVCRNTLTARKISESSLLMESKIVPAGVVEIARLQFEGYAYIKP
  RVAVHLDER EKAALAL RNTKNLLEGLAGVEVEVVAHADGVEELRTGSPQAALTAQLADRGVRFVVCENTLRSRNLSEKDFPGYVGTVPSAIVELVVRQAEGWQYLRP
DYRVVFHIDEDDESRVLLLISNVRNLMADLESVRIEVVAYSMGVNVLRRDSEYSGDVSELTGQGVRFCACSNTLRASGMDGDDLLEGVDVVSSGVGHIVRRQTEGWAYIRP
```

```
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  KVVVQIKDFDKVPQAL  RSVINLYNDIKDAEIEVVLHQSAIKAL KDSDTRSIIEDLIKKNILIVGCENSIRSQNLSHDQLIPGIKIVTSGVGEIVRKQSEGWIYL
  KIIVHIDEMAKWPMVLNNLNHLAQAYPAPNNQIELLVNGDAVMGV   KEAEKIRHALTSQIVIAV CQNSLTQRKITTEDLLNNSTIVASGVVELVEKQALGYHYLRP
  KLVFHINEPDKWQRVIMNINNFLNDVGQGNADIEVVANGEAVSAFQTNKMLIEQMQKLAEIGVNFVACQNALKAQSIAKESLPEFVTVVPAGITEIARKQTEGFAYIKP
QDKVAYHVNEAQTQALATL RNIRNHLDTDPSAQITVVTHANGVDFLPNGGEYAATVSALVSRGVKFEICEITLKNRNLKKEQFIQEATFTPSGVVRLTKMQLQGYAYIKP
    MYHLTEGIEEAVRAM RNVRNHLDADPTAKIVVVANGAGIDFLKNGNPFDAIVQDLVTRHVEFRACRNTLTTRNIDPSKLLPEATLVQSGVAEAARLQAEGFAYLRP
 YKVVYQISEGTEQAVRAI GNLRNHLNGAPGTRIVVVALGRGIDFLDKGRSFDAPVAALASMGVEFRVCHNSLAAFKVPEDKLLLEAKVVPAGVVEITRLQQEGFAYLKP
  KVVYQLSEGIDQAVRAM GNLRNHLNGAPGTKIVVVAFGYGVDFLSRGNTFEGPVGALASAGVEFRVCRNTLTARKISESSLLMESKIVPAGVVEIARLQFEGYAYIKP
  RVAVHLDER EKAALAL RNTKNLLEGLAGVEVEVVAHADGVEELRTGSPQAALTAQLADRGVRFVVCENTLRSRNLSEKDFPGYVGTVPSAIVELVVRQAEGWQYLRP
DYRVVFHIDEDDESRVLLLISNVRNLMADLESVRIEVVAYSMGVNVLRRDSEYSGDVSELTGQGVRFCACSNTLRASGMDGDDLLEGVDVVSSGVGHIVRRQTEGWAYIRP
```

```
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  KVVVQIKDFDKVPQAL  RSVINLYNDIKDAEIEVVLHQSAIKAL KDSDTRSIIEDLIKKNILIVGCENSIRSQNLSHDQLIPGIKIVTSGVGEIVRKQSEGWIYL
  KIIVHIDEMAKWPMVLNNLNHLAQAYPAPNNQIELLVNGDAVMGV   KEAEKIRHALTSQIVIAV CQNSLTQRKITTEDLLNNSTIVASGVVELVEKQALGYHYLRP
  KLVFHINEPDKWQRVIMNINNFLNDVGQGNADIEVVANGEAVSAFQTNKMLIEQMQKLAEIGVNFVACQNALKAQSIAKESLPEFVTVVPAGITEIARKQTEGFAYIKP
QDKVAYHVNEAQTQALATL RNIRNHLDTDPSAQITVVTHANGVDFLPNGGEYAATVSALVSRGVKFEICEITLKNRNLKKEQFIQEATFTPSGVVRLTKMQLQGYAYIKP
    MYHLTEGIEEAVRAM RNVRNHLDADPTAKIVVVANGAGIDFLKNGNPFDAIVQDLVTRHVEFRACRNTLTTRNIDPSKLLPEATLVQSGVAEAARLQAEGFAYLRP
 YKVVYQISEGTEQAVRAI GNLRNHLNGAPGTRIVVVALGRGIDFLDKGRSFDAPVAALASMGVEFRVCHNSLAAFKVPEDKLLLEAKVVPAGVVEITRLQQEGFAYLKP
  KVVYQLSEGIDQAVRAM GNLRNHLNGAPGTKIVVVAFGYGVDFLSRGNTFEGPVGALASAGVEFRVCRNTLTARKISESSLLMESKIVPAGVVEIARLQFEGYAYIKP
  RVAVHLDER EKAALAL RNTKNLLEGLAGVEVEVVAHADGVEELRTGSPQAALTAQLADRGVRFVVCENTLRSRNLSEKDFPGYVGTVPSAIVELVVRQAEGWQYLRP
DYRVVFHIDEDDESRVLLLISNVRNLMADLESVRIEVVAYSMGVNVLRRDSEYSGDVSELTGQGVRFCACSNTLRASGMDGDDLLEGVDVVSSGVGHIVRRQTEGWAYIRP
```

```
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  KVVVQIKDFDKVPQAL  RSVINLYNDIKDAEIEVVLHQSAIKAL KDSDTRSIIEDLIKKNILIVGCENSIRSQNLSHDQLIPGIKIVTSGVGEIVRKQSEGWIYL
  KIIVHIDEMAKWPMVLNNLNHLAQAYPAPNNQIELLVNGDAVMGV   KEAEKIRHALTSQIVIAV CQNSLTQRKITTEDLLNNSTIVASGVVELVEKQALGYHYLRP
  KLVFHINEPDKWQRVIMNINNFLNDVGQGNADIEVVANGEAVSAFQTNKMLIEQMQKLAEIGVNFVACQNALKAQSIAKESLPEFVTVVPAGITEIARKQTEGFAYIKP
QDKVAYHVNEAQTQALATL RNIRNHLDTDPSAQITVVTHANGVDFLPNGGEYAATVSALVSRGVKFEICEITLKNRNLKKEQFIQEATFTPSGVVRLTKMQLQGYAYIKP
    MYHLTEGIEEAVRAM RNVRNHLDADPTAKIVVVANGAGIDFLKNGNPFDAIVQDLVTRHVEFRACRNTLTTRNIDPSKLLPEATLVQSGVAEAARLQAEGFAYLRP
 YKVVYQISEGTEQAVRAI GNLRNHLNGAPGTRIVVVALGRGIDFLDKGRSFDAPVAALASMGVEFRVCHNSLAAFKVPEDKLLLEAKVVPAGVVEITRLQQEGFAYLKP
  KVVYQLSEGIDQAVRAM GNLRNHLNGAPGTKIVVVAFGYGVDFLSRGNTFEGPVGALASAGVEFRVCRNTLTARKISESSLLMESKIVPAGVVEIARLQFEGYAYIKP
  RVAVHLDER EKAALAL RNTKNLLEGLAGVEVEVVAHADGVEELRTGSPQAALTAQLADRGVRFVVCENTLRSRNLSEKDFPGYVGTVPSAIVELVVRQAEGWQYLRP
DYRVVFHIDEDDESRVLLLISNVRNLMADLESVRIEVVAYSMGVNVLRRDSEYSGDVSELTGQGVRFCACSNTLRASGMDGDDLLEGVDVVSSGVGHIVRRQTEGWAYIRP
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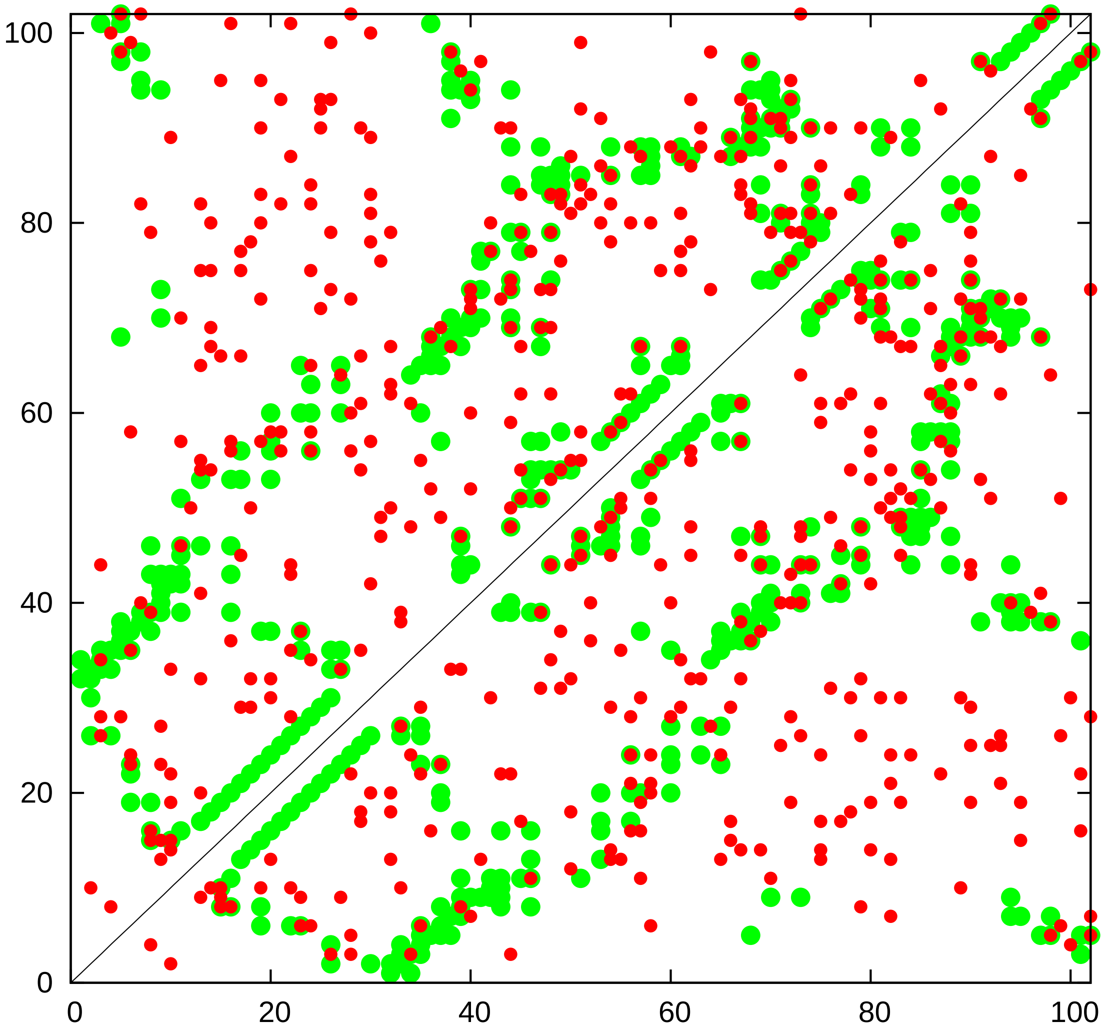

0
20
40
60
80
100
0
20
40
60
80
100

```
wtaylor@mull1:~/fewpred/pred1l1sA$ head folds.sort

build1l1sA/folds/fold-9-5-1:REMARK Build  Rank   1 Fold     70   711.217 40.79 17.43  aABbcCFfeEdD aBcFed +B+0.-A+0.+B-1.-A-1.+B-2.+a+0. 710.779
build1l1sA/folds/fold-9-5-2:REMARK Build  Rank   2 Fold     99   710.411 40.79 17.41  EefFCcbBAaDd EfCbAD +B+0.-A+0.+B-1.-A-1.+B-2.+a+0. 709.809
build1l1sA/folds/fold-9-4-3:REMARK Build  Rank   3 Fold     69   710.078 36.78 19.31  aABbcCFfeEDd aBcFeD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0. 709.296
build1l1sA/folds/fold-9-5-3:REMARK Build  Rank   3 Fold     69   710.078 36.78 19.31  aABbcCFfeEDd aBcFeD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0. 708.416
build1l1sA/folds/fold-9-4-4:REMARK Build  Rank   4 Fold     98   709.352 36.78 19.29  EefFCcbBAadD EfCbAd +B+0.-A+0.+B-1.-A-1.+B-2.-a+0. 708.352
build1l1sA/folds/fold-9-5-4:REMARK Build  Rank   4 Fold     98   709.352 36.78 19.29  EefFCcbBAadD EfCbAd +B+0.-A+0.+B-1.-A-1.+B-2.-a+0. 707.902
build1l1sA/folds/fold-9-5-6:REMARK Build  Rank   6 Fold    100   623.324 40.35 15.45  EefFCcbBaADd EfCbaD +B+0.-A+0.+B-1.-A-1.-B-2.+a+0. 621.322
build1l1sA/folds/fold-9-3-2:REMARK Build  Rank   2 Fold     23   608.719 37.84 16.09  eEFfcCDdaAbB eFcDab +B+0.-A+0.+B-1.-A-1.+B-2.+a+0. 607.525
build1l1sA/folds/fold-18-1-1:REMARK Build  Rank   1 Fold    362   603.768 24.43 24.72  CcbBEefFGgiIHhdDAa CbEfGiHdA +B+0.-A+0.+B-1.-A-1.+B-2.-A-2.+B-3.-a+0.+B+1. 603.202
build1l1sA/folds/fold-18-0-1:REMARK Build  Rank   1 Fold    362   603.768 24.43 24.72  CcbBEefFGgiIHhdDAa CbEfGiHdA +B+0.-A+0.+B-1.-A-1.+B-2.-A-2.+B-3.-a+0.+B+1. 603.065
```

```
wtaylor@mull1:~/fewpred/pred1l1sA$ head folds.best

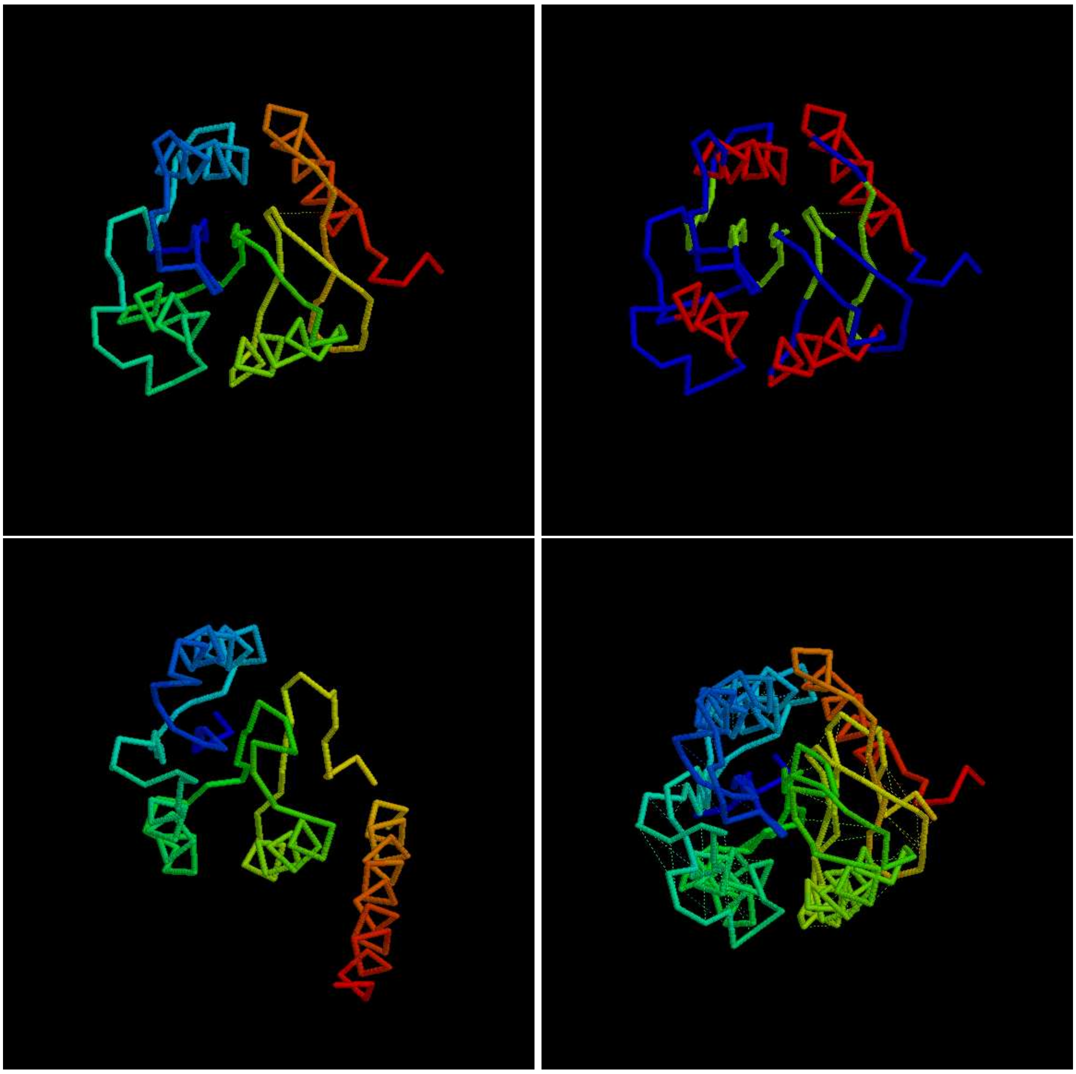
fold-9-5-1 Build Rank 1 Fold 70 711.217 40.79 17.43 aABbcCFfeEdD aBcFed +B+0.-A+0.+B-1.-A-1.+B-2.+a+0. 4936.69
fold-9-5-2 Build Rank 2 Fold 99 710.411 40.79 17.41 EefFCcbBAaDd EfCbAD +B+0.-A+0.+B-1.-A-1.+B-2.+a+0. 3123.17
fold-9-4-3 Build Rank 3 Fold 69 710.078 36.78 19.31 aABbcCFfeEDd aBcFeD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0. 2306.36
fold-9-5-3 Build Rank 3 Fold 69 710.078 36.78 19.31 aABbcCFfeEDd aBcFeD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0. 2180.46
fold-9-4-4 Build Rank 4 Fold 98 709.352 36.78 19.29 EefFCcbBAadD EfCbAd +B+0.-A+0.+B-1.-A-1.+B-2.-a+0. 3217.71
fold-9-5-4 Build Rank 4 Fold 98 709.352 36.78 19.29 EefFCcbBAadD EfCbAd +B+0.-A+0.+B-1.-A-1.+B-2.-a+0. 2820.8
fold-9-5-6 Build Rank 6 Fold 100 623.324 40.35 15.45 EefFCcbBaADd EfCbaD +B+0.-A+0.+B-1.-A-1.-B-2.+a+0. 3709.19
fold-9-3-2 Build Rank 2 Fold 23 608.719 37.84 16.09 eEFfcCDdaAbB eFcDab +B+0.-A+0.+B-1.-A-1.+B-2.+a+0. 3371.93
fold-18-1-1 Build Rank 1 Fold 362 603.768 24.43 24.72 CcbBEefFGgiIHhdDAa CbEfGiHdA +B+0.-A+0.+B-1.-A-1.+B-2.-A-2.+B-3.-a+0.+B+1. 2188.78
fold-18-0-1 Build Rank 1 Fold 362 603.768 24.43 24.72 CcbBEefFGgiIHhdDAa CbEfGiHdA +B+0.-A+0.+B-1.-A-1.+B-2.-A-2.+B-3.-a+0.+B+1. 2072.08
```

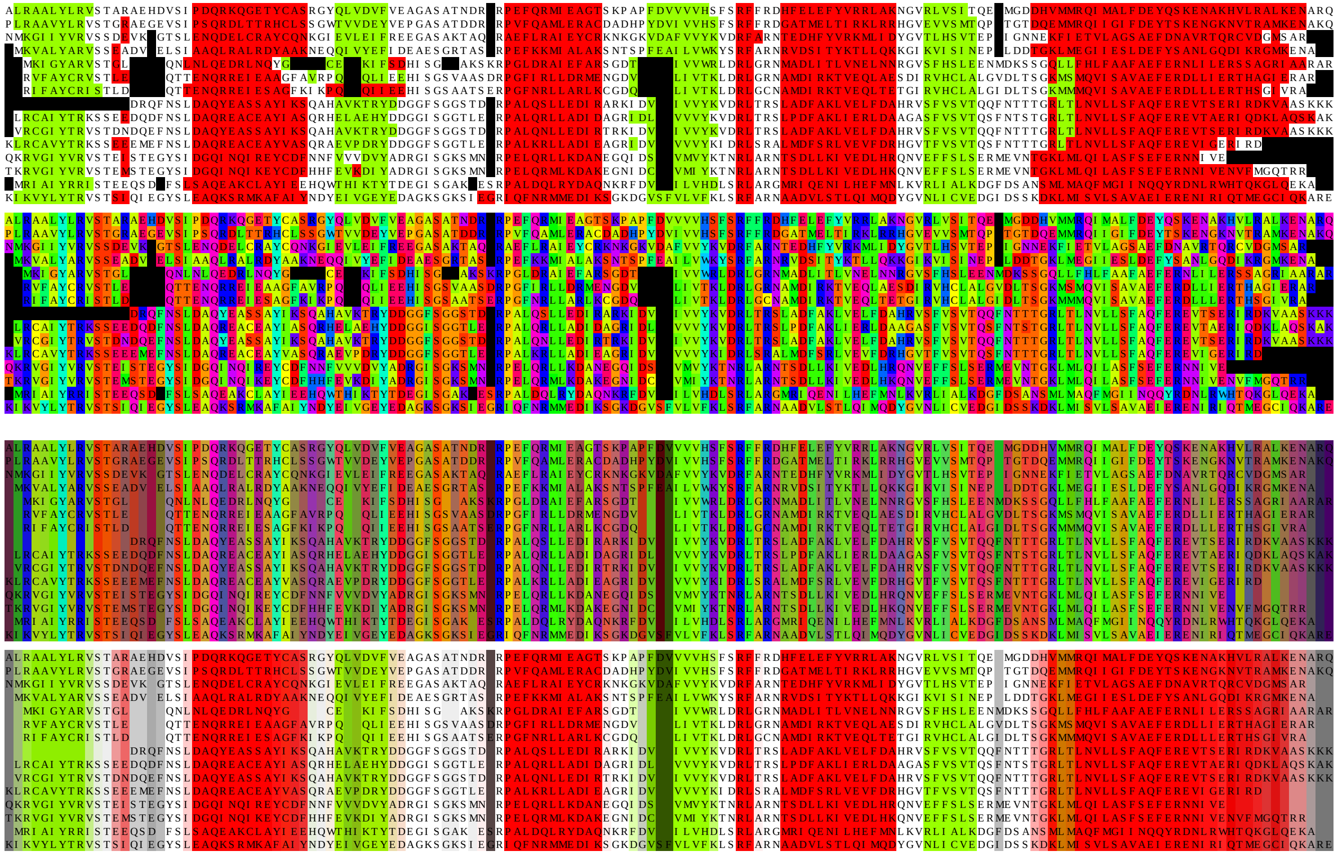
```
wtaylor@mull1:~/fewpred/pred1l1sA$ sort -nr -k9 folds.best | head

fold-15-17-1 Build Rank 1 Fold 406 560.596 18.70 29.97 BbcCDdgGFfHheEAa BcDgFHeA +B+0.-A+0.+B-1.-A-1.+B-2.+B-3.-a+0.+B+1. 2287.64
fold-26-17-1 Build Rank 1 Fold 838 548.242 18.70 29.31 BbcCDdgGFfHheEAa BcDgFHeA +B+0.-A+0.+B-1.-A-1.+B-2.+B-3.-a+0.+B+1. 3783.01
fold-26-16-1 Build Rank 1 Fold 838 548.242 18.70 29.31 BbcCDdgGFfHheEAa BcDgFHeA +B+0.-A+0.+B-1.-A-1.+B-2.+B-3.-a+0.+B+1. 3291.21
fold-4-0-7 Build Rank 14 Fold 103 386.648 14.59 26.51 GghHIiFfbBAaCcdDEe GhIFbACdE +B+0.-A+0.+B-1.+a+0.-a+1.+B+3.+B+2.-A+1.+B+1. 1551.03
fold-4-0-6 Build Rank 11 Fold 449 386.652 14.59 26.51 CcbBAaDdhHIiGgfFEe CbADhIGfE +B+0.-A+0.+B-1.+a+0.-a+1.+B+3.+B+2.-A+1.+B+1. 1606.33
fold-26-17-4 Build Rank 6 Fold 21 426.427 17.07 24.98 AacCDdgGFfHheEBb AcDgFHeB +B+0.-A+0.+B-2.-A-1.+B-3.+B-4.-a+0.+B-1. 2274.83
fold-26-16-4 Build Rank 6 Fold 21 426.427 17.07 24.98 AacCDdgGFfHheEBb AcDgFHeB +B+0.-A+0.+B-2.-A-1.+B-3.+B-4.-a+0.+B-1. 3439.67
fold-8-9-1 Build Rank 1 Fold 26 530.064 21.42 24.74 BbcCDdgGFfeEAa BcDgFeA +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1. 3925.81
fold-8-8-1 Build Rank 1 Fold 26 530.064 21.42 24.74 BbcCDdgGFfeEAa BcDgFeA +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1. 3000.81
fold-18-1-1 Build Rank 1 Fold 362 603.768 24.43 24.72 CcbBEefFGgiIHhdDAa CbEfGiHdA +B+0.-A+0.+B-1.-A-1.+B-2.-A-2.+B-3.-a+0.+B+1. 2188.78
```

`3guvA (149) = +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.(-A+1)`

**A resolvase family site-specific recombinase from Streptococcus pneumoniae**. Under all rankings, the top folds corresponded to the native with the exception of the orientation of the long terminal $\alpha$-helix which does not pack on the $\beta$-sheet but forms a coiled-coil in the dimeric native structure. Excluding this helix after the chain break in the structure (leaving 121 residues) the top models were all correct.

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MKVALYARVSSEADVELSIAAQLRALRDYAAKNEQQIVYEFIDEAESGRTASRPEFKKMIALAKSNTSPFEAILVWKYSRFARNRVDSITYKTLLQKKGIKVISINEPLDDTGKLMEGIIESLDEFYSANLGQDIKRGMKENA
MKIGYARVSTGLQNLNLQEDRLNQYGCEKIFSDHISGAKSKRPGLDRAIEFARSGDTIVVWRLDRLGRNMADLITLVNELNNRGVSFHSLEENMDKSSGQLLFHLFAAFAEFERNLILERSSAGRIAARAR
RVFAYCRVSTLEQTTENQRREIEAAGFAVRPQQLIEEHISGSVAASDRPGFIRLLDRMENGDVLIVTKLDRLGRNAMDIRKTVEQLAESDIRVHCLALGVDLTSGKMSMQVISAVAEFERDLLIERTHAGIERAR
RIFAYCRISTLDQTTENQRREIESAGFKIKPQQIIEEHISGSAATSERPGFNRLLARLKCGDQLIVTKLDRLGCNAMDIRKTVEQLTETGIRVHCLALGIDLTSGKMMMQVISAVAEFERDLLLERTHSGIVRA
DRQFNSLDAQYEASSAYIKSQAHAVKTRYDDGGFSGGSTDRPALQSLLEDIRARKIDVIVVYKVDRLTRSLADFAKLVELFDAHRVSFVSVTQQFNTTTGRLTLNVLLSFAQFEREVTSERIRDKVAASKKK
LRCAIYTRKSSEEDQDFNSLDAQREACEAYIASQRHELAEHYDDGGISGGTLERPALQRLLADIDAGRIDLVVVYKVDRLTRSLPDFAKLIERLDAAGASFVSVTQSFNTSTGRLTLNVLLSFAQFEREVTAERIQDKLAQSKAK
VRCGIYTRVSTDNDQEFNSLDAQYEASSAYIKSQAHAVKTRYDDGGFSGGSTDRPALQNLLEDIRTRKIDVIVVYKVDRLTRSLADFAKLVELFDAHRVSFVSVTQQFNTTTGRLTLNVLLSFAQFEREVTSERIRDKVAASKKK
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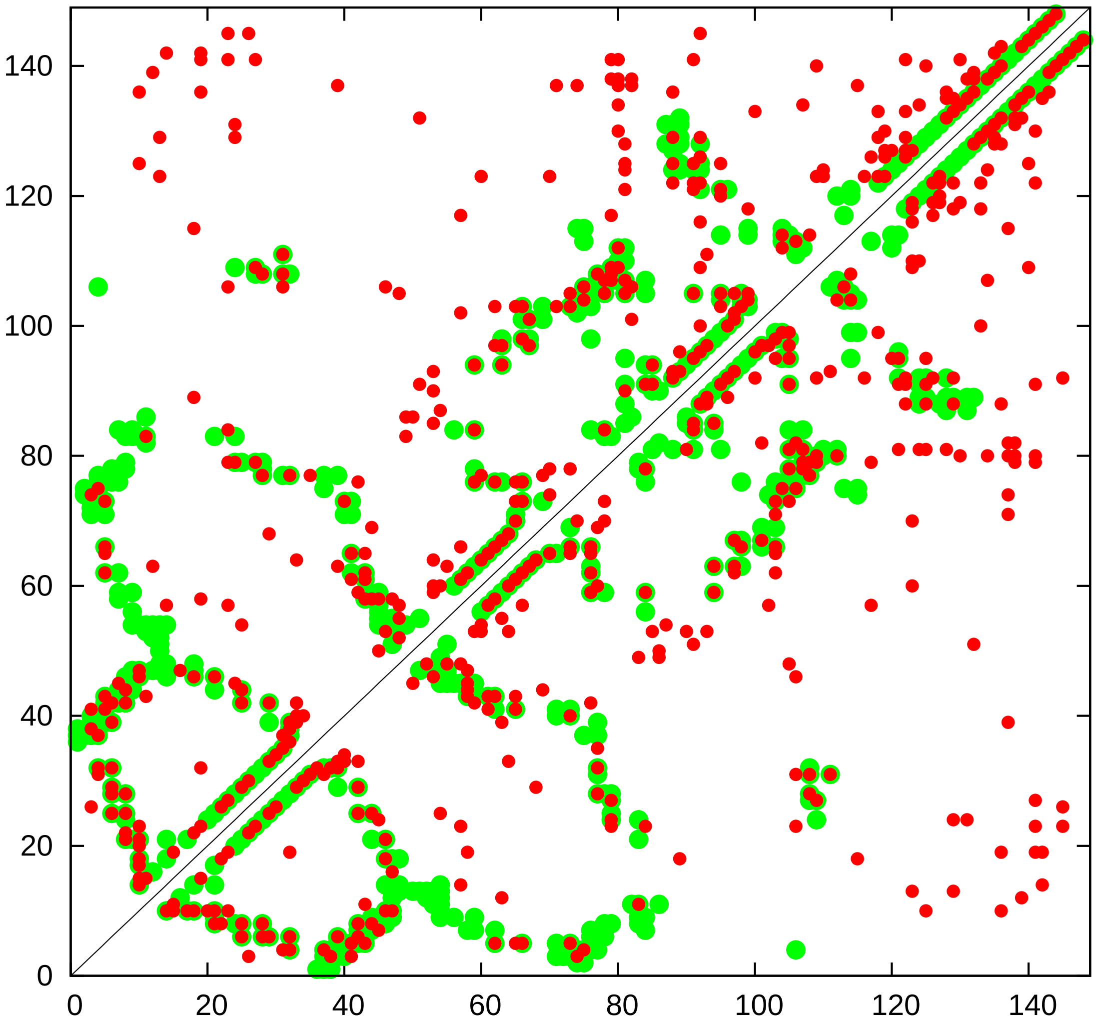
MRIAIYRRISTEEQSDFSLSAQEAKCLAYIEEHQWTHIKTYTDEGISGAKESRPALDQLRYDAQNKRFDVILVHDLSRLARGMRIQENILHEFMNLKVRLIALKDGFDSANSMLMAQFMGIINQQYRDNLRWHTQKGLQEKA
KIKVYLYTRVSTSIQIEGYSLEAQKSRMKAFAIYNDYEIVGEYEDAGKSGKSIEGRIQFNRMMEDIKSGKDGVSFVLVFKLSRFARNAADVLSTLQIMQDYGVNLICVEDGIDSSKDKLMISVLSAVAEIERENIRIQTMEGCIQKARE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100
120
140

```
wtaylor@mull1:~/fewpred/pred3guvA$ head folds.sort

build3guvA/folds/fold-4-1-1:REMARK Build  Rank   1 Fold      1  1669.002 34.45 48.45  CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1668.22
build3guvA/folds/fold-4-0-1:REMARK Build  Rank   1 Fold      1  1669.002 34.45 48.45  CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1668.13
build3guvA/folds/fold-0-0-1:REMARK Build  Rank   1 Fold      1  1649.208 39.22 42.05  CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1648.87
build3guvA/folds/fold-0-1-1:REMARK Build  Rank   1 Fold      1  1649.208 39.22 42.05  CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1648.37
build3guvA/folds/fold-0-4-1:REMARK Build  Rank   1 Fold      1  1634.165 38.89 42.02  CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1633.77
build3guvA/folds/fold-0-5-1:REMARK Build  Rank   1 Fold      1  1634.165 38.89 42.02  CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1633.2
build3guvA/folds/fold-0-5-2:REMARK Build  Rank   2 Fold    298  1618.097 38.89 41.61  EehHGgfFCcbBAadD EhGfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1617.53
build3guvA/folds/fold-0-4-2:REMARK Build  Rank   2 Fold    298  1618.097 38.89 41.61  EehHGgfFCcbBAadD EhGfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1616.77
build3guvA/folds/fold-5-1-1:REMARK Build  Rank   1 Fold      1  1612.850 34.75 46.41  CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1612.08
build3guvA/folds/fold-5-0-1:REMARK Build  Rank   1 Fold      1  1612.850 34.75 46.41  CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 1612.03
```

```
wtaylor@mull1:~/fewpred/pred3guvA$ head folds.best

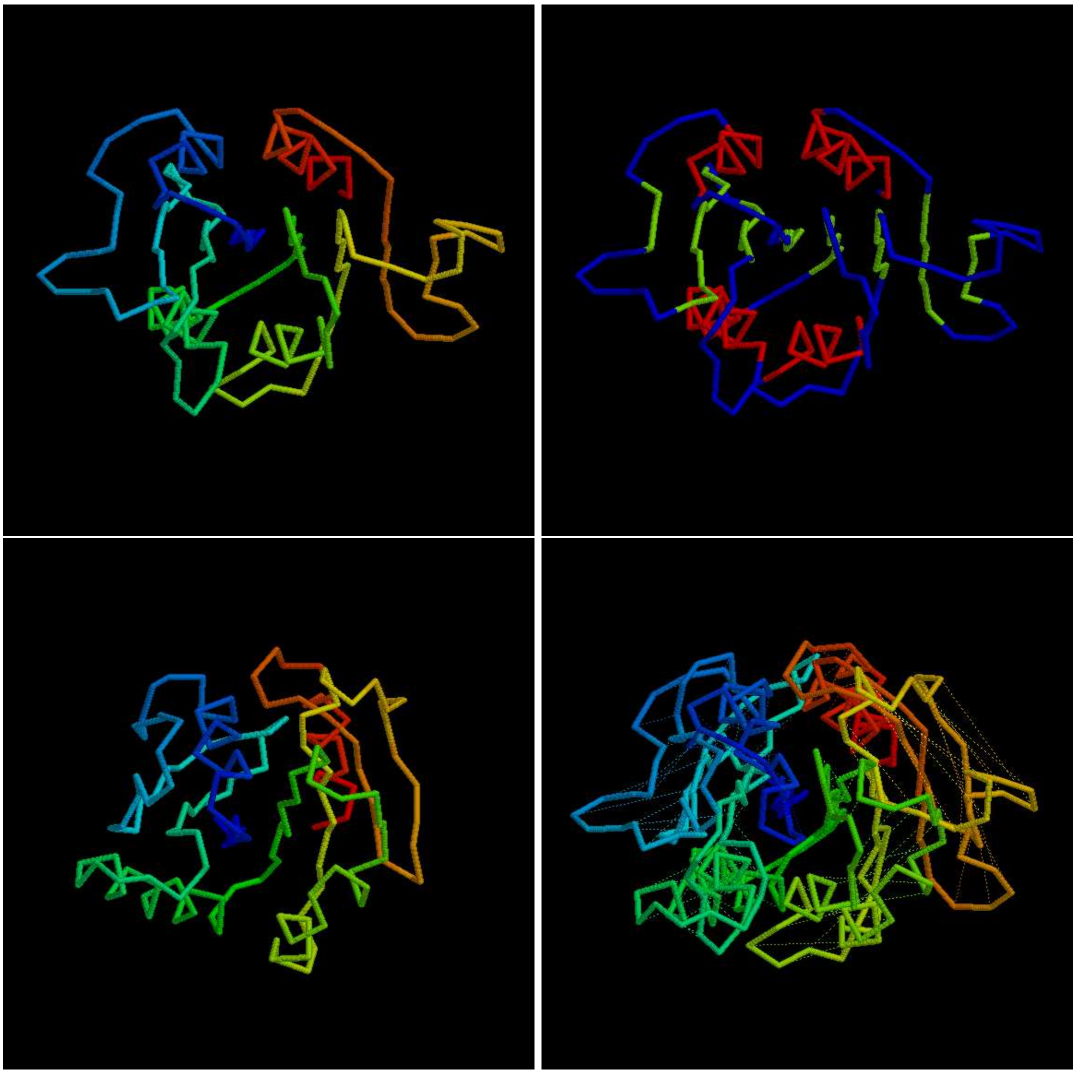
fold-4-1-1 Build Rank 1 Fold 1 1669.002 34.45 48.45 CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 8298.47
fold-4-0-1 Build Rank 1 Fold 1 1669.002 34.45 48.45 CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 7118.46
fold-0-1-1 Build Rank 1 Fold 1 1649.208 39.22 42.05 CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 5440.91
fold-0-5-1 Build Rank 1 Fold 1 1634.165 38.89 42.02 CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 5123.67
fold-5-1-1 Build Rank 1 Fold 1 1612.850 34.75 46.41 CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 6635.97
fold-5-0-1 Build Rank 1 Fold 1 1612.850 34.75 46.41 CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 6516.16
fold-0-2-1 Build Rank 1 Fold 182 1579.885 42.41 37.26 cCBbaADdeEHhgGFf cBaDeHgF +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 3172.21
fold-0-3-1 Build Rank 1 Fold 182 1579.885 42.41 37.26 cCBbaADdeEHhgGFf cBaDeHgF +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 4102.83
fold-4-5-1 Build Rank 1 Fold 130 1526.779 33.16 46.04 CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 4052.71
fold-4-4-1 Build Rank 1 Fold 130 1526.779 33.16 46.04 CcbBAadDEehHGgfF CbAdEhGf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-A+1. 8989.51
```

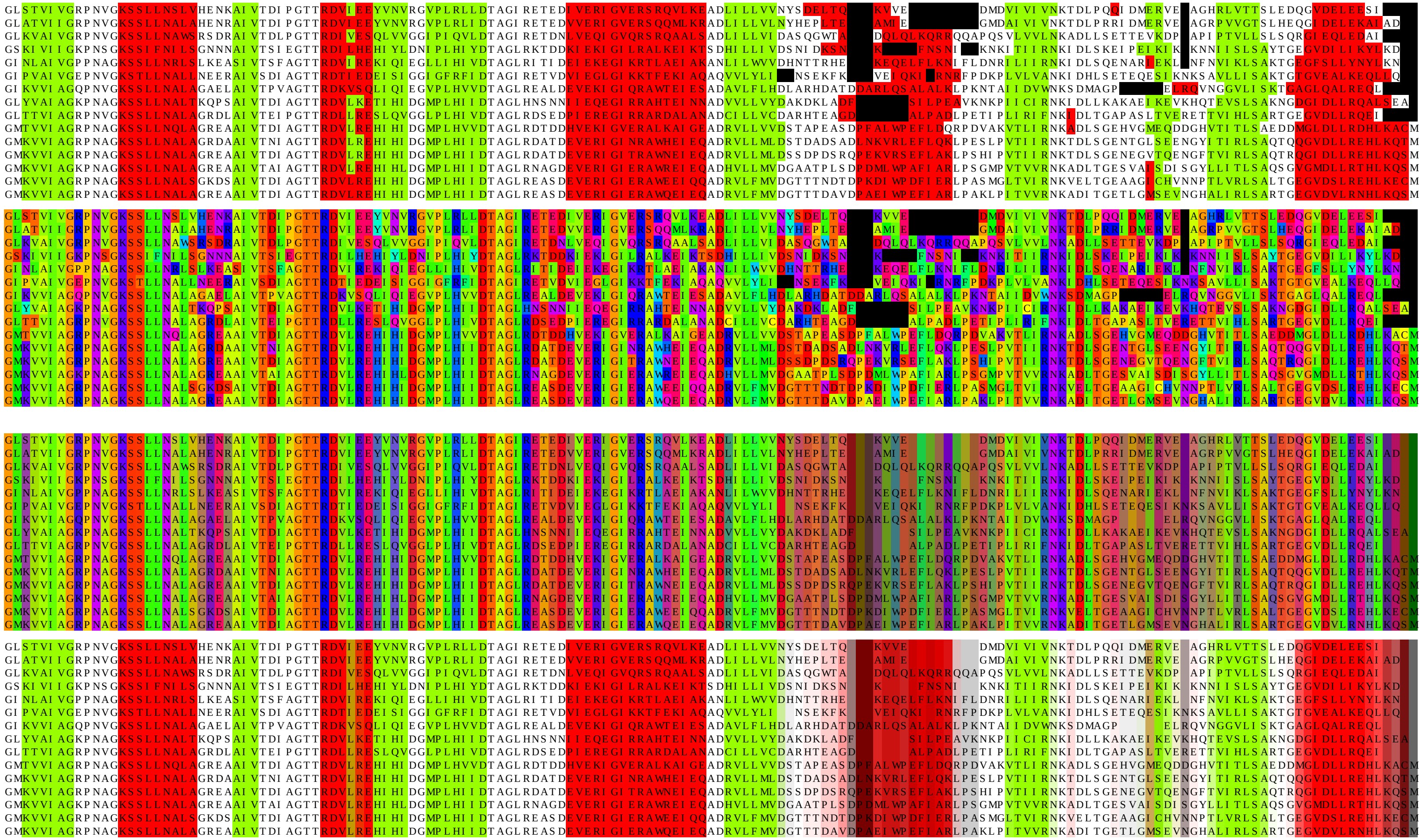
```
wtaylor@mull1:~/fewpred/pred3guvA$ sort -nr -k9 folds.best | head

fold-12-1-7 Build Rank 16 Fold 661 1145.056 20.22 56.64 GghHIifFEebBCcAadD GhIfEbCAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.+B+3.-A+1. 3771.82
fold-12-1-6 Build Rank 13 Fold 125 1145.072 20.22 56.64 CcbBAadDEehHGgIifF CbAdEhGIf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.+B+3.-A+1. 4255.23
fold-12-0-7 Build Rank 16 Fold 661 1145.056 20.22 56.64 GghHIifFEebBCcAadD GhIfEbCAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.+B+3.-A+1. 4074.39
fold-12-0-6 Build Rank 13 Fold 125 1145.072 20.22 56.64 CcbBAadDEehHGgIifF CbAdEhGIf +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.+B+3.-A+1. 5004.49
fold-7-1-14 Build Rank 27 Fold 1158 990.032 18.38 53.85 GghHIifFEebBCcAadD GhIfEbCAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.+B+3.-A+1. 3617.54
fold-7-0-14 Build Rank 27 Fold 1158 990.032 18.38 53.85 GghHIifFEebBCcAadD GhIfEbCAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.+B+3.-A+1. 3046.71
fold-7-1-6 Build Rank 12 Fold 1157 1112.760 20.69 53.78 GghHIifFEebBCcaADd GhIfEbCaD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+3.+A+1. 3393.4
fold-7-0-6 Build Rank 12 Fold 1157 1112.760 20.69 53.78 GghHIifFEebBCcaADd GhIfEbCaD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+3.+A+1. 3487.3
fold-45-3-5 Build Rank 5 Fold 167 795.299 14.87 53.49 CcbBAadDEegGFfHhiI CbAdEgFHi +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.+B+3.-a+2. 1495.9
fold-45-2-5 Build Rank 5 Fold 167 795.299 14.87 53.49 CcbBAadDEegGFfHhiI CbAdEgFHi +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.+B+3.-a+2. 2731.42
```

`2gj8A (161) = +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1`

**The MnmE G-domain from Escherichia coli.** The top models under the combined score were a good approximations to this ras-like protein except that the irregular amino terminal edge of the domain had been predicted in a more regular (Rossmann-like) way. The reranked best list however, reproduced the ras-type topology on this edge with the one slight deviation of linking an exposed loop as a short extra strand on the edge of the sheet.

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GLATVIIGRPNVGKSSLLNALAHENRAIVTDIPGTTRDVIEEYVNVRGVPLRLIDTAGIRETEDVVERIGVERSQQMLKRADLILLVLNYHEPLTE AMIE GMDAIVIVNKTDLPRRIDMERVE AGRPVVGTSLHEQGIDELEKAIAD
GLKVAIVGRPNVGKSSLLNAWSRSDRAIVTDLPGTTRDIVESQLVVGGIPIQVLDTAGIRETDNLVEQIGVQRSRQAALSADLILLVIDASQGWTA DQLQLKQRRQQAPQSVLVVLNKADLLSETTEVKDP APIPTVLLSLSQRGIEQLEDAI
GSKIVIIGKPNSGKSSIFNILSGNNNAIVTSIEGTTRDILHEHIYLDNIPLHIYDTAGLRKTDDKIEKIGILRALKEIKTSDHILLIVDSNIDKSN K FNSNI KNKITIIRNKIDLSKEIPEIKIK KNNIISLSAYTGEGVDILIKYLKD
GINLAIVGPPNAGKSSLLNRLSLKEASIVTSFAGTTRDVIREKIQIEGLLIHIVDTAGLRITIDEIEKEGIKRTLAEIAKANLILWVVDHNTTRHE KEQELFLKNIFLDNRILIIRNKIDLSQENARIEKL NFNVIKLSAKTGEGFSLLYNYLKN
GIPVAIVGEPNVGKSTLLNALLNEERAIVSDIAGTTRDTIEDEISIGGIGFRFIDTAGIRETVDVIEGLGIKKTFEKIAQAQVVLYLI NSEKFK VEIQKI RNRFPDKPLVLVANKIDHLSETEQESIKNKSAVLLISAKTGTGVEALKEQLLQ
GIKVVIAGQPNVGKSSLLNALAGAELAIVTPVAGTTRDKVSQLIQIEGVPLHVVDTAGLREALDEVEKIGIQRAWTEIESADAVLFLHDLARHDATDDARLQSALALKLPKNTAIIDVWNKSDMAGP ELRQVNGGVLISKTGAGLQALREQL
GLYVAIAGKPNAGKSSLLNALTKQPSAIVTDIAGTTRDVLKETIHIDGMPLHIIDTAGLHNSNNIIEQEGIRRAHTEINNADVVLLVYDAKDKLADF SILPEAVKNKPIICIRNKIDLLKAKAEIKEVKHQTEVSLSAKNGDGIDLLRQALSEA
GLTTVIAGRPNVGKSSLLNALAGRDLAIVTEIPGTTRDLLRESLQVGGLPLHIVDTAGLRDSEDPIEREGIRRARDALANADCILLVCDARHTEAGD ALPADLPETIPLIRIFNKIDLTGAPASLTVERETTVIHLSARTGEGVDLLRQEI
GMTVVIAGRPNAGKSSLLNQLAGREAAIVTDIAGTTRDVLREHIHIDGMPLHVVDTAGLRDTDDHVEKIGVERALKAIGEADRVLLVVDSTAPEASDPFALWPEFLDQRPDVAKVTLIRNKADLSGEHVGMEQDDGHVTITLSAEDDMGLDLLRDHLKACM
GMKVVIAGRPNAGKSSLLNALAGRDAAIVTNIAGTTRDVLREHIHIDGMPLHIIDTAGLRDATDEVERIGINRAWHEIEQADRVLLMLDSTDADSADLNKVRLEFLQKLPESLPVTIIRNKTDLSGENTGLSEENGYITIRLSAQTQQGVDLLREHLKQTM
GMKVVIAGRPNAGKSSLLNALAGREAAIVTDIAGTTRDVLREHIHIDGMPLHIIDTAGLRDATDEVERIGITRAWNEIEQADRVLLMLDSSDPDSRQPEKVRSEFLAKLPSHIPVTIIRNKTDLSGENEGVTQENGFTVIRLSAQTRQGIDLLREHLKQSM
GMKVVIAGKPNAGKSSLLNALAGREAAIVTAIAGTTRDVLREHIHLDGMPLHIIDTAGLRNAGDEVERIGIERAWREIEQADHVLLMVDGAATPLSDPDMLWPAFIARLPSGMPVTVVRNKADLTGESVAISDISGYLLITLSAQSGVGMDLLRTHLKQSM
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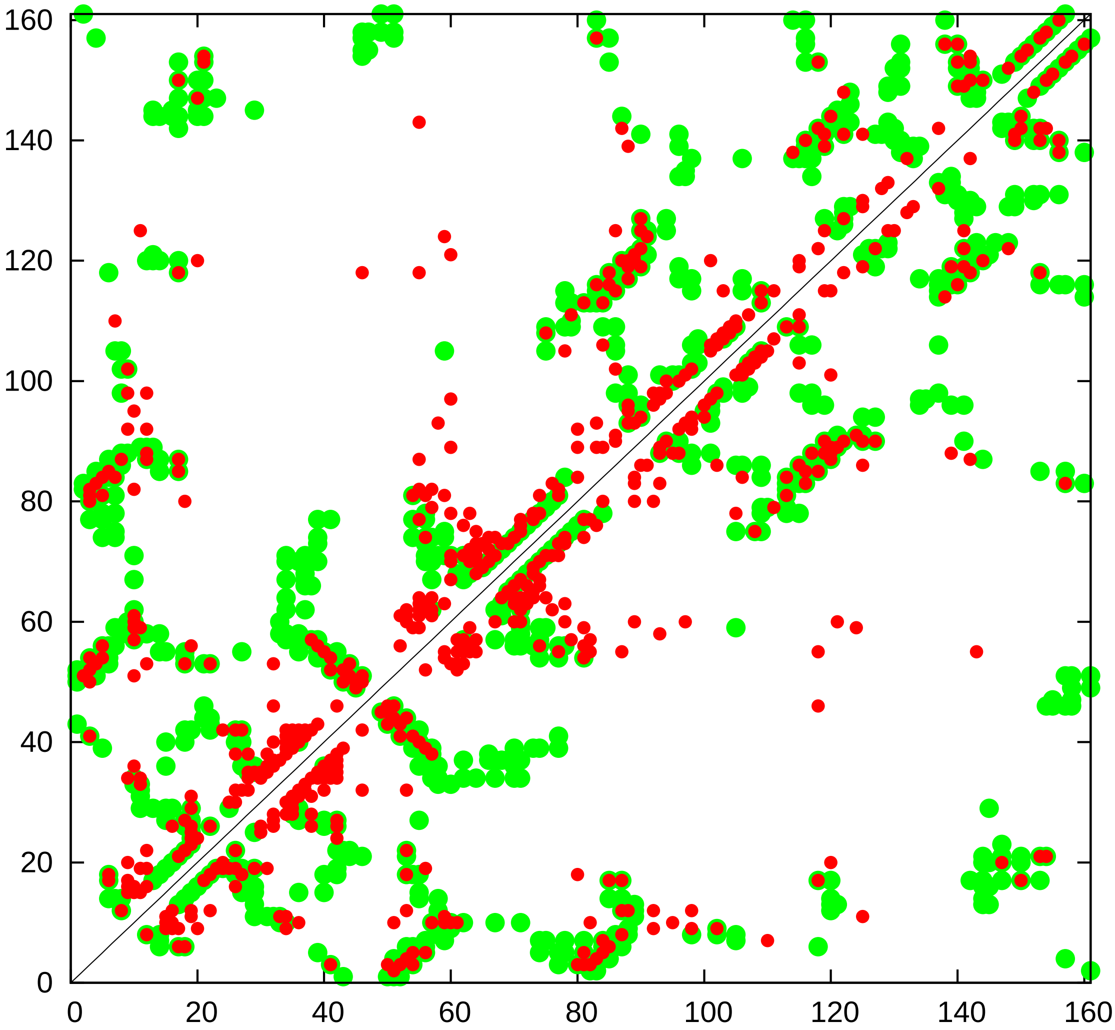
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wtaylor@mull1:~/fewpred/pred2gj8A$ head folds.sort

build2gj8A/folds/fold-30-22-1:REMARK Build  Rank   1 Fold    833  2648.630 51.80 51.13  gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 2648.22
build2gj8A/folds/fold-31-22-1:REMARK Build  Rank   1 Fold    839  2624.941 50.71 51.77  gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 2624.08
build2gj8A/folds/fold-31-23-1:REMARK Build  Rank   1 Fold    839  2624.941 50.71 51.77  gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 2624.03
build2gj8A/folds/fold-44-3-1:REMARK Build  Rank   1 Fold    763  2590.722 51.16 50.64  eEFfcCBbaADdgGHhiILlkKJj eFcBaDgHiLkJ +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 2590.18
build2gj8A/folds/fold-44-2-1:REMARK Build  Rank   1 Fold    763  2590.722 51.16 50.64  eEFfcCBbaADdgGHhiILlkKJj eFcBaDgHiLkJ +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 2590.01
build2gj8A/folds/fold-32-23-1:REMARK Build  Rank   1 Fold    796  2585.012 50.01 51.69  gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 2584.48
build2gj8A/folds/fold-32-22-1:REMARK Build  Rank   1 Fold    796  2585.012 50.01 51.69  gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 2584.22
build2gj8A/folds/fold-36-23-1:REMARK Build  Rank   1 Fold    833  2576.206 51.41 50.11  gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 2575.99
build2gj8A/folds/fold-36-22-1:REMARK Build  Rank   1 Fold    833  2576.206 51.41 50.11  gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 2575.71
build2gj8A/folds/fold-28-22-1:REMARK Build  Rank   1 Fold    636  2552.804 52.11 48.99  gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 2552.77
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wtaylor@mull1:~/fewpred/pred2gj8A$ head folds.best

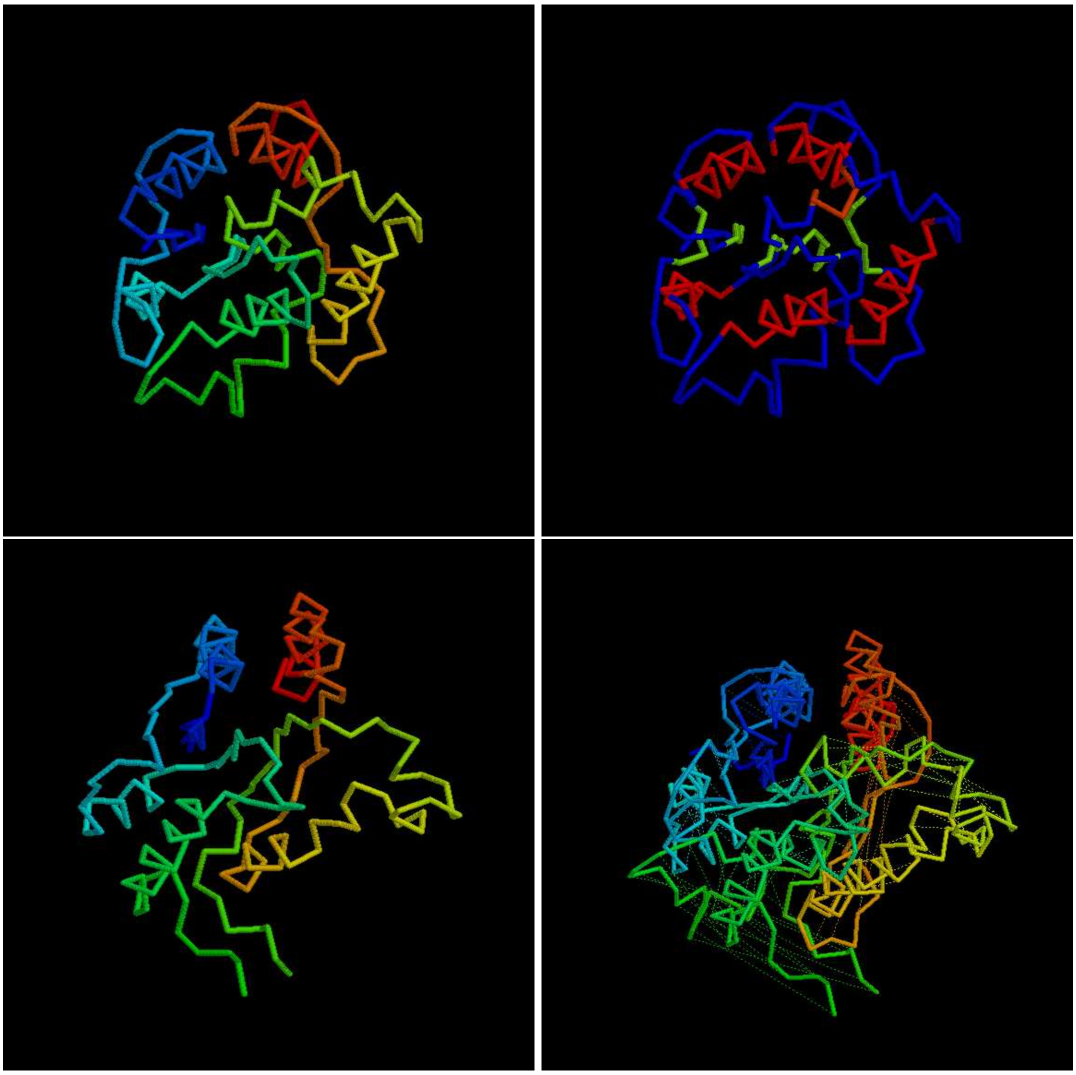
fold-30-22-1 Build Rank 1 Fold 833 2648.630 51.80 51.13 gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 8770.46
fold-31-22-1 Build Rank 1 Fold 839 2624.941 50.71 51.77 gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 13244.4
fold-31-23-1 Build Rank 1 Fold 839 2624.941 50.71 51.77 gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 11494.8
fold-44-3-1 Build Rank 1 Fold 763 2590.722 51.16 50.64 eEFfcCBbaADdgGHhiILlkKJj eFcBaDgHiLkJ +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 12808.6
fold-44-2-1 Build Rank 1 Fold 763 2590.722 51.16 50.64 eEFfcCBbaADdgGHhiILlkKJj eFcBaDgHiLkJ +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 12682.6
fold-32-23-1 Build Rank 1 Fold 796 2585.012 50.01 51.69 gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 13715.2
fold-32-22-1 Build Rank 1 Fold 796 2585.012 50.01 51.69 gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 8855.32
fold-36-23-1 Build Rank 1 Fold 833 2576.206 51.41 50.11 gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 8351.6
fold-36-22-1 Build Rank 1 Fold 833 2576.206 51.41 50.11 gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 8319.07
fold-28-22-1 Build Rank 1 Fold 636 2552.804 52.11 48.99 gGHhiILlkKJjeEFfcCAabBDd gHiLkJeFcAbD +B+0.-A+0.+B-1.-A-1.+B-2.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 10144.1
```

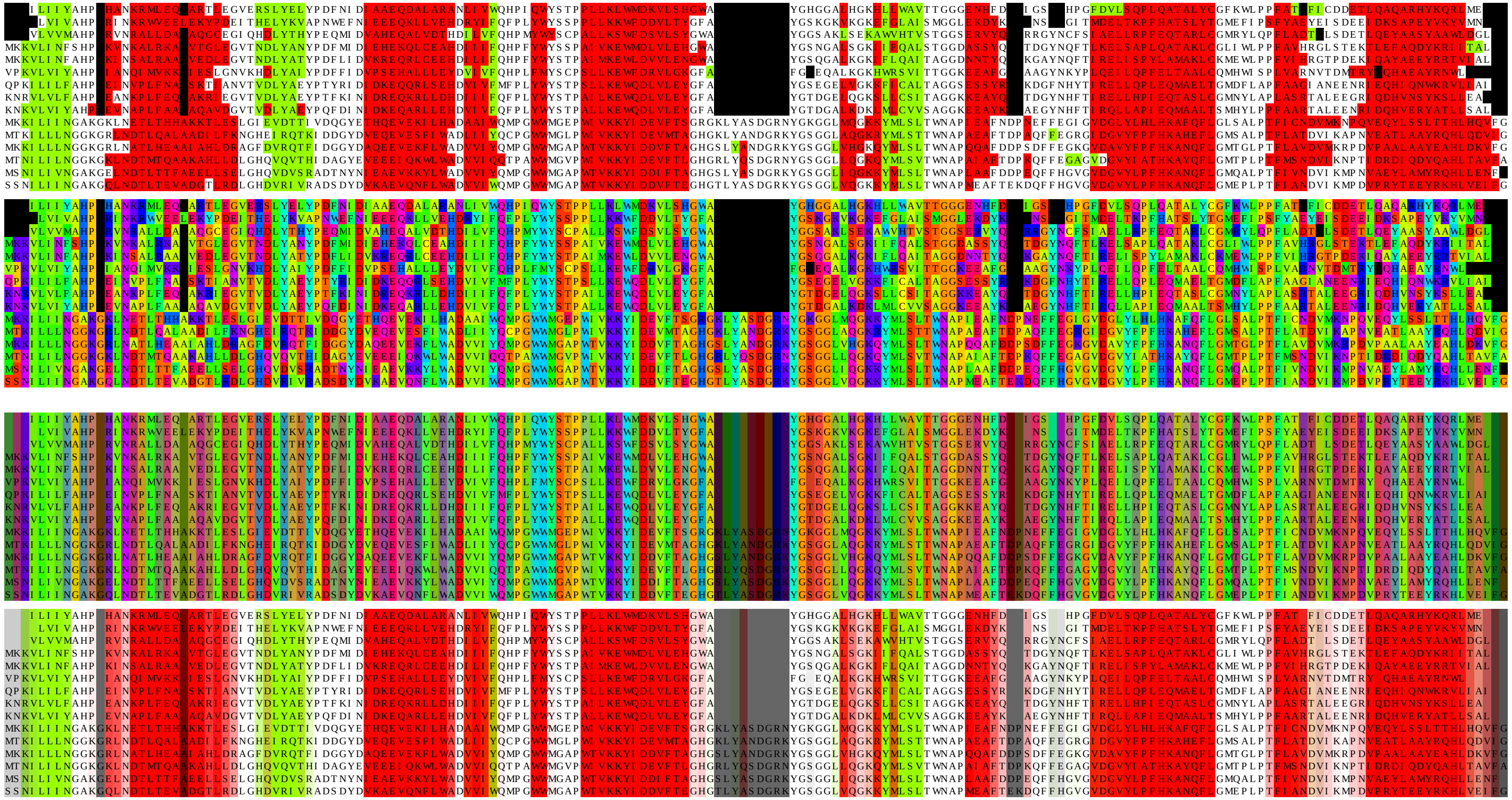
```
wtaylor@mull1:~/fewpred/pred2gj8A$ sort -nr -k9 folds.best | head

fold-9-1-2 Build Rank 4 Fold 774 2274.048 34.50 65.92 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 9550.56
fold-9-0-2 Build Rank 4 Fold 774 2274.048 34.50 65.92 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 11506.9
fold-11-21-3 Build Rank 3 Fold 7299 2246.004 34.23 65.62 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 8351.02
fold-11-20-3 Build Rank 3 Fold 7299 2246.004 34.23 65.62 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 7015.96
fold-2-21-3 Build Rank 3 Fold 8653 2245.654 34.23 65.61 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 8288.47
fold-2-20-3 Build Rank 3 Fold 8653 2245.654 34.23 65.61 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 11043.1
fold-11-1-2 Build Rank 4 Fold 322 2259.926 34.46 65.59 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 9133.88
fold-11-0-2 Build Rank 4 Fold 322 2259.926 34.46 65.59 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 9867.85
fold-2-1-2 Build Rank 4 Fold 336 2257.542 34.46 65.52 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 9615.78
fold-2-0-2 Build Rank 4 Fold 336 2257.542 34.46 65.52 GgjJLlkKIihHEedDCcaABbfF GjLkIhEdCaBf +B+0.-A+0.+B-3.-B-2.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.+B+3.-A+1. 10923
```

`2amjA (180) = +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1`

**A modulator of drug activity B from Escherichia coli.** The same model was ranked top of both the full and best lists and had the correct fold. The top folds in the reranked best list, however, all included an extra edge strand resulting in a rearrangement on the C-terminal edge of the domain with the correct fold being displaced to rank 60.





```
   ILIIYAHP HANKRMLEQ ARTLEGVERSLYELYPDFNIDIAAEQDALARANLIVWQHPIQWYSTPPLLKLWMDKVLSHGWA         YGHGGALHGKHLLWAVTTGGGENHFD  IGS  HPGFDVLSQPLQATALYCGFKWLPPFAT FICDDETLQAQARHYKQRLME   
    LVIVAHP RINKRWVEELEKYPDEITHELYKVAPNWEFNIEEEQKLLVEHDRYIFQFPLYWYSSPPLLKKWFDDVLTYGFA         YGSKGKVKGKEFGLAISMGGLEKDYK   NS  GITMDELTKPFHATSLYTGMEFIPSFYAEYEISDEEIDKSAPEYVKYVMN   
   VLVVMAHP RVNRALLDA AQGCEGIQHDLYTHYPEQMIDVAHEQALVDTHDILVFQHPMYWYSCPALLKSWFDSVLSYGWA         YGGSAKLSEKAWVHTVSTGGSERVYQ  RRGYNCFSIAELLRPFEQTARLCGMRYLQPFLADT LSDETLQEYAASYAAWLDGL  
MKKVLINFSHP KVNKALRKA VTGLEGVTNDLYANYPDFMIDIEHEKQLCEAHDIIIFQHPFYWYSSPAIVKEWMDLVLEHGWA         YGSNGALSGKIIFQALSTGGDASSYQ  TDGYNQFTLKELSAPLQATAKLCGLIWLPPFAVHRGLSTEKTLEFAQDYKRIITAL  
MKKVLINFAHP KINSALRAA VEDLEGVTNDLYATYPDFLIDVKREQRLCEEHDILIFQHPFYWYSTPAIMKEWLDVVLENGWA         YGSQGALKGKIFLQAITAGGDNNTYQ  KGAYNQFTIRELISPYLAMAKLCKMEWLPPFVIHRGTPDEKIQAYAEEYRRTVIAL  
VPKVLVIYAHP IANQIMVKK IESLGNVKHDLYAIYPDFFIDVPSEHALLLEYDVIVFQHPLFMYSCPSLLKEWFDRVLGKGFA         FG EQALKGKHWRSVITTGGKEEAFG  AAGYNKYPLQEILQPFELTAALCQMHWISPLVARNVTDMTRY QHAEAYRNWL     
QPKILILFAHP EINVPLFNA SKTIANVTVDLYAEYPTYRIDIDKEQQRLSEHDVIVFMFPLYWYSTPSLLKEWQDLVLEYGFA         YGSEGELVGKKFICALTAGGSESSYR  KDGFNHYTIRELLQPLEQMAELTGMDFLAPFAAGIANEENRIEQHIQNWKRVLIAI  
KNRVLVLFAHP EANKPLFEQ AKRIEGVTVDLYAEYPTFKINIDREQKRLLDHDIIIFQFPLYWYSTPAILKEWQDLVLEYGFA         YGTDGELQGKSLLCSITAGGKKEAYQ  TDGYNHFTIRELLHPIEQTASLCGMNYLAPLASRTALEEGRIQDHVNSYKSLLEA   
KNKVLVIYAHP EVNAPLFAA AQAVDGVTVDLYAEYPQFDINIDKEQARLLEHDVIVFQFPLYWYSTPALLKEWQDLVLEYGFA         YGTDGALKDKLMLCVVSAGGKEEAYK  AEGYNHFTIRQLLAPIEQMAALTSMHYLPPFAARTALEENRIDQHVERYATLLSAL  
MKKILIINGAKGKLNETLTHHAKKTLESLGIEVDTTIVDQGYETHQEVEKILHADAAIWQMPGWWMGEPWIVKKYIDEVFTSGRGKLYASDGRNYGKGGLMQGKKYMLSLTWNAPIEAFNDPNEFFEGIGVDGLYLHLHKAFQFLGLSALPTFICNDVMKNPQVEQYLSSLTTHLHQVFG
MTKILLLNGGKGRLNDTLQALAADILFKNGHEIRQTKIDDGYDVEQEVESFIWADLIIYQCPGWWMGLPWIVKKYIDEVMTAGHGKLYANDGRKYGSGGLAQGKRYMLSTTWNAPAEAFTDPAQFFEGRGIDGVYFPFHKAHEFLGMSALPTFLATDVIKAPNVEATLAAYRQHLQDVIG
MKKILLLNGGKGRLNATLHEAAIAHLDRAGFDVRQTFIDGGYDAQEEVEKFLWADVVIYQMPGWWMGAPWTVKKYIDDVFTAGHGSLYANDGRKYGSGGLVHGKQYMLSLTWNAPQQAFDDPSDFFEGKGVDAVYFPFHKANQFLGMTGLPTFLAVDVMKRPDVPAALAAYEAHLDKVFG
MTNILILNGGKGKLNDTMTQAAKAHLLDLGHQVQVTHIDAGYEVEEEIQKWLWADVVIQQTPAWWMGVPWIVKKYIDEVFTLGHGRLYQSDGRNYGSGGLLQGKQYMLSVTWNAPAIAFTDPKQFFEGAGVDGVYIATHKAYQFLGMTPLPTFMSNDVIKNPTIDRDIQDYQAHLTAVFA
MSNILIVNGAKGELNDTLTTFAEELLSELGHQVDVSRADTNYNIEAEVKKYLWADVVIYQMPGWWMGAPWTVKKYIDDIFTAGHGSLYASDGRKYGSGGLIQGKKYMLSLTWNAPLAAFDDPEQFFHGVGVDGVYLPFHKANQFLGMQALPTFIVNDVIKMPNVAEYLAMYRQHLLENF 
SSNILIINGAKGQLNDTLTEVADGTLRDLGHDVRIVRADSDYDVKAEVQNFLWADVVIWQMPGWWMGAPWTVKKYIDDVFTEGHGTLYASDGRKYGSGGLVQGKKYMLSLTWNAPMEAFTEKDQFFHGVGVDGVYLPFHKANQFLGMEPLPTFIANDVIKMPDVPRYTEEYRKHLVEIFG
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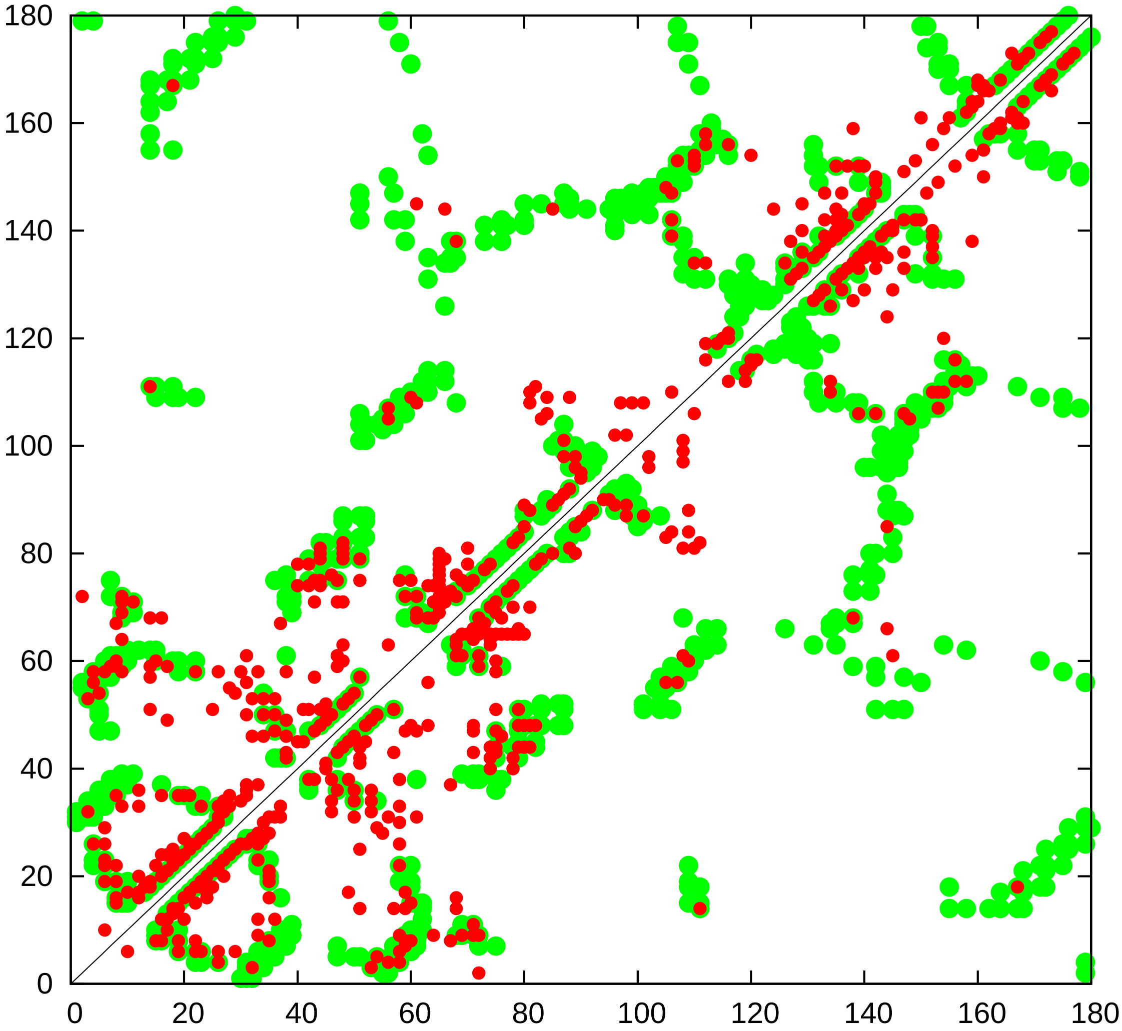

180
160
140
120
100
80
60
40
20
0
0
20
40
60
80
100
120
140
160
180

```
wtaylor@mull1:~/fewpred/pred2amjA$ head folds.full

build2amjA/folds/fold-12-4-1:REMARK Build  Rank   1 Fold   3353  1211.596 26.53 45.67  cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 1210.81
build2amjA/folds/fold-12-5-1:REMARK Build  Rank   1 Fold   3353  1211.596 26.53 45.67  cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 1210.72
build2amjA/folds/fold-12-5-2:REMARK Build  Rank   2 Fold    529  1211.193 32.24 37.57  eEDdaABbcCFfiIHhgGJj eDaBcFiHgJ +B+0.-A+0.+B-2.-a+0.+B-1.-a+1.+B+2.-A+1.+B+1.-a+2. 1210.11
build2amjA/folds/fold-12-4-2:REMARK Build  Rank   2 Fold    529  1211.193 32.24 37.57  eEDdaABbcCFfiIHhgGJj eDaBcFiHgJ +B+0.-A+0.+B-2.-a+0.+B-1.-a+1.+B+2.-A+1.+B+1.-a+2. 1209.9
build2amjA/folds/fold-12-4-3:REMARK Build  Rank   3 Fold   1203  1207.525 26.53 45.51  GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 1206.21
build2amjA/folds/fold-12-5-3:REMARK Build  Rank   3 Fold   1203  1207.525 26.53 45.51  GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 1205.84
build2amjA/folds/fold-12-4-4:REMARK Build  Rank   4 Fold   3363  1205.505 31.15 38.70  cCDdaABbeEFfiIHhgGJj cDaBeFiHgJ +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+3.-A+1.+B+2.-a+2. 1204.02
build2amjA/folds/fold-12-5-4:REMARK Build  Rank   4 Fold   3363  1205.505 31.15 38.70  cCDdaABbeEFfiIHhgGJj cDaBeFiHgJ +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+3.-A+1.+B+2.-a+2. 1203.61
build2amjA/folds/fold-12-4-5:REMARK Build  Rank   5 Fold    328  1205.298 32.24 37.39  EehHIijJGgfFAadDCcbB EhIjGfAdCb +B+0.-A+0.+B-2.-a+0.+B-1.-a+1.+B+2.-A+1.+B+1.-a+2. 1203.52
build2amjA/folds/fold-12-5-5:REMARK Build  Rank   5 Fold    328  1205.298 32.24 37.39  EehHIijJGgfFAadDCcbB EhIjGfAdCb +B+0.-A+0.+B-2.-a+0.+B-1.-a+1.+B+2.-A+1.+B+1.-a+2. 1203.21
```

```
wtaylor@mull1:~/fewpred/pred2amjA$ head folds.best

fold-12-4-1 Build Rank 1 Fold 3353 1211.596 26.53 45.67 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 4574.76
fold-12-5-1 Build Rank 1 Fold 3353 1211.596 26.53 45.67 cCDdaABbeEFfgGJjiIHh cDaBeFgJiH +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 4903.27
fold-12-4-3 Build Rank 3 Fold 1203 1207.525 26.53 45.51 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 4393.73
fold-12-5-3 Build Rank 3 Fold 1203 1207.525 26.53 45.51 GghHIijJEefFCcbBAadD GhIjEfCbAd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 4443.93
fold-12-4-9 Build Rank 9 Fold 3354 1150.657 25.20 45.67 cCDdaABbeEFfgGJjiIhH cDaBeFgJih +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 3271.71
fold-12-5-9 Build Rank 9 Fold 3354 1150.657 25.20 45.67 cCDdaABbeEFfgGJjiIhH cDaBeFgJih +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 5239.77
fold-12-5-10 Build Rank 10 Fold 1204 1146.785 25.20 45.51 GghHIijJEefFCcbBAaDd GhIjEfCbAD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.+A+1. 5206.45
fold-12-4-12 Build Rank 12 Fold 731 1120.151 30.65 36.55 eEJjiIHhgGDdaABbcCFf eJiHgDaBcF +B+0.-A+0.+B-2.-a+0.+B-1.-a+1.+B+2.-A+2.+B+1.-A+1. 3719.28
fold-12-0-3 Build Rank 3 Fold 3212 1102.119 26.45 41.67 gGHhiIJjeEFfcCBbaADd gHiJeFcBaD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 4107.96
fold-12-1-3 Build Rank 3 Fold 3212 1102.119 26.45 41.67 gGHhiIJjeEFfcCBbaADd gHiJeFcBaD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-a+2.+B+3.-A+1. 3695.68
```

```
wtaylor@mull1:~/fewpred/pred2amjA$ sort -nr -k9 folds.best | head

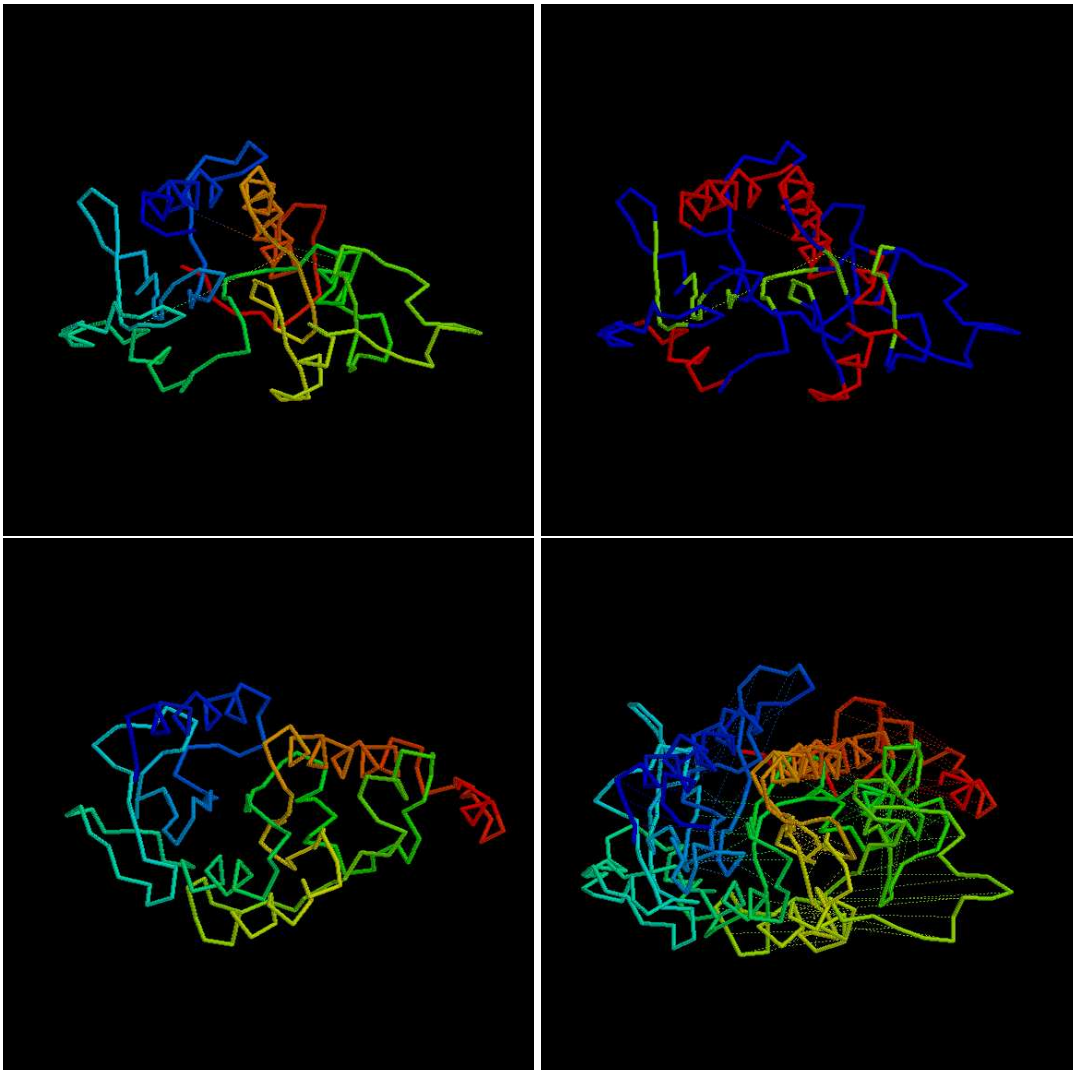
fold-0-23-2 Build Rank 2 Fold 4180 853.203 17.21 49.58 hHIijJKkfFGgeEAaBbcCDd hIjKfGeABcD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-A+1.+B+3.-a+2. 2316.54
fold-0-22-2 Build Rank 2 Fold 4180 853.203 17.21 49.58 hHIijJKkfFGgeEAaBbcCDd hIjKfGeABcD +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-A+1.+B+3.-a+2. 1998.52
fold-0-22-19 Build Rank 19 Fold 4181 774.795 15.63 49.58 hHIijJKkfFGgeEAaBbcCdD hIjKfGeABcd +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-A+1.+B+3.+a+2. 2580.23
fold-0-11-3 Build Rank 3 Fold 1032 851.767 17.36 49.07 CcbBAadDEegGFfjJiIHhkK CbAdEgFjiHk +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-A+1.+B+3.-a+2. 3059.01
fold-0-11-17 Build Rank 17 Fold 1033 776.677 15.83 49.07 CcbBAadDEegGFfjJiIHhKk CbAdEgFjiHK +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-A+1.+B+3.+a+2. 2641.51
fold-0-11-10 Build Rank 10 Fold 1036 810.713 16.52 49.07 CcbBAadDEegGFfjJkKHhiI CbAdEgFjkHi +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-a+2.+B+3.-A+1. 3624.17
fold-0-10-3 Build Rank 3 Fold 1032 851.767 17.36 49.07 CcbBAadDEegGFfjJiIHhkK CbAdEgFjiHk +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-A+1.+B+3.-a+2. 2597.66
fold-0-10-17 Build Rank 17 Fold 1033 776.677 15.83 49.07 CcbBAadDEegGFfjJiIHhKk CbAdEgFjiHK +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-A+1.+B+3.+a+2. 2337.25
fold-0-10-10 Build Rank 10 Fold 1036 810.713 16.52 49.07 CcbBAadDEegGFfjJkKHhiI CbAdEgFjkHi +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-a+2.+B+3.-A+1. 3976.79
fold-0-23-10 Build Rank 10 Fold 4185 787.909 16.21 48.60 hHIijJKkfFGgeEAaDdcCBb hIjKfGeADcB +B+0.-A+0.+B-1.-a+0.+B+1.-a+1.+B+2.-B+4.-a+2.+B+3.-A+1. 2407.44
```

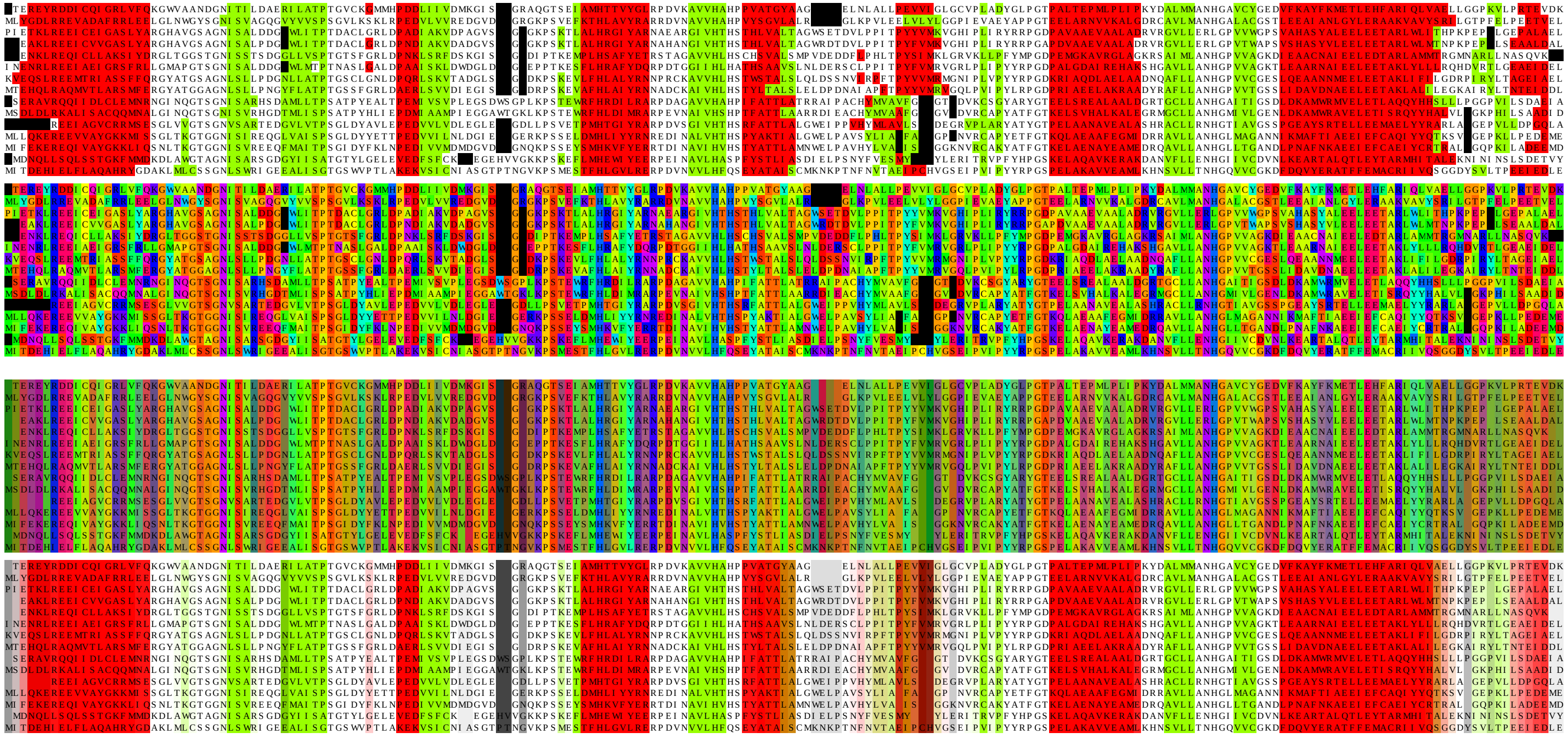
`1vjnA (194)`

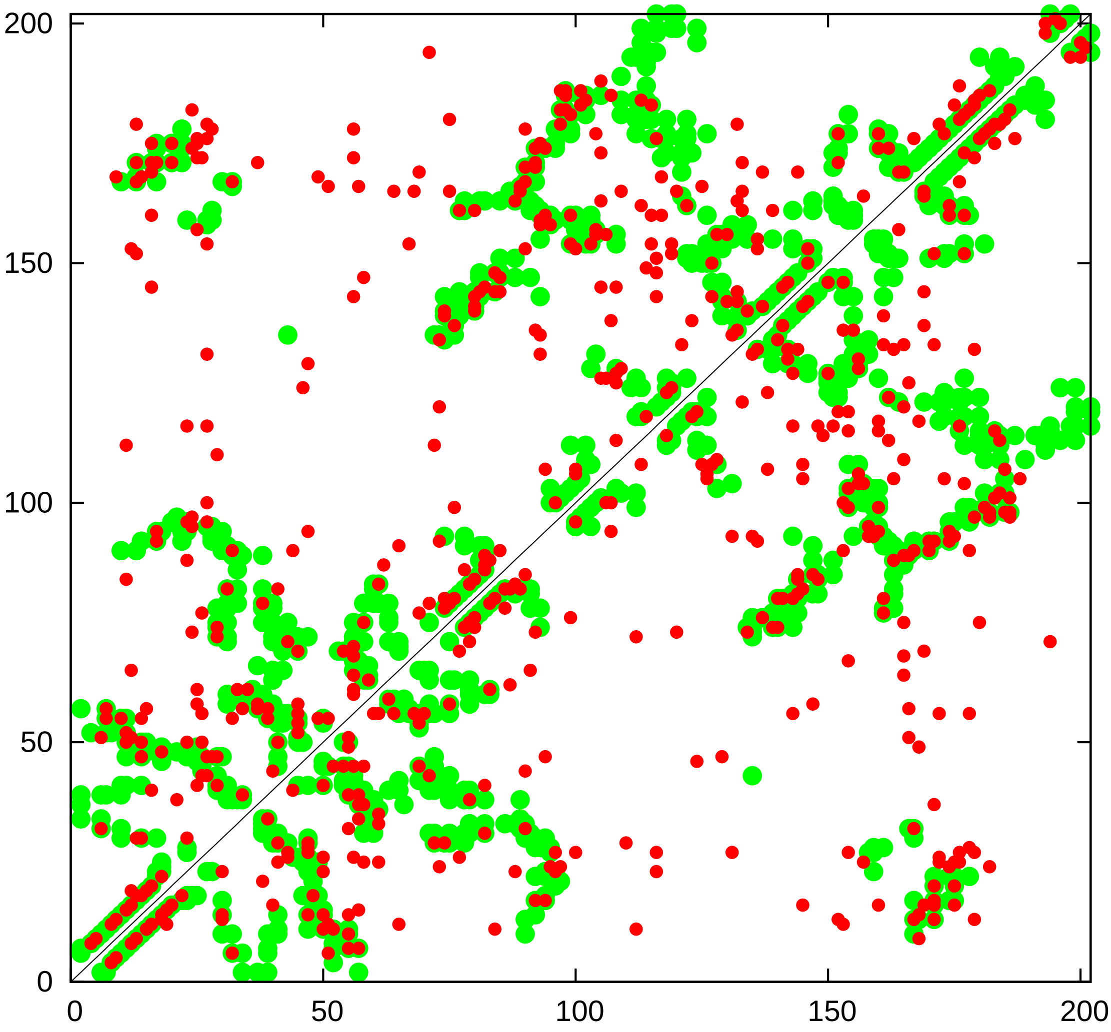
**A putative Zn-dependent hydrolase of the metallo-beta-lactamase superfamily from thermotoga maritima**. Unlike the proteins considered above, `1vjnA` has two $\beta$-sheets, forming a three-layer $\beta\beta\alpha$ architecture (0-6+7-3), with a $3_{10}$ helix on the empty face bringing it close to a 4-layer architecture. The PLATO server considered all three and four layer Forms with the dominant selections being the 4-layer $\alpha\beta\beta\alpha$ architecture, resulting from the prediction of the $3_{10}$ helix and some other loops as $\alpha$-helices. The combinations of almost 20 secondary structure elements over this size of Form are 'astronomic' and the correct fold was not found.

`1opiA (202) = -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.-A+2.+B+4.-a+1.-B+2.+B+3.-A+1`

**L-fuculose-1-phosphate aldolase from Bacteroides thetaiotaomicron**. The same fold was top of both the full and best list and was a good approximation to the native fold with the exception of a swap between the first and third (edge) $\beta$-strands. Although this seems reasonable on the basis of their relative hydrophobicity, the predicted contacts linked the first strand to deeper SSEs and in the reranked topology the top fold corresponded to the native.






200
150
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50
0
0
50
100
150
200

```
wtaylor@mull1:~/newpred/pred2opiA$ head folds.sort

build2opiA/folds/fold-7-1-1:REMARK Build  Rank   1 Fold   2088  1211.513 31.16 38.89  CcaABbdDeEFfkKLliIJjhHGg CaBdeFkLiJhG -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+A+2.-B+6.+a+1.-B+5.+B+4.-A+1. 1211.24
build2opiA/folds/fold-7-0-1:REMARK Build  Rank   1 Fold   2088  1211.513 31.16 38.89  CcaABbdDeEFfkKLliIJjhHGg CaBdeFkLiJhG -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+A+2.-B+6.+a+1.-B+5.+B+4.-A+1. 1210.7
build2opiA/folds/fold-7-1-2:REMARK Build  Rank   2 Fold   2091  1183.490 31.39 37.70  CcaABbdDeEFfkKLliIHhjJGg CaBdeFkLiHjG -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+A+2.-B+6.+a+1.-B+4.+B+5.-A+1. 1182.96
build2opiA/folds/fold-7-0-2:REMARK Build  Rank   2 Fold   2091  1183.490 31.39 37.70  CcaABbdDeEFfkKLliIHhjJGg CaBdeFkLiHjG -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+A+2.-B+6.+a+1.-B+4.+B+5.-A+1. 1182.78
build2opiA/folds/fold-3-0-1:REMARK Build  Rank   1 Fold   2735  1136.571 31.20 36.42  jJIikKlLHhgGDdaABbcCEefF jIklHgDaBcEf -A+0.+B+0.-B+1.-a+0.+a-1.-B-1.+a-2.-B-4.+A-2.-B-3.+B-2.-A-1. 1136.04
build2opiA/folds/fold-3-1-1:REMARK Build  Rank   1 Fold   2735  1136.571 31.20 36.42  jJIikKlLHhgGDdaABbcCEefF jIklHgDaBcEf -A+0.+B+0.-B+1.-a+0.+a-1.-B-1.+a-2.-B-4.+A-2.-B-3.+B-2.-A-1. 1135.65
build2opiA/folds/fold-7-8-1:REMARK Build  Rank   2 Fold   3369  1129.653 28.23 40.02  KklLJjhHiIFfbBAadDCceEGg KlJhiFbAdCeG -A+0.+B+0.-B-1.+B-2.+a+0.-B-3.+a-1.-B-6.+A-2.-B-5.+B-4.-A-1. 1129.23
build2opiA/folds/fold-7-9-1:REMARK Build  Rank   2 Fold   3369  1129.653 28.23 40.02  KklLJjhHiIFfbBAadDCceEGg KlJhiFbAdCeG -A+0.+B+0.-B-1.+B-2.+a+0.-B-3.+a-1.-B-6.+A-2.-B-5.+B-4.-A-1. 1128.33
build2opiA/folds/fold-7-9-2:REMARK Build  Rank   3 Fold   5093  1085.273 25.84 41.99  KkhHLljJiIFfbBAadDCceEGg KhLjiFbAdCeG -A+0.+B+0.-B+2.+B+1.+a+0.-B-1.+a-1.-B-4.+A-2.-B-3.+B-2.-A-1. 1084.29
build2opiA/folds/fold-7-8-2:REMARK Build  Rank   3 Fold   5093  1085.273 25.84 41.99  KkhHLljJiIFfbBAadDCceEGg KhLjiFbAdCeG -A+0.+B+0.-B+2.+B+1.+a+0.-B-1.+a-1.-B-4.+A-2.-B-3.+B-2.-A-1. 1083.74
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wtaylor@mull1:~/newpred/pred2opiA$ head folds.best

fold-7-1-1 Build Rank 1 Fold 2088 1211.513 31.16 38.89 CcaABbdDeEFfkKLliIJjhHGg CaBdeFkLiJhG -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+A+2.-B+6.+a+1.-B+5.+B+4.-A+1. 2881.99
fold-7-0-1 Build Rank 1 Fold 2088 1211.513 31.16 38.89 CcaABbdDeEFfkKLliIJjhHGg CaBdeFkLiJhG -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+A+2.-B+6.+a+1.-B+5.+B+4.-A+1. 2467.89
fold-7-1-2 Build Rank 2 Fold 2091 1183.490 31.39 37.70 CcaABbdDeEFfkKLliIHhjJGg CaBdeFkLiHjG -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+A+2.-B+6.+a+1.-B+4.+B+5.-A+1. 3553.46
fold-7-0-2 Build Rank 2 Fold 2091 1183.490 31.39 37.70 CcaABbdDeEFfkKLliIHhjJGg CaBdeFkLiHjG -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+A+2.-B+6.+a+1.-B+4.+B+5.-A+1. 2625.47
fold-7-8-1 Build Rank 2 Fold 3369 1129.653 28.23 40.02 KklLJjhHiIFfbBAadDCceEGg KlJhiFbAdCeG -A+0.+B+0.-B-1.+B-2.+a+0.-B-3.+a-1.-B-6.+A-2.-B-5.+B-4.-A-1. 3032.97
fold-7-9-1 Build Rank 2 Fold 3369 1129.653 28.23 40.02 KklLJjhHiIFfbBAadDCceEGg KlJhiFbAdCeG -A+0.+B+0.-B-1.+B-2.+a+0.-B-3.+a-1.-B-6.+A-2.-B-5.+B-4.-A-1. 4708.56
fold-7-9-2 Build Rank 3 Fold 5093 1085.273 25.84 41.99 KkhHLljJiIFfbBAadDCceEGg KhLjiFbAdCeG -A+0.+B+0.-B+2.+B+1.+a+0.-B-1.+a-1.-B-4.+A-2.-B-3.+B-2.-A-1. 3736.25
fold-7-8-2 Build Rank 3 Fold 5093 1085.273 25.84 41.99 KkhHLljJiIFfbBAadDCceEGg KhLjiFbAdCeG -A+0.+B+0.-B+2.+B+1.+a+0.-B-1.+a-1.-B-4.+A-2.-B-3.+B-2.-A-1. 4846.5
fold-39-20-2 Build Rank 2 Fold 7539 1081.934 28.72 37.67 dDAabBCcFfeEGgmMJjiIKkhHLl dAbCFeGmJiKhL -A+0.+B+0.-B+1.+B+2.+a+0.-B+3.+B+4.-B+7.+a+1.-B+5.+B+6.-A+1.+A+2. 3530.43
fold-39-20-3 Build Rank 3 Fold 16 1078.719 25.37 42.52 dDCcaABbFfeEGgmMJjiIKkhHlL dCaBFeGmJiKhl -A+0.+B+0.-B-2.+B-1.+a+0.-B+1.+B+2.-B+5.+a+1.-B+3.+B+4.-A+1.-A+2. 2490.77
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wtaylor@mull1:~/newpred/pred2opiA$ sort -nr -k9 folds.best | head

fold-7-8-10 Build Rank 14 Fold 2649 918.080 18.40 49.91 DdeECcaAbBFfKklLIiHhjJGg DeCabFKlIHjG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.-A+2.+B+4.-a+1.-B+2.+B+3.-A+1. 2342.34
fold-7-8-14 Build Rank 18 Fold 2646 906.669 18.82 48.19 DdeECcaAbBFfKklLIiJjhHGg DeCabFKlIJhG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.-A+2.+B+4.-a+1.-B+3.+B+2.-A+1. 2551.55
fold-7-9-25 Build Rank 32 Fold 2652 752.583 15.77 47.72 DdeECcaAbBFfKkhHiILljJGg DeCabFKhiLjG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.-A+2.+B+2.+a+1.-B+4.+B+3.-A+1. 2426.79
fold-7-8-25 Build Rank 32 Fold 2652 752.583 15.77 47.72 DdeECcaAbBFfKkhHiILljJGg DeCabFKhiLjG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.-A+2.+B+2.+a+1.-B+4.+B+3.-A+1. 2630.92
fold-7-9-33 Build Rank 43 Fold 2658 736.725 15.86 46.44 DdeECcaAbBFfKkjJiILlhHGg DeCabFKjiLhG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.-A+2.+B+3.+a+1.-B+4.+B+2.-A+1. 2148.3
fold-7-8-33 Build Rank 43 Fold 2658 736.725 15.86 46.44 DdeECcaAbBFfKkjJiILlhHGg DeCabFKjiLhG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.-A+2.+B+3.+a+1.-B+4.+B+2.-A+1. 1763.38
fold-7-9-13 Build Rank 17 Fold 2679 908.129 20.39 44.54 DdeECcaAbBFfiIlLKkJjhHGg DeCabFilKJhG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.+a+1.+B+4.-A+2.-B+3.+B+2.-A+1. 3455.72
fold-7-8-13 Build Rank 17 Fold 2679 908.129 20.39 44.54 DdeECcaAbBFfiIlLKkJjhHGg DeCabFilKJhG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.+a+1.+B+4.-A+2.-B+3.+B+2.-A+1. 3037.65
fold-7-9-47 Build Rank 60 Fold 2685 698.849 15.70 44.50 DdeECcaAbBFfiIjJKkLlhHGg DeCabFijKLhG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.+a+1.+B+3.-A+2.-B+4.+B+2.-A+1. 2469.99
fold-7-9-5 Build Rank 6 Fold 2670 989.248 22.55 43.86 DdeECcaAbBFfkKLliIHhjJGg DeCabFkLiHjG -A+0.+B+0.-B-1.+B-2.+a+0.-B+1.+A+2.-B+4.+a+1.-B+2.+B+3.-A+1. 3016.37
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