

MODELLER

VISALINI R

21BBT053

1. BUILD_PROFILE.py

```
File Edit View
Z: 1 7.35000 0.00000 0.00006
Z: 1 7.45000 0.00271 0.00005
Z: 1 7.55000 0.00090 0.00004
Z: 1 7.65000 0.00090 0.00004
Z: 1 7.75000 0.00090 0.00003
Z: 1 7.85000 0.00090 0.00003
Z: 1 7.95000 0.00271 0.00003
Z: 1 8.05000 0.00000 0.00002

HITS FOUND IN ITERATION: 1

Dynamically allocated memory at amaxprofile [B,KiB,MiB]: 1112098 1086.033 1.061
> 1shfA 1 58 4800 59 592 35.29 0.28E-03 2 51 539 589 6 56
> 1cnuA 1 439 4400 134 592 27.16 0.53E-02 3 79 50 129 45 125
> 1ark 1 649 6400 60 592 42.00 0.98E-07 4 50 539 588 8 57
> 1azeA 1 777 4500 56 592 39.62 0.12E-02 5 51 537 590 3 55
> 1bu1A 1 1428 4300 57 592 34.00 0.32E-02 6 50 539 589 5 54
> 1fmk 1 3385 5100 437 592 33.33 0.66E-03 7 51 539 589 7 57
> 1g83A 1 3682 4800 161 592 35.29 0.90E-03 8 51 539 589 5 55
> 1gcqA 1 3740 4950 56 592 40.38 0.12E-03 9 52 536 589 3 54
> 1gl5A 1 3845 4500 67 592 40.00 0.14E-02 10 50 539 589 7 56
> 1gr1A 1 3921 5500 211 592 38.33 0.38E-04 11 60 528 589 146 205
> 1hqz1 1 4317 36200 139 592 100.00 0.0 12 139 3 141 1 139
> 1hsq 1 4341 5100 71 592 46.04 0.77E-04 13 48 530 588 11 59
> 1jo8A 1 5152 16000 58 592 100.00 0.0 14 58 535 592 1 58
> 1semA 1 5389 5250 58 592 40.74 0.29E-04 15 54 533 588 1 54
> 1nloC 1 6537 5050 56 592 33.33 0.75E-04 16 51 539 589 4 54
> 1ut1A 1 6750 5500 57 592 40.38 0.81E-05 17 52 536 589 3 54
> 1ootA 1 8041 5000 58 592 38.60 0.10E-03 18 55 534 590 1 57
> 1ud1A 1 8461 6250 98 592 47.76 0.37E-06 19 66 520 590 22 88
> 1h3hA 1 9785 5500 60 592 40.38 0.86E-05 20 52 536 589 5 56
> 1j3tA 1 9952 4800 74 592 40.00 0.36E-03 21 55 533 590 9 63
> 1uhcA 1 10135 4900 79 592 42.31 0.24E-03 22 48 539 588 18 69
> 1uhfA 1 10144 4950 69 592 42.55 0.16E-03 23 47 539 588 13 59
> 1uj0A 1 10164 6000 58 592 48.98 0.69E-06 24 49 539 589 7 55

profile iteration -> Weight Matrix [sec]: 0.000000
profile iteration -> Score Collection [sec]: 7.734375
profile iteration -> Score Collection/Seq [sec]: 0.000698
nonprofile iteration -> DP Stems per seq [all/seq]: 1432.436401

Ln 1, Col 1 18,831 characters 100% Windows (CRLF) UTF-8
```

2. COMPARE.PY

```
File Edit View
159 -----
160 -----
161 -----
162 -----
163 -----
164 -----
165 -----
166 -----

Sequence identity comparison (ID_TABLE):
Diagonal ... number of residues;
Upper triangle ... number of identical residues;
Lower triangle ... % sequence identity, id/min(length).

1g83A @21gcqA @11j08A @11semA @2
1g83A @2 161 19 19 17
1gcqA @1 34 56 21 31
1j08A @1 33 38 58 20
1semA @2 29 55 34 58

Weighted pair-group average clustering based on a distance matrix:
----- 1g83A @2.6 67.7500
|----- 1gcqA @1.7 45.0000
|----- 1semA @2.0 64.5000
|----- 1j08A @1.3

+-----+
68.6600 64.5650 60.4700 56.3750 52.2800 48.1850 44.0900
66.6125 62.5175 58.4225 54.3275 50.2325 46.1375

Total CPU time [seconds] : 0.06

Ln 861, Col 65 35,067 characters 100% Windows (CRLF) UTF-8
```

3. MODEL-SINGLE.PY (DOPE SCORE)

```
File Edit View
427 16478 529K 530K C N 4107 4109 -79.09 -70.20 34.51 2.29 -62.90 146.35 19.93
427 530K 530K N CA 4109 4110 173.74 140.40 -40.80
428 16480 531P 532K C N 4123 4125 -76.93 -70.20 9.47 0.57 -62.90 172.72 23.22
428 532K 532K N CA 4125 4126 147.05 140.40 -40.80
429 16481 532K 533E C N 4132 4134 -101.28 -117.80 24.04 1.29 -63.60 169.67 24.75
429 533E 533E N CA 4134 4135 154.26 136.80 -40.30
430 16482 533E 534N C N 4141 4143 -113.95 -119.90 14.40 0.50 -63.20 172.61 19.24
430 534N 534N N CA 4143 4144 123.89 137.00 -41.10
431 16496 547E 548D C N 4255 4257 -63.90 -63.30 1.61 0.17 -70.90 171.34 8.79
431 548D 548D N CA 4257 4258 -38.50 -40.00 150.30
432 16497 548D 549N C N 4263 4265 -67.45 -63.20 10.32 1.12 55.90 142.42 17.56
432 549N 549N N CA 4265 4266 -31.70 -41.10 39.50
433 16512 563E 564F C N 4308 4309 -116.99 -124.20 96.56 4.37 -63.20 105.98 12.02
433 564F 564F N CA 4308 4309 47.01 143.30 -44.30
434 16523 574L 575E C N 4487 4489 141.32 -117.80 101.33 3.49 54.60 135.30 16.68
434 575E 575E N CA 4489 4490 146.26 136.80 42.40
435 16539 590L 591G C N 4609 4611 44.49 78.70 43.43 1.19 82.20 152.58 9.23
435 591G 591G N CA 4611 4612 -139.34 -166.10 8.50

report_____> Distribution of short non-bonded contacts:

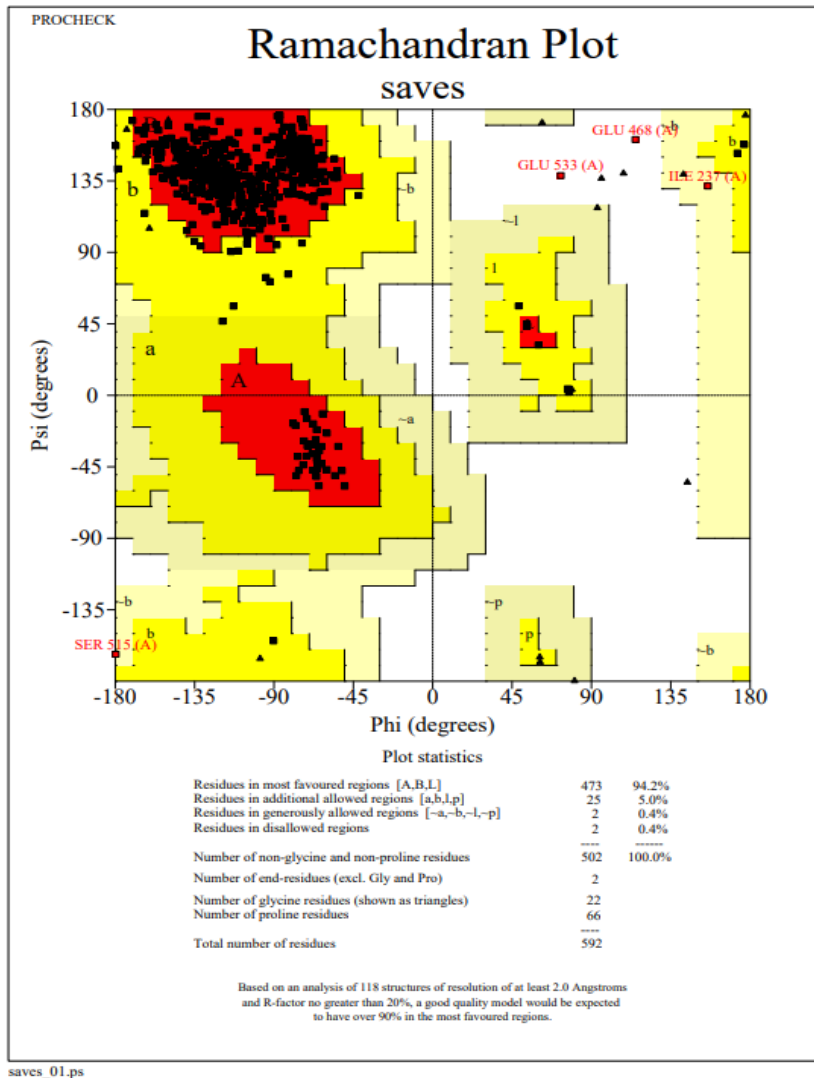
DISTANCE1: 0.00 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40
DISTANCE2: 2.10 2.20 2.30 2.40 2.50 2.60 2.70 2.80 2.90 3.00 3.10 3.20 3.30 3.40 3.50
FREQUENCY: 0 0 0 0 0 0 11 32 135 152 171 252 318 282 318 367

<< end of ENERGY.
|
>> Summary of successfully produced models:
Filename molpdf DOPE score G4341 score
-----
P15891.899990001.pdb 2909.69214 -17794.63086 0.91611
P15891.899990002.pdb 2776.51855 -18146.82031 0.70451
P15891.899990003.pdb 3021.52100 -17469.49805 0.95531
P15891.899990004.pdb 2910.89233 -17878.05859 0.83139
P15891.899990005.pdb 2898.23535 -17747.46680 0.98353

Total CPU time [seconds] : 114.72

Ln 5230, Col 1 4,42,909 characters 100% Windows (CRLF) UTF-8
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4. RAMACHANDRAN PLOT:



INFERENCE:

- The Ramachandran plot analysis of the protein structure indicates that 94.2% of the residues are in the most favored regions, with only 0.4% in disallowed regions.
- The model is of good quality, as it exceeds the general benchmark of having over 90% of residues in the most favored regions.