MODELLER 9.25, 2020/09/03, r11894

PROTEIN STRUCTURE MODELLING BY SATISFACTION OF SPATIAL RESTRAINTS

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Kind, OS, HostName, Kernel, Processor: 4, Windows Vista build 9200, LAPTOP-REA0J2HD, SMP, unknown

Date and time of compilation : 2020/09/03 08:23:39

MODELLER executable type : x86\_64-w64

Job starting time (YY/MM/DD HH:MM:SS): 2021/01/25 12:27:21

check\_ali\_\_\_> Checking the sequence-structure alignment.

Implied intrachain target CA(i)-CA(i+1) distances longer than 8.0 angstroms:

ALN\_POS TMPL RID1 RID2 NAM1 NAM2 DIST

----------------------------------------------

102 1 102 137 S K 19.491

END OF TABLE

read\_to\_681\_> topology.submodel read from topology file: 3

patch\_s\_522\_> Number of disulfides patched in MODEL: 3

mdtrsr\_\_446W> A potential that relies on one protein is used, yet you have at

least one known structure available. MDT, not library, potential is used.

0 atoms in HETATM/BLK residues constrained

to protein atoms within 2.30 angstroms

and protein CA atoms within 10.00 angstroms

0 atoms in residues without defined topology

constrained to be rigid bodies

condens\_443\_> Restraints marked for deletion were removed.

Total number of restraints before, now: 61167 56994

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_484W> Dihedral still outside +-90: 90.1808

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: SER:OXT SER

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 985621

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -66957.1719

<< end of ENERGY.

DOPE score : -66957.171875

>> Model assessment by GA341 potential

Surface library : C:\Program Files\Modeller9.25/modlib/surf5.de

Pair library : C:\Program Files\Modeller9.25/modlib/pair9.de

Chain identifier : \_

% sequence identity : 90.875000

Sequence length : 581

Compactness : 0.124941

Native energy (pair) : -441.860827

Native energy (surface) : -31.283203

Native energy (combined) : -12.055779

Z score (pair) : -12.350094

Z score (surface) : -10.753749

Z score (combined) : -16.814140

GA341 score : 1.000000

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 9862

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 3926.8628

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 4703 0 3 0.006 0.006 52.849 1.000

2 Bond angle potential : 6399 0 23 2.067 2.067 538.62 1.000

3 Stereochemical cosine torsion poten: 3170 0 93 46.395 46.395 1047.4 1.000

4 Stereochemical improper torsion pot: 1995 0 1 1.260 1.260 78.036 1.000

5 Soft-sphere overlap restraints : 9862 0 0 0.002 0.002 3.8119 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 12335 9 29 0.208 0.208 462.24 1.000

10 Distance restraints 2 (N-O) : 12118 9 15 0.232 0.232 545.81 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 580 0 7 4.153 4.153 117.94 1.000

14 Sidechain Chi\_1 dihedral restraints: 486 0 4 55.592 55.592 55.512 1.000

15 Sidechain Chi\_2 dihedral restraints: 367 0 0 59.693 59.693 96.252 1.000

16 Sidechain Chi\_3 dihedral restraints: 161 0 0 67.213 67.213 96.300 1.000

17 Sidechain Chi\_4 dihedral restraints: 49 0 0 88.142 88.142 33.142 1.000

18 Disulfide distance restraints : 3 0 0 0.008 0.008 0.30405E-01 1.000

19 Disulfide angle restraints : 6 0 0 1.379 1.379 0.25181 1.000

20 Disulfide dihedral angle restraints: 3 0 0 28.101 28.101 2.3090 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 8505 0 0 0.379 0.379 219.59 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 579 47 62 25.933 51.899 291.74 1.000

26 Distance restraints 4 (SDCH-SDCH) : 5535 0 2 0.606 0.606 285.06 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

# Heavy relative violation of each residue is written to: ache2.V99990001

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 54932.3359

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 9 : Distance restraints 1 (CA-CA)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 18964 17R 102S CA CA 121 810 12.92 10.70 2.22 4.54 10.70 2.22 4.54

2 18987 18A 102S CA CA 132 810 10.35 8.11 2.24 4.80 8.11 2.24 4.80

3 21378 103K 227E CA CA 816 1756 14.62 9.12 5.50 9.22 9.12 5.50 9.22

4 21379 103K 228W CA CA 816 1765 11.94 8.11 3.83 7.50 8.11 3.83 7.50

5 21384 103K 515T CA CA 816 4037 14.92 9.99 4.93 9.46 9.99 4.93 9.46

6 21385 103K 516G CA CA 816 4044 17.35 12.62 4.72 9.44 12.62 4.72 9.44

-------------------------------------------------------------------------------------------------

Feature 10 : Distance restraints 2 (N-O)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 32964 103K 227E N O 815 1763 15.51 9.48 6.03 8.84 9.48 6.03 8.84

2 32966 103K 513A N O 815 4026 13.44 9.72 3.72 7.18 9.72 3.72 7.18

3 32967 103K 514K N O 815 4035 13.82 7.08 6.74 13.01 7.08 6.74 13.01

4 32968 103K 515T N O 815 4042 17.96 10.56 7.39 12.85 10.56 7.39 12.85

5 35489 227E 103K N O 1755 823 12.86 9.12 3.74 5.53 9.12 3.74 5.53

6 35513 228W 103K N O 1764 823 11.71 8.58 3.14 5.50 8.58 3.14 5.50

-------------------------------------------------------------------------------------------------

Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 16280 1I 2T C N 7 9 -69.78 -78.10 13.24 0.83 -63.20 157.94 20.69

1 2T 2T N CA 9 10 160.10 149.80 -42.10

2 16281 2T 3D C N 14 16 -58.39 -70.90 35.43 1.24 -63.30 157.22 19.71

2 3D 3D N CA 16 17 117.15 150.30 -40.00

3 16318 39V 40D C N 296 298 47.53 -63.30 130.97 16.38 -70.90 154.95 12.76

3 40D 40D N CA 298 299 -109.78 -40.00 150.30

4 16380 101P 102S C N 807 809 -91.87 -136.60 74.50 2.61 -64.10 129.63 8.16

4 102S 102S N CA 809 810 91.62 151.20 -35.00

5 16381 102S 103K C N 813 815 -74.53 -70.20 83.62 6.16 56.60 132.40 14.62

5 103K 103K N CA 815 816 56.89 140.40 38.60

6 16382 103K 104A C N 822 824 -147.54 -134.00 14.87 0.73 -62.50 -162.52 36.92

6 104A 104A N CA 824 825 140.87 147.00 -40.90

7 16383 104A 105R C N 827 829 -130.34 -125.20 7.69 0.42 -63.00 -171.58 21.84

7 105R 105R N CA 829 830 134.88 140.60 -41.10

8 16385 106L 107R C N 846 848 141.73 -125.20 99.34 4.85 -63.00 -146.22 25.53

8 107R 107R N CA 848 849 105.85 140.60 -41.10

9 16386 107R 108H C N 857 859 -151.25 -125.60 34.94 0.86 -63.20 178.42 27.99

9 108H 108H N CA 859 860 162.52 138.80 -42.30

10 16387 108H 109G C N 867 869 -146.64 -167.20 22.95 0.35 82.20 -156.27 15.33

10 109G 109G N CA 869 870 164.39 174.60 8.50

11 16388 109G 110R C N 871 873 -105.07 -125.20 30.78 1.70 -63.00 160.63 24.61

11 110R 110R N CA 873 874 163.88 140.60 -41.10

12 16389 110R 111G C N 882 884 -82.54 -80.20 54.77 2.27 82.20 -161.42 7.85

12 111G 111G N CA 884 885 119.38 174.10 8.50

13 16390 111G 112A C N 886 888 -87.59 -68.20 44.65 2.96 -62.50 135.92 23.58

13 112A 112A N CA 888 889 -174.48 145.30 -40.90

14 16391 112A 113N C N 891 893 -56.52 -71.20 36.01 1.96 -63.20 151.17 19.27

14 113N 113N N CA 893 894 109.92 142.80 -41.10

15 16392 113N 114G C N 899 901 -67.02 -80.20 31.80 0.75 82.20 -157.66 6.66

15 114G 114G N CA 901 902 145.16 174.10 8.50

16 16394 115V 116E C N 910 912 -152.72 -117.80 35.66 1.15 -63.60 -163.04 31.23

16 116E 116E N CA 912 913 144.05 136.80 -40.30

17 16395 116E 117H C N 919 921 -106.07 -125.60 41.87 1.19 -63.20 150.30 16.58

17 117H 117H N CA 921 922 101.76 138.80 -42.30

18 16397 118A 119A C N 934 936 -74.22 -68.20 6.07 0.54 -62.50 174.98 29.26

18 119A 119A N CA 936 937 144.52 145.30 -40.90

19 16398 119A 120K C N 939 941 -78.75 -70.20 9.02 0.72 -62.90 179.04 22.43

19 120K 120K N CA 941 942 137.53 140.40 -40.80

20 16399 120K 121T C N 948 950 -134.42 -124.80 39.16 1.41 -63.20 153.92 24.35

20 121T 121T N CA 950 951 -178.55 143.50 -42.10

21 16400 121T 122D C N 955 957 -60.72 -70.90 18.27 0.63 -63.30 175.14 21.77

21 122D 122D N CA 957 958 135.12 150.30 -40.00

22 16402 123P 124D C N 970 972 -165.96 -96.50 71.59 2.91 -63.30 171.12 18.48

22 124D 124D N CA 972 973 96.90 114.20 -40.00

23 16403 124D 125H C N 978 980 -112.79 -125.60 54.72 1.82 -63.20 137.18 14.81

23 125H 125H N CA 980 981 85.60 138.80 -42.30

24 16406 127I 128H C N 1004 1006 -118.06 -125.60 12.68 0.33 -63.20 179.50 19.67

24 128H 128H N CA 1006 1007 128.60 138.80 -42.30

25 16407 128H 129S C N 1014 1016 -148.64 -136.60 12.50 0.58 -64.10 -163.72 20.27

25 129S 129S N CA 1016 1017 147.86 151.20 -35.00

26 16408 129S 130A C N 1020 1022 -155.34 -134.00 22.14 0.96 -62.50 -159.25 37.87

26 130A 130A N CA 1022 1023 141.11 147.00 -40.90

27 16409 130A 131T C N 1025 1027 -146.34 -124.80 22.05 1.04 -63.20 -171.03 29.64

27 131T 131T N CA 1027 1028 148.20 143.50 -42.10

28 16411 132P 133Q C N 1039 1041 -83.18 -73.00 17.49 1.33 -63.80 167.91 23.71

28 133Q 133Q N CA 1041 1042 126.49 140.70 -40.30

29 16412 133Q 134N C N 1048 1050 -105.97 -119.90 33.21 1.16 -63.20 154.01 17.26

29 134N 134N N CA 1050 1051 106.85 137.00 -41.10

30 16413 134N 135T C N 1056 1058 -133.42 -124.80 14.48 0.45 -63.20 177.26 27.34

30 135T 135T N CA 1058 1059 155.14 143.50 -42.10

31 16415 136T 137N C N 1070 1072 -113.29 -119.90 88.51 3.87 55.90 169.44 18.59

31 137N 137N N CA 1072 1073 48.74 137.00 39.50

32 16472 193P 194G C N 1497 1499 65.23 82.20 27.37 2.04 -62.40 130.71 24.28

32 194G 194G N CA 1499 1500 -12.97 8.50 -41.20

33 16496 217E 218N C N 1690 1692 -108.08 -63.20 85.44 9.18 -63.20 85.44 9.18

33 218N 218N N CA 1692 1693 31.60 -41.10 -41.10

34 16506 227E 228W C N 1762 1764 -80.35 -63.00 69.20 7.81 -63.00 69.20 7.81

34 228W 228W N CA 1764 1765 22.79 -44.20 -44.20

35 16513 234E 235S C N 1823 1825 70.75 -72.40 157.89 12.60 -64.10 171.51 15.34

35 235S 235S N CA 1825 1826 -140.97 152.40 -35.00

36 16614 335G 336A C N 2560 2562 -81.10 -62.50 36.30 6.94 -62.50 36.30 6.94

36 336A 336A N CA 2562 2563 -72.07 -40.90 -40.90

37 16651 372D 373F C N 2852 2854 -94.06 -63.20 63.08 7.17 -63.20 63.08 7.17

37 373F 373F N CA 2854 2855 10.71 -44.30 -44.30

38 16715 436F 437F C N 3385 3387 -96.18 -63.20 37.51 6.74 -63.20 37.51 6.74

38 437F 437F N CA 3387 3388 -62.17 -44.30 -44.30

39 16847 568S 569W C N 4479 4481 -55.49 -63.00 11.21 1.31 -124.90 178.16 9.92

39 569W 569W N CA 4481 4482 -52.52 -44.20 143.40

40 16850 571G 572S C N 4504 4506 -81.43 -72.40 9.76 0.77 -64.10 177.16 13.94

40 572S 572S N CA 4506 4507 148.68 152.40 -35.00

41 16851 572S 573E C N 4510 4512 -78.50 -69.30 10.00 0.88 -63.60 179.50 23.15

41 573E 573E N CA 4512 4513 138.58 142.50 -40.30

42 16853 574C 575E C N 4525 4527 -82.43 -69.30 39.96 2.58 -63.60 140.72 19.82

42 575E 575E N CA 4527 4528 -179.76 142.50 -40.30

43 16854 575E 576N C N 4534 4536 -54.79 -71.20 22.20 1.21 -63.20 169.15 21.61

43 576N 576N N CA 4536 4537 127.84 142.80 -41.10

44 16855 576N 577N C N 4542 4544 -130.34 -119.90 31.26 1.16 -63.20 166.57 24.62

44 577N 577N N CA 4544 4545 166.46 137.00 -41.10

45 16856 577N 578N C N 4550 4552 -74.96 -71.20 21.66 1.29 -63.20 155.22 20.06

45 578N 578N N CA 4552 4553 164.13 142.80 -41.10

46 16857 578N 579A C N 4558 4560 -66.64 -68.20 5.67 0.51 -62.50 168.40 27.80

46 579A 579A N CA 4560 4561 150.75 145.30 -40.90

47 16858 579A 580A C N 4563 4565 -69.34 -68.20 4.64 0.33 -62.50 169.44 28.11

47 580A 580A N CA 4565 4566 149.80 145.30 -40.90

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 28 72 215 286 400 416 521 672 720 798

<< end of ENERGY.

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: SER:OXT SER

>> ENERGY; Differences between the model's features and restraints:

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Number of non-bonded pairs (excluding 1-2,1-3,1-4): 984585

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -66902.8281

<< end of ENERGY.

DOPE score : -66902.828125

>> Model assessment by GA341 potential

Surface library : C:\Program Files\Modeller9.25/modlib/surf5.de

Pair library : C:\Program Files\Modeller9.25/modlib/pair9.de

Chain identifier : \_

% sequence identity : 90.875000

Sequence length : 581

Compactness : 0.188547

Native energy (pair) : -441.777993

Native energy (surface) : -29.656038

Native energy (combined) : -11.400718

Z score (pair) : -11.544038

Z score (surface) : -10.815771

Z score (combined) : -14.683325

GA341 score : 1.000000

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 9860

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 4063.1013

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 4703 0 3 0.006 0.006 56.121 1.000

2 Bond angle potential : 6399 0 27 2.099 2.099 557.36 1.000

3 Stereochemical cosine torsion poten: 3170 0 99 46.073 46.073 1038.0 1.000

4 Stereochemical improper torsion pot: 1995 0 1 1.257 1.257 78.017 1.000

5 Soft-sphere overlap restraints : 9860 0 0 0.002 0.002 3.6806 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 12335 9 29 0.210 0.210 467.91 1.000

10 Distance restraints 2 (N-O) : 12118 14 35 0.251 0.251 668.63 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 580 0 6 4.188 4.188 119.95 1.000

14 Sidechain Chi\_1 dihedral restraints: 486 0 1 54.394 54.394 51.990 1.000

15 Sidechain Chi\_2 dihedral restraints: 367 0 2 60.898 60.898 110.54 1.000

16 Sidechain Chi\_3 dihedral restraints: 161 0 0 60.387 60.387 91.218 1.000

17 Sidechain Chi\_4 dihedral restraints: 49 0 0 103.203 103.203 33.984 1.000

18 Disulfide distance restraints : 3 0 0 0.008 0.008 0.31967E-01 1.000

19 Disulfide angle restraints : 6 0 0 1.420 1.420 0.26729 1.000

20 Disulfide dihedral angle restraints: 3 0 0 27.376 27.376 2.2159 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 8505 0 1 0.331 0.331 167.22 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 579 51 71 26.790 51.943 324.67 1.000

26 Distance restraints 4 (SDCH-SDCH) : 5535 0 3 0.614 0.614 291.32 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

# Heavy relative violation of each residue is written to: ache2.V99990002

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 55309.7148

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 9 : Distance restraints 1 (CA-CA)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 18964 17R 102S CA CA 121 810 12.94 10.70 2.24 4.58 10.70 2.24 4.58

2 18987 18A 102S CA CA 132 810 10.36 8.11 2.25 4.83 8.11 2.25 4.83

3 21378 103K 227E CA CA 816 1756 14.59 9.12 5.47 9.18 9.12 5.47 9.18

4 21379 103K 228W CA CA 816 1765 11.94 8.11 3.83 7.51 8.11 3.83 7.51

5 21384 103K 515T CA CA 816 4037 14.88 9.99 4.90 9.40 9.99 4.90 9.40

6 21385 103K 516G CA CA 816 4044 17.32 12.62 4.70 9.39 12.62 4.70 9.39

-------------------------------------------------------------------------------------------------

Feature 10 : Distance restraints 2 (N-O)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 32410 80E 476H N O 625 3720 13.33 10.58 2.75 5.72 10.58 2.75 5.72

2 32457 83W 476H N O 651 3720 12.59 10.24 2.34 4.65 10.24 2.34 4.65

3 32964 103K 227E N O 815 1763 15.52 9.48 6.04 8.86 9.48 6.04 8.86

4 32966 103K 513A N O 815 4026 13.44 9.72 3.72 7.18 9.72 3.72 7.18

5 32967 103K 514K N O 815 4035 13.79 7.08 6.71 12.96 7.08 6.71 12.96

6 32968 103K 515T N O 815 4042 17.94 10.56 7.37 12.81 10.56 7.37 12.81

7 35489 227E 103K N O 1755 823 12.92 9.12 3.80 5.62 9.12 3.80 5.62

8 35513 228W 103K N O 1764 823 11.86 8.58 3.28 5.76 8.58 3.28 5.76

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Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 16280 1I 2T C N 7 9 -69.30 -78.10 10.66 0.45 -63.20 174.22 22.74

1 2T 2T N CA 9 10 143.78 149.80 -42.10

2 16281 2T 3D C N 14 16 -126.19 -96.50 30.85 1.27 -63.30 174.29 18.71

2 3D 3D N CA 16 17 122.55 114.20 -40.00

3 16318 39V 40D C N 296 298 59.89 -63.30 144.20 18.17 -70.90 161.50 13.45

3 40D 40D N CA 298 299 -114.95 -40.00 150.30

4 16327 48V 49P C N 376 378 -64.35 -58.70 34.85 2.45 -64.50 143.31 10.69

4 49P 49P N CA 378 379 3.89 -30.50 147.20

5 16328 49P 50A C N 383 385 70.59 -68.20 139.86 11.25 -68.20 139.86 11.25

5 50A 50A N CA 385 386 128.03 145.30 145.30

6 16380 101P 102S C N 807 809 -92.69 -136.60 74.05 2.61 -64.10 129.76 8.15

6 102S 102S N CA 809 810 91.57 151.20 -35.00

7 16381 102S 103K C N 813 815 -69.70 -70.20 54.81 3.96 56.60 134.76 12.95

7 103K 103K N CA 815 816 85.59 140.40 38.60

8 16383 104A 105R C N 827 829 77.02 57.30 27.68 1.81 -63.00 152.21 27.58

8 105R 105R N CA 829 830 18.58 38.00 -41.10

9 16384 105R 106L C N 838 840 -103.38 -108.50 14.29 0.81 -63.50 177.50 27.08

9 106L 106L N CA 840 841 145.84 132.50 -41.20

10 16386 107R 108H C N 857 859 -173.53 -125.60 67.85 1.68 -63.20 171.18 28.25

10 108H 108H N CA 859 860 -173.18 138.80 -42.30

11 16387 108H 109G C N 867 869 -63.10 -80.20 44.68 1.07 82.20 -168.77 6.55

11 109G 109G N CA 869 870 132.82 174.10 8.50

12 16388 109G 110R C N 871 873 -169.43 -125.20 54.35 1.60 -63.00 -178.75 31.46

12 110R 110R N CA 873 874 172.19 140.60 -41.10

13 16389 110R 111G C N 882 884 -134.68 -167.20 38.00 0.63 82.20 -155.23 15.67

13 111G 111G N CA 884 885 154.95 174.60 8.50

14 16390 111G 112A C N 886 888 -68.86 -68.20 1.18 0.08 -62.50 172.93 28.66

14 112A 112A N CA 888 889 146.29 145.30 -40.90

15 16391 112A 113N C N 891 893 -100.17 -119.90 30.07 0.90 -63.20 159.74 18.18

15 113N 113N N CA 893 894 114.30 137.00 -41.10

16 16394 115V 116E C N 910 912 -135.31 -117.80 75.46 3.42 -63.60 130.89 21.36

16 116E 116E N CA 912 913 -149.80 136.80 -40.30

17 16395 116E 117H C N 919 921 -53.53 -67.60 14.39 0.99 -63.20 179.52 23.05

17 117H 117H N CA 921 922 136.96 140.00 -42.30

18 16396 117H 118A C N 929 931 -119.16 -134.00 16.70 0.38 -62.50 -171.49 33.91

18 118A 118A N CA 931 932 139.32 147.00 -40.90

19 16397 118A 119A C N 934 936 -132.12 -134.00 2.85 0.09 -62.50 -172.36 34.48

19 119A 119A N CA 936 937 144.86 147.00 -40.90

20 16398 119A 120K C N 939 941 -118.01 -118.00 6.80 0.33 -62.90 -178.34 21.25

20 120K 120K N CA 941 942 132.30 139.10 -40.80

21 16399 120K 121T C N 948 950 -145.47 -124.80 30.59 0.97 -63.20 172.70 27.46

21 121T 121T N CA 950 951 166.05 143.50 -42.10

22 16400 121T 122D C N 955 957 -101.52 -96.50 5.04 0.21 -63.30 158.43 17.59

22 122D 122D N CA 957 958 113.75 114.20 -40.00

23 16404 125H 126L C N 988 990 -99.39 -108.50 12.02 0.54 -63.50 169.71 21.78

23 126L 126L N CA 990 991 124.67 132.50 -41.20

24 16406 127I 128H C N 1004 1006 -148.73 -125.60 62.72 1.90 -63.20 147.85 23.90

24 128H 128H N CA 1006 1007 -162.90 138.80 -42.30

25 16407 128H 129S C N 1014 1016 -71.85 -72.40 18.04 1.08 -64.10 154.76 11.69

25 129S 129S N CA 1016 1017 170.43 152.40 -35.00

26 16408 129S 130A C N 1020 1022 -68.65 -68.20 18.19 1.45 -62.50 155.74 25.83

26 130A 130A N CA 1022 1023 163.48 145.30 -40.90

27 16409 130A 131T C N 1025 1027 -59.78 -78.10 19.19 1.00 -63.20 173.85 22.07

27 131T 131T N CA 1027 1028 144.08 149.80 -42.10

28 16410 131T 132P C N 1032 1034 -59.95 -58.70 19.02 1.67 -64.50 163.39 12.43

28 132P 132P N CA 1034 1035 -49.47 -30.50 147.20

29 16411 132P 133Q C N 1039 1041 -171.68 -121.10 65.90 2.08 -63.80 174.97 31.02

29 133Q 133Q N CA 1041 1042 -178.06 139.70 -40.30

30 16412 133Q 134N C N 1048 1050 -126.74 -119.90 30.19 1.20 -63.20 165.21 24.26

30 134N 134N N CA 1050 1051 166.40 137.00 -41.10

31 16413 134N 135T C N 1056 1058 -78.83 -78.10 26.38 1.10 -63.20 142.58 19.32

31 135T 135T N CA 1058 1059 176.17 149.80 -42.10

32 16415 136T 137N C N 1070 1072 -121.93 -119.90 84.40 3.88 55.90 178.31 19.39

32 137N 137N N CA 1072 1073 52.63 137.00 39.50

33 16472 193P 194G C N 1497 1499 65.25 82.20 26.49 1.99 -62.40 130.98 24.36

33 194G 194G N CA 1499 1500 -11.85 8.50 -41.20

34 16496 217E 218N C N 1690 1692 -108.84 -63.20 87.33 9.39 -63.20 87.33 9.39

34 218N 218N N CA 1692 1693 33.35 -41.10 -41.10

35 16506 227E 228W C N 1762 1764 -80.90 -63.00 70.98 8.01 -63.00 70.98 8.01

35 228W 228W N CA 1764 1765 24.49 -44.20 -44.20

36 16513 234E 235S C N 1823 1825 71.84 -72.40 159.11 12.70 -64.10 172.04 15.47

36 235S 235S N CA 1825 1826 -140.43 152.40 -35.00

37 16614 335G 336A C N 2560 2562 -80.74 -62.50 36.24 6.91 -62.50 36.24 6.91

37 336A 336A N CA 2562 2563 -72.22 -40.90 -40.90

38 16651 372D 373F C N 2852 2854 -93.92 -63.20 63.19 7.19 -63.20 63.19 7.19

38 373F 373F N CA 2854 2855 10.92 -44.30 -44.30

39 16715 436F 437F C N 3385 3387 -94.99 -63.20 37.01 6.67 -63.20 37.01 6.67

39 437F 437F N CA 3387 3388 -63.24 -44.30 -44.30

40 16754 475L 476H C N 3709 3711 -12.50 -67.60 129.11 11.27 -67.60 129.11 11.27

40 476H 476H N CA 3711 3712 -103.24 140.00 140.00

41 16755 476H 477G C N 3719 3721 -60.76 -62.40 38.62 5.85 82.20 143.39 10.01

41 477G 477G N CA 3721 3722 -2.62 -41.20 8.50

42 16799 520V 521D C N 4072 4074 -62.82 -63.30 9.59 1.16 -70.90 160.33 8.30

42 521D 521D N CA 4074 4075 -49.58 -40.00 150.30

43 16800 521D 522G C N 4080 4082 -65.16 -62.40 3.44 0.50 82.20 154.87 11.73

43 522G 522G N CA 4082 4083 -39.15 -41.20 8.50

44 16849 570V 571G C N 4500 4502 94.51 78.70 30.23 0.47 82.20 160.10 8.39

44 571G 571G N CA 4502 4503 168.13 -166.10 8.50

45 16850 571G 572S C N 4504 4506 -83.59 -72.40 24.35 1.13 -64.10 152.22 12.29

45 572S 572S N CA 4506 4507 174.03 152.40 -35.00

46 16851 572S 573E C N 4510 4512 -70.98 -69.30 10.22 0.72 -63.60 167.28 22.71

46 573E 573E N CA 4512 4513 152.59 142.50 -40.30

47 16853 574C 575E C N 4525 4527 -75.43 -69.30 16.33 1.03 -63.60 162.50 22.32

47 575E 575E N CA 4527 4528 157.63 142.50 -40.30

48 16854 575E 576N C N 4534 4536 -81.11 -71.20 27.52 1.52 -63.20 151.49 19.95

48 576N 576N N CA 4536 4537 168.47 142.80 -41.10

49 16855 576N 577N C N 4542 4544 -68.06 -71.20 20.05 1.20 -63.20 164.17 20.26

49 577N 577N N CA 4544 4545 123.00 142.80 -41.10

50 16857 578N 579A C N 4558 4560 -62.65 -68.20 5.92 0.43 -62.50 175.89 28.83

50 579A 579A N CA 4560 4561 143.21 145.30 -40.90

51 16858 579A 580A C N 4563 4565 -75.69 -68.20 10.08 0.64 -62.50 167.57 28.13

51 580A 580A N CA 4565 4566 152.05 145.30 -40.90

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 27 65 220 286 430 458 520 621 739 742

<< end of ENERGY.

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: SER:OXT SER

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 991172

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -66755.7734

<< end of ENERGY.

DOPE score : -66755.773438

>> Model assessment by GA341 potential

Surface library : C:\Program Files\Modeller9.25/modlib/surf5.de

Pair library : C:\Program Files\Modeller9.25/modlib/pair9.de

Chain identifier : \_

% sequence identity : 90.875000

Sequence length : 581

Compactness : 0.155265

Native energy (pair) : -426.972454

Native energy (surface) : -28.614181

Native energy (combined) : -11.176466

Z score (pair) : -11.725996

Z score (surface) : -10.579478

Z score (combined) : -14.646024

GA341 score : 1.000000

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 9776

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 3996.1636

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

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1 Bond length potential : 4703 0 2 0.006 0.006 54.250 1.000

2 Bond angle potential : 6399 0 25 2.119 2.119 565.21 1.000

3 Stereochemical cosine torsion poten: 3170 0 94 46.004 46.004 1039.3 1.000

4 Stereochemical improper torsion pot: 1995 0 1 1.299 1.299 81.691 1.000

5 Soft-sphere overlap restraints : 9776 0 0 0.002 0.002 3.9225 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 12335 8 29 0.209 0.209 468.70 1.000

10 Distance restraints 2 (N-O) : 12118 12 23 0.243 0.243 610.75 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 580 0 8 4.300 4.300 126.45 1.000

14 Sidechain Chi\_1 dihedral restraints: 486 0 3 53.984 53.984 48.043 1.000

15 Sidechain Chi\_2 dihedral restraints: 367 0 3 57.204 57.204 100.27 1.000

16 Sidechain Chi\_3 dihedral restraints: 161 0 0 68.226 68.226 93.421 1.000

17 Sidechain Chi\_4 dihedral restraints: 49 0 0 87.065 87.065 32.286 1.000

18 Disulfide distance restraints : 3 0 0 0.022 0.022 0.24101 1.000

19 Disulfide angle restraints : 6 0 0 1.824 1.824 0.44085 1.000

20 Disulfide dihedral angle restraints: 3 0 0 26.165 26.165 1.9483 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 8505 0 0 0.331 0.331 164.17 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 579 54 69 25.281 52.683 292.94 1.000

26 Distance restraints 4 (SDCH-SDCH) : 5535 0 2 0.646 0.646 312.13 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

# Heavy relative violation of each residue is written to: ache2.V99990003

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 55171.4180

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

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Feature 9 : Distance restraints 1 (CA-CA)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 18987 18A 102S CA CA 132 810 10.29 8.11 2.18 4.68 8.11 2.18 4.68

2 21378 103K 227E CA CA 816 1756 14.62 9.12 5.50 9.22 9.12 5.50 9.22

3 21379 103K 228W CA CA 816 1765 11.94 8.11 3.83 7.51 8.11 3.83 7.51

4 21384 103K 515T CA CA 816 4037 14.99 9.99 5.01 9.61 9.99 5.01 9.61

5 21385 103K 516G CA CA 816 4044 17.35 12.62 4.73 9.45 12.62 4.73 9.45

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Feature 10 : Distance restraints 2 (N-O)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 32964 103K 227E N O 815 1763 15.52 9.48 6.05 8.86 9.48 6.05 8.86

2 32966 103K 513A N O 815 4026 13.46 9.72 3.74 7.23 9.72 3.74 7.23

3 32967 103K 514K N O 815 4035 13.92 7.08 6.84 13.20 7.08 6.84 13.20

4 32968 103K 515T N O 815 4042 17.97 10.56 7.41 12.87 10.56 7.41 12.87

5 35489 227E 103K N O 1755 823 13.07 9.12 3.95 5.84 9.12 3.95 5.84

6 35513 228W 103K N O 1764 823 11.97 8.58 3.39 5.94 8.58 3.39 5.94

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Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 16280 1I 2T C N 7 9 -115.75 -124.80 10.63 0.40 -63.20 -172.50 27.54

1 2T 2T N CA 9 10 137.92 143.50 -42.10

2 16281 2T 3D C N 14 16 -84.78 -96.50 19.85 0.83 -63.30 139.84 16.07

2 3D 3D N CA 16 17 98.18 114.20 -40.00

3 16318 39V 40D C N 296 298 50.29 -63.30 134.42 16.79 -70.90 155.75 12.87

3 40D 40D N CA 298 299 -111.87 -40.00 150.30

4 16380 101P 102S C N 807 809 -88.22 -136.60 76.44 2.61 -64.10 129.29 8.24

4 102S 102S N CA 809 810 92.01 151.20 -35.00

5 16381 102S 103K C N 813 815 -64.12 -70.20 62.91 4.41 56.60 126.92 12.58

5 103K 103K N CA 815 816 77.78 140.40 38.60

6 16382 103K 104A C N 822 824 -129.64 -134.00 32.35 1.73 -62.50 169.69 25.52

6 104A 104A N CA 824 825 114.94 147.00 -40.90

7 16383 104A 105R C N 827 829 -107.97 -125.20 28.09 0.91 -63.00 165.73 19.77

7 105R 105R N CA 829 830 118.41 140.60 -41.10

8 16384 105R 106L C N 838 840 -122.60 -108.50 20.92 1.18 -63.50 168.93 20.93

8 106L 106L N CA 840 841 117.05 132.50 -41.20

9 16385 106L 107R C N 846 848 -169.17 -125.20 61.60 1.87 -63.00 171.87 30.10

9 107R 107R N CA 848 849 -176.26 140.60 -41.10

10 16386 107R 108H C N 857 859 -67.23 -67.60 11.08 0.86 -63.20 166.67 21.09

10 108H 108H N CA 859 860 151.07 140.00 -42.30

11 16387 108H 109G C N 867 869 -137.88 -167.20 35.34 0.62 82.20 -157.52 15.46

11 109G 109G N CA 869 870 154.87 174.60 8.50

12 16388 109G 110R C N 871 873 -125.11 -125.20 6.45 0.31 -63.00 -177.27 28.97

12 110R 110R N CA 873 874 147.05 140.60 -41.10

13 16389 110R 111G C N 882 884 94.96 78.70 60.10 1.09 82.20 128.18 6.86

13 111G 111G N CA 884 885 136.04 -166.10 8.50

14 16390 111G 112A C N 886 888 -172.30 -134.00 46.91 1.17 -62.50 -178.10 35.57

14 112A 112A N CA 888 889 174.08 147.00 -40.90

15 16391 112A 113N C N 891 893 -73.27 -71.20 4.08 0.32 -63.20 179.90 23.05

15 113N 113N N CA 893 894 139.28 142.80 -41.10

16 16392 113N 114G C N 899 901 100.90 78.70 68.58 1.14 82.20 121.95 6.84

16 114G 114G N CA 901 902 129.01 -166.10 8.50

17 16394 115V 116E C N 910 912 -112.87 -117.80 17.50 0.77 -63.60 167.71 20.09

17 116E 116E N CA 912 913 120.00 136.80 -40.30

18 16395 116E 117H C N 919 921 -115.49 -125.60 39.92 1.69 -63.20 149.71 22.14

18 117H 117H N CA 921 922 177.42 138.80 -42.30

19 16396 117H 118A C N 929 931 -109.03 -134.00 26.20 1.18 -62.50 170.62 30.43

19 118A 118A N CA 931 932 154.95 147.00 -40.90

20 16397 118A 119A C N 934 936 -70.64 -68.20 33.58 2.79 -62.50 152.93 24.68

20 119A 119A N CA 936 937 111.81 145.30 -40.90

21 16398 119A 120K C N 939 941 -141.59 -118.00 52.80 2.15 -62.90 154.42 24.74

21 120K 120K N CA 941 942 -173.67 139.10 -40.80

22 16400 121T 122D C N 955 957 -65.28 -70.90 7.98 0.64 -63.30 164.05 20.37

22 122D 122D N CA 957 958 155.97 150.30 -40.00

23 16402 123P 124D C N 970 972 -91.59 -70.90 32.93 1.20 -63.30 146.84 19.93

23 124D 124D N CA 972 973 175.91 150.30 -40.00

24 16403 124D 125H C N 978 980 -113.45 -125.60 13.39 0.36 -63.20 -177.48 20.20

24 125H 125H N CA 980 981 133.17 138.80 -42.30

25 16404 125H 126L C N 988 990 -80.82 -70.70 33.02 2.89 -63.50 152.36 20.23

25 126L 126L N CA 990 991 110.17 141.60 -41.20

26 16406 127I 128H C N 1004 1006 -128.58 -125.60 3.50 0.09 -63.20 -171.24 27.88

26 128H 128H N CA 1006 1007 140.63 138.80 -42.30

27 16407 128H 129S C N 1014 1016 -69.43 -72.40 5.04 0.23 -64.10 176.75 13.13

27 129S 129S N CA 1016 1017 148.33 152.40 -35.00

28 16408 129S 130A C N 1020 1022 -151.49 -134.00 23.75 0.68 -62.50 179.63 34.19

28 130A 130A N CA 1022 1023 163.06 147.00 -40.90

29 16409 130A 131T C N 1025 1027 -124.45 -124.80 1.66 0.08 -63.20 -176.68 27.57

29 131T 131T N CA 1027 1028 145.12 143.50 -42.10

30 16411 132P 133Q C N 1039 1041 -127.21 -63.80 65.20 11.47 -63.80 65.20 11.47

30 133Q 133Q N CA 1041 1042 -55.45 -40.30 -40.30

31 16412 133Q 134N C N 1048 1050 -58.45 -71.20 13.60 1.08 -63.20 171.44 21.18

31 134N 134N N CA 1050 1051 147.52 142.80 -41.10

32 16413 134N 135T C N 1056 1058 -136.94 -124.80 22.19 0.69 -63.20 172.40 26.92

32 135T 135T N CA 1058 1059 162.07 143.50 -42.10

33 16415 136T 137N C N 1070 1072 -74.90 -63.20 14.47 1.71 55.90 149.35 18.43

33 137N 137N N CA 1072 1073 -32.58 -41.10 39.50

34 16472 193P 194G C N 1497 1499 64.98 82.20 26.33 1.99 -62.40 130.82 24.34

34 194G 194G N CA 1499 1500 -11.42 8.50 -41.20

35 16496 217E 218N C N 1690 1692 -108.68 -63.20 85.14 9.15 -63.20 85.14 9.15

35 218N 218N N CA 1692 1693 30.88 -41.10 -41.10

36 16506 227E 228W C N 1762 1764 -79.34 -63.00 70.46 8.00 -63.00 70.46 8.00

36 228W 228W N CA 1764 1765 24.34 -44.20 -44.20

37 16513 234E 235S C N 1823 1825 71.48 -72.40 158.50 12.65 -64.10 172.17 15.43

37 235S 235S N CA 1825 1826 -141.11 152.40 -35.00

38 16614 335G 336A C N 2560 2562 -80.87 -62.50 35.97 6.87 -62.50 35.97 6.87

38 336A 336A N CA 2562 2563 -71.82 -40.90 -40.90

39 16651 372D 373F C N 2852 2854 -93.55 -63.20 61.97 7.05 -63.20 61.97 7.05

39 373F 373F N CA 2854 2855 9.73 -44.30 -44.30

40 16699 420P 421G C N 3257 3259 20.30 78.70 86.09 1.81 -80.20 130.37 9.42

40 421G 421G N CA 3259 3260 -102.85 -166.10 174.10

41 16700 421G 422Y C N 3261 3263 -75.59 -63.50 16.20 2.27 55.90 149.96 18.50

41 422Y 422Y N CA 3263 3264 -32.61 -43.40 39.50

42 16715 436F 437F C N 3385 3387 -95.06 -63.20 37.05 6.67 -63.20 37.05 6.67

42 437F 437F N CA 3387 3388 -63.22 -44.30 -44.30

43 16799 520V 521D C N 4072 4074 -63.20 -63.30 9.67 1.19 -70.90 160.22 8.28

43 521D 521D N CA 4074 4075 -49.66 -40.00 150.30

44 16800 521D 522G C N 4080 4082 -65.34 -62.40 3.42 0.52 82.20 155.14 11.75

44 522G 522G N CA 4082 4083 -39.45 -41.20 8.50

45 16847 568S 569W C N 4479 4481 -54.44 -63.00 9.25 1.64 -124.90 -170.52 10.51

45 569W 569W N CA 4481 4482 -40.70 -44.20 143.40

46 16849 570V 571G C N 4500 4502 164.48 -167.20 28.48 0.48 82.20 -171.96 12.89

46 571G 571G N CA 4502 4503 177.59 174.60 8.50

47 16850 571G 572S C N 4504 4506 -80.62 -72.40 16.06 0.74 -64.10 159.65 12.62

47 572S 572S N CA 4506 4507 166.20 152.40 -35.00

48 16851 572S 573E C N 4510 4512 -99.19 -117.80 19.22 0.60 -63.60 175.95 21.70

48 573E 573E N CA 4512 4513 132.02 136.80 -40.30

49 16853 574C 575E C N 4525 4527 -105.47 -117.80 26.97 1.06 -63.60 158.74 19.18

49 575E 575E N CA 4527 4528 112.81 136.80 -40.30

50 16854 575E 576N C N 4534 4536 -153.62 -119.90 65.34 2.12 -63.20 155.03 24.31

50 576N 576N N CA 4536 4537 -167.03 137.00 -41.10

51 16855 576N 577N C N 4542 4544 -64.27 -71.20 39.60 2.35 -63.20 144.91 18.06

51 577N 577N N CA 4544 4545 103.81 142.80 -41.10

52 16856 577N 578N C N 4550 4552 -90.00 -71.20 23.51 1.31 -63.20 164.19 22.04

52 578N 578N N CA 4552 4553 156.91 142.80 -41.10

53 16857 578N 579A C N 4558 4560 -123.19 -134.00 11.21 0.49 -62.50 179.70 32.69

53 579A 579A N CA 4560 4561 149.96 147.00 -40.90

54 16858 579A 580A C N 4563 4565 -70.44 -68.20 12.56 0.93 -62.50 161.64 26.89

54 580A 580A N CA 4565 4566 157.66 145.30 -40.90

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 26 58 204 290 426 422 539 641 728 778

<< end of ENERGY.

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: SER:OXT SER

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 985434

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -67085.4922

<< end of ENERGY.

DOPE score : -67085.492188

>> Model assessment by GA341 potential

Surface library : C:\Program Files\Modeller9.25/modlib/surf5.de

Pair library : C:\Program Files\Modeller9.25/modlib/pair9.de

Chain identifier : \_

% sequence identity : 90.875000

Sequence length : 581

Compactness : 0.138773

Native energy (pair) : -427.796482

Native energy (surface) : -29.181024

Native energy (combined) : -11.065727

Z score (pair) : -11.740248

Z score (surface) : -10.448792

Z score (combined) : -14.224600

GA341 score : 1.000000

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 9774

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 3992.4519

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 4703 1 2 0.006 0.006 53.642 1.000

2 Bond angle potential : 6399 0 25 2.093 2.093 550.96 1.000

3 Stereochemical cosine torsion poten: 3170 0 88 46.540 46.540 1055.4 1.000

4 Stereochemical improper torsion pot: 1995 0 1 1.287 1.287 80.263 1.000

5 Soft-sphere overlap restraints : 9774 0 0 0.002 0.002 4.1323 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 12335 10 28 0.208 0.208 467.86 1.000

10 Distance restraints 2 (N-O) : 12118 9 15 0.232 0.232 551.75 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 580 0 8 4.097 4.097 114.81 1.000

14 Sidechain Chi\_1 dihedral restraints: 486 0 3 56.091 56.091 61.358 1.000

15 Sidechain Chi\_2 dihedral restraints: 367 0 5 62.617 62.617 111.61 1.000

16 Sidechain Chi\_3 dihedral restraints: 161 0 0 69.941 69.941 94.108 1.000

17 Sidechain Chi\_4 dihedral restraints: 49 0 0 104.513 104.513 32.719 1.000

18 Disulfide distance restraints : 3 0 0 0.008 0.008 0.31394E-01 1.000

19 Disulfide angle restraints : 6 0 0 2.182 2.182 0.63076 1.000

20 Disulfide dihedral angle restraints: 3 0 0 26.092 26.092 1.9132 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 8505 0 0 0.344 0.344 180.37 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 579 46 66 25.594 50.371 291.10 1.000

26 Distance restraints 4 (SDCH-SDCH) : 5535 0 2 0.658 0.658 339.81 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

# Heavy relative violation of each residue is written to: ache2.V99990004

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 55070.2578

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 841 102S 103K C N 813 815 1.47 1.35 0.13 4.57 1.35 0.13 4.57

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Feature 9 : Distance restraints 1 (CA-CA)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 18987 18A 102S CA CA 132 810 10.32 8.11 2.21 4.74 8.11 2.21 4.74

2 21377 103K 226P CA CA 816 1749 13.56 11.05 2.51 4.64 11.05 2.51 4.64

3 21378 103K 227E CA CA 816 1756 14.75 9.12 5.62 9.43 9.12 5.62 9.43

4 21379 103K 228W CA CA 816 1765 12.08 8.11 3.97 7.77 8.11 3.97 7.77

5 21383 103K 514K CA CA 816 4028 11.61 9.36 2.26 4.53 9.36 2.26 4.53

6 21384 103K 515T CA CA 816 4037 15.01 9.99 5.03 9.65 9.99 5.03 9.65

7 21385 103K 516G CA CA 816 4044 17.47 12.62 4.85 9.69 12.62 4.85 9.69

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Feature 10 : Distance restraints 2 (N-O)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 32964 103K 227E N O 815 1763 15.52 9.48 6.05 8.86 9.48 6.05 8.86

2 32966 103K 513A N O 815 4026 13.47 9.72 3.74 7.23 9.72 3.74 7.23

3 32967 103K 514K N O 815 4035 13.84 7.08 6.76 13.05 7.08 6.76 13.05

4 32968 103K 515T N O 815 4042 17.95 10.56 7.39 12.84 10.56 7.39 12.84

5 35489 227E 103K N O 1755 823 12.94 9.12 3.83 5.65 9.12 3.83 5.65

6 35513 228W 103K N O 1764 823 11.84 8.58 3.26 5.72 8.58 3.26 5.72

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Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 16280 1I 2T C N 7 9 -89.55 -78.10 19.58 1.21 -63.20 177.97 21.18

1 2T 2T N CA 9 10 133.91 149.80 -42.10

2 16281 2T 3D C N 14 16 -81.42 -96.50 18.06 0.74 -63.30 165.13 19.35

2 3D 3D N CA 16 17 124.14 114.20 -40.00

3 16318 39V 40D C N 296 298 55.03 -63.30 138.87 17.46 -70.90 158.97 13.19

3 40D 40D N CA 298 299 -112.68 -40.00 150.30

4 16380 101P 102S C N 807 809 -91.90 -136.60 75.53 2.66 -64.10 128.35 8.08

4 102S 102S N CA 809 810 90.31 151.20 -35.00

5 16381 102S 103K C N 813 815 -75.43 -70.20 79.54 5.89 56.60 133.92 14.55

5 103K 103K N CA 815 816 61.03 140.40 38.60

6 16382 103K 104A C N 822 824 -159.09 -134.00 29.19 1.53 -62.50 -161.89 29.68

6 104A 104A N CA 824 825 132.07 147.00 -40.90

7 16383 104A 105R C N 827 829 174.91 -125.20 61.95 2.10 -63.00 -156.78 35.42

7 105R 105R N CA 829 830 156.45 140.60 -41.10

8 16384 105R 106L C N 838 840 -110.19 -108.50 43.51 2.37 -63.50 138.34 17.18

8 106L 106L N CA 840 841 89.02 132.50 -41.20

9 16385 106L 107R C N 846 848 -119.30 -125.20 17.17 0.68 -63.00 174.88 20.49

9 107R 107R N CA 848 849 124.47 140.60 -41.10

10 16386 107R 108H C N 857 859 -127.09 -125.60 12.53 0.45 -63.20 178.30 26.47

10 108H 108H N CA 859 860 151.24 138.80 -42.30

11 16387 108H 109G C N 867 869 -64.10 -80.20 36.90 0.86 82.20 -162.69 6.54

11 109G 109G N CA 869 870 140.89 174.10 8.50

12 16388 109G 110R C N 871 873 -74.51 -72.10 3.17 0.21 -63.00 175.32 24.47

12 110R 110R N CA 873 874 143.96 141.90 -41.10

13 16389 110R 111G C N 882 884 94.74 78.70 50.39 0.84 82.20 138.20 7.34

13 111G 111G N CA 884 885 146.13 -166.10 8.50

14 16390 111G 112A C N 886 888 -129.10 -134.00 4.90 0.17 -62.50 -175.73 33.76

14 112A 112A N CA 888 889 147.29 147.00 -40.90

15 16391 112A 113N C N 891 893 -115.07 -119.90 7.48 0.22 -63.20 -179.98 20.11

15 113N 113N N CA 893 894 131.29 137.00 -41.10

16 16392 113N 114G C N 899 901 85.73 78.70 29.45 0.56 82.20 156.84 7.79

16 114G 114G N CA 901 902 165.30 -166.10 8.50

17 16394 115V 116E C N 910 912 -125.25 -117.80 15.35 0.59 -63.60 -179.66 27.53

17 116E 116E N CA 912 913 150.22 136.80 -40.30

18 16395 116E 117H C N 919 921 -70.03 -67.60 6.79 0.45 -63.20 171.49 21.87

18 117H 117H N CA 921 922 146.34 140.00 -42.30

19 16396 117H 118A C N 929 931 -111.81 -134.00 27.78 0.72 -62.50 178.13 27.23

19 118A 118A N CA 931 932 130.28 147.00 -40.90

20 16398 119A 120K C N 939 941 67.01 56.60 21.74 1.10 -62.90 143.23 25.01

20 120K 120K N CA 941 942 19.52 38.60 -40.80

21 16400 121T 122D C N 955 957 110.14 54.50 63.65 8.26 -63.30 -153.64 35.17

21 122D 122D N CA 957 958 71.81 40.90 -40.00

22 16402 123P 124D C N 970 972 -59.69 -70.90 12.12 0.72 -63.30 174.36 21.31

22 124D 124D N CA 972 973 145.68 150.30 -40.00

23 16403 124D 125H C N 978 980 -81.56 -63.20 87.64 9.94 -63.20 87.64 9.94

23 125H 125H N CA 980 981 43.39 -42.30 -42.30

24 16404 125H 126L C N 988 990 -143.15 -108.50 39.84 1.76 -63.50 -175.31 30.57

24 126L 126L N CA 990 991 152.16 132.50 -41.20

25 16406 127I 128H C N 1004 1006 -83.49 -67.60 16.38 1.35 -63.20 179.48 21.24

25 128H 128H N CA 1006 1007 136.03 140.00 -42.30

26 16407 128H 129S C N 1014 1016 -97.85 -72.40 35.69 2.84 -64.10 165.85 10.49

26 129S 129S N CA 1016 1017 127.38 152.40 -35.00

27 16412 133Q 134N C N 1048 1050 -156.87 -119.90 52.37 1.53 -63.20 172.48 26.73

27 134N 134N N CA 1050 1051 174.08 137.00 -41.10

28 16413 134N 135T C N 1056 1058 -76.23 -78.10 1.94 0.13 -63.20 168.07 22.42

28 135T 135T N CA 1058 1059 150.34 149.80 -42.10

29 16415 136T 137N C N 1070 1072 -80.64 -63.20 24.31 2.73 55.90 150.65 18.59

29 137N 137N N CA 1072 1073 -24.16 -41.10 39.50

30 16473 194G 195F C N 1501 1503 -60.56 -63.20 45.99 6.56 -63.20 45.99 6.56

30 195F 195F N CA 1503 1504 1.61 -44.30 -44.30

31 16496 217E 218N C N 1690 1692 -109.00 -63.20 87.06 9.36 -63.20 87.06 9.36

31 218N 218N N CA 1692 1693 32.94 -41.10 -41.10

32 16506 227E 228W C N 1762 1764 -80.25 -63.00 69.93 7.91 -63.00 69.93 7.91

32 228W 228W N CA 1764 1765 23.58 -44.20 -44.20

33 16513 234E 235S C N 1823 1825 62.75 -72.40 152.56 12.23 -64.10 162.67 14.43

33 235S 235S N CA 1825 1826 -136.82 152.40 -35.00

34 16614 335G 336A C N 2560 2562 -81.33 -62.50 35.56 6.83 -62.50 35.56 6.83

34 336A 336A N CA 2562 2563 -71.06 -40.90 -40.90

35 16651 372D 373F C N 2852 2854 -94.73 -63.20 63.86 7.26 -63.20 63.86 7.26

35 373F 373F N CA 2854 2855 11.23 -44.30 -44.30

36 16715 436F 437F C N 3385 3387 -95.69 -63.20 37.08 6.67 -63.20 37.08 6.67

36 437F 437F N CA 3387 3388 -62.15 -44.30 -44.30

37 16811 532D 533P C N 4174 4176 -80.78 -58.70 71.23 4.40 -64.50 111.18 9.18

37 533P 533P N CA 4176 4177 37.22 -30.50 147.20

38 16849 570V 571G C N 4500 4502 94.31 78.70 40.30 0.62 82.20 148.74 7.83

38 571G 571G N CA 4502 4503 156.75 -166.10 8.50

39 16850 571G 572S C N 4504 4506 -142.43 -136.60 22.16 0.99 -64.10 171.37 18.04

39 572S 572S N CA 4506 4507 172.58 151.20 -35.00

40 16851 572S 573E C N 4510 4512 -64.62 -69.30 14.73 0.96 -63.60 168.84 22.46

40 573E 573E N CA 4512 4513 128.54 142.50 -40.30

41 16853 574C 575E C N 4525 4527 -65.34 -69.30 4.58 0.27 -63.60 179.51 24.03

41 575E 575E N CA 4527 4528 140.19 142.50 -40.30

42 16854 575E 576N C N 4534 4536 -109.85 -119.90 11.22 0.35 -63.20 179.28 20.20

42 576N 576N N CA 4536 4537 132.01 137.00 -41.10

43 16855 576N 577N C N 4542 4544 -120.68 -119.90 16.74 0.74 -63.20 174.89 25.14

43 577N 577N N CA 4544 4545 153.73 137.00 -41.10

44 16856 577N 578N C N 4550 4552 -66.31 -71.20 11.70 0.64 -63.20 173.30 21.50

44 578N 578N N CA 4552 4553 132.17 142.80 -41.10

45 16857 578N 579A C N 4558 4560 -168.37 -134.00 44.43 1.19 -62.50 178.69 34.85

45 579A 579A N CA 4560 4561 175.15 147.00 -40.90

46 16858 579A 580A C N 4563 4565 -62.91 -68.20 6.85 0.44 -62.50 178.14 29.21

46 580A 580A N CA 4565 4566 140.96 145.30 -40.90

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 28 56 215 289 405 411 540 659 716 752

<< end of ENERGY.

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

iupac\_m\_397W> Atoms were not swapped because of the uncertainty of how to handle the H atom.

>> Model assessment by DOPE potential

iatmcls\_286W> MODEL atom not classified: SER:OXT SER

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 983132

Dynamic pairs routine : 1, NATM x NATM double loop

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 1 9999

NLOGN\_USE : 15

CONTACT\_SHELL : 15.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T F F F T

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : -67099.7812

<< end of ENERGY.

DOPE score : -67099.781250

>> Model assessment by GA341 potential

Surface library : C:\Program Files\Modeller9.25/modlib/surf5.de

Pair library : C:\Program Files\Modeller9.25/modlib/pair9.de

Chain identifier : \_

% sequence identity : 90.875000

Sequence length : 581

Compactness : 0.175940

Native energy (pair) : -454.092029

Native energy (surface) : -30.522091

Native energy (combined) : -11.700688

Z score (pair) : -11.687965

Z score (surface) : -10.928697

Z score (combined) : -14.717052

GA341 score : 1.000000

>> ENERGY; Differences between the model's features and restraints:

Number of all residues in MODEL : 581

Number of all, selected real atoms : 4576 4576

Number of all, selected pseudo atoms : 0 0

Number of all static, selected restraints : 56994 56994

COVALENT\_CYS : F

NONBONDED\_SEL\_ATOMS : 1

Number of non-bonded pairs (excluding 1-2,1-3,1-4): 9734

Dynamic pairs routine : 2, NATM x NATM cell sorting

Atomic shift for contacts update (UPDATE\_DYNAMIC) : 0.390

LENNARD\_JONES\_SWITCH : 6.500 7.500

COULOMB\_JONES\_SWITCH : 6.500 7.500

RESIDUE\_SPAN\_RANGE : 0 99999

NLOGN\_USE : 15

CONTACT\_SHELL : 4.000

DYNAMIC\_PAIRS,\_SPHERE,\_COULOMB,\_LENNARD,\_MODELLER : T T F F F

SPHERE\_STDV : 0.050

RADII\_FACTOR : 0.820

Current energy : 3948.1548

Summary of the restraint violations:

NUM ... number of restraints.

NUMVI ... number of restraints with RVIOL > VIOL\_REPORT\_CUT[i].

RVIOL ... relative difference from the best value.

NUMVP ... number of restraints with -Ln(pdf) > VIOL\_REPORT\_CUT2[i].

RMS\_1 ... RMS(feature, minimally\_violated\_basis\_restraint, NUMB).

RMS\_2 ... RMS(feature, best\_value, NUMB).

MOL.PDF ... scaled contribution to -Ln(Molecular pdf).

# RESTRAINT\_GROUP NUM NUMVI NUMVP RMS\_1 RMS\_2 MOL.PDF S\_i

------------------------------------------------------------------------------------------------------

1 Bond length potential : 4703 1 3 0.006 0.006 53.265 1.000

2 Bond angle potential : 6399 0 26 2.067 2.067 539.96 1.000

3 Stereochemical cosine torsion poten: 3170 0 93 46.393 46.393 1044.9 1.000

4 Stereochemical improper torsion pot: 1995 0 1 1.256 1.256 77.857 1.000

5 Soft-sphere overlap restraints : 9734 0 0 0.002 0.002 3.5771 1.000

6 Lennard-Jones 6-12 potential : 0 0 0 0.000 0.000 0.0000 1.000

7 Coulomb point-point electrostatic p: 0 0 0 0.000 0.000 0.0000 1.000

8 H-bonding potential : 0 0 0 0.000 0.000 0.0000 1.000

9 Distance restraints 1 (CA-CA) : 12335 10 29 0.209 0.209 470.57 1.000

10 Distance restraints 2 (N-O) : 12118 9 24 0.240 0.240 583.49 1.000

11 Mainchain Phi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

12 Mainchain Psi dihedral restraints : 0 0 0 0.000 0.000 0.0000 1.000

13 Mainchain Omega dihedral restraints: 580 0 7 4.163 4.163 118.53 1.000

14 Sidechain Chi\_1 dihedral restraints: 486 0 4 55.297 55.297 51.641 1.000

15 Sidechain Chi\_2 dihedral restraints: 367 0 2 58.402 58.402 107.48 1.000

16 Sidechain Chi\_3 dihedral restraints: 161 0 0 62.975 62.975 99.723 1.000

17 Sidechain Chi\_4 dihedral restraints: 49 0 0 112.105 112.105 34.545 1.000

18 Disulfide distance restraints : 3 0 0 0.007 0.007 0.27468E-01 1.000

19 Disulfide angle restraints : 6 0 0 2.033 2.033 0.54757 1.000

20 Disulfide dihedral angle restraints: 3 0 0 23.421 23.421 1.6160 1.000

21 Lower bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

22 Upper bound distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

23 Distance restraints 3 (SDCH-MNCH) : 8505 0 0 0.339 0.339 168.38 1.000

24 Sidechain Chi\_5 dihedral restraints: 0 0 0 0.000 0.000 0.0000 1.000

25 Phi/Psi pair of dihedral restraints: 579 54 72 26.472 53.965 322.92 1.000

26 Distance restraints 4 (SDCH-SDCH) : 5535 0 0 0.598 0.598 269.11 1.000

27 Distance restraints 5 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

28 NMR distance restraints 6 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

29 NMR distance restraints 7 (X-Y) : 0 0 0 0.000 0.000 0.0000 1.000

30 Minimal distance restraints : 0 0 0 0.000 0.000 0.0000 1.000

31 Non-bonded restraints : 0 0 0 0.000 0.000 0.0000 1.000

32 Atomic accessibility restraints : 0 0 0 0.000 0.000 0.0000 1.000

33 Atomic density restraints : 0 0 0 0.000 0.000 0.0000 1.000

34 Absolute position restraints : 0 0 0 0.000 0.000 0.0000 1.000

35 Dihedral angle difference restraint: 0 0 0 0.000 0.000 0.0000 1.000

36 GBSA implicit solvent potential : 0 0 0 0.000 0.000 0.0000 1.000

37 EM density fitting potential : 0 0 0 0.000 0.000 0.0000 1.000

38 SAXS restraints : 0 0 0 0.000 0.000 0.0000 1.000

39 Symmetry restraints : 0 0 0 0.000 0.000 0.0000 1.000

# Heavy relative violation of each residue is written to: ache2.V99990005

# The profile is NOT normalized by the number of restraints.

# The profiles are smoothed over a window of residues: 1

# The sum of all numbers in the file: 55292.7188

List of the violated restraints:

A restraint is violated when the relative difference

from the best value (RVIOL) is larger than CUTOFF.

ICSR ... index of a restraint in the current set.

RESNO ... residue numbers of the first two atoms.

ATM ... IUPAC atom names of the first two atoms.

FEAT ... the value of the feature in the model.

restr ... the mean of the basis restraint with the smallest

difference from the model (local minimum).

viol ... difference from the local minimum.

rviol ... relative difference from the local minimum.

RESTR ... the best value (global minimum).

VIOL ... difference from the best value.

RVIOL ... relative difference from the best value.

-------------------------------------------------------------------------------------------------

Feature 1 : Bond length potential

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 841 102S 103K C N 813 815 1.47 1.35 0.13 4.53 1.35 0.13 4.53

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Feature 9 : Distance restraints 1 (CA-CA)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 18964 17R 102S CA CA 121 810 12.92 10.70 2.22 4.54 10.70 2.22 4.54

2 18987 18A 102S CA CA 132 810 10.37 8.11 2.25 4.83 8.11 2.25 4.83

3 21377 103K 226P CA CA 816 1749 13.53 11.05 2.48 4.57 11.05 2.48 4.57

4 21378 103K 227E CA CA 816 1756 14.65 9.12 5.53 9.27 9.12 5.53 9.27

5 21379 103K 228W CA CA 816 1765 12.00 8.11 3.89 7.63 8.11 3.89 7.63

6 21384 103K 515T CA CA 816 4037 14.96 9.99 4.97 9.55 9.99 4.97 9.55

7 21385 103K 516G CA CA 816 4044 17.41 12.62 4.79 9.57 12.62 4.79 9.57

-------------------------------------------------------------------------------------------------

Feature 10 : Distance restraints 2 (N-O)

List of the RVIOL violations larger than : 4.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 32964 103K 227E N O 815 1763 15.50 9.48 6.02 8.82 9.48 6.02 8.82

2 32966 103K 513A N O 815 4026 13.47 9.72 3.74 7.23 9.72 3.74 7.23

3 32967 103K 514K N O 815 4035 13.83 7.08 6.75 13.02 7.08 6.75 13.02

4 32968 103K 515T N O 815 4042 17.96 10.56 7.40 12.85 10.56 7.40 12.85

5 35489 227E 103K N O 1755 823 12.68 9.12 3.57 5.27 9.12 3.57 5.27

6 35513 228W 103K N O 1764 823 11.55 8.58 2.97 5.22 8.58 2.97 5.22

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Feature 25 : Phi/Psi pair of dihedral restraints

List of the RVIOL violations larger than : 6.5000

# ICSR RESNO1/2 ATM1/2 INDATM1/2 FEAT restr viol rviol RESTR VIOL RVIOL

1 16280 1I 2T C N 7 9 -106.68 -124.80 24.99 0.82 -63.20 173.91 19.74

1 2T 2T N CA 9 10 126.29 143.50 -42.10

2 16281 2T 3D C N 14 16 -68.60 -70.90 14.15 0.59 -63.30 176.42 21.46

2 3D 3D N CA 16 17 136.34 150.30 -40.00

3 16318 39V 40D C N 296 298 43.82 -63.30 126.35 15.82 -70.90 153.98 12.61

3 40D 40D N CA 298 299 -106.99 -40.00 150.30

4 16353 74F 75P C N 591 593 -57.70 -58.70 13.07 1.00 -64.50 169.41 13.00

4 75P 75P N CA 593 594 -43.53 -30.50 147.20

5 16354 75P 76G C N 598 600 -80.47 -62.40 21.31 3.21 82.20 167.14 12.38

5 76G 76G N CA 600 601 -29.90 -41.20 8.50

6 16380 101P 102S C N 807 809 -92.73 -136.60 74.62 2.64 -64.10 129.06 8.10

6 102S 102S N CA 809 810 90.84 151.20 -35.00

7 16381 102S 103K C N 813 815 -80.92 -70.20 74.66 5.66 56.60 140.33 14.97

7 103K 103K N CA 815 816 66.51 140.40 38.60

8 16382 103K 104A C N 822 824 -152.26 -134.00 18.29 0.57 -62.50 -166.74 36.47

8 104A 104A N CA 824 825 147.96 147.00 -40.90

9 16383 104A 105R C N 827 829 128.05 -125.20 112.32 3.67 -63.00 -138.42 40.08

9 105R 105R N CA 829 830 175.53 140.60 -41.10

10 16384 105R 106L C N 838 840 -73.60 -70.70 7.58 0.48 -63.50 170.49 24.26

10 106L 106L N CA 840 841 148.61 141.60 -41.20

11 16385 106L 107R C N 846 848 -67.75 -72.10 17.59 1.26 -63.00 166.02 22.11

11 107R 107R N CA 848 849 124.85 141.90 -41.10

12 16386 107R 108H C N 857 859 -124.80 -125.60 38.50 1.48 -63.20 153.33 23.19

12 108H 108H N CA 859 860 177.29 138.80 -42.30

13 16387 108H 109G C N 867 869 88.15 78.70 11.08 0.36 82.20 179.72 9.02

13 109G 109G N CA 869 870 -171.88 -166.10 8.50

14 16388 109G 110R C N 871 873 -133.57 -125.20 26.52 1.07 -63.00 168.62 27.60

14 110R 110R N CA 873 874 165.76 140.60 -41.10

15 16389 110R 111G C N 882 884 -138.06 -167.20 31.31 0.46 82.20 -151.57 15.82

15 111G 111G N CA 884 885 163.15 174.60 8.50

16 16390 111G 112A C N 886 888 -62.67 -68.20 8.75 0.55 -62.50 179.42 29.39

16 112A 112A N CA 888 889 138.52 145.30 -40.90

17 16391 112A 113N C N 891 893 -135.62 -119.90 21.54 0.63 -63.20 -177.81 26.88

17 113N 113N N CA 893 894 151.72 137.00 -41.10

18 16392 113N 114G C N 899 901 -133.54 -167.20 41.60 0.77 82.20 -157.83 15.53

18 114G 114G N CA 901 902 150.15 174.60 8.50

19 16395 116E 117H C N 919 921 -153.20 -125.60 31.16 1.35 -63.20 -170.61 20.14

19 117H 117H N CA 921 922 124.34 138.80 -42.30

20 16396 117H 118A C N 929 931 -74.38 -68.20 6.97 0.48 -62.50 170.99 28.62

20 118A 118A N CA 931 932 148.53 145.30 -40.90

21 16397 118A 119A C N 934 936 -107.15 -134.00 41.18 1.35 -62.50 162.91 24.92

21 119A 119A N CA 936 937 115.77 147.00 -40.90

22 16398 119A 120K C N 939 941 -138.21 -118.00 77.74 3.98 -62.90 129.09 15.03

22 120K 120K N CA 941 942 64.04 139.10 -40.80

23 16399 120K 121T C N 948 950 -153.41 -124.80 56.31 1.76 -63.20 154.89 25.49

23 121T 121T N CA 950 951 -168.00 143.50 -42.10

24 16400 121T 122D C N 955 957 -72.80 -70.90 7.46 0.28 -63.30 162.77 20.68

24 122D 122D N CA 957 958 157.51 150.30 -40.00

25 16403 124D 125H C N 978 980 -141.98 -125.60 46.58 1.43 -63.20 156.55 24.65

25 125H 125H N CA 980 981 -177.59 138.80 -42.30

26 16404 125H 126L C N 988 990 -100.33 -63.50 51.28 6.64 -63.50 51.28 6.64

26 126L 126L N CA 990 991 -5.52 -41.20 -41.20

27 16406 127I 128H C N 1004 1006 -100.07 -125.60 32.21 0.79 -63.20 165.61 18.69

27 128H 128H N CA 1006 1007 119.15 138.80 -42.30

28 16407 128H 129S C N 1014 1016 -78.09 -72.40 11.66 0.54 -64.10 163.02 12.70

28 129S 129S N CA 1016 1017 162.58 152.40 -35.00

29 16408 129S 130A C N 1020 1022 -126.34 -134.00 7.66 0.25 -62.50 -176.36 33.51

29 130A 130A N CA 1022 1023 146.92 147.00 -40.90

30 16409 130A 131T C N 1025 1027 -135.70 -124.80 30.41 1.01 -63.20 163.02 25.62

30 131T 131T N CA 1027 1028 171.89 143.50 -42.10

31 16411 132P 133Q C N 1039 1041 -70.69 -73.00 2.77 0.17 -63.80 179.61 26.05

31 133Q 133Q N CA 1041 1042 139.18 140.70 -40.30

32 16412 133Q 134N C N 1048 1050 -80.54 -71.20 34.60 1.98 -63.20 143.84 18.96

32 134N 134N N CA 1050 1051 176.11 142.80 -41.10

33 16413 134N 135T C N 1056 1058 -78.99 -78.10 64.00 2.76 -63.20 128.88 15.53

33 135T 135T N CA 1058 1059 85.81 149.80 -42.10

34 16414 135T 136T C N 1063 1065 -132.09 -63.20 100.14 10.90 -78.10 130.88 7.40

34 136T 136T N CA 1065 1066 30.58 -42.10 149.80

35 16415 136T 137N C N 1070 1072 -115.20 -119.90 69.34 3.04 55.90 173.42 17.98

35 137N 137N N CA 1072 1073 67.82 137.00 39.50

36 16472 193P 194G C N 1497 1499 66.39 82.20 27.32 2.01 -62.40 131.68 24.44

36 194G 194G N CA 1499 1500 -13.77 8.50 -41.20

37 16496 217E 218N C N 1690 1692 -108.92 -63.20 87.71 9.43 -63.20 87.71 9.43

37 218N 218N N CA 1692 1693 33.75 -41.10 -41.10

38 16506 227E 228W C N 1762 1764 -80.98 -63.00 71.49 8.07 -63.00 71.49 8.07

38 228W 228W N CA 1764 1765 24.99 -44.20 -44.20

39 16513 234E 235S C N 1823 1825 70.90 -72.40 158.17 12.62 -64.10 171.44 15.36

39 235S 235S N CA 1825 1826 -140.66 152.40 -35.00

40 16600 321Y 322S C N 2465 2467 -124.93 -136.60 43.54 1.93 -64.10 156.56 9.73

40 322S 322S N CA 2467 2468 109.25 151.20 -35.00

41 16601 322S 323G C N 2471 2473 109.10 78.70 55.62 0.89 -80.20 172.78 12.20

41 323G 323G N CA 2473 2474 147.32 -166.10 174.10

42 16614 335G 336A C N 2560 2562 -80.62 -62.50 36.11 6.88 -62.50 36.11 6.88

42 336A 336A N CA 2562 2563 -72.13 -40.90 -40.90

43 16651 372D 373F C N 2852 2854 -93.02 -63.20 63.03 7.19 -63.20 63.03 7.19

43 373F 373F N CA 2854 2855 11.23 -44.30 -44.30

44 16715 436F 437F C N 3385 3387 -95.08 -63.20 36.99 6.66 -63.20 36.99 6.66

44 437F 437F N CA 3387 3388 -63.05 -44.30 -44.30

45 16811 532D 533P C N 4174 4176 -80.67 -58.70 71.40 4.42 -64.50 110.94 9.15

45 533P 533P N CA 4176 4177 37.44 -30.50 147.20

46 16849 570V 571G C N 4500 4502 88.04 78.70 12.67 0.31 82.20 176.92 8.88

46 571G 571G N CA 4502 4503 -174.67 -166.10 8.50

47 16850 571G 572S C N 4504 4506 -103.64 -72.40 31.27 2.19 -64.10 175.67 15.41

47 572S 572S N CA 4506 4507 153.83 152.40 -35.00

48 16851 572S 573E C N 4510 4512 -114.45 -117.80 11.40 0.62 -63.60 179.36 26.79

48 573E 573E N CA 4512 4513 147.70 136.80 -40.30

49 16853 574C 575E C N 4525 4527 -61.47 -69.30 17.06 1.52 -63.60 162.06 21.49

49 575E 575E N CA 4527 4528 157.65 142.50 -40.30

50 16854 575E 576N C N 4534 4536 -55.83 -71.20 15.37 1.11 -63.20 176.40 21.66

50 576N 576N N CA 4536 4537 142.66 142.80 -41.10

51 16855 576N 577N C N 4542 4544 -123.00 -119.90 29.53 1.27 -63.20 163.84 23.88

51 577N 577N N CA 4544 4545 166.37 137.00 -41.10

52 16856 577N 578N C N 4550 4552 -64.49 -71.20 10.37 0.55 -63.20 176.00 21.93

52 578N 578N N CA 4552 4553 134.89 142.80 -41.10

53 16857 578N 579A C N 4558 4560 -146.35 -134.00 26.45 1.10 -62.50 170.72 32.46

53 579A 579A N CA 4560 4561 170.39 147.00 -40.90

54 16858 579A 580A C N 4563 4565 -62.20 -68.20 6.12 0.56 -62.50 172.60 28.27

54 580A 580A N CA 4565 4566 146.51 145.30 -40.90

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 23 71 215 270 383 428 524 679 709 736

<< end of ENERGY.

>> Summary of successfully produced models:

Filename molpdf DOPE score GA341 score

----------------------------------------------------------------------

ache2.B99990001.pdb 3926.86279 -66957.17188 1.00000

ache2.B99990002.pdb 4063.10132 -66902.82813 1.00000

ache2.B99990003.pdb 3996.16357 -66755.77344 1.00000

ache2.B99990004.pdb 3992.45190 -67085.49219 1.00000

ache2.B99990005.pdb 3948.15479 -67099.78125 1.00000

Total CPU time [seconds] : 223.41