SAVES v5.0

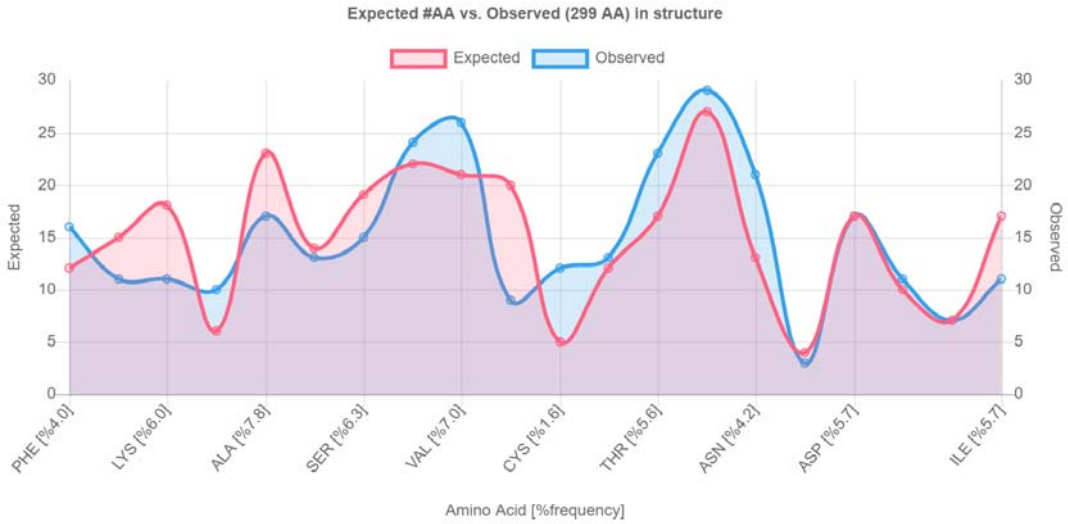
WHATCHECK • PROCHECK • ERRAT • Verify3D • PROVE • CRYST • pdbU [?]

New Job

VERIFY	ERRAT	PROVE	PROCHECK	WHATCHECK
92.98% of the residues have averaged 3D-1D score >= 0.2 **Pass**	Overall Quality Factor **A: 98.9437**	Buried outlier protein atoms total from 1 Model: 3.7% Warning	Out of 8 evaluations • **Errors: 2** • Warning: 4 • Pass: 2	1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47

Job results for:3CL_model_01.pdb | Link to this job:518828
Interactive Ramachandran Plot | View Structure

finished: Mar 11th, 2020 [8:31 AM]
Amino acid distributions determined from 160,252 PDB structures (2020/03/11)



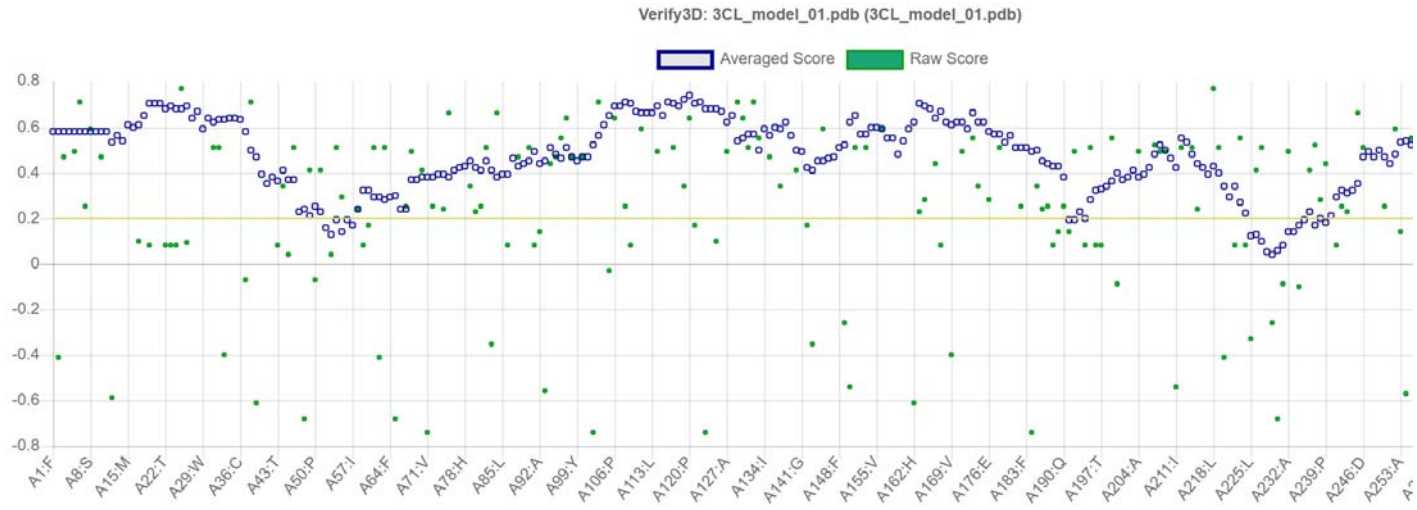
Verify 3D results

↑ TOP

92.98% of the residues have averaged 3D-1D score >= 0.2

Pass

At least 80% of the amino acids have scored >= 0.2 in the 3D/1D profile.



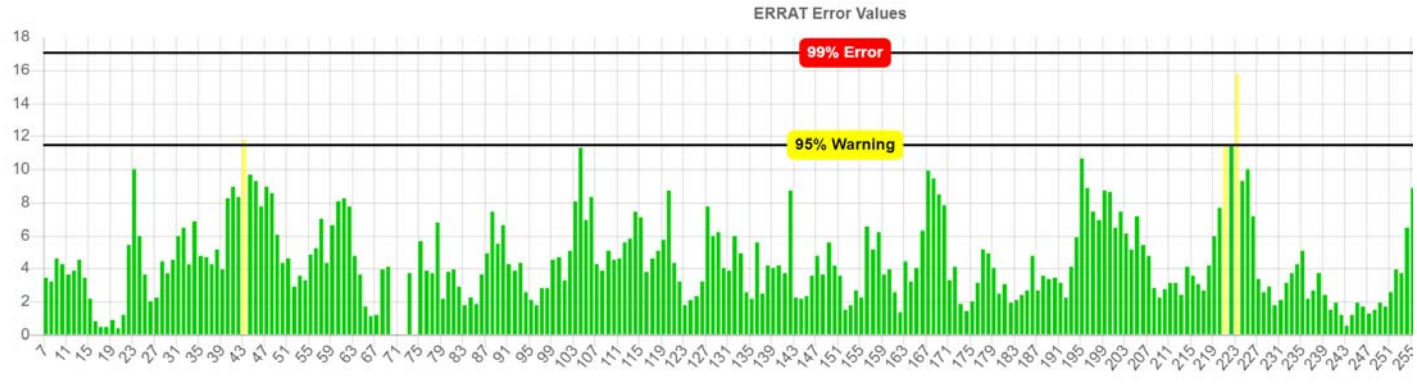
Save as image | Save data to file

ERRAT results

↑ TOP

Input: 3CL_model_01.pdb (3CL_model_01.pdb)
Moleman is used to identify chains and separate into files. Each pdb chain file is linked below for each plot. For an explanation on how the chains were found, here is the moleman logfile

Quality Factor: A: 98.9437 | PDF | PostScript | Log | PDB chain file used



Save as image

PROVE results

↑ TOP

Input file: **3CL_model_01.pdb**
Model : 42 buried outlier protein atoms, 3.7% Warning
Job Run Report | Labeled pdb

- **Job output**
- **Plot PS | Plot PDF**
- **Job run log**

PROCHECK results

↑ TOP

Out of 8 evaluations

- **Errors: 2**
- Warning: 4
- Pass: 2

1. **Main Ramachandran plot**
2. **All-residue Ramachandran plots**
3. **All-residue chi1-chi2 plots**
4. **Main-chain parameters**
5. **Side-chain parameters**
6. **Residue properties plot**
7. **Main-chain bond lengths**
8. **Main-chain bond angles**
9. **RMS distances from planarity**
10. **Distorted geometry**
11. **Results Summary**
12. **Program Output**

Remaining log and data files

1. 3218001.nb
2. pplot.log
3. tplot.log
4. 3218001.new
5. anglen.log
6. 3218001.sum
7. fort.27
8. 3218001.out
9. 3218001.pln
10. procheck_run.out
11. procheck.prm
12. 3218001.sdh
13. 3218001.sco
14. 3218001.lan
15. 3218001.rin
16. bplot.log
17. clean.log
18. nb.log
19. secstr.log

WHATCHECK results

↑ TOP

1. Error: Missing unit cell information **Error** ↑ TOP

No SCALE matrix is given in the PDB file.

2. Error: Missing symmetry information **Error** ↑ TOP

Problem: No CRYST1 card is given in the PDB file.

3. Note: No rounded coordinates detected Pass ↑ TOP

No significant rounding of atom coordinates has been detected.

4. Note: Valine nomenclature OK Pass ↑ TOP

No errors were detected in valine nomenclature.

5. Note: Threonine nomenclature OK Pass ↑ TOP

No errors were detected in threonine nomenclature.

6. Note: Isoleucine nomenclature OK Pass ↑ TOP

No errors were detected in isoleucine nomenclature.

7. Note: Leucine nomenclature OK Pass ↑ TOP

```
No errors were detected in leucine nomenclature.
```

8. Warning: Arginine nomenclature problem Warning

↑ TOP

```
The arginine residues listed in the table below have their N-H-1
and N-H-2 swapped.

 186 ARG  (188 ) A
```

9. Warning: Tyrosine convention problem Warning

↑ TOP

```
The tyrosine residues listed in the table below have their chi-2
not between -90.0 and 90.0

  35 TYR  (37  ) A
  52 TYR  (54  ) A
  99 TYR  (101 ) A
 116 TYR  (118 ) A
 124 TYR  (126 ) A
 207 TYR  (209 ) A
 235 TYR  (237 ) A
```

10. Warning: Phenylalanine convention problem Warning

↑ TOP

```
The phenylalanine residues listed in the table below have their
chi-2 not between -90.0 and 90.0.

 110 PHE  (112 ) A
 138 PHE  (140 ) A
 148 PHE  (150 ) A
 292 PHE  (294 ) A
```

11. Warning: Aspartic acid convention problem Warning

↑ TOP

```
The aspartic acid residues listed in the table below have their
chi-2 not between -90.0 and 90.0.

  32 ASP  (34  ) A
 153 ASP  (155 ) A
```

12. Warning: Glutamic acid convention problem Warning

↑ TOP

```
The glutamic acid residues listed in the table below have their
chi-3 outside the -90.0 to 90.0 range.

  45 GLU  (47  ) A
 176 GLU  (178 ) A
 286 GLU  (288 ) A
```

13. Note: L or D conformation checked OK Pass

↑ TOP

```
All amino acids in the structure have the L conformation.
```

14. Note: Chain names are unique Pass

↑ TOP

```
All chain names assigned to polymer molecules are unique.
```

15. Note: Weights checked OK Pass

↑ TOP

```
All atomic occupancy factors ('weights') fall in the 0.0--1.0 range.
```

16. Note: No missing atoms detected Pass

↑ TOP

```
All expected atoms are present.
```

17. Note: All bond lengths OK Pass

↑ TOP

```
All bond lengths are in agreement with standard bond lengths using
a tolerance of 4 sigma (both standard values and sigma for amino acid
residues have been taken from Engh and Huber [REF])
```

18. Note: Normal bond length variability Pass

↑ TOP

```
Bond lengths were found to deviate normally from the standard bond
lengths (values for Protein residues were taken from Engh and Huber
[REF]).

 Z-score for bond lengths: 0.669
```

```
 RMS-deviation in bond distances: 0.015
```

19. Warning: Directionality in bond lengths Warning

↑ TOP

```
Comparison of bond distances with Engh and Huber [REF] standard
values shows a significant systematic deviation. The bonds in one
direction are systematically longer than in other directions.

If this is not an XRAY structure this effect is hard to explain.
Otherwise you will have seen symmetry problems earlier. Please
correct these and rerun this check to see the implications on the
cell axes.
```

20. Warning: Unusual bond angles Warning

↑ TOP

```
The bond angles listed in the table below were found to deviate
more than 4 sigma from standard bond angles (both standard values
and sigma have been taken from Engh and Huber [REF]).  In the table
below for each strange angle the bond angle and the number of
standard deviations it differs from the Engh and Huber values is
given. Please note that only bond angles within protein residues
are taken into account: disulphide bridges and peptide bonds are
neglected.

   6 PHE  (8   ) A CA   CB   CG   109.204  -4.6
  31 ASP  (33  ) A CA   CB   CG   108.430  -4.2
  39 HIS  (41  ) A CD2  CG   ND1  110.610   4.5
  46 ASP  (48  ) A CA   CB   CG   117.276   4.7
  70 ASN  (72  ) A CA   CB   CG   117.595   5.0
  90 ASP  (92  ) A CA   CB   CG   119.479   6.9
 111 SER  (113 ) A C    CA   CB   101.317  -4.6
 161 HIS  (163 ) A CD2  CG   ND1  110.879   4.8
 162 HIS  (164 ) A CD2  CG   ND1  110.333   4.2
 170 HIS  (172 ) A CA   CB   CG   109.248  -4.6
 170 HIS  (172 ) A CD2  CG   ND1  110.453   4.4
 185 ASP  (187 ) A CA   CB   CG   116.787   4.2
 233 MET  (235 ) A CG   SD   CE    84.896  -7.3
 287 ASP  (289 ) A CA   CB   CG   119.282   6.7
```

21. Note: Normal bond angle variability Pass

↑ TOP

```
Bond angles were found to deviate normally from the mean Engh and
Huber [REF] standard bond angles. The RMS Z-score given below is
expected to be around 1.0 for a normally restrained data set, and
this is indeed observed for very high resolution X-ray structures.
More common values are around 1.55

 Z-score for bond angles: 1.140
 RMS-deviation in bond angles: 2.107
```

22. Error: Side chain planarity problems Error

↑ TOP

```
The side chains of the residues listed in the table below contain a
planar group that was found to deviate from planarity by more than
4.0 times the expected value.  For an amino acid residue that has a
side chain with a planar group, the RMS deviation of the atoms to a
least squares plane was determined. The number in the table is the
number of standard deviations this RMS value deviates from the
expected value (0.0).

  90 ASP  (92  ) A   4.886
```

23. Note: Atoms connected to aromatic rings OK Pass

↑ TOP

```
All of the atoms that are connected to planar aromatic rings in side
chains of amino-acid residues are in the plane within expected RMS
deviations.
```

24. Note: PRO puckering amplitude OK Pass

↑ TOP

```
Puckering amplitudes for all PRO residues are within normal ranges.
```

25. Note: PRO puckering phases OK Pass

↑ TOP

```
Puckering phases for all PRO residues are normal
```

26. Warning: Torsion angle evaluation shows unusual residues Warning

↑ TOP

```
The residues listed in the table below contain bad or abnormal
torsion angles.

These scores give an impression of how ``normal'' the torsion
angles in protein residues are. All torsion angles except omega are
used for calculating a `normality' score. Average values and
standard deviations were obtained from the residues in the WHAT IF
database. These are used to calculate Z-scores.  A residue with a
Z-score of below -2.0 is poor, and a score of less than -3.0 is
worrying.  For such residues more than one torsion angle is in a
highly unlikely position.
```

```
 152 TYR  (154 ) A -2.8555
 182 PRO  (184 ) A -2.5876
 186 ARG  (188 ) A -2.0958
  25 LEU  (27  ) A -2.0908
 137 SER  (139 ) A -2.0475
```

27. Warning: Backbone torsion angle evaluation shows unusual conformations Warning

↑ TOP

```
The residues listed in the table below have abnormal backbone torsion
angles.

Residues with ``forbidden'' phi-psi combinations are listed, as
well as residues with unusual omega angles (deviating by more than
3 sigma from the normal value). Please note that it is normal if
about 5 percent of the residues is listed here as having unusual
phi-psi combinations.

   5 ALA  (7   ) A omega poor
   7 PRO  (9   ) A omega poor
  31 ASP  (33  ) A Poor phi/psi
  45 GLU  (47  ) A omega poor
  46 ASP  (48  ) A omega poor
  50 PRO  (52  ) A omega poor
  82 ASN  (84  ) A Poor phi/psi
  84 VAL  (86  ) A omega poor
  97 PRO  (99  ) A omega poor
 105 GLN  (107 ) A PRO omega poor
 127 ALA  (129 ) A omega poor
 132 PHE  (134 ) A Poor phi/psi
 153 ASP  (155 ) A Poor phi/psi
 158 CYS  (160 ) A Poor phi/psi
 159 TYR  (161 ) A omega poor
 173 THR  (175 ) A omega poor
 179 PHE  (181 ) A omega poor
 182 PRO  (184 ) A Poor PRO-phi
 212 ASN  (214 ) A omega poor
 236 ASN  (238 ) A Poor phi/psi
 280 LEU  (282 ) A Poor phi/psi
```

28. Note: Ramachandran Z-score OK Pass

↑ TOP

```
The score expressing how well the backbone conformations of all residues
are corresponding to the known allowed areas in the Ramachandran plot is
within expected ranges for well-refined structures.

 Ramachandran Z-score : -0.782
```

29. Warning: Omega angle restraints not strong enough Warning

↑ TOP

```
The omega angles for trans-peptide bonds in a structure is
expected to give a gaussian distribution with the average around
+178 degrees, and a standard deviation around 5.5. In the current
structure the standard deviation of this distribution is above 7.0,
which indicates that the omega values have been under-constrained.

 Standard deviation of omega values : 7.149
```

30. Note: chi-1/chi-2 angle correlation Z-score OK Pass

↑ TOP

```
The score expressing how well the chi-1/chi-2 angles of all residues
are corresponding to the populated areas in the database is
within expected ranges for well-refined structures.

 chi-1/chi-2 correlation Z-score : -1.151
```

31. Note: Ramachandran plot Pass

↑ TOP

```
In this Ramachandran plot large crosses represent glycines and
small crosses represent the other residues. If too many small crosses
fall outside the boxed areas then the molecule is poorly refined (or
worse).

In the TeX file, a plot has been inserted here

 Chain identifier: A
```

32. Note: Secondary structure Pass

↑ TOP

```
This is the secondary structure according to DSSP. Only helix (H), strand
(S), turn (T) and coil (blank) are shown. [REF]

 Secondary structure assignment
The DSSP executable was not found
/software/what/whattest/dssp/DSSP.EXE
WARNING. You don`t have the DSSP program installed. Therefore
the emulator will be used. This emulator gives rather poor results,
but it prevents WHAT IF from crashing. See the writeup about this.
                    10        20        30        40        50        60
                     |         |         |         |         |         |
    1 -  60  FRKMAFPSGKVEGCMVQVTCGTTTLNGLWLDDVVYCPRHVICTSEDMLNPNYEDLLIRKS
    1 -  60         HH 33H3TSSSST  T SSSS T  TSSST3333TT  3  T THH HHH T3
                    70        80        90       100       110       120
```

```
                |         |         |         |         |         |
  61 - 120  NHNFLVQAGNVQLRVIGHSMQNCVLKLKVDTANPKTPKYKFVRIQPGQTFSVLACYNGSP
  61 - 120  3 3TSSST  T      SS T  TSSSS    T  T SSSSS  T TT SSSSS TTTT
                130       140       150       160       170       180
                |         |         |         |         |         |
 121 - 180  SGVYQCAMRPNFTIKGSFLNGSCGSVGFNIDYDCVSFCYMHHMELPTGVHAGTDLEGNFY
 121 - 180   SSSSS  T  T S    T T3 TT SSS TTTTSSS SS  S T  T SSSST  T
                190       200       210       220       230       240
                |         |         |         |         |         |
 181 - 240  GPFVDRQTAQAAGTDTTITVNVLAWLYAAVINGDRWFLNRFTTTLNDFNLVAMKYNYEPL
 181 - 240                  STHHHHHHHHHHHHHHT 3  T     THHHHHH3333TTSS
                250       260       270       280       290
                |         |         |         |         |
 241 - 299  TQDHVDILGPLSAQTGIAVLDMCASLKELLQNGMNGRTILGSALLEDEFTPFDVVRQCS
 241 - 299  THHHHHHHHHHHHHHHT THHHHHHHHHHHHHH 3TTT TTTT       THHHHHHHHH
```

33. Error: Abnormally short interatomic distances **Error**

↑ TOP

The pairs of atoms listed in the table below have an unusually short distance.

The contact distances of all atom pairs have been checked. Two atoms are said to `bump' if they are closer than the sum of their Van der Waals radii minus 0.40 Angstrom. For hydrogen bonded pairs a tolerance of 0.55 Angstrom is used. The first number in the table tells you how much shorter that specific contact is than the acceptable limit. The second distance is the distance between the centers of the two atoms.

The last text-item on each line represents the status of the atom pair. The text `INTRA' means that the bump is between atoms that are explicitly listed in the PDB file. `INTER' means it is an inter-symmetry bump. If a line contains the text 'HB', the bump criterium was relaxed because there could be a hydrogen bond. If the text 'BF' is present, the sum of the B-factors of the atoms is higher than 80, which makes the appearance of the bump somewhat less severe because the atoms probably aren't there anyway.

Bumps between atoms for which the sum of their occupancies is lower than one are not reported. In any case, each bump is listed in only one direction.

```
  42 CYS  (44  ) A SG    --   52 TYR  (54  ) A CE1     0.101   3.299 INTRA
  10 LYS  (12  ) A NZ    --  153 ASP  (155 ) A OD1     0.000   2.550 INTRA HB
```

34. Warning: Abnormal packing environment for some residues Warning

↑ TOP

The residues listed in the table below have an unusual packing environment.

The packing environment of the residues is compared with the average packing environment for all residues of the same type in good PDB files. A low packing score can indicate one of several things: Poor packing, misthreading of the sequence through the density, crystal contacts, contacts with a co-factor, or the residue is part of the active site. It is not uncommon to see a few of these, but in any case this requires further inspection of the residue.

```
 152 TYR  (154 ) A  -7.77
 220 ARG  (222 ) A  -6.95
 254 GLN  (256 ) A  -5.51
  95 LYS  (97  ) A  -5.50
 271 GLN  (273 ) A  -5.43
 139 LEU  (141 ) A  -5.40
 272 ASN  (274 ) A  -5.39
 103 ARG  (105 ) A  -5.31
 212 ASN  (214 ) A  -5.19
 135 LYS  (137 ) A  -5.11
 105 GLN  (107 ) A  -5.04
 187 GLN  (189 ) A  -5.03
  63 ASN  (65  ) A  -5.03
 140 ASN  (142 ) A  -5.03
 221 PHE  (223 ) A  -5.01
```

35. Note: No series of residues with bad packing environment Pass

↑ TOP

There are no stretches of three or more residues each having a quality control score worse than -4.0.

36. Note: Structural average packing environment OK Pass

↑ TOP

The structural average quality control value is within normal ranges.

Average for range 1 - 299 : -0.890

37. Note: Backbone oxygen evaluation OK Pass

↑ TOP

All residues for which the local backbone conformation could be found in the WHAT IF database have a normal backbone oxygen position.

38. Note: Rotamers checked OK Pass

↑ TOP

```
None of the residues that have a normal backbone environment have
abnormal rotamers.
```

39. Warning: Unusual backbone conformations Warning

↑ TOP

```
For the residues listed in the table below, the backbone formed by
itself and two neighboring residues on either side is in a
conformation that is not seen very often in the database of solved
protein structures.  The number given in the table is the number of
similar backbone conformations in the database with the same amino
acid in the center.

For this check, backbone conformations are compared with database
structures using C-alpha superpositions with some restraints on the
backbone oxygen positions.

A residue mentioned in the table can be part of a strange loop, or
there might be something wrong with it or its directly surrounding
residues. There are a few of these in every protein, but in any
case it is worth looking at!

   3 LYS  (5   ) A  0
   4 MET  (6   ) A  0
   5 ALA  (7   ) A  0
   6 PHE  (8   ) A  0
   7 PRO  (9   ) A  0
   8 SER  (10  ) A  0
   9 GLY  (11  ) A  0
  10 LYS  (12  ) A  0
  11 VAL  (13  ) A  0
  12 GLU  (14  ) A  0
  13 GLY  (15  ) A  0
  14 CYS  (16  ) A  0
  15 MET  (17  ) A  0
  16 VAL  (18  ) A  0
  17 GLN  (19  ) A  0
  18 VAL  (20  ) A  0
  19 THR  (21  ) A  0
  20 CYS  (22  ) A  0
  21 GLY  (23  ) A  0
  22 THR  (24  ) A  0
  23 THR  (25  ) A  0
  24 THR  (26  ) A  0
  25 LEU  (27  ) A  0
  26 ASN  (28  ) A  0
  27 GLY  (29  ) A  0
And so on for a total of   295 lines
```

40. Error: Backbone conformation Z-score very low Error

↑ TOP

```
A comparison of the backbone conformation with database proteins
shows that the backbone fold in this structure is very unusual.

 Backbone conformation Z-score : -26.447
```

41. Note: Symmetry related water molecules check not performed Pass

↑ TOP

```
Since there is no symmetry, the position check for symmetry related
water molecules can not be performed
```

42. Error: Average B-factor error Error

↑ TOP

```
The average B-factor for all buried protein atoms normally lies between
10--20. Values around 3--5 are expected for X-ray studies performed
at liquid nitrogen temperature.

Because of the extreme value for the average B-factor, no further analysis
of the B-factors is performed.

Average B-factor for buried atoms :  0.935
```

43. Error: HIS, ASN, GLN side chain flips Error

↑ TOP

```
Listed here are Histidine, Asparagine or Glutamine residues for which
the assignment or orientation determined from hydrogen bonding analysis
are different from the assignment given in the input. Either they could
form energetically more favorable hydrogen bonds if the terminal group
was rotated by 180 degrees, or there is no assignment in the input
file (atom type 'A') but an assignment could be made.

  70 ASN  (72  ) A
 178 ASN  (180 ) A
 212 ASN  (214 ) A
 244 HIS  (246 ) A
```

44. Note: Histidine type assignments Pass

↑ TOP

```
For all complete HIS residues in the structure a tentative
assignment to HIS-D (protonated on ND1), HIS-E (protonated on NE2),
or HIS-H (protonated on both ND1 and NE2, positively charged) is
made based on the hydrogen bond network.  A second assignment is
```

```
made based on which of the Engh and Huber [REF] histidine
geometries fits best to the structure.

In the table below all normal histidine residues are listed. The
assignment based on the geometry of the residue is listed first,
together with the RMS Z-score for the fit to the Engh and Huber
parameters.  For all residues where the H-bond assignment is
different, the assignment is listed in the last columns, together
with its RMS Z-score to the Engh and Huber parameters.

As always, the RMS Z-scores should be close to 1.0 if the residues
were restrained to the Engh and Huber parameters during refinement.

Please note that because the differences between the geometries of
the different types are small it is possible that the geometric
assignment given here does not correspond to the type used in
refinement.  This is especially true if the Z-scores are much higher
than 1.0.

If the two assignments differ, or the ``geometry'' Z-score is high,
it is advisable to verify the hydrogen bond assignment, check the
HIS type used during the refinement and possibly adjust it.

  39 HIS  (41  ) A HIS-E   0.30
  62 HIS  (64  ) A HIS-E   0.47 HIS-D   1.49
  78 HIS  (80  ) A HIS-E   0.40 HIS-D   1.43
 161 HIS  (163 ) A HIS-E   0.45
 162 HIS  (164 ) A HIS-E   0.36 HIS-H   1.65
 170 HIS  (172 ) A HIS-E   0.51
 244 HIS  (246 ) A HIS-E   0.31
```

45. Warning: Buried unsatisfied hydrogen bond donors Warning

↑ TOP

```
The buried hydrogen bond donors listed in the table below have a
hydrogen atom that is not involved in a hydrogen bond in the
optimized hydrogen bond network.

Hydrogen bond donors that are buried inside the protein normally
use all of their hydrogens to form hydrogen bonds within the
protein.  If there are any non hydrogen bonded buried hydrogen bond
donors in the structure they will be listed here.  In very good
structures the number of listed atoms will tend to zero.

  39 HIS  (41  ) A N
  47 MET  (49  ) A N
  48 LEU  (50  ) A N
  58 ARG  (60  ) A N
  66 VAL  (68  ) A N
  91 THR  (93  ) A N
 124 TYR  (126 ) A OH
 143 CYS  (145 ) A N
 146 VAL  (148 ) A N
 150 ILE  (152 ) A N
 169 VAL  (171 ) A N
 172 GLY  (174 ) A N
 196 THR  (198 ) A N
 217 PHE  (219 ) A N
 261 ASP  (263 ) A N
 286 GLU  (288 ) A N
 289 PHE  (291 ) A N
 290 THR  (292 ) A OG1
```

46. Note: Buried hydrogen bond acceptors OK Pass

↑ TOP

```
All buried polar side-chain hydrogen bond acceptors are involved in a
hydrogen bond in the optimized hydrogen bond network.
```

47. Note: Overall summary report Pass

↑ TOP

```
This is an attempt to create an overall summary of the quality of the
structure.  We do not recommend anyone to look at these numbers, please
look at the complete report instead.

 Structure Z-scores, positive is better than average:
  1st generation packing quality :  -0.975
  Ramachandran plot appearance   :  -0.782
  chi-1/chi-2 rotamer normality  :  -1.151
  Backbone conformation          : -26.447 (bad)

 RMS Z-scores, should be close to 1.0:
  Bond lengths                   :   0.669
  Bond angles                    :   1.140
  Omega angle restraints         :   1.300 (loose)
  Side chain planarity           :   1.151

REFERENCES
==========

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```

```
DSSP
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