



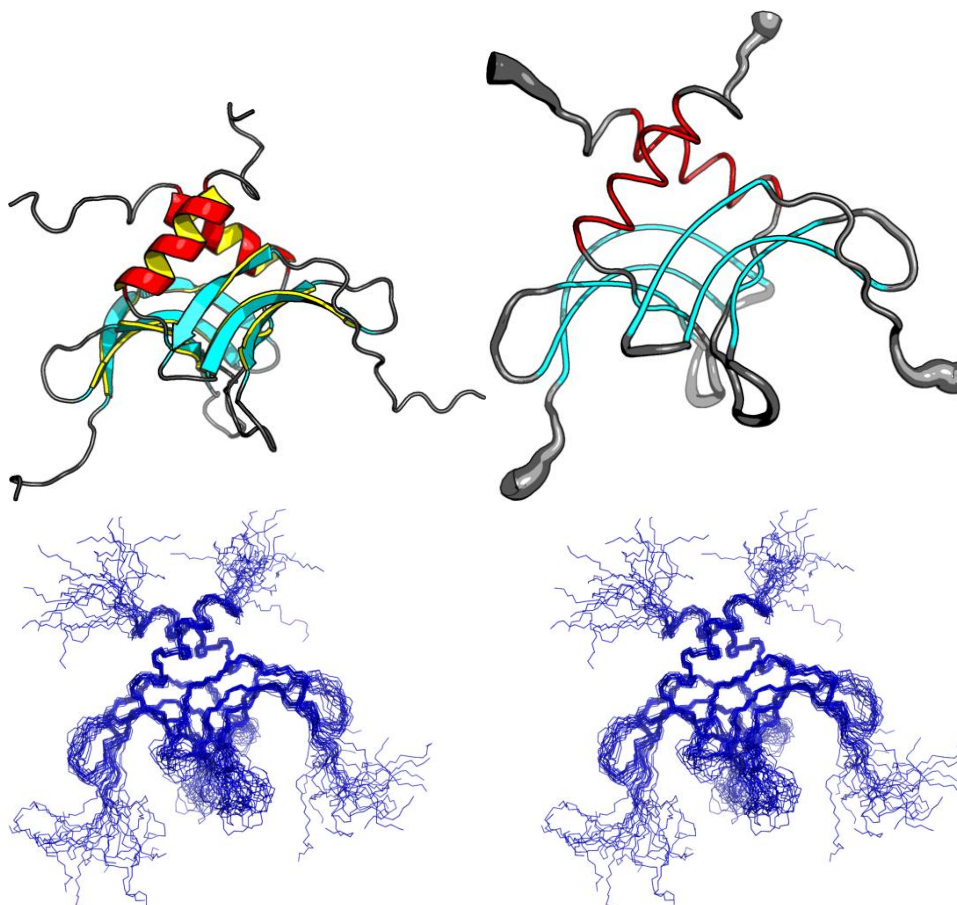
Structure Quality Analysis for NAME

Analyses performed for user defined residues.

The constraints analysis is based on the following files: NOE distance constraints file. Angular constraints file. H-bond constraints file.

Procheck analysis, RMSD calculation and structure superimposition are based on: User defined residues

NESG ID: NAME
PDB ID:
Deposition date:
Common Name:
Class:
Length (a.a.): 164
Organism:
SwissProt /
TrEMBL ID:
models: 20
Oligomerization: dimer
Molecular
weight: 19131



Secondary Structure Elements:

Inter-chain break(s) between 82 & 93

alpha helices: 61A-72A, 61B-73B

beta strands: 9E-21E, 25P-34P, 39A-46A, 57E-59E, 9E-21E, 25P-34P, 40S-46S, 57E-59E

Total number of restricting constraints per restrained residue: 26.0

Restricting long range constraints per restrained residue: 9.1

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

3.25 0.2 0



Structure Quality Analysis for NAME

Dihedral angle violations per model

1 - 10° > 10°

5 0

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score

0.966 0.926 0.946 0.835

RMSD *All residues* *Ordered residues*² *Selected residues*³

All backbone atoms 2.8 Å 0.6 Å 0.6 Å

All heavy atoms 3.5 Å 1.1 Å 1.1 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions *Additionally allowed regions* *Generously allowed regions* *Disallowed regions*

92.6% 7.4% 0.0% 0.0%

Ramachandran Plot Summary for selected residues³ from Richardson Lab's Molprobity

Most favoured regions *Allowed regions* *Disallowed regions* [View plot](#) [View model summary](#)

97% 3% 0%

Global quality scores

Program *Verify3D* *ProsaII (-ve)* *Procheck (phi-psi)*³ *Procheck (all)*³ *MolProbity Clashscore*

-Raw score 0.27 0.24 -0.38 -0.32 25.93

*Z-score*¹ -3.05 -1.70 -1.18 -1.89 -2.92

Generalized linear model RMSD prediction: 2.11

Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 & Åring for H atoms, 2.2 & Åring for heavy atoms): 86

RMS deviation for bond angles: 0.6°

RMS deviation for bond lengths: 0.004 Å

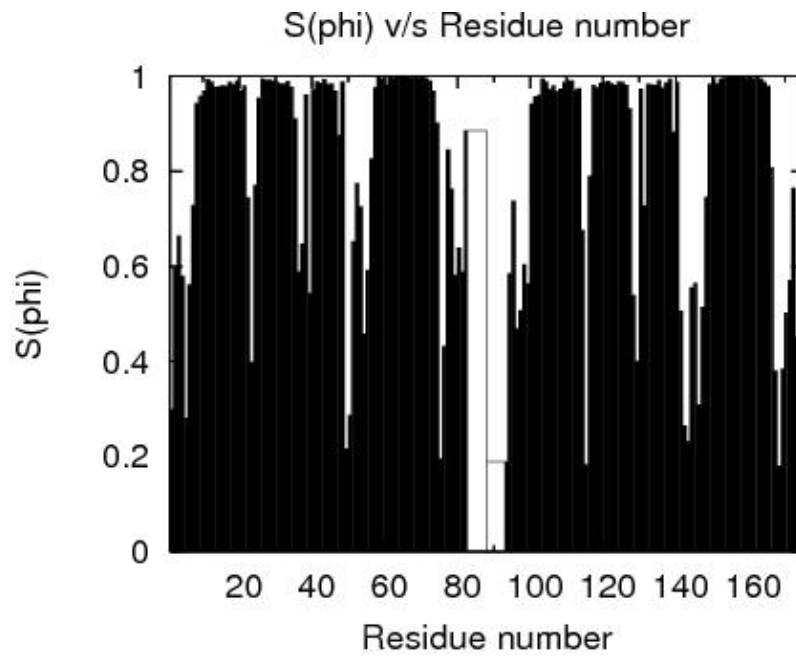
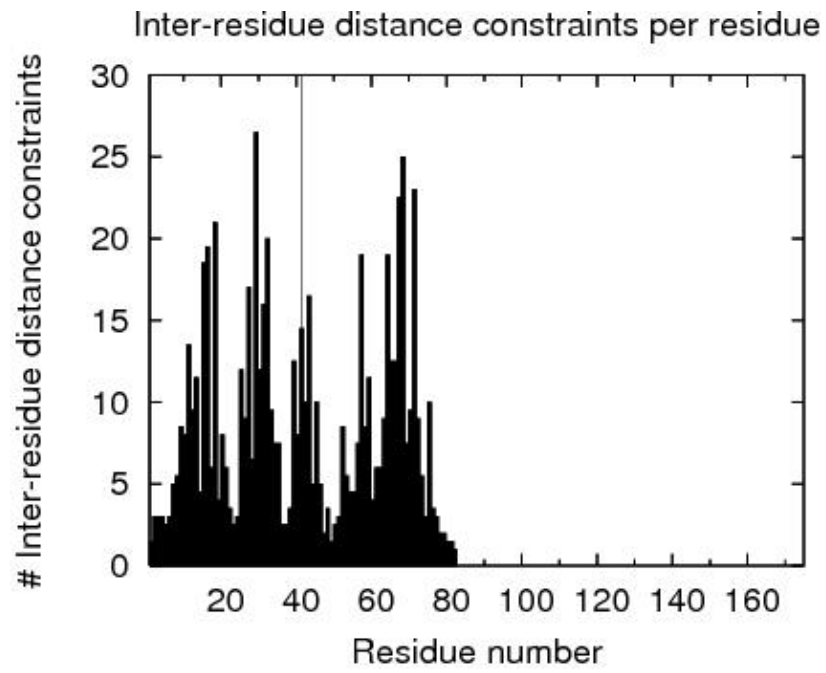
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 8A-21A,25A-34A,40A-46A,57A-73A,8B-21B,25B-34B,40B-47B,57B-73B

³Selected residues: 8A-21A,25A-34A,40A-46A,57A-73A,8B-21B,25B-34B,40B-47B,57B-73B

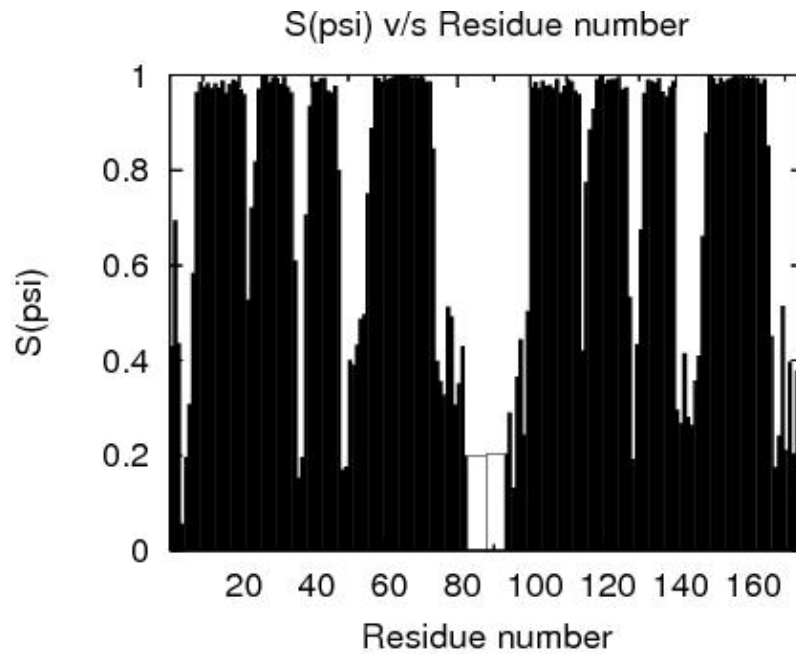


Structure Quality Analysis for NAME





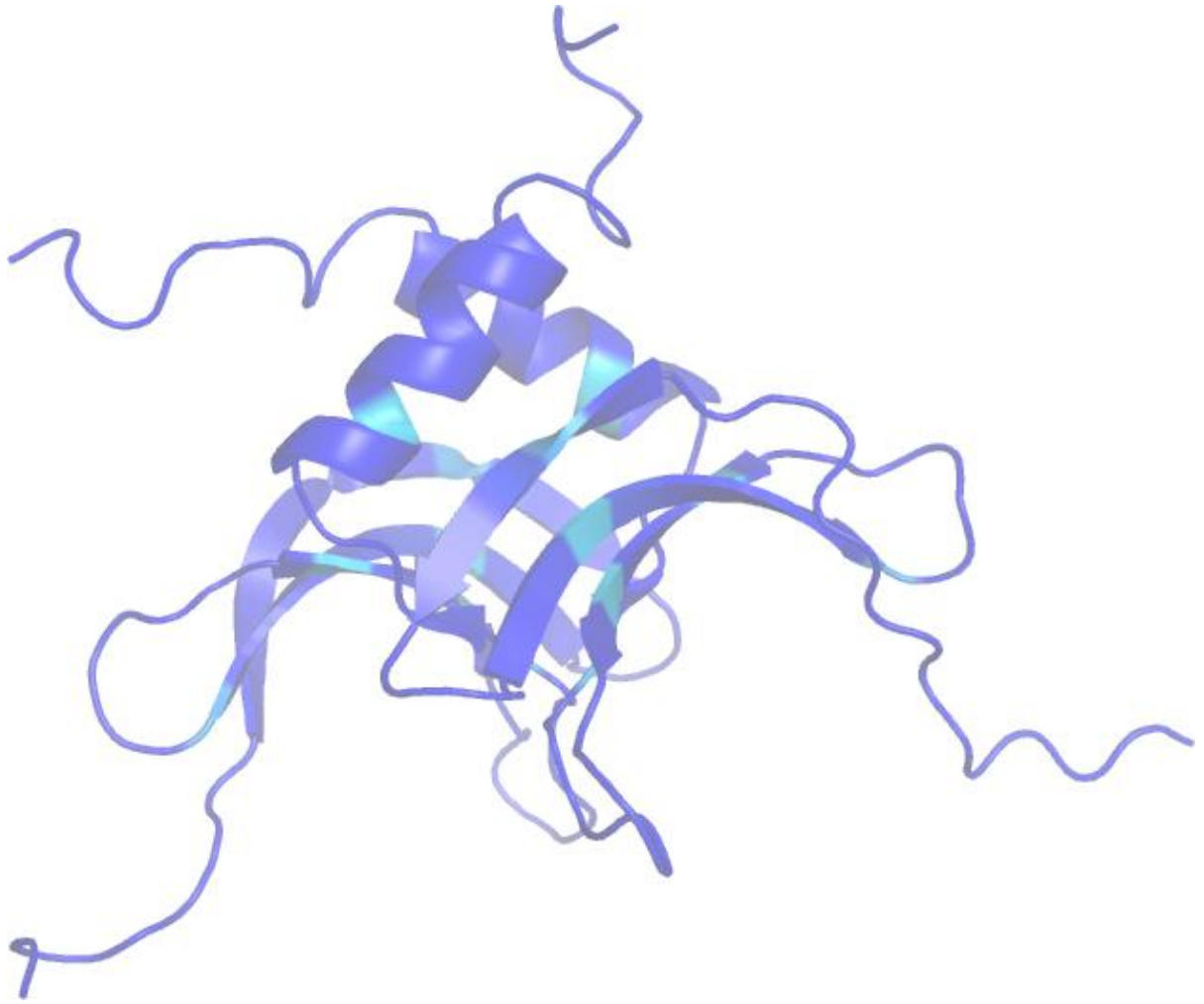
Structure Quality Analysis for NAME



RPF Precision Map



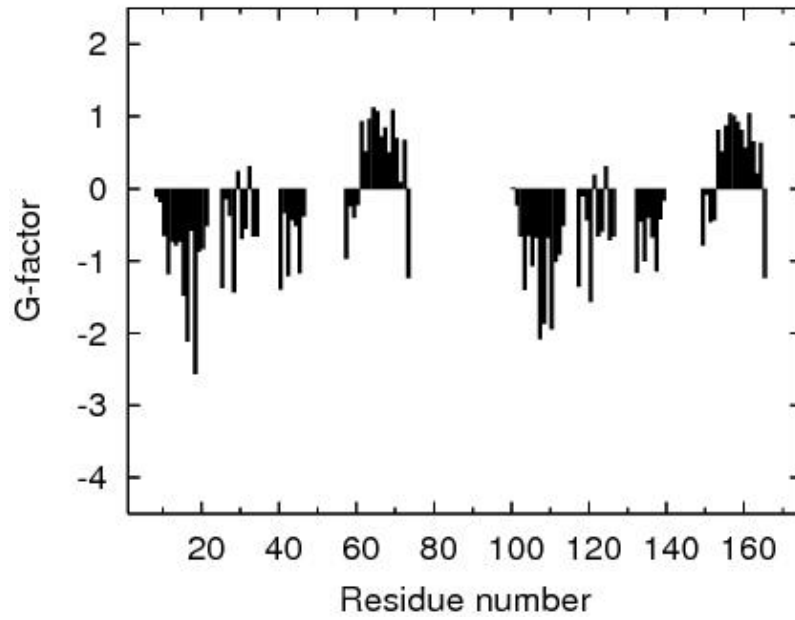
Structure Quality Analysis for NAME



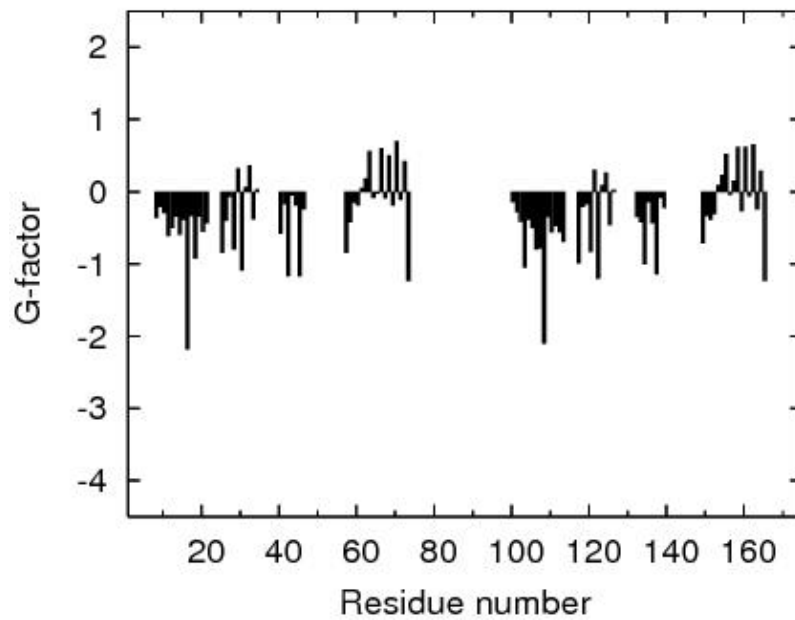


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

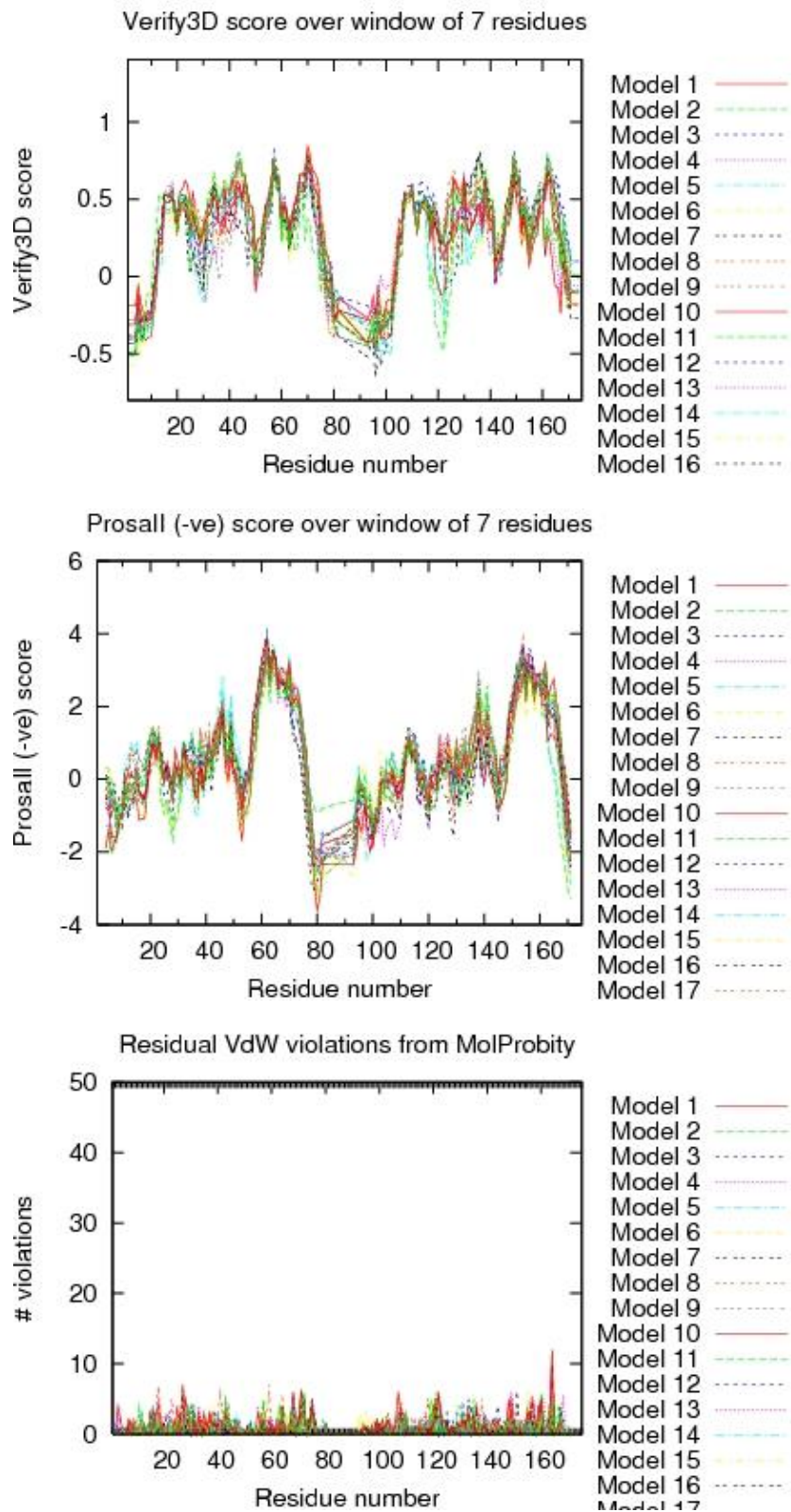


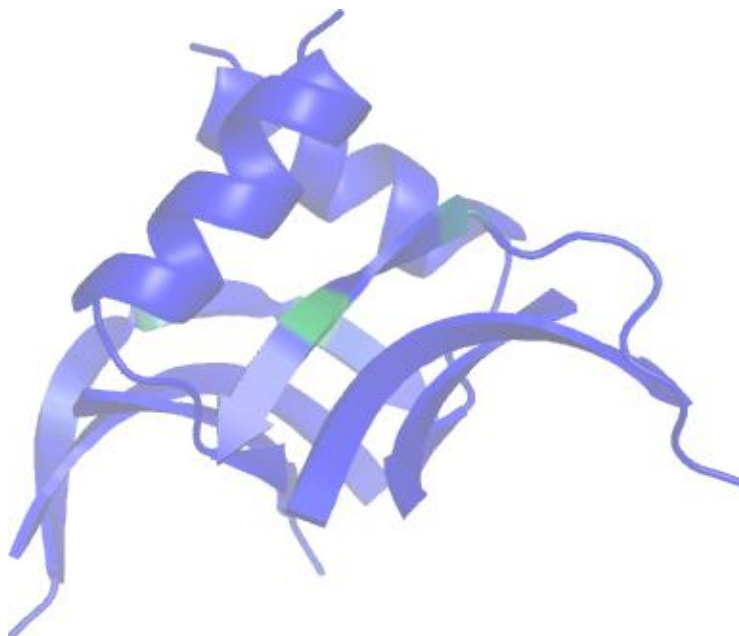
Procheck G-factor for all dihedral angles





Structure Quality Analysis for NAME





Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobit)

References:

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3. Sippl M J, "Recognition of Errors in Three-Dimensional Structures of Proteins", Proteins 17 (1993): 355-362
4. Sippl M J, "Calculation of Conformation Ensembles from Potentials of Mean Force", J Mol Biol 213 (1990): 859-883
5. Laskowski R Ai et al, "AQUA and PROCHECK_NMR: Programs for checking the quality of proteins structures solved by NMR", J Biomolec NMR 8 (1996): 477-486
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8. Word J M et al, "Asparagine and Glutamine: Using Hydrogen Atom Contacts in the Choice of Side-chain Amide Orientation", J Mol Biol 285 (1999): 1735-1747
9. Word J M et al, "Visualizing and Quantifying Molecular Goodness-of-Fit: Small-probe Contact Dots with Explicit Hydrogens", J Mol Biol 285 (1999): 1711-1733
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11. Luthy R, McLachlan A D and Eisenberg D, "Secondary Structure-Based Profiles: Use of Structure-Conserving Scoring Tables in Searching Protein Sequence Databases for Structural Similarities", Proteins 10 (1991): 229-239
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17. Bagaria, A., Jaravine, V., Huang, Y.J., Montelione, G.T., and Guntert, P. "Protein structure validation by generalized linear model root-mean-square deviation prediction". Protein Sci 21(2012), 229-238.

Analysed by on May-10-2013 using PSVS 1.3



Software Environment

Software for structure quality evaluation:

DSSP	DsspCMBI-April-2000
pdbstat	PdbStat-5.4 Version
AutoAssign	Version 2.4.0 (uses only AVS scripts)
RPF analysis	ASDP-1.0
PDB validation	Version 8.061
Verify3D	Version 1.0 corrected by Aneerban
ProsaII	Prosa2003
PROCHECK	Version 3.5.4
MolMol	Version 2K.2

MolProbit programs:

cluster	1999
clashlistcluster	1999 (corrected by Aneerban)
mage	Version 6.35.040409
prekin	Version 6.35.040406
reduce	Version 2.14
probe	Version 2.6

Other Software:

PERL	Version 5.8.0
convert	ImageMagick 5.5.6
ps2pdf	Ghostscript 7.05
htmldoc	v1.9



Structure Quality Analysis for NAME

```
gnuplot      Version 3.7 patchlevel 3
jpegtopnm   year 2000
pnmcrop      year 2000
pnmtojpeg   year 2000
```