



# 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.

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.): 108

Organism:

SwissProt /  
TrEMBL ID:

# models: 20

Oligomerization: monomer

Molecular  
weight: 12029

Secondary Structure Elements:

alpha helices:

beta strands: 6U-11U, 22A-30A, 62U-69U, 15L-17L, 98L-106L, 75Y-83Y, 36L-45L, 48R-57R

Total number of restricting constraints per restrained residue: 26.7

Restricting long range constraints per restrained residue: 11.5

Distance violations per model

Calculated using sum over  $r^{-6}$

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

30.7 73.55 168.05

Dihedral angle violations per model

1 - 10 ° > 10 °

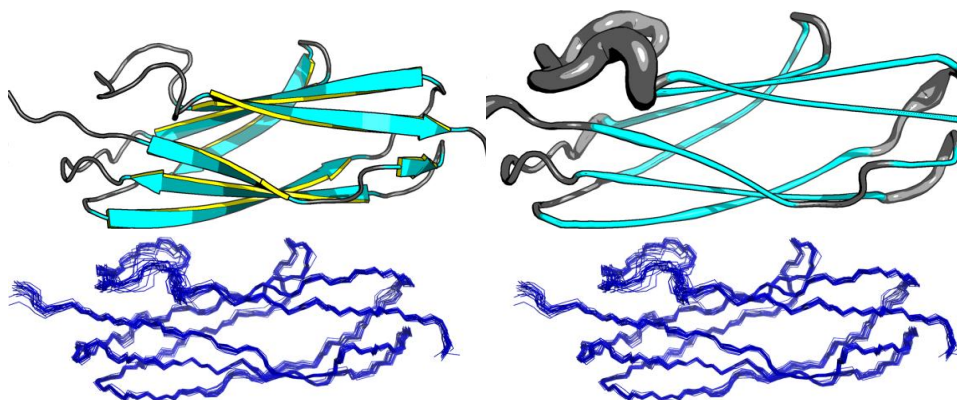
32.15 26.9

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score

0.958 0.946 0.952 0.854





## Structure Quality Analysis for NAME

RMSD	All residues	Ordered residues <sup>2</sup>	Selected residues <sup>3</sup>
All backbone atoms	0.4 Å	0.4 Å	0.4 Å
All heavy atoms	0.8 Å	0.7 Å	0.7 Å

Ramachandran Plot Summary for selected residues<sup>3</sup> from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
91.6%	8.4%	0.0%	0.0%

Ramachandran Plot Summary for selected residues<sup>3</sup> from Richardson Lab's Molprobit

Most favoured regions	Allowed regions	Disallowed regions	<a href="#">View plot</a>	<a href="#">View model summary</a>
98.3%	1.7%	0%		

### Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) <sup>3</sup>	Procheck (all) <sup>3</sup>	MolProbit Clashscore
-Raw score	0.43	0.42	-0.38	-0.02	2.90
Z-score <sup>1</sup>	-0.48	-0.95	-1.18	-0.12	1.03

### Generalized linear model RMSD prediction: 1.40

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):	0
RMS deviation for bond angles:	0.6 °
RMS deviation for bond lengths:	0.011 Å

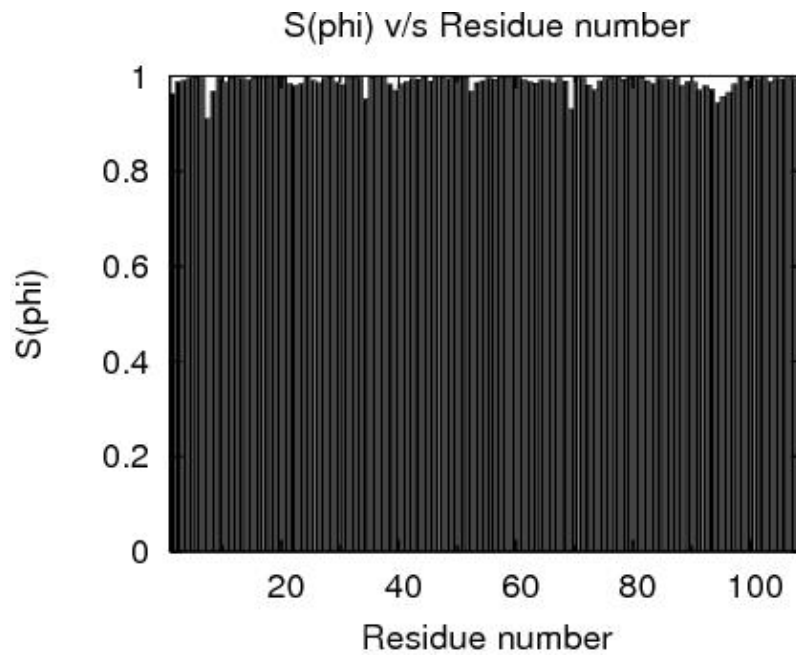
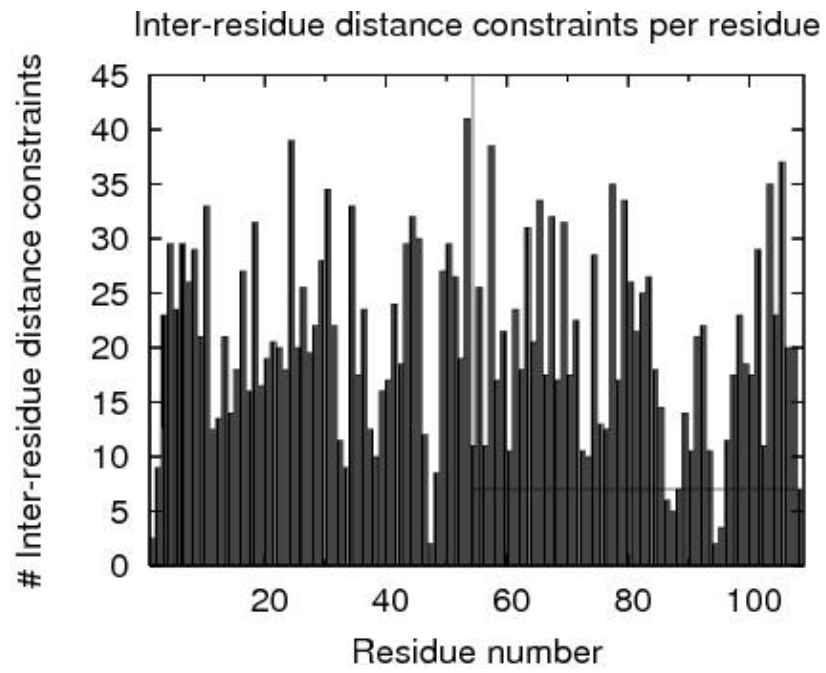
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

<sup>2</sup>Order residues: 1A-107A

<sup>3</sup>Selected residues: 2A-107A

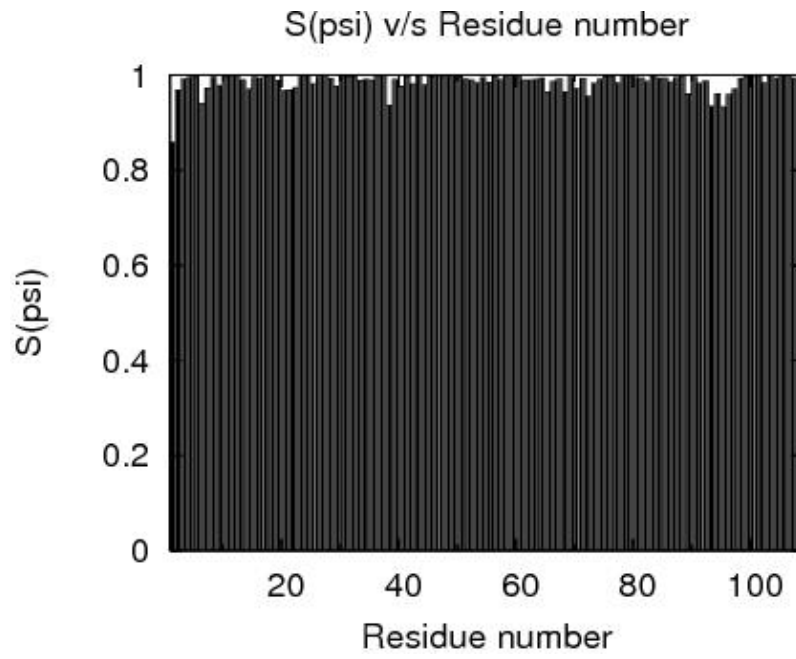


# Structure Quality Analysis for NAME

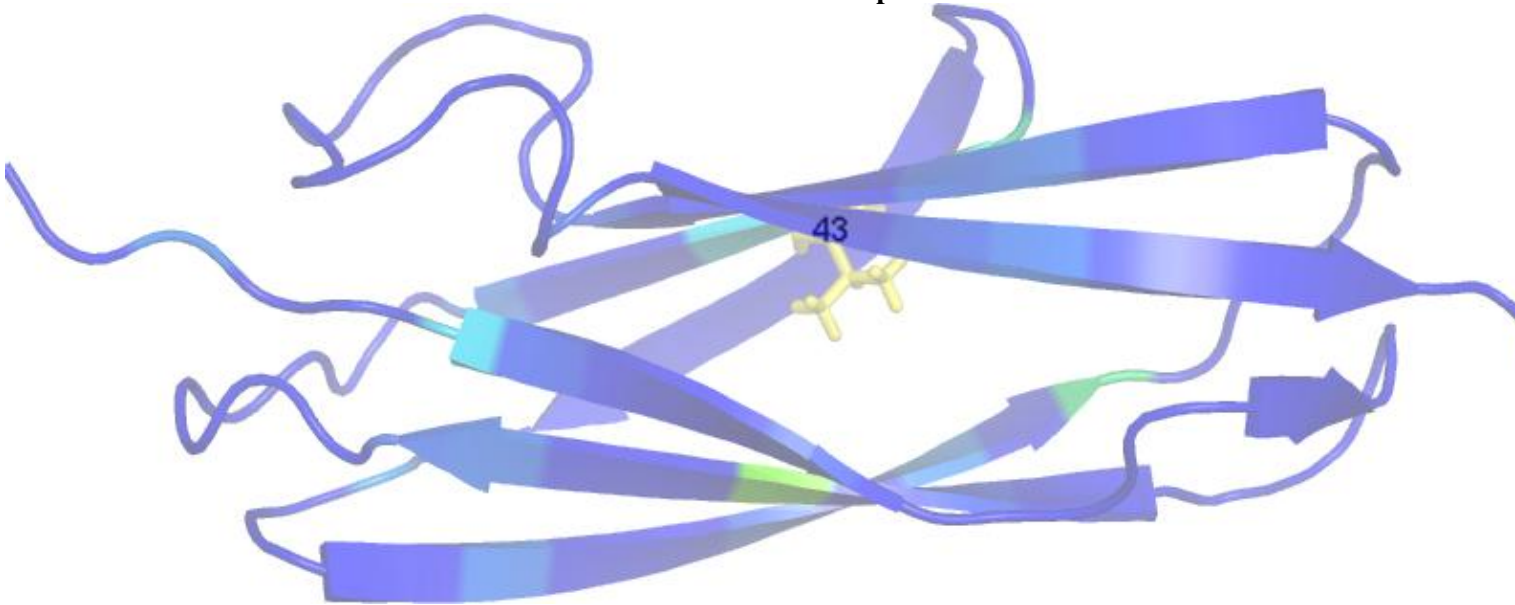




# Structure Quality Analysis for NAME



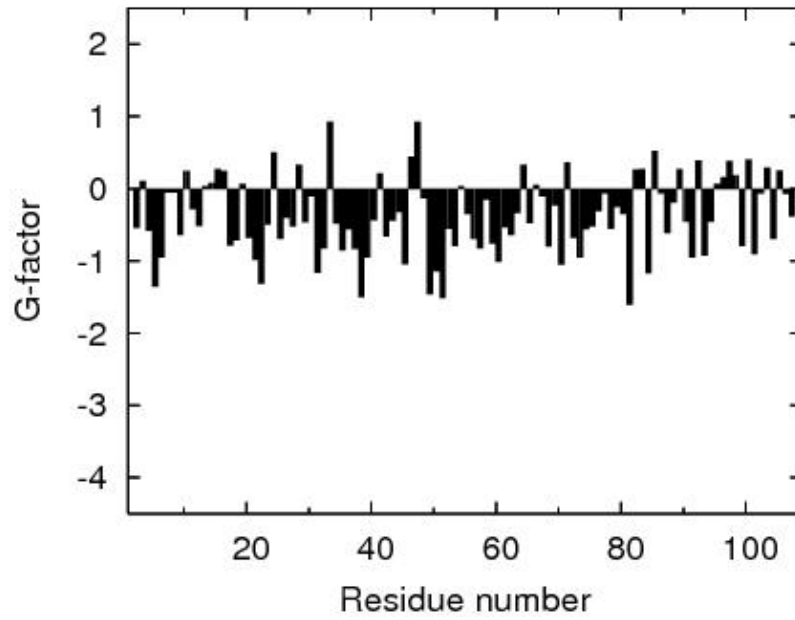
### RPF Precision Map



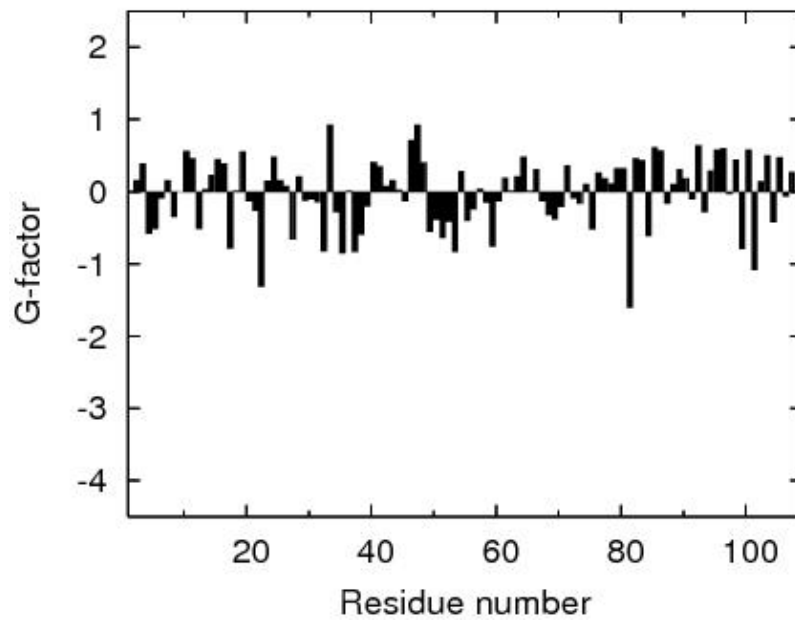


## Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

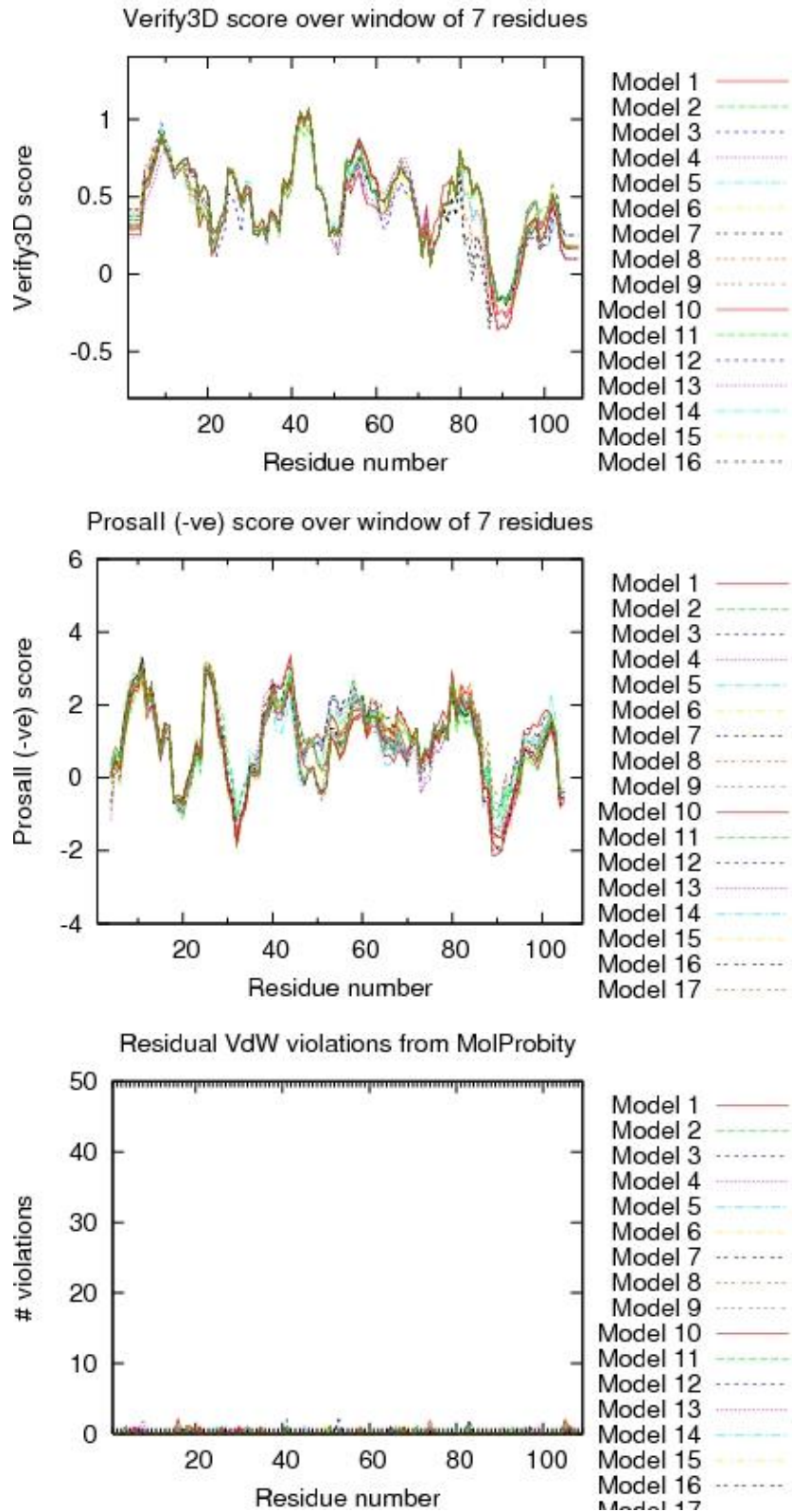


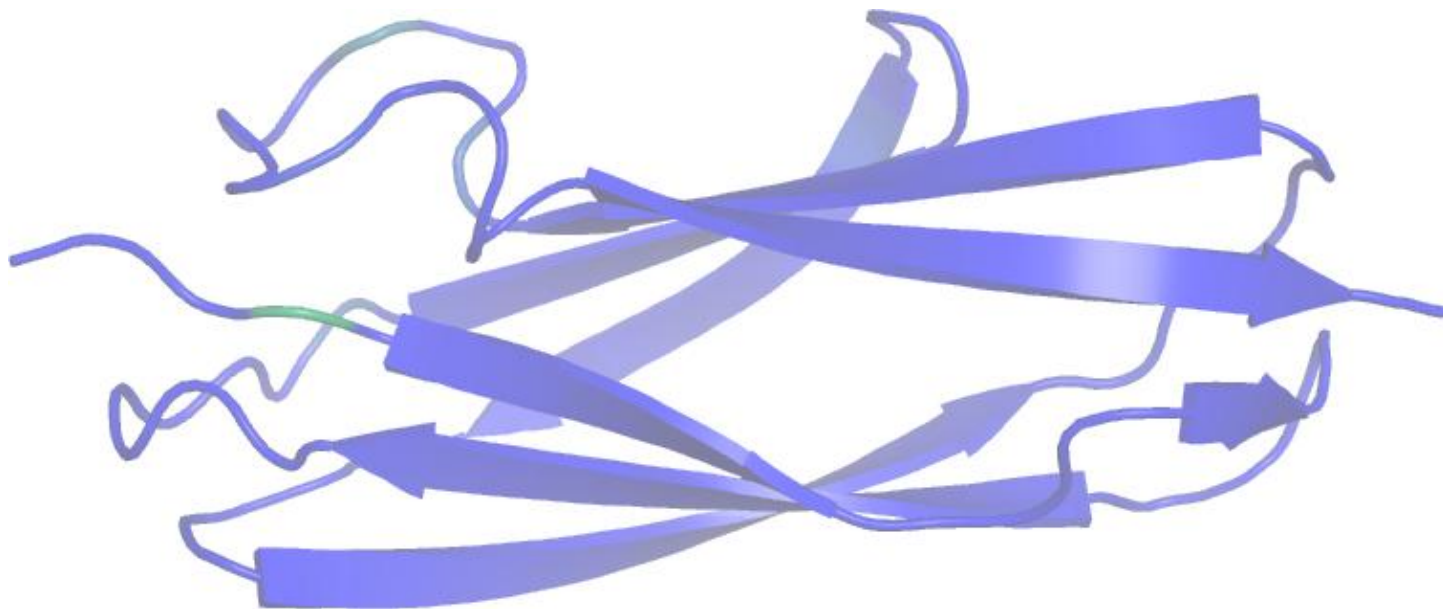
Procheck G-factor for all dihedral angles





# Structure Quality Analysis for NAME





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

**References:**

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2. Bowie J U, Luthy R and Eisenberg D, "A Method to Identify Protein Sequences that Fold into a Known Three-Dimensional Structure", Science 253 (1991): 164-169
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 A et al, "AQUA and PROCHECK\_NMR: Programs for checking the quality of proteins structures solved by NMR", J Biomolec NMR 8 (1996): 477-486
6. Laskowski R A et al "PROCHECK: a program to check the stereochemical quality of protein structures" J Appl Cryst, 26 (1993): 283-291
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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
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10. Tejero R and Montelione G T, "PDBStat", unpublished
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13. Koradi, R, et al, "MOLMOL: a program for display and analysis of macromolecular structures ", J Mol



Graphics 14 (1996): 51-55.

14. Güntert, P, Mumenthaler, C & Wüthrich, K "Torsion angle dynamics for NMR structure calculation with the new program DYANA", J. Mol. Biol 273 (1997): 283-298

15. Lovell S C et al, "Structure validation by Calpha geometry: phi,psi and Cbeta deviation" Proteins (2003) 50: 437-450

16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features", Biopolymers (1983) 22: 2577-2637

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



## Structure Quality Analysis for NAME

```
htmldoc          v1.9
gnuplot          Version 3.7 patchlevel 3
jpegtopnm       year 2000
pnmcrop         year 2000
pnmtojpeg       year 2000
```