



# 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.): 99

Organism:

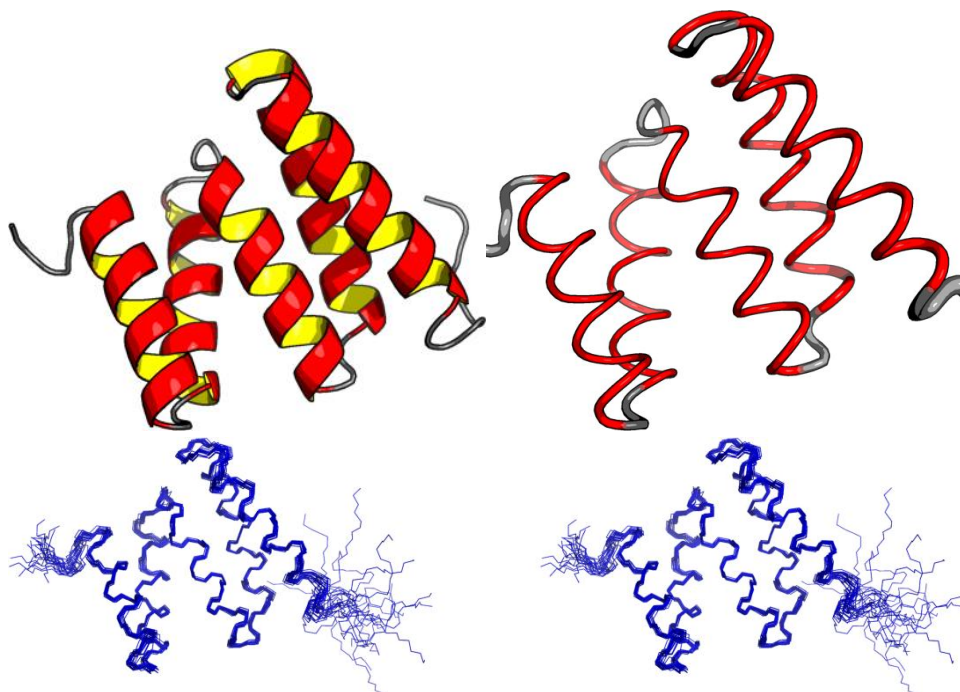
SwissProt /

TrEMBL ID:

# models: 20

Oligomerization: monomer

Molecular weight: 11468



Secondary Structure Elements:

alpha helices: 6A-18A, 22A-35A, 40A-52A, 56A-72A, 76A-89A

beta strands:

Total number of restricting constraints per restrained residue: 34.8

Restricting long range constraints per restrained residue: 8.5

Distance violations per model

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

0.1 - 0.2 Å   0.2 - 0.5 Å   > 0.5 Å

3            0.1            0

Dihedral angle violations per model

1 - 10 °   > 10 °

7.2        0.65

FIDs deposited in the BMRB? no



## Structure Quality Analysis for NAME

### RPF Scores

Recall Precision F-measure DP-score

0.931 0.971 0.95 0.828

RMSD *All residues* *Ordered residues*<sup>2</sup> *Selected residues*<sup>3</sup>

*All backbone atoms* 1.6 Å 0.4 Å 0.4 Å

*All heavy atoms* 2.2 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*

91.7% 8.2% 0.1% 0.0%

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

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

97.1% 2.9% 0%

### Global quality scores

Program *Verify3D* *ProsaII (-ve)* *Procheck (phi-psi)*<sup>3</sup> *Procheck (all)*<sup>3</sup> *MolProbability Clashscore*

*-Raw score* 0.35 0.81 0.39 0.22 12.91

*Z-score*<sup>1</sup> -1.77 0.66 1.85 1.30 -0.69

### Generalized linear model RMSD prediction: 0.68

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

Number of close contacts (within 1.6 & Å for H atoms, 2.2 & Å for heavy atoms): 5

RMS deviation for bond angles: 1.1 °

RMS deviation for bond lengths: 0.018 Å

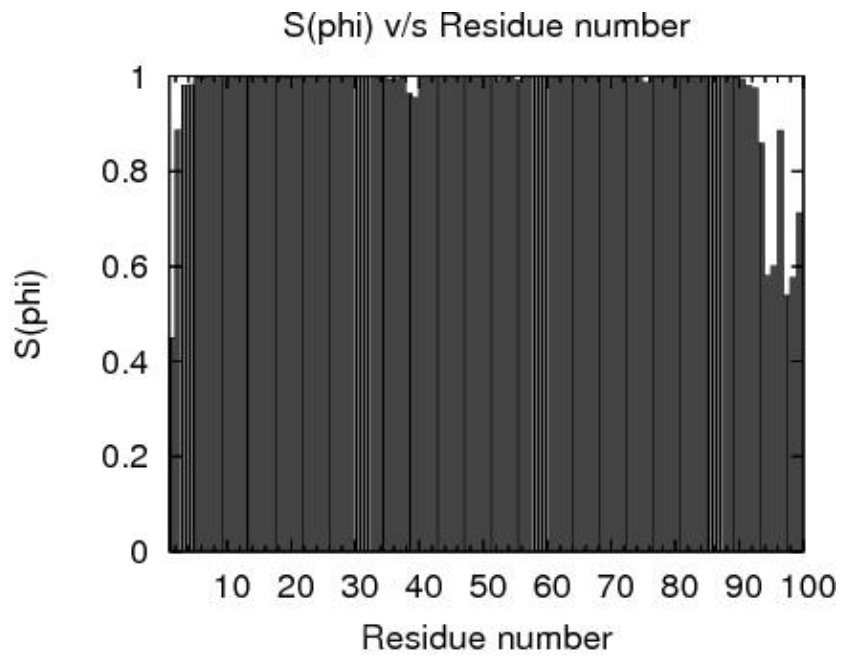
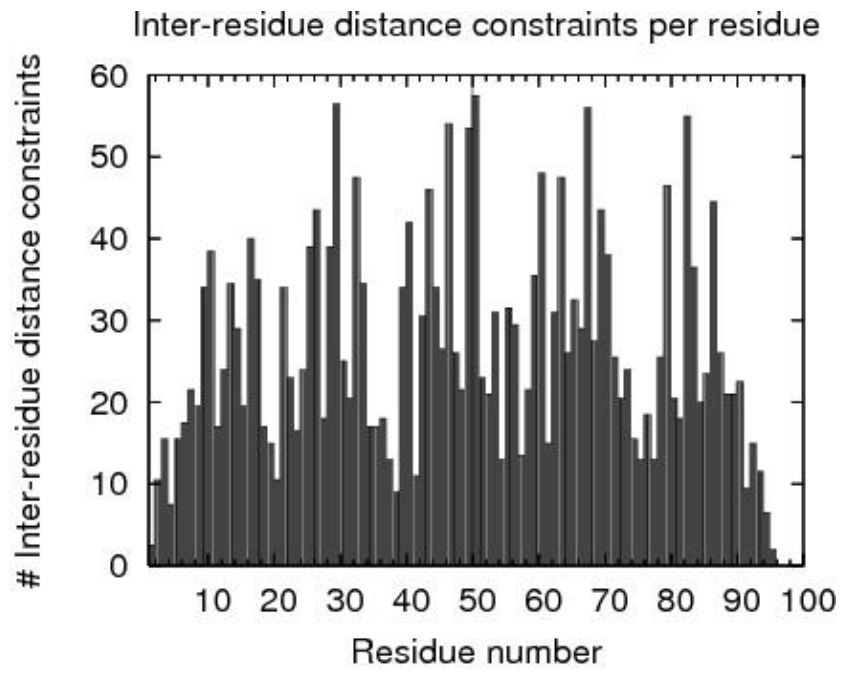
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

<sup>2</sup>Order residues: 2A-92A

<sup>3</sup>Selected residues: 2A-92A

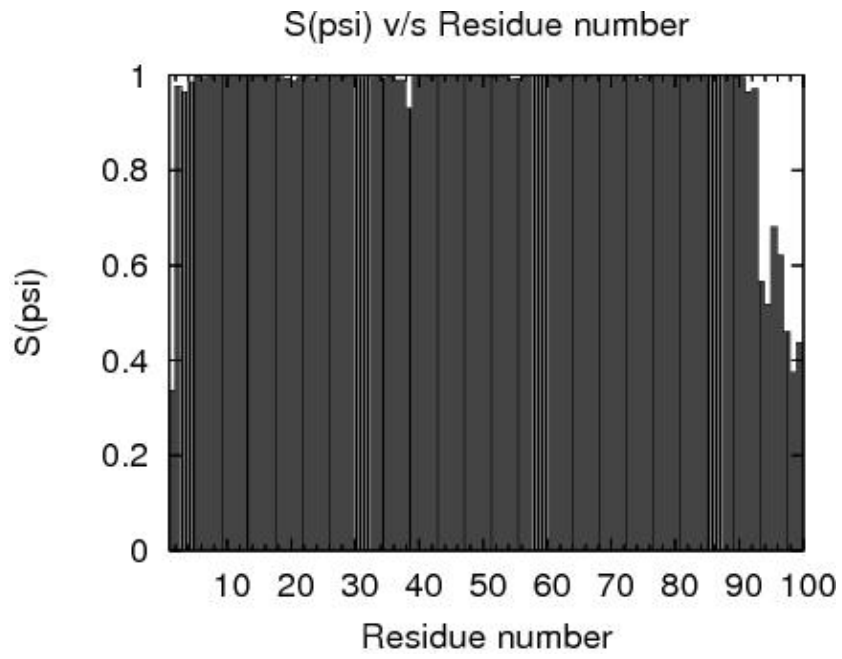


# Structure Quality Analysis for NAME

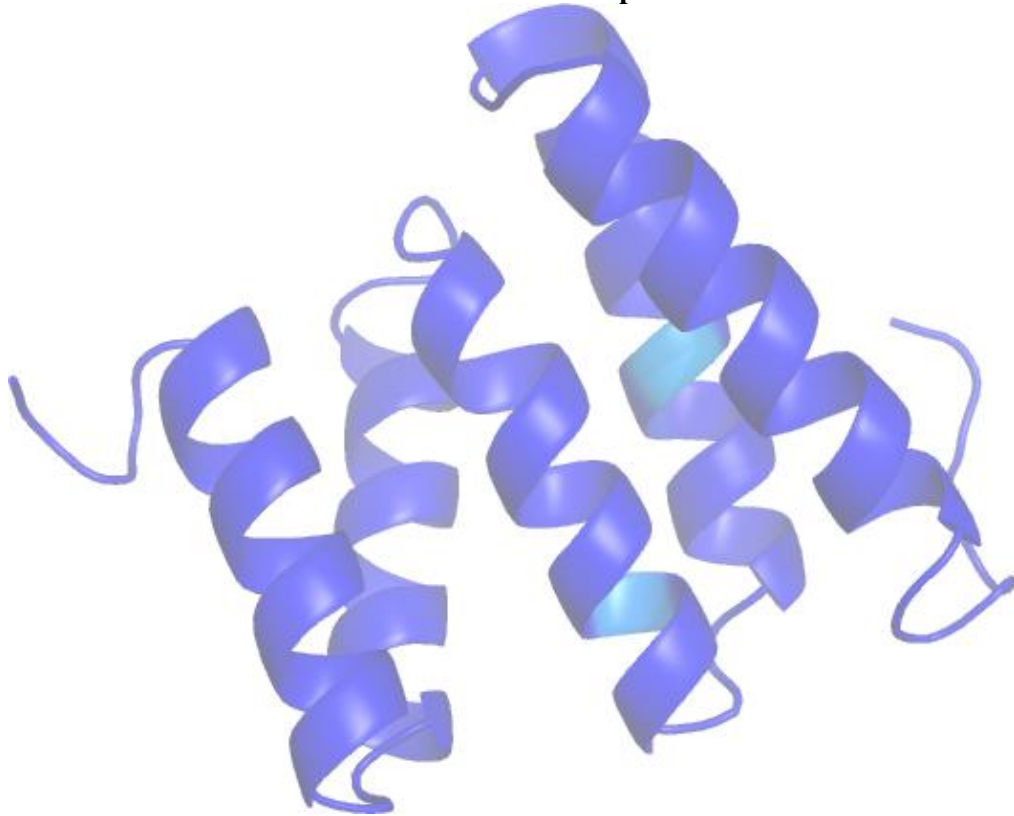




# Structure Quality Analysis for NAME



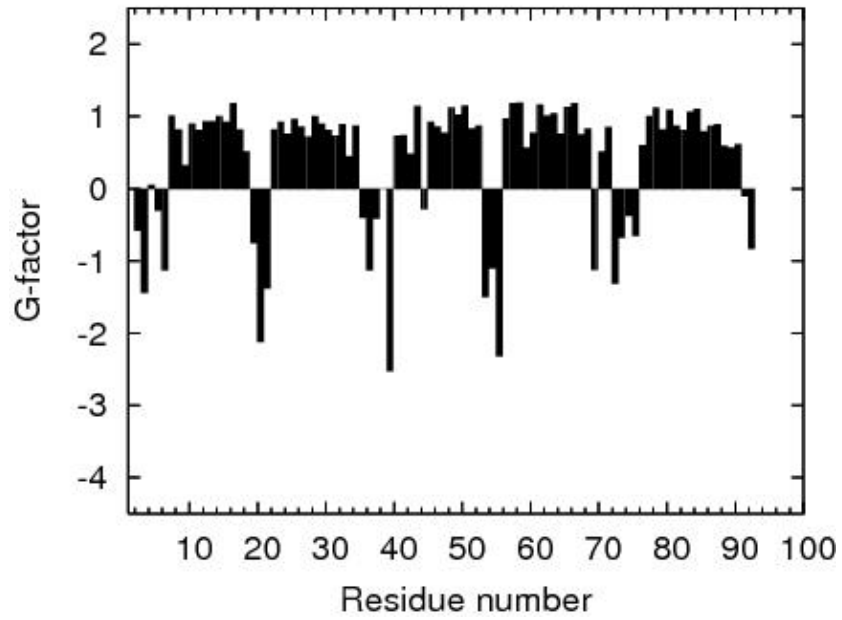
**RPF Precision Map**



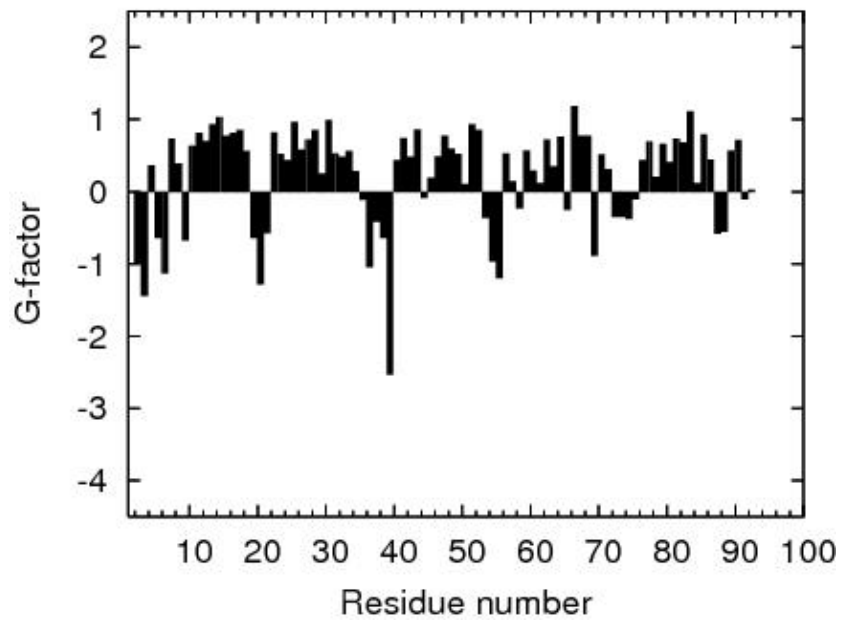


## Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

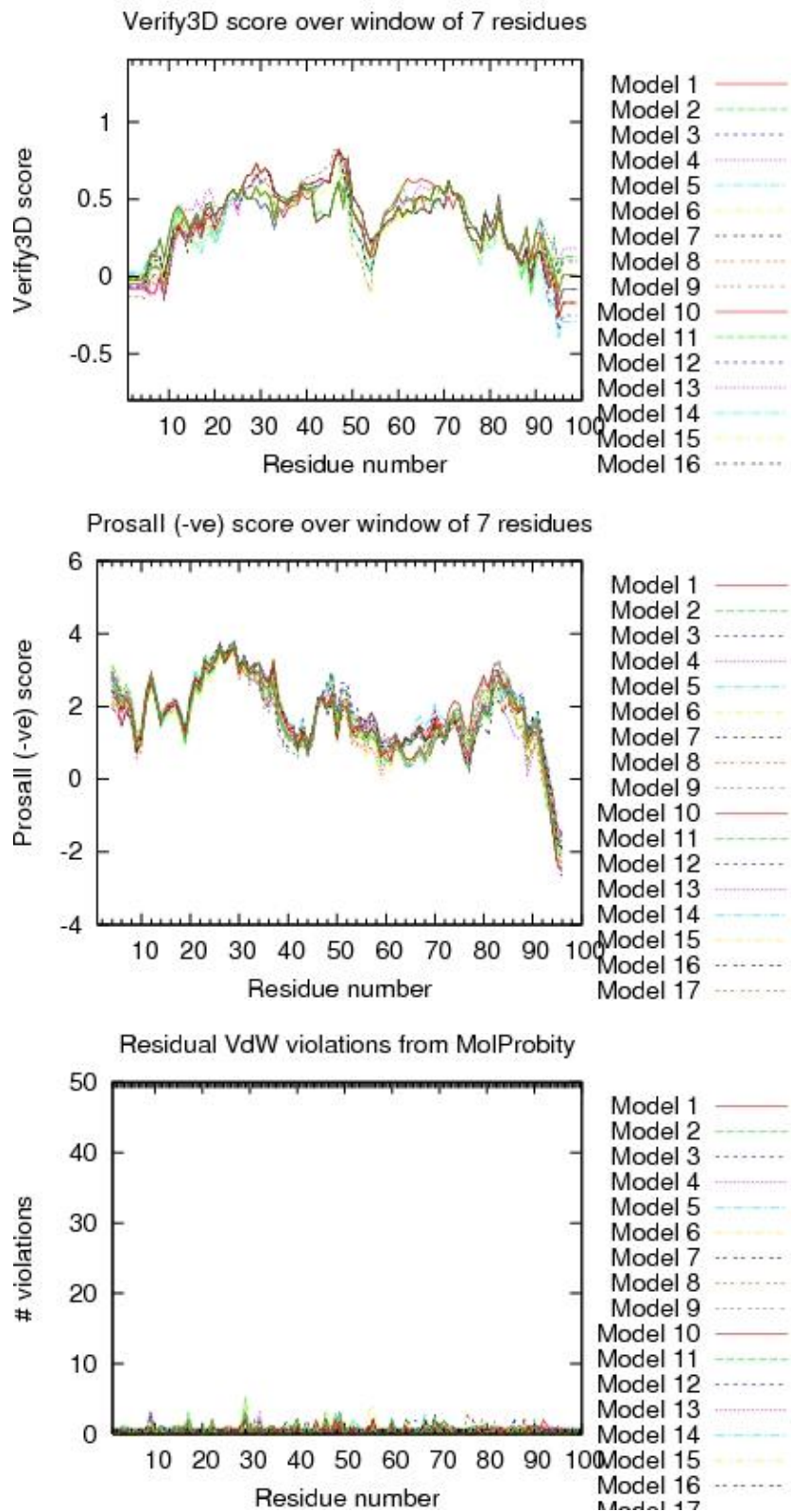


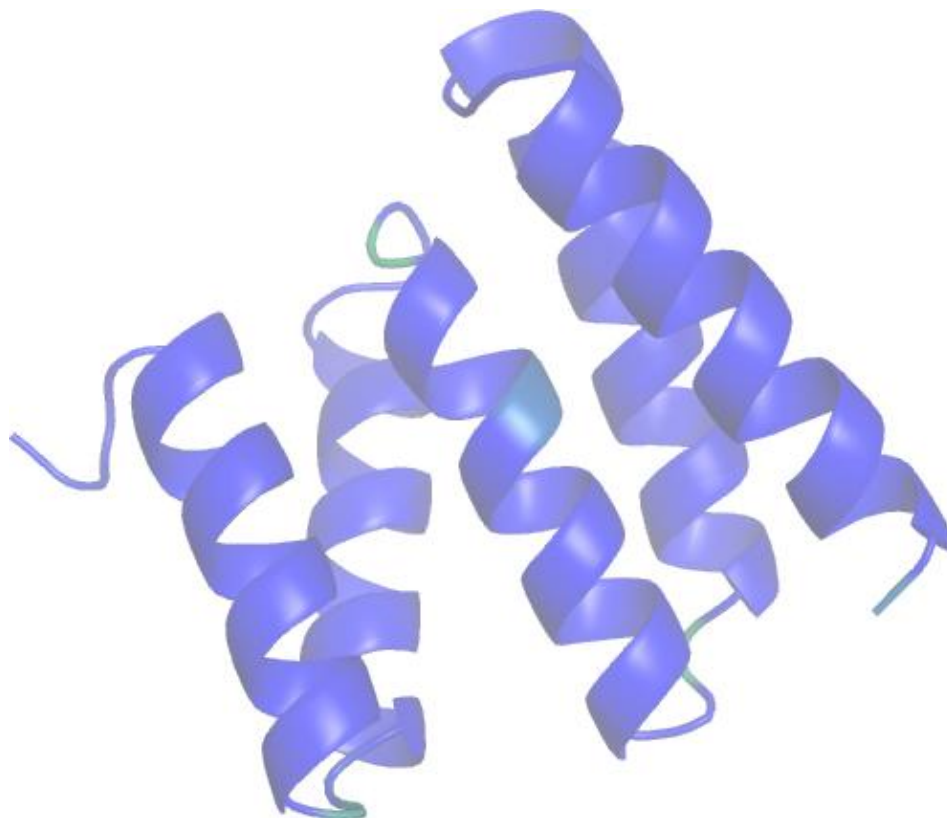
Procheck G-factor for all dihedral angles





## Structure Quality Analysis for NAME





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

***References:***

1. Luthy R, Bowie J U and Eisenberg D, "Assessment of protein models with three-dimensional profiles", Nature 356 (1992): 83-85
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
7. Word J M et al, "Exploring steric constraints on protein mutations using MAGE / PROBE", Prot Sci 9 (2000): 2251-2259
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
10. Tejero R and Montelione G T, "PDBStat", unpublished
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

12. Richardson D C, Richardson J S, "The kinemage: a tool for scientific communication", Prot Sci 1(1) (1992): 3-9

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