



# 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.): 96

Organism:

SwissProt /

TrEMBL ID:

# models: 20

Oligomerization: monomer

Molecular weight: 10776

Secondary Structure Elements:

alpha helices:

beta strands: 10R-13R, 33L-36L, 15U-18U, 51A-54A, 67L-69L, 24R-26R, 84L-91L, 61Y-66Y, 37R-38R, 76S-77S

Total number of restricting constraints per restrained residue: 10.5

Restricting long range constraints per restrained residue: 4.4

Distance violations per model

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

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

6.7 17.05 32.1

Dihedral angle violations per model

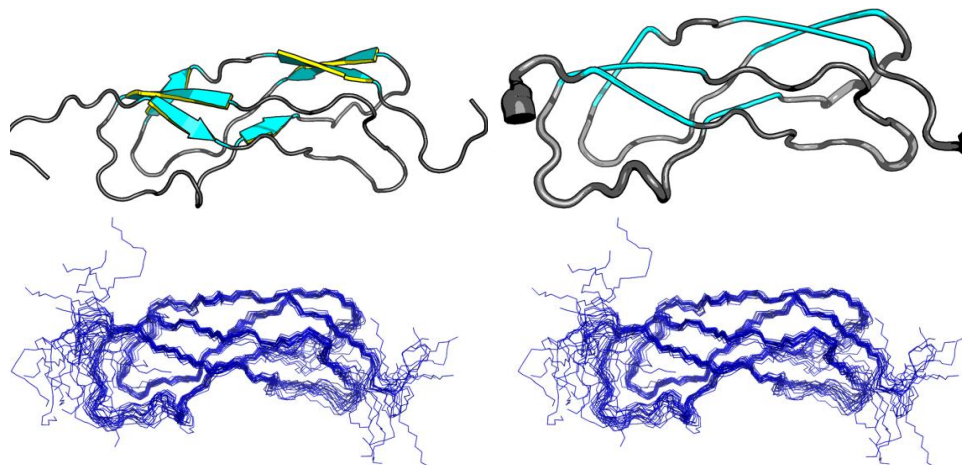
1 - 10° > 10°

1.8 1.3

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score





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0.949 0.863 0.904 0.832

RMSD	All residues	Ordered residues <sup>2</sup>	Selected residues <sup>3</sup>
All backbone atoms	2.2 Å	0.7 Å	0.7 Å
All heavy atoms	2.7 Å	1.2 Å	1.2 Å

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

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
92.7%	7.3%	0.0%	0.0%

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

Most favoured regions	Allowed regions	Disallowed regions	<a href="#">View plot</a>	<a href="#">View model summary</a>
99.4%	0.4%	0.2%		

### Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) <sup>3</sup>	Procheck (all) <sup>3</sup>	MolProbability Clashscore
-Raw score	0.41	0.56	-0.42	-0.00	2.79
Z-score <sup>1</sup>	-0.80	-0.37	-1.34	-0.00	1.05

### Generalized linear model RMSD prediction: 1.39

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):	0
RMS deviation for bond angles:	0.7 °
RMS deviation for bond lengths:	0.010 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

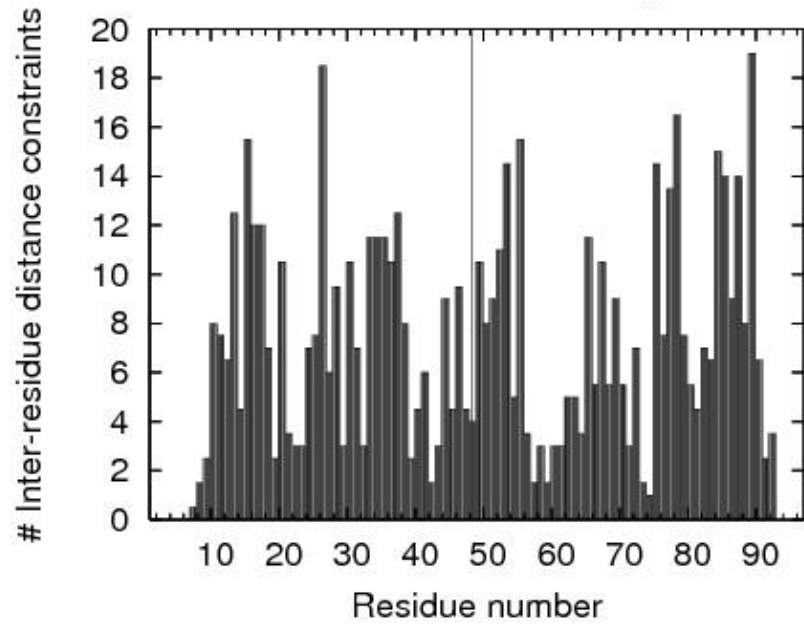
<sup>2</sup>Order residues: 9A-17A,24A-42A,45A-55A,59A-72A,75A-91A

<sup>3</sup>Selected residues: 9A-17A,24A-42A,45A-55A,59A-72A,75A-91A

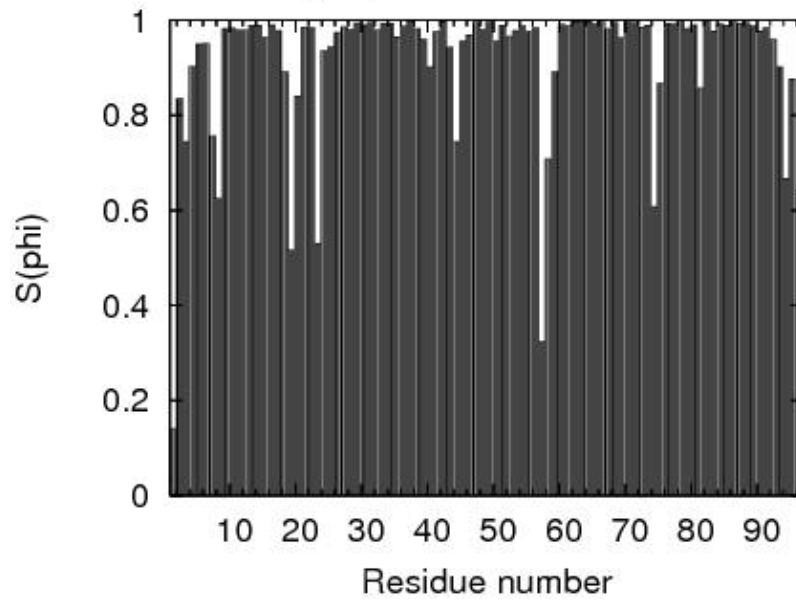


# Structure Quality Analysis for NAME

## Inter-residue distance constraints per residue

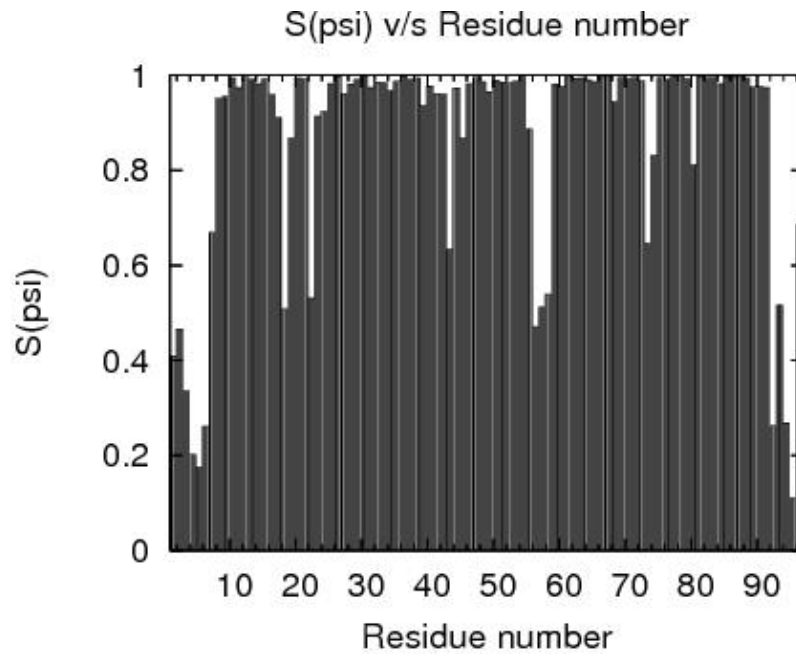


## S(phi) v/s Residue number

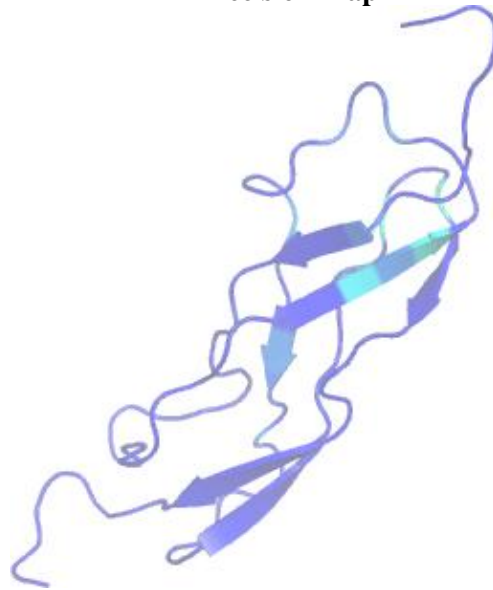




# Structure Quality Analysis for NAME



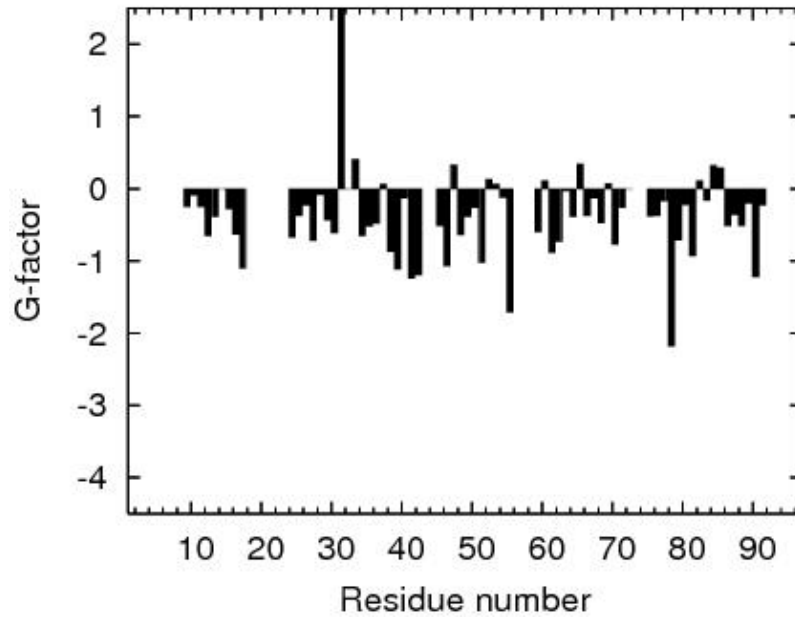
RPF Precision Map



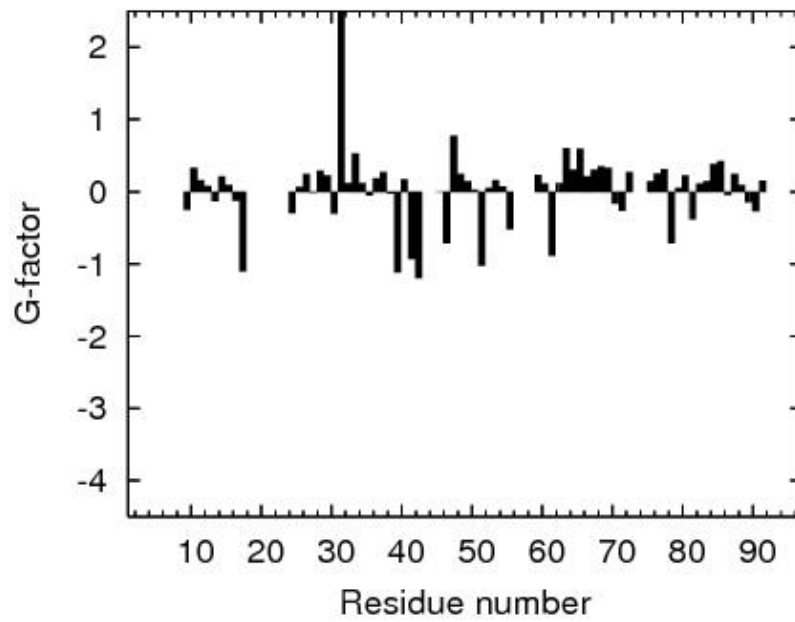


# Structure Quality Analysis for NAME

## Procheck G-factor for phi-psi

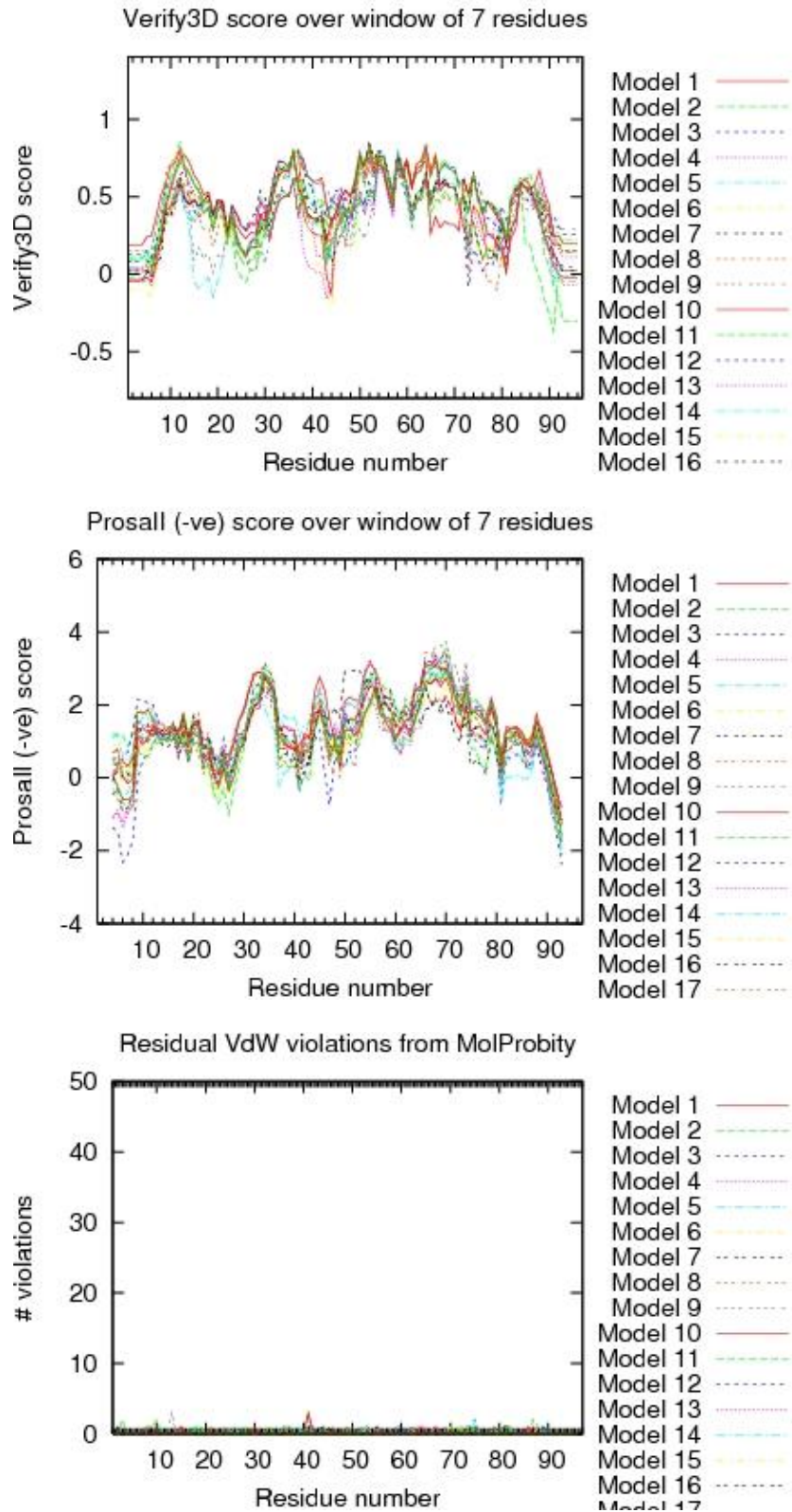


## Procheck G-factor for all dihedral angles





# Structure Quality Analysis for NAME





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

**References:**

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 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
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 constrains 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

### MolProbity 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