



# 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.): 142

Organism:

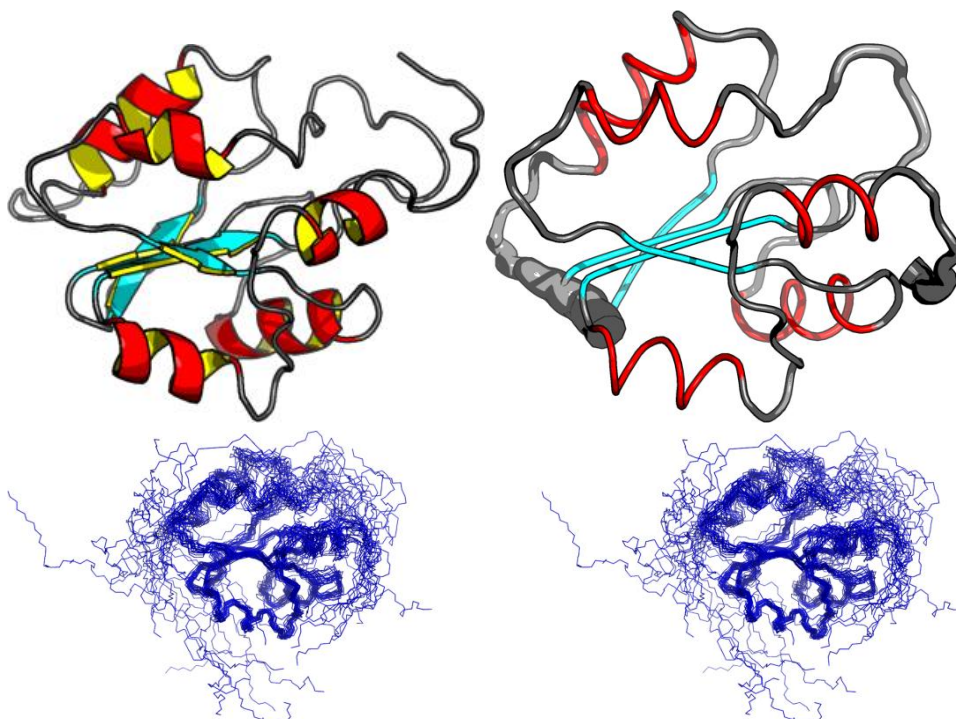
SwissProt /

TrEMBL ID:

# models: 20

Oligomerization: monomer

Molecular weight: 16126



Secondary Structure Elements:

alpha helices: 9A-17A, 27A-34A, 58A-62A, 80A-86A, 115A-124A

beta strands: 20N-22N, 71N-75N, 37Y-40Y, 94A-99A, 102S-108S

Total number of restricting constraints per restrained residue: 16.1

Restricting long range constraints per restrained residue: 3.8

Distance violations per model

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

0.1 - 0.2 Å   0.2 - 0.5 Å   > 0.5 Å

18.05      29.85      75.7

Dihedral angle violations per model

1 - 10 °   > 10 °

21.55    11.2

FIDs deposited in the BMRB? no



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RMSD	All residues	Ordered residues <sup>2</sup>	Selected residues <sup>3</sup>
All backbone atoms	5.4 Å	1.0 Å	1.0 Å
All heavy atoms	6.1 Å	1.4 Å	1.4 Å

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

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
93.8%	6.1%	0.1%	0.0%

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

Most favoured regions	Allowed regions	Disallowed regions	<a href="#">View plot</a>	<a href="#">View model summary</a>
98.9%	1.1%	0%		

### Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) <sup>3</sup>	Procheck (all) <sup>3</sup>	MolProbity Clashscore
-Raw score	0.42	0.54	0.01	0.20	4.42
Z-score <sup>1</sup>	-0.64	-0.45	0.35	1.18	0.77

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):	1
RMS deviation for bond angles:	0.7 °
RMS deviation for bond lengths:	0.010 Å

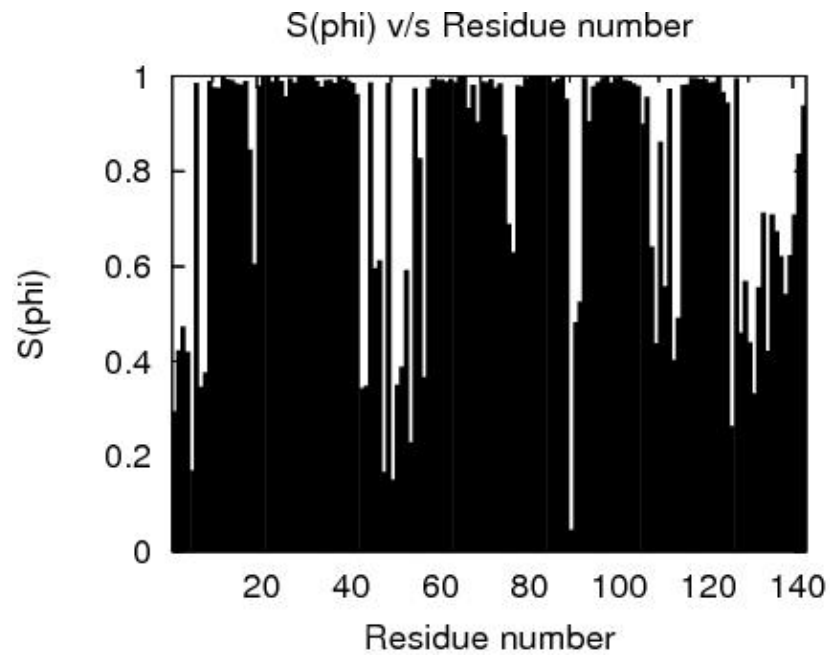
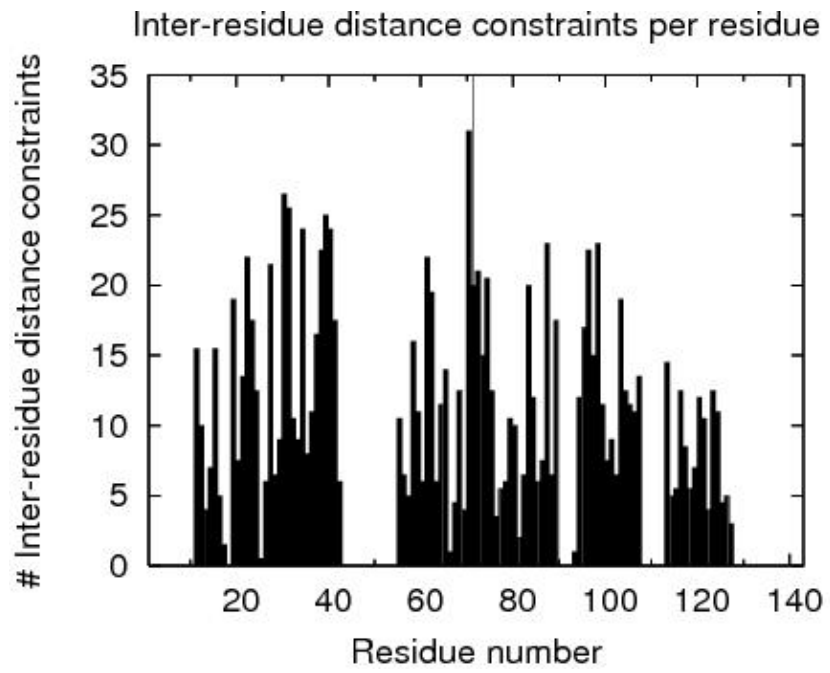
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

<sup>2</sup>Order residues: 9A-17A,20A-41A,58A-65A,67A-74A,78A-88A,93A-106A,115A-125A

<sup>3</sup>Selected residues: 9A-17A,20A-41A,58A-74A,78A-88A,93A-106A,115A-125A

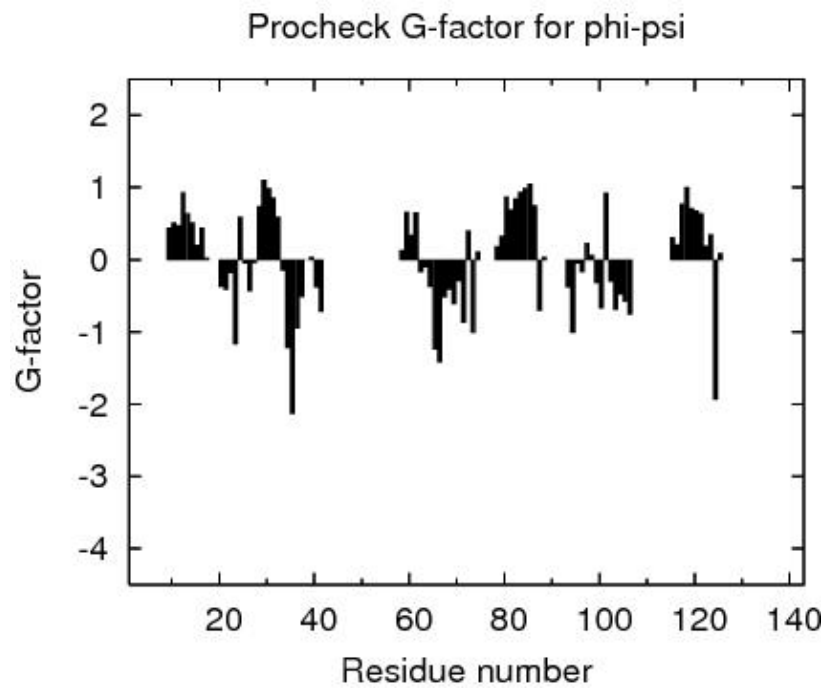
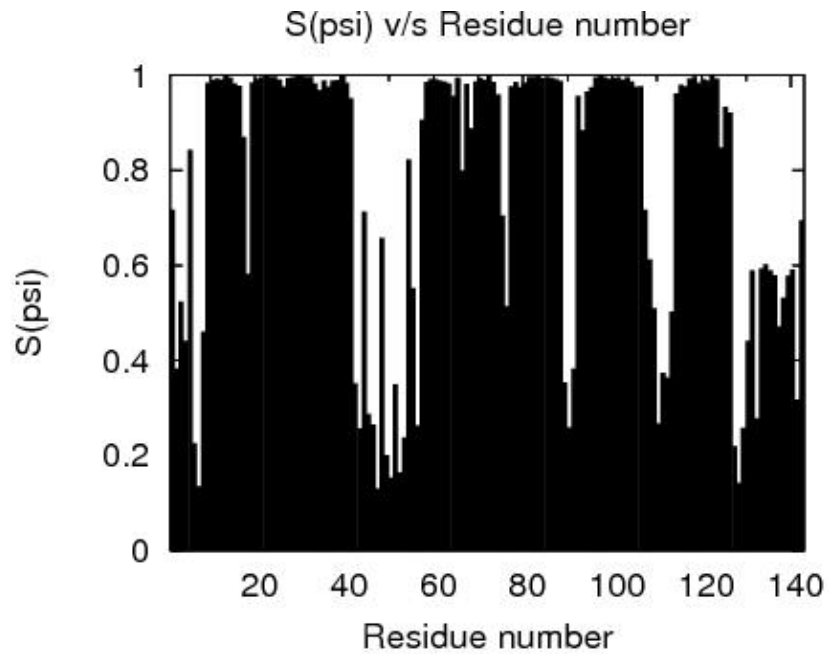


# Structure Quality Analysis for NAME





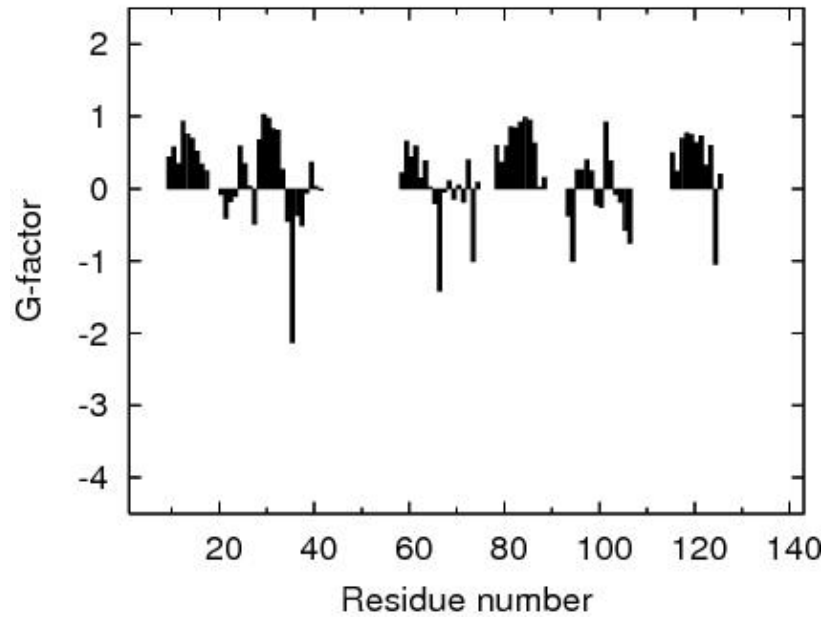
# Structure Quality Analysis for NAME



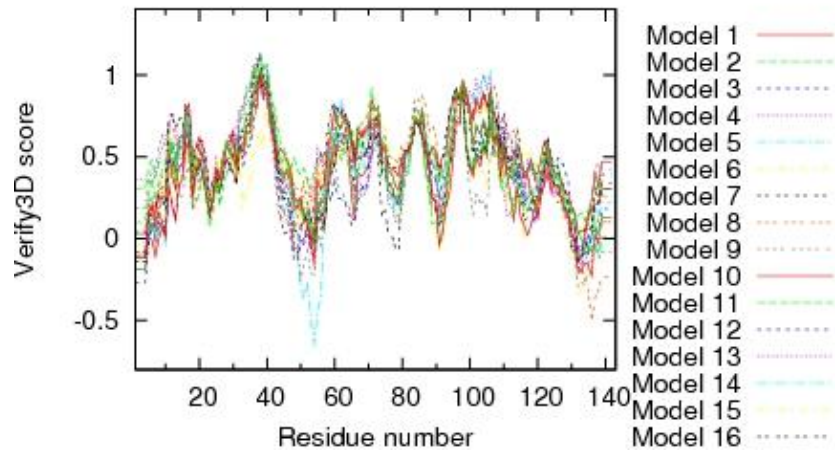


# Structure Quality Analysis for NAME

## Procheck G-factor for all dihedral angles

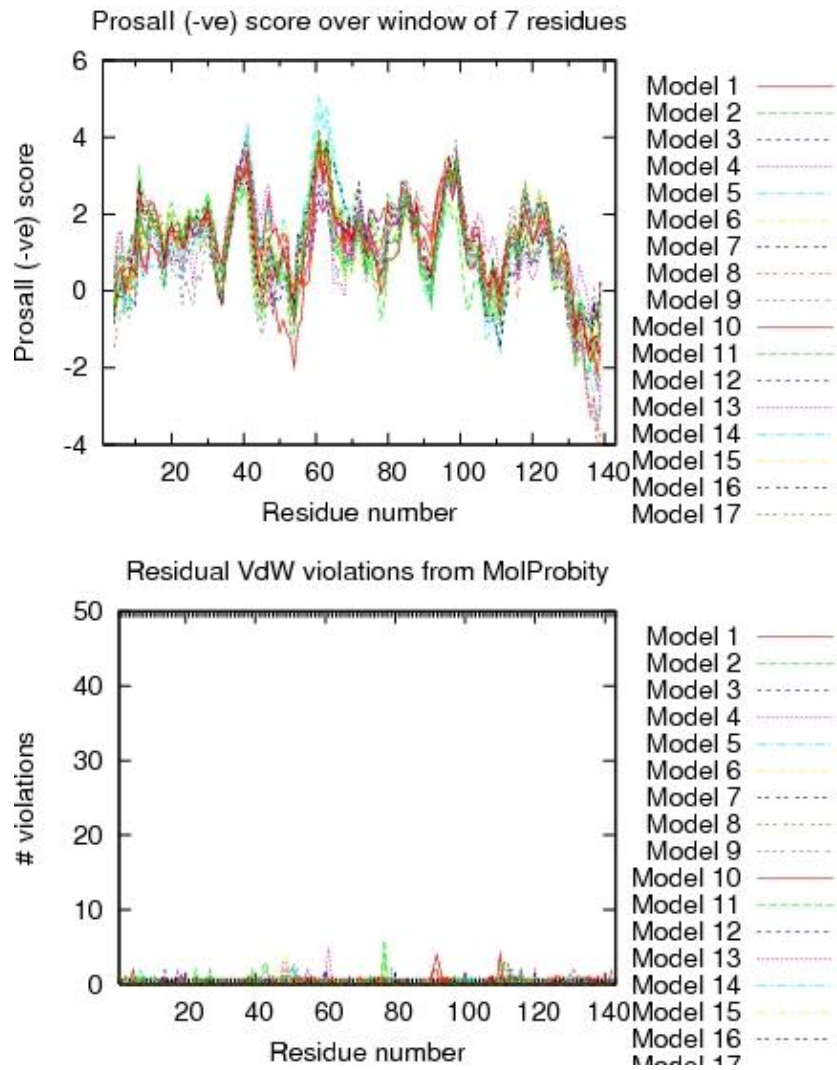


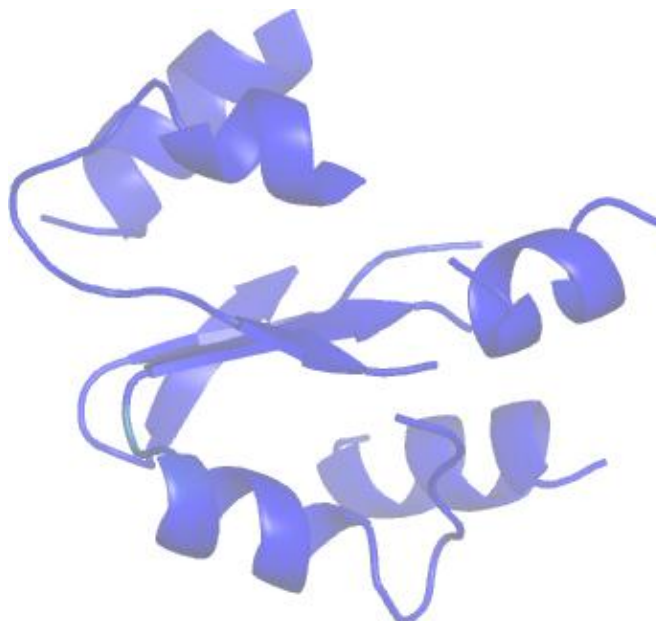
## Verify3D score over window of 7 residues





# Structure Quality Analysis for NAME





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

**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
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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
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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-11-2013 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
```