



# 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.): 134

Organism:

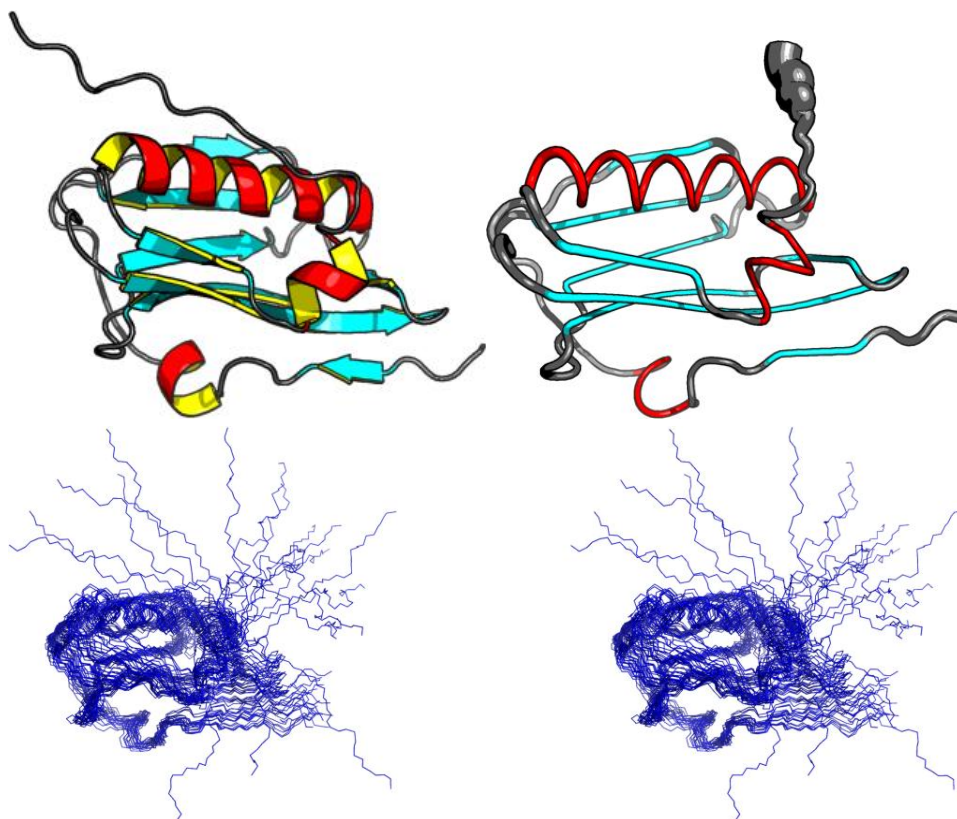
SwissProt /

TrEMBL ID:

# models: 20

Oligomerization: monomer

Molecular weight: 15090



Secondary Structure Elements:

alpha helices: 12A-15A, 88A-104A, 113A-118A

beta strands: 5G-8G, 44N-54N, 108R-111R, 24O-29O, 32U-37U, 57G-68G, 73E-79E

Total number of restricting constraints per restrained residue: 18.5

Restricting long range constraints per restrained residue: 5.5

Distance violations per model

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

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

9.7 2.5 0

Dihedral angle violations per model

1 - 10 ° > 10 °



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7.75 0

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score

0.973 0.883 0.926 0.749

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

*All backbone atoms* 5.4 Å 4.1 Å 4.1 Å

*All heavy atoms* 5.6 Å 4.0 Å 4.0 Å

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

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

87.9% 12.1% 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* [View plot](#) [View model summary](#)

96.4% 3.6% 0%

### Global quality scores

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

*-Raw score* 0.34 0.41 -0.46 -0.31 17.27

*Z-score*<sup>1</sup> -1.93 -0.99 -1.49 -1.83 -1.44

### Generalized linear model RMSD prediction: 2.14

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): 13

RMS deviation for bond angles: 1.2 °

RMS deviation for bond lengths: 0.019 Å

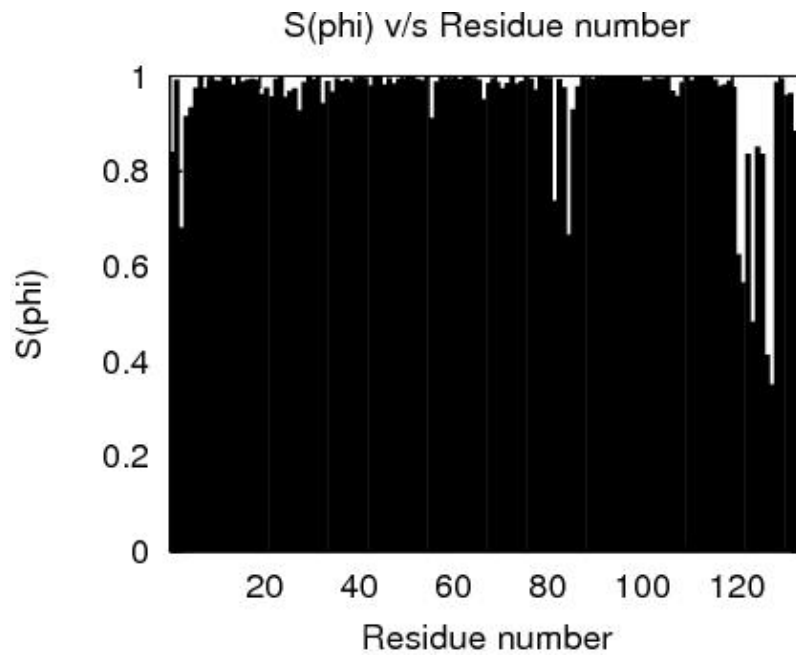
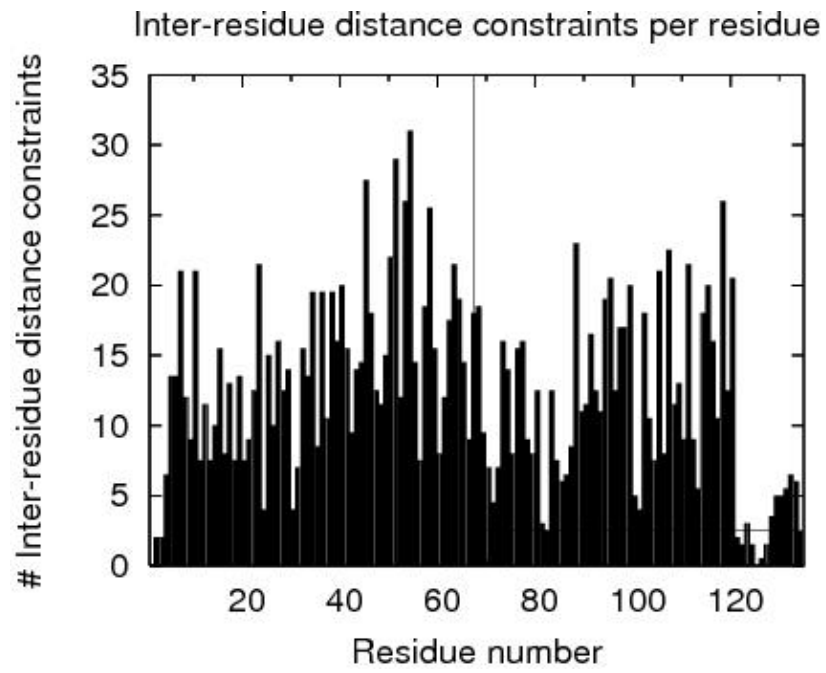
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

<sup>2</sup>Order residues: 4A-80A,86A-119A,129A-132A

<sup>3</sup>Selected residues: 4A-80A,86A-119A,129A-132A

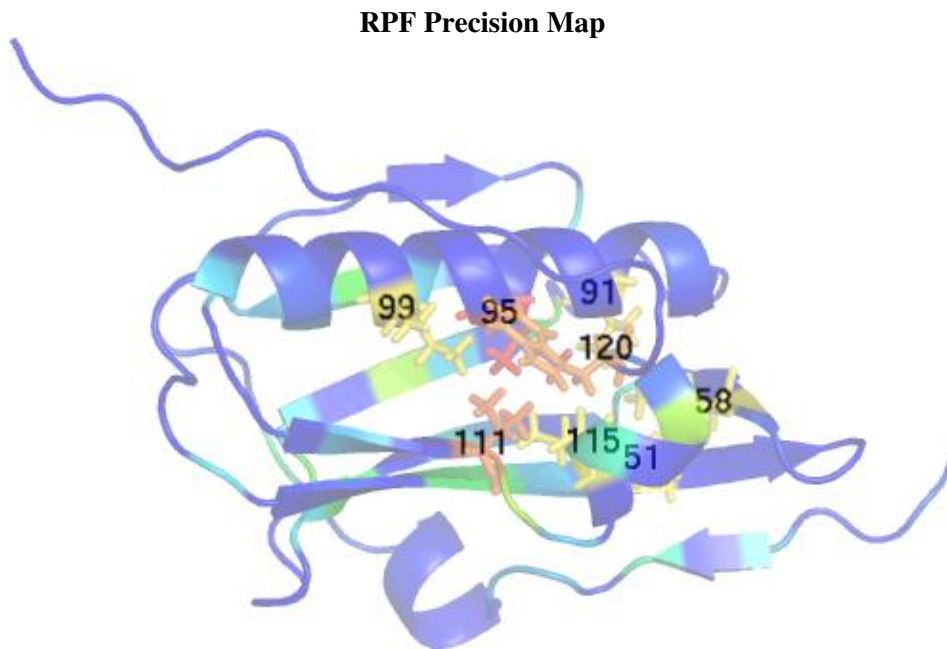
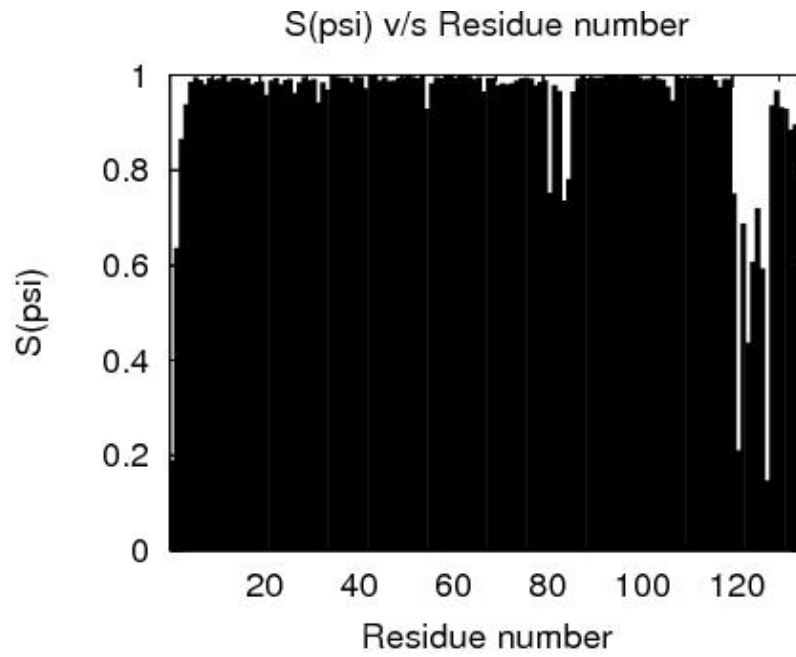


# Structure Quality Analysis for NAME





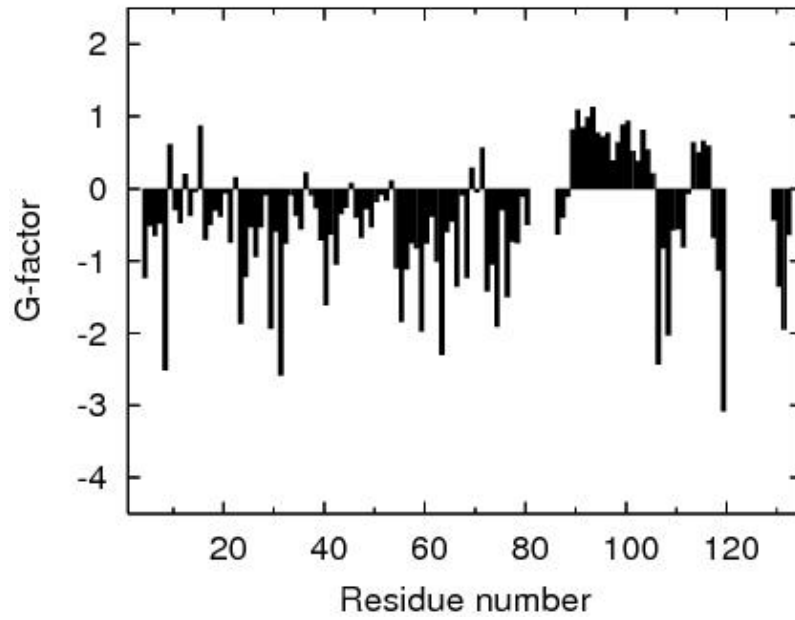
# Structure Quality Analysis for NAME



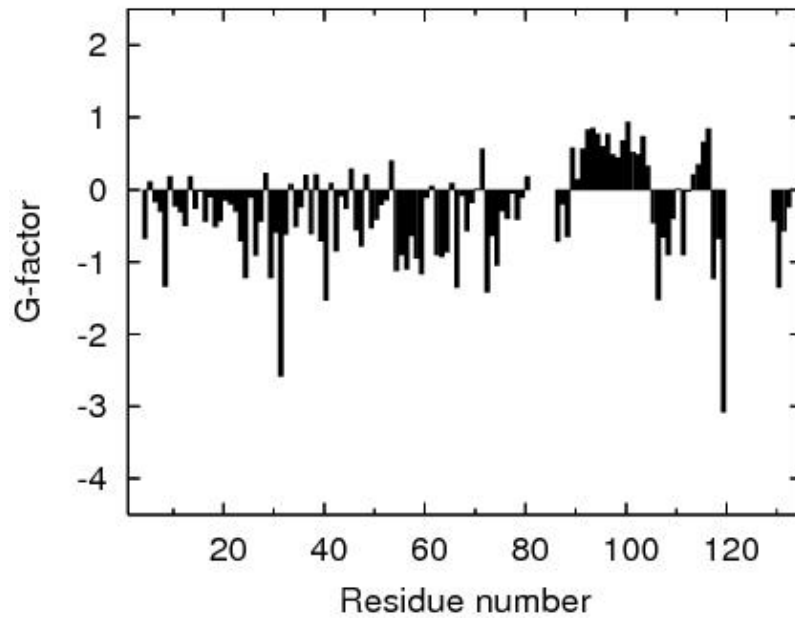


## Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

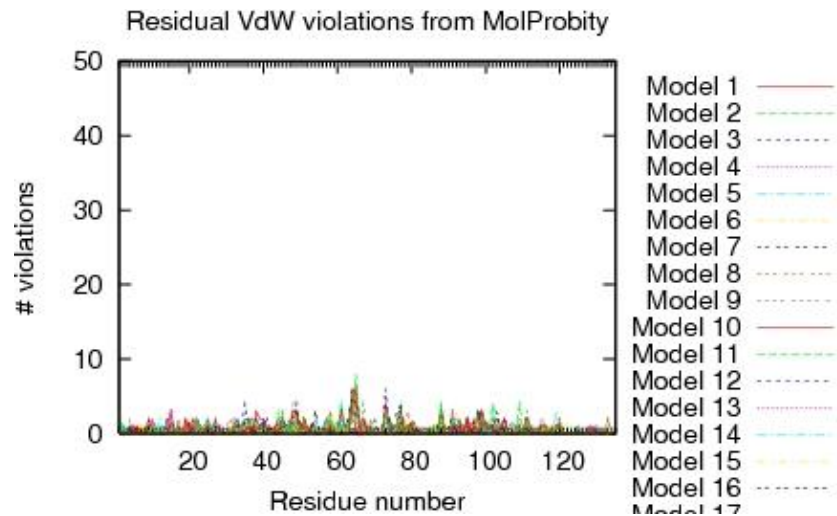
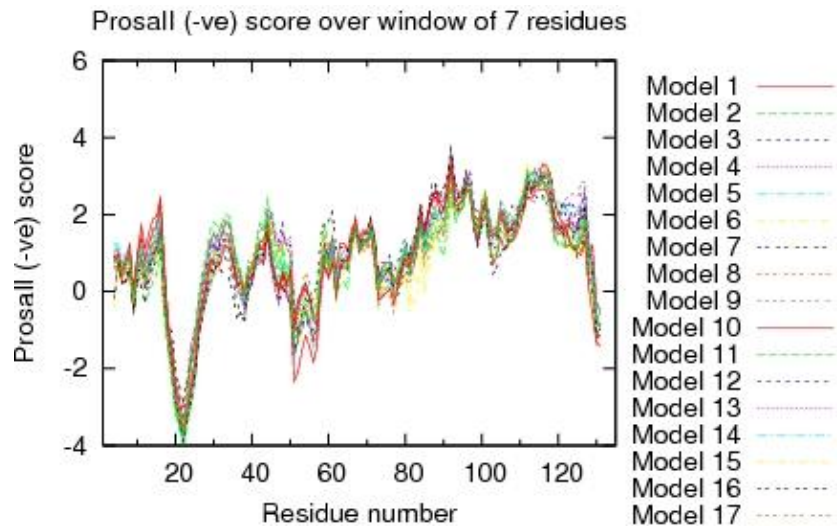
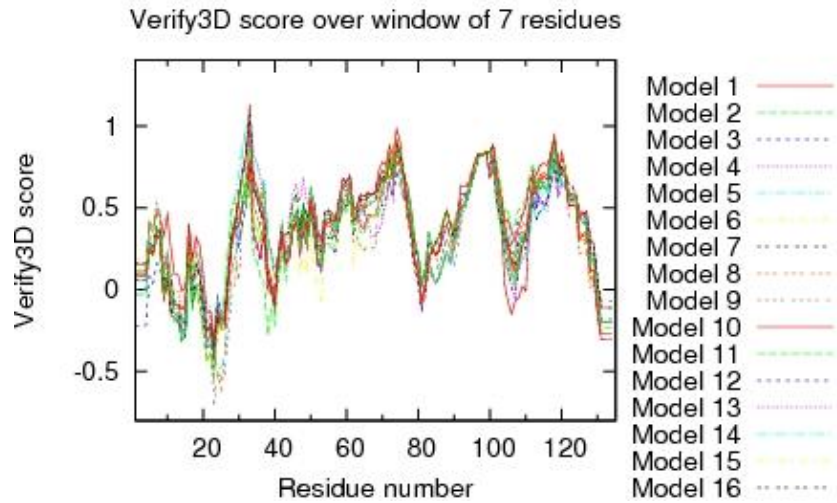


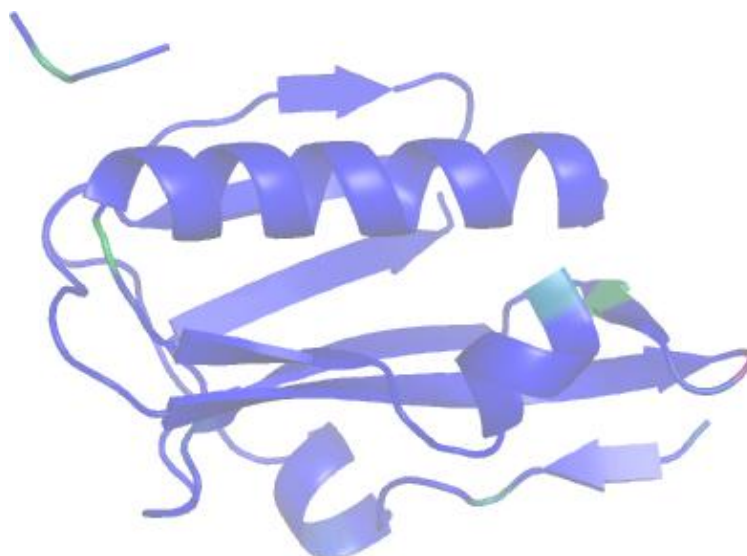
Procheck G-factor for all dihedral angles





# Structure Quality Analysis for NAME





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

### 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



## Structure Quality Analysis for NAME

pnmcrop  
pnmtjpeg

year 2000  
year 2000