



# 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.): 91

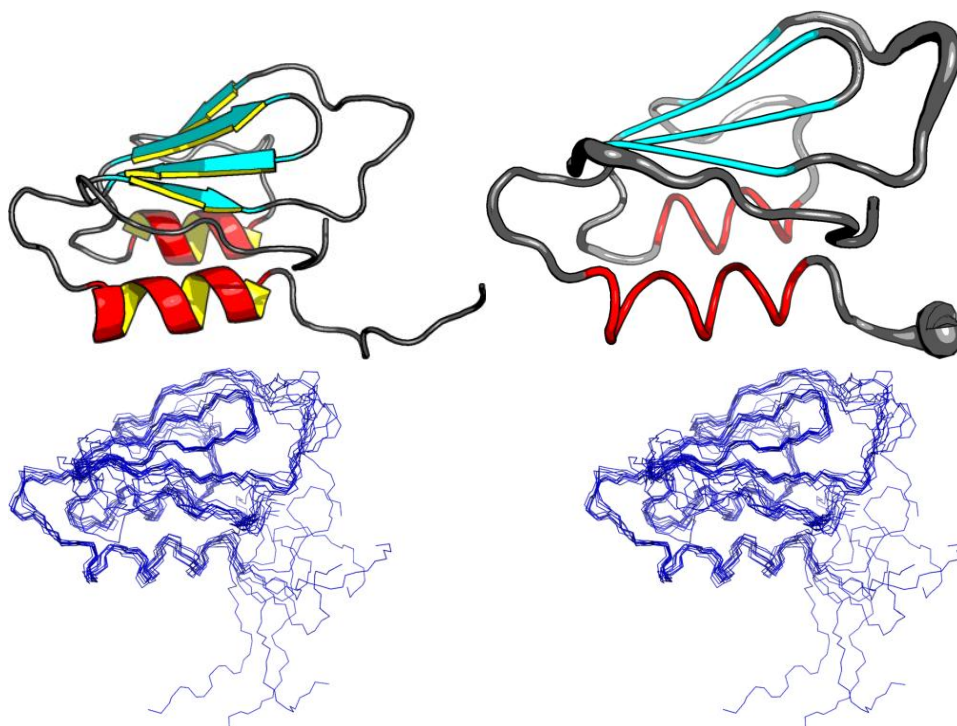
Organism:

SwissProt /  
TrEMBL ID:

# models: 10

Oligomerization: monomer

Molecular  
weight: 10472



Secondary Structure Elements:

alpha helices: 40A-47A, 71A-81A

beta strands: 5R-6R, 14R-18R, 60E-64E, 53R-57R, 28R-31R

Total number of restricting constraints per restrained residue: 15.7

Restricting long range constraints per restrained residue: 5.1

Distance violations per model

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

0.1 - 0.2 Å   0.2 - 0.5 Å   > 0.5 Å

7.5            3.1            2.1

Dihedral angle violations per model

1 - 10 °   > 10 °

1.2        0.4

FIDs deposited in the BMRB? no



## Structure Quality Analysis for NAME

### RPF Scores

Recall Precision F-measure DP-score

0.928 0.781 0.848 0.764

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

*All backbone atoms* 2.7 Å 0.6 Å 0.6 Å

*All heavy atoms* 3.4 Å 0.8 Å 0.8 Å

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

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

90.8% 7.1% 1.2% 0.8%

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

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

95.5% 4.3% 0.2%

### Global quality scores

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

*-Raw score* 0.36 0.55 -0.11 0.11 9.96

*Z-score*<sup>1</sup> -1.61 -0.41 -0.12 0.65 -0.18

### Generalized linear model RMSD prediction: 1.29

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: 0.6 °

RMS deviation for bond lengths: 0.011 Å

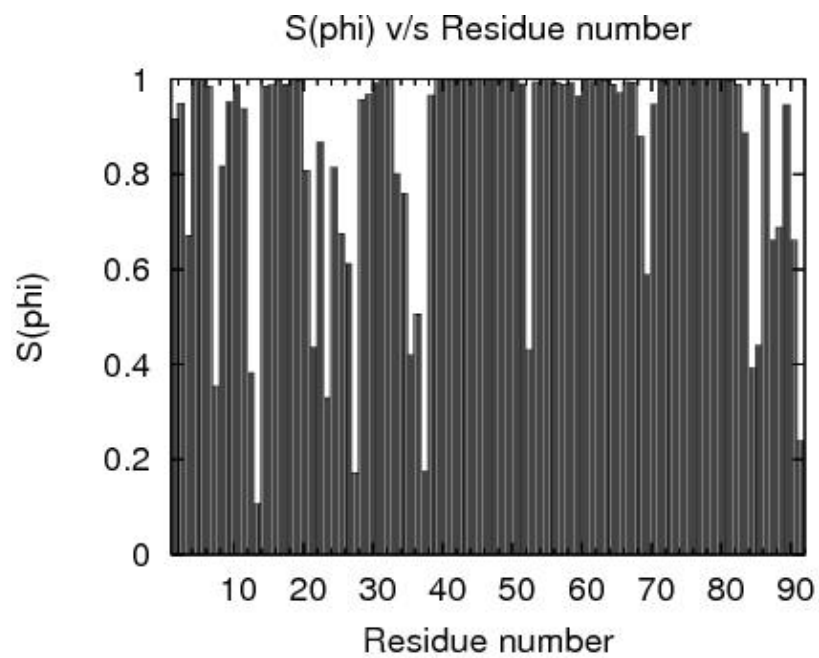
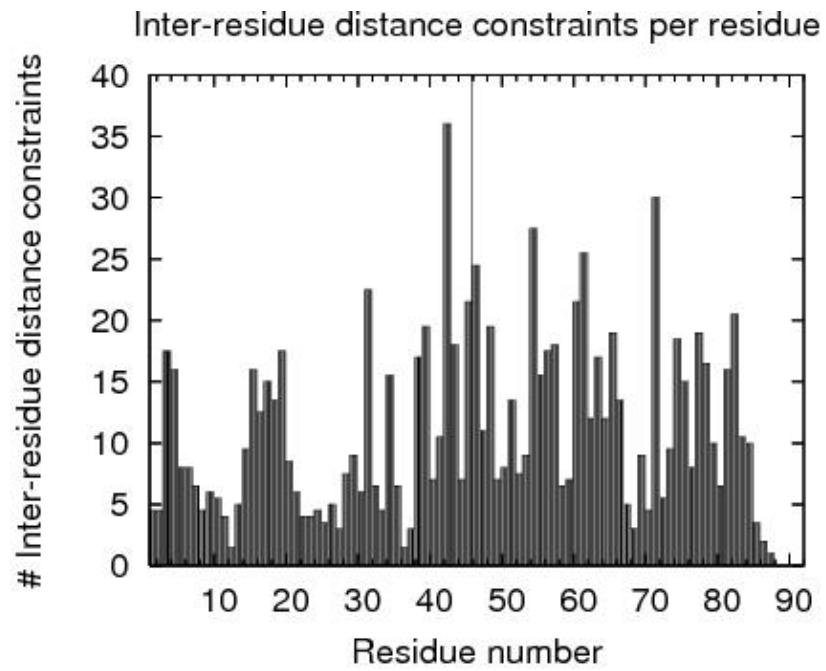
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

<sup>2</sup> Order residues: 14A-18A,28A-32A,38A-50A,53A-68A,70A-82A

<sup>3</sup> Selected residues: 14A-18A,28A-32A,38A-50A,53A-67A,70A-82A

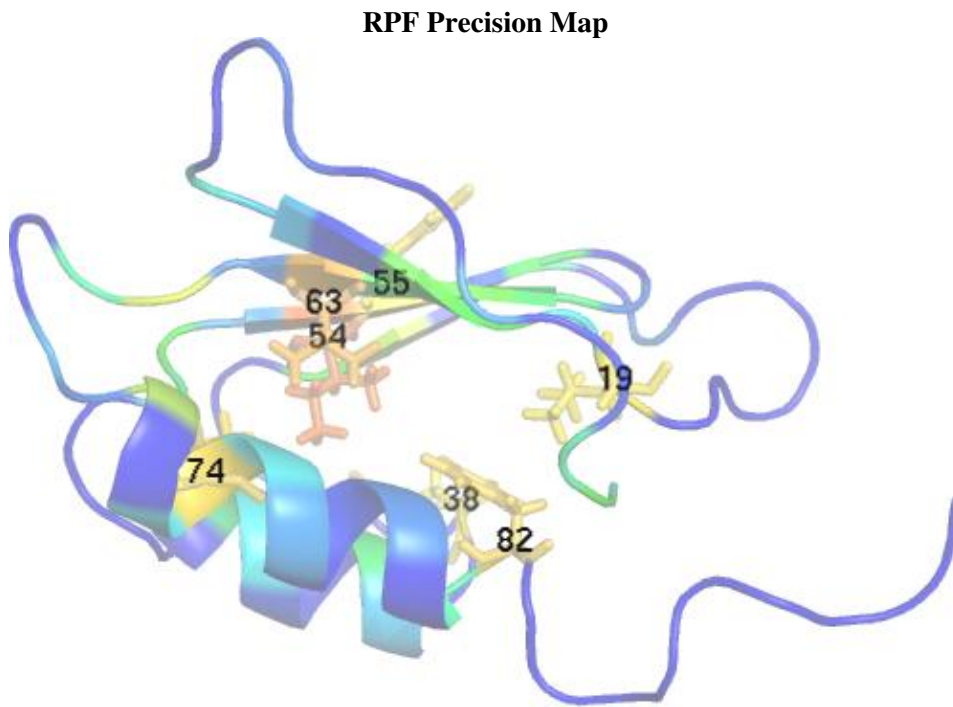
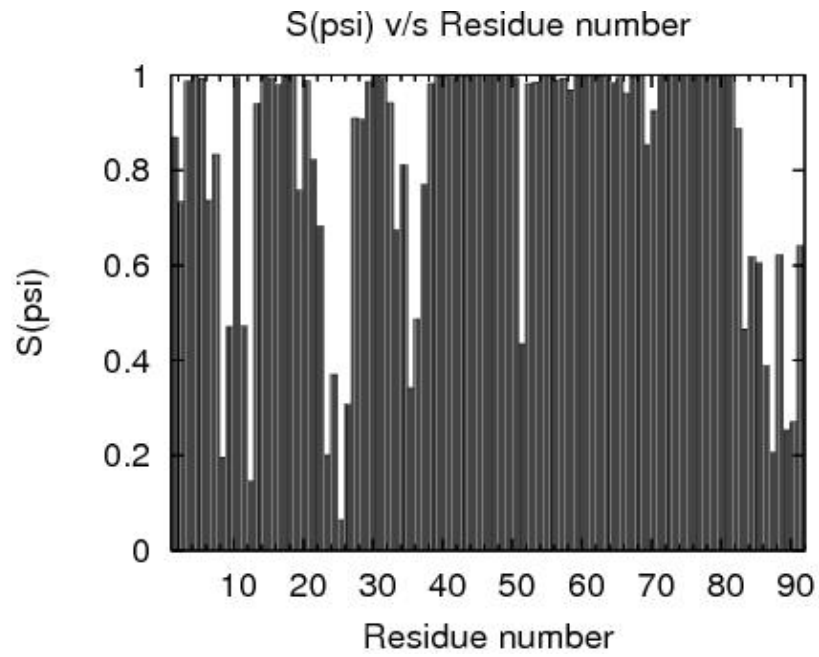


# Structure Quality Analysis for NAME





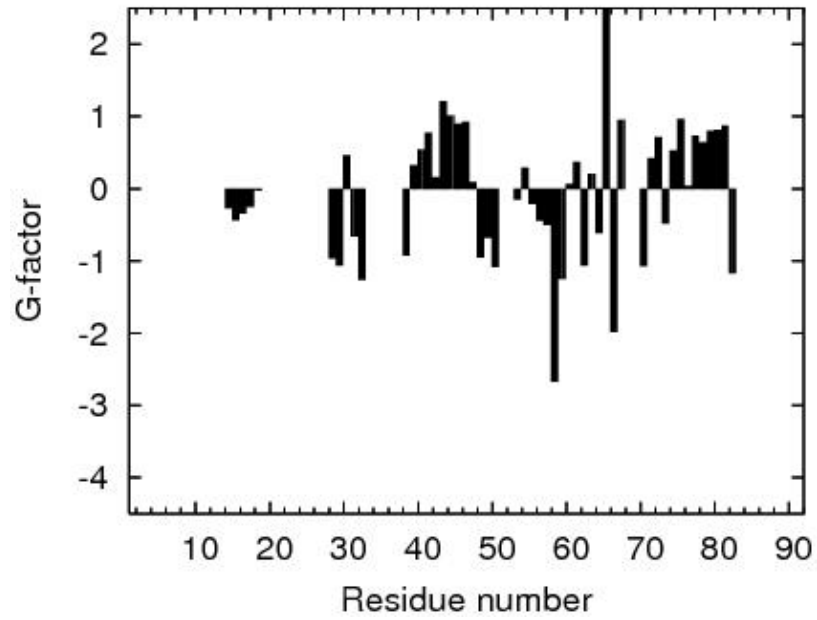
# Structure Quality Analysis for NAME



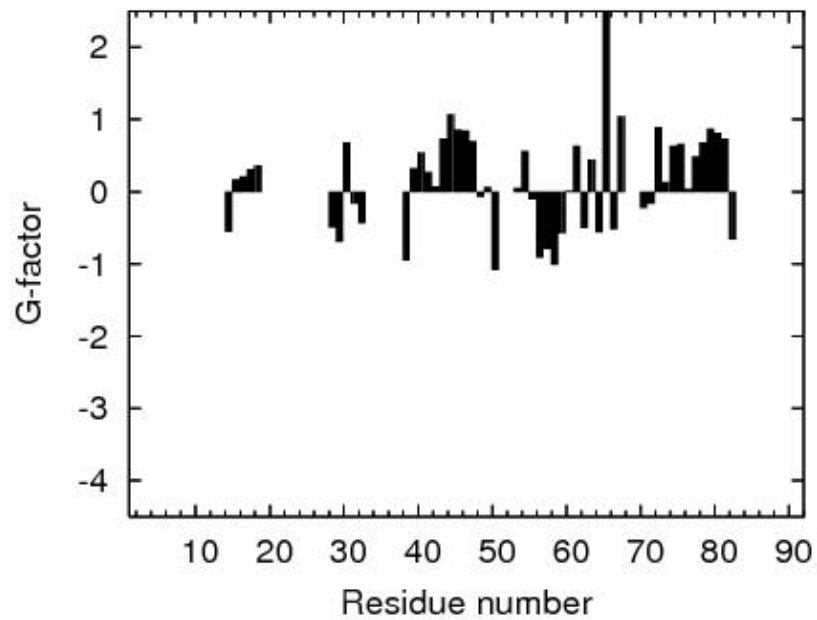


# Structure Quality Analysis for NAME

## Procheck G-factor for phi-psi

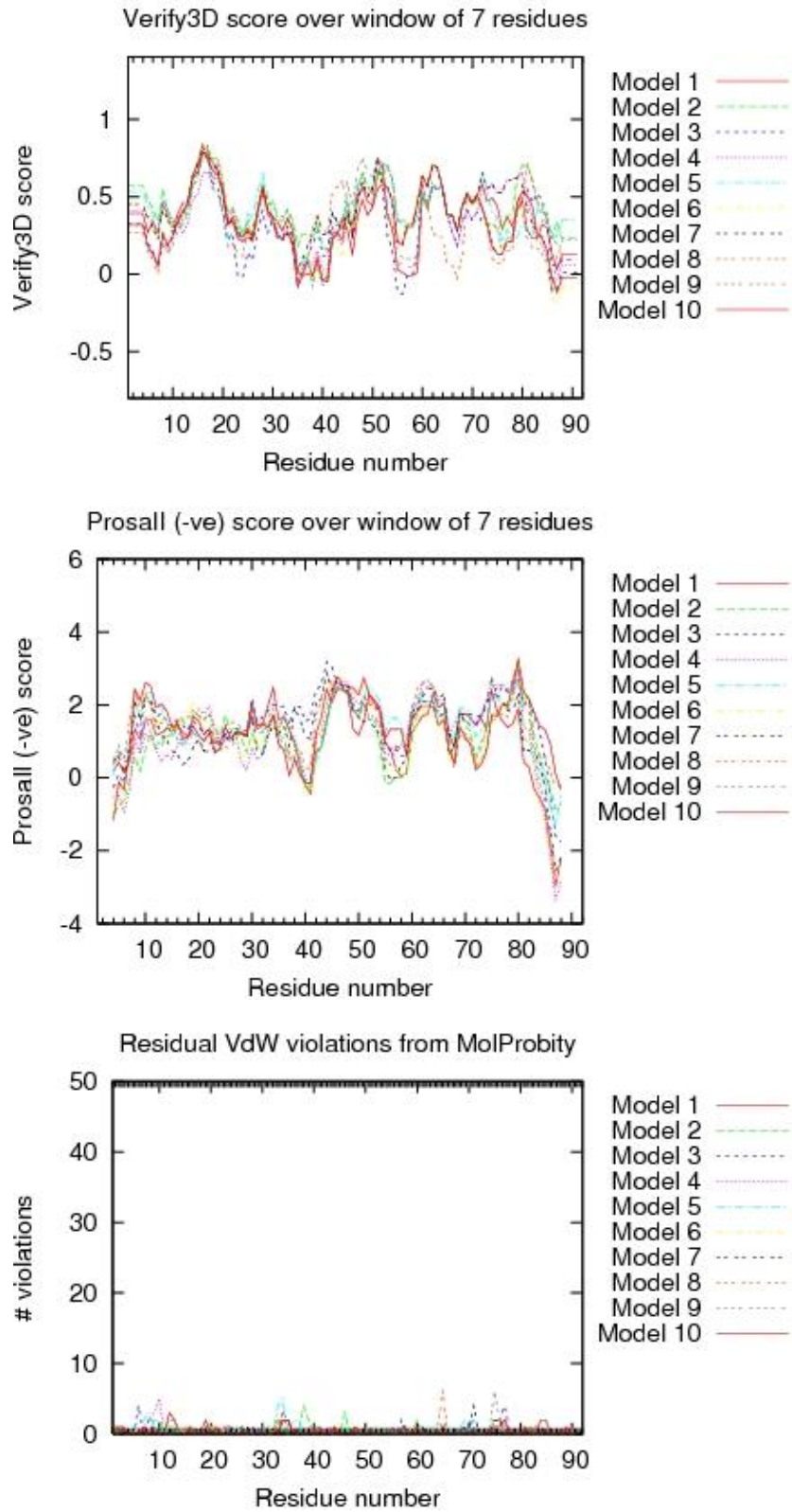


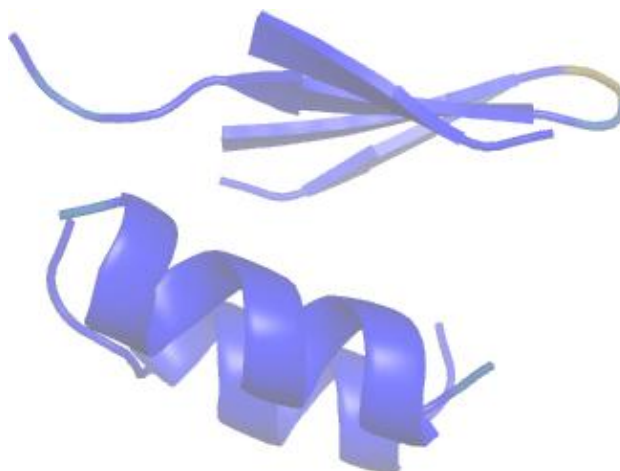
## Procheck G-factor for all dihedral angles





# Structure Quality Analysis for NAME





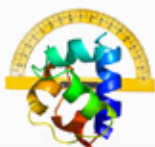
### **Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobity)**

#### ***References:***

1. Luthy R, Bowie J U and Eisenberg D, "Assessment of protein models with three-dimensional profiles", *Nature* 356 (1992): 83-85
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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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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.



## Protein Structure Validation Suite (PSVS)



### 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