



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.): 86

Organism:

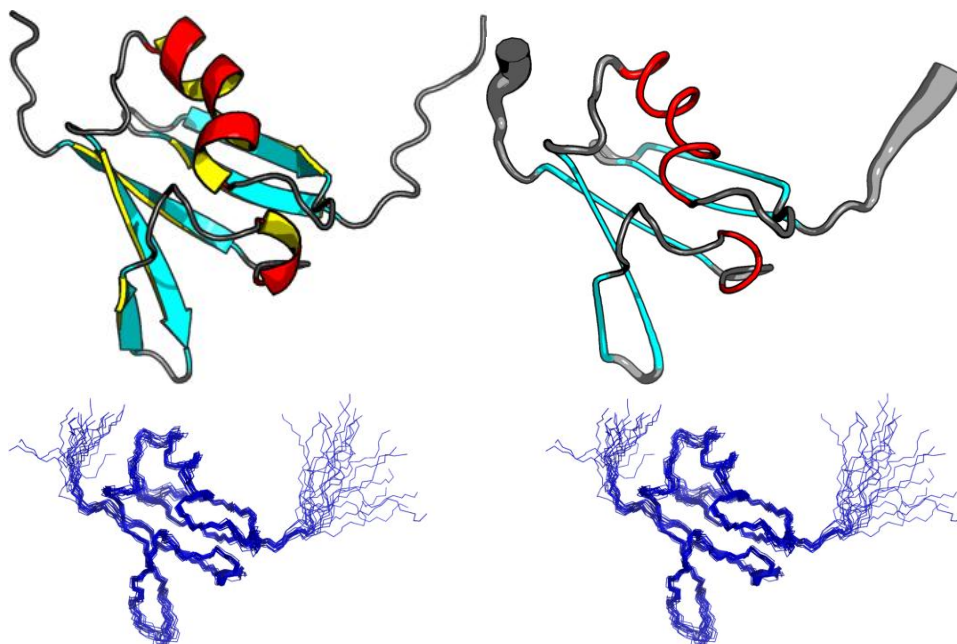
SwissProt /

TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular weight: 9763



Secondary Structure Elements:

alpha helices: 31A-42A

beta strands: 19N-24N, 10E-15E, 75U-80U, 49S-55S, 58U-62U

Total number of restricting constraints per restrained residue: 22.1

Restricting long range constraints per restrained residue: 6.4

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

0.5 0.05 0

Dihedral angle violations per model

1 - 10 ° > 10 °

1.25 0

FIDs deposited in the BMRB? no

RPF Scores



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Recall Precision F-measure DP-score

0.982 0.931 0.956 0.824

RMSD *All residues* *Ordered residues*² *Selected residues*³

All backbone atoms 1.6 Å 0.6 Å 0.6 Å

All heavy atoms 2.0 Å 1.0 Å 1.0 Å

Ramachandran Plot Summary for selected residues³ from Procheck

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

91.9% 8.0% 0.1% 0.0%

Ramachandran Plot Summary for selected residues³ from Richardson Lab's Molprobit

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

98.7% 1.3% 0%

Global quality scores

Program *Verify3D* *ProsaII (-ve)* *Procheck (phi-psi)*³ *Procheck (all)*³ *MolProbit Clashscore*

-Raw score 0.38 0.61 -0.36 -0.15 14.51

*Z-score*¹ -1.28 -0.17 -1.10 -0.89 -0.96

Generalized linear model RMSD prediction: 1.28

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): 2

RMS deviation for bond angles: 0.6 °

RMS deviation for bond lengths: 0.009 Å

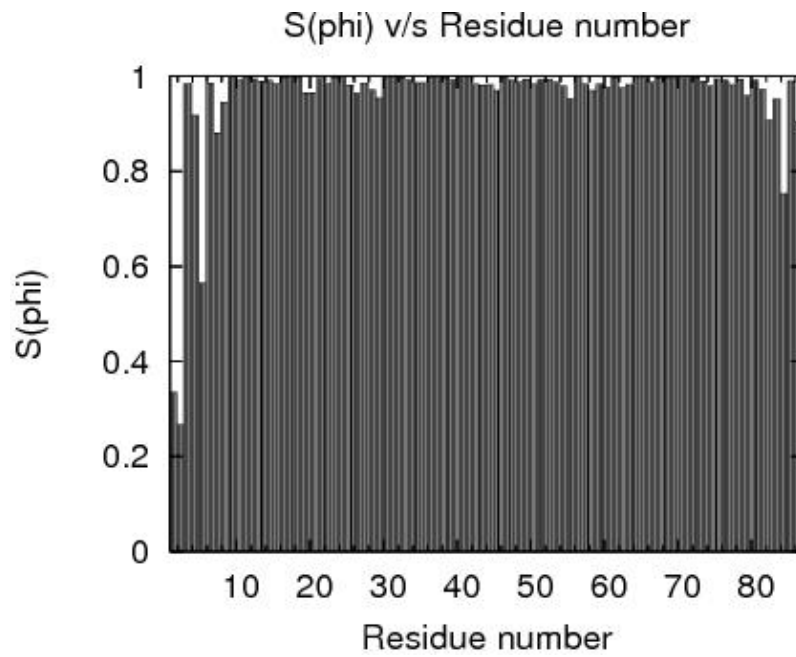
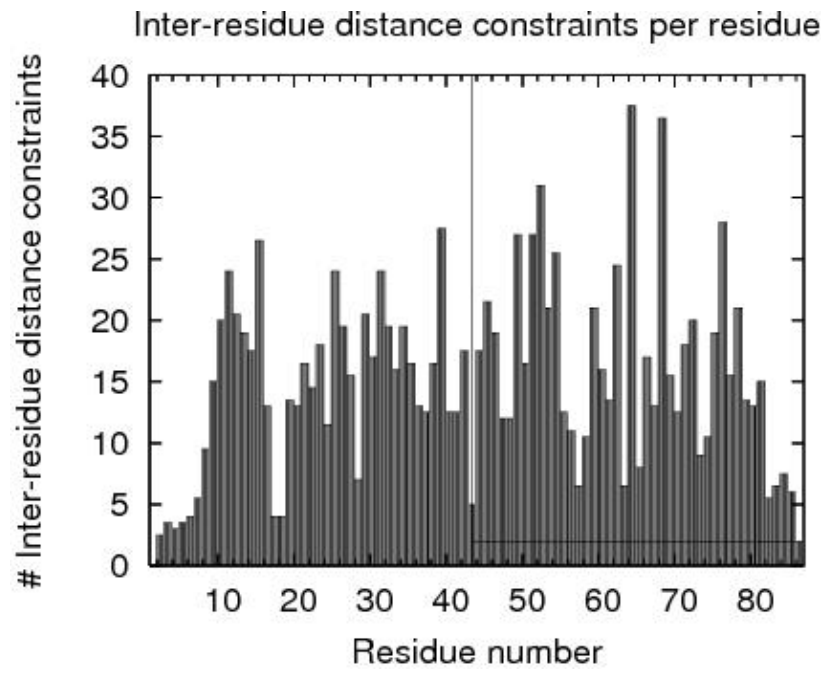
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 8A-82A

³Selected residues: 8A-82A

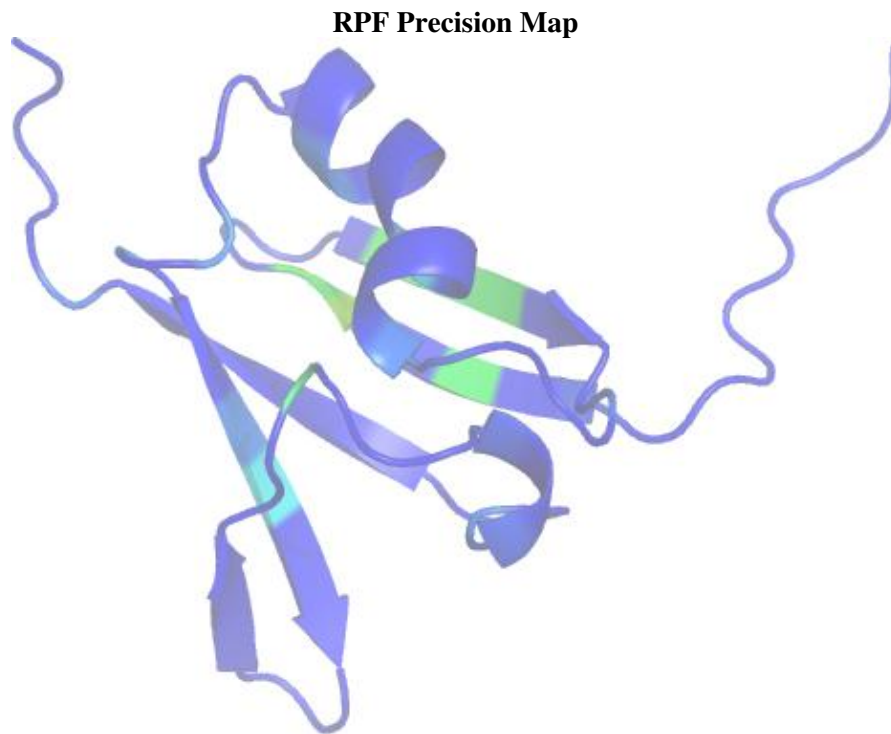
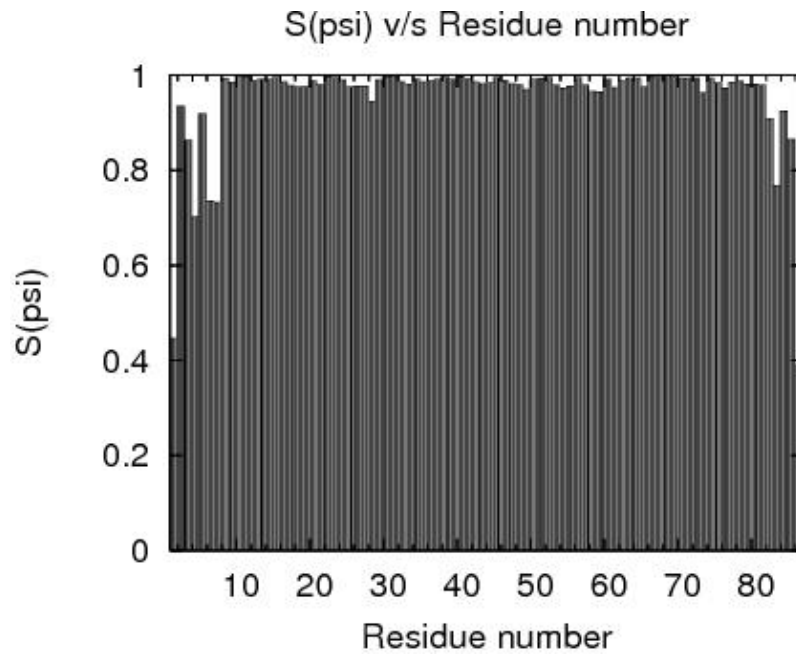


Structure Quality Analysis for NAME





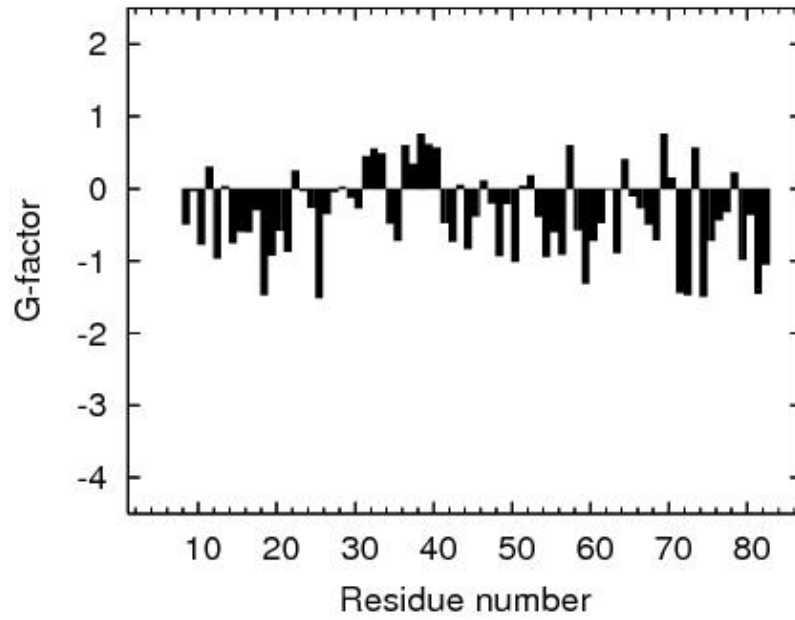
Structure Quality Analysis for NAME



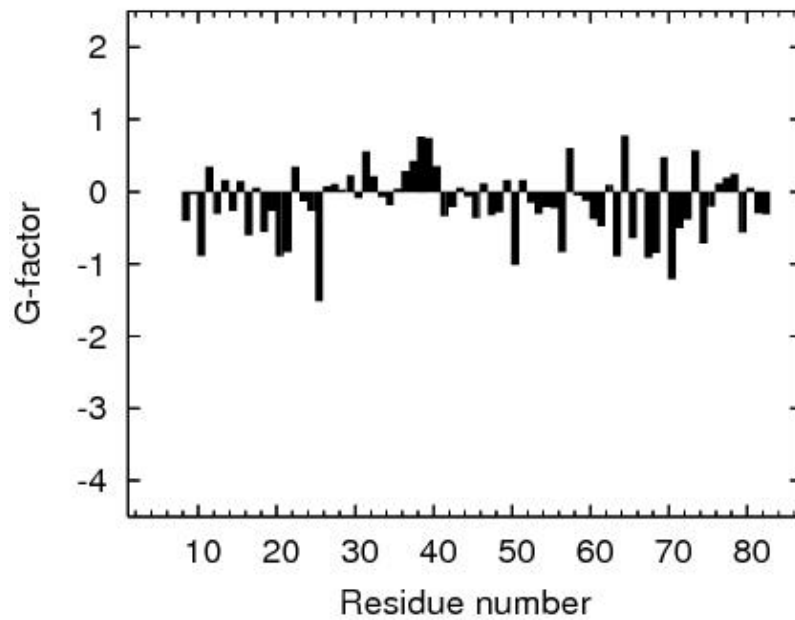


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi



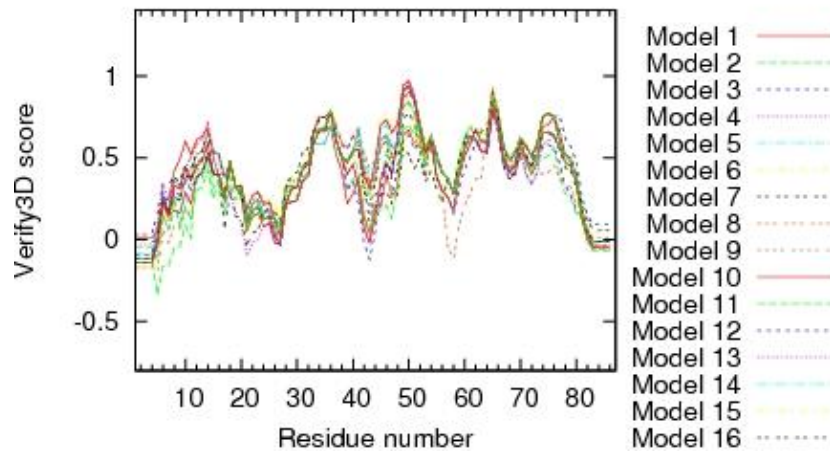
Procheck G-factor for all dihedral angles



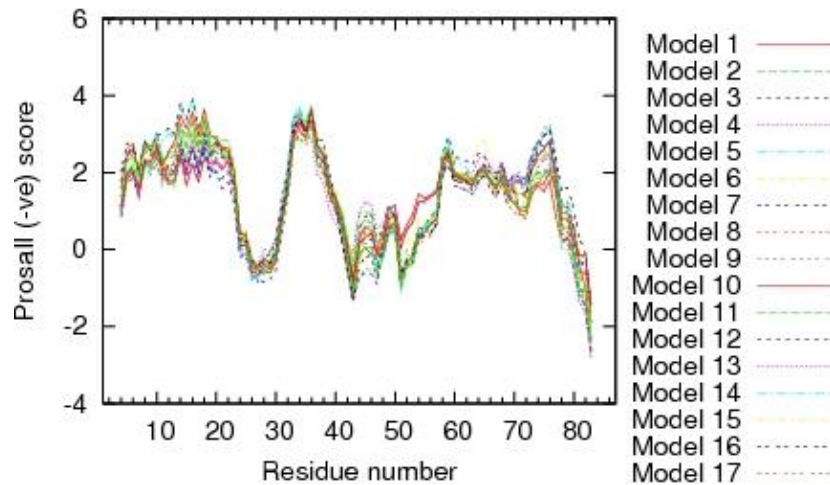


Structure Quality Analysis for NAME

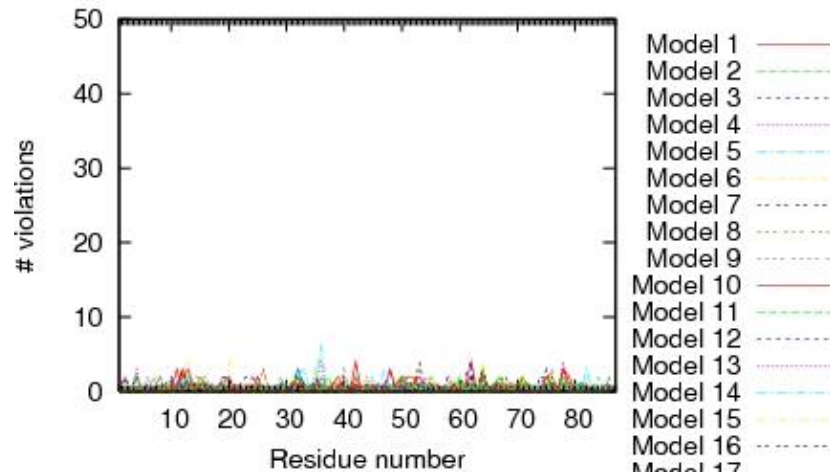
Verify3D score over window of 7 residues



ProsaII (-ve) score over window of 7 residues



Residual VdW violations from MolProbity





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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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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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
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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
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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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
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```
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
```