



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.): 78

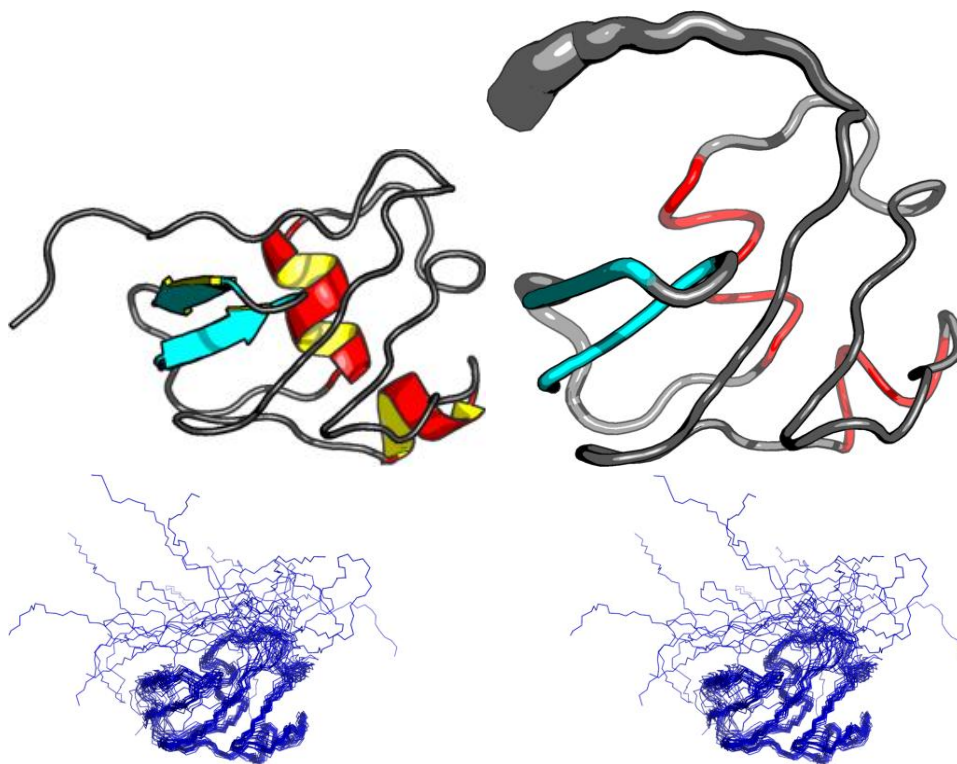
Organism:

SwissProt /
TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular
weight: 8519



Secondary Structure Elements:

alpha helices: 20A-26A, 48A-51A

beta strands: 2N-5N, 8S-11S, 17R-19R, 53R-55R, 42U-44U, 37L-39L, 60L-62L

Total number of restricting constraints per restrained residue: 14.4

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

8.6 14.9 34.9

Dihedral angle violations per model

1 - 10 ° > 10 °

1.45 0.5



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FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score

0.971 0.928 0.949 0.827

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

All backbone atoms 4.8 Å 0.9 Å 0.9 Å

All heavy atoms 5.5 Å 1.3 Å 1.3 Å

Ramachandran Plot Summary for selected residues³ from Procheck

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

93.1% 6.7% 0.0% 0.2%

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

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

98.3% 1.5% 0.2%

Global quality scores

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

-Raw score 0.37 0.56 -0.26 0.13 3.51

*Z-score*¹ -1.44 -0.37 -0.71 0.77 0.92

Generalized linear model RMSD prediction: 1.06

Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 & Åring for H atoms, 2.2 & Åring for heavy atoms): 0

RMS deviation for bond angles: 0.6 °

RMS deviation for bond lengths: 0.011 Å

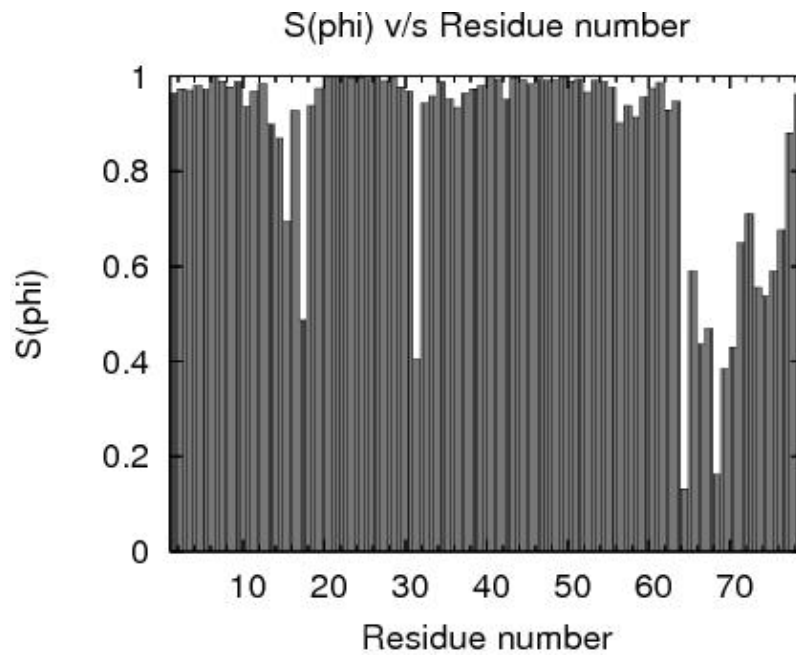
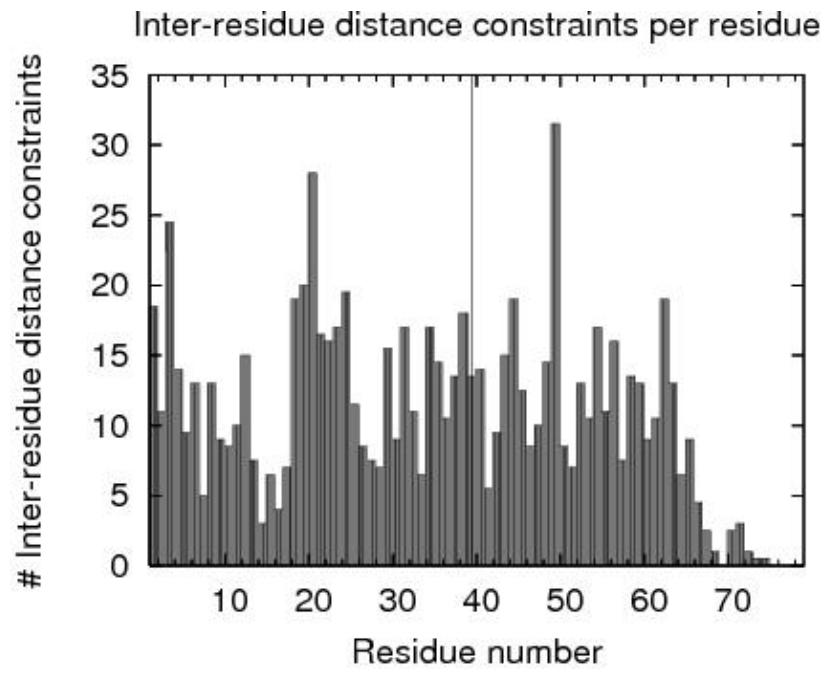
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 2A-13A,18A-29A,32A-63A

³Selected residues: 1A-13A,18A-29A,32A-63A

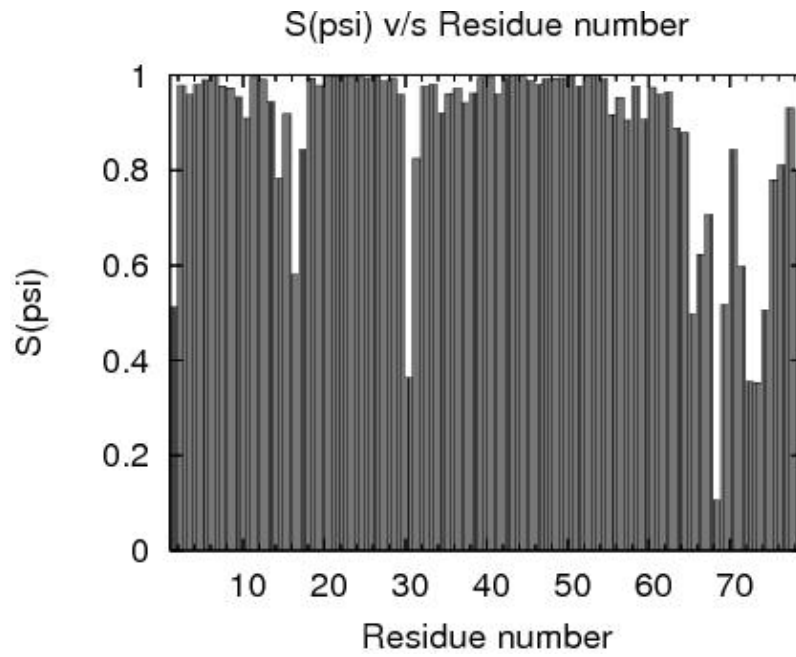


Structure Quality Analysis for NAME

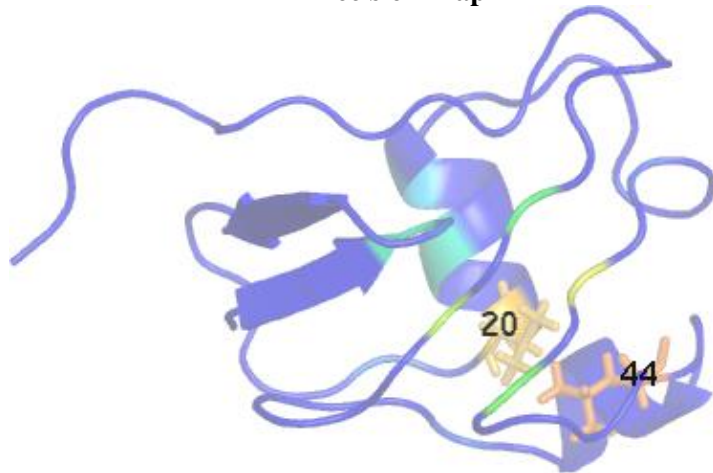




Structure Quality Analysis for NAME



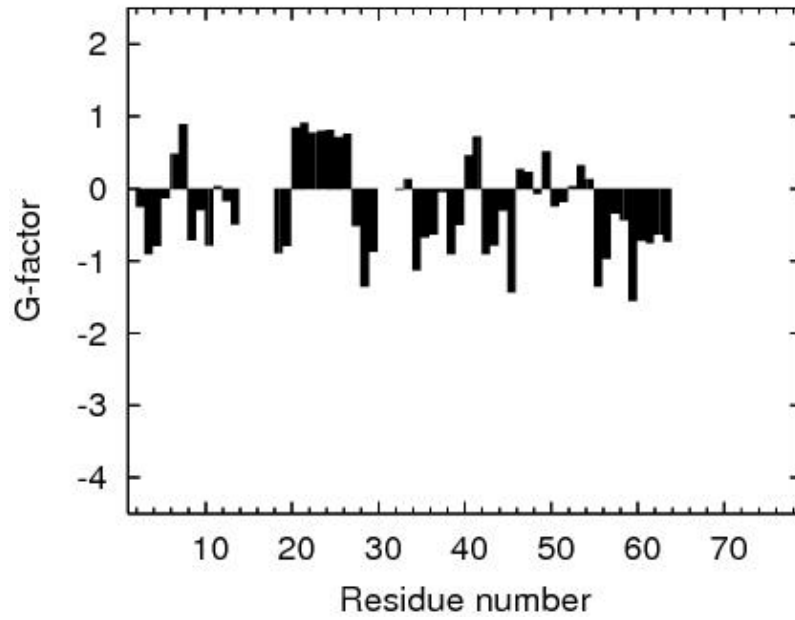
RPF Precision Map



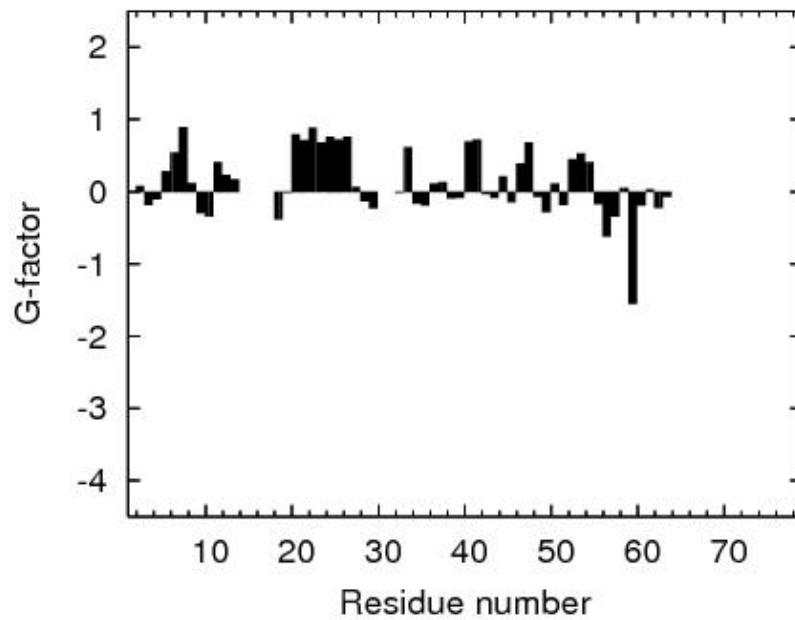


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi



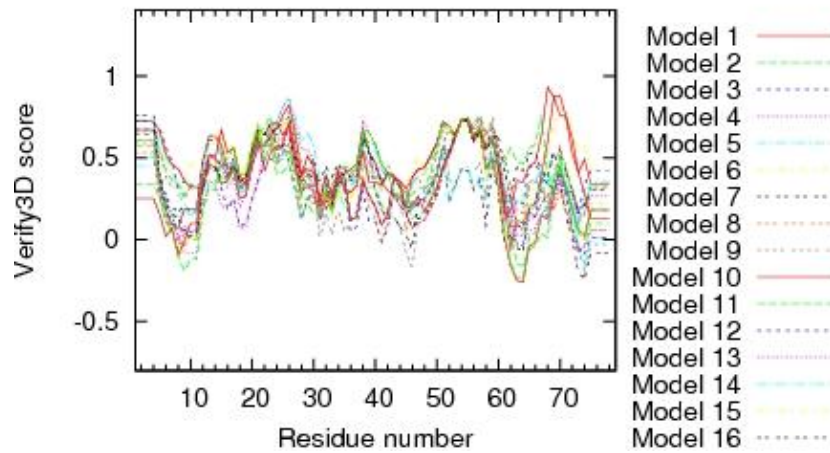
Procheck G-factor for all dihedral angles



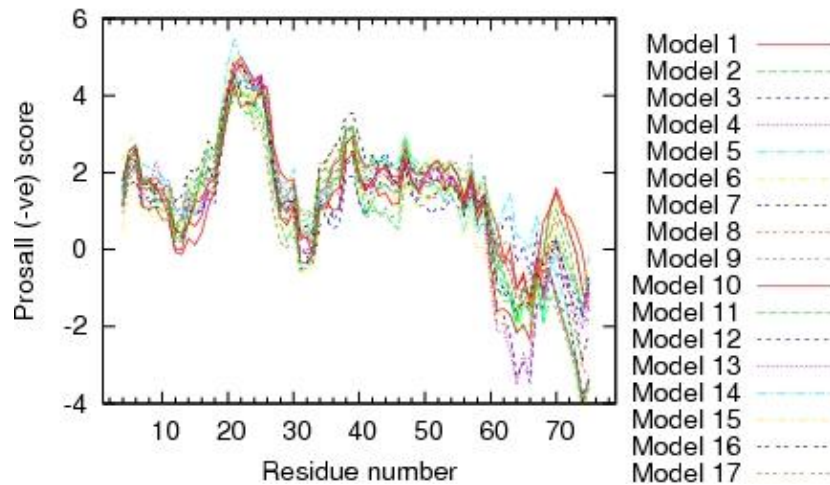


Structure Quality Analysis for NAME

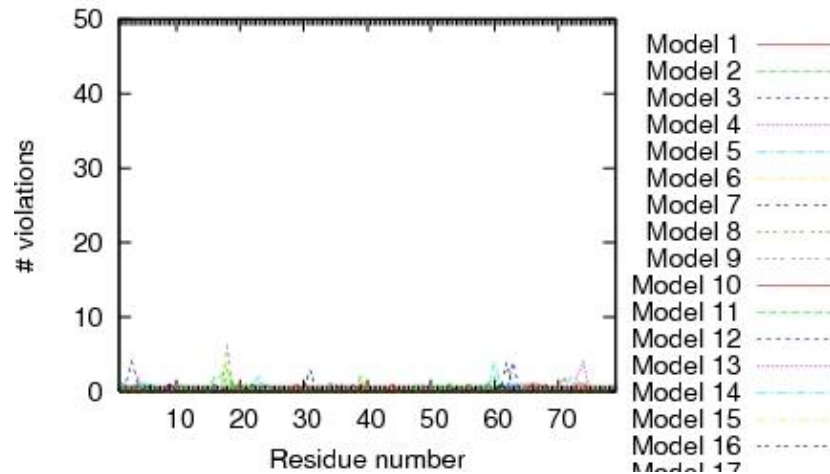
Verify3D score over window of 7 residues

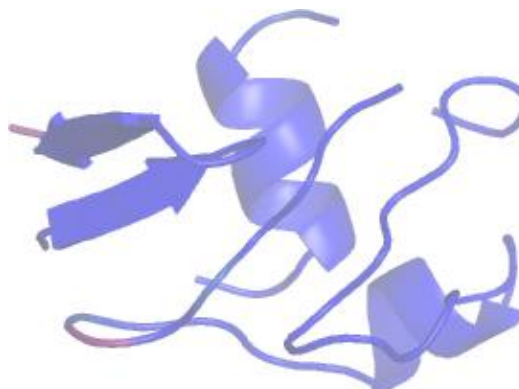


ProsaII (-ve) score over window of 7 residues



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
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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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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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

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