



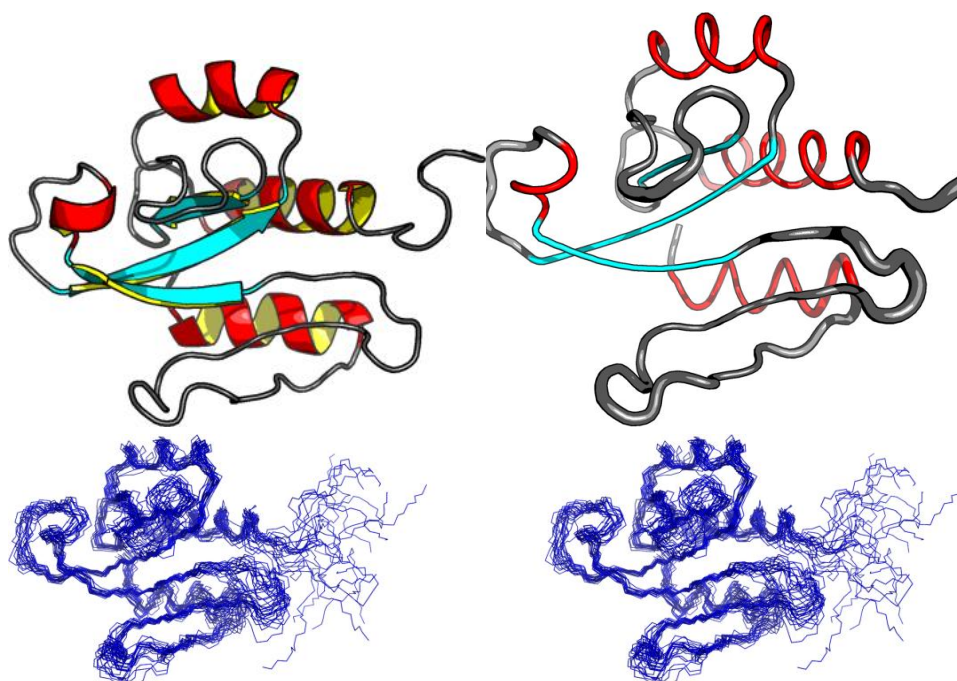
Structure Quality Analysis for NAME

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.): 125
Organism:
SwissProt /
TrEMBL ID:
models: 20
Oligomerization: monomer
Molecular
weight: 14802



Secondary Structure Elements:

alpha helices: 3A-14A, 68A-76A, 102A-115A

beta strands: 29A-33A, 38S-47S, 58G-65G, 91P-95P, 80E-82E

Total number of restricting constraints per restrained residue: 17.0

Restricting long range constraints per restrained residue: 4.9

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

21.3 41.2 125.15

Dihedral angle violations per model

1 - 10° > 10°

9.75 7.1

FIDs deposited in the BMRB? no

RPF Scores



Structure Quality Analysis for NAME

Recall Precision F-measure DP-score

0.884 0.845 0.864 0.707

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

All backbone atoms 2.2 Å 1.1 Å 1.1 Å

All heavy atoms 2.9 Å 1.6 Å 1.6 Å

Ramachandran Plot Summary for selected residues³ from Procheck

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

91.9% 8.1% 0.0% 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](#)

99.4% 0.5% 0%

Global quality scores

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

-Raw score 0.44 0.78 0.01 0.22 4.35

*Z-score*¹ -0.32 0.54 0.35 1.30 0.78

Generalized linear model RMSD prediction: 1.71

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: 1.0 °

RMS deviation for bond lengths: 0.018 Å

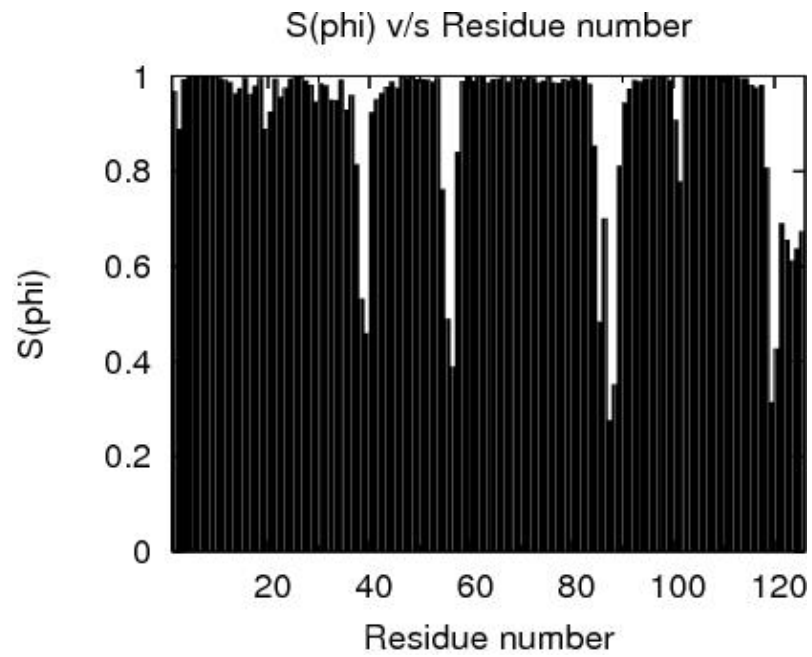
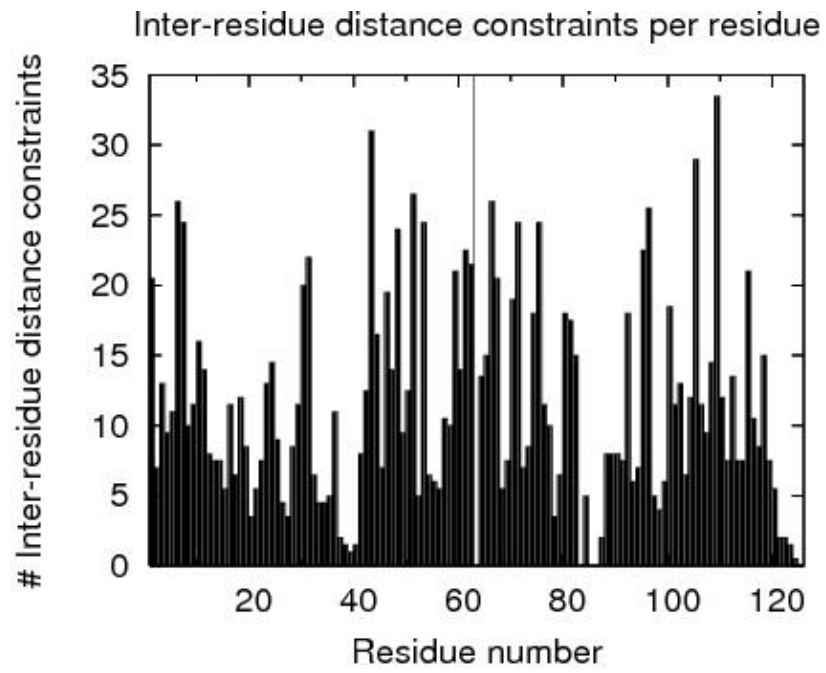
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 2A-18A,20A-36A,40A-53A,57A-83A,90A-99A,102A-117A

³Selected residues: 2A-36A,40A-53A,57A-83A,90A-99A,101A-116A

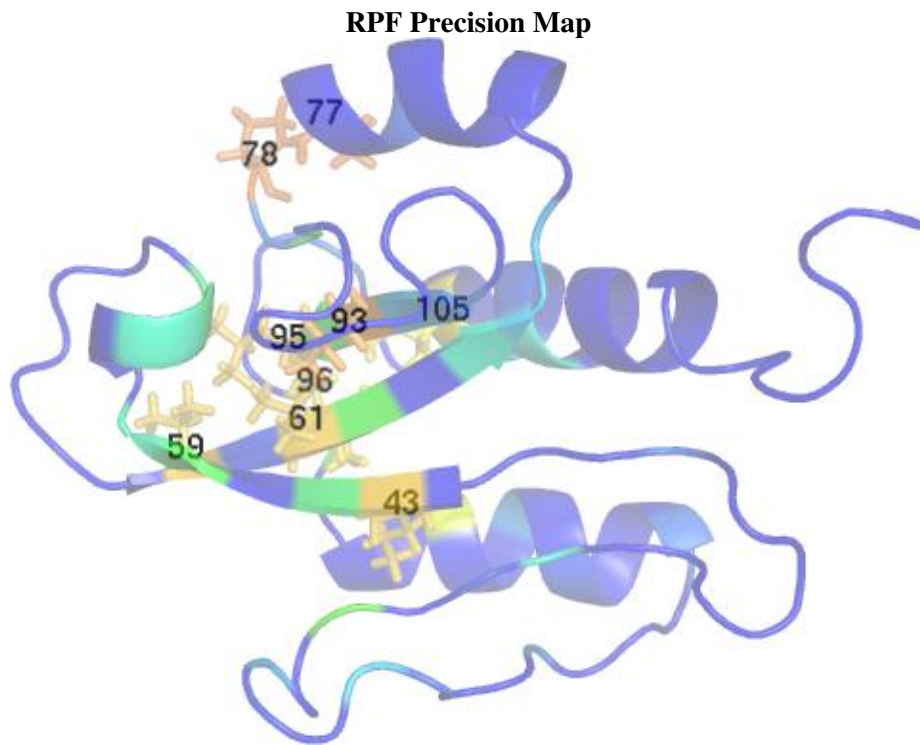
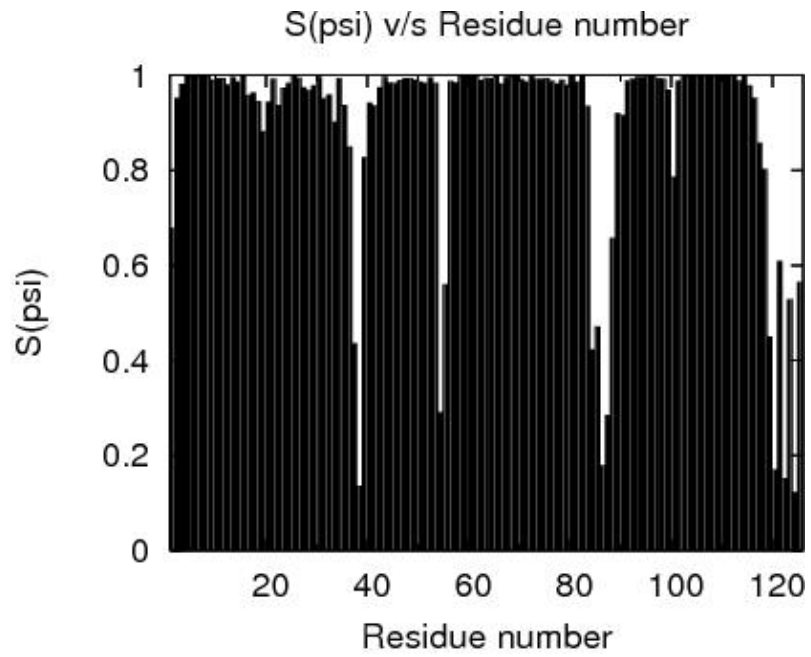


Structure Quality Analysis for NAME





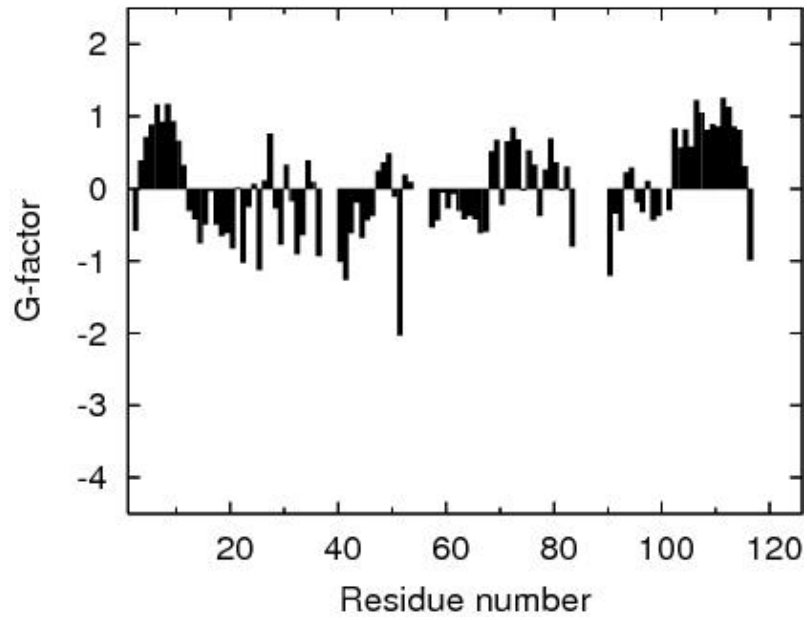
Structure Quality Analysis for NAME



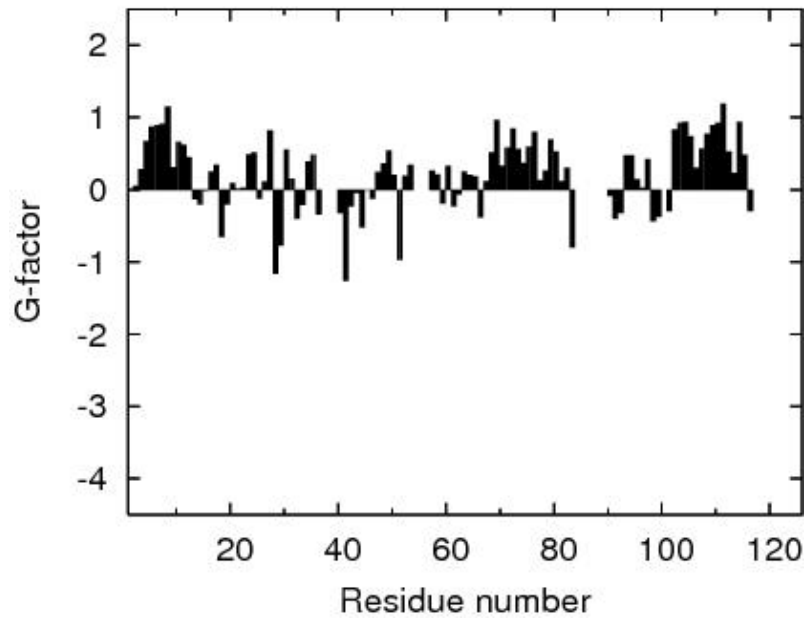


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

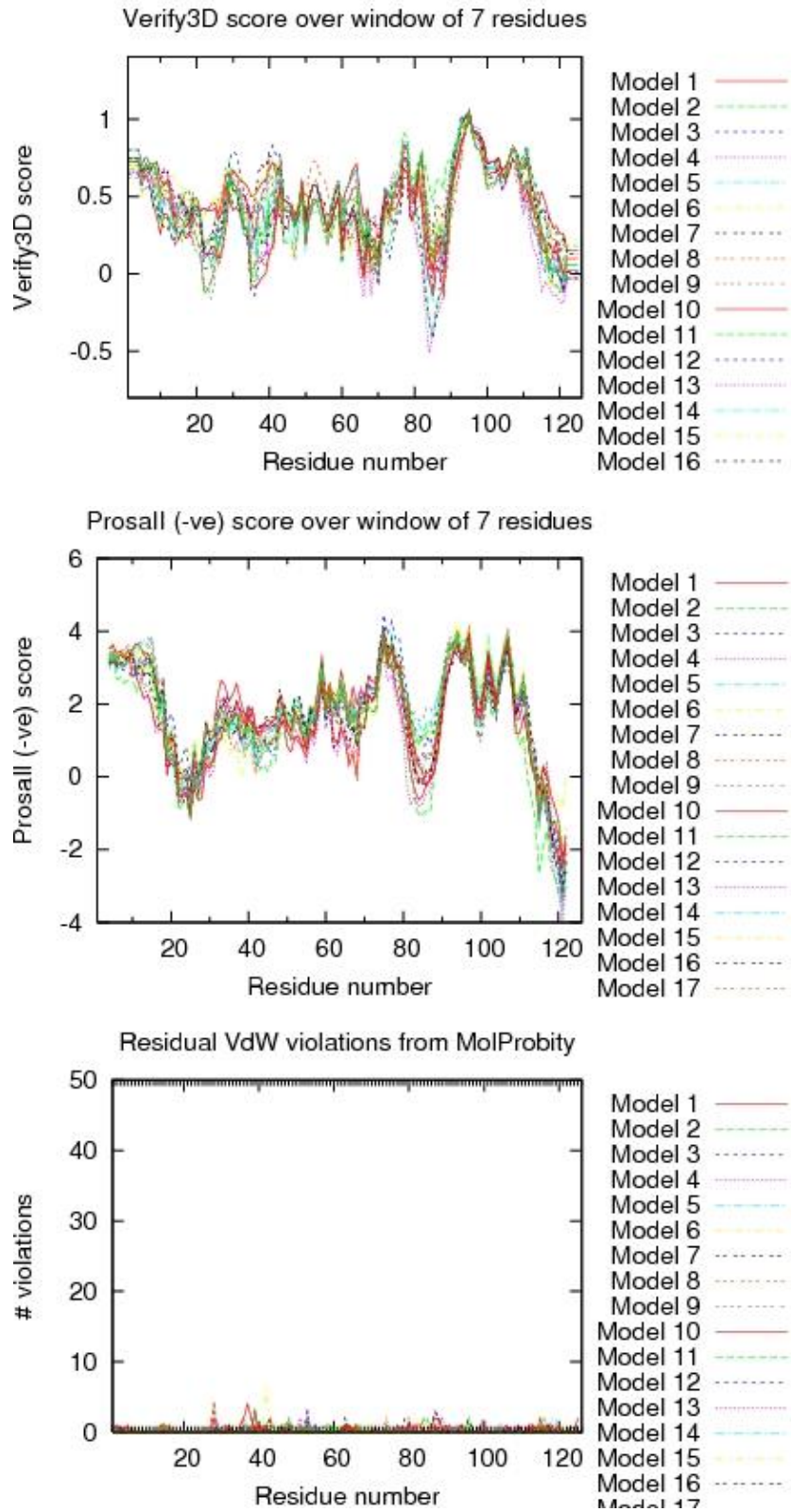


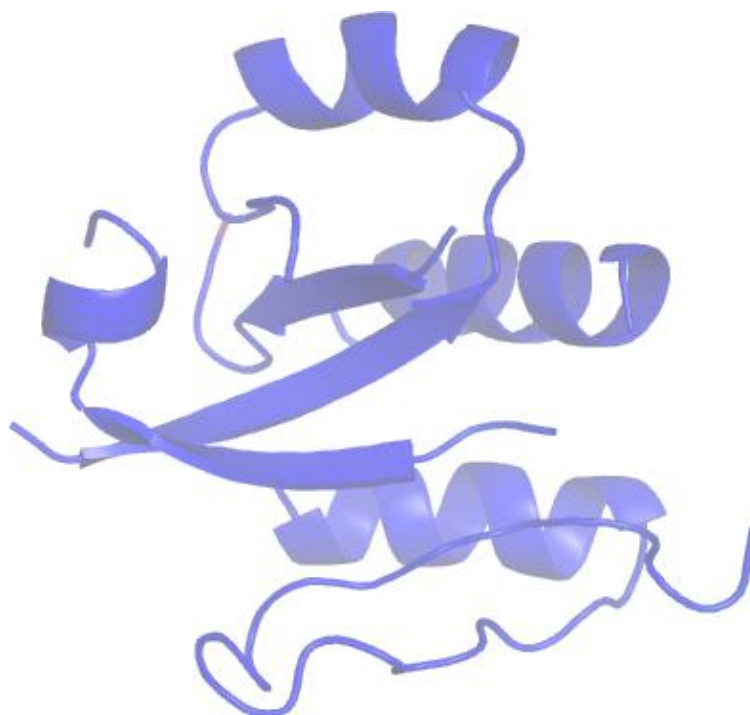
Procheck G-factor for all dihedral angles





Structure Quality Analysis for NAME





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

References:

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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