



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.): 78

Organism:

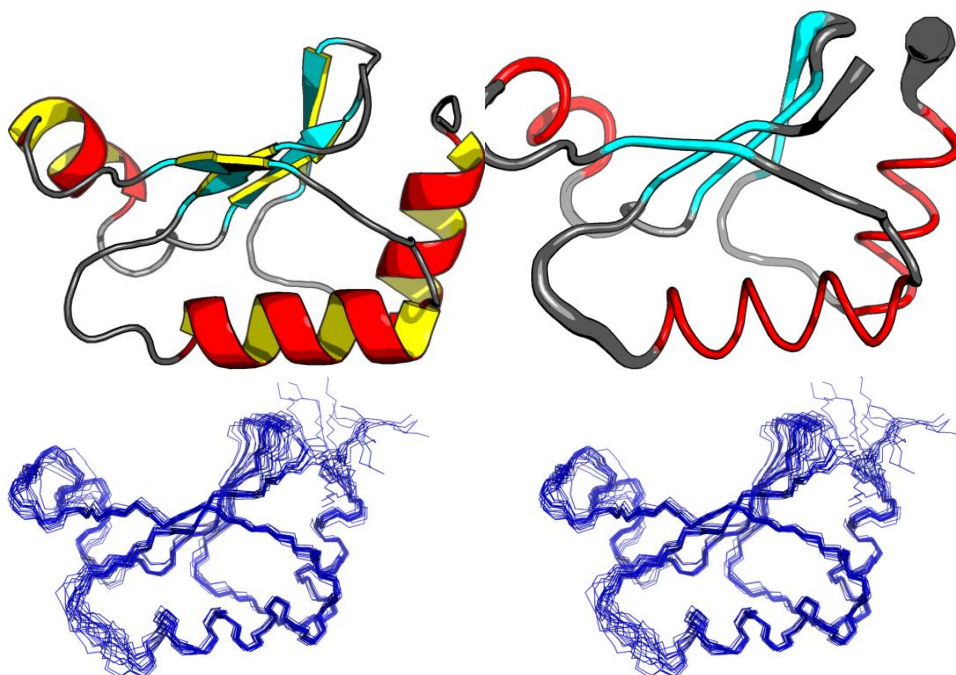
SwissProt /

TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular weight: 8704



Secondary Structure Elements:

alpha helices: 13A-24A, 38A-44A, 65A-74A

beta strands: 30A-33A, 4A-7A, 51A-52A, 58A-59A

Total number of restricting constraints per restrained residue: 22.7

Restricting long range constraints per restrained residue: 6.2

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

12.2 4.7 1.65

Dihedral angle violations per model

1 - 10 ° > 10 °

1.5 2

FIDs deposited in the BMRB? no

RPF Scores



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Recall Precision F-measure DP-score

0.962 0.916 0.939 0.796

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

All backbone atoms 1.3 Å 0.4 Å 0.4 Å

All heavy atoms 1.6 Å 0.6 Å 0.6 Å

Ramachandran Plot Summary for selected residues³ from Procheck

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

93.9% 6.1% 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](#)

95.4% 4.6% 0%

Global quality scores

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

-Raw score 0.39 0.61 0.04 0.13 15.86

*Z-score*¹ -1.12 -0.17 0.47 0.77 -1.20

Generalized linear model RMSD prediction: 0.91

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: 1.2 °

RMS deviation for bond lengths: 0.012 Å

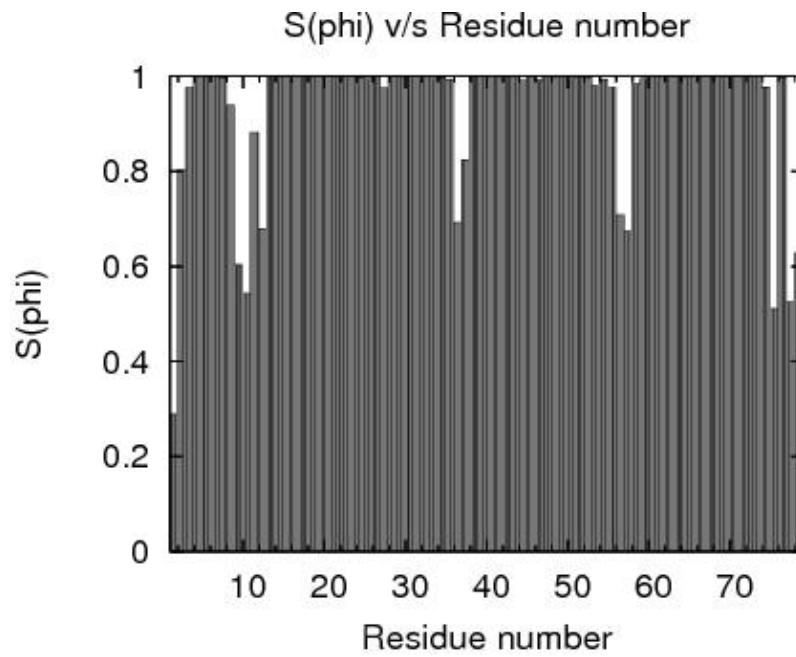
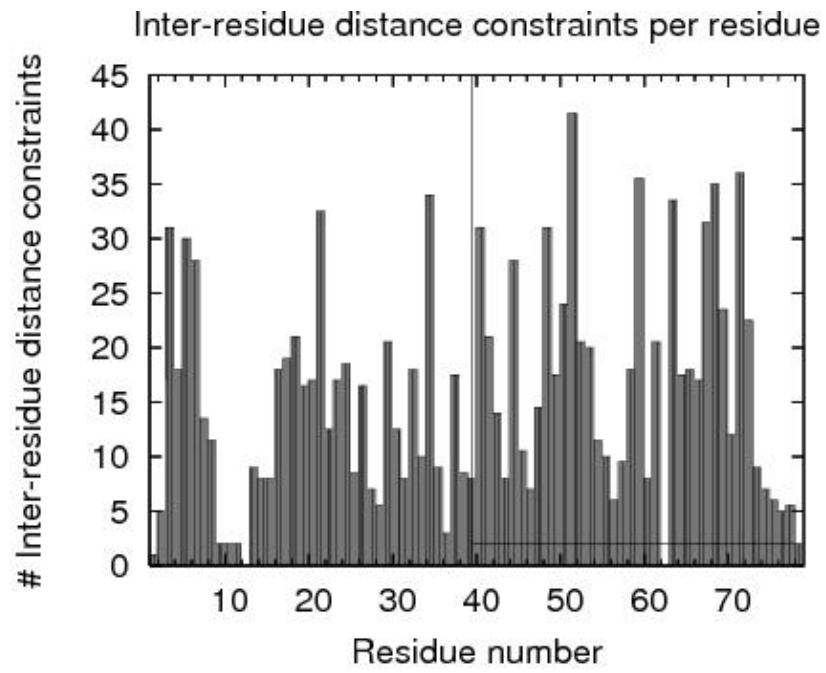
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 3A-7A,13A-34A,37A-55A,58A-74A

³Selected residues: 3A-7A,13A-34A,38A-55A,58A-74A

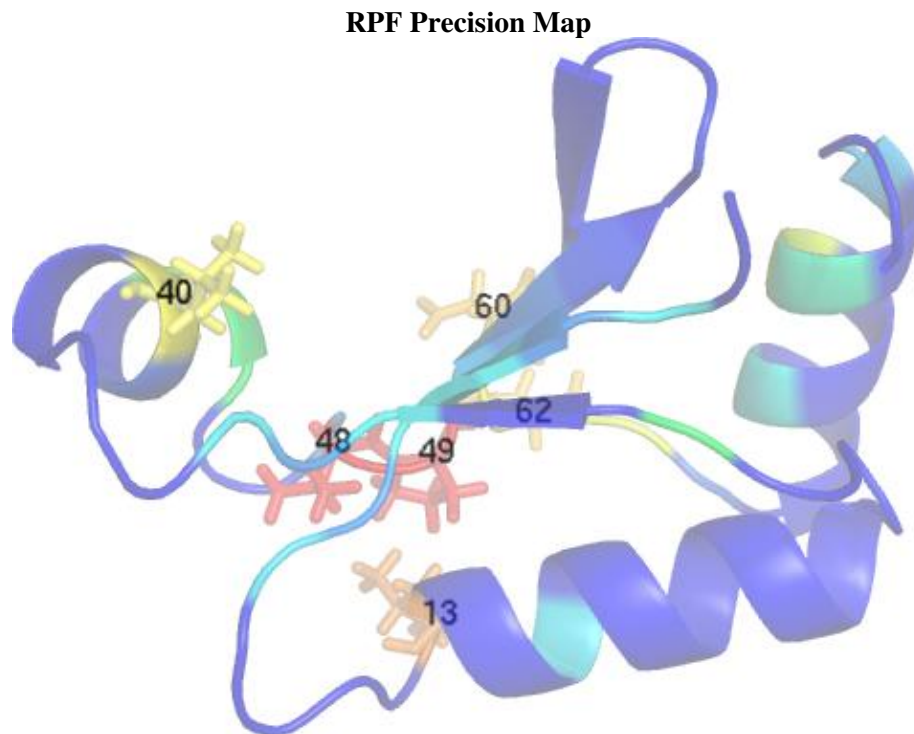
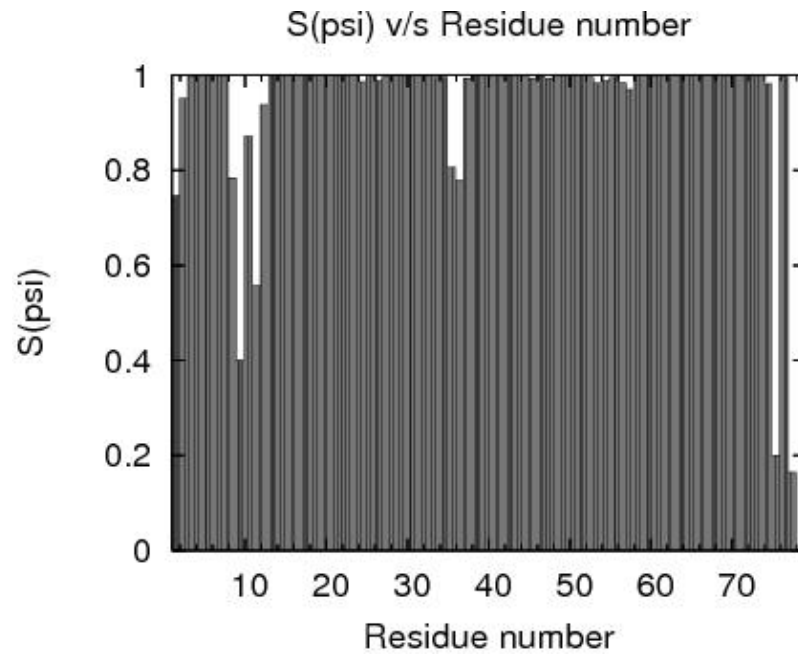


Structure Quality Analysis for NAME





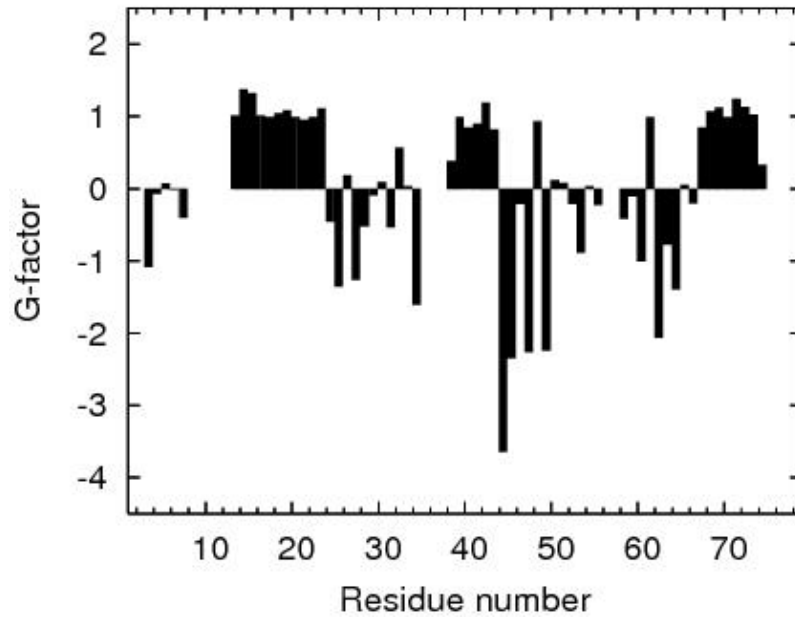
Structure Quality Analysis for NAME



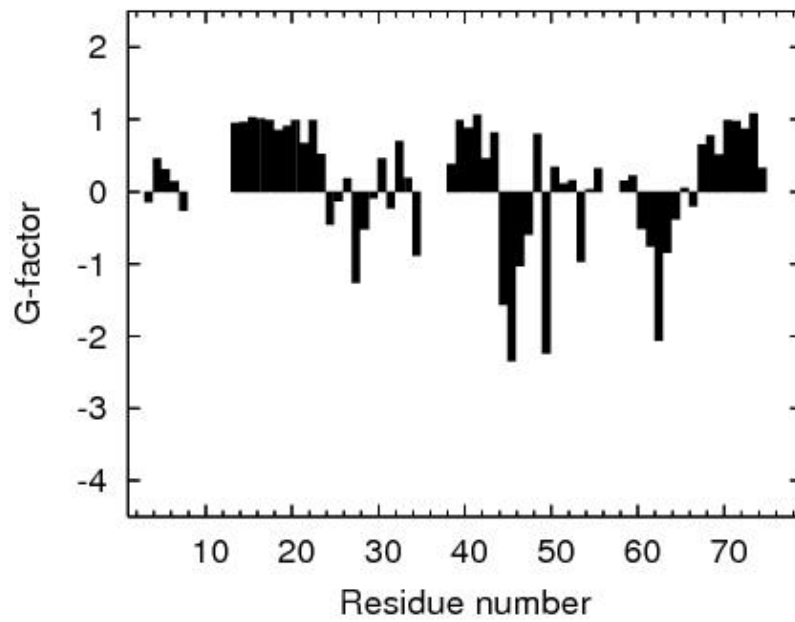


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi



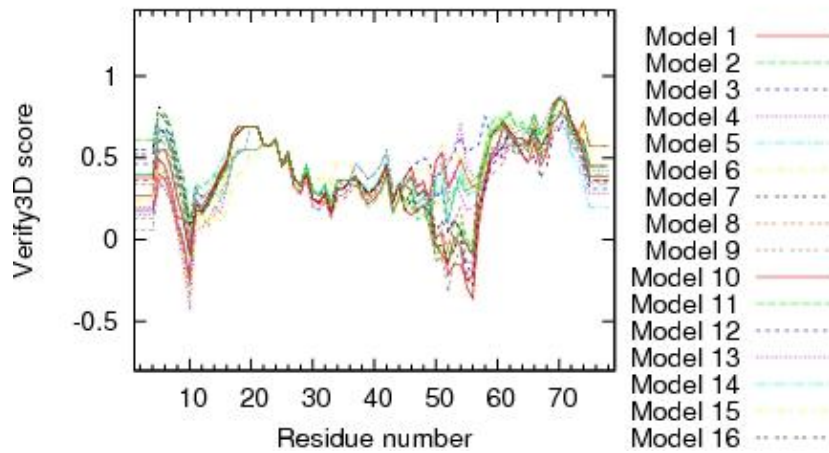
Procheck G-factor for all dihedral angles



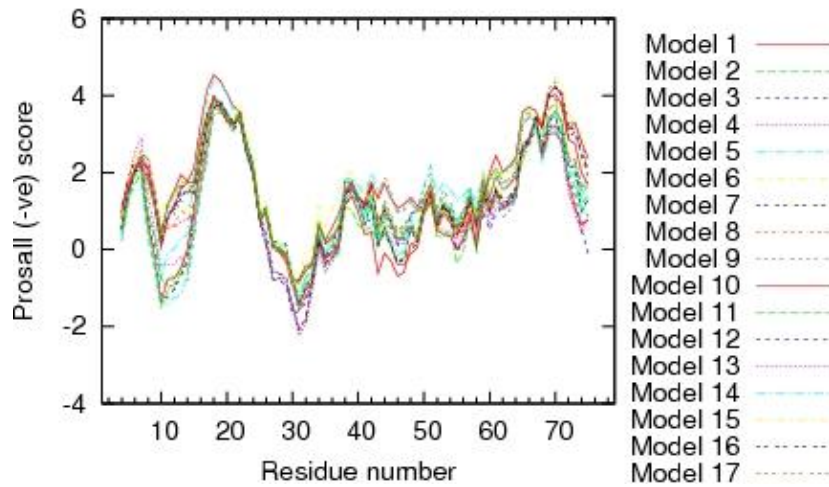


Structure Quality Analysis for NAME

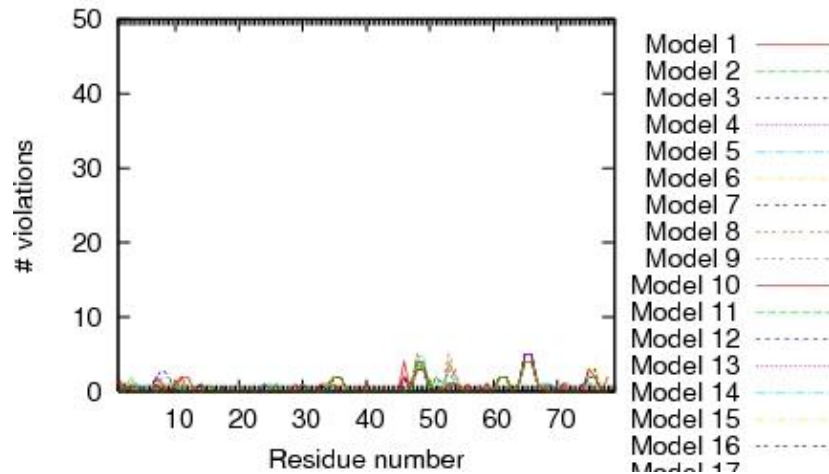
Verify3D score over window of 7 residues

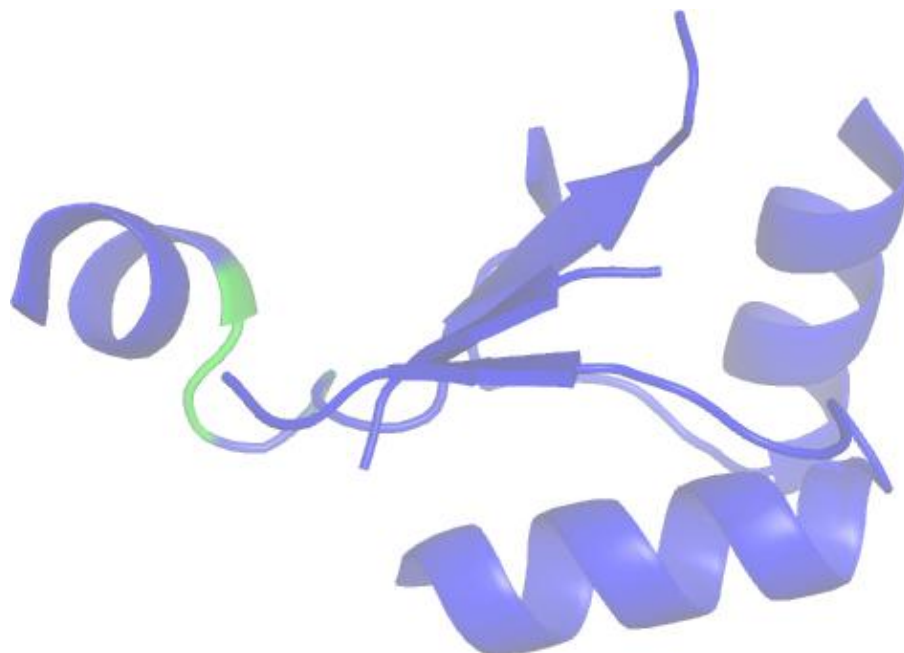


ProsaII (-ve) score over window of 7 residues



Residual VdW violations from MolProbity





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

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
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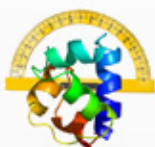
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15. Lovell S C et al, "Structure validation by Calpha geometry: phi,psi and Cbeta deviation" Proteins (2003) 50: 437-450

16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features", Biopolymers (1983) 22: 2577-2637

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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



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pnmcrop
pnmtjpeg

year 2000
year 2000