



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: 20

Oligomerization: monomer

Molecular weight: 10166

Secondary Structure Elements:

alpha helices: 19A-26A, 64A-79A

beta strands: 31S-38S, 45G-52G, 55N-61N

Total number of restricting constraints per restrained residue: 32.3

Restricting long range constraints per restrained residue: 10.7

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

24.85 59.75 132.3

Dihedral angle violations per model

1 - 10° > 10°

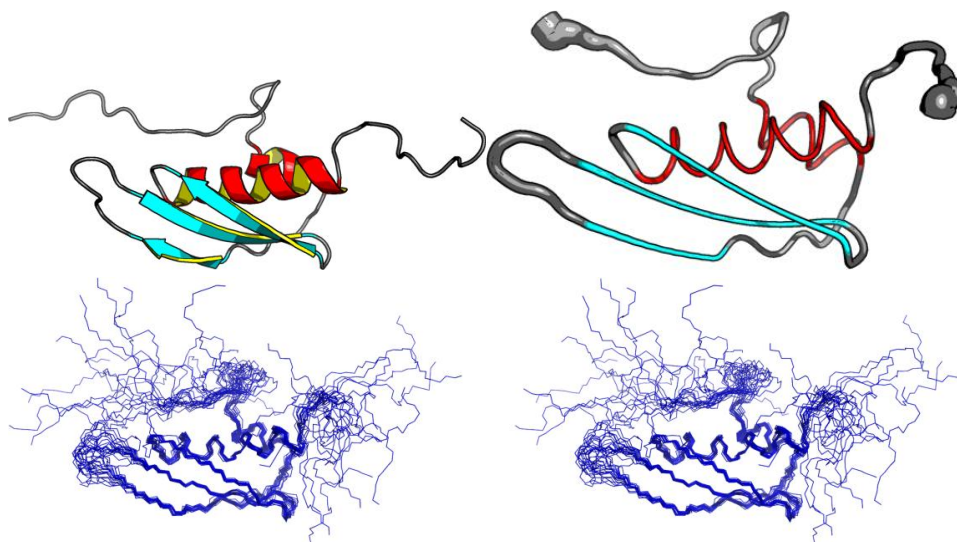
2.1 0.3

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score

0.963 0.975 0.969 0.879





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RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	4.3 Å	0.5 Å	0.5 Å
All heavy atoms	4.7 Å	0.9 Å	0.9 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
91.8%	8.1%	0.0%	0.1%

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

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
99.1%	0.8%	0.1%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbity Clashscore
-Raw score	0.30	0.59	-0.07	0.21	2.72
Z-score ¹	-2.57	-0.25	0.04	1.24	1.06

Generalized linear model RMSD prediction: 0.84

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

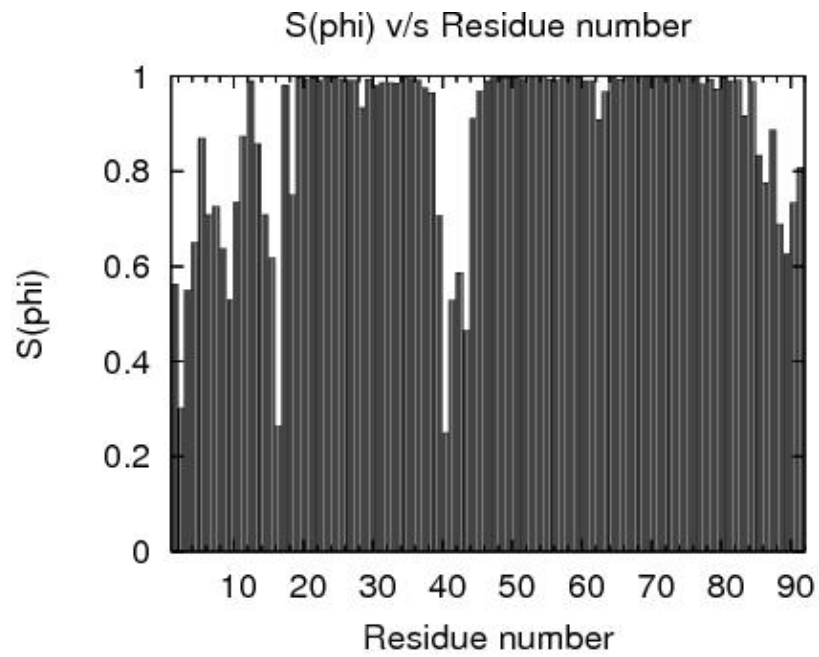
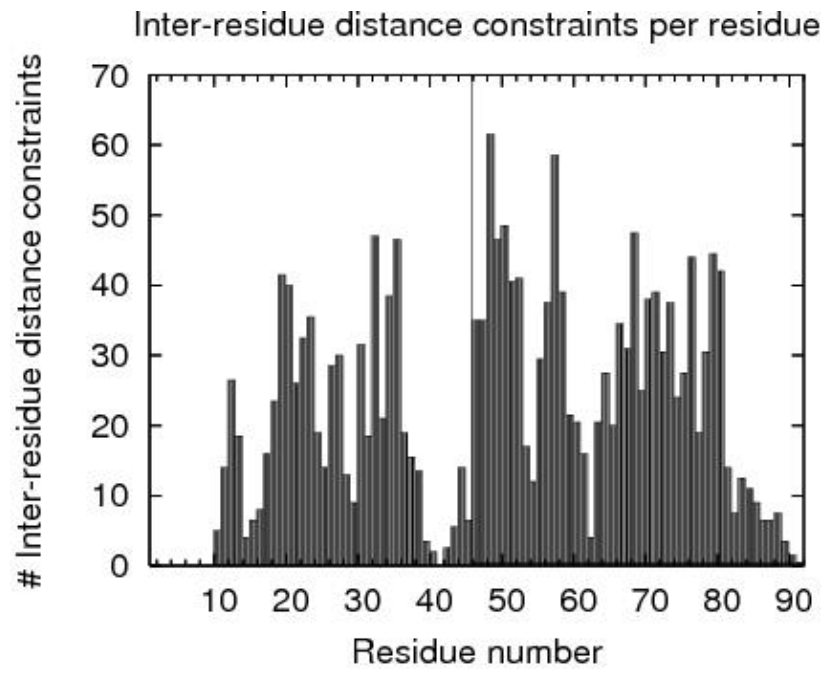
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 19A-38A,44A-81A

³Selected residues: 19A-38A,44A-81A

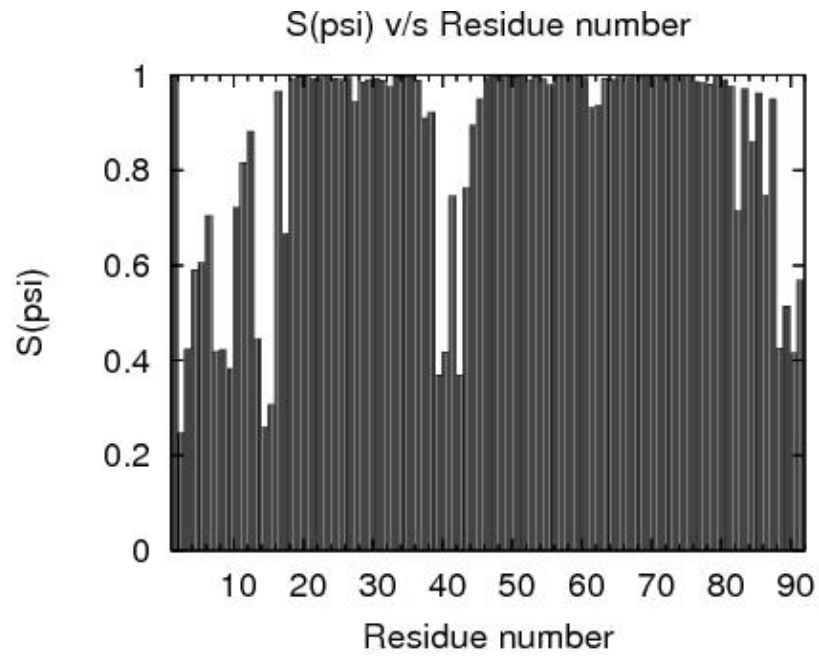


Structure Quality Analysis for NAME

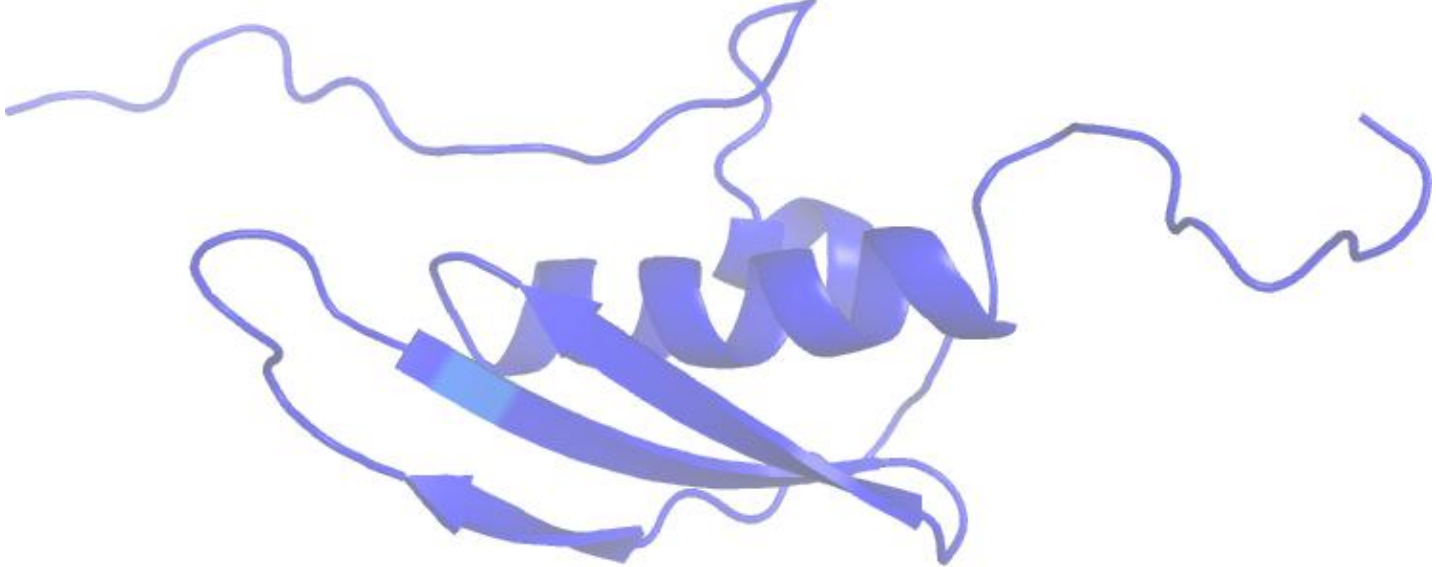




Structure Quality Analysis for NAME



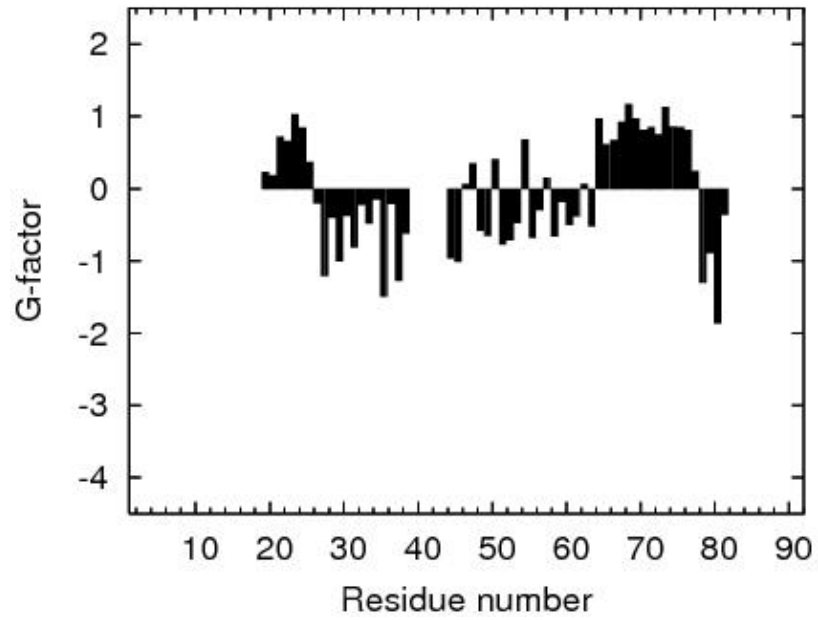
RPF Precision Map



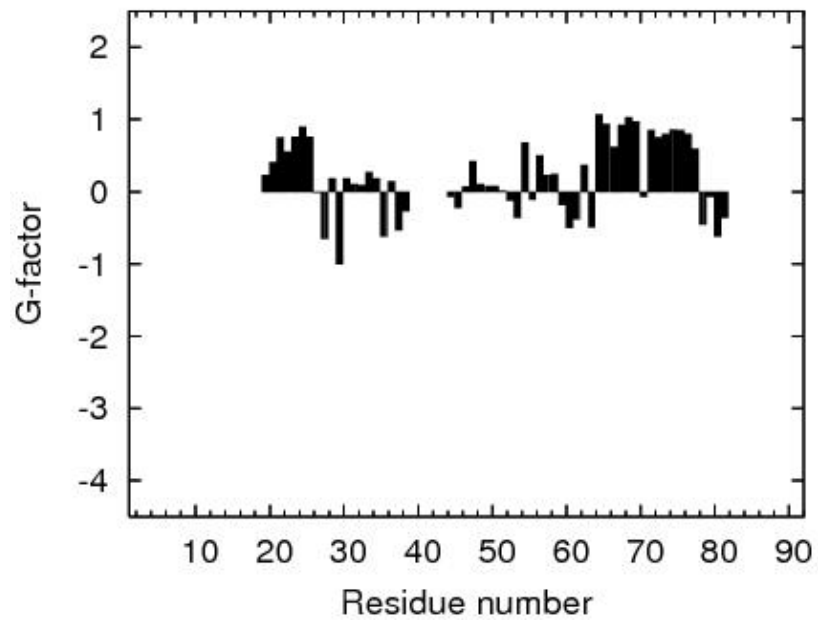


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi



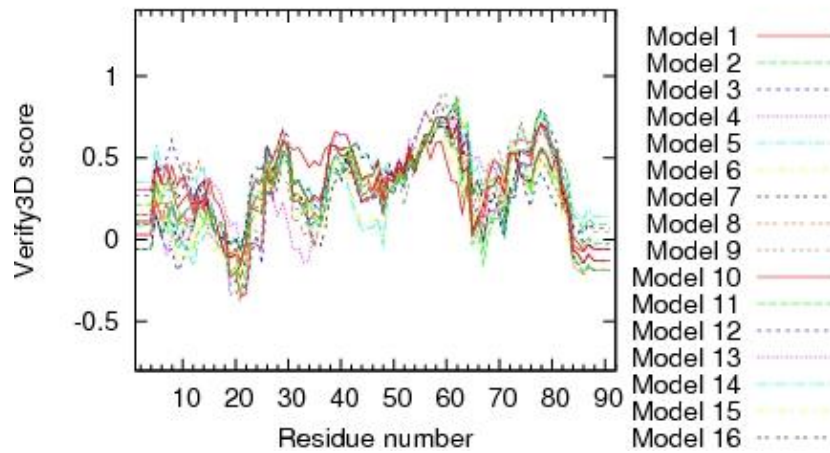
Procheck G-factor for all dihedral angles



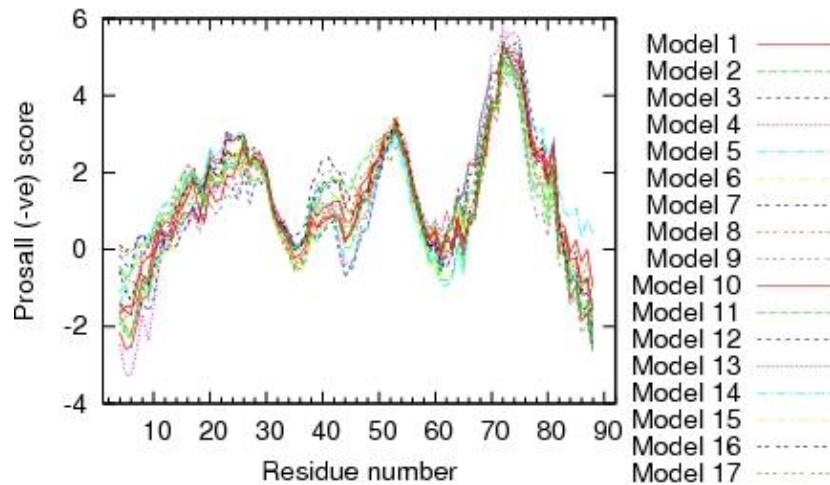


Structure Quality Analysis for NAME

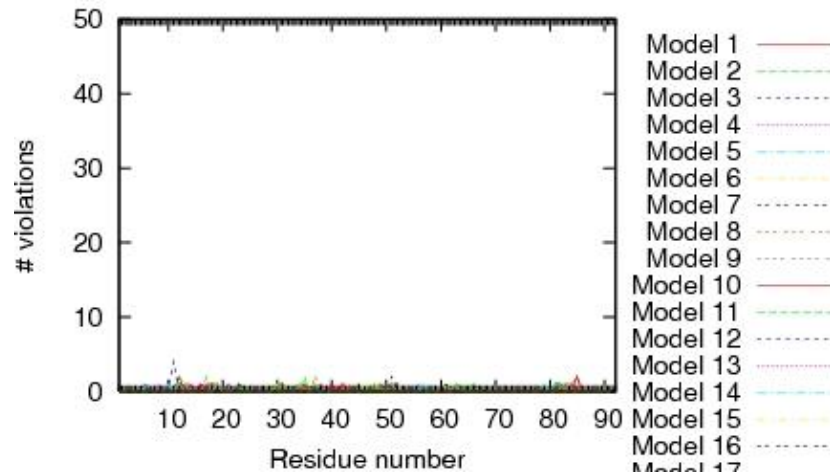
Verify3D score over window of 7 residues

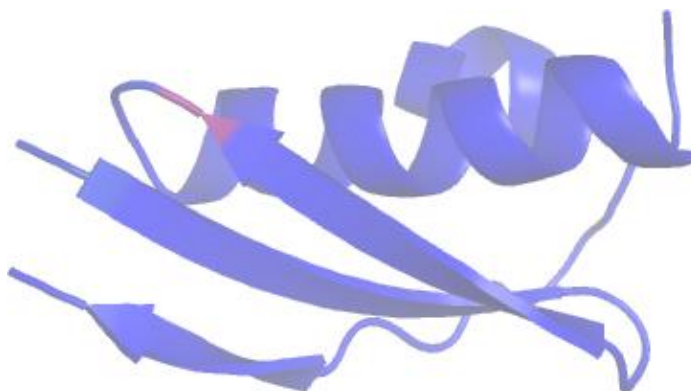


ProsaII (-ve) score over window of 7 residues



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
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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
pdostat	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