



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.): 121

Organism:

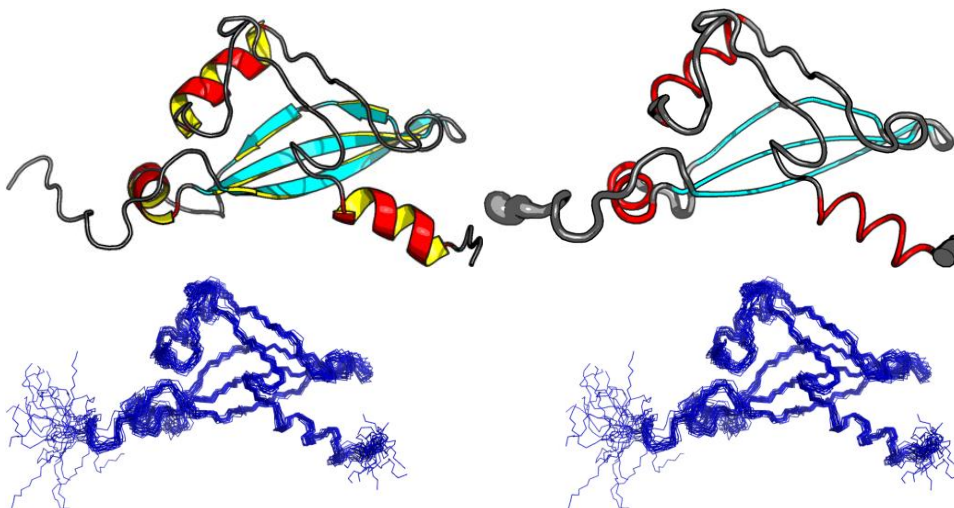
SwissProt /

TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular weight: 14335



Secondary Structure Elements:

alpha helices: 6A-14A, 39A-43A, 75A-81A

beta strands: 22E-26E, 50E-54E, 61U-62U, 83R-92R, 65E-69E, 98L-106L

Total number of restricting constraints per restrained residue: 18.9

Restricting long range constraints per restrained residue: 5.4

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

0.9 0.1 0

Dihedral angle violations per model

1 - 10 ° > 10 °

3.6 0

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score

0.911 0.93 0.92 0.753



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RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	1.6 Å	0.7 Å	0.7 Å
All heavy atoms	2.1 Å	1.1 Å	1.1 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
85.1%	14.5%	0.4%	0.0%

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

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
94.2%	5%	0.8%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbity Clashscore
-Raw score	0.26	0.43	-0.42	-0.40	22.04
Z-score ¹	-3.21	-0.91	-1.34	-2.37	-2.26

Generalized linear model RMSD prediction: 1.97

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):	10
RMS deviation for bond angles:	0.6 °
RMS deviation for bond lengths:	0.008 Å

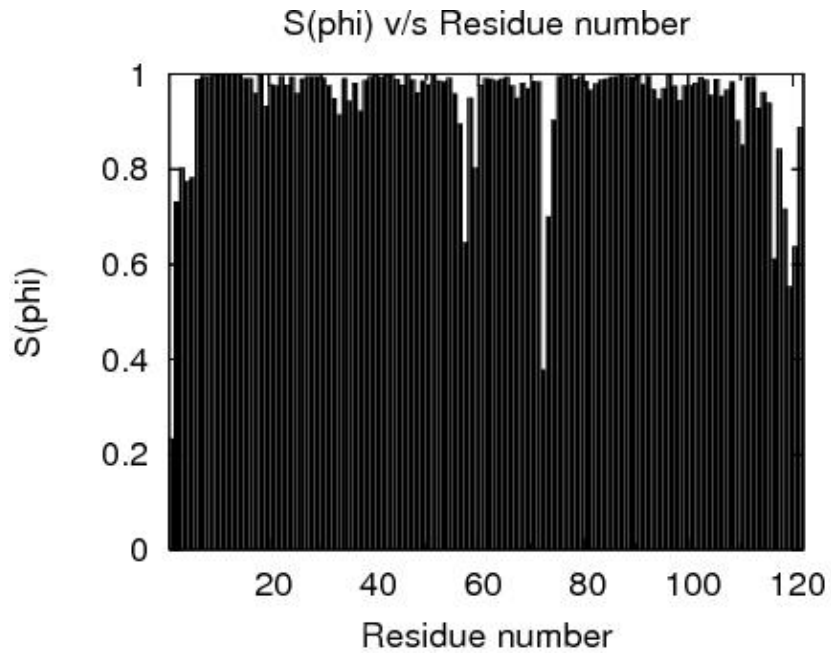
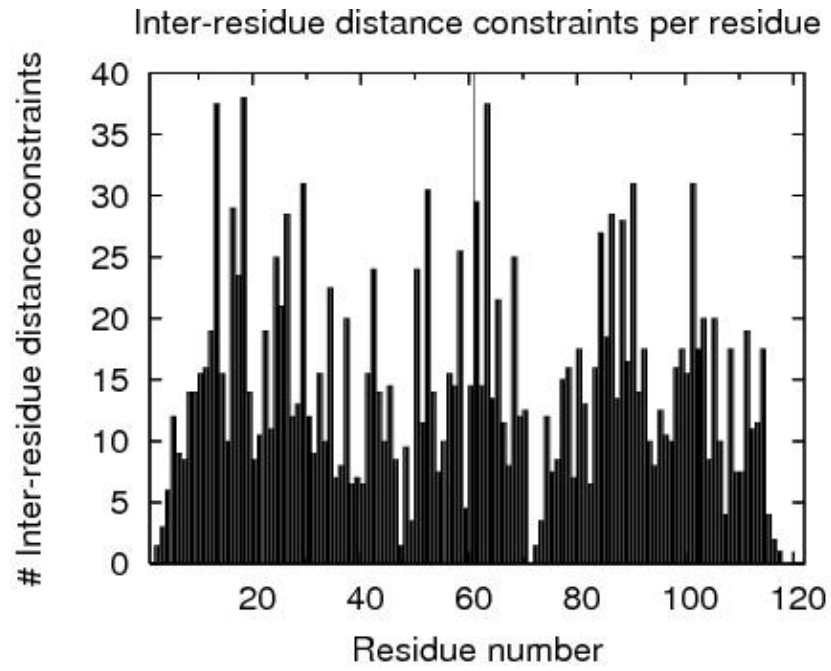
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 6A-55A,60A-70A,74A-108A,110A-114A

³Selected residues: 6A-55A,60A-70A,74A-108A,110A-114A

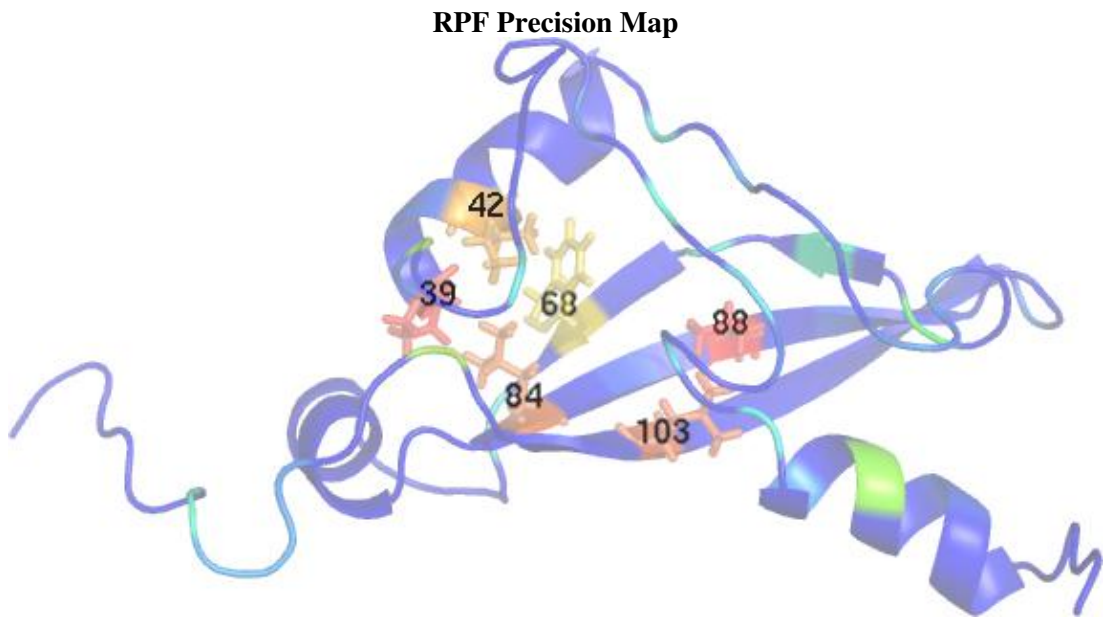
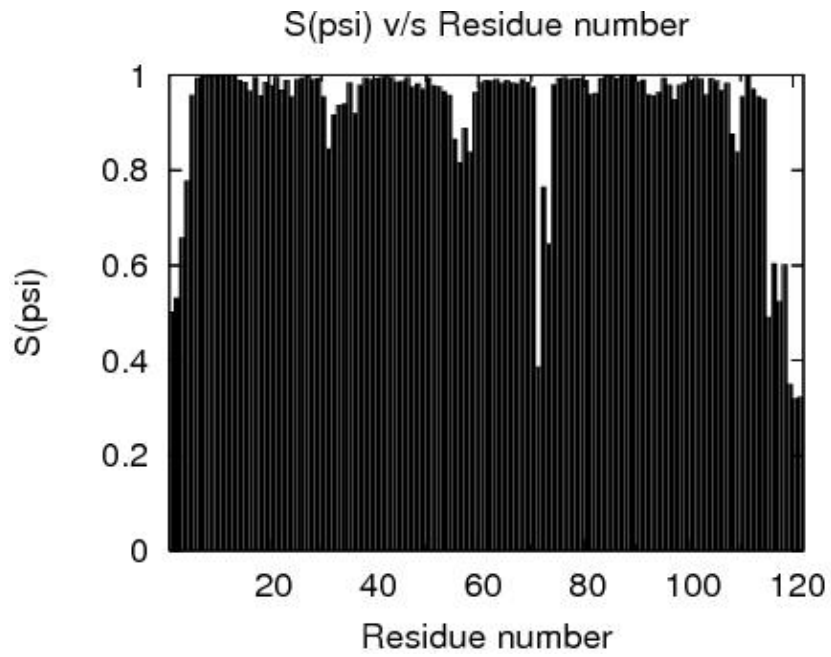


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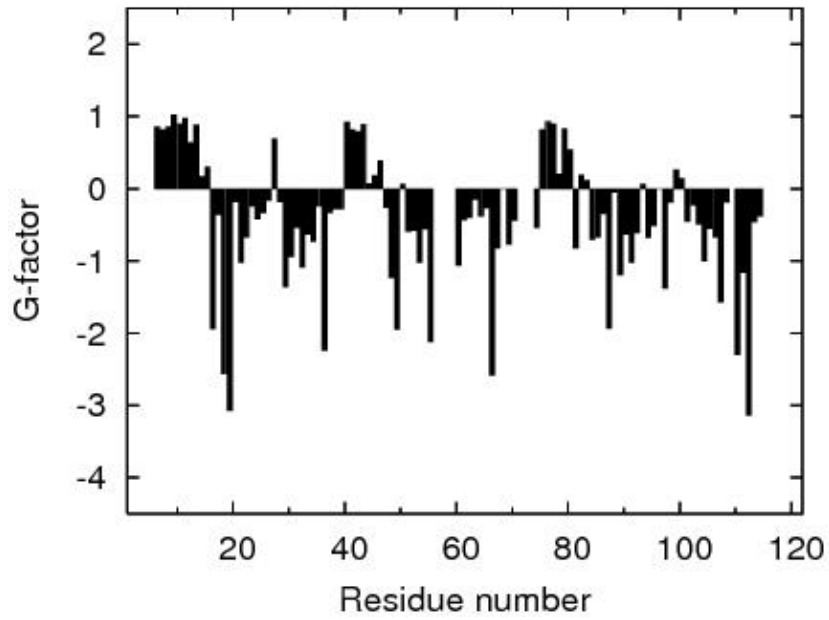
Structure Quality Analysis for NAME



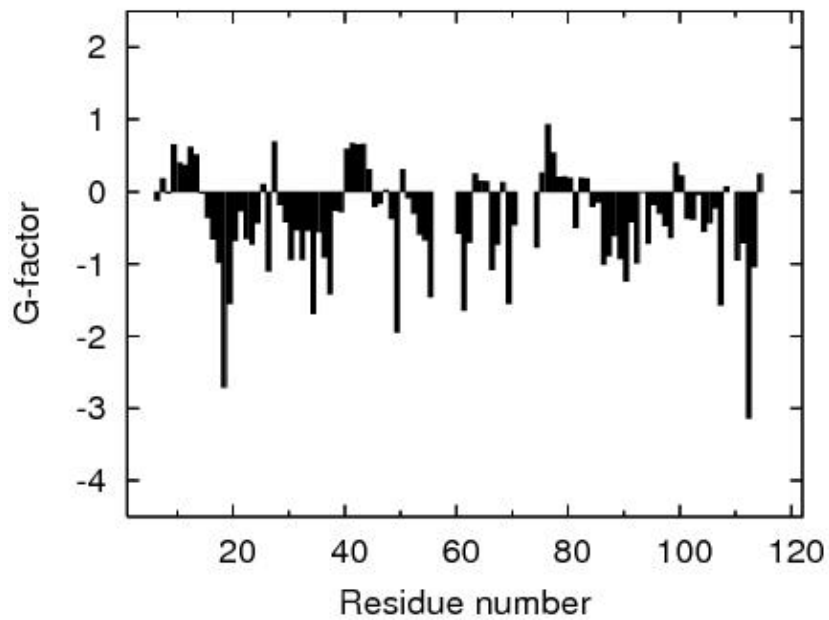


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

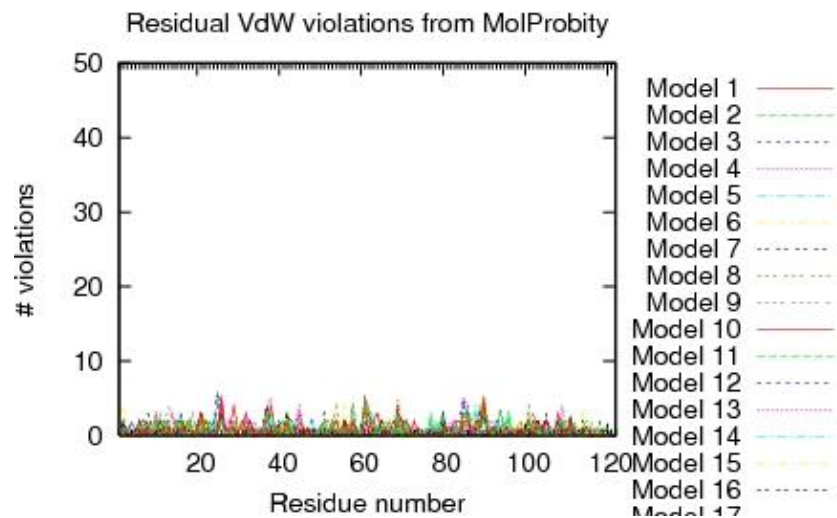
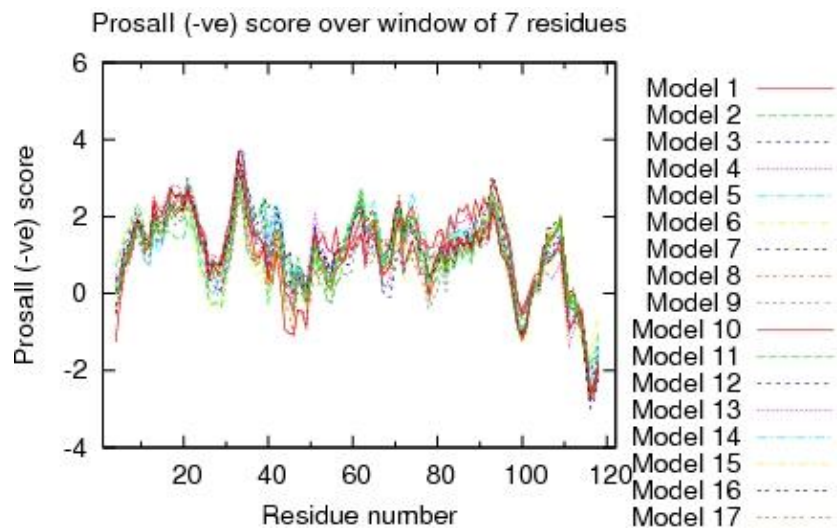
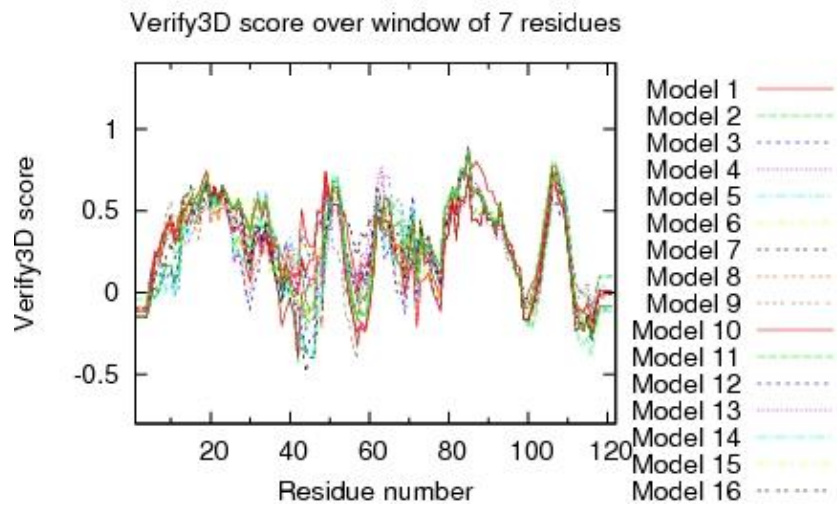


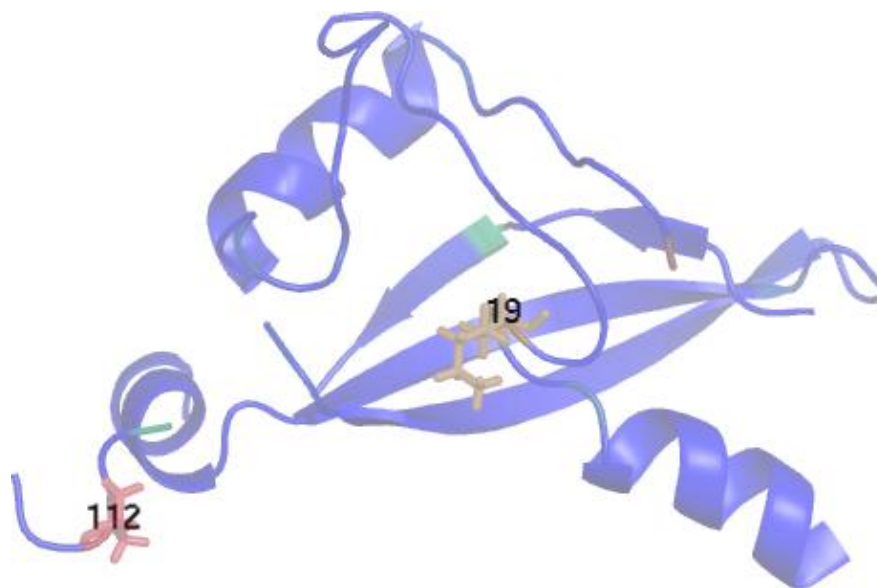
Procheck G-factor for all dihedral angles





Structure Quality Analysis for NAME





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

References:

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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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5. Laskowski R Ai 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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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-11-2013 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
convert	ImageMagick 5.5.6
ps2pdf	Ghostscript 7.05
htmldoc	v1.9
gnuplot	Version 3.7 patchlevel 3



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jpegtopnm	year 2000
pnmcrop	year 2000
pnmtjpeg	year 2000