



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.): 109

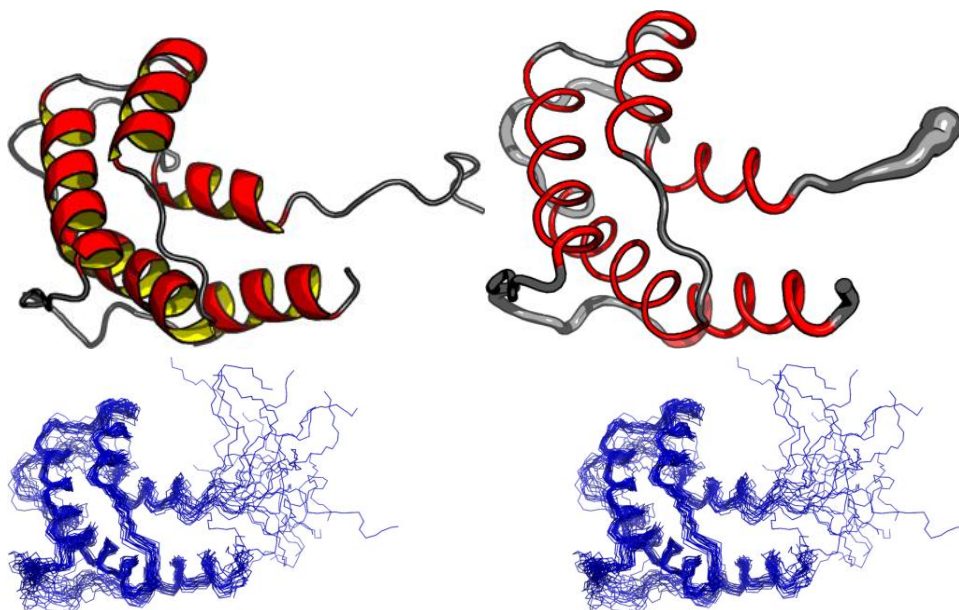
Organism:

SwissProt /
TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular
weight: 12107



Secondary Structure Elements:

alpha helices: 11A-20A, 35A-47A, 53A-63A, 67A-82A, 96A-107A

beta strands:

Total number of restricting constraints per restrained residue: 13.2

Restricting long range constraints per restrained residue: 2.4

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

2.3 0.6 0

Dihedral angle violations per model

1 - 10° > 10°

0.3 0

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score



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0.9806 0.899107 0.938 0.8

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	2.7 Å	0.8 Å	0.8 Å
All heavy atoms	3.2 Å	1.2 Å	1.2 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
96.1%	3.9%	0.0%	0.0%

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

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
96.1%	3.9%	0%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbability Clashscore
-Raw score	0.30	0.67	0.36	0.19	19.93
Z-score ¹	-2.57	0.08	1.73	1.12	-1.89

Generalized linear model RMSD prediction: 0.93

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):	41
RMS deviation for bond angles:	0.6 °
RMS deviation for bond lengths:	0.004 Å

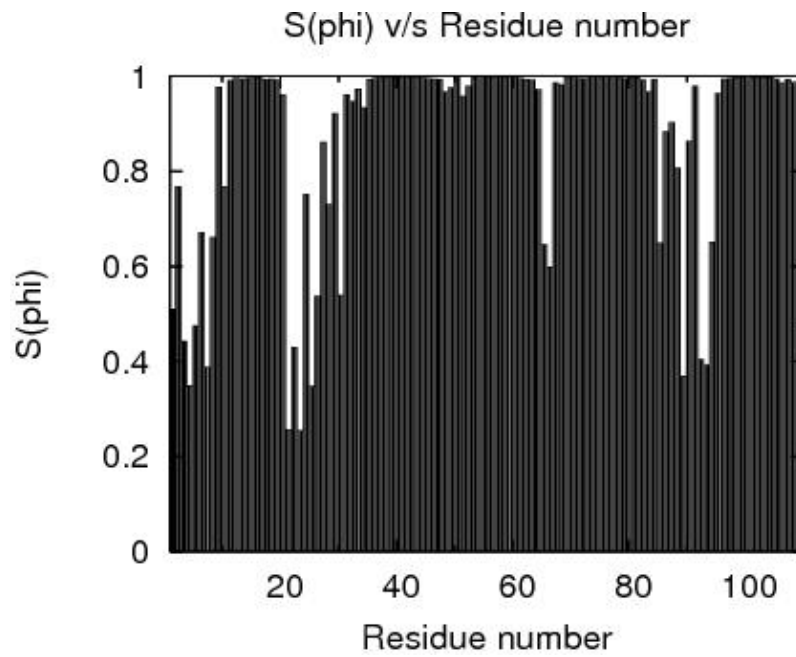
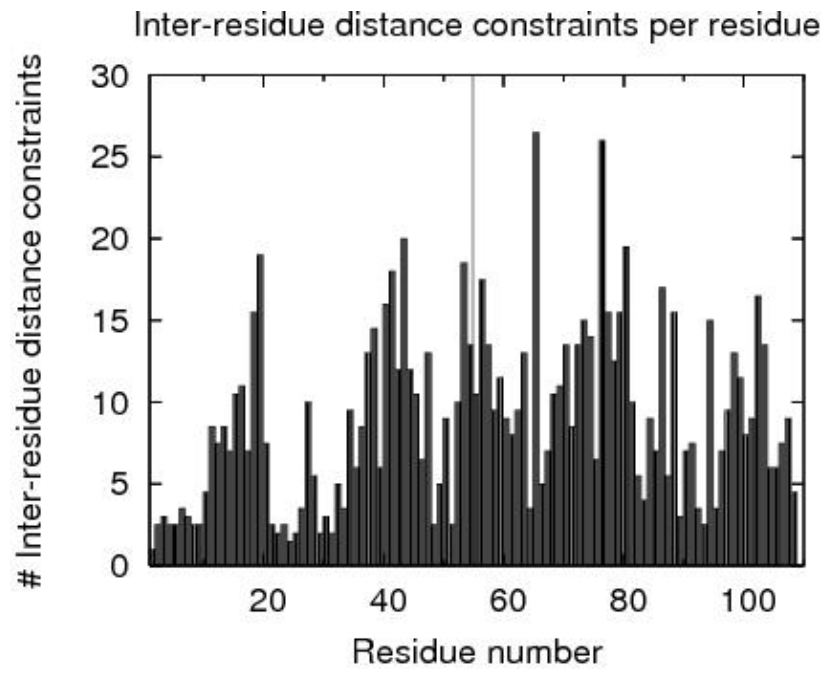
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 11A-19A,31A-63A,67A-83A,95A-108A

³Selected residues: 11A-19A,31A-63A,67A-83A,95A-108A

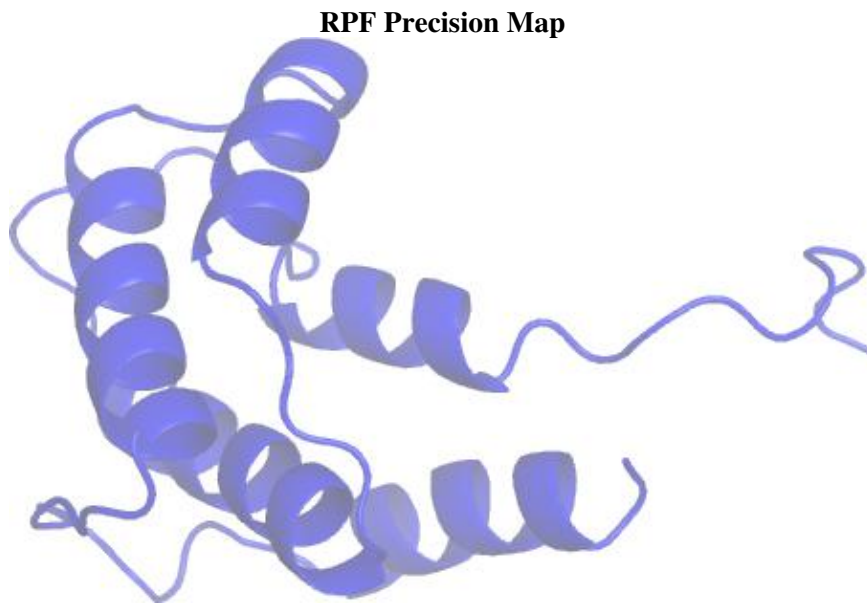
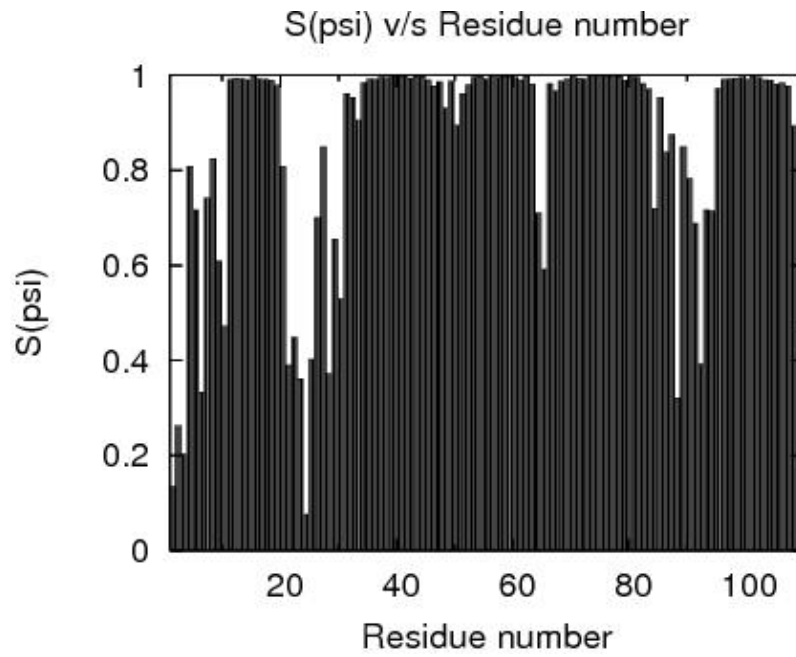


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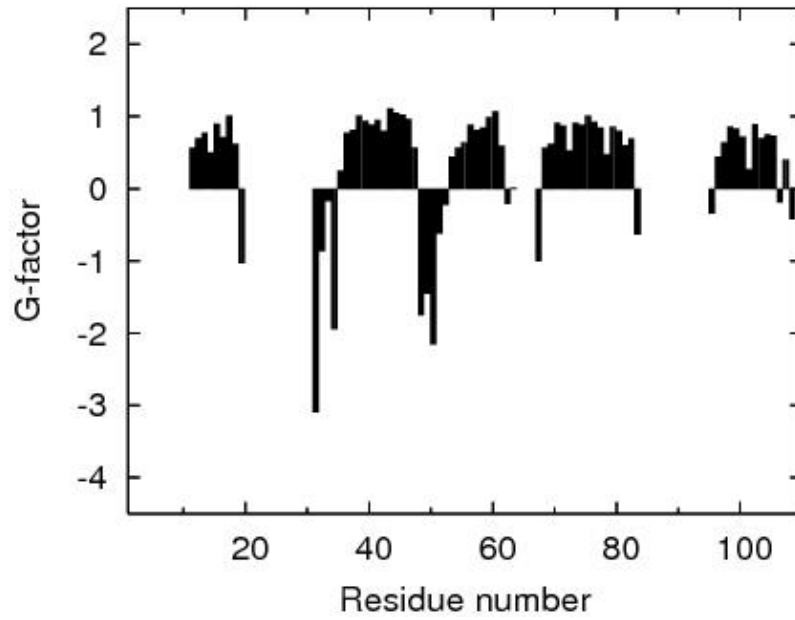
Structure Quality Analysis for NAME



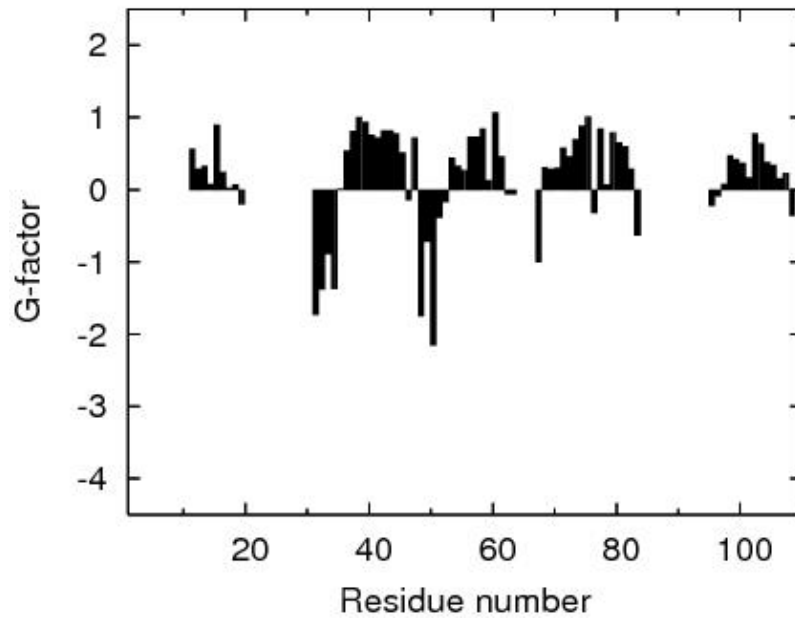


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

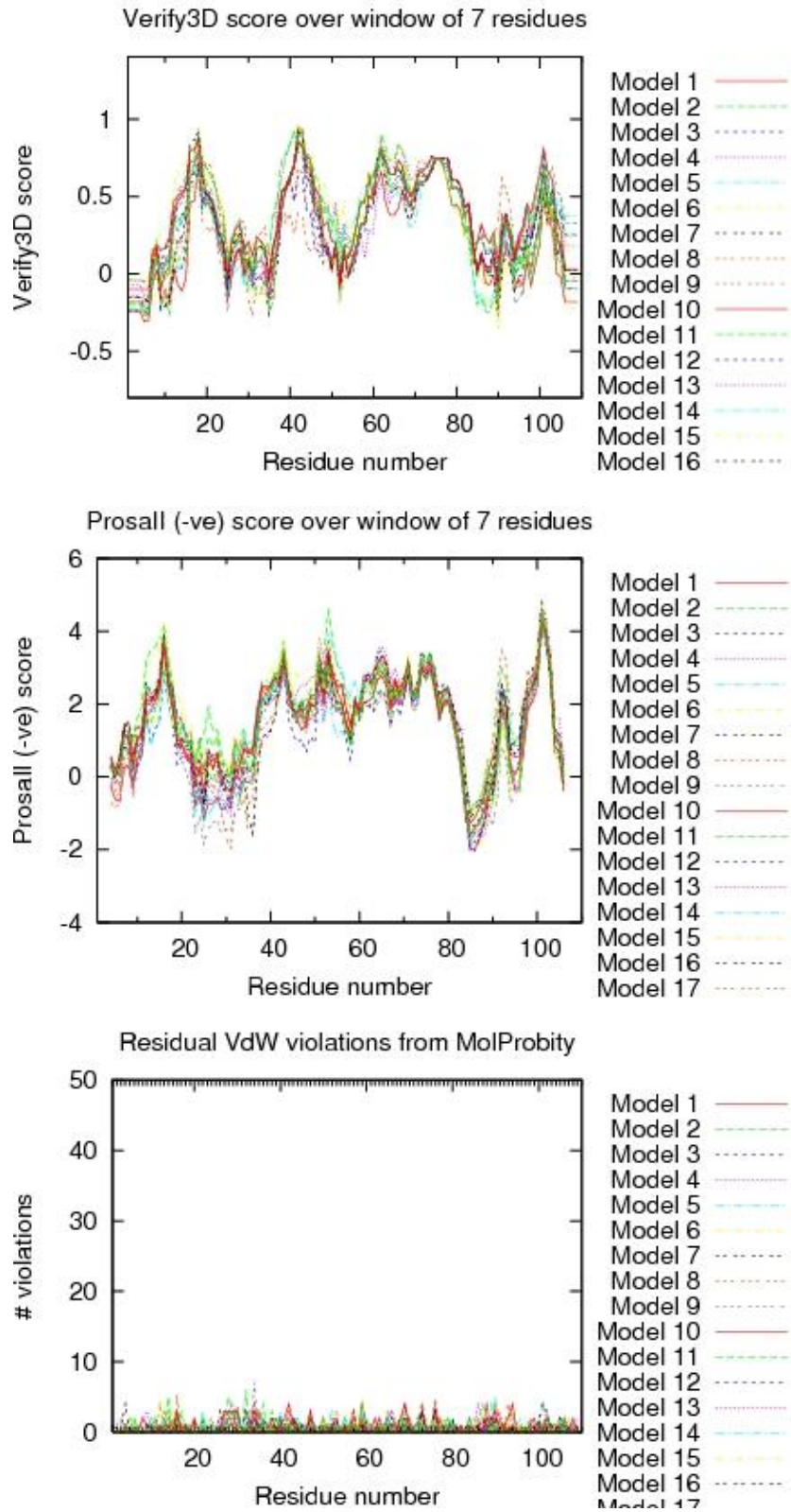


Procheck G-factor for all dihedral angles





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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
4. Sippl M J, "Calculation of Conformation Ensembles from Potentials of Mean Force", J Mol Biol 213 (1990): 859-883
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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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
9. Word J M et al, "Visualizing and Quantifying Molecular Goodness-of-Fit: Small-probe Contact Dots with Explicit Hydrogens", J Mol Biol 285 (1999): 1711-1733
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11. Luthy R, McLachlan A D and Eisenberg D, "Secondary Structure-Based Profiles: Use of Structure-Conserving Scoring Tables in Searching Protein Sequence Databases for Structural Similarities", Proteins 10 (1991): 229-239
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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

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