



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.): 175

Organism:

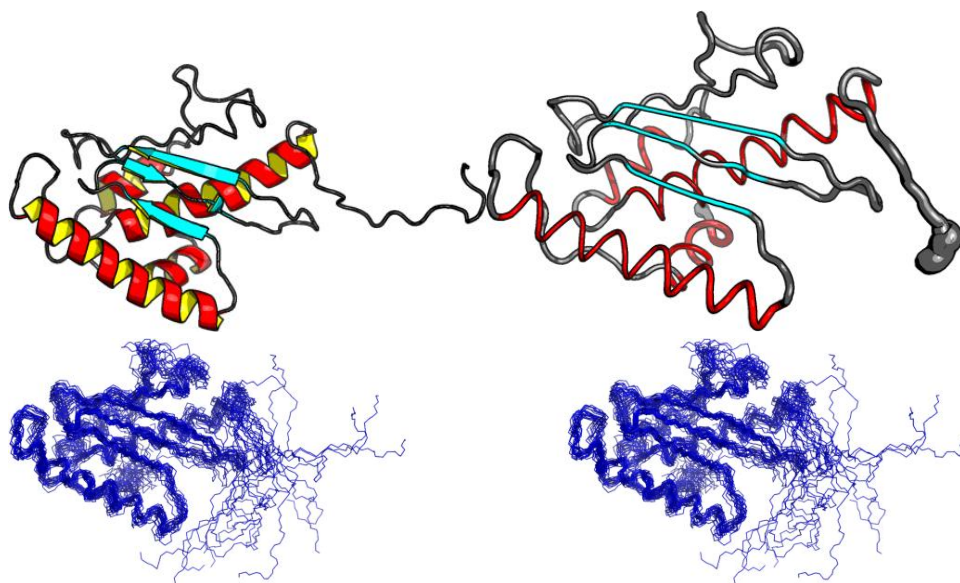
SwissProt /

TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular weight: 20523



Secondary Structure Elements:

alpha helices: 4A-9A, 25A-48A, 100A-105A, 122A-126A, 134A-140A, 142A-156A

beta strands: 57U-58U, 64G-73G, 76U-85U, 96U-97U

Total number of restricting constraints per restrained residue: 23.4

Restricting long range constraints per restrained residue: 6.6

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

21.35 45.7 99.65

Dihedral angle violations per model

1 - 10 ° > 10 °

13.25 7.8

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score



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0.92 0.961 0.94 0.78

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	3.7 Å	1.2 Å	1.2 Å
All heavy atoms	4.3 Å	1.7 Å	1.6 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
93.0%	6.8%	0.1%	0.1%

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

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
97.2%	2.7%	0.1%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbability Clashscore
-Raw score	0.39	0.42	-0.08	0.16	3.94
Z-score ¹	-1.12	-0.95	0.00	0.95	0.85

Generalized linear model RMSD prediction: 2.07

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):	0
RMS deviation for bond angles:	0.7 °
RMS deviation for bond lengths:	0.010 Å

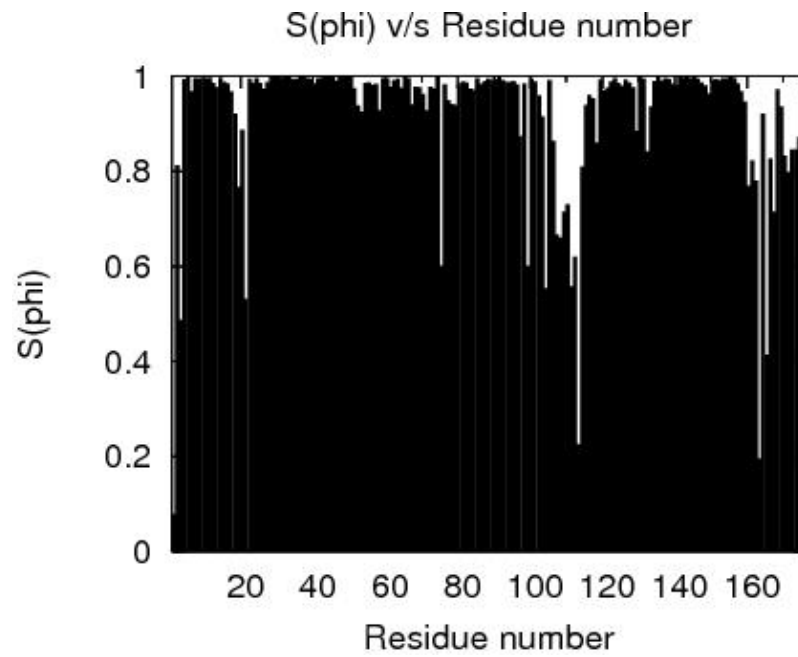
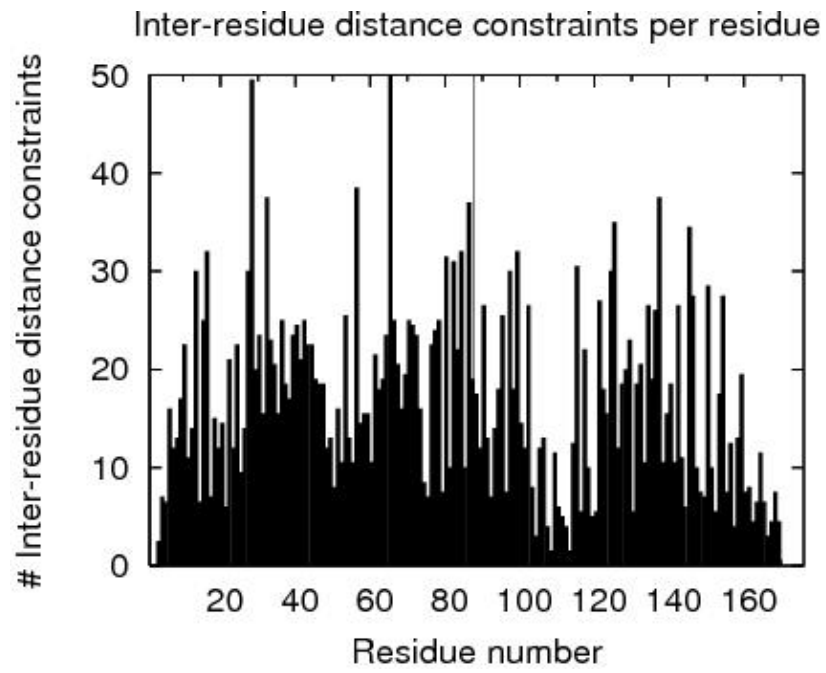
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 4A-17A,22A-73A,76A-97A,100A-102A,119A-131A,133A-159A

³Selected residues: 4A-17A,22A-52A,54A-73A,76A-97A,100A-102A,115A-159A

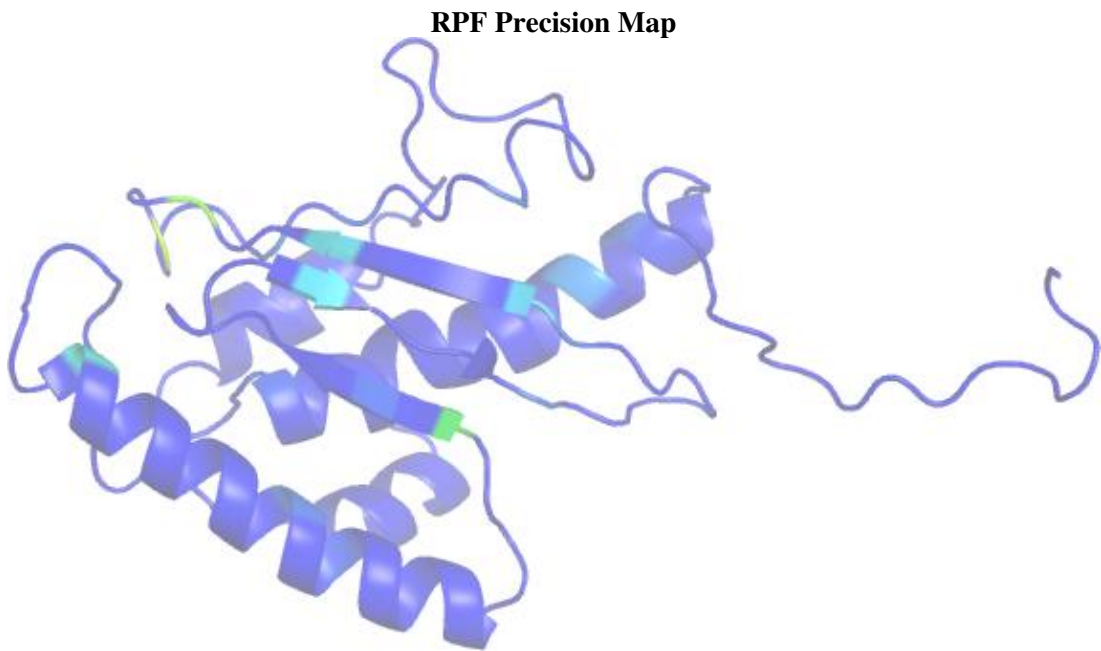
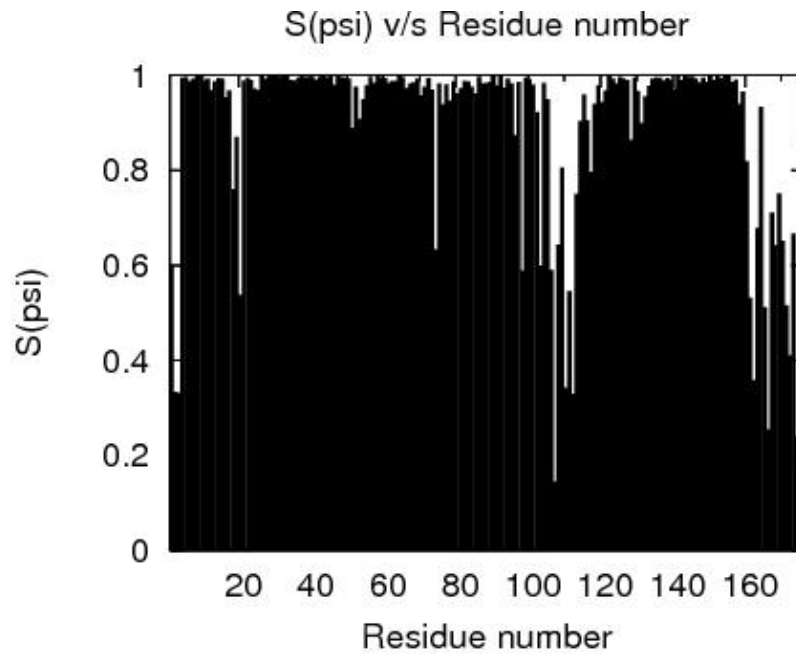


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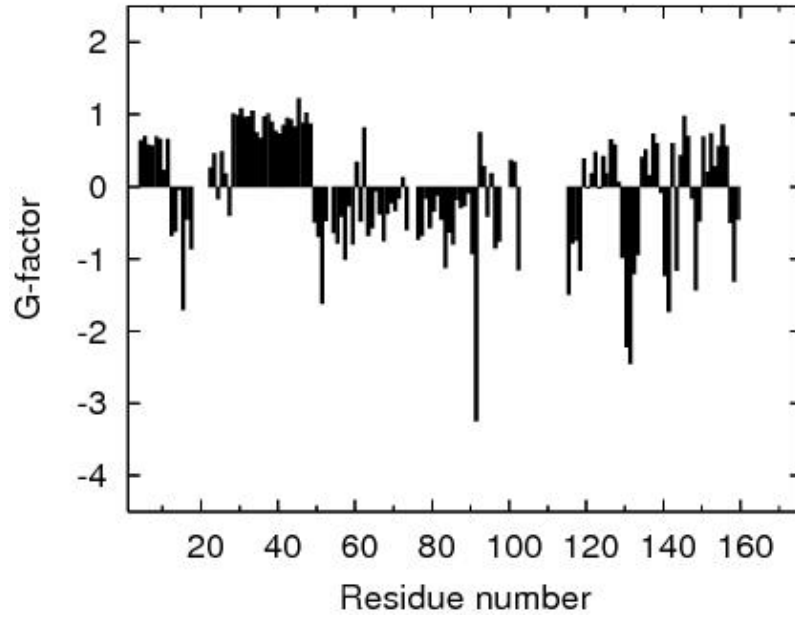
Structure Quality Analysis for NAME



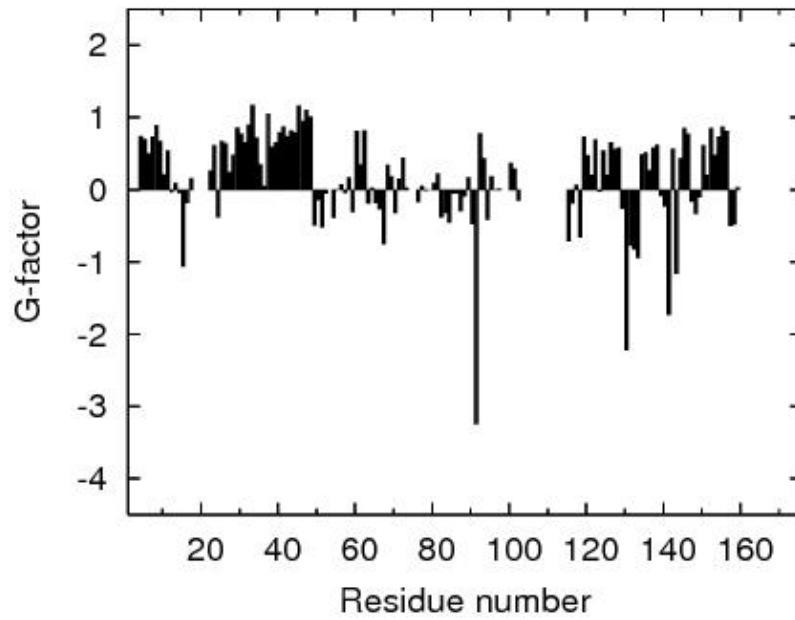


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

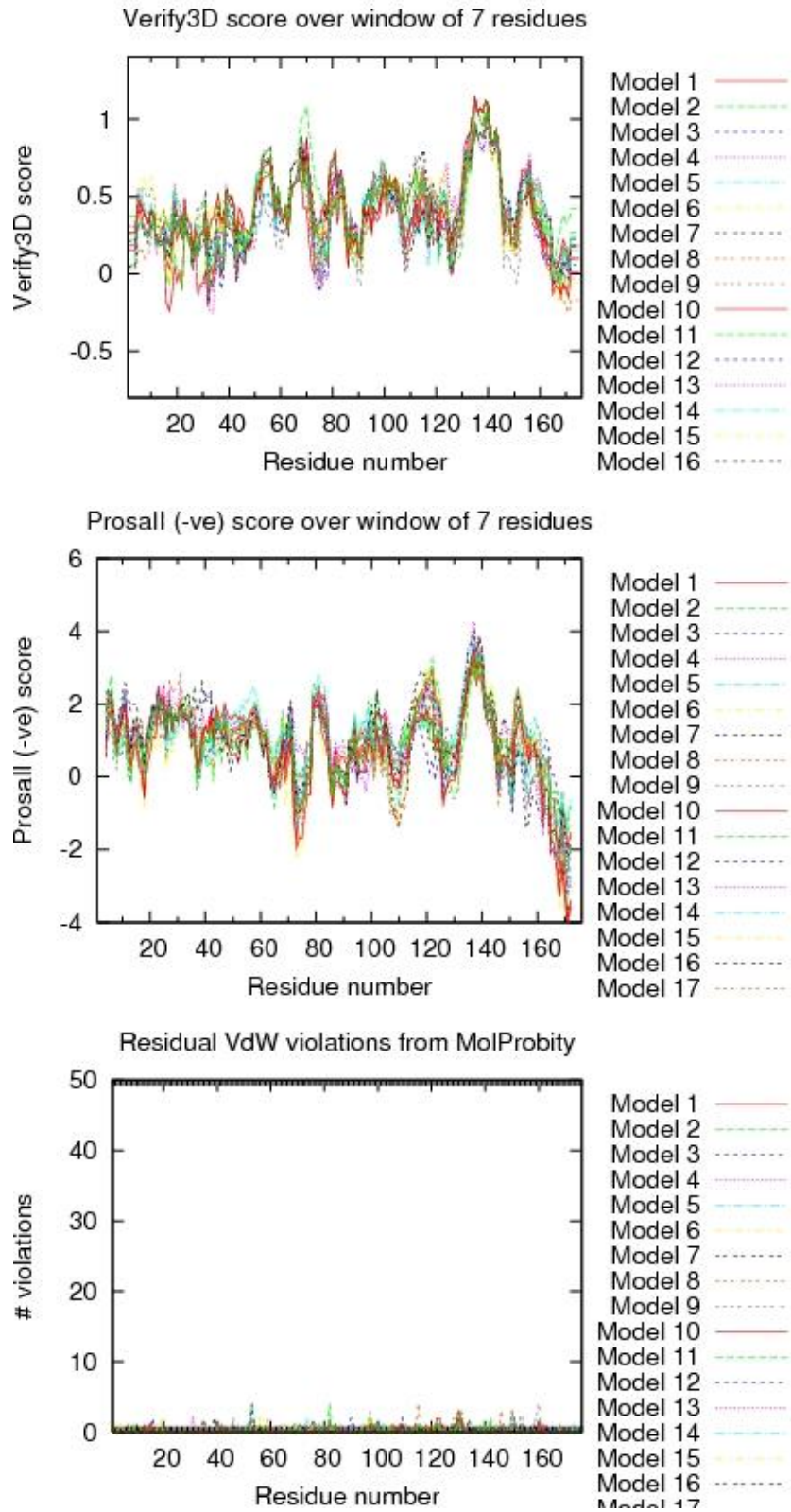


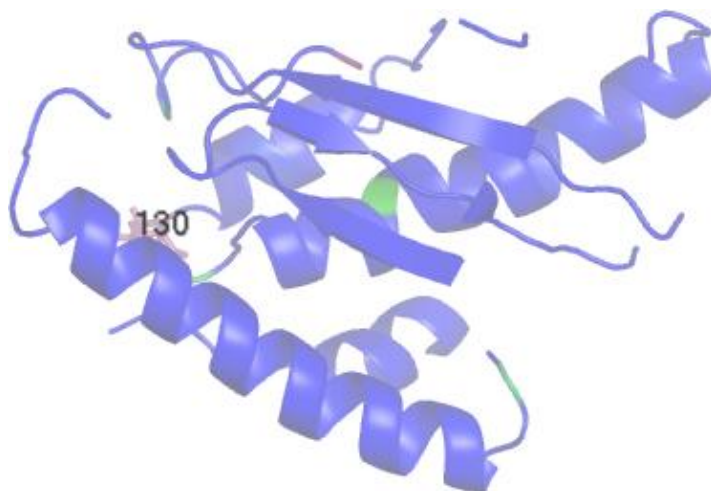
Procheck G-factor for all dihedral angles





Structure Quality Analysis for NAME





Residue Plot of Ramachandran analysis(based on data from Richardson Lab's 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
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 A 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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13. Koradi, R, et al, "MOLMOL: a program for display and analysis of macromolecular structures ", J Mol Graphics 14 (1996): 51-55.
14. Güntert, P, Mumenthaler, C & Wüthrich, K "Torsion angle dynamics for NMR structure calculation with the new program DYANA", J. Mol. Biol 273 (1997): 283-298
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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
pnmtjpeg	year 2000