



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.): 142

Organism:

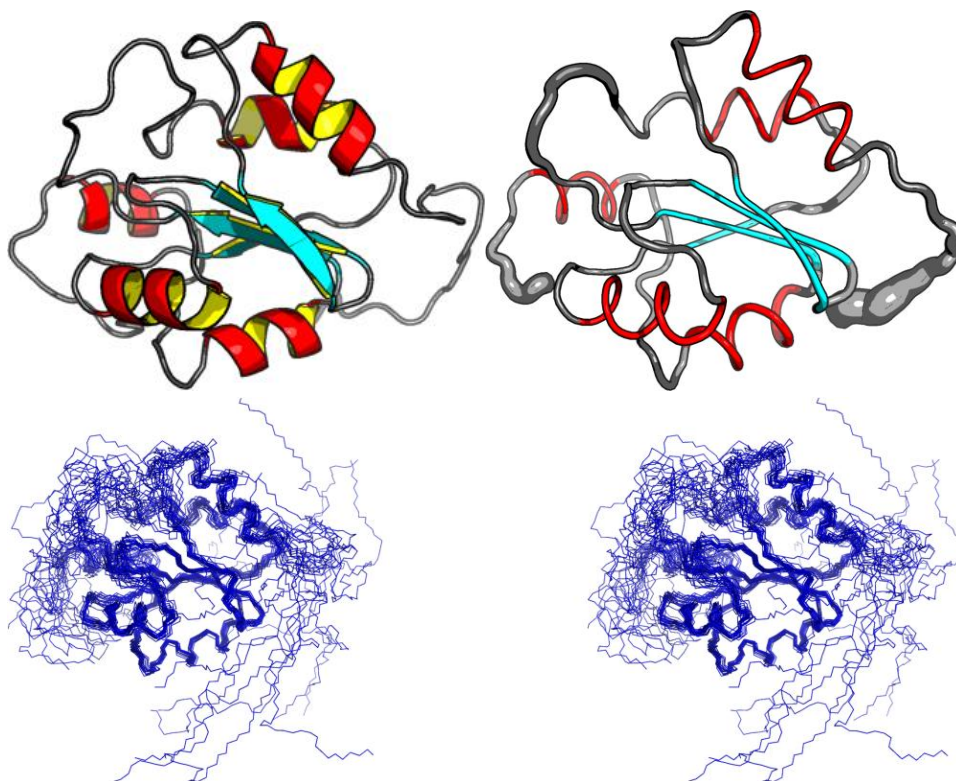
SwissProt /

TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular weight: 16126



Secondary Structure Elements:

alpha helices: 9A-16A, 27A-34A, 58A-62A, 78A-87A, 115A-123A

beta strands: 20N-21N, 72L-74L, 37Y-40Y, 95R-99R, 102S-106S

Total number of restricting constraints per restrained residue: 16.1

Restricting long range constraints per restrained residue: 3.8

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

13.15 11.65 2.45

Dihedral angle violations per model

1 - 10 ° > 10 °

1.55 0.9



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FIDs deposited in the BMRB? no

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	5.4 Å	0.7 Å	0.7 Å
All heavy atoms	6.1 Å	1.0 Å	1.0 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
94.9%	5.0%	0.1%	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
99.6%	0.4%	0%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbity Clashscore
-Raw score	0.41	0.52	0.16	0.21	7.29
Z-score ¹	-0.80	-0.54	0.94	1.24	0.27

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):	2
RMS deviation for bond angles:	0.7 °
RMS deviation for bond lengths:	0.010 Å

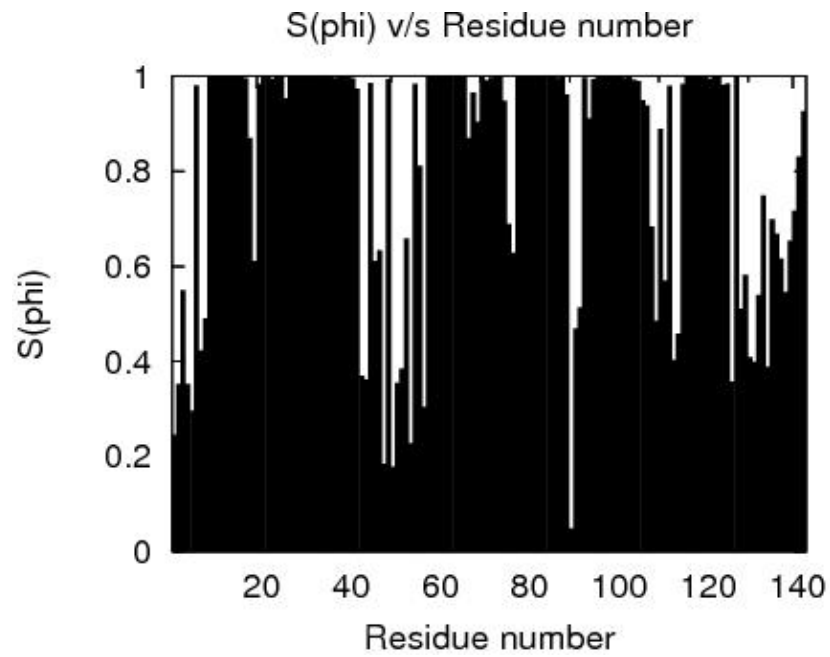
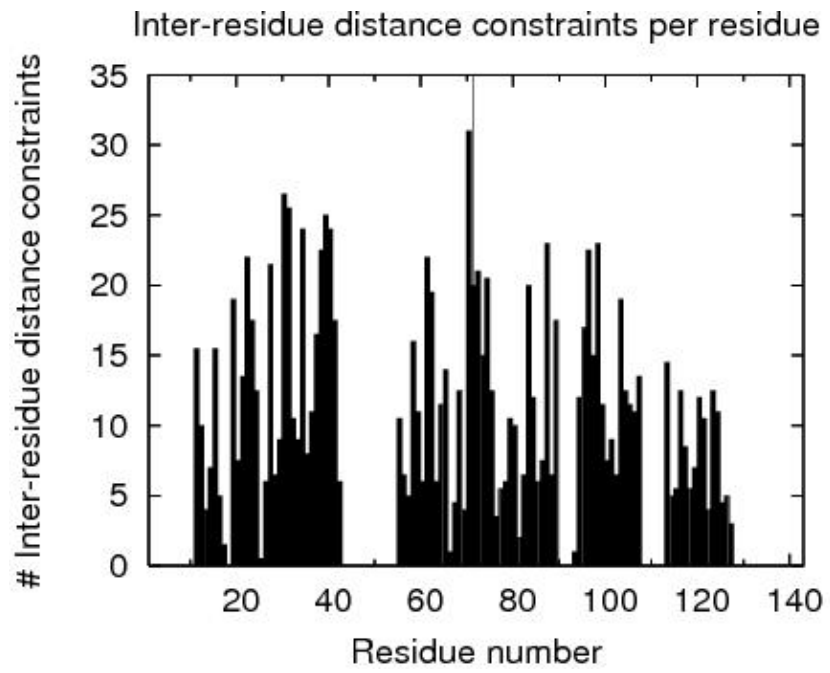
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 9A-17A,20A-41A,58A-74A,78A-88A,93A-106A,115A-125A

³Selected residues: 9A-17A,20A-41A,58A-74A,78A-88A,93A-106A,115A-125A

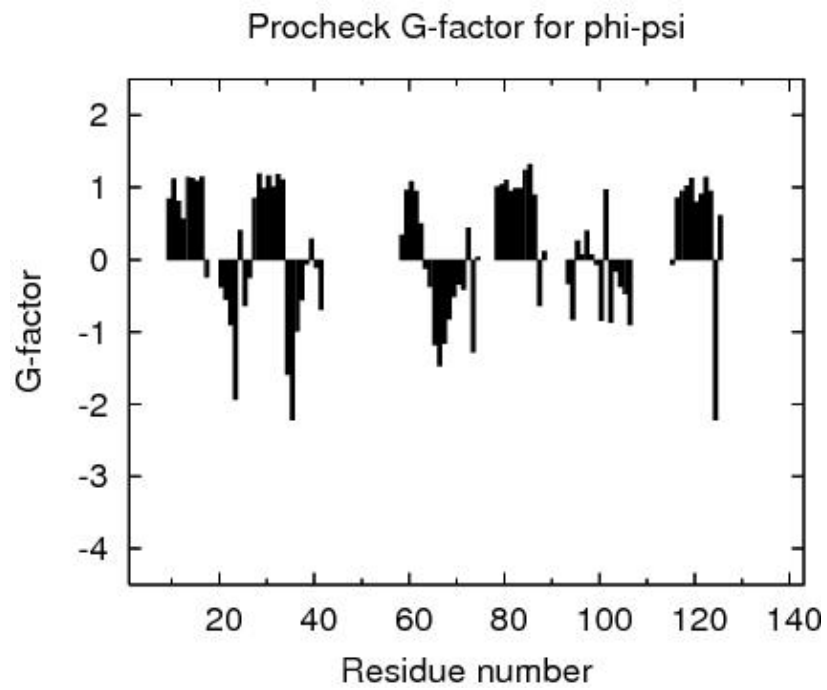
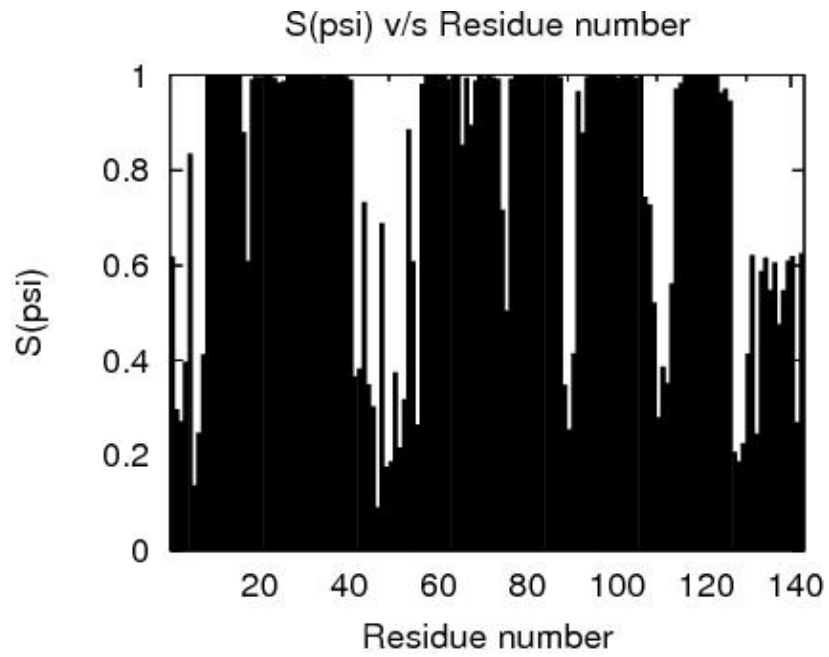


Structure Quality Analysis for NAME





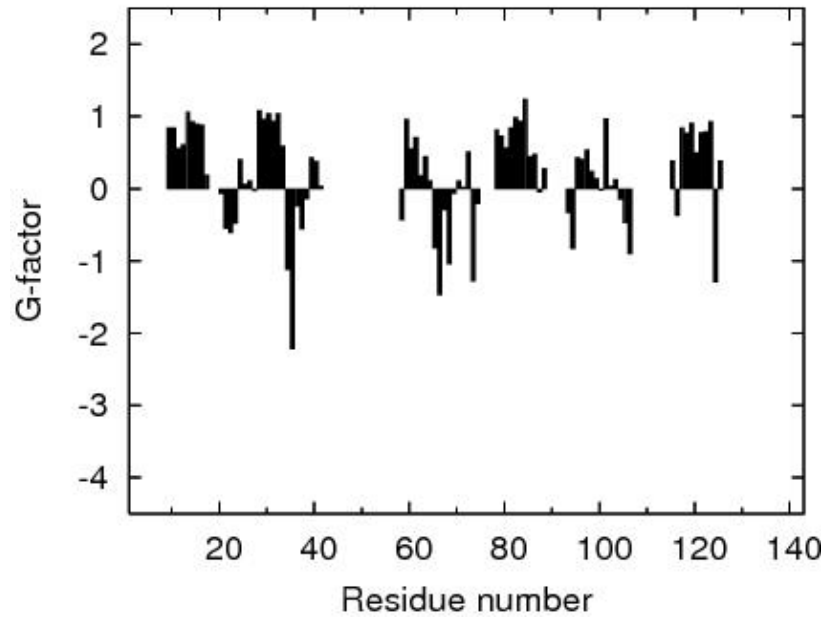
Structure Quality Analysis for NAME



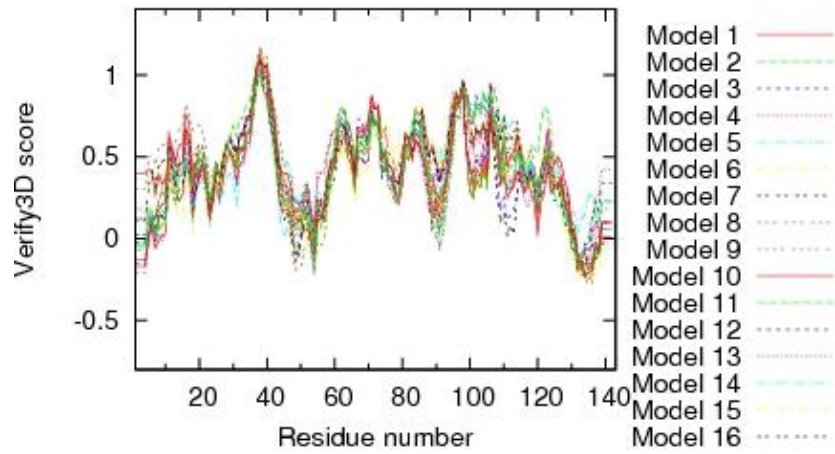


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Procheck G-factor for all dihedral angles

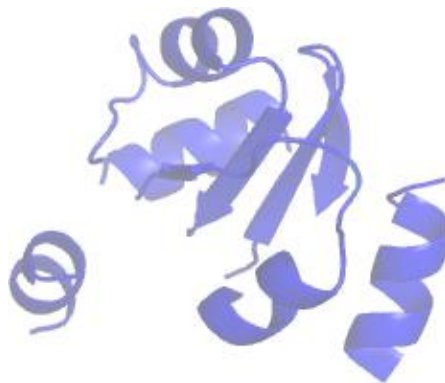
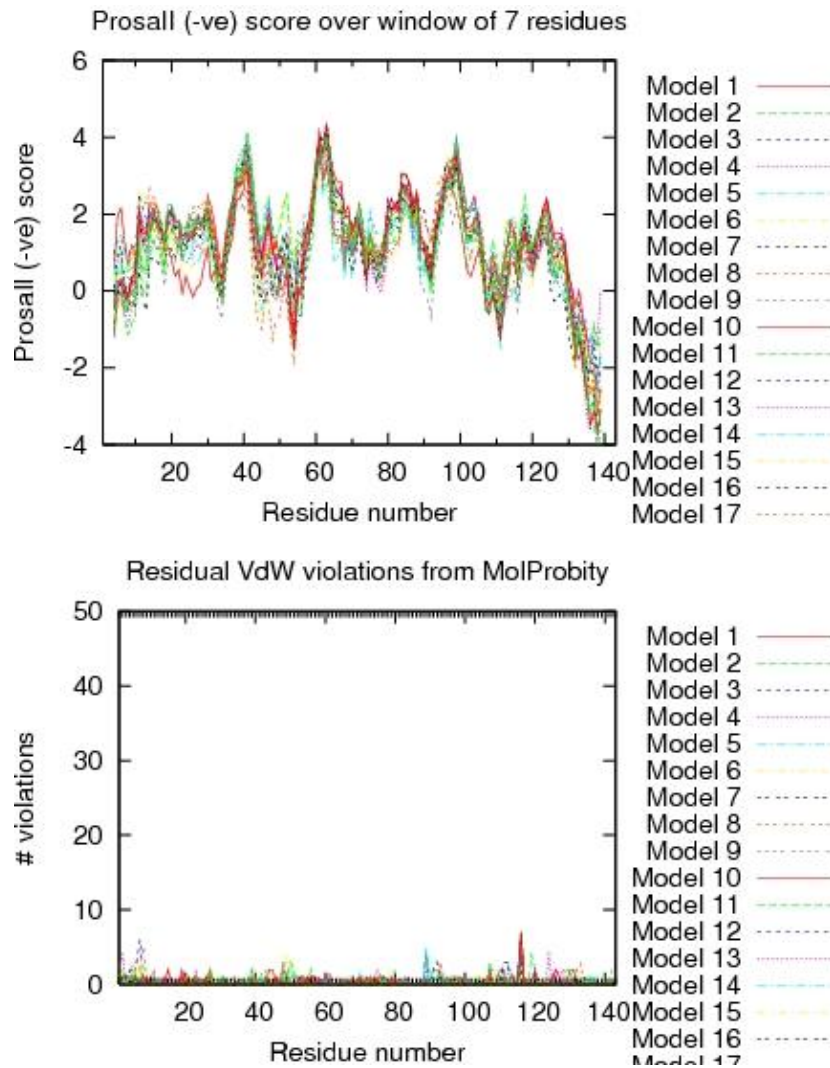


Verify3D score over window of 7 residues





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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 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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7. Word J M et al, "Exploring steric constraints on protein mutations using MAGE / PROBE", *Prot Sci* 9 (2000): 2251-2259
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12. Richardson D C, Richardson J S, "The kinemage: a tool for scientific communication", *Prot Sci* 1(1) (1992): 3-9
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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16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features", *Biopolymers* (1983) 22: 2577-2637
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
jpegtopnm	year 2000
pnmcrop	year 2000
pnmtojpeg	year 2000