



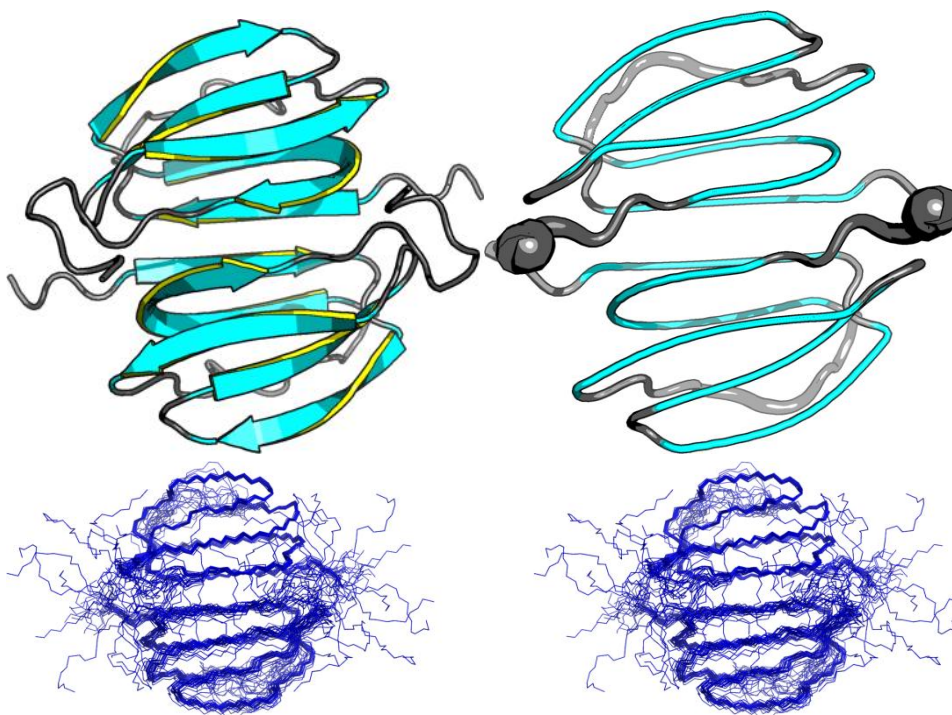
Structure Quality Analysis for NAME

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.): 142
Organism:
SwissProt /
TrEMBL ID:
models: 20
Oligomerization: dimer
Molecular
weight: 15958



Secondary Structure Elements:

Inter-chain break(s) between 71 & 82

alpha helices:

beta strands: 5N-10N, 50N-61N, 30Y-41Y, 22U-27U, 12L-19L, 5N-10N, 50N-61N, 30Y-41Y, 22U-27U, 12L-19L

Total number of restricting constraints per restrained residue: 31.8

Restricting long range constraints per restrained residue: 13.4

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

4.9 0.6 0.5

Dihedral angle violations per model

1 - 10 ° > 10 °

3 2.4



Structure Quality Analysis for NAME

FIDs deposited in the BMRB? no

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	2.9 Å	0.4 Å	0.3 Å
All heavy atoms	3.7 Å	0.7 Å	0.6 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
86.7%	13.3%	0.0%	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
98.9%	1.1%	0%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbity Clashscore
-Raw score	0.34	0.34	-0.60	-0.17	5.75
Z-score ¹	-1.93	-1.28	-2.05	-1.01	0.54

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:	0.6 °
RMS deviation for bond lengths:	0.009 Å

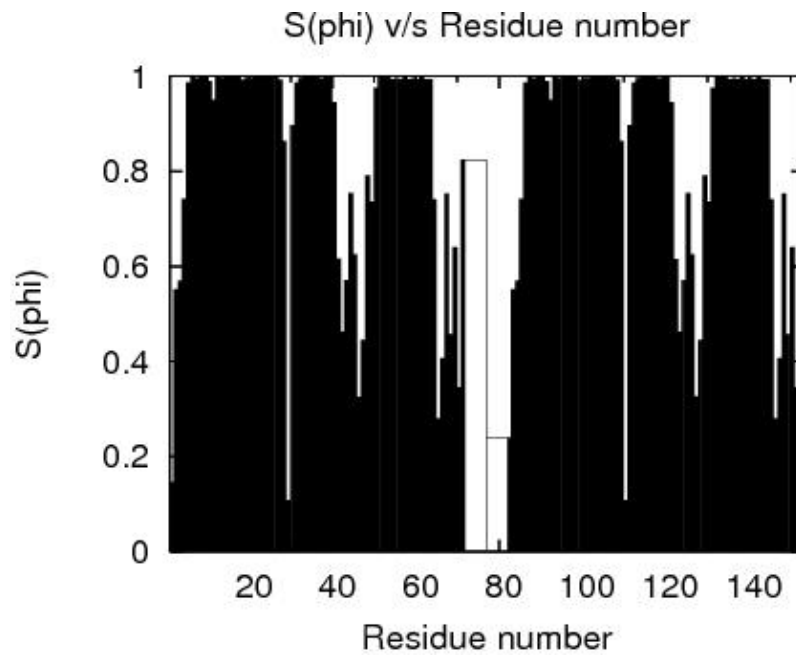
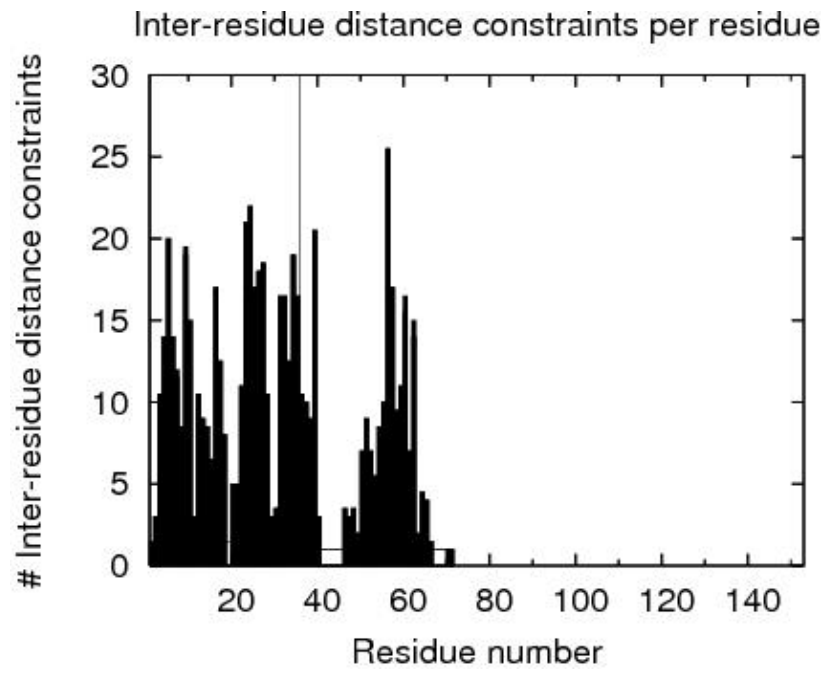
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 5A-27A,30A-40A,50A-62A,5B-27B,30B-40B,50B-62B

³Selected residues: 5A-27A,30A-40A,50A-62A

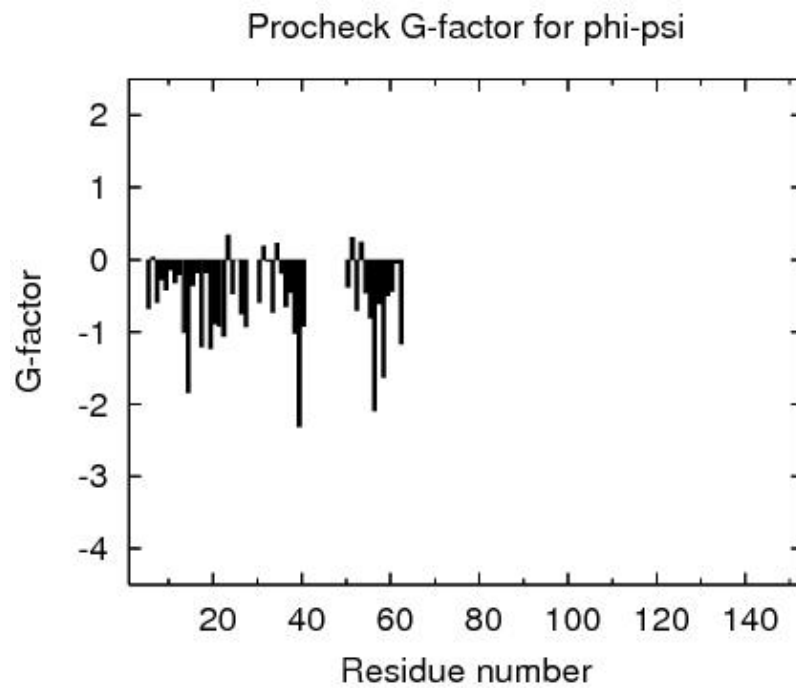
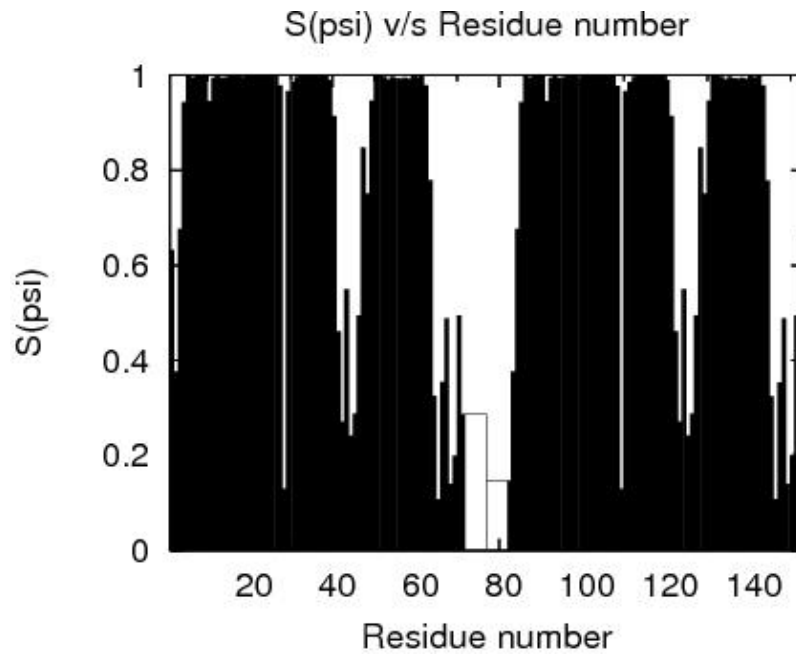


Structure Quality Analysis for NAME





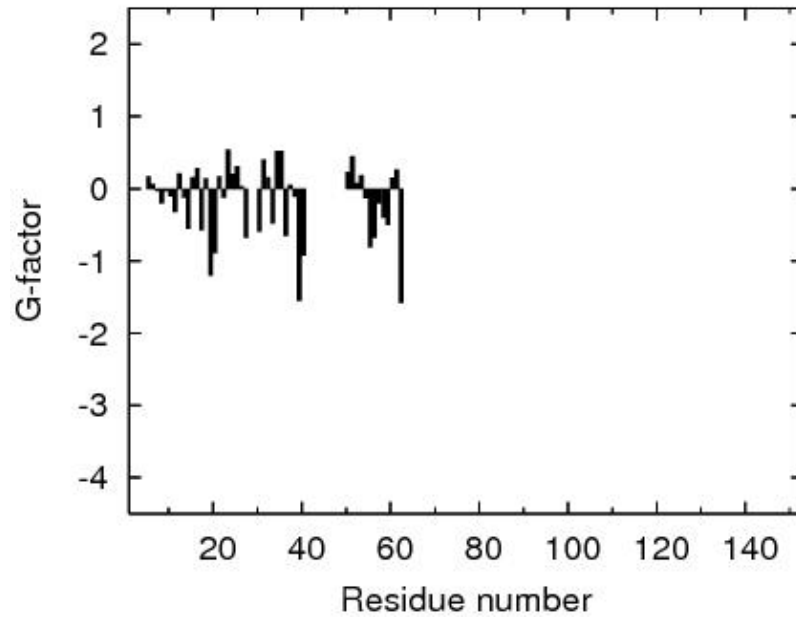
Structure Quality Analysis for NAME



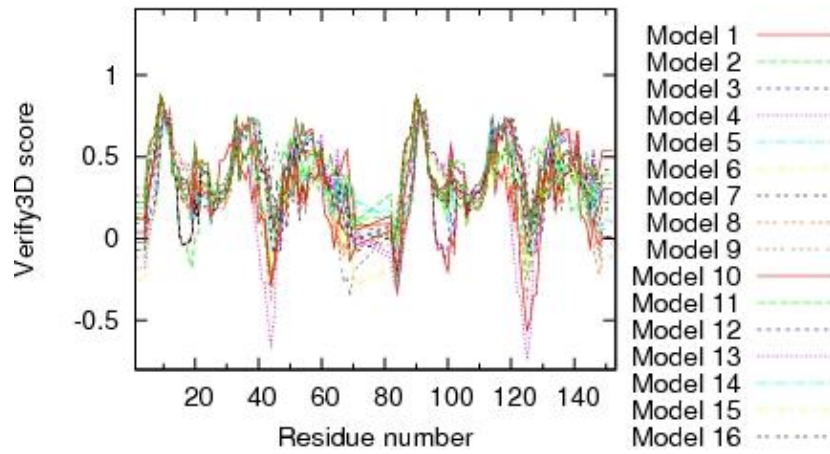


Structure Quality Analysis for NAME

Procheck G-factor for all dihedral angles

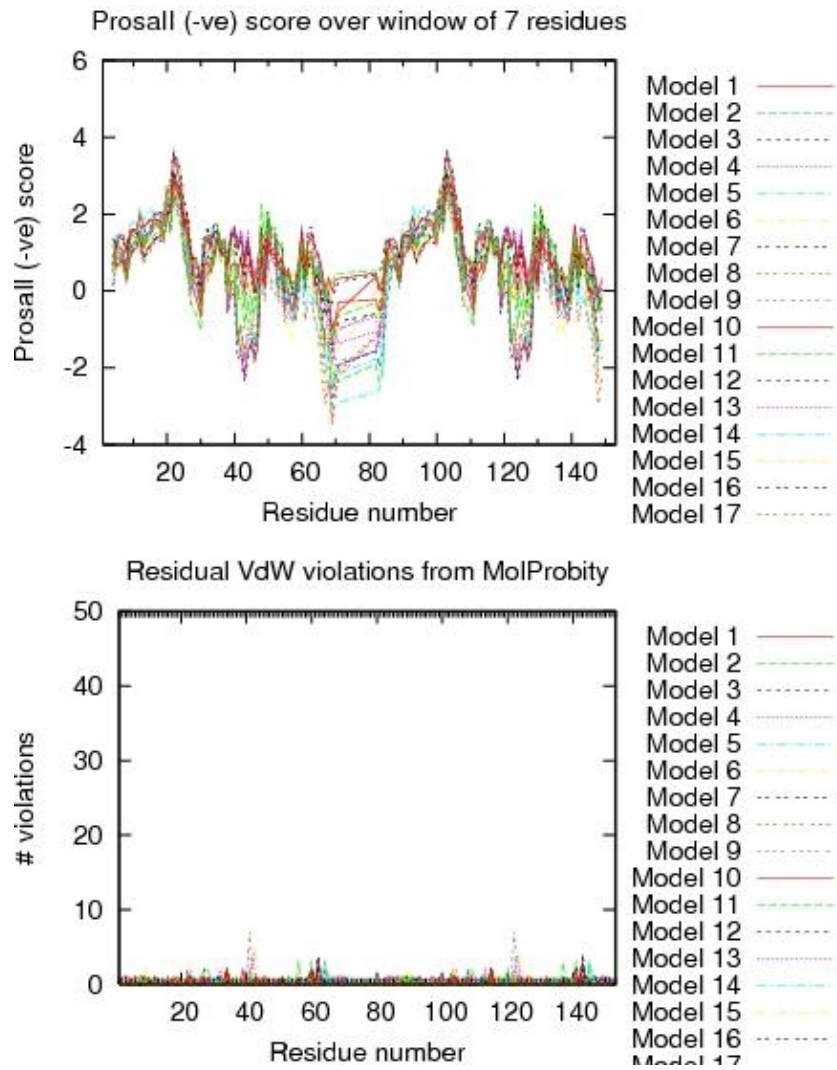


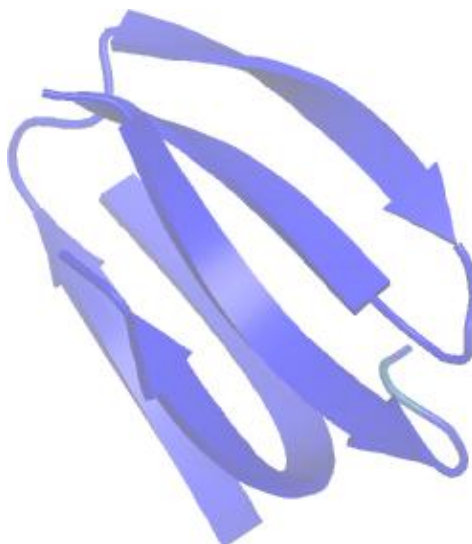
Verify3D score over window of 7 residues





Structure Quality Analysis for NAME





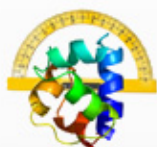
Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobity)

References:

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3. Sippl M J, "Recognition of Errors in Three-Dimensional Structures of Proteins", Proteins 17 (1993): 355-362
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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.



Protein Structure Validation Suite (PSVS)



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
pnmtojpeg	year 2000