

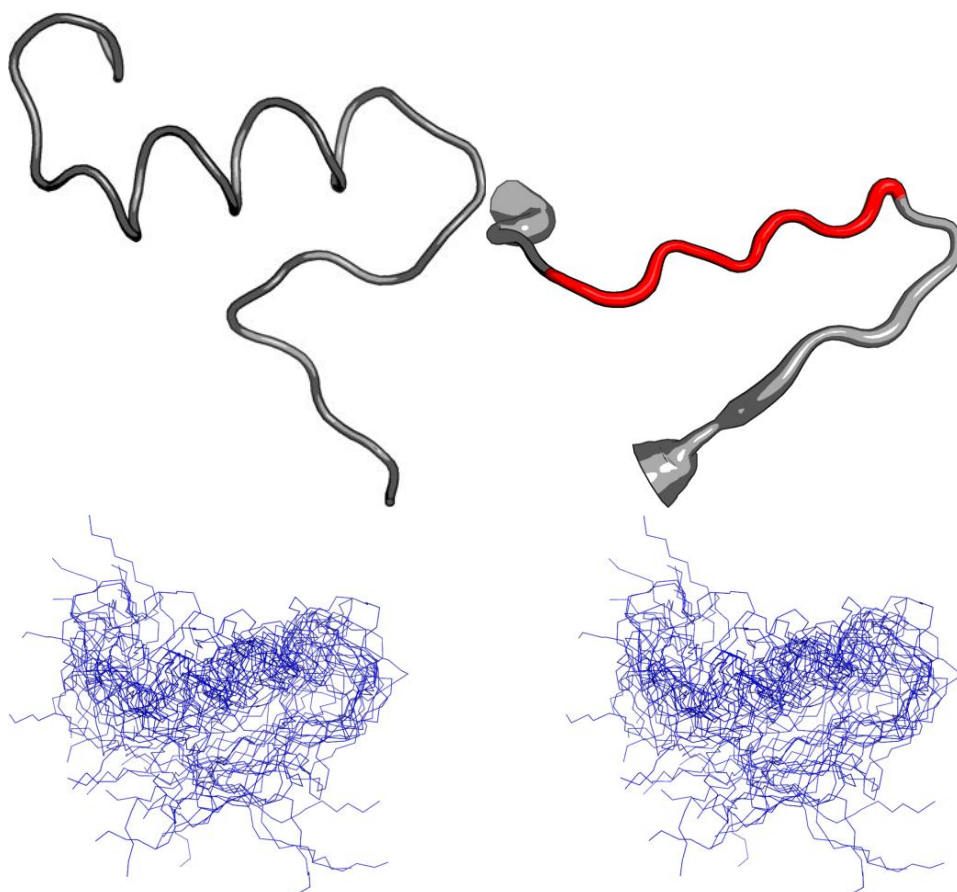


Structure Quality Analysis for NAME

Analyses performed for all residues.

Procheck analysis, RMSD calculation and structure superimposition are based on: all residues

NESG ID: NAME
PDB ID:
Deposition date:
Common Name:
Class:
Length (a.a.): 28
Organism:
SwissProt /
TrEMBL ID:
models: 22
Oligomerization: monomer
Molecular
weight: 3245



Secondary Structure Elements:

alpha helices: 7A-17A

beta strands:

FIDs deposited in the BMRB? no

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	4.0 Å	1.3 Å	4.0 Å
All heavy atoms	5.3 Å	2.5 Å	5.3 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
95.2%	4.8%	0.0%	0.0%

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



Structure Quality Analysis for NAME

Most favoured regions *Allowed regions* *Disallowed regions* [View plot](#) [View model summary](#)

99.5% 0.5% 0%

Global quality scores

Program *Verify3D* *ProsaII (-ve)* *Procheck (phi-psi)³* *Procheck (all)³* *MolProbity Clashscore*

-Raw score 0.24 0.60 0.13 0.29 3.01

Z-score¹ -3.53 -0.21 0.83 1.71 1.01

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): 0

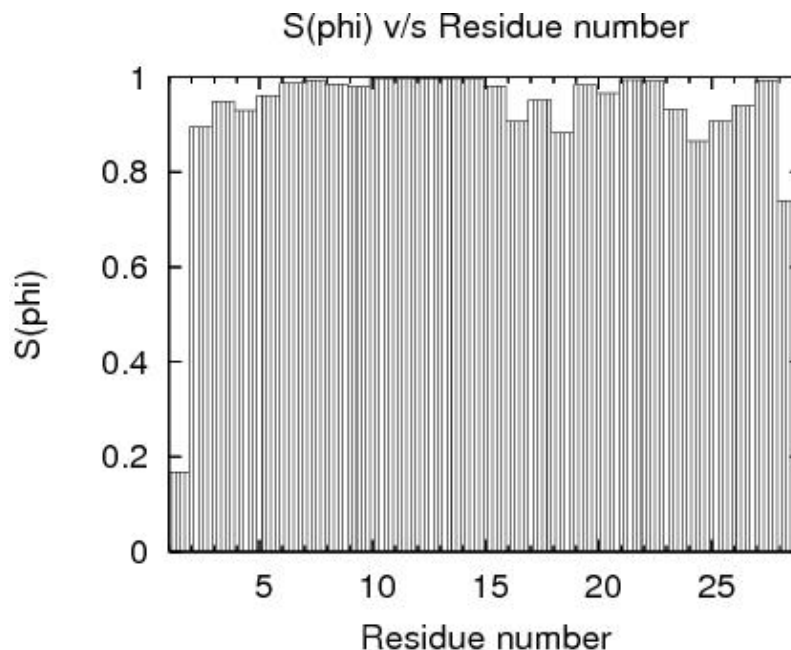
RMS deviation for bond angles: 0.7 °

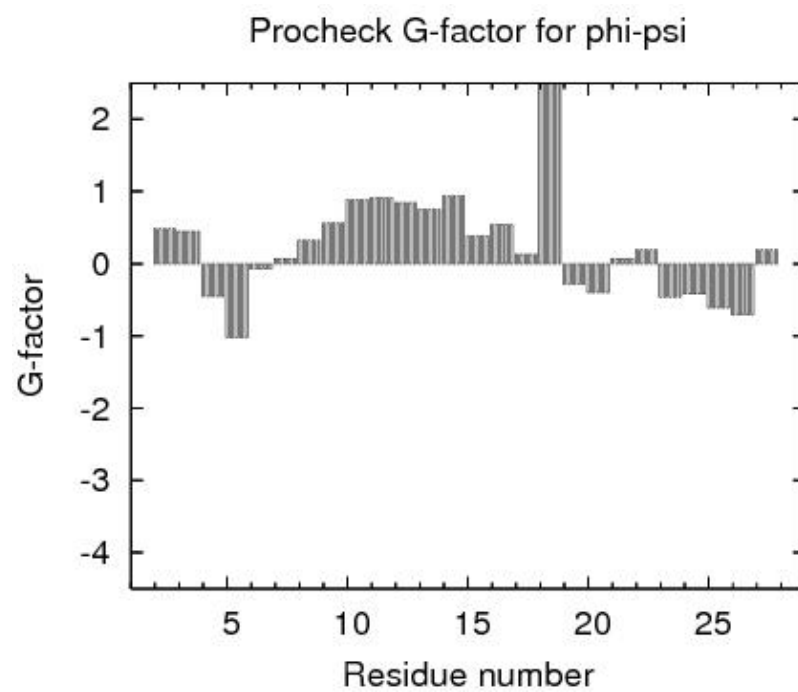
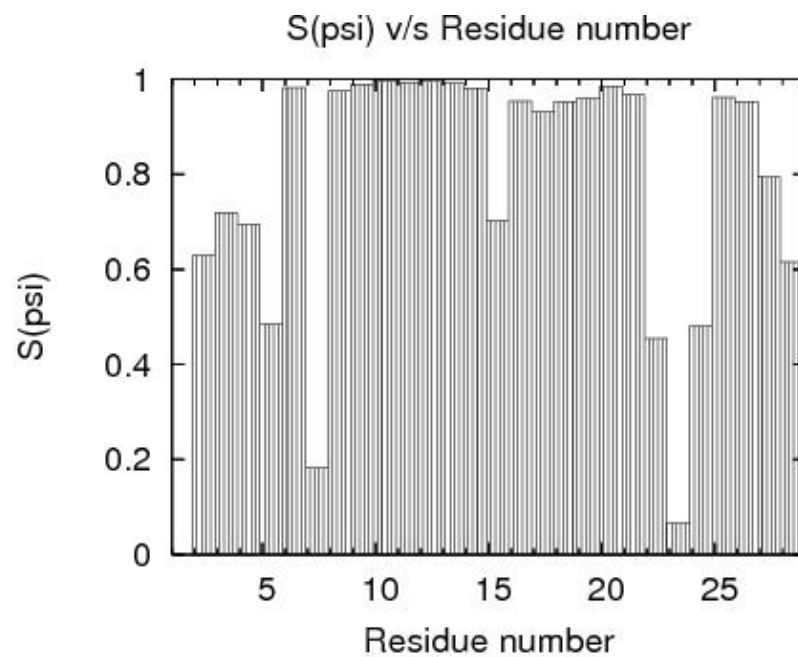
RMS deviation for bond lengths: 0.017 Å

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: HASH(0xd7f3c0)

³Selected residues: all

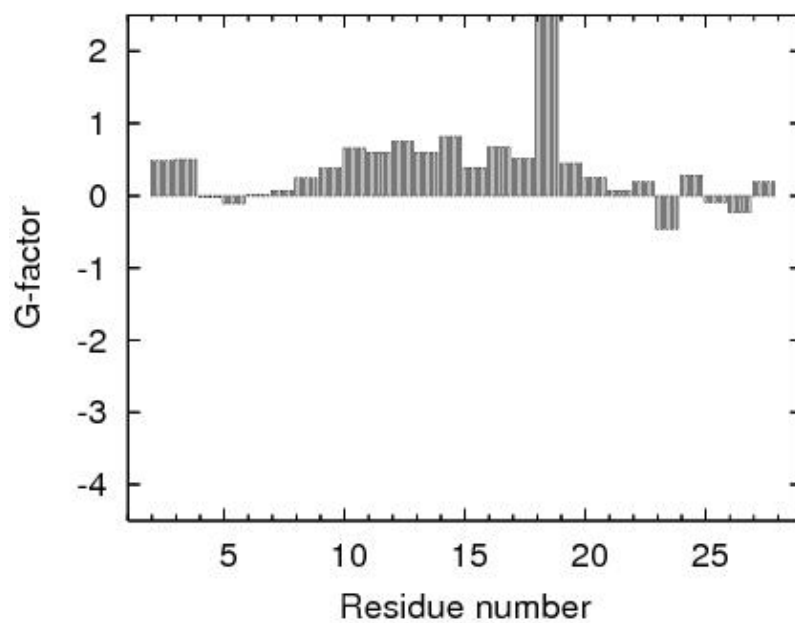




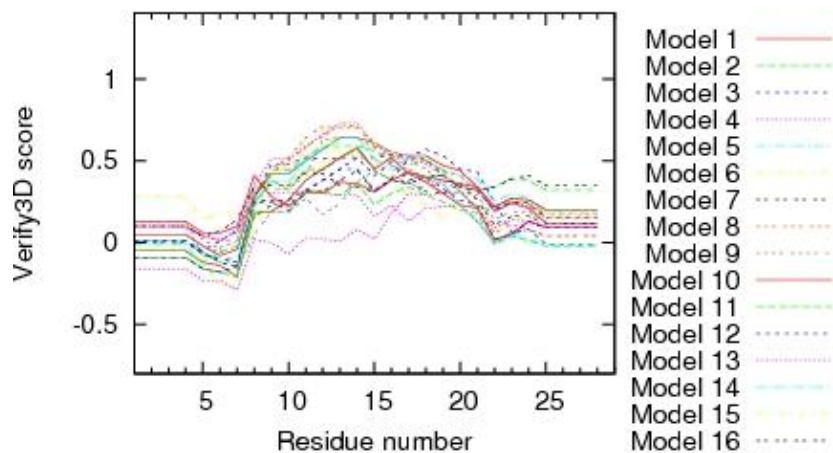


Structure Quality Analysis for NAME

Procheck G-factor for all dihedral angles

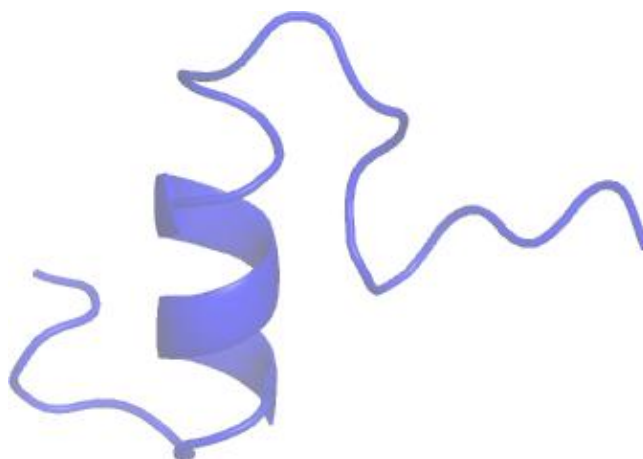
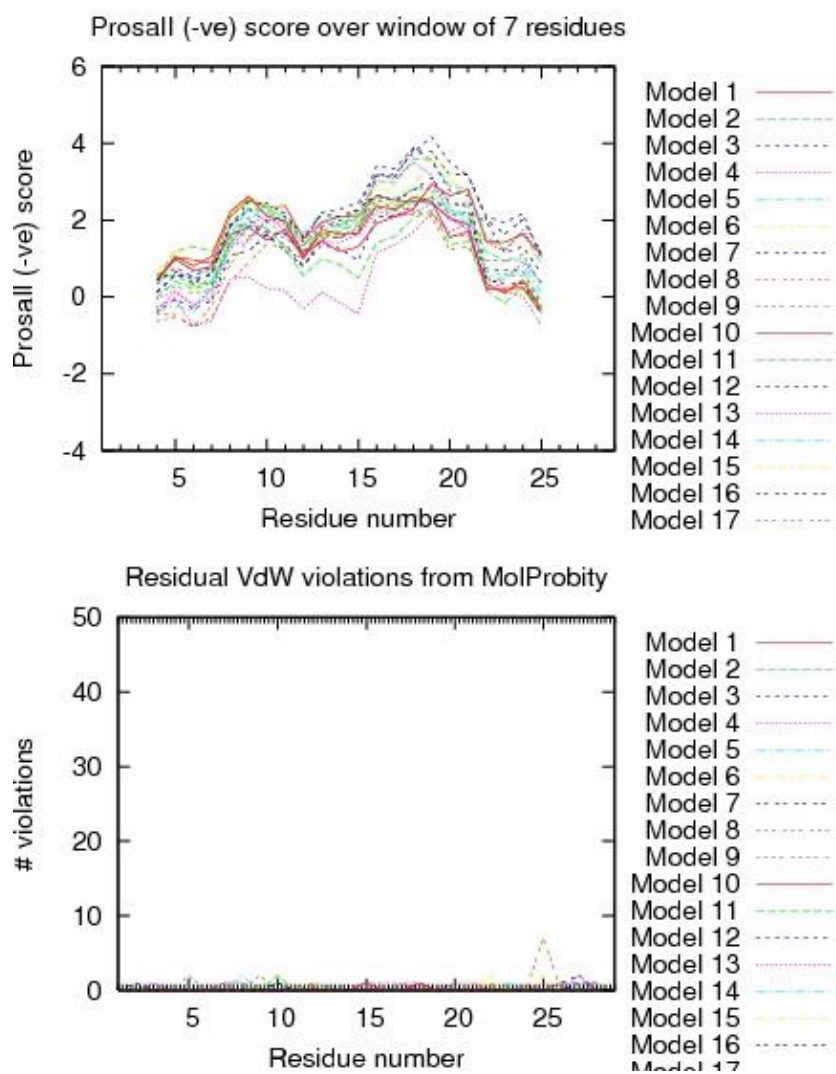


Verify3D score over window of 7 residues





Structure Quality Analysis for NAME

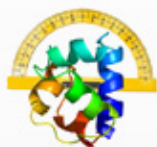


Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobity)



References:

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Protein Structure Validation Suite (PSVS)





Software Environment

Software for structure quality evaluation:

DSSP	DsspCMBI-April-2000
pdbstat	PdbStat-5.9 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