



Structure Quality Analysis for NAME

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.): 94

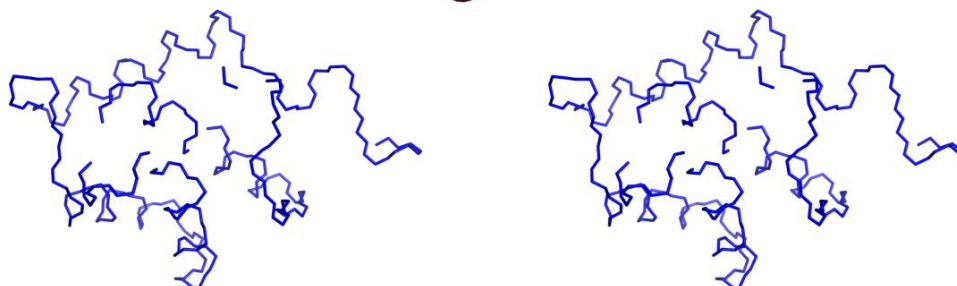
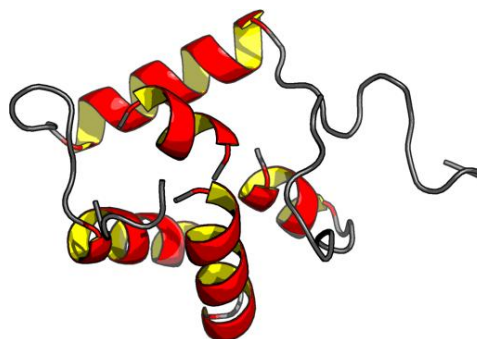
Organism:

SwissProt /

TrEMBL ID:

Oligomerization: monomer

Molecular weight: 10451



Secondary Structure Elements:

alpha helices: 19A-31A, 41A-48A, 55A-65A, 75A-89A

beta strands: 39E-40E, 72G-73G

Resolution: 1.450 Å R-factor: 0.160 R-free: 0.176

Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

<i>Most favoured regions</i>	<i>Additionally allowed regions</i>	<i>Generously allowed regions</i>	<i>Disallowed regions</i>
95.8%	4.2%	0.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobability

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	View plot	View model summary
100%	0%	0%		

Global quality scores

Program	<i>Verify3D</i>	<i>ProsaII (-ve)</i>	<i>Procheck (phi-psi)</i>	<i>Procheck (all)</i>	<i>MolProbability</i>	<i>Clashscore</i>
-Raw score	0.44	0.50	0.43	0.31	4.10	
Z-score ¹	-0.32	-0.62	2.01	1.83	0.82	

Close Contacts and Deviations from Ideal Geometry (from PDB validation software)



Structure Quality Analysis for NAME

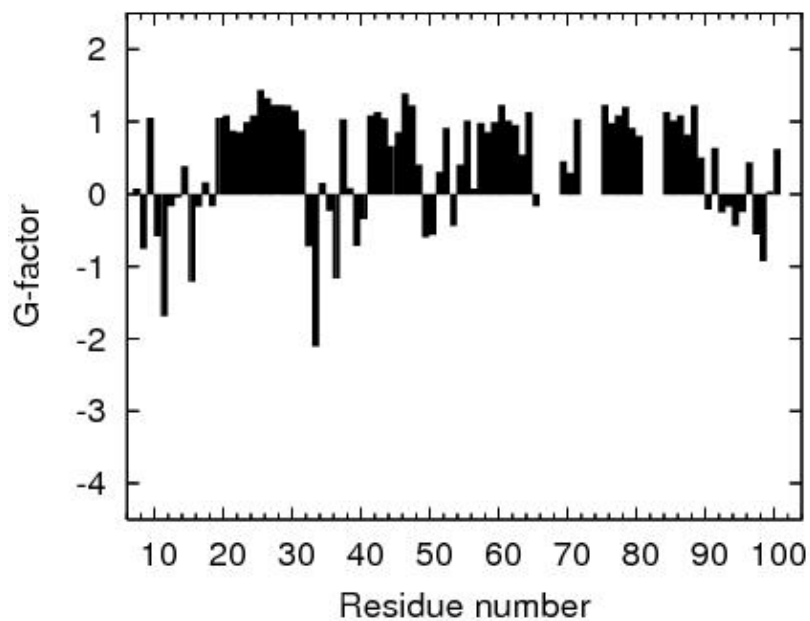
Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 0.8 °

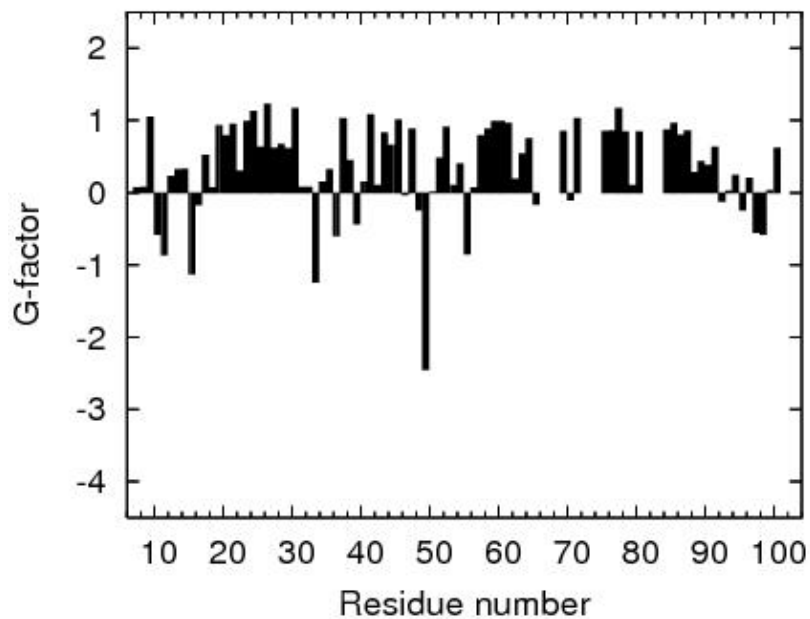
RMS deviation for bond lengths: 0.005 Å

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

Procheck G-factor for phi-psi

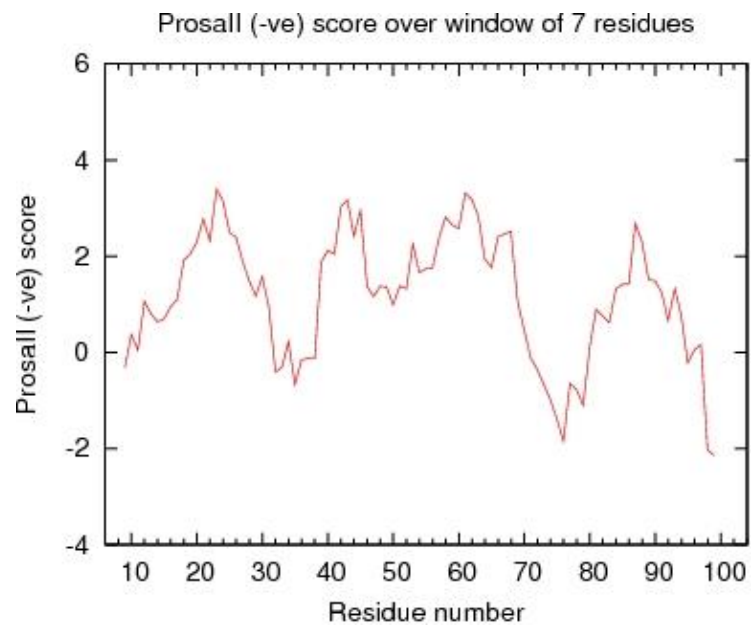
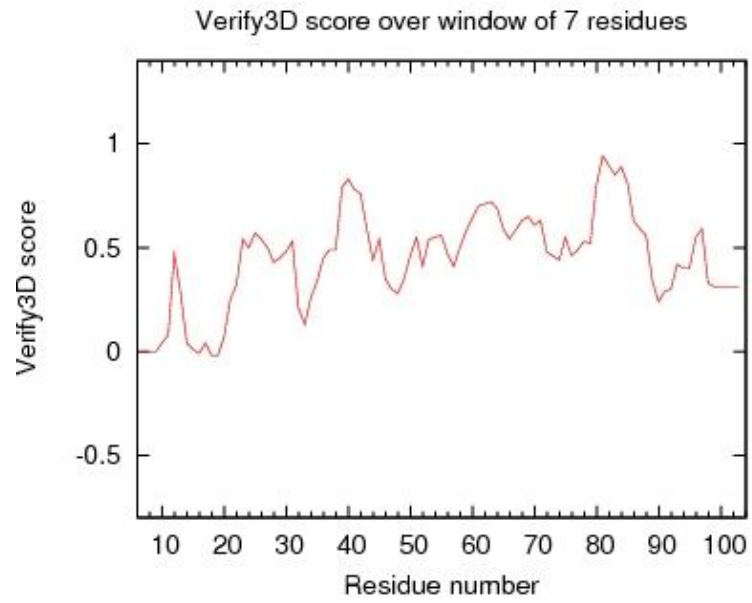


Procheck G-factor for all dihedral angles



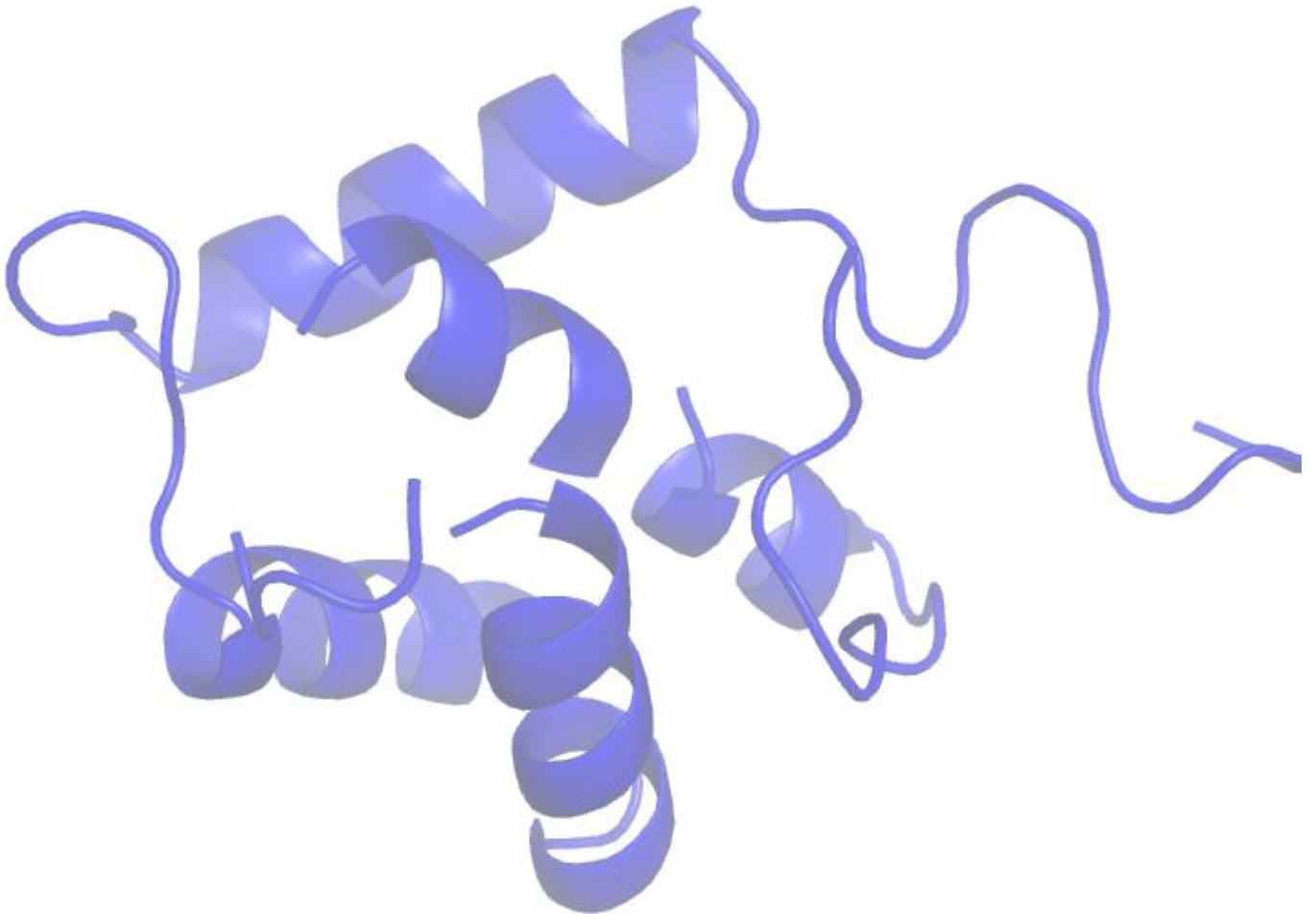
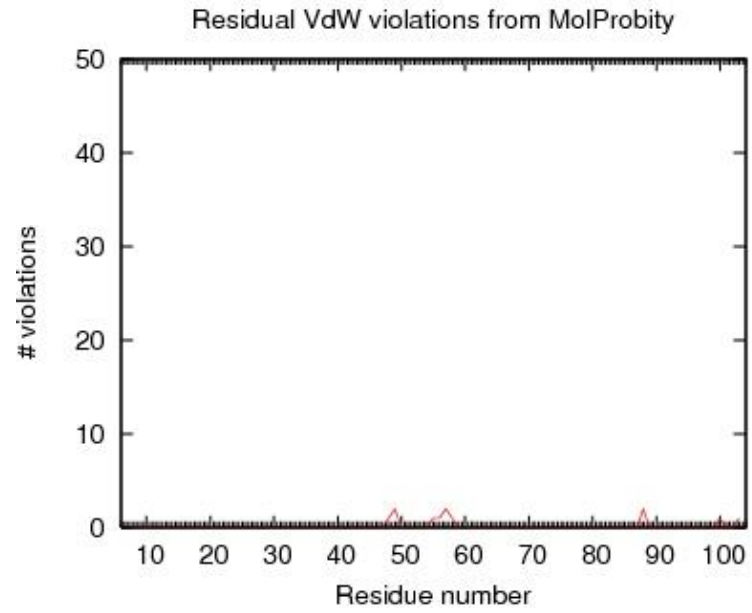


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Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobity)

References:

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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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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
pnmtojpeg	year 2000