



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.): 66

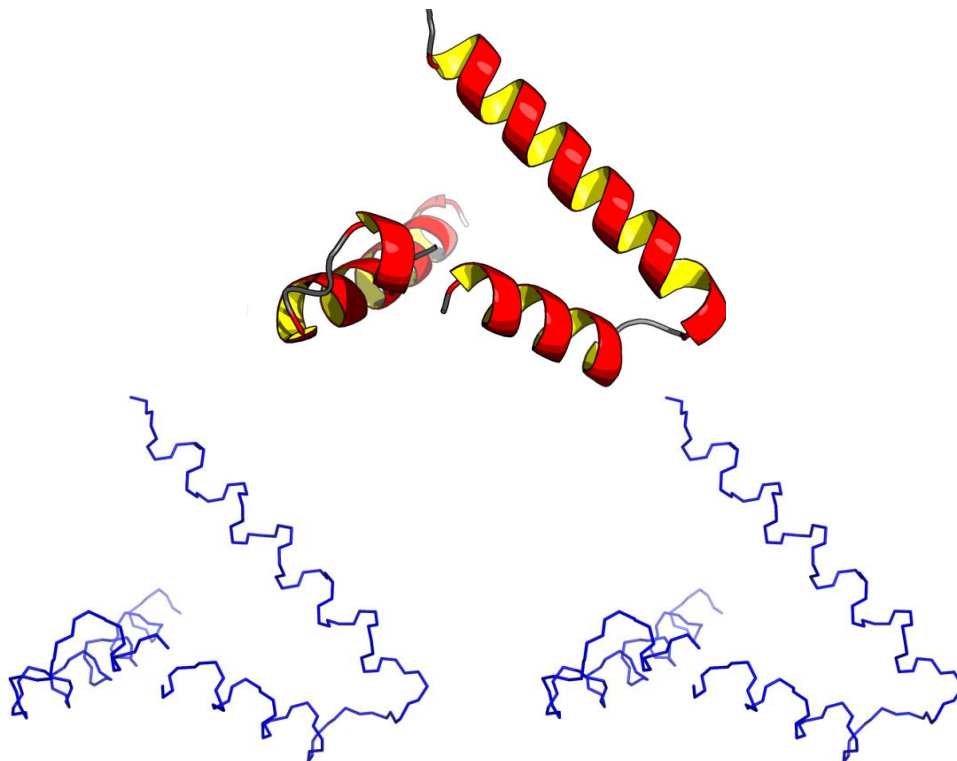
Organism:

SwissProt /

TrEMBL ID:

Oligomerization: monomer

Molecular weight: 7154



Secondary Structure Elements:

alpha helices: 9A-26A, 30A-48A, 51A-72A

beta strands:

Resolution: 2.300 Å R-factor: 0.223 R-free: 0.232

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>
94.9%	5.1%	0.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobit

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	View plot	View model summary
96.9%	3.1%	0%		

Global quality scores

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



Structure Quality Analysis for NAME

-Raw score 0.16 -0.02 0.56 0.34 14.07
Z-score¹ -4.82 -2.77 2.52 2.01 -0.89

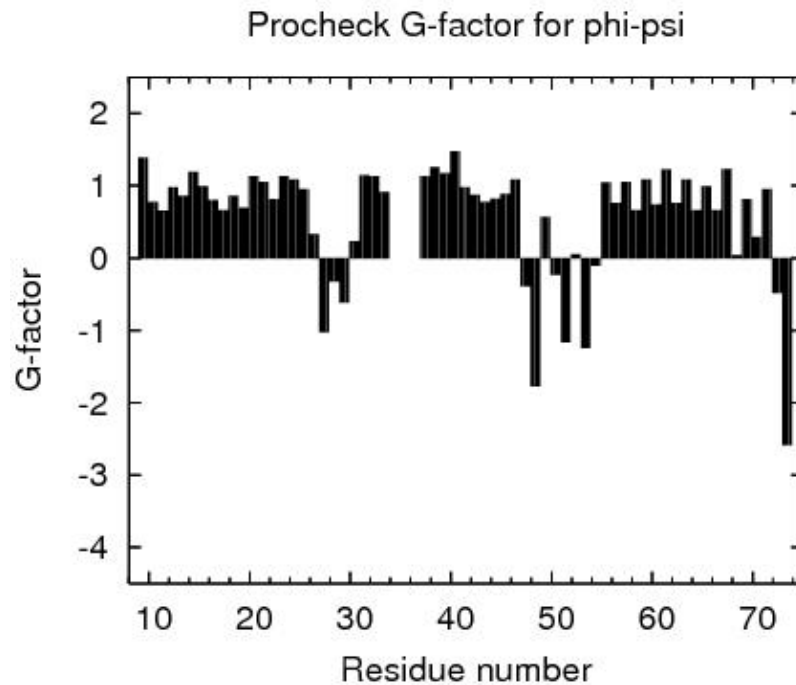
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.0 °

RMS deviation for bond lengths: 0.005 Å

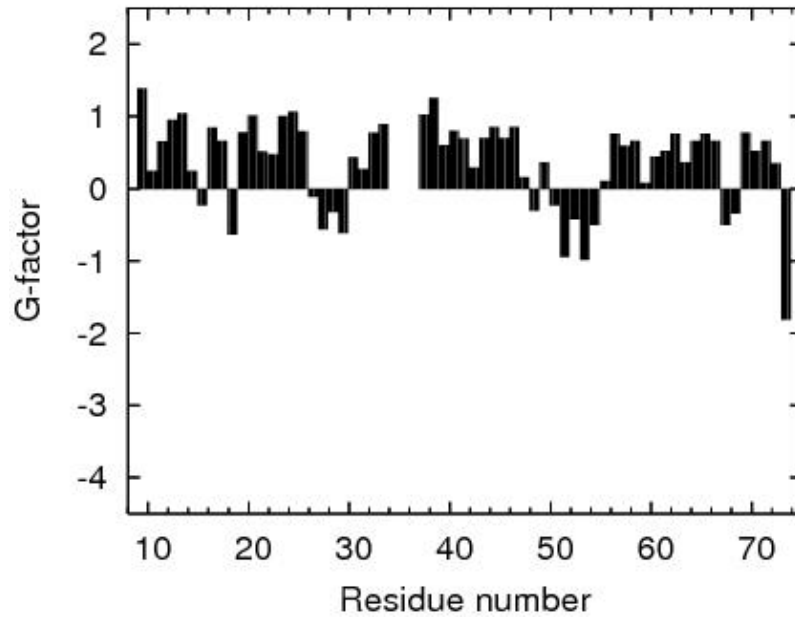
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score



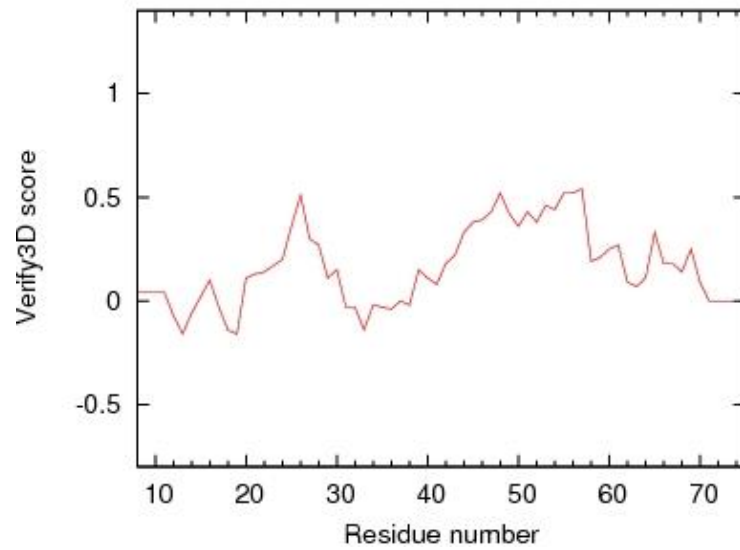


Structure Quality Analysis for NAME

Procheck G-factor for all dihedral angles

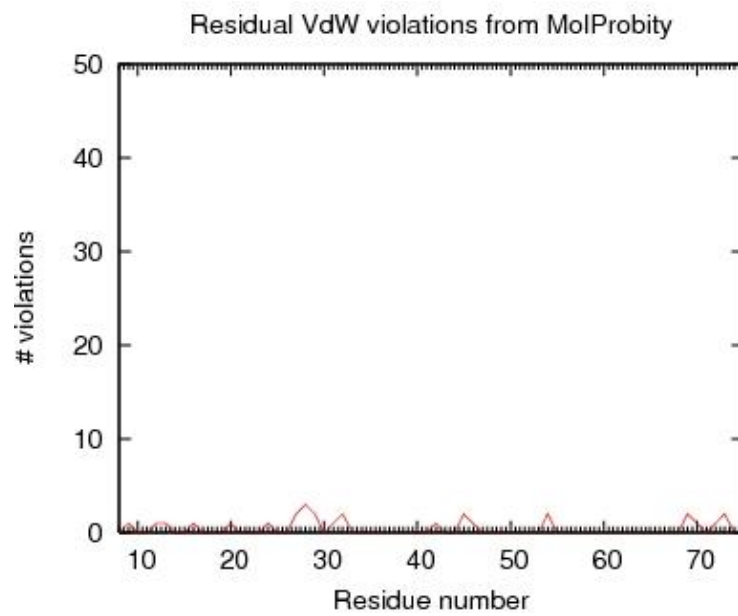
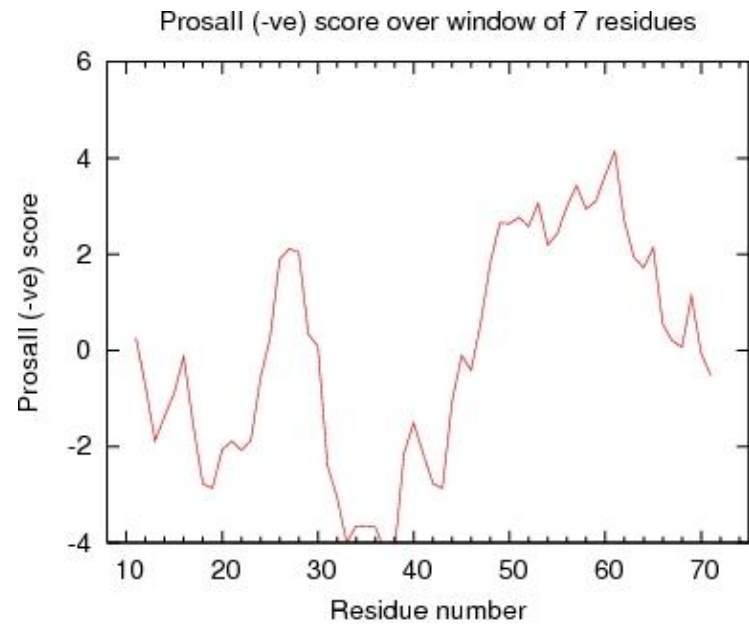


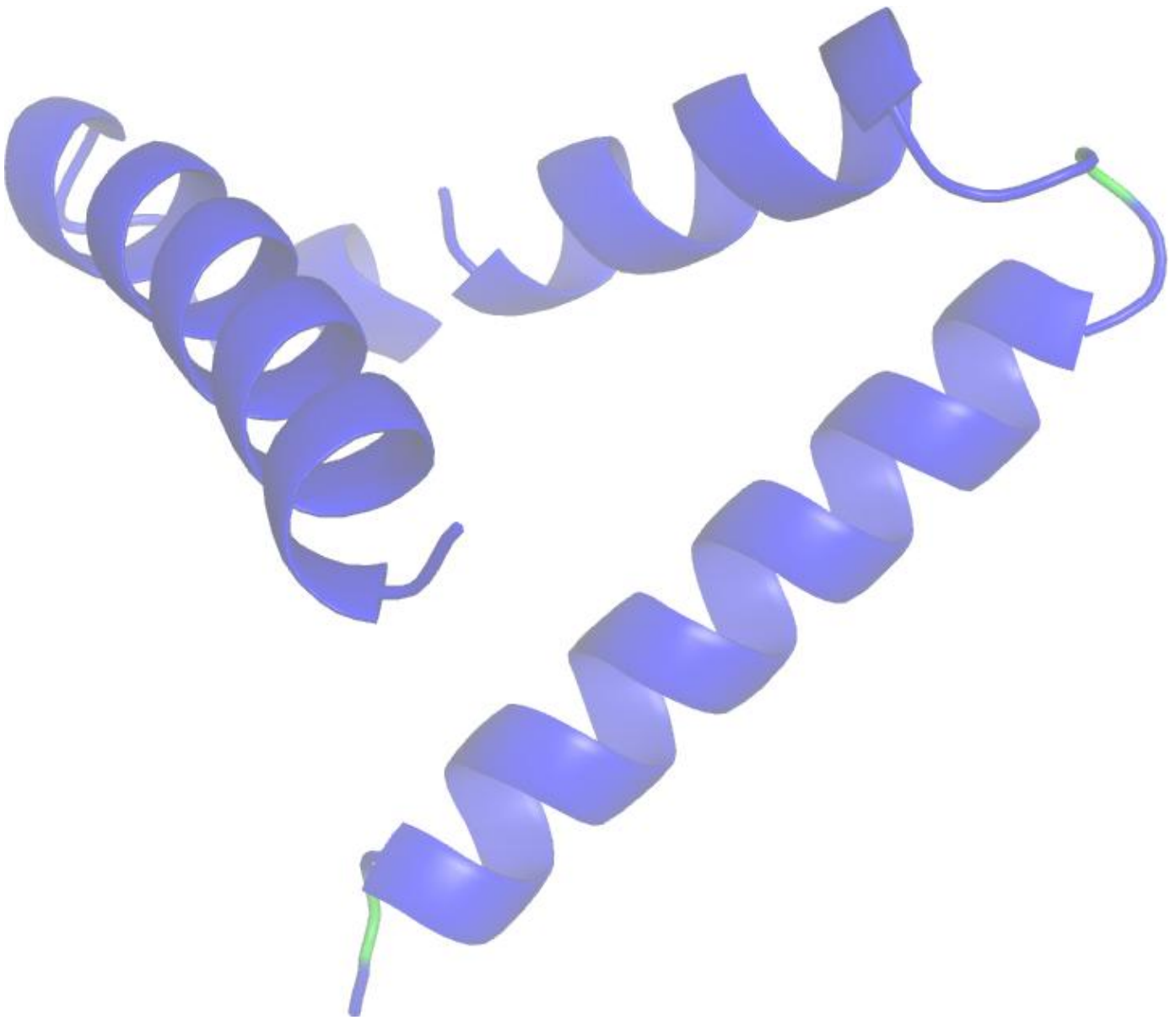
Verify3D score over window of 7 residues





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

References:

1. Luthy R, Bowie J U and Eisenberg D, "Assessment of protein models with three-dimensional profiles", Nature 356 (1992): 83-85
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 Ai et al, "AQUA and PROCHECK_NMR: Programs for checking the quality of proteins



- structures solved by NMR", *J Biomolec NMR* 8 (1996): 477-486
6. Laskowski R A et al "PROCHECK: a program to check the stereochemical quality of protein structures" *J Appl Cryst*, 26 (1993): 283-291
 7. Word J M et al, "Exploring steric constrains on protein mutations using MAGE / PROBE", *Prot Sci* 9 (2000): 2251-2259
 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
 10. Tejero R and Montelione G T, "PDBStat", unpublished
 11. Luthy R, McLachlan A D and Eisenberg D, "Secondary Structure-Based Profiles: Use of Structure-Conserving Scoring Tables in Searching Protein Sequence Databases for Structural Similarities", *Proteins* 10 (1991): 229-239
 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
 15. Lovell S C et al, "Structure validation by Calpha geometry: phi,psi and Cbeta deviation" *Proteins* (2003) 50: 437-450
 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-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

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