



# 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.): 114

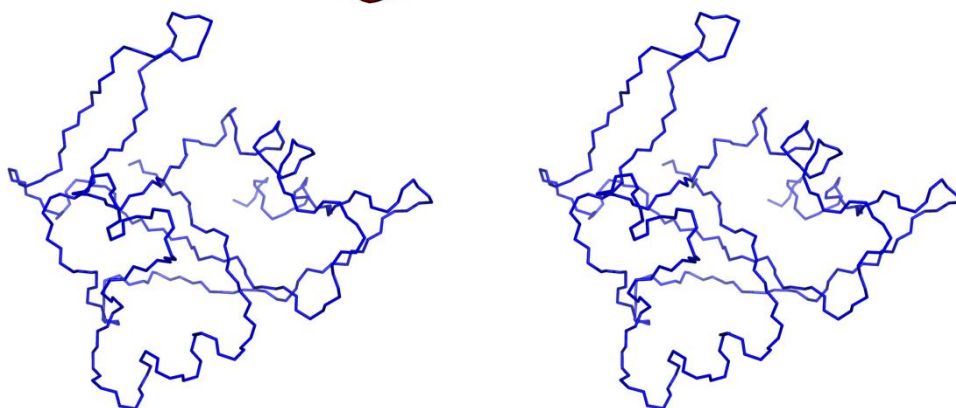
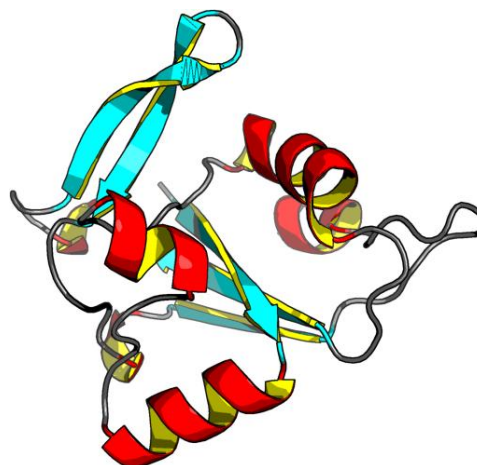
Organism:

SwissProt /

TrEMBL ID:

Oligomerization: monomer

Molecular weight: 12426



Secondary Structure Elements:

alpha helices: 10A-19A, 26A-31A, 39A-49A, 110A-114A

beta strands: 37R-38R, 3U-9U, 56U-62U, 93L-98L, 21G-22G, 88U-89U, 34E-35E, 80G-84G, 70U-74U

Resolution: 1.800 Å R-factor: 0.222 R-free: 0.252

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>
92.9%	6.1%	1.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobit

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	<a href="#">View plot</a>	<a href="#">View model summary</a>
97.3%	2.7%	0%		

**Global quality scores**



## Structure Quality Analysis for NAME

Program	<i>Verify3D</i>	<i>ProsaII</i> (-ve)	<i>Procheck</i> (phi-psi)	<i>Procheck</i> (all)	<i>MolProbity</i> Clashscore
-Raw score	0.44	0.66	-0.11	-0.02	11.01
Z-score <sup>1</sup>	-0.32	0.04	-0.12	-0.12	-0.36

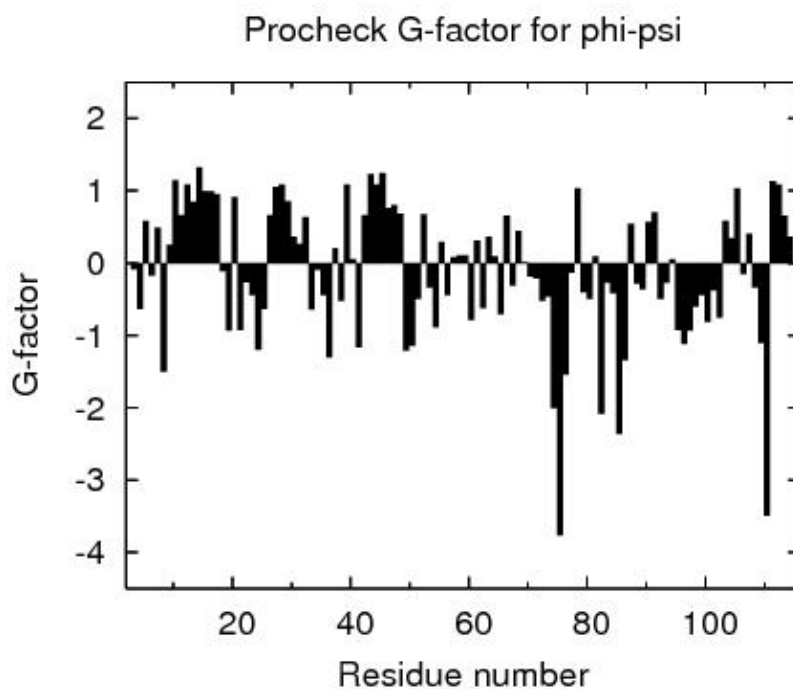
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.3 °

RMS deviation for bond lengths: 0.005 Å

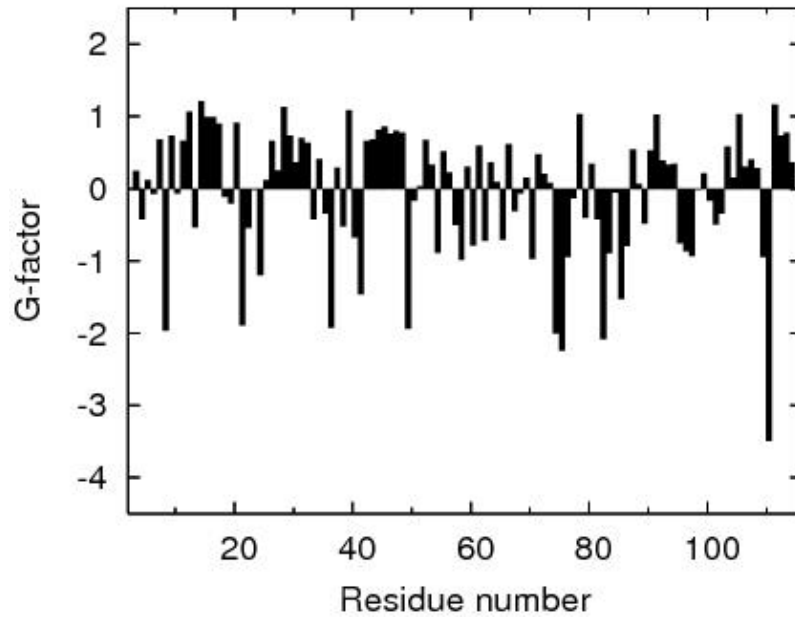
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution ≤ 1.80 Å, R-factor ≤ 0.25 and R-free ≤ 0.28; a positive value indicates a 'better' score



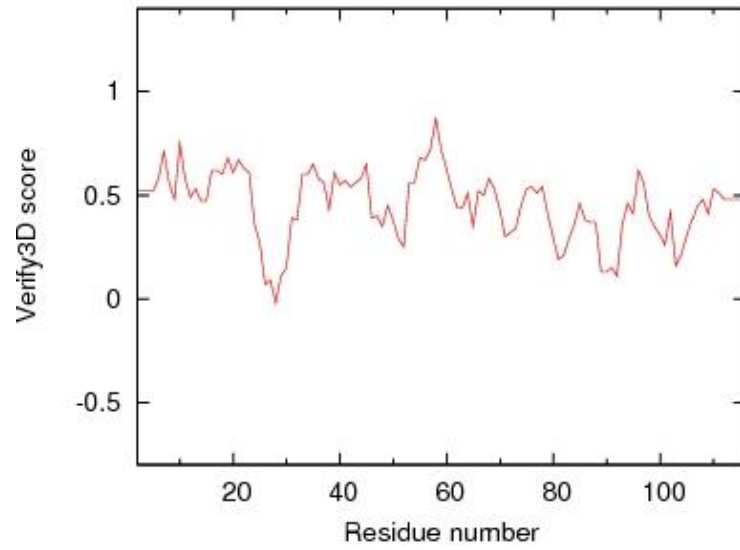


# Structure Quality Analysis for NAME

## Procheck G-factor for all dihedral angles

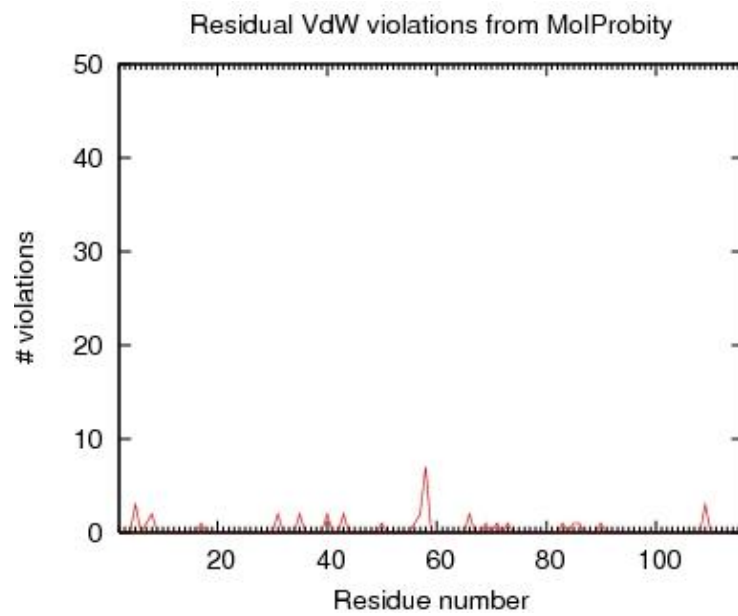
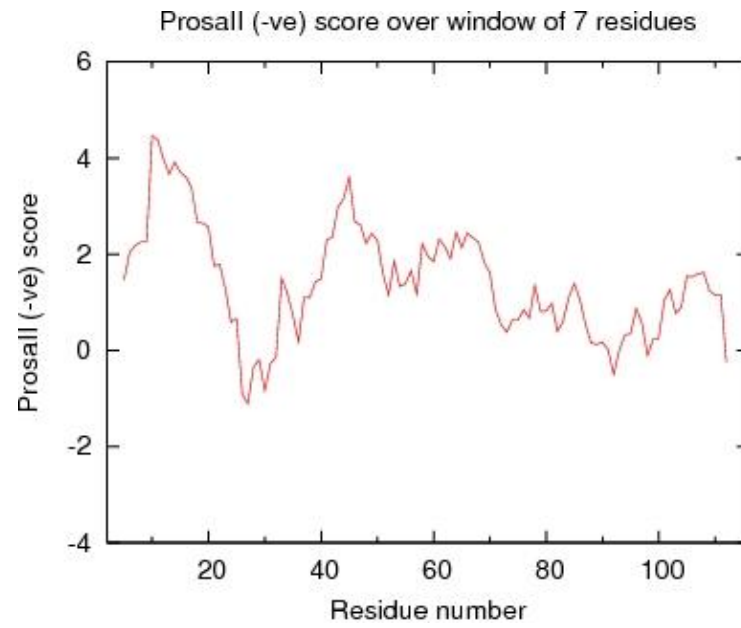


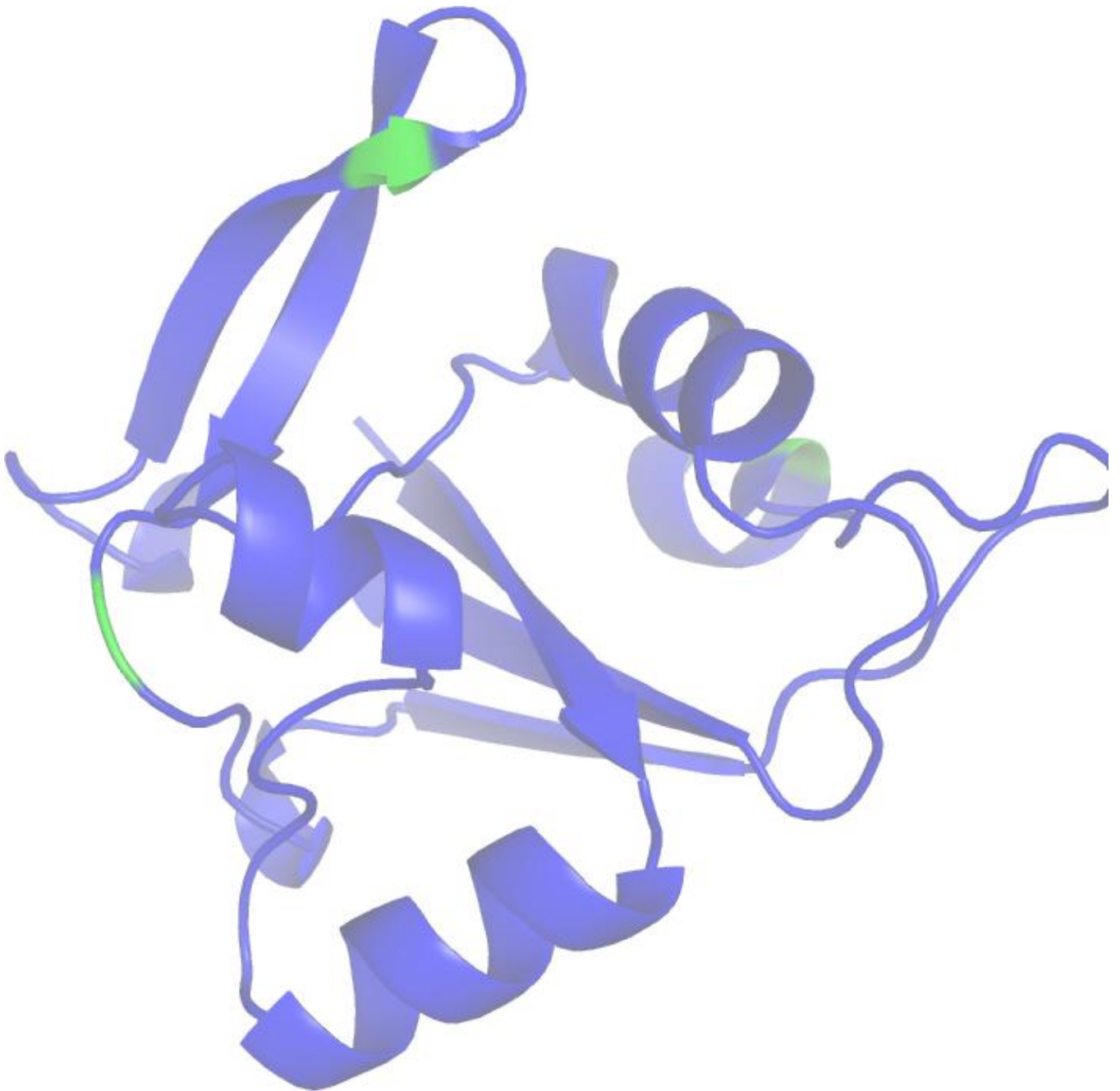
## Verify3D score over window of 7 residues





## Structure Quality Analysis for NAME





**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
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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
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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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-9-2013 using PSVS 1.3



## Software Environment

### Software for structure quality evaluation:

DSSP  
pdbstat

DsspCMBI-April-2000  
PdbStat-5.4 Version



## Structure Quality Analysis for NAME

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