



# 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.): 215

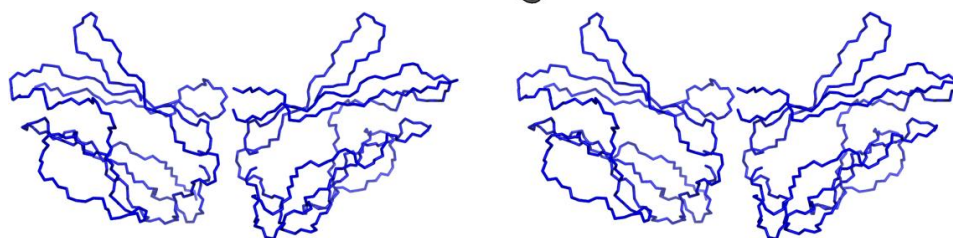
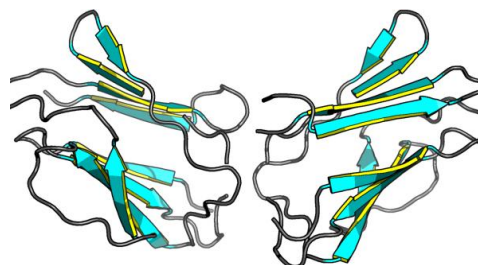
Organism:

SwissProt /

TrEMBL ID:

Oligomerization: dimer

Molecular weight: 23688



Secondary Structure Elements:

*Inter-chain break(s) between 131 & 142*

alpha helices:

beta strands: 28L-33L, 39E-44E, 81R-86R, 98P-101P, 50N-51N, 75L-76L, 64R-69R, 56U-61U, 114S-118S, 124U-129U, 28L-33L, 39E-44E, 81R-85R, 98P-100P, 50N-51N, 75L-76L, 64R-69R, 56U-61U, 113L-118L, 124U-129U

Resolution: 2.392 Å R-factor: 0.238 R-free: 0.245

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>
83.0%	17.0%	0.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobitry

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	<a href="#">View plot</a>	<a href="#">View model summary</a>
94.7%	5.3%	0%		

## Global quality scores

Program	<i>Verify3D</i>	<i>ProsaII (-ve)</i>	<i>Procheck (phi-psi)</i>	<i>Procheck (all)</i>	<i>MolProbitry Clashscore</i>
-Raw score	0.39	0.54	-0.59	-0.33	18.77
Z-score <sup>1</sup>	-1.12	-0.45	-2.01	-1.95	-1.70

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



## Structure Quality Analysis for NAME

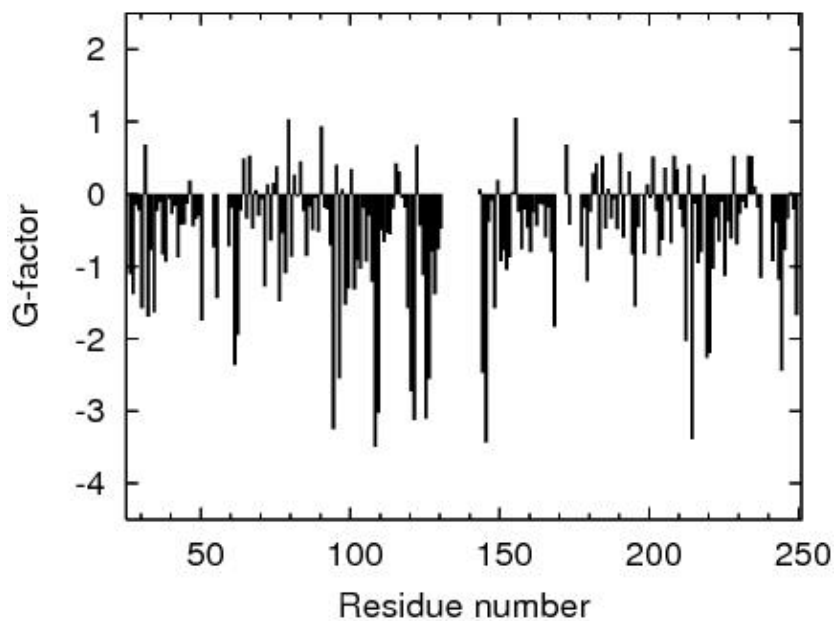
Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.3 °

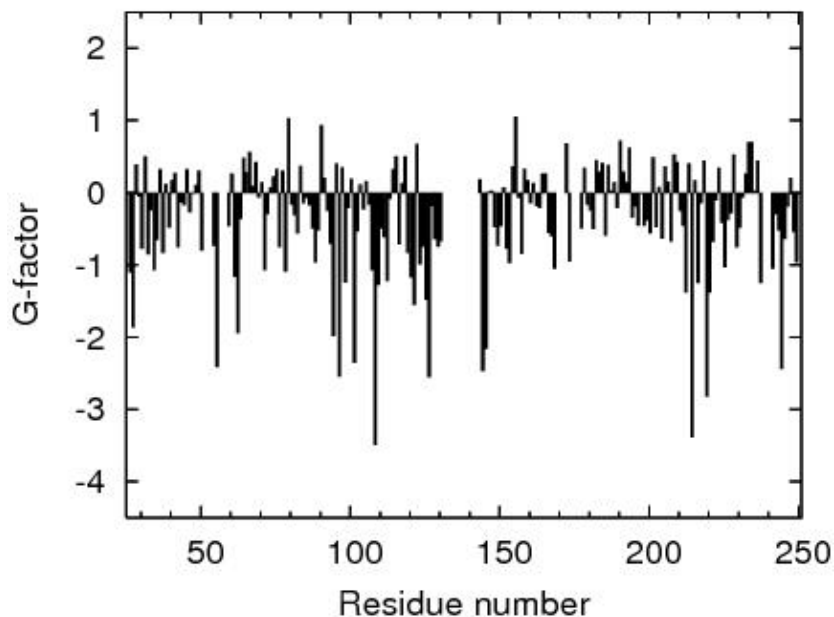
RMS deviation for bond lengths: 0.007 Å

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

Procheck G-factor for phi-psi

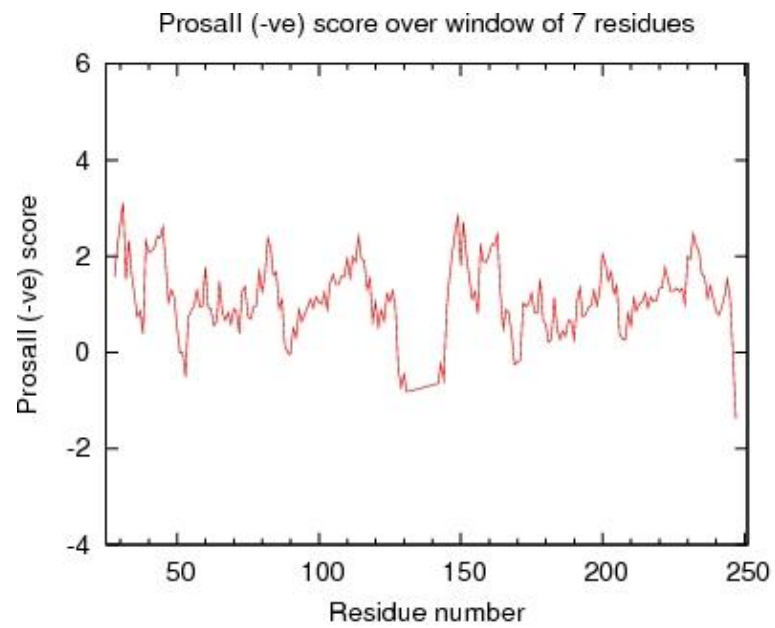
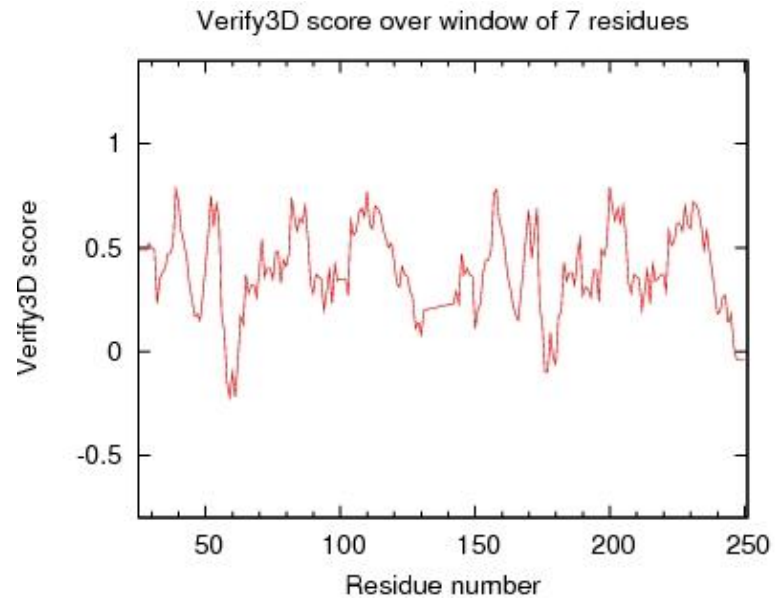


Procheck G-factor for all dihedral angles



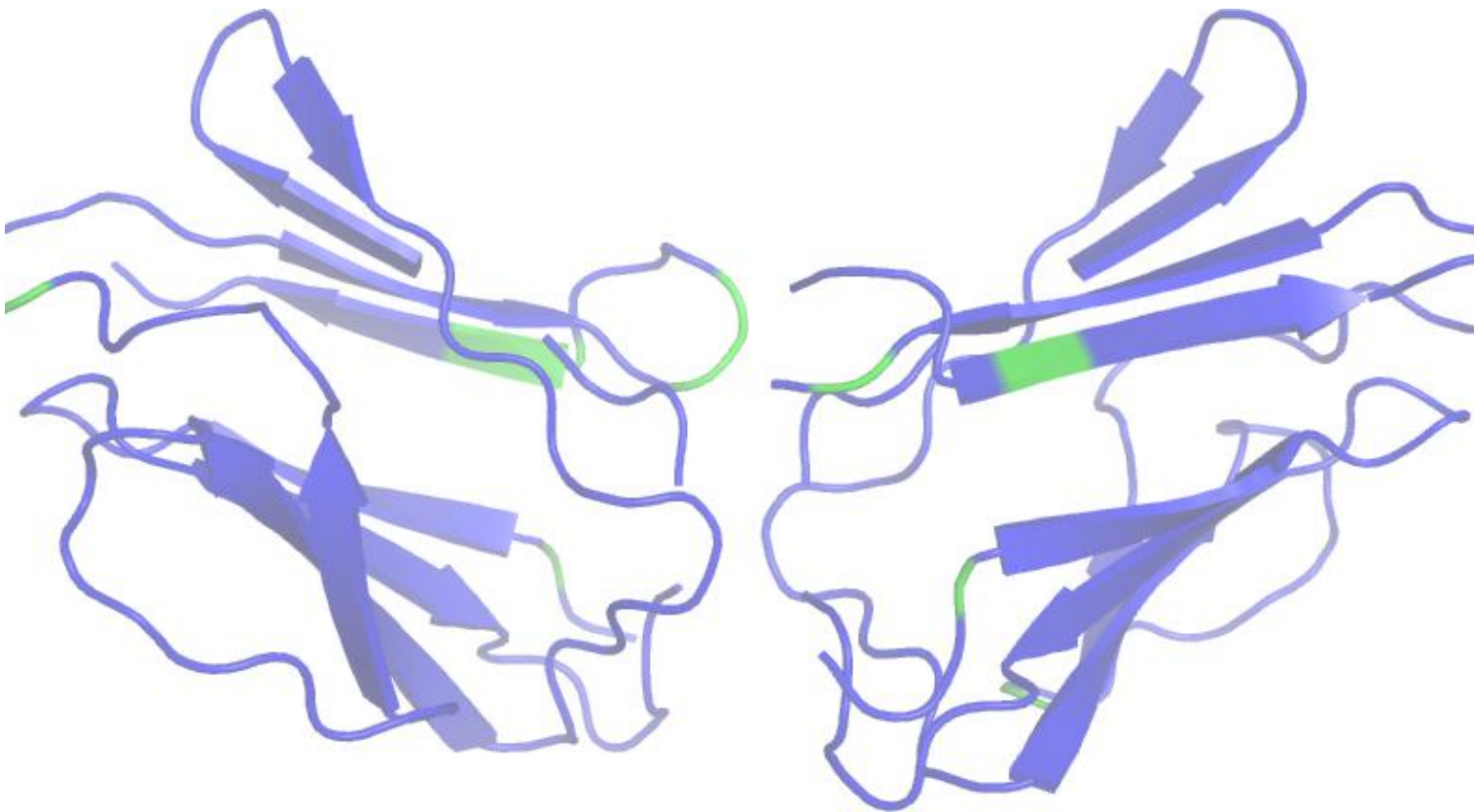
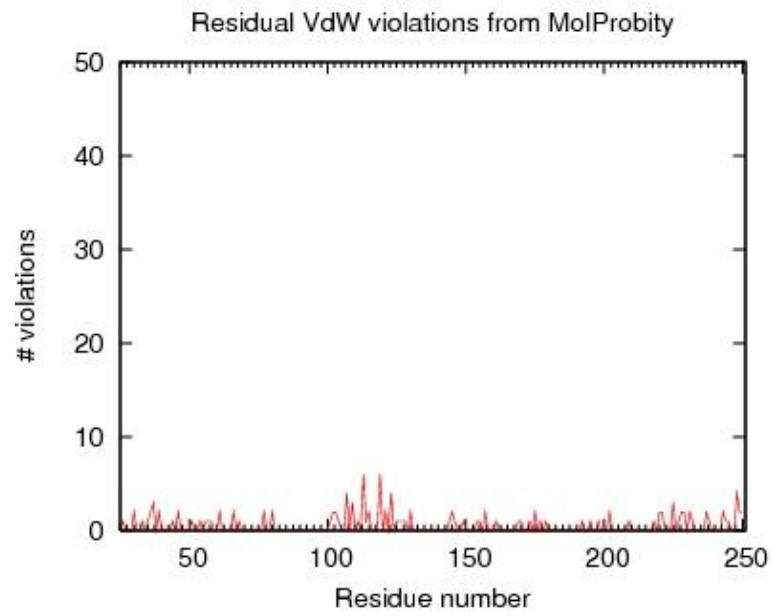


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### Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobity)

#### *References:*

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 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
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 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
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 C $\alpha$  geometry: phi,psi and C $\beta$  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