



# 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.): 136

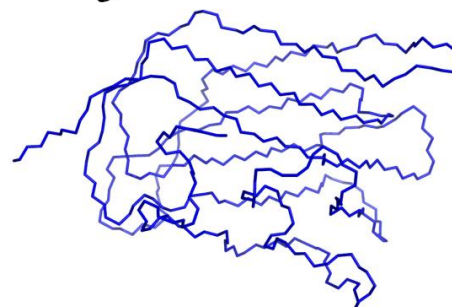
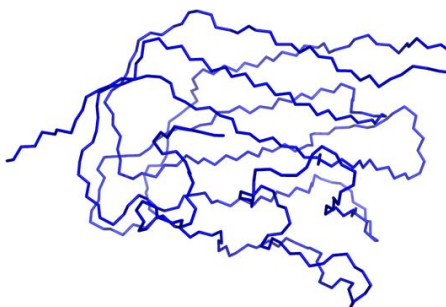
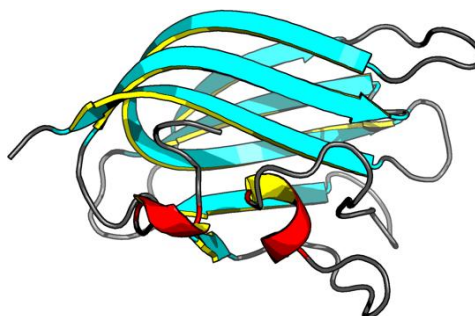
Organism:

SwissProt /

TrEMBL ID:

Oligomerization: monomer

Molecular weight: 15365



Secondary Structure Elements:

alpha helices:

beta strands: 14U-16U, 47N-67N, 128R-139R, 39P-40P, 69L-77L, 86U-92U, 101N-105N, 110Y-122Y

Resolution: 1.400 Å R-factor: 0.215 R-free: 0.244

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>
85.4%	13.8%	0.8%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobrity

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	<a href="#">View plot</a>	<a href="#">View model summary</a>
96.3%	3.7%	0%		

## Global quality scores

Program	<i>Verify3D</i>	<i>ProsaII (-ve)</i>	<i>Procheck (phi-psi)</i>	<i>Procheck (all)</i>	<i>MolProbrity</i>	<i>Clashscore</i>
-Raw score	0.48	0.29	-0.50	-0.26	15.08	
Z-score <sup>1</sup>	0.32	-1.49	-1.65	-1.54	-1.06	

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



## Structure Quality Analysis for NAME

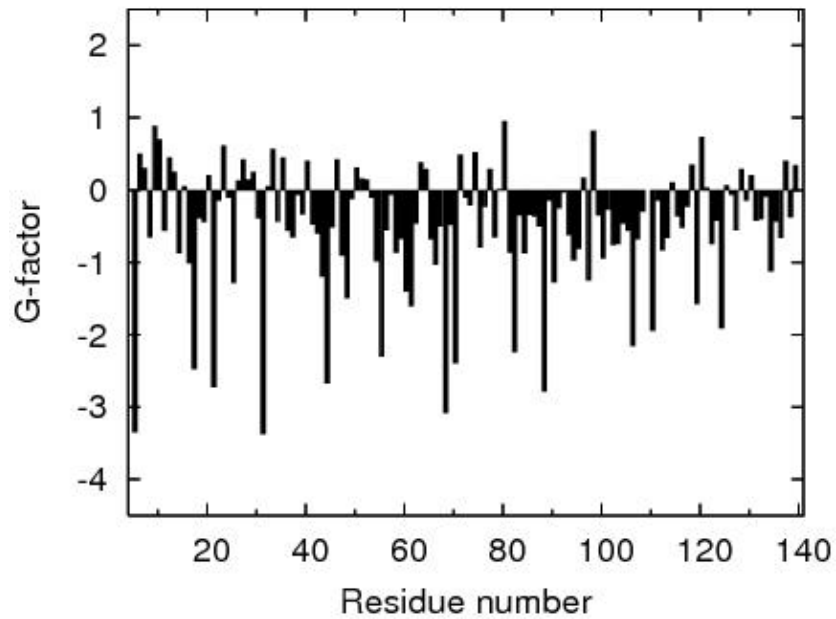
Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.3 °

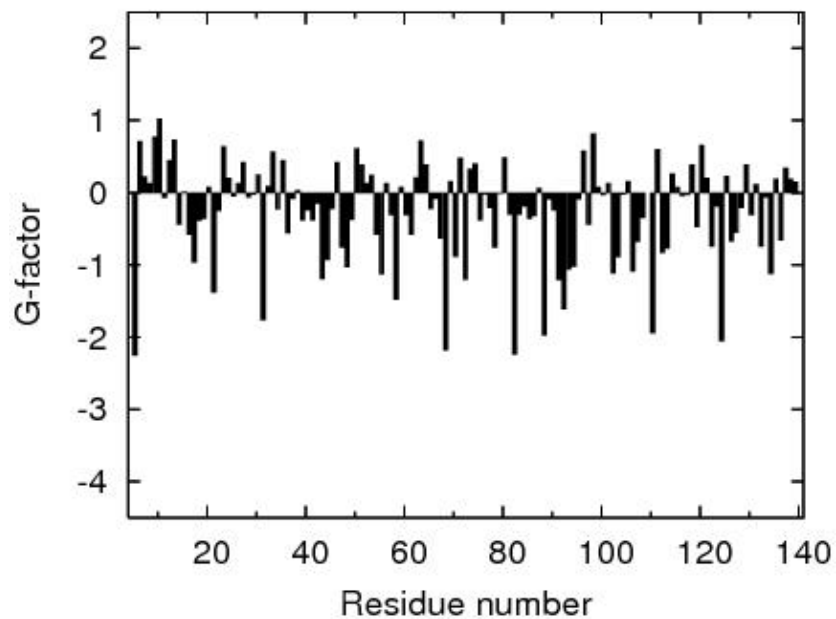
RMS deviation for bond lengths: 0.005 Å

<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

Procheck G-factor for phi-psi

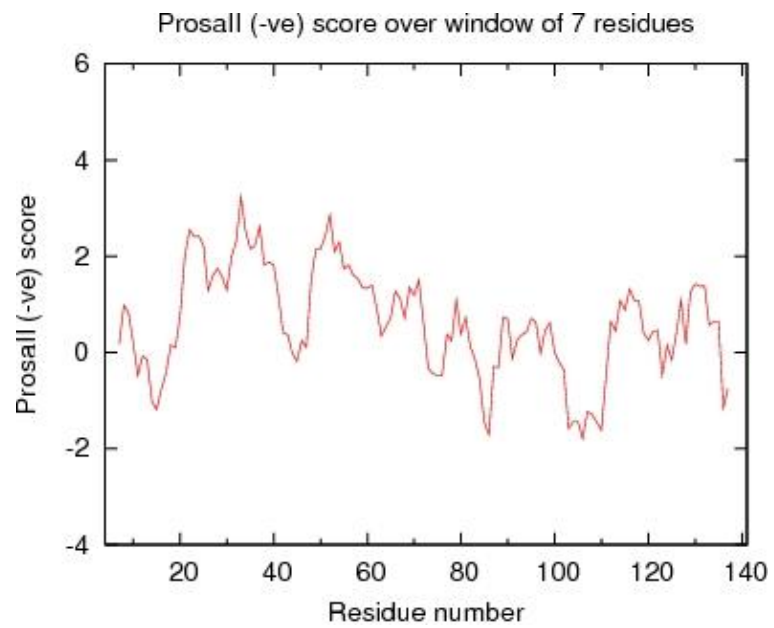
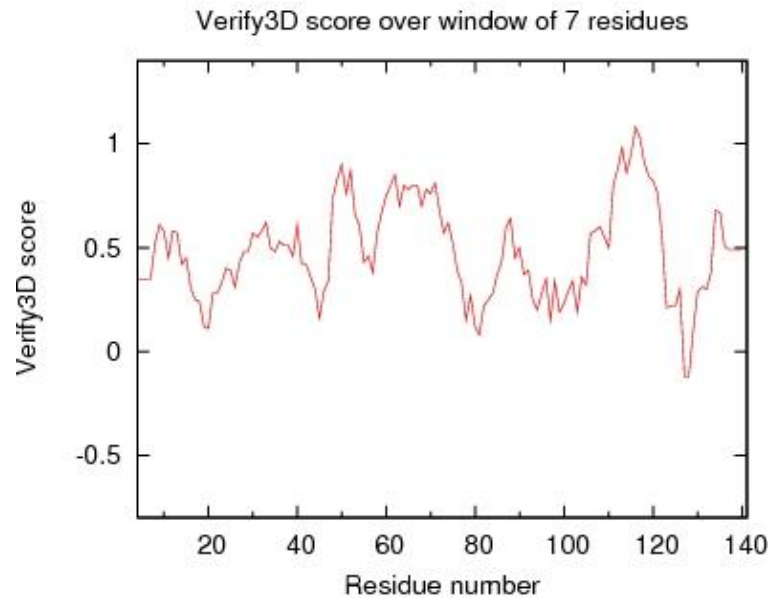


Procheck G-factor for all dihedral angles



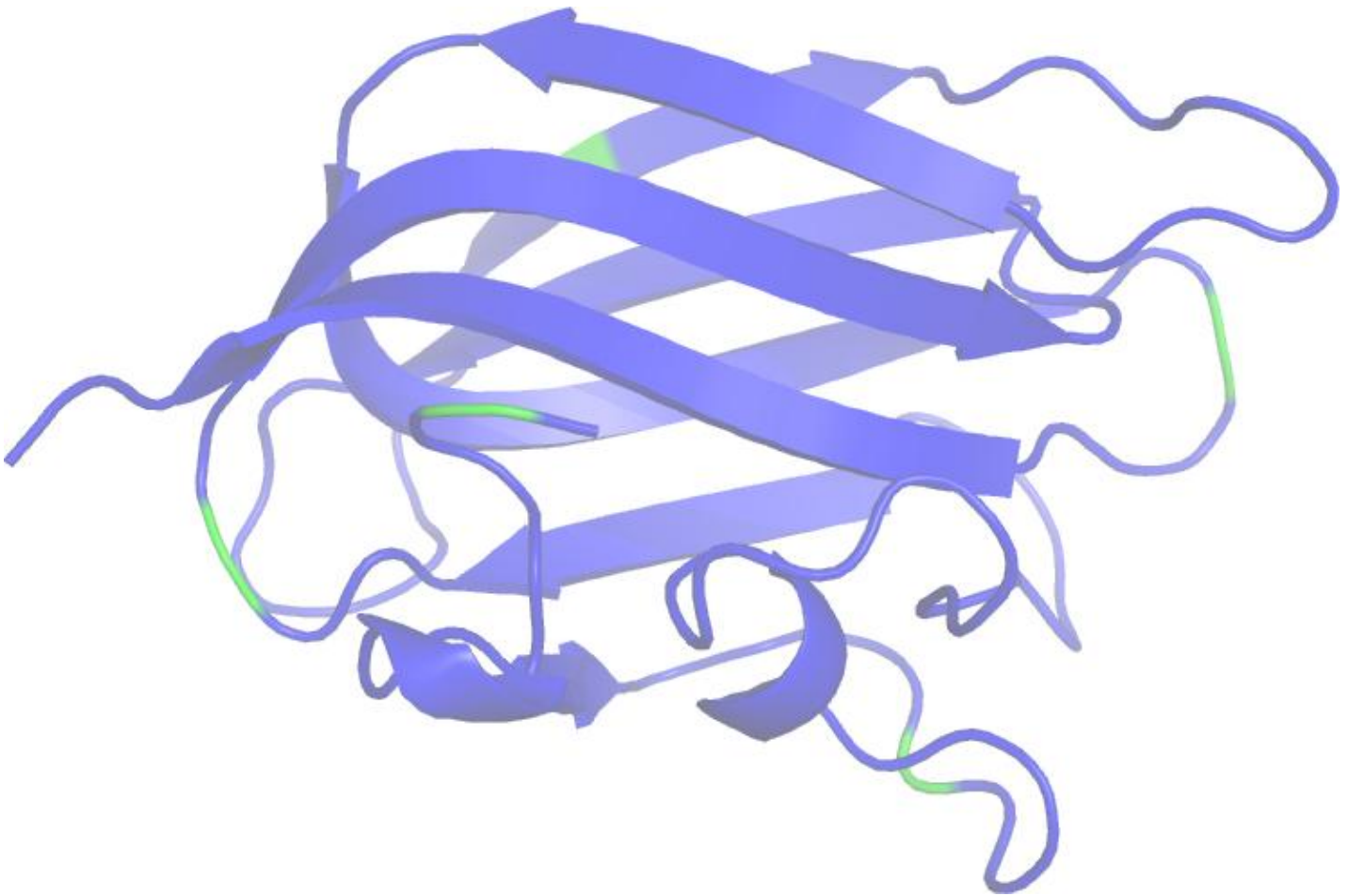
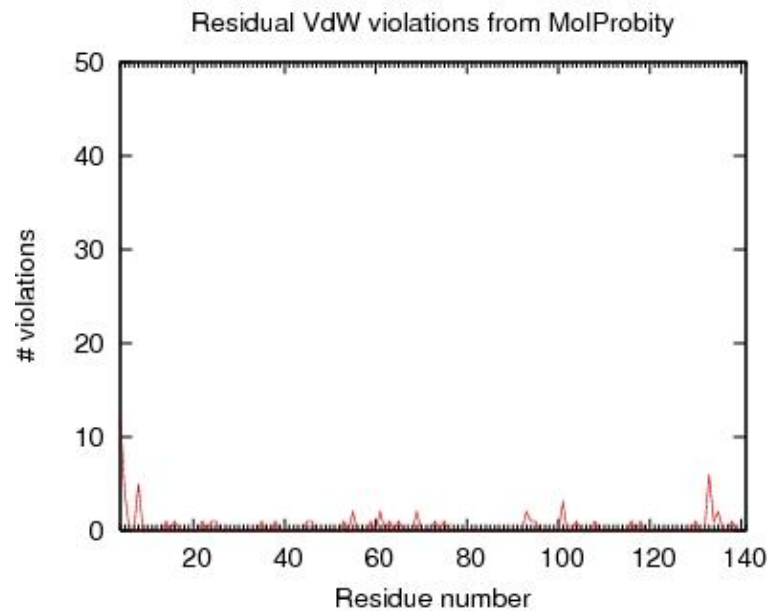


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**Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobity)**

**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
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Analysed by on May-10-2013 using PSVS 1.3



**Protein Structure Validation Suite  
(PSVS)**





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## 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