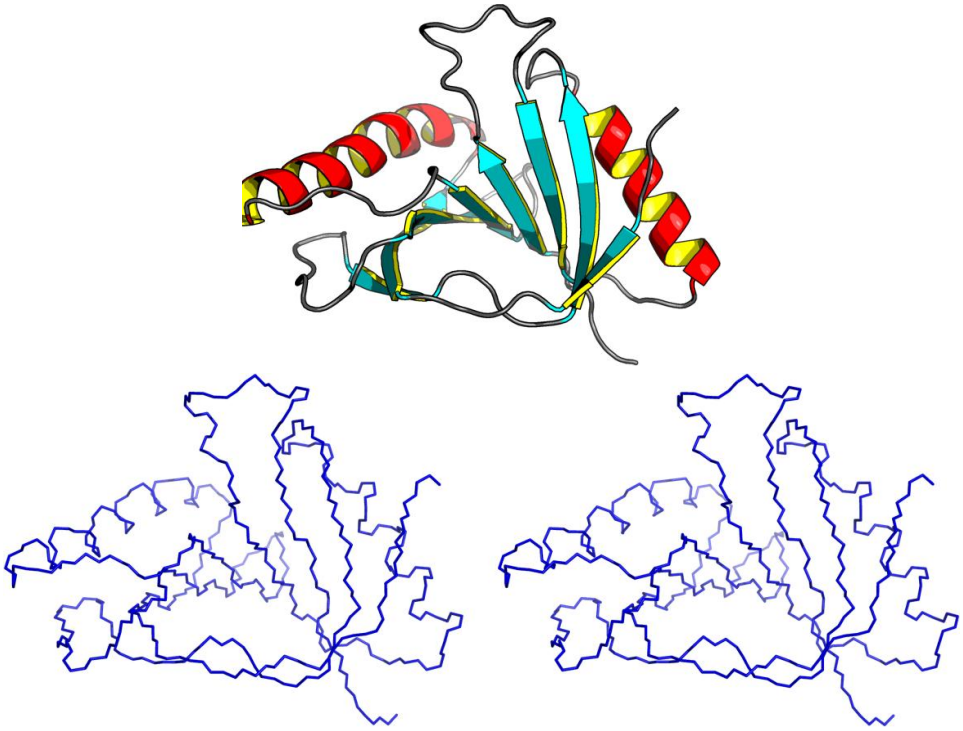
Structure Quality Analysis for NAME

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.):	153
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	monomer
Molecular weight:	16458



Secondary Structure Elements:
alpha helices: 28A-48A, 110A-122A
beta strands: 9S-14S, 95Y-103Y, 148G-155G, 127U-135U, 58E-62E, 69E-76E, 18O-26O, 88L-91L

Resolution: 1.800 Å R-factor: 0.210 R-free: 0.234
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
95.9%	4.1%	0.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
98.7%	1.3%	0%		

Global quality scores

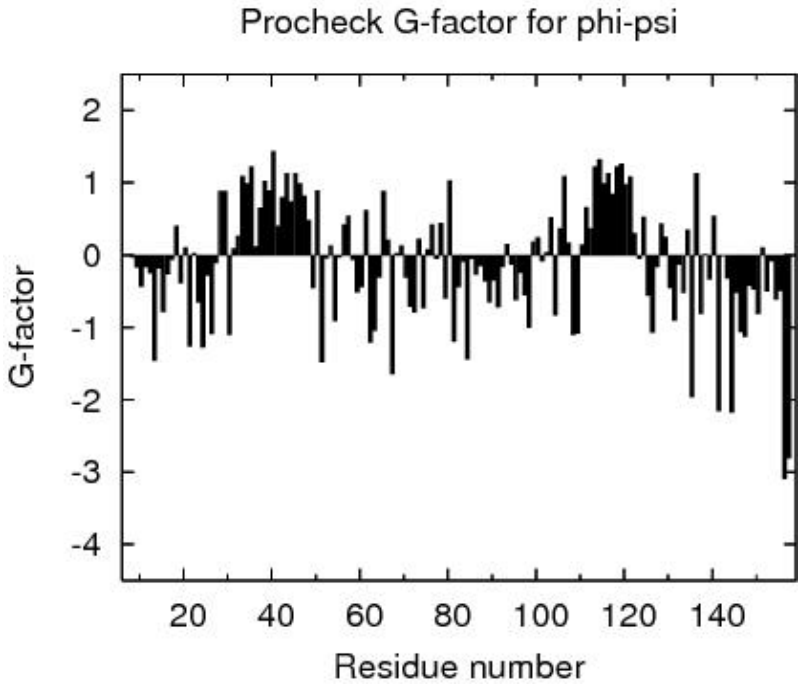
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*
-Raw score	0.47	0.55	-0.11	-0.07	10.64

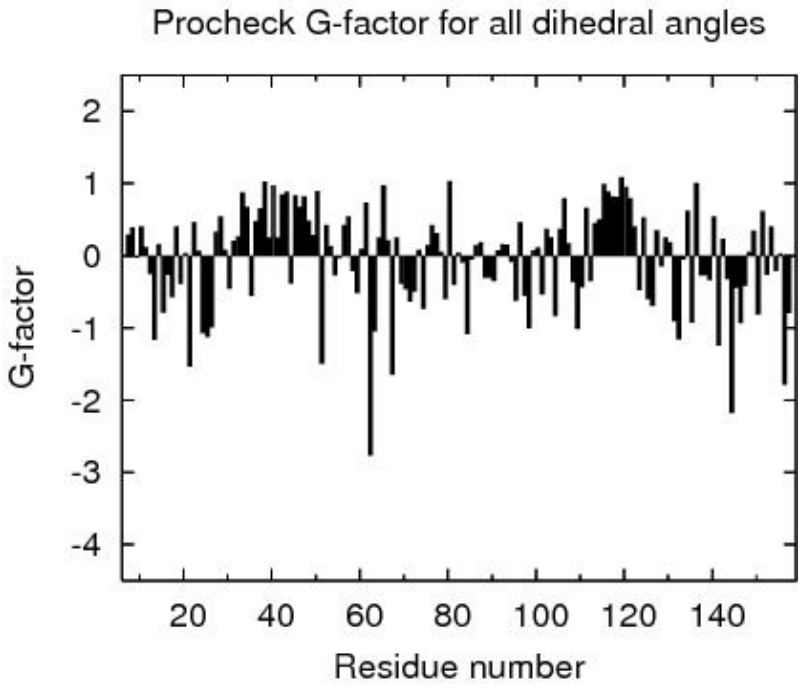
Z-score[1]	0.16	-0.41	-0.12	-0.41	-0.30

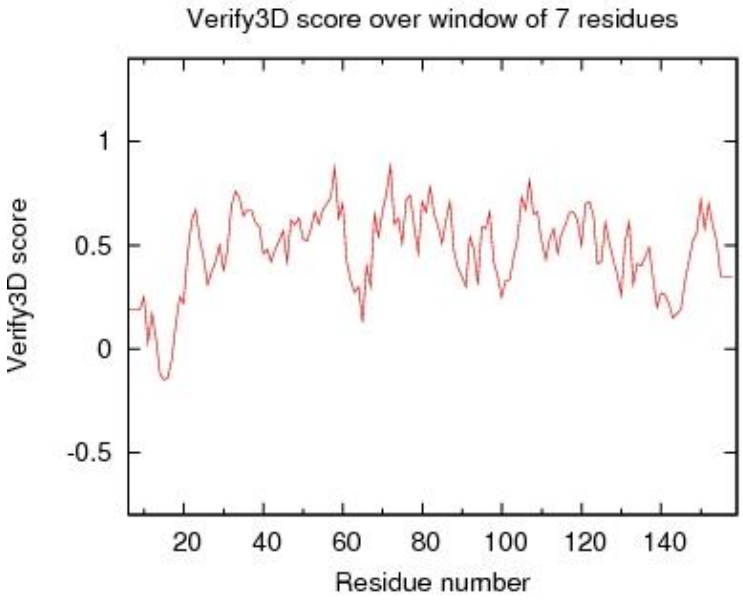
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

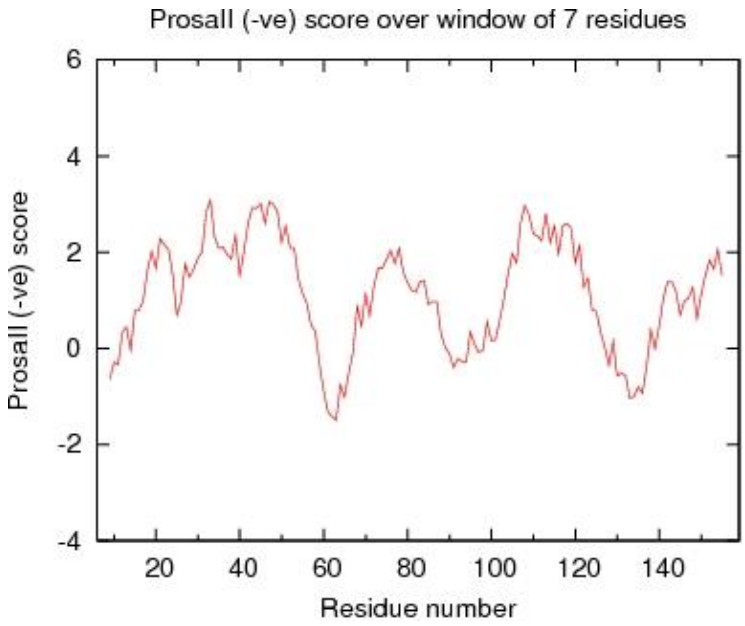
Number of close contacts (within 2.2 Å):	0
RMS deviation for bond angles:	1.4 °
RMS deviation for bond lengths:	0.006 Å

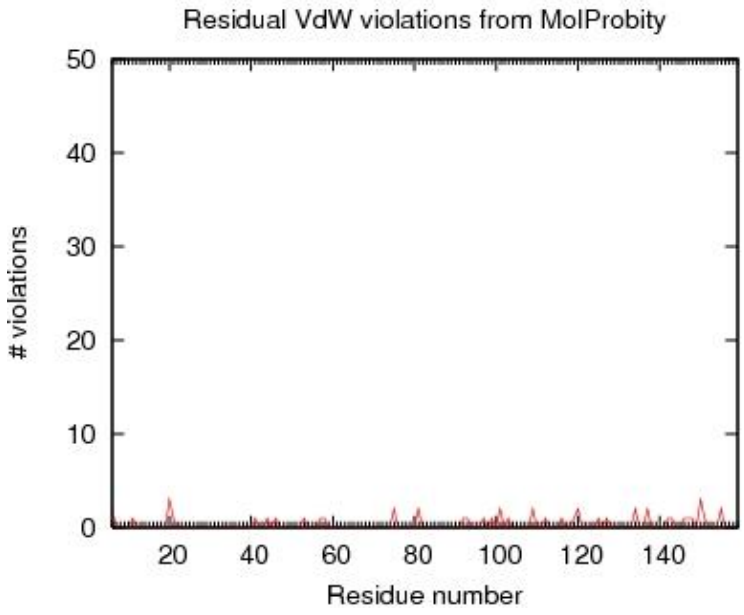
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

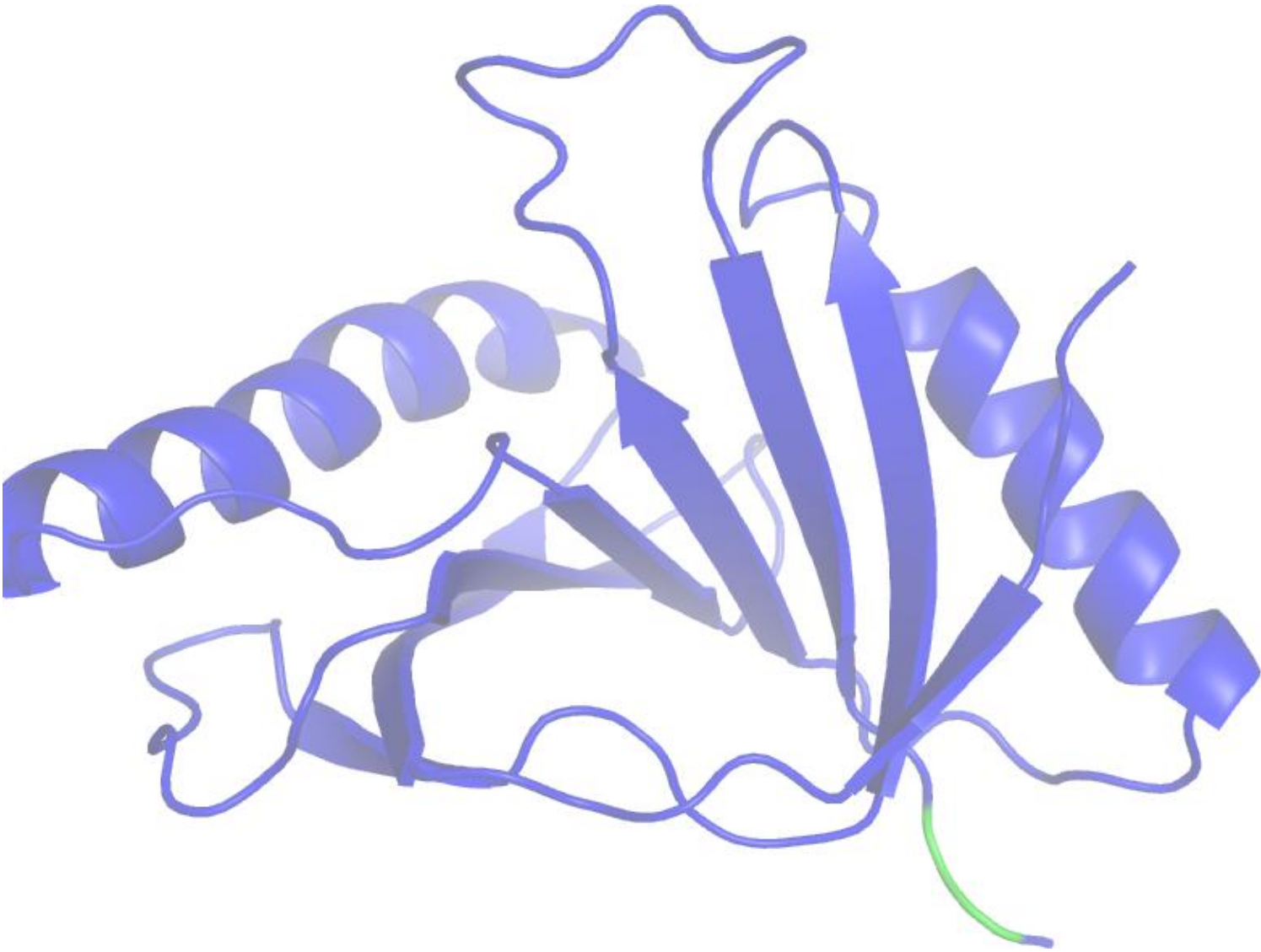



Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
20
40
60
80
100
120
140
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
20
40
60
80
100
120
140
Residue number


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
20
40
60
80
100
120
140
Residue number


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
20
40
60
80
100
120
140
Residue number



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

References:

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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 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
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Analysed by on May-9-2013 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
```