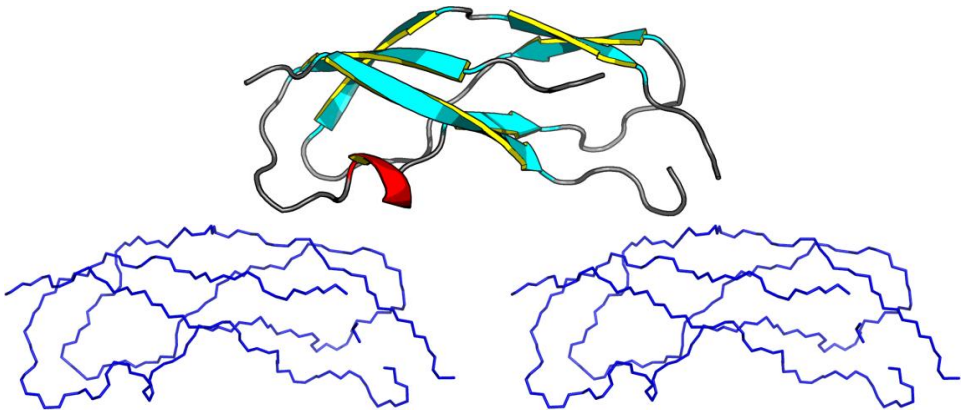
Structure Quality Analysis for NAME

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.):	84
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	monomer
Molecular weight:	9333



Secondary Structure Elements:
alpha helices:
beta strands: 62S-63S, 44E-48E, 4R-12R, 26R-33R, 69E-75E, 18R-20R, 78L-85L, 55Y-60Y

Resolution: 1.800 Å R-factor: 0.224 R-free: 0.258
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
91.2%	7.4%	1.5%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
95.2%	2.4%	2.4%		

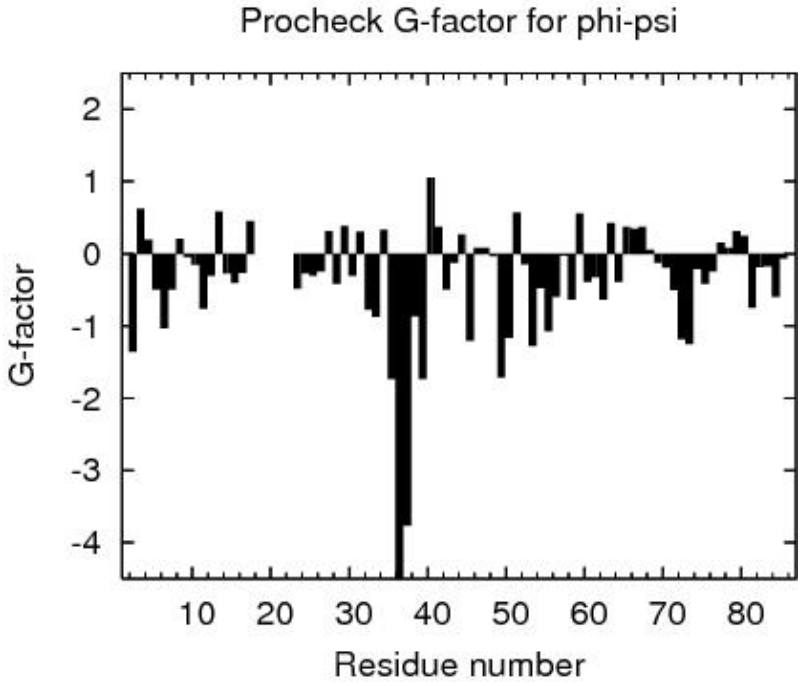
Global quality scores

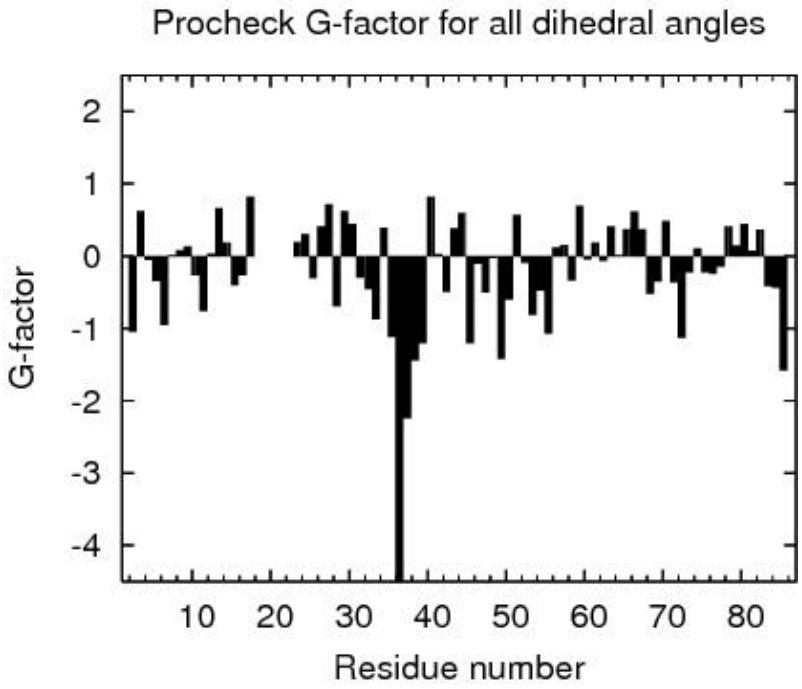
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*
-Raw score	0.51	0.37	-0.38	-0.20	22.09
Z-score[1]	0.80	-1.16	-1.18	-1.18	-2.27

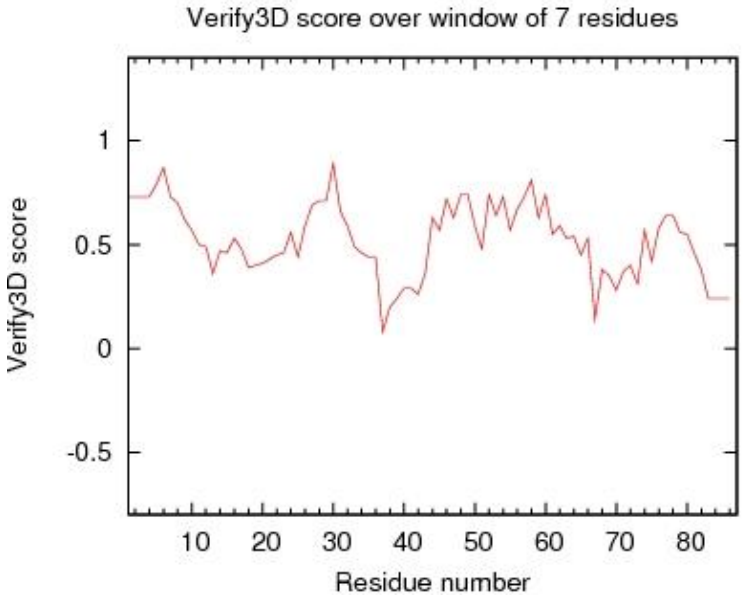
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

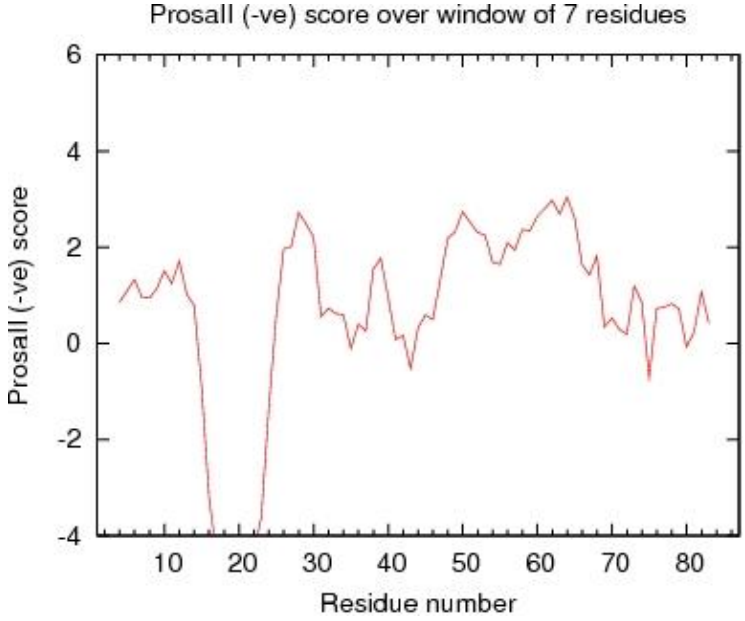
Number of close contacts (within 2.2 Å):	0
RMS deviation for bond angles:	1.3 °
RMS deviation for bond lengths:	0.005 Å

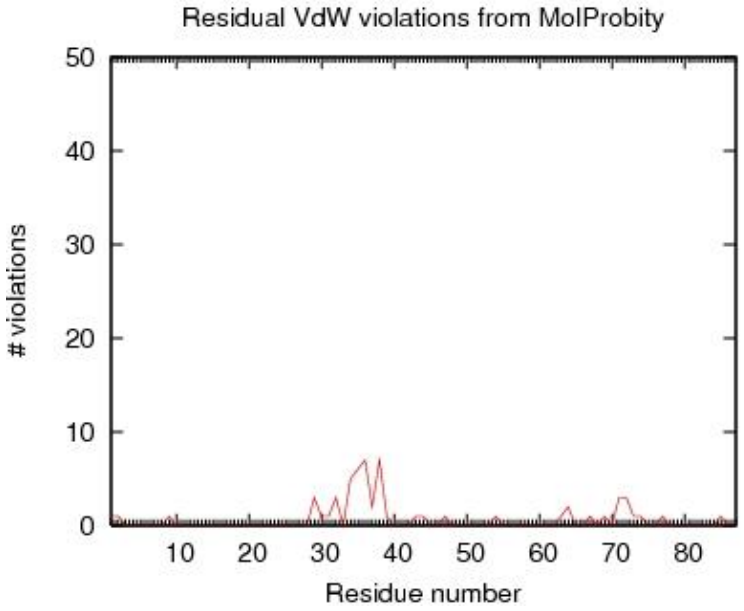
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

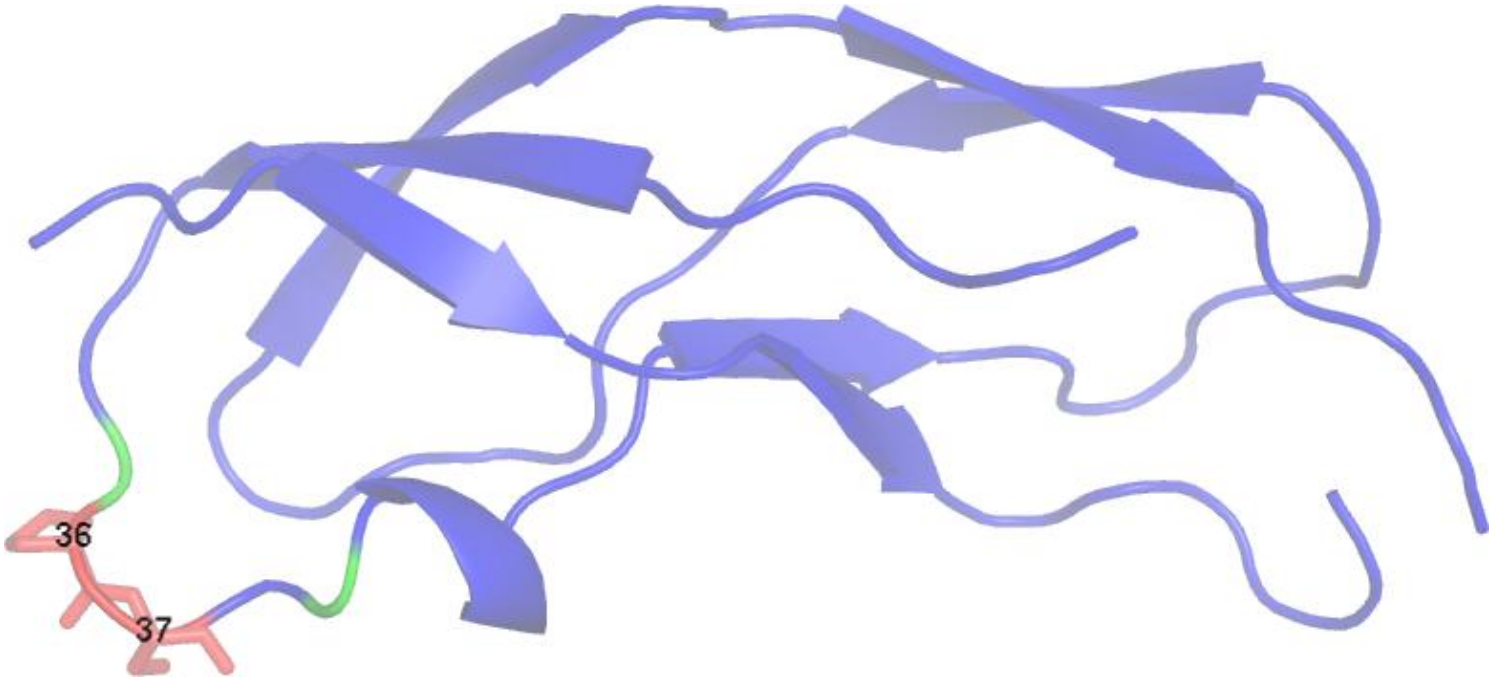





Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
10
20
30
40
50
60
70
80
Residue number


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
10
20
30
40
50
60
70
80
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
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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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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
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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
```

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
```