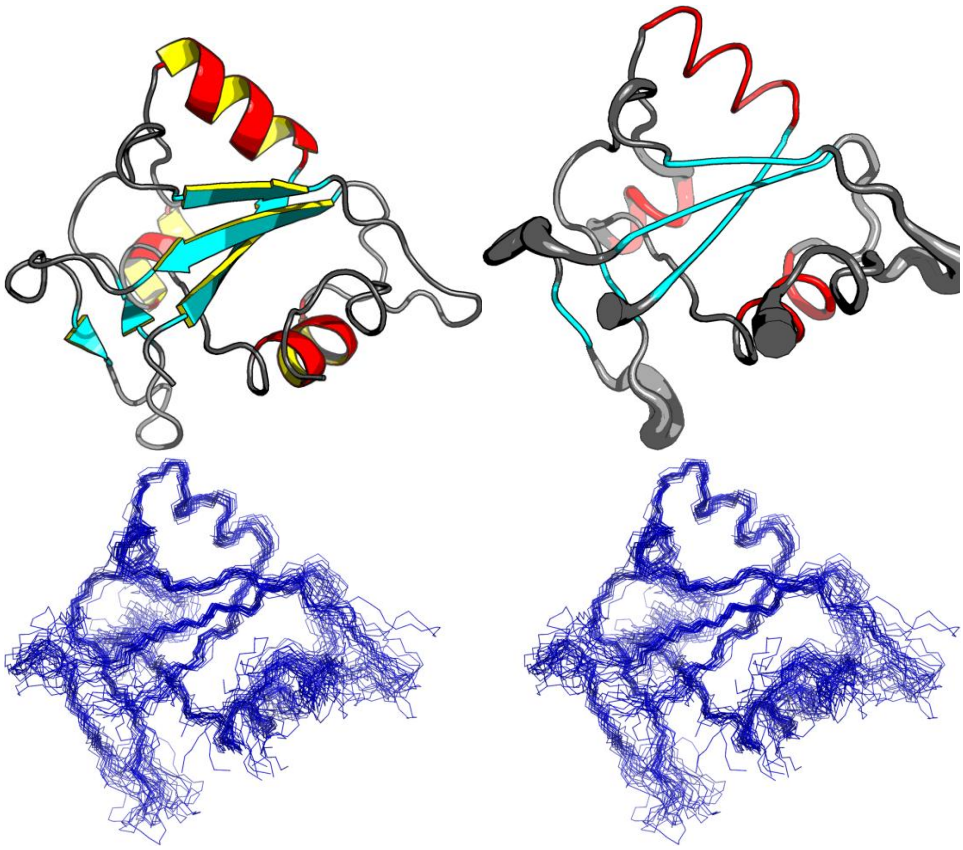
Structure Quality Analysis for NAME

Analyses performed for user defined residues.
The constraints analysis is based on the following files: NOE distance constraints file. Angular constraints file. H-bond constraints file.
Procheck analysis,RMSD calculation and structure superimposition are based on: User defined residues

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	116
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	monomer
Molecular weight:	12686



Secondary Structure Elements:
alpha helices: 10A-19A, 26A-32A, 39A-48A, 109A-112A
beta strands: 37R-38R, 3U-9U, 56U-62U, 95G-99G, 21G-22G, 88U-89U, 34E-35E, 80G-84G, 70U-74U

Total number of restricting constraints per restrained residue:	12.1
Restricting long range constraints per restrained residue:	3.6

Distance violations per model
Calculated using sum over r^-6

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
10.1	20.2	57.4

Dihedral angle violations per model

1 - 10 °	> 10 °
1.85	1.2

FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score
0.93	0.859	0.893	0.882

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	1.6 Å	1.0 Å	1.0 Å
All heavy atoms	2.0 Å	1.4 Å	1.4 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
96.0%	4.0%	0.0%	0.0%

Ramachandran Plot Summary for selected residues[3] from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
99.6%	0.4%	0%		

Global quality scores

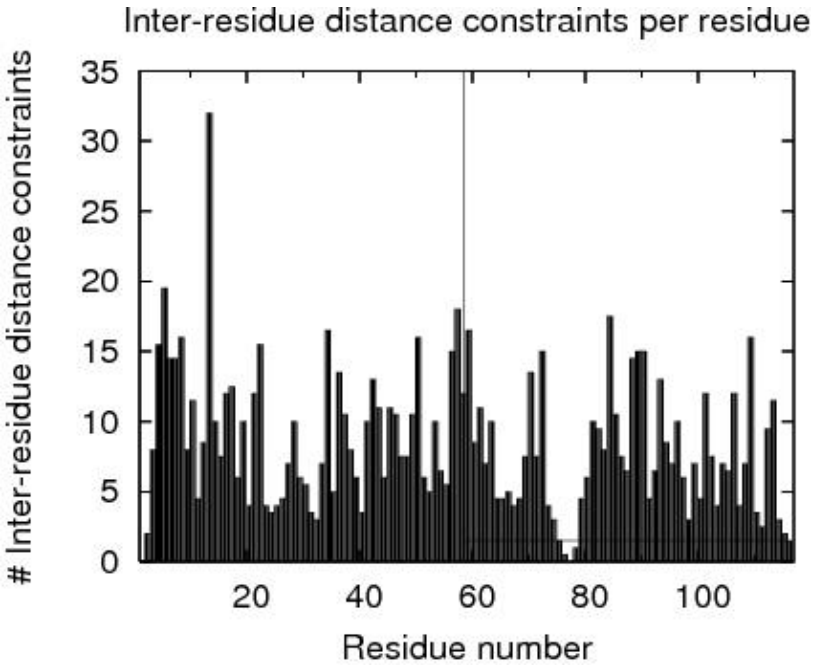
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.42	0.53	-0.03	0.21	5.71
Z-score[1]	-0.64	-0.50	0.20	1.24	0.55

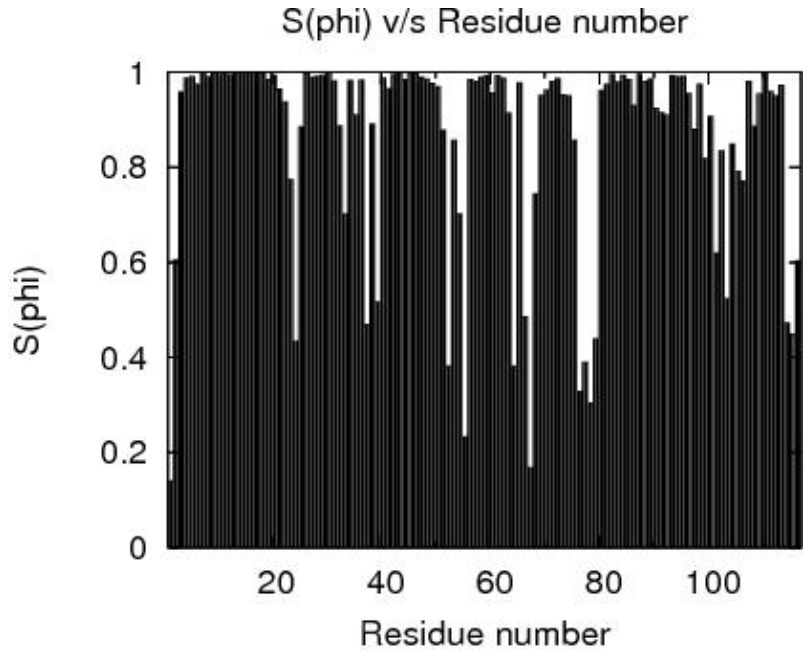
Generalized linear model RMSD prediction: 1.06

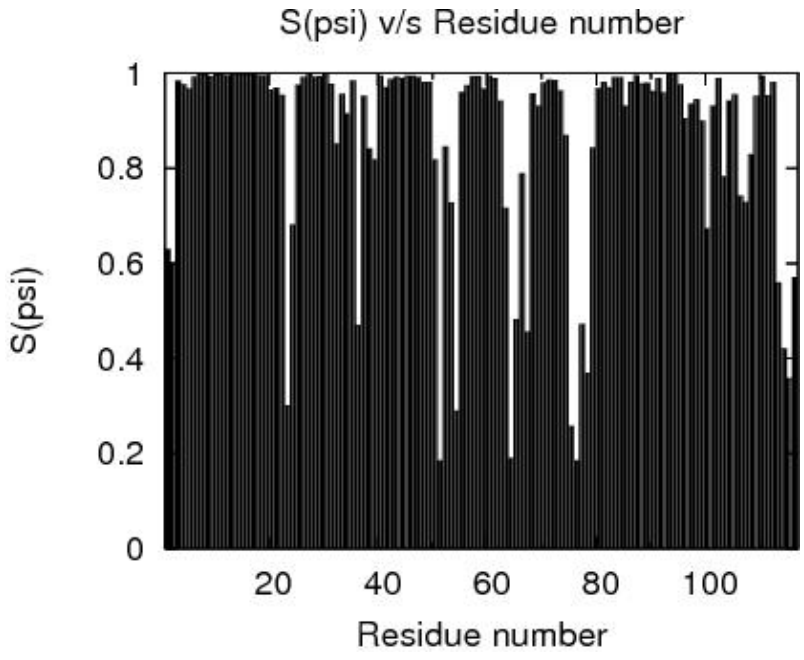
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	0
RMS deviation for bond angles:	0.7 °
RMS deviation for bond lengths:	0.012 Å

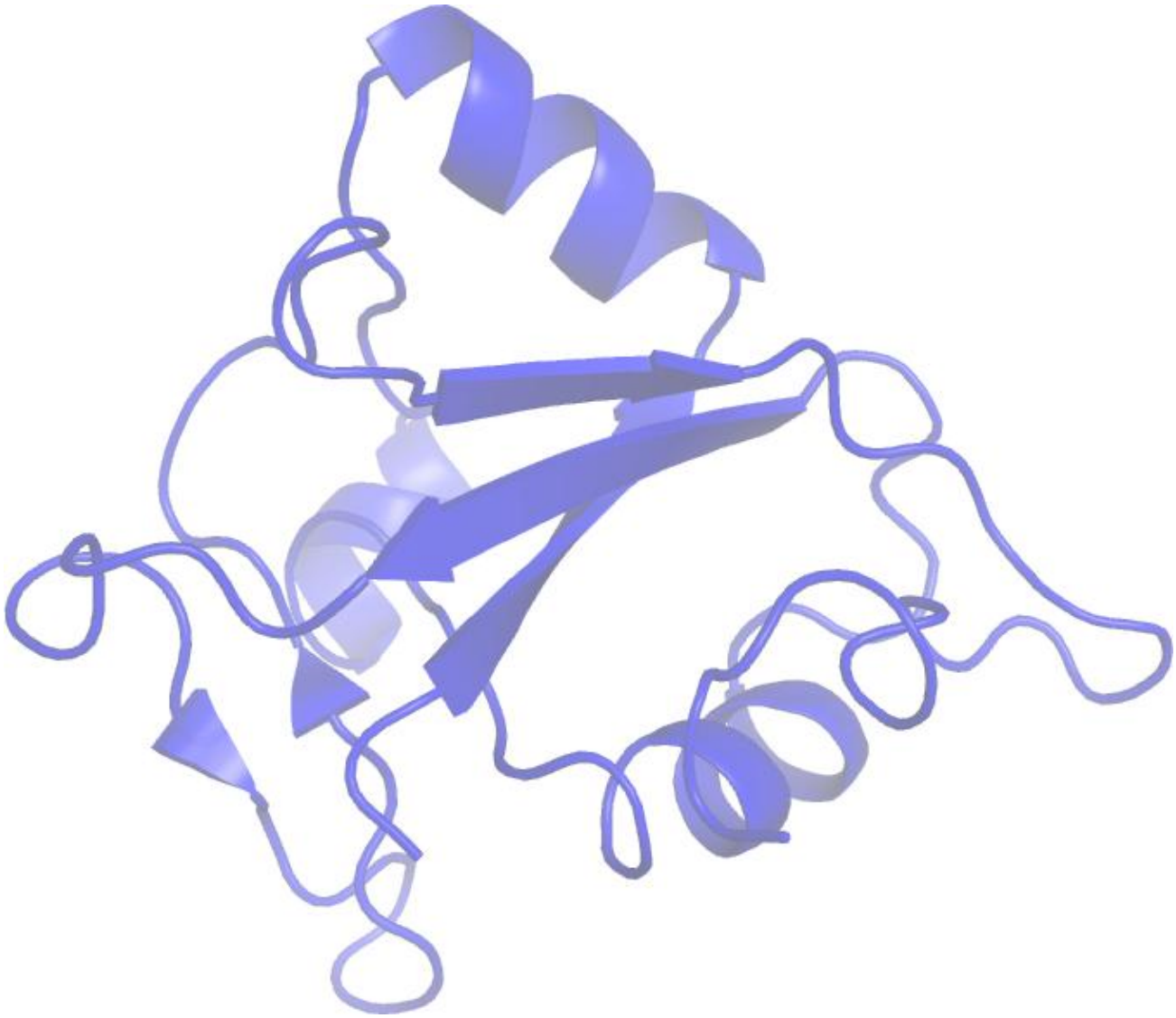
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 3A-22A,25A-31A,40A-49A,56A-62A,69A-74A,80A-98A,109A-112A
[3]Selected residues: 3A-22A,26A-31A,40A-49A,56A-62A,69A-73A,80A-96A,109A-112A


Inter-residue distance constraints per residue
Inter-residue distance constraints
0
5
10
15
20
25
30
35
20
40
60
80
100
Residue number

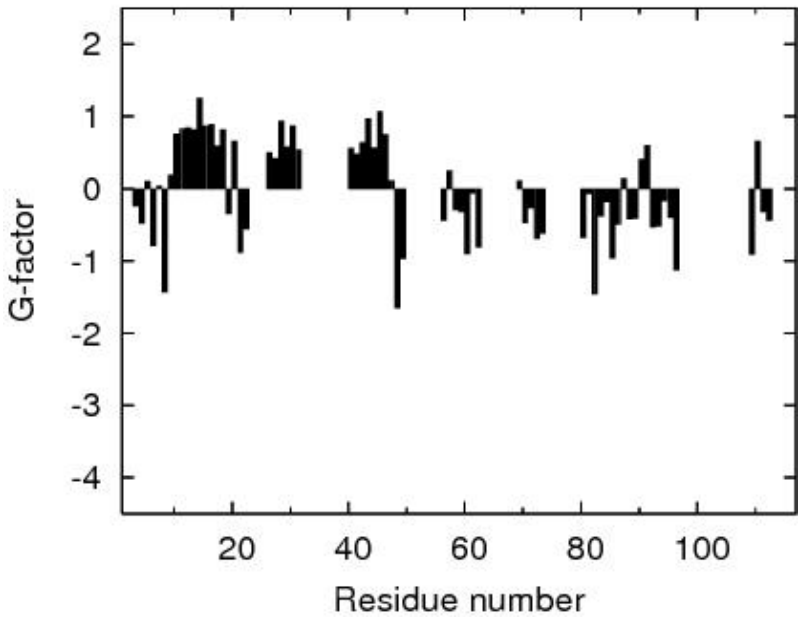

S(phi) v/s Residue number
S(phi)
0
0.2
0.4
0.6
0.8
1
20
40
60
80
100
Residue number



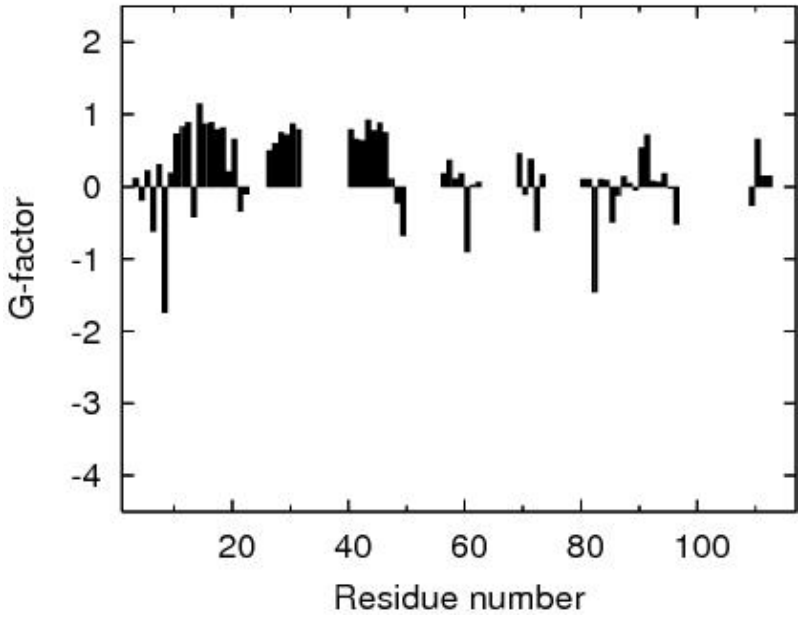
RPF Precision Map



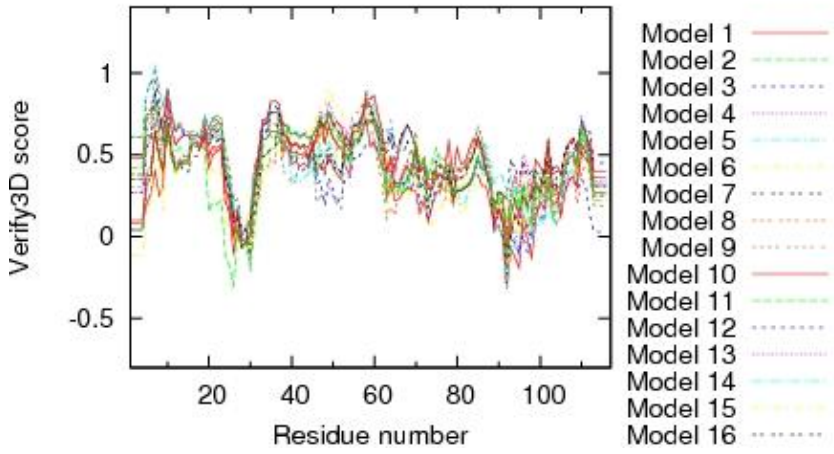
Procheck G-factor for phi-psi



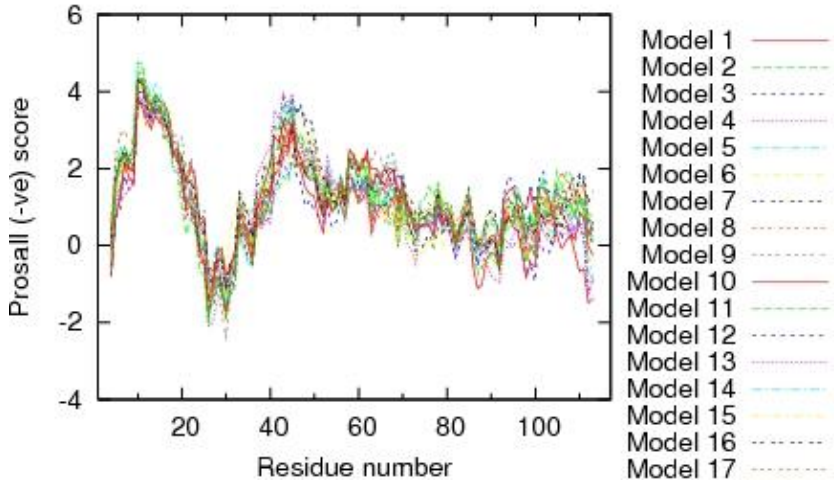
Procheck G-factor for all dihedral angles



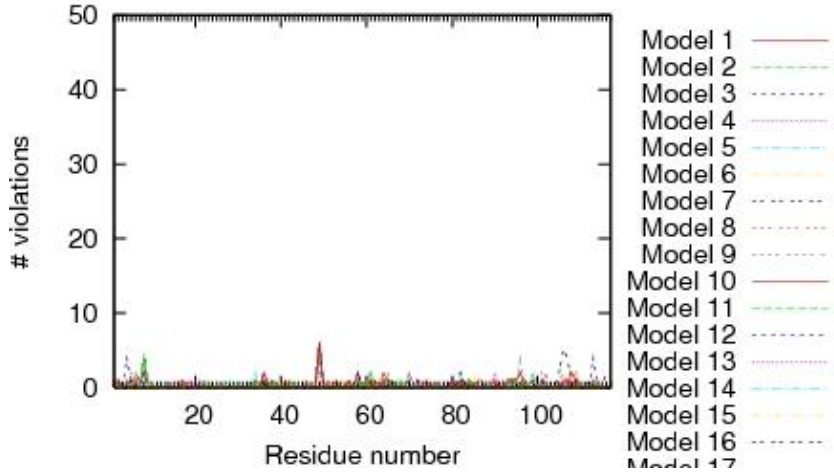
Verify3D score over window of 7 residues

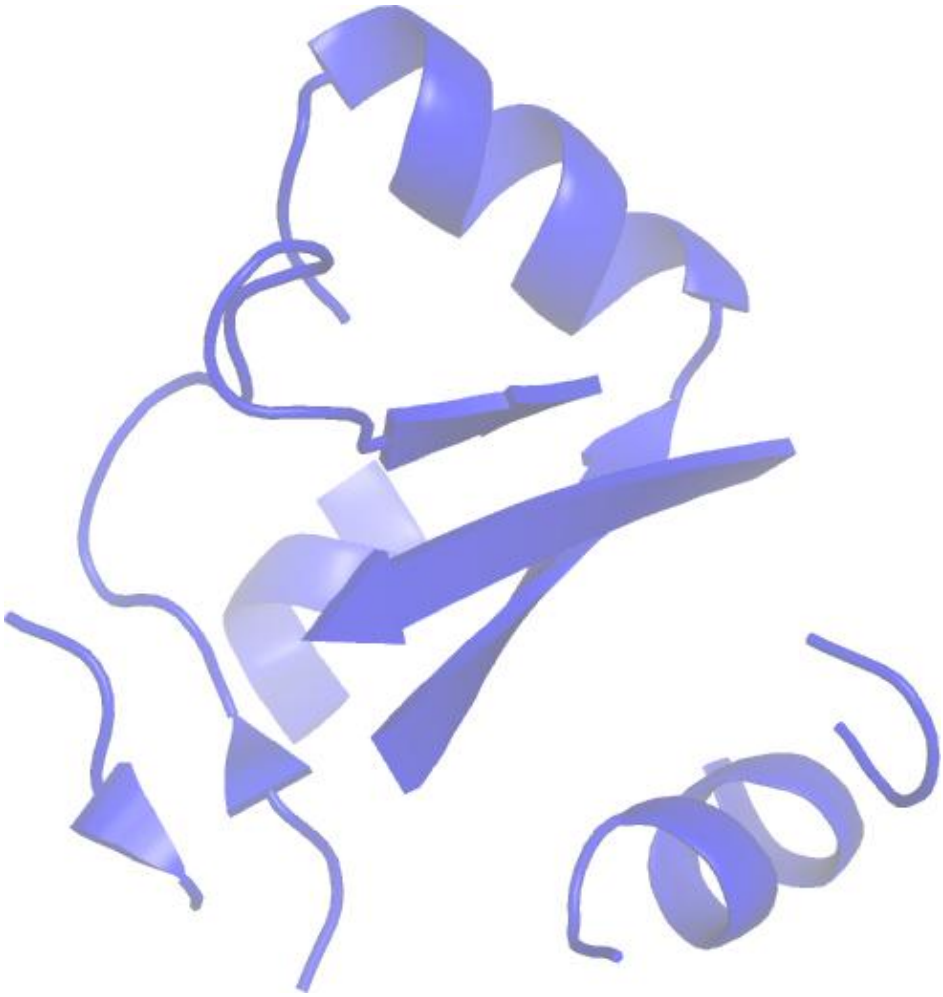


Prosall (-ve) score over window of 7 residues



Residual VdW violations from MolProbity





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

References:

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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 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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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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13. Koradi, R, et al, "MOLMOL: a program for display and analysis of macromolecular structures ", J Mol Graphics 14 (1996): 51-55.
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15. Lovell S C et al, "Structure validation by Calpha geometry: phi,psi and Cbeta deviation" Proteins (2003) 50: 437-450
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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-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
```