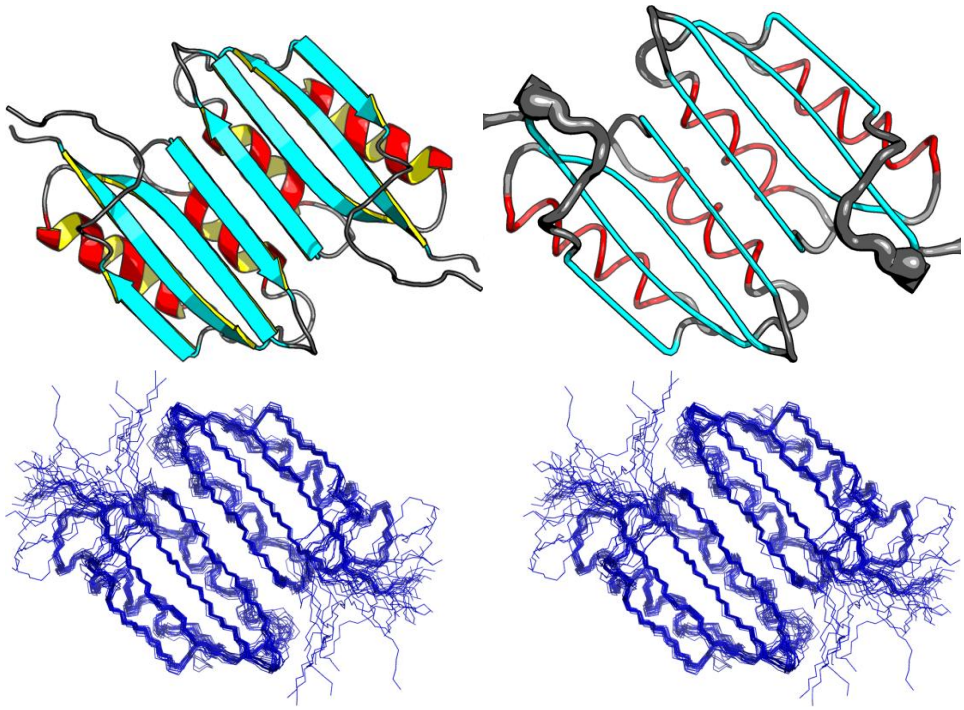
Structure Quality Analysis for NAME

Analyses performed for user defined residues.
The constraints analysis is based on the following files: NOE distance constraints file. Angular constraints file.
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.):	176
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	dimer
Molecular weight:	20049



Secondary Structure Elements:
Inter-chain break(s) between 88 & 99
alpha helices: 18A-27A, 56A-66A, 18B-27B, 56B-66B
beta strands: 33E-41E, 44E-53E, 4E-13E, 72L-78L, 33E-41E, 44E-53E, 4E-13E, 72L-78L

Total number of restricting constraints per restrained residue:	32.3
Restricting long range constraints per restrained residue:	11.8

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

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
40.65	97.45	260.35

Dihedral angle violations per model

1 - 10 °	> 10 °
11.35	3.5

FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score
0.876	0.845	0.86	0.773

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	1.9 Å	0.7 Å	0.6 Å
All heavy atoms	2.5 Å	1.0 Å	1.0 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
91.7%	8.2%	0.1%	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

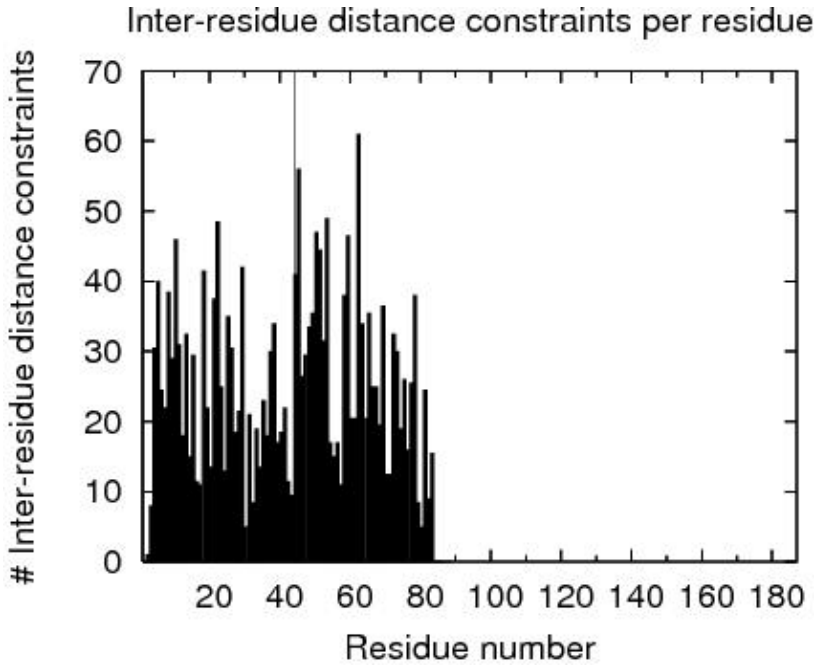
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.46	0.64	-0.14	0.15	5.86
Z-score[1]	0.00	-0.04	-0.24	0.89	0.52

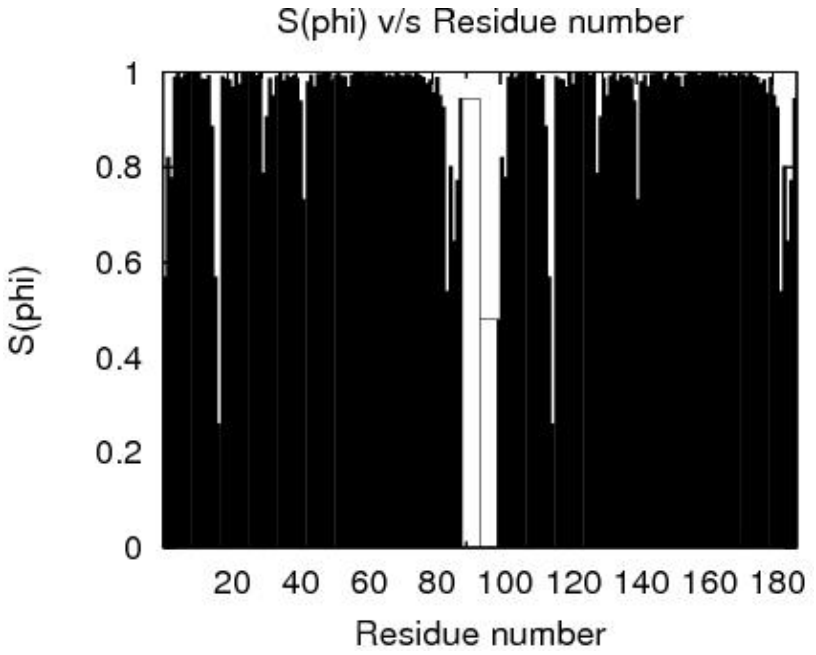
Generalized linear model RMSD prediction: 2.17

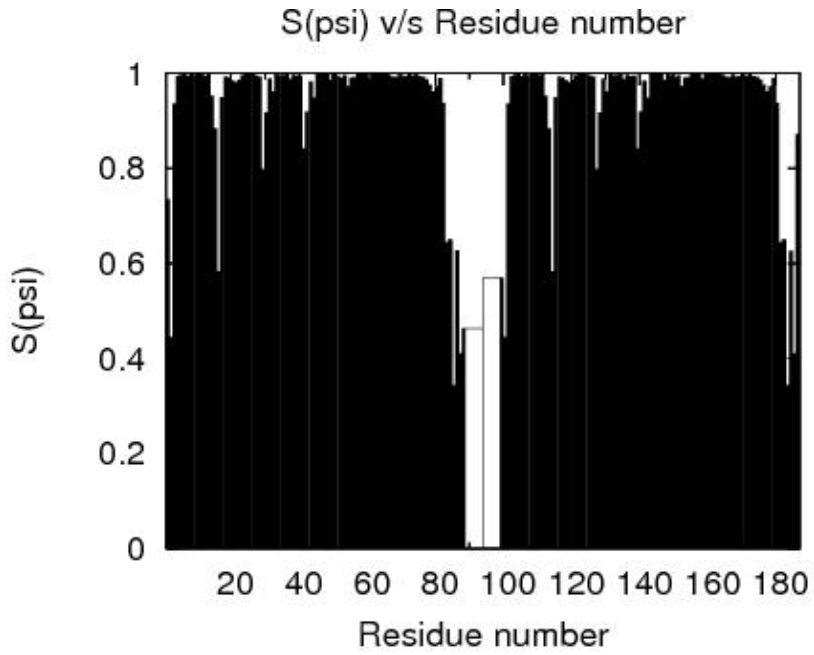
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

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:	0.010 Å

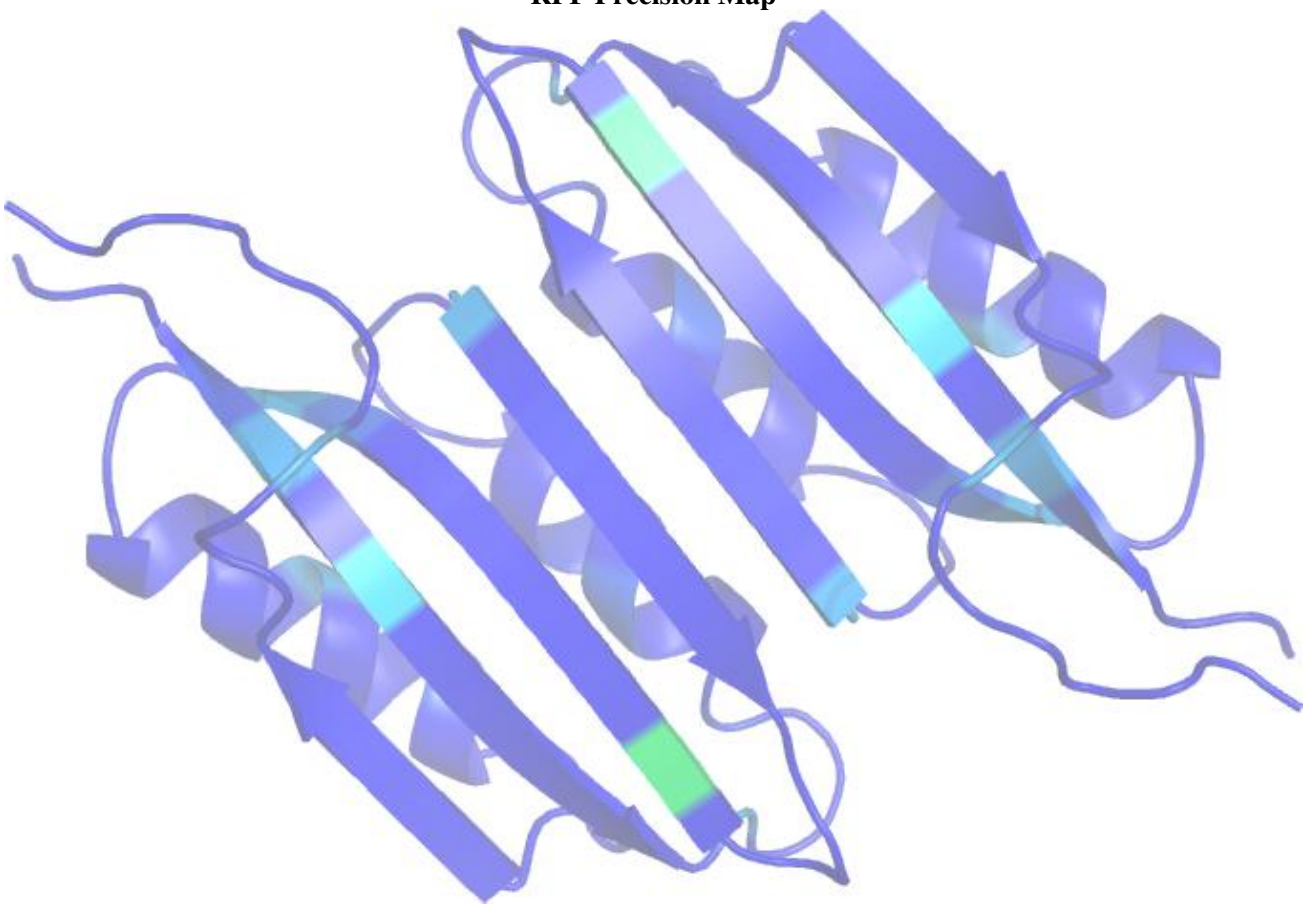
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 4A-14A,18A-28A,31A-40A,43A-82A,4B-14B,18B-28B,31B-40B,43B-82B
[3]Selected residues: 4A-15A,18A-28A,31A-41A,43A-82A,3B-15B,18B-41B,43B-77B


Inter-residue distance constraints per residue
Inter-residue distance constraints
70
60
50
40
30
20
10
0
20 40 60 80 100 120 140 160 180
Residue number

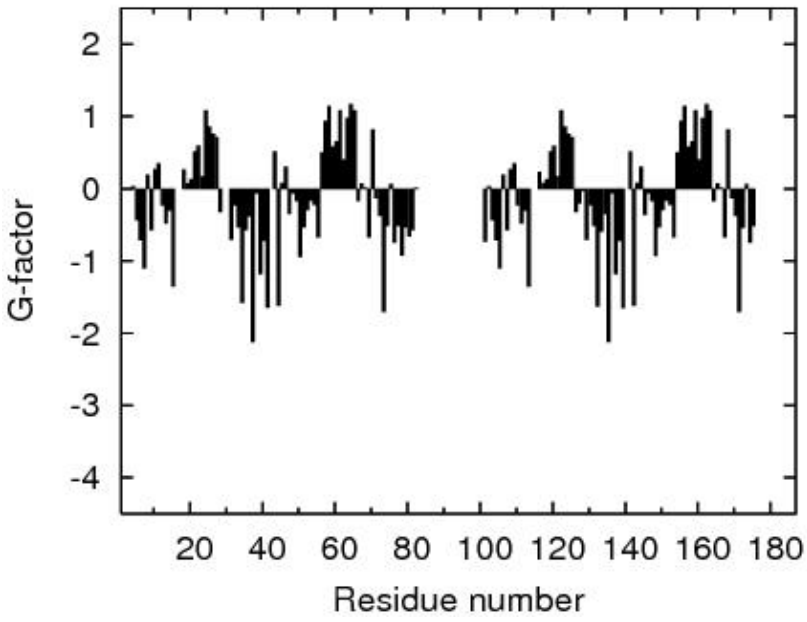

S(phi) v/s Residue number
S(phi)
1
0.8
0.6
0.4
0.2
0
20 40 60 80 100 120 140 160 180
Residue number



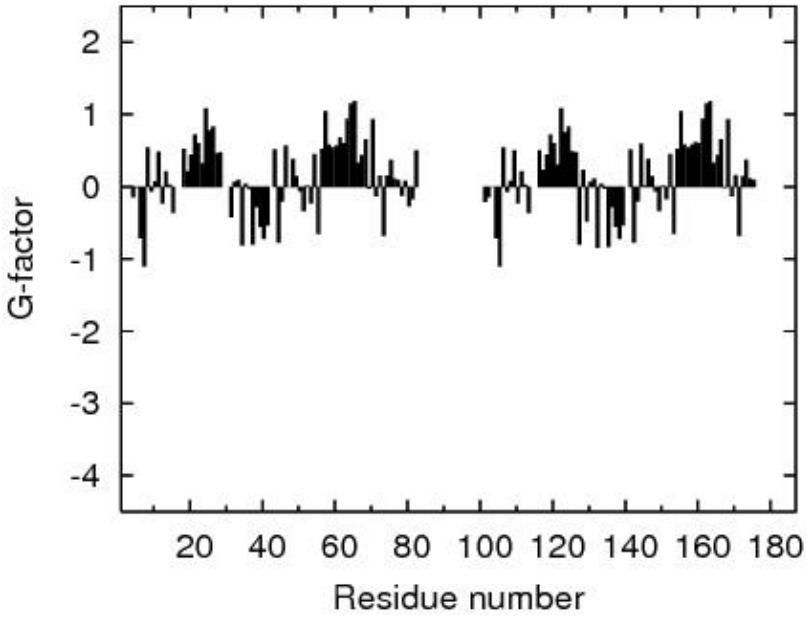
RPF Precision Map



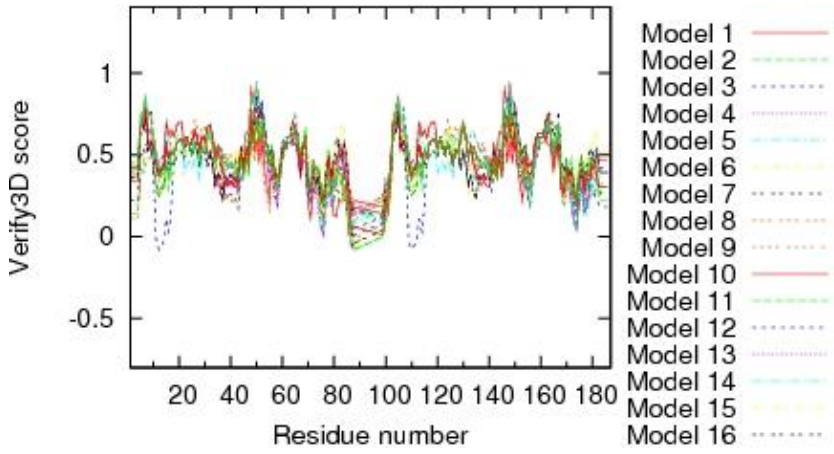
Procheck G-factor for phi-psi



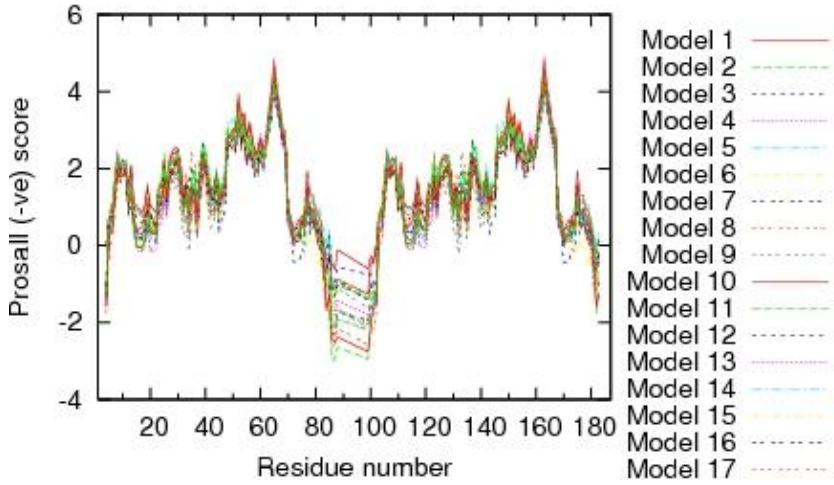
Procheck G-factor for all dihedral angles



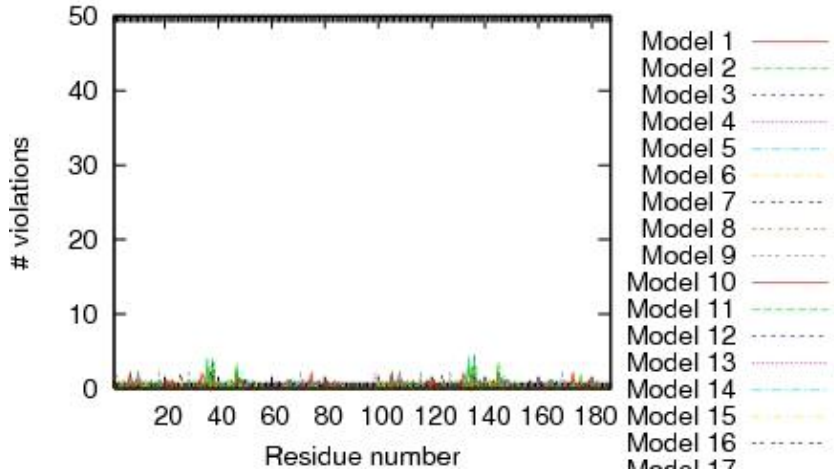
Verify3D score over window of 7 residues

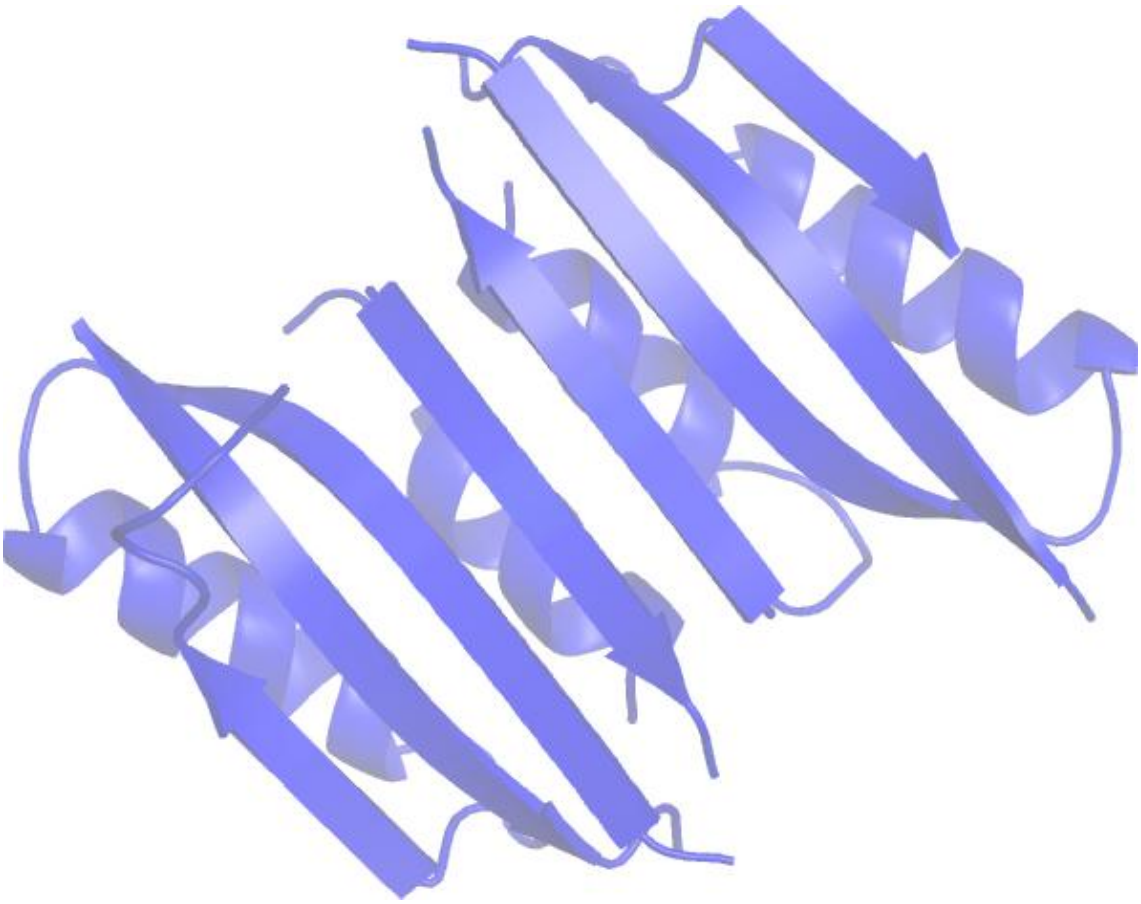


Prosall (-ve) score over window of 7 residues



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
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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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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
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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
```