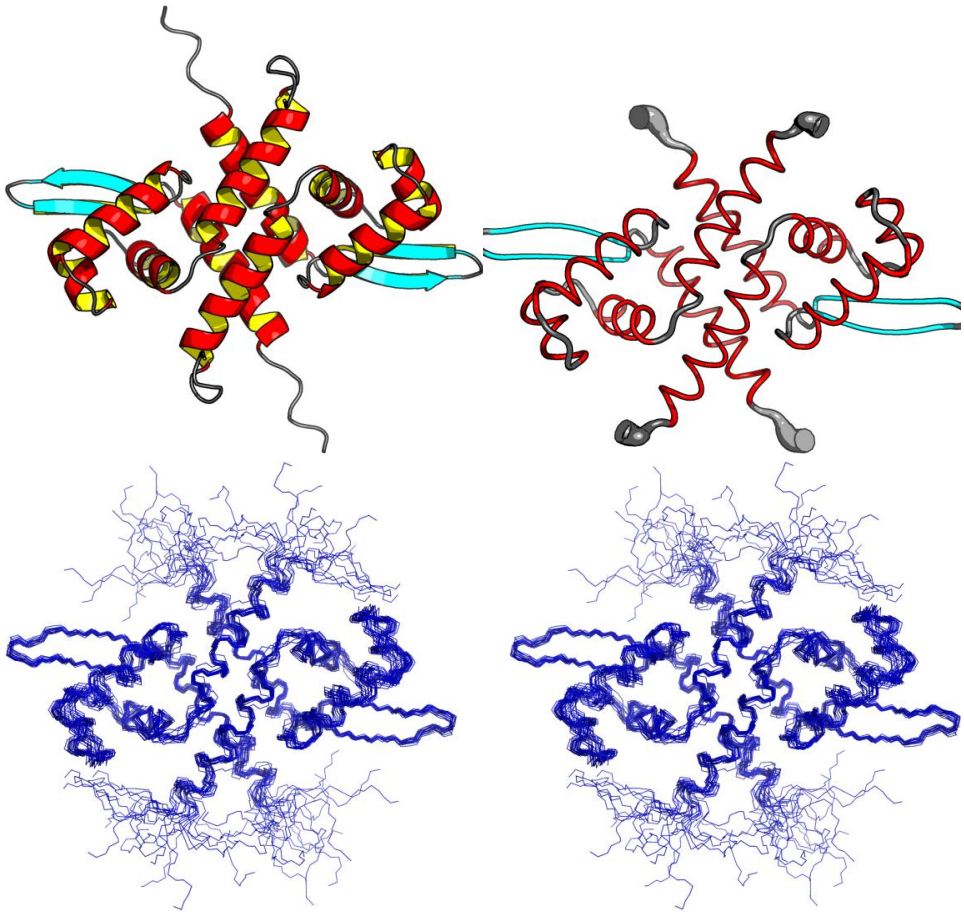
Structure Quality Analysis for NAME

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.):	216
Organism:	
SwissProt / TrEMBL ID:	
# models:	18
Oligomerization:	dimer
Molecular weight:	23434



Secondary Structure Elements:
Inter-chain break(s) between 108 & 119
alpha helices: 7A-22A, 27A-34A, 41A-48A, 52A-64A, 84A-101A, 7B-22B, 27B-34B, 41B-48B, 52B-64B, 84B-101B
beta strands: 39G-40G, 76G-81G, 68L-73L, 39G-40G, 76G-81G, 68L-73L

Total number of restricting constraints per restrained residue:	29.2
Restricting long range constraints per restrained residue:	6.7

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

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å

4.67 1.56 1
Dihedral angle violations per model

1 - 10 ° > 10 °
0 0
FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score
0.955	0.839	0.894	0.77

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	2.8 Å	0.7 Å	0.7 Å
All heavy atoms	3.2 Å	1.1 Å	1.1 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
99.7%	0.3%	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
99.9%	0.1%	0%		

Global quality scores

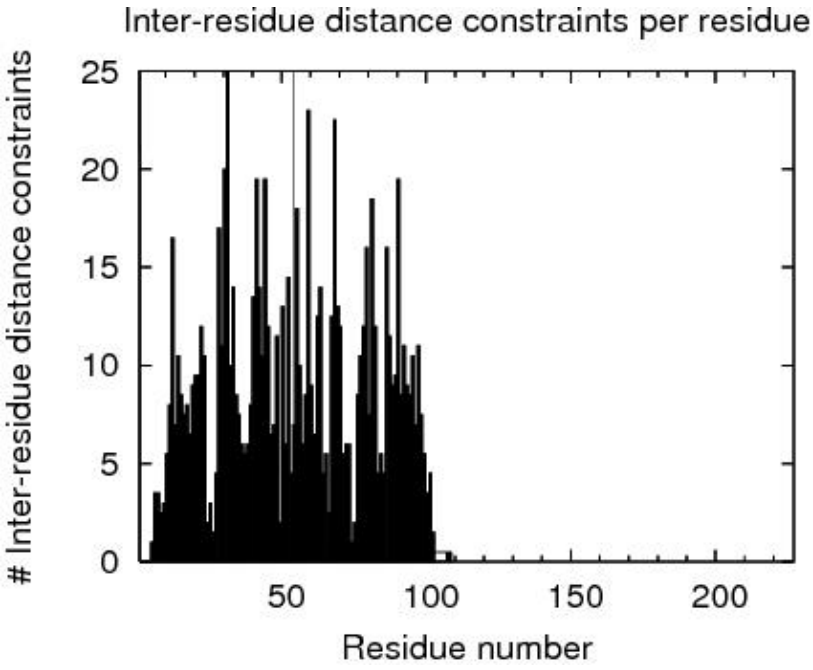
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.42	0.88	0.49	0.52	4.11
Z-score[1]	-0.64	0.95	2.24	3.08	0.82

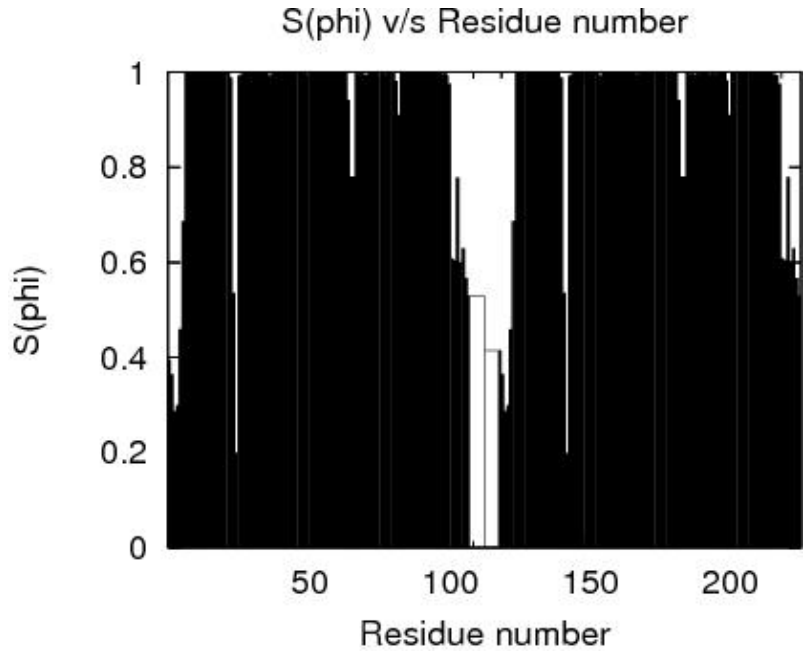
Generalized linear model RMSD prediction: 1.99

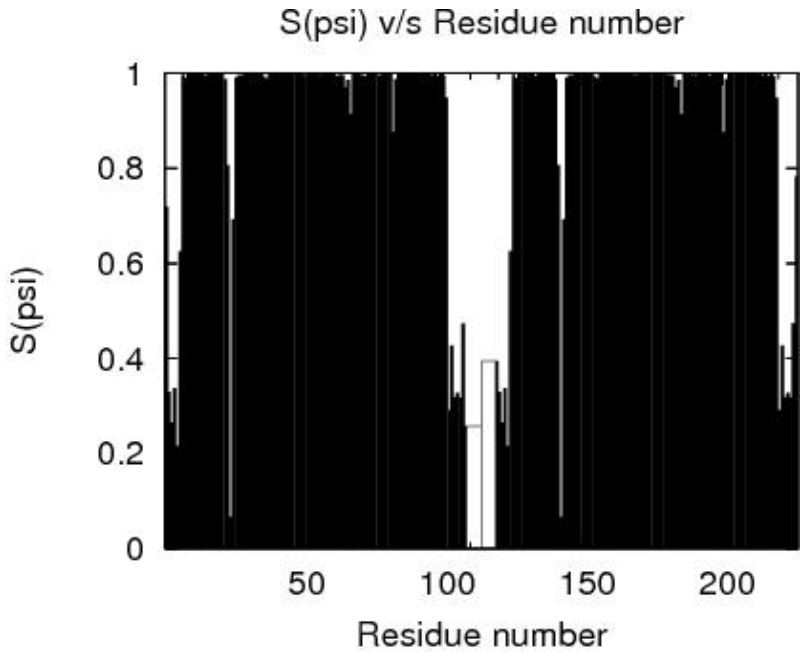
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

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:	0.009 Å

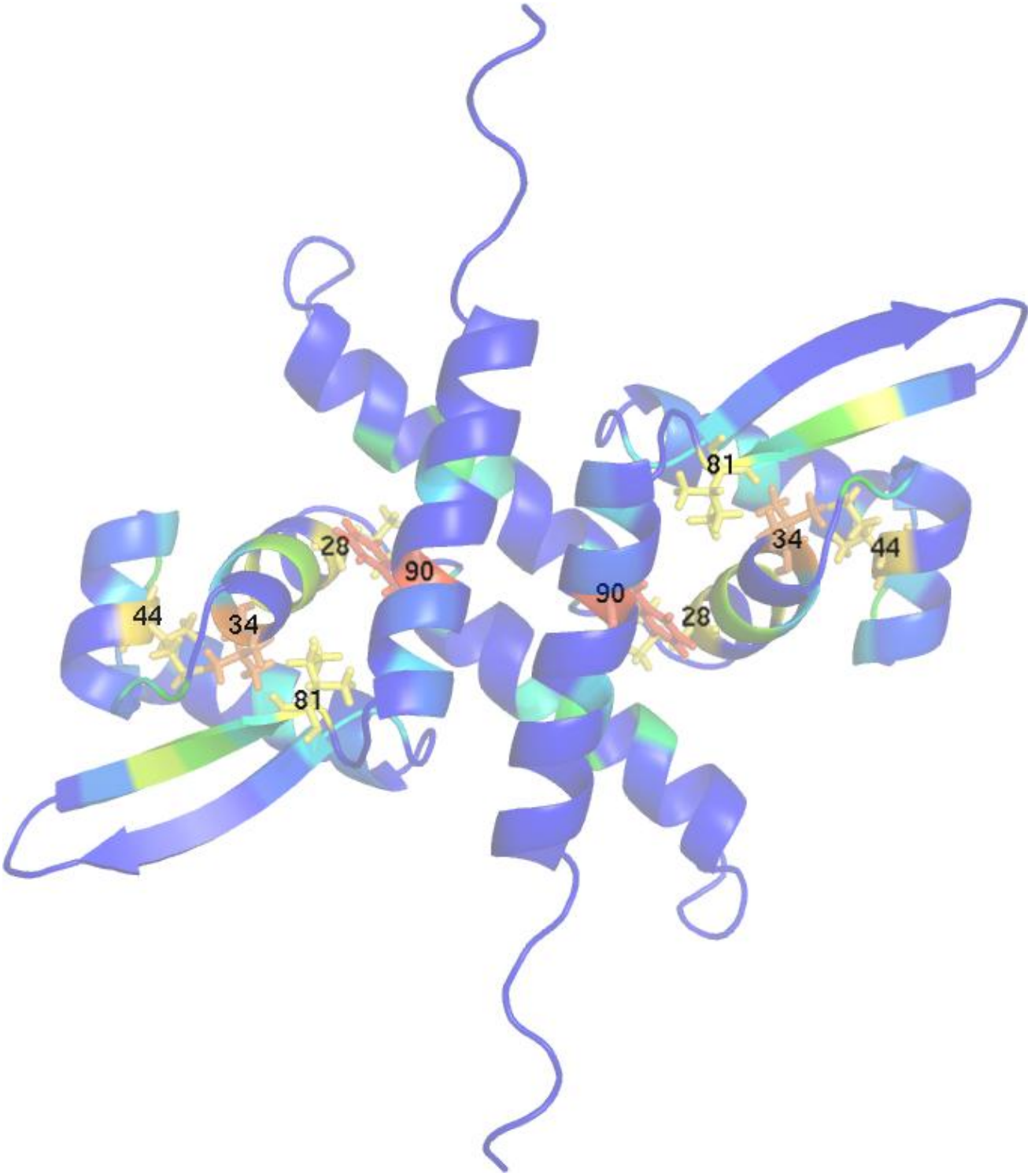
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 7A-22A,26A-65A,68A-101A,7B-22B,26B-65B,68B-101B
[3]Selected residues: 7A-22A,26A-65A,68A-101A,7B-22B,26B-100B

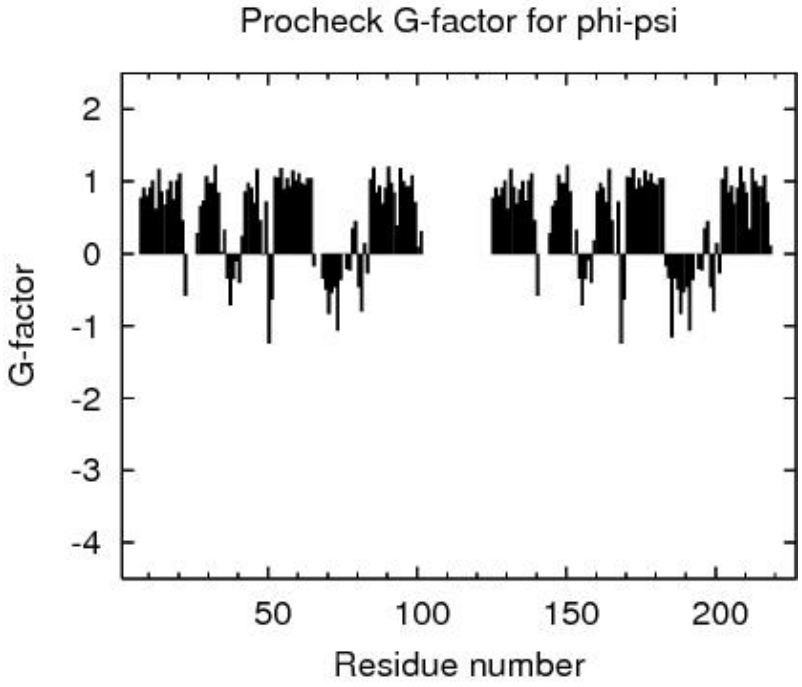

Inter-residue distance constraints per residue
Inter-residue distance constraints
25
20
15
10
5
0
50
100
150
200
Residue number

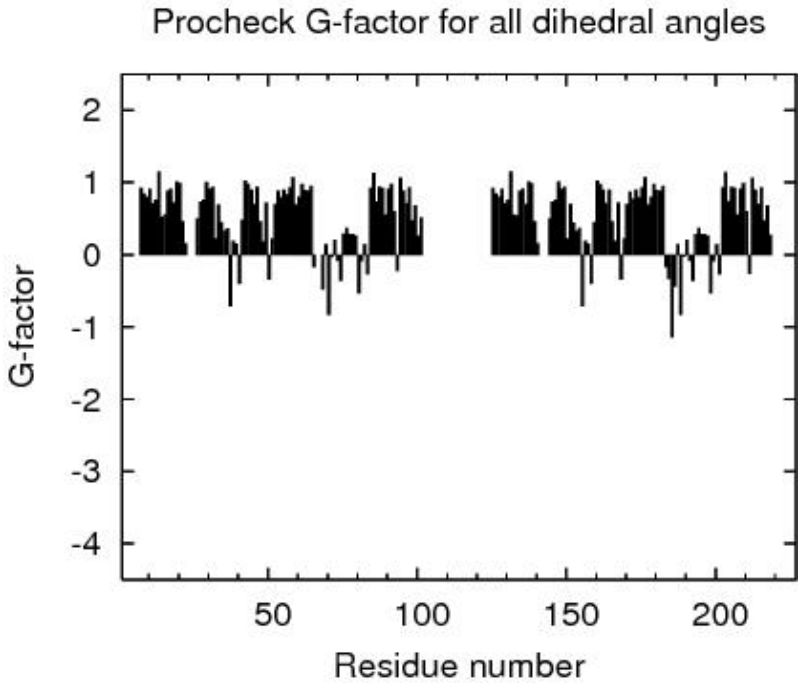

S(phi) v/s Residue number
S(phi)
1
0.8
0.6
0.4
0.2
0
50
100
150
200
Residue number

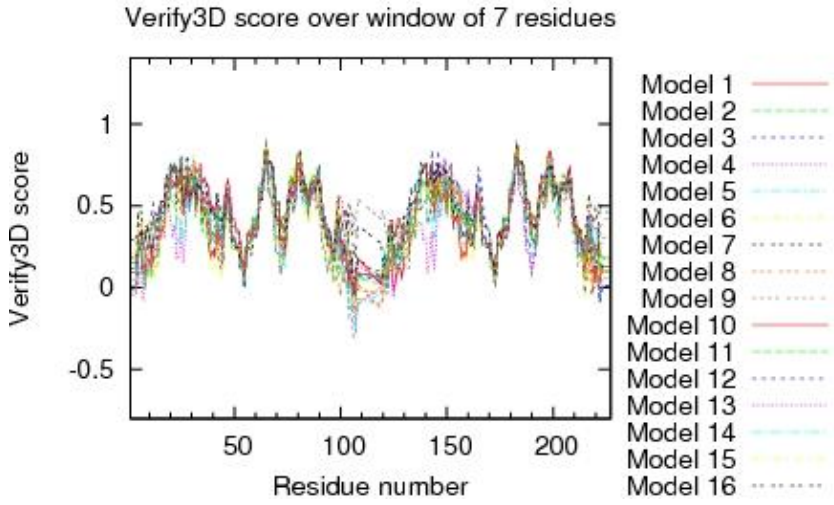


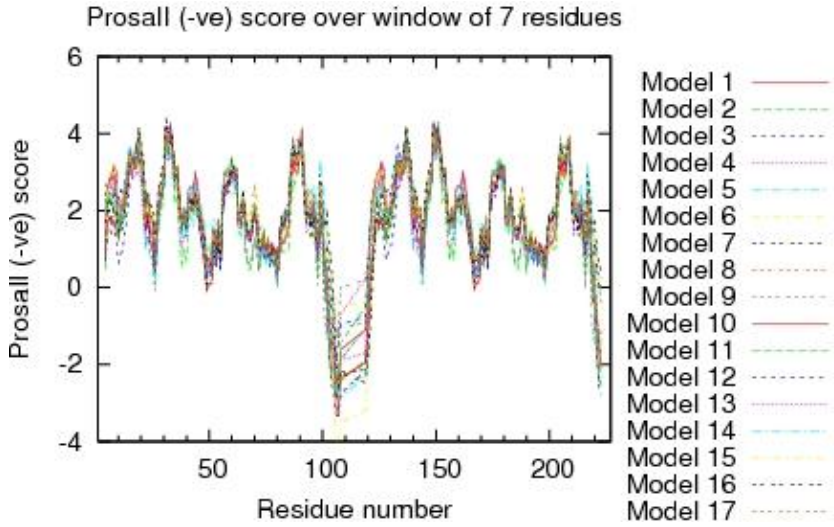
RPF Precision Map

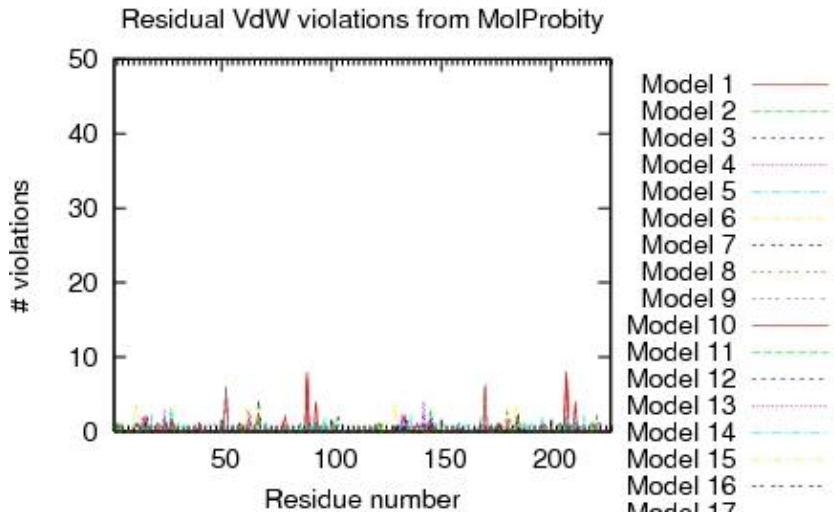

81
34
44
28
90
90
28
44
34
81

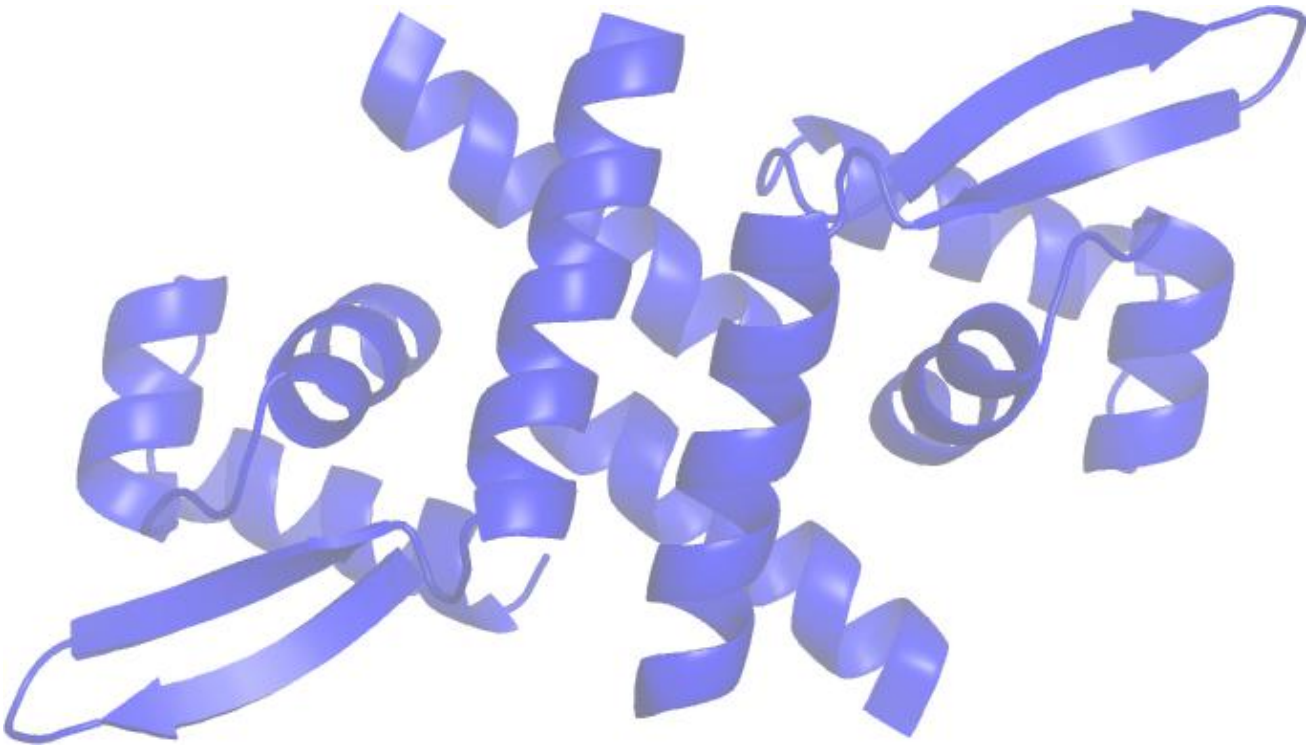

Procheck G-factor for phi-psi
G-factor
2
1
0
-1
-2
-3
-4
50
100
150
200
Residue number


Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
50
100
150
200
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
50
100
150
200
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10
Model 11
Model 12
Model 13
Model 14
Model 15
Model 16


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
50
100
150
200
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10
Model 11
Model 12
Model 13
Model 14
Model 15
Model 16
Model 17


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
50
100
150
200
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10
Model 11
Model 12
Model 13
Model 14
Model 15
Model 16



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

References:

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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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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.

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
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