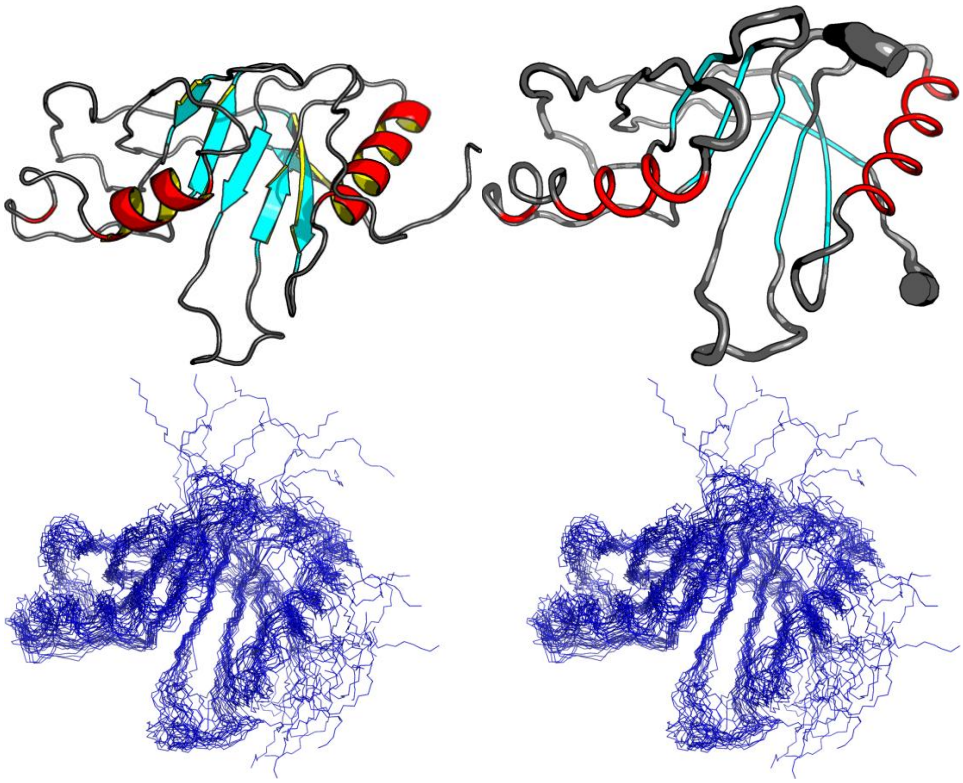
Structure Quality Analysis for NAME

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.):	166
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	monomer
Molecular weight:	18119



Secondary Structure Elements:
alpha helices: 28A-40A, 110A-123A
beta strands: 10U-13U, 96S-103S, 148G-153G, 131A-134A, 58E-62E, 68R-72R, 23G-27G, 75E-76E, 18O-22O, 87L-91L

Total number of restricting constraints per restrained residue:	11.4
Restricting long range constraints per restrained residue:	2.6

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

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
6.25	0.95	0

Dihedral angle violations per model

1 - 10 °	> 10 °

16.15 0
FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score
0.974	0.938	0.955	0.734

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	3.8 Å	1.5 Å	1.5 Å
All heavy atoms	4.5 Å	1.9 Å	1.9 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
92.7%	6.5%	0.1%	0.7%

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

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
96.8%	3.1%	0.1%		

Global quality scores

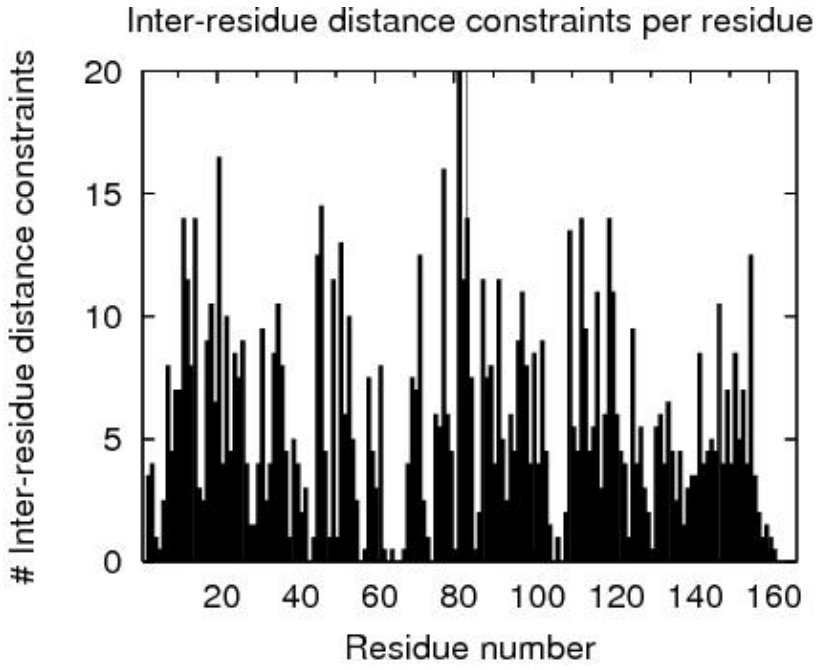
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.36	0.28	-0.41	-0.51	32.05
Z-score[1]	-1.61	-1.53	-1.30	-3.02	-3.97

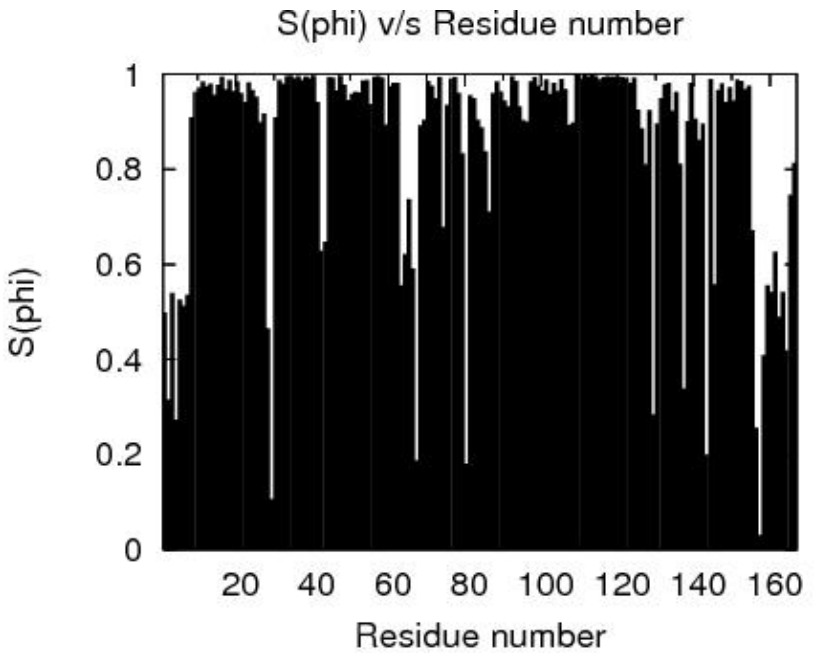
Generalized linear model RMSD prediction: 2.52

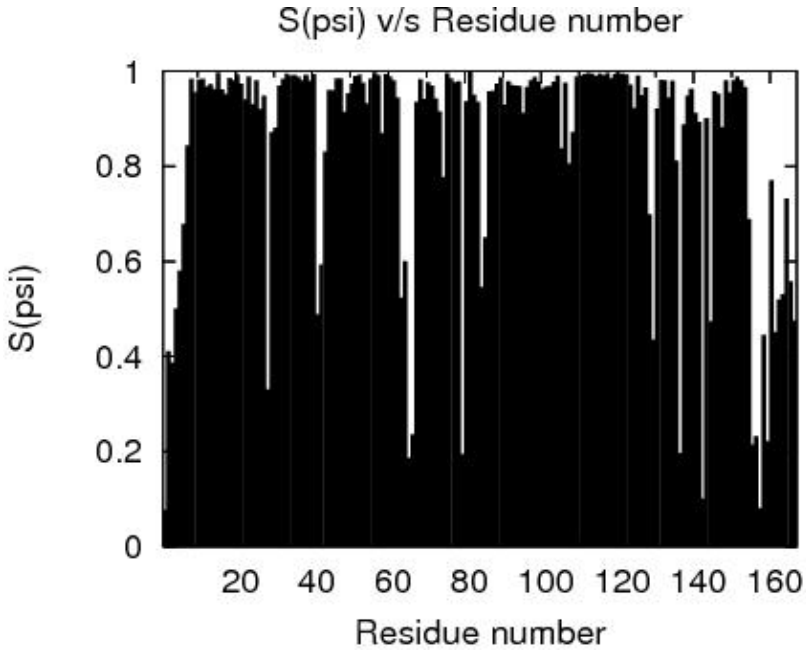
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	165
RMS deviation for bond angles:	0.7 °
RMS deviation for bond lengths:	0.004 Å

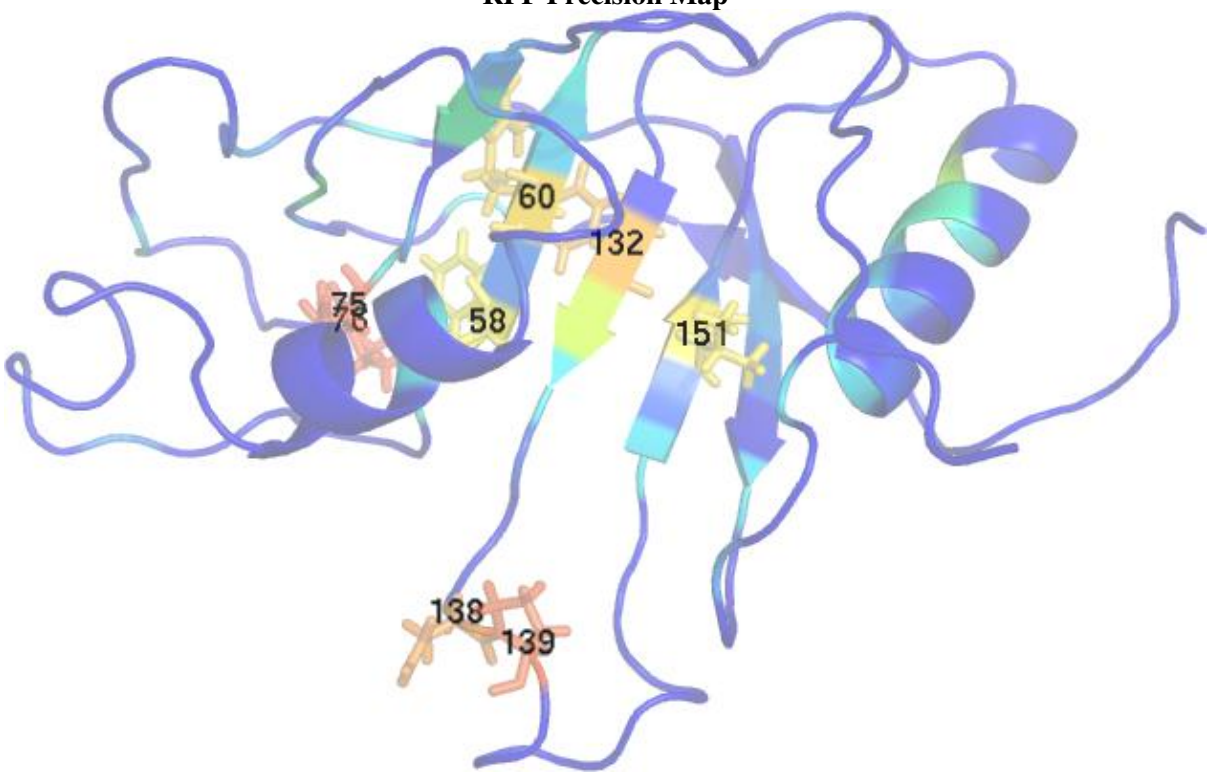
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues:
8A-27A,31A-40A,44A-62A,68A-73A,75A-78A,81A-83A,87A-106A,109A-126A,130A-134A,138A-140A,146A-153A
[3]Selected residues:
8A-27A,31A-40A,44A-62A,68A-73A,75A-78A,81A-83A,87A-106A,109A-126A,130A-134A,138A-140A,146A-153A


Inter-residue distance constraints per residue
Inter-residue distance constraints
0
5
10
15
20
20
40
60
80
100
120
140
160
Residue number

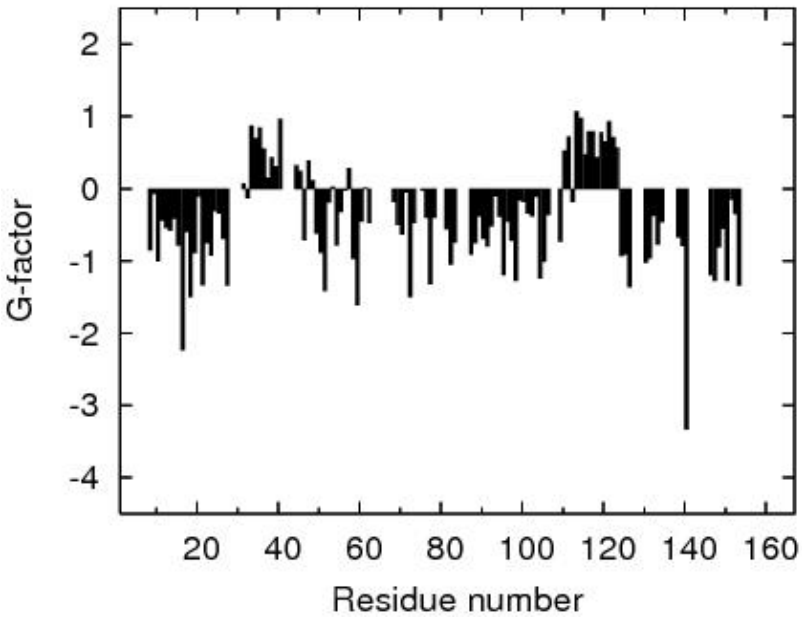

S(phi) v/s Residue number
S(phi)
0
0.2
0.4
0.6
0.8
1
20
40
60
80
100
120
140
160
Residue number



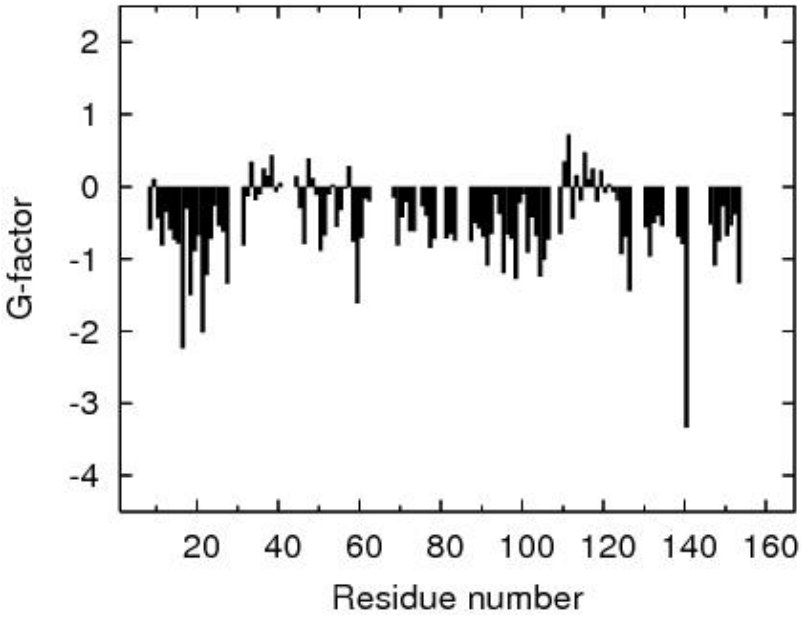
RPF Precision Map

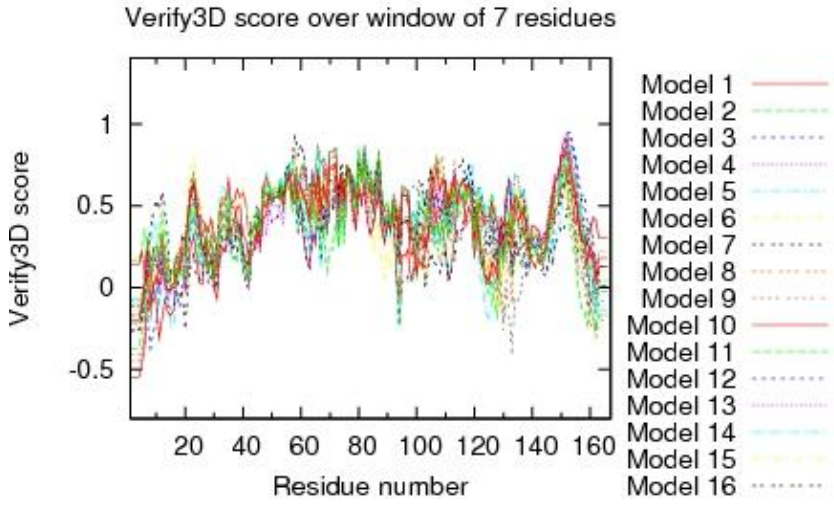


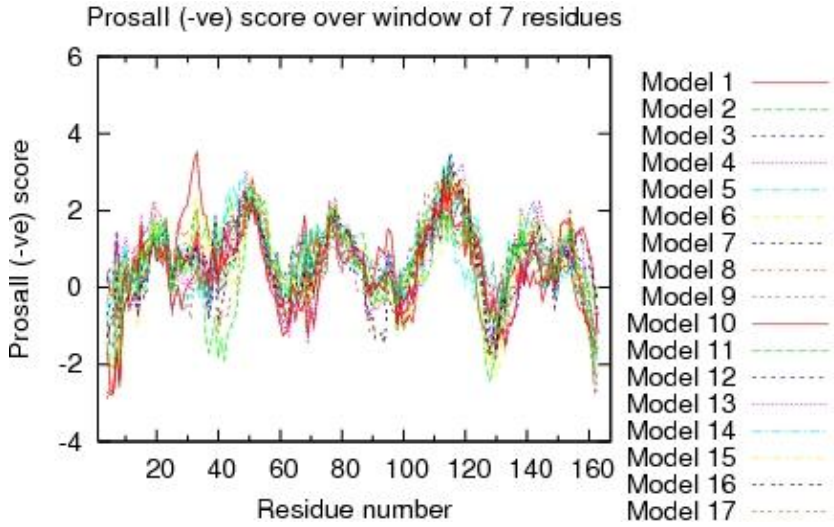
Procheck G-factor for phi-psi

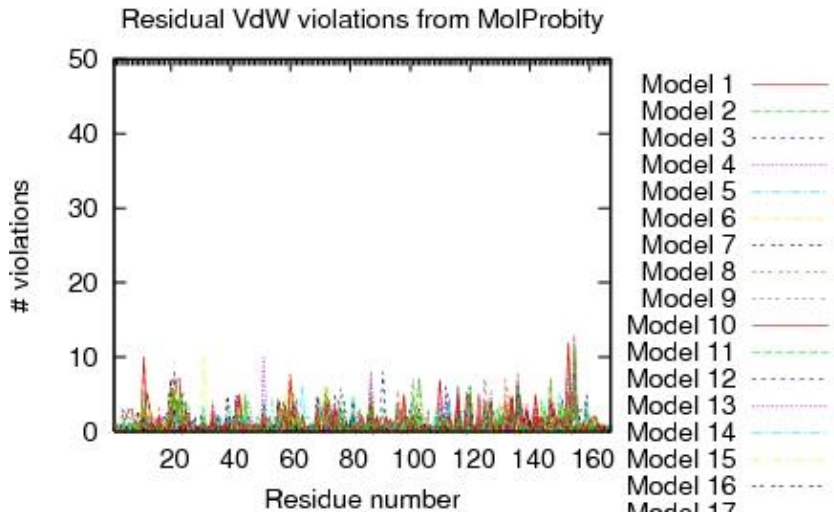


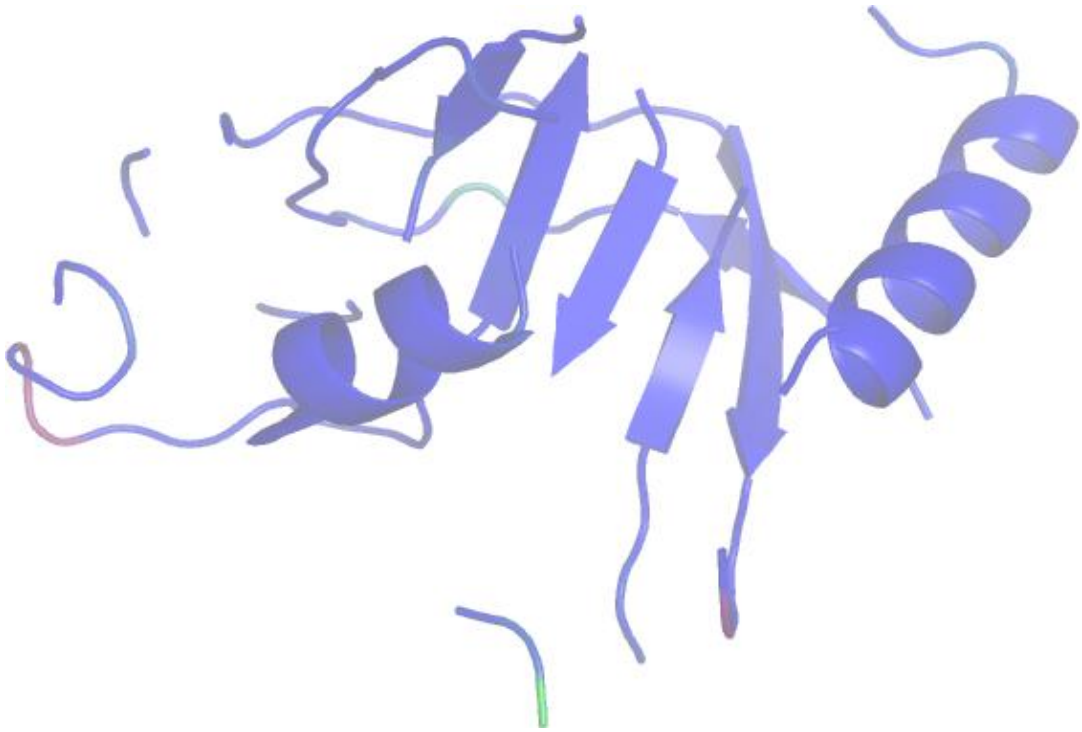
Procheck G-factor for all dihedral angles




Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
20 40 60 80 100 120 140 160
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
20 40 60 80 100 120 140 160
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
20 40 60 80 100 120 140 160
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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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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11. Luthy R, McLachlan A D and Eisenberg D, "Secondary Structure-Based Profiles: Use of Structure-Conserving Scoring Tables in Searching Protein Sequence Databases for Structural Similarities", Proteins 10 (1991): 229-239
12. Richardson D C, Richardson J S, "The kinemage: a tool for scientific communication", Prot Sci 1(1)

(1992): 3-9
13. Koradi, R, et al, "MOLMOL: a program for display and analysis of macromolecular structures ", J Mol Graphics 14 (1996): 51-55.
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
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
```