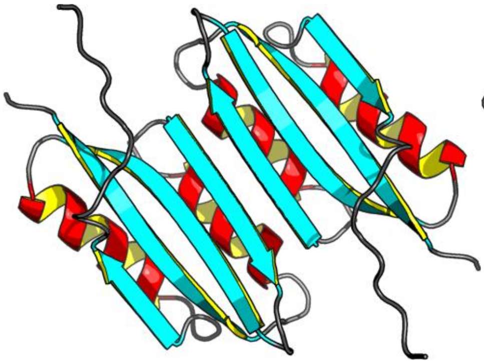
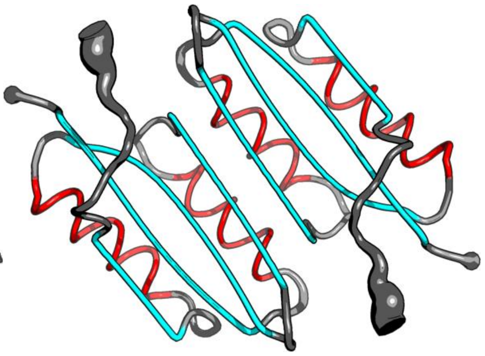
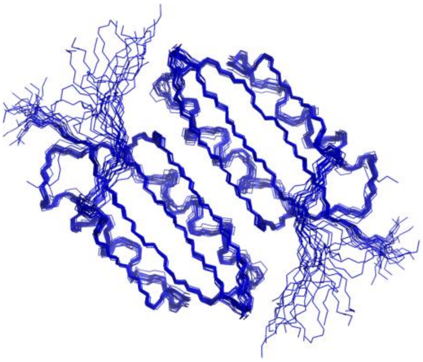
Structure Quality Analysis for NAME

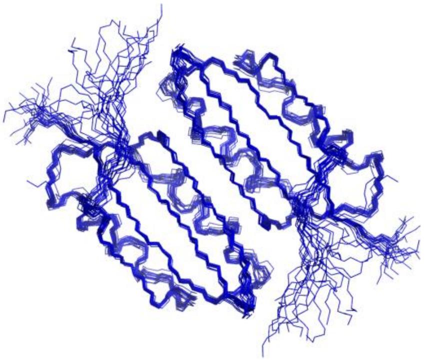
Analyses performed for user defined residues.
The constraints analysis is based on the following files: NOE distance constraints file. Angular constraints file.
Procheck analysis,RMSD calculation and structure superimposition are based on: User defined residues

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-40E, 44E-53E, 4E-13E, 72L-78L, 33E-40E, 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
20.5	10.75	2.35

Dihedral angle violations per model

1 - 10 °	> 10 °
0.25	0

FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score
0.911	0.844	0.876	0.824

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	1.6 Å	0.5 Å	0.4 Å
All heavy atoms	2.0 Å	0.6 Å	0.6 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
96.1%	3.8%	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	0.45	0.70	0.02	0.02	9.13
Z-score[1]	-0.16	0.21	0.39	0.12	-0.04

Generalized linear model RMSD prediction: 1.85

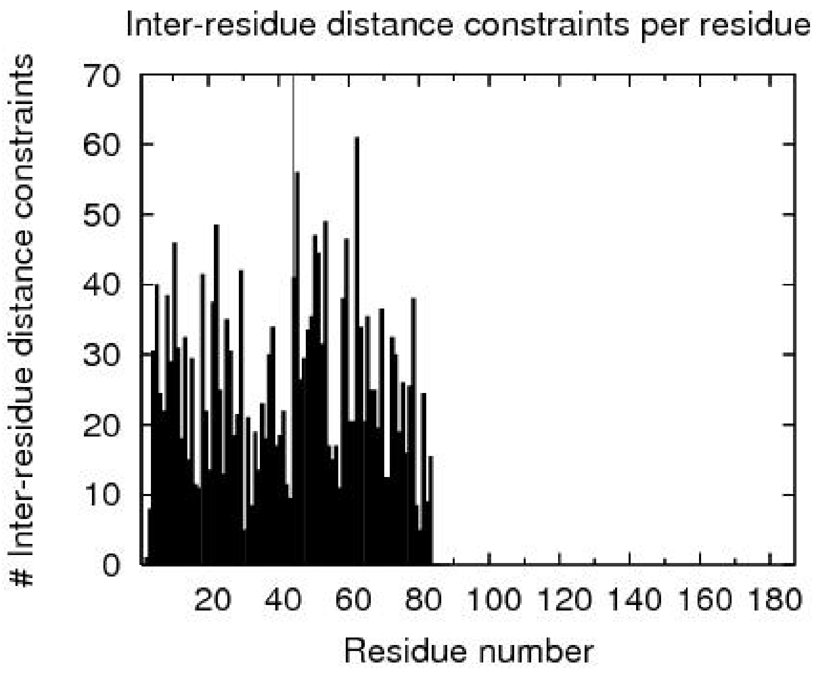
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

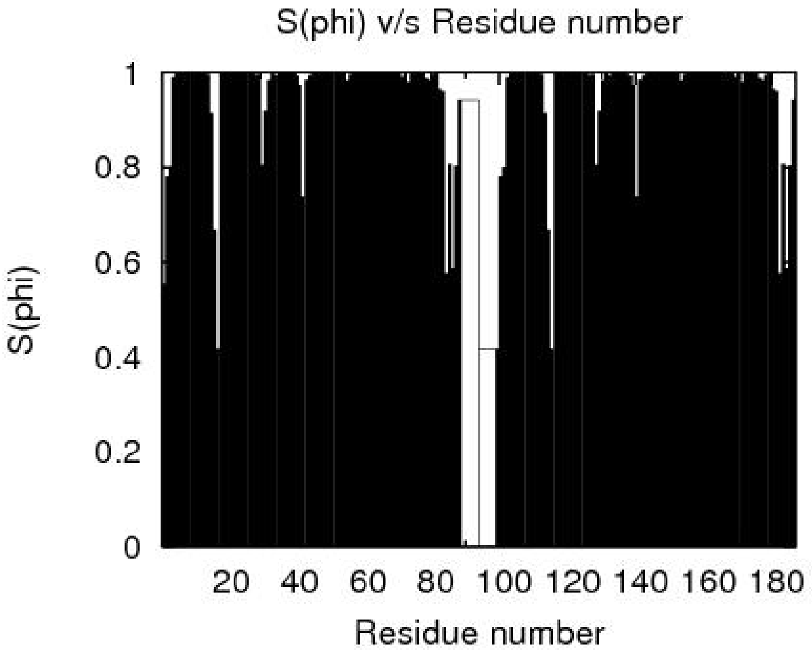
Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	0
RMS deviation for bond angles:	0.7 °
RMS deviation for bond lengths:	0.010 Å

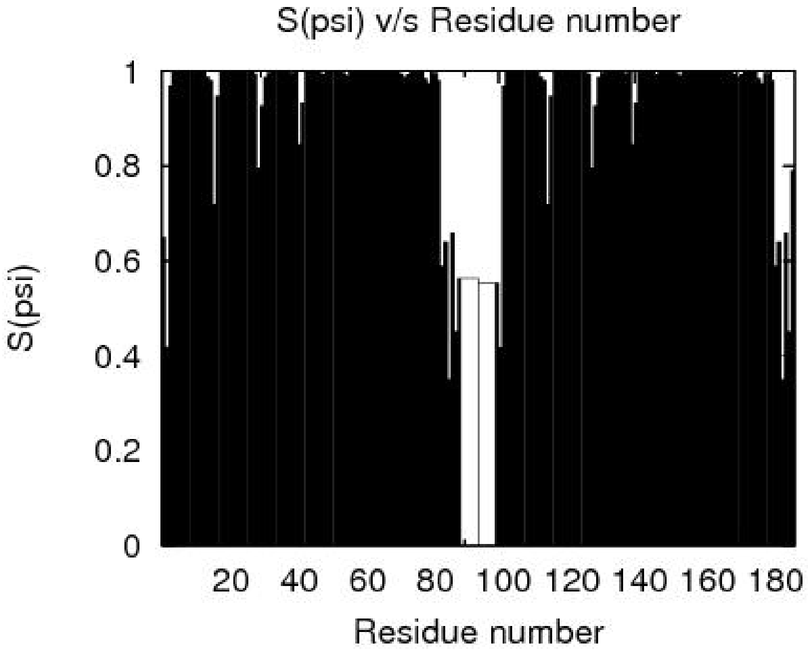
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

[2] Order residues: 4A-15A,18A-28A,31A-41A,43A-82A,4B-15B,18B-28B,31B-41B,43B-82B

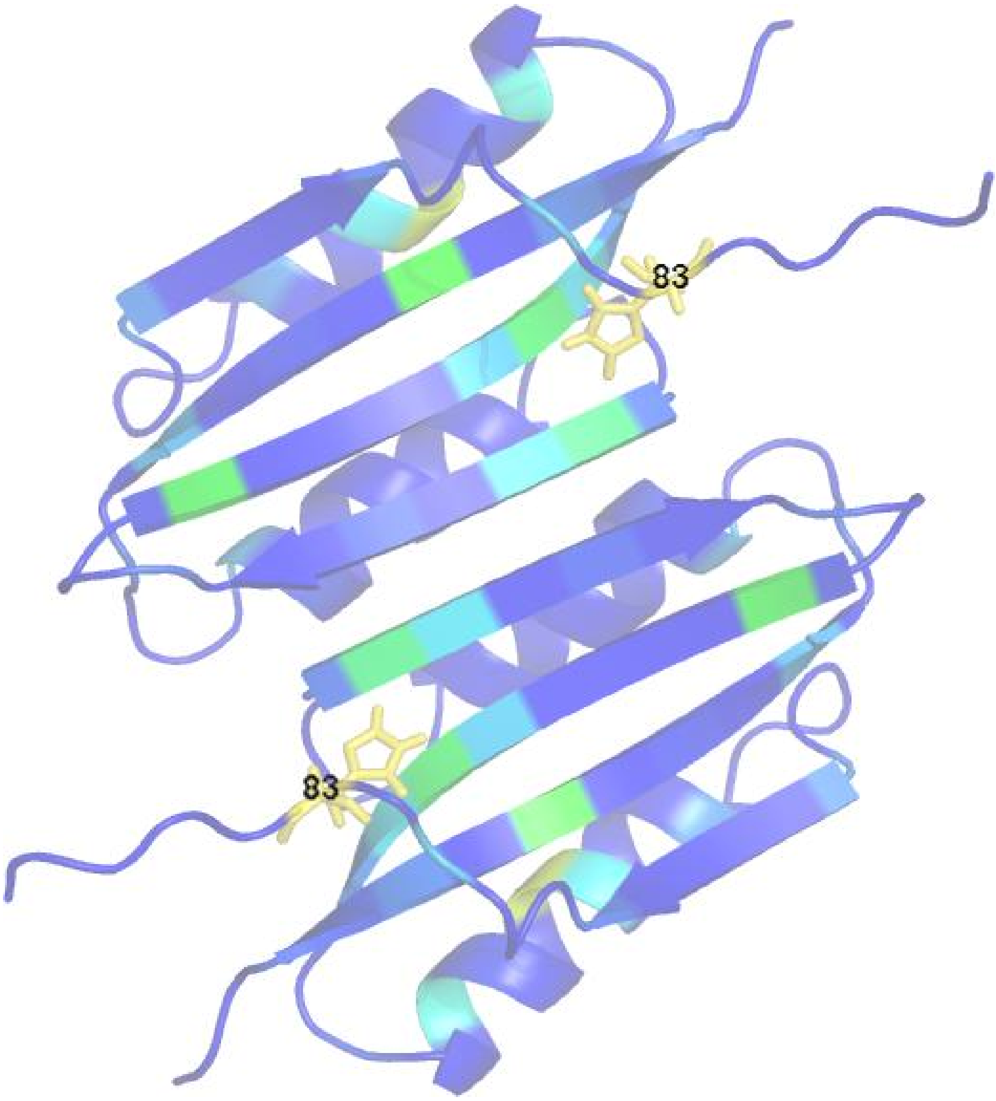
[3] Selected residues: 4A-15A,18A-28A,31A-41A,43A-82A,3B-15B,18B-41B,43B-77B


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

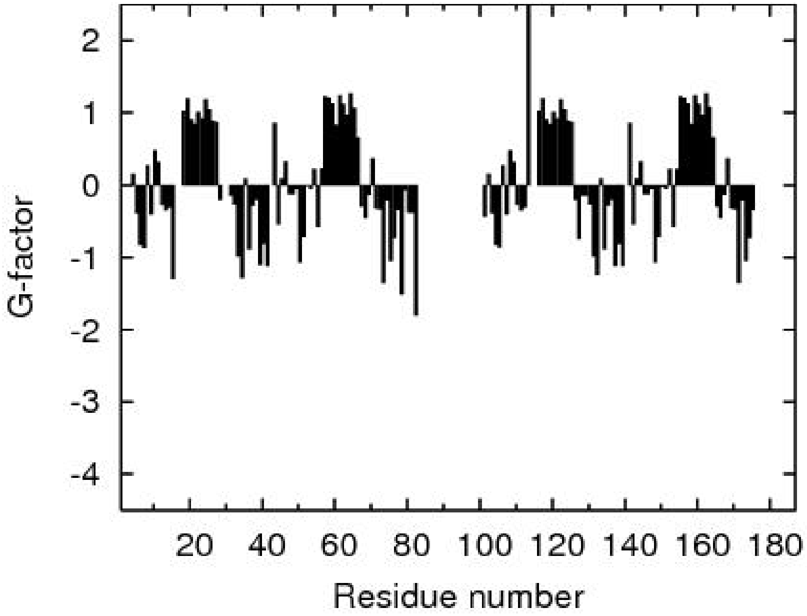

S(phi) v/s Residue number
S(phi)
0
0.2
0.4
0.6
0.8
1
20
40
60
80
100
120
140
160
180
Residue number



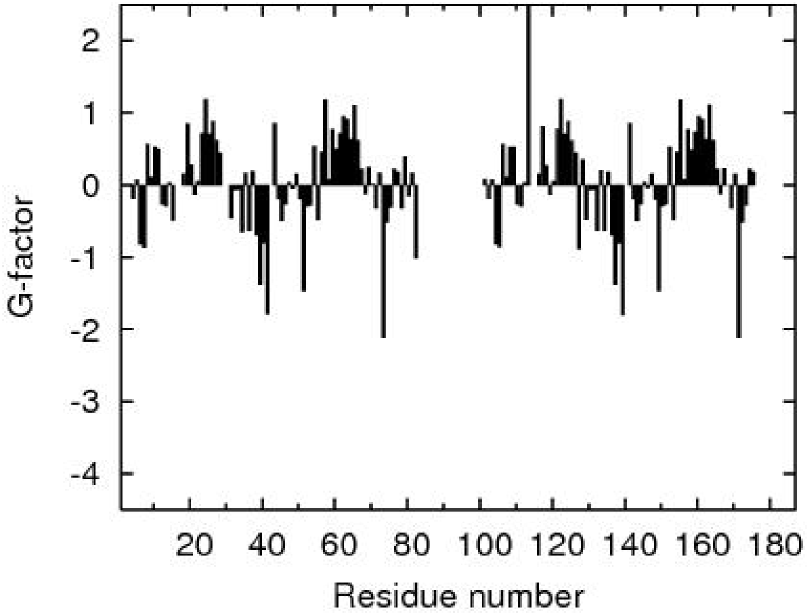
RPF Precision Map

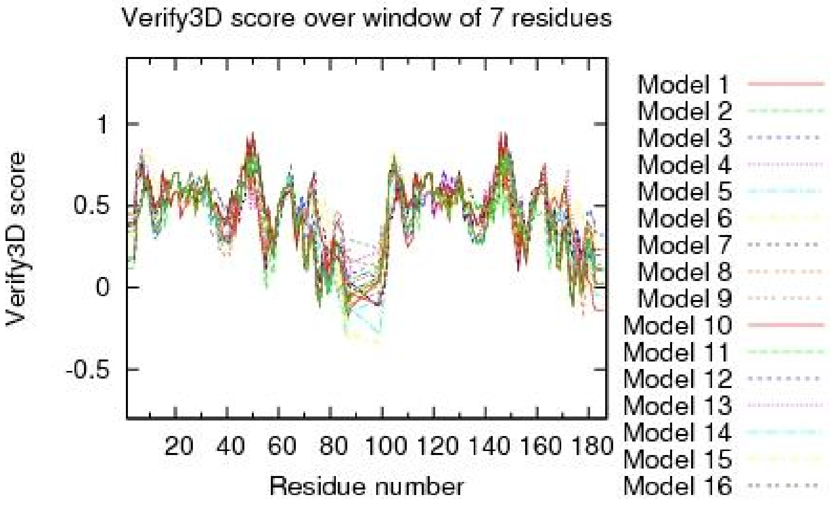

83
83

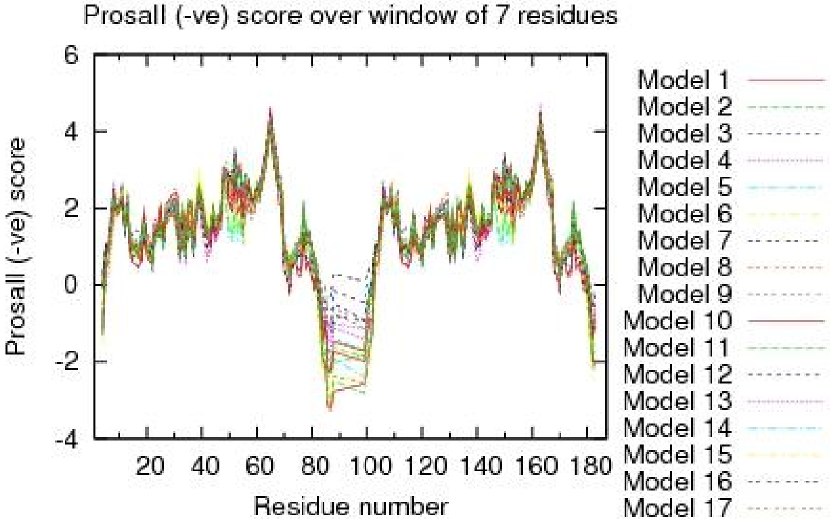
Procheck G-factor for phi-psi

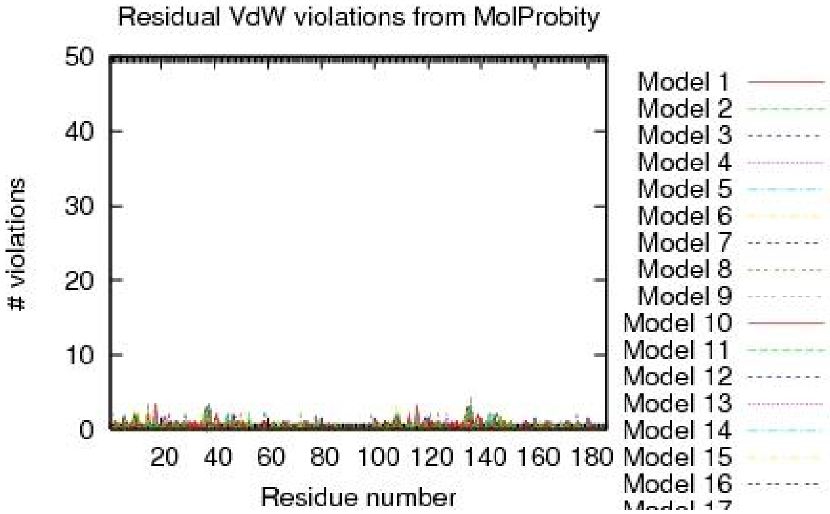


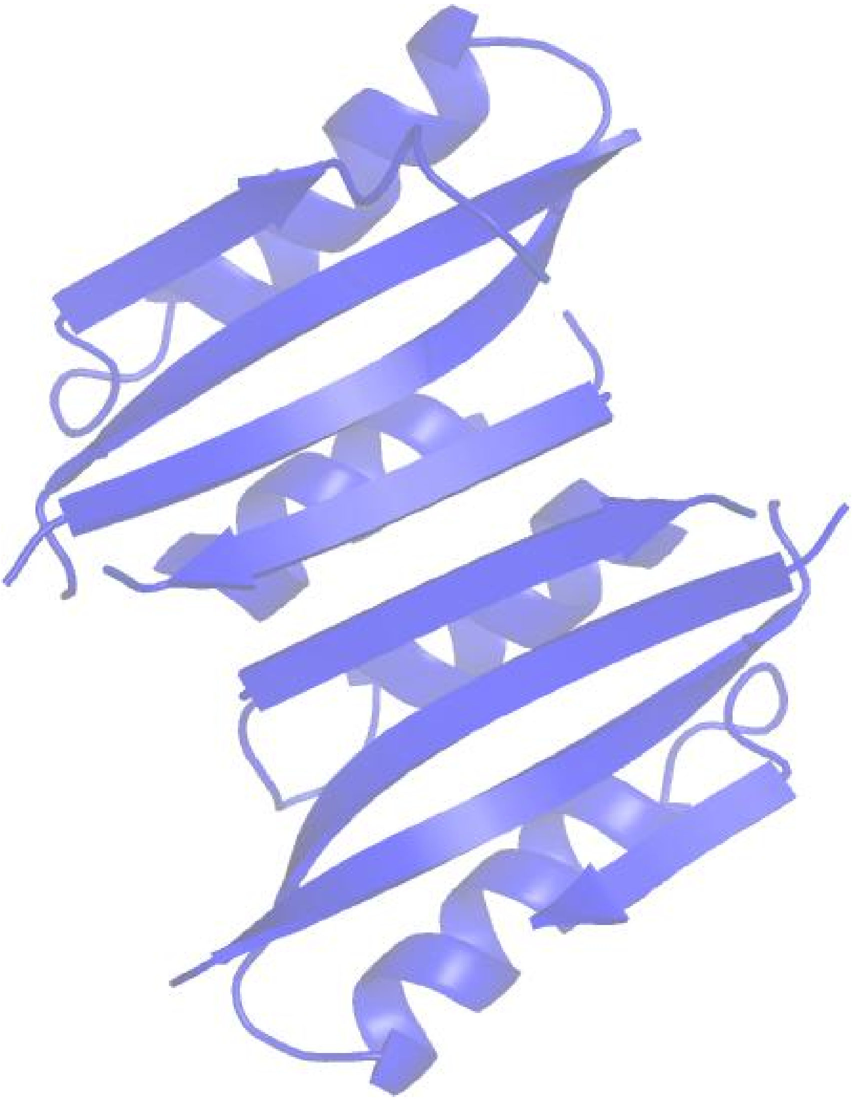
Procheck G-factor for all dihedral angles




Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
20
40
60
80
100
120
140
160
180
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
180
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
180
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:

1. Luthy R, Bowie J U and Eisenberg D, "Assessment of protein models with three-dimensional profiles", Nature 356 (1992): 83-85
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
6. Laskowski R A et al "PROCHECK: a program to check the stereochemical quality of protein structures" J Appl Cryst, 26 (1993): 283-291

7. Word J M et al, "Exploring steric constrains on protein mutations using MAGE / PROBE", Prot Sci 9 (2000): 2251-2259
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
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
10. Tejero R and Montelione G T, "PDBStat", unpublished
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
16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features", Biopolymers (1983) 22: 2577-2637
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.

Protein Structure Validation Suite (PSVS)

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
```