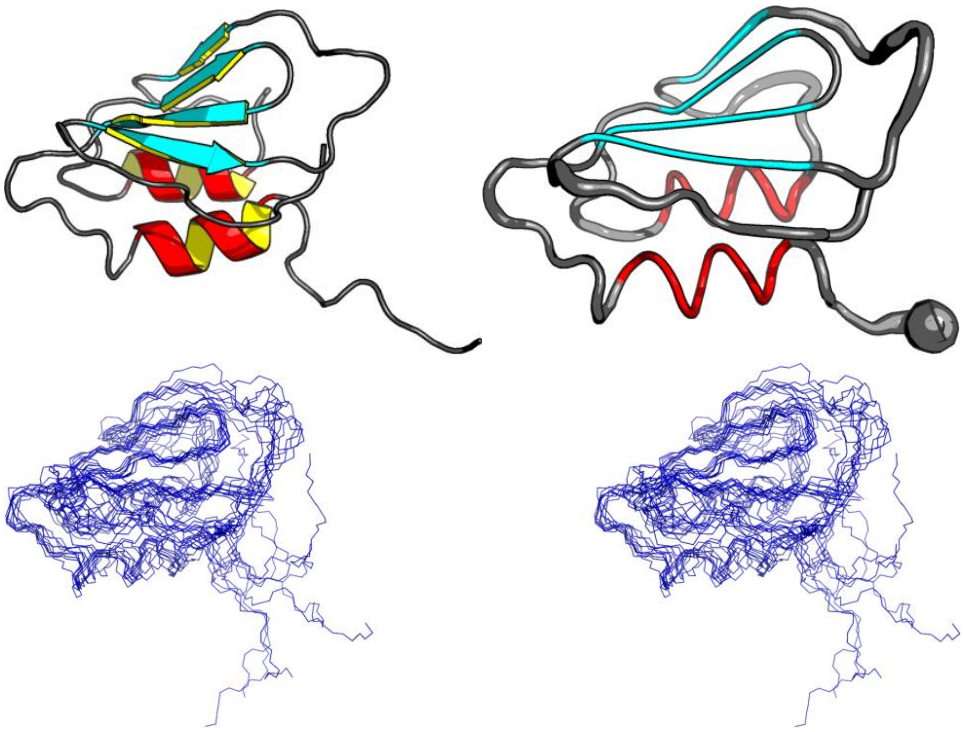
Structure Quality Analysis for NAME

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.):	91
Organism:	
SwissProt / TrEMBL ID:	
# models:	10
Oligomerization:	monomer
Molecular weight:	10472



Secondary Structure Elements:
alpha helices: 40A-46A, 71A-80A
beta strands: 3E-6E, 14R-19R, 60E-64E, 54E-57E, 28R-31R

Total number of restricting constraints per restrained residue:	15.7
Restricting long range constraints per restrained residue:	5.1

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

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
12.6	20.4	69.8

Dihedral angle violations per model

1 - 10 °	> 10 °
6.4	6.5

FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score
0.89	0.787	0.835	0.723

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	2.8 Å	1.2 Å	1.2 Å
All heavy atoms	3.6 Å	1.7 Å	1.7 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
88.8%	9.2%	0.6%	1.5%

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

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
95.9%	3.9%	0.2%		

Global quality scores

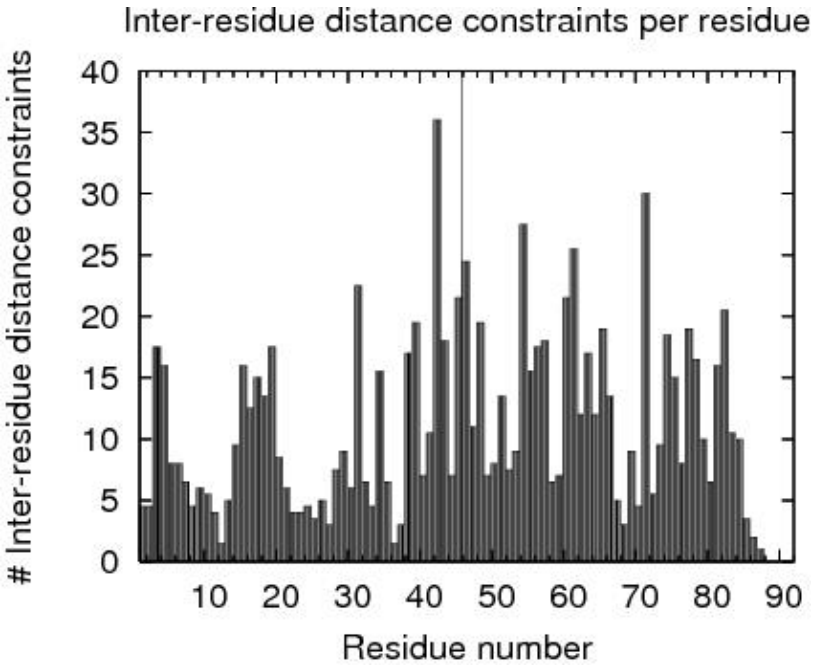
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.35	0.57	-0.28	0.07	7.45
Z-score[1]	-1.77	-0.33	-0.79	0.41	0.25

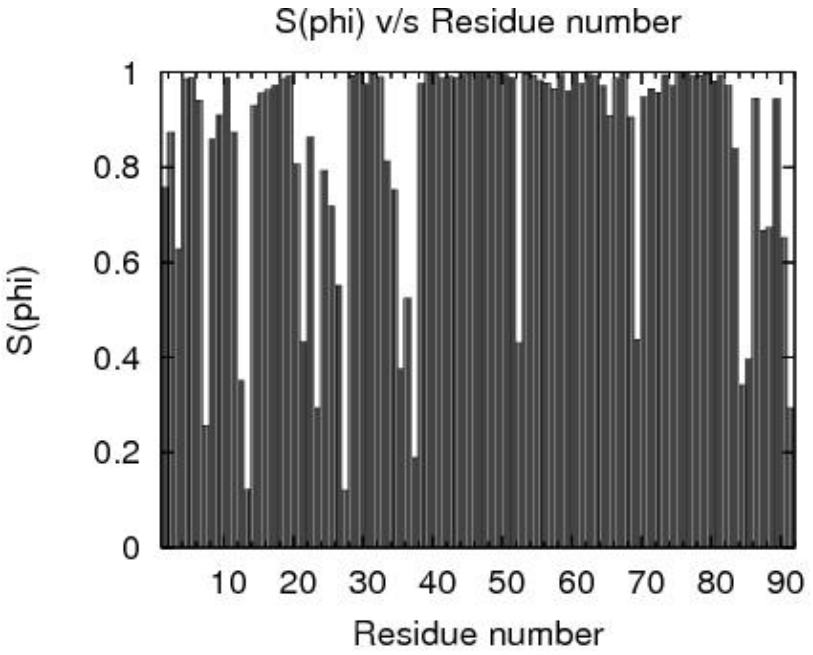
Generalized linear model RMSD prediction: 1.58

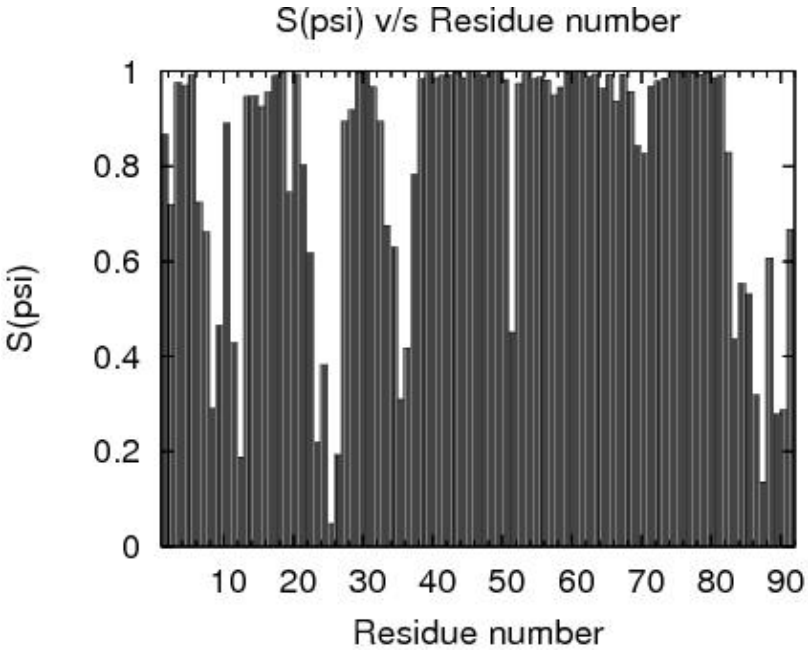
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	1
RMS deviation for bond angles:	0.5 °
RMS deviation for bond lengths:	0.010 Å

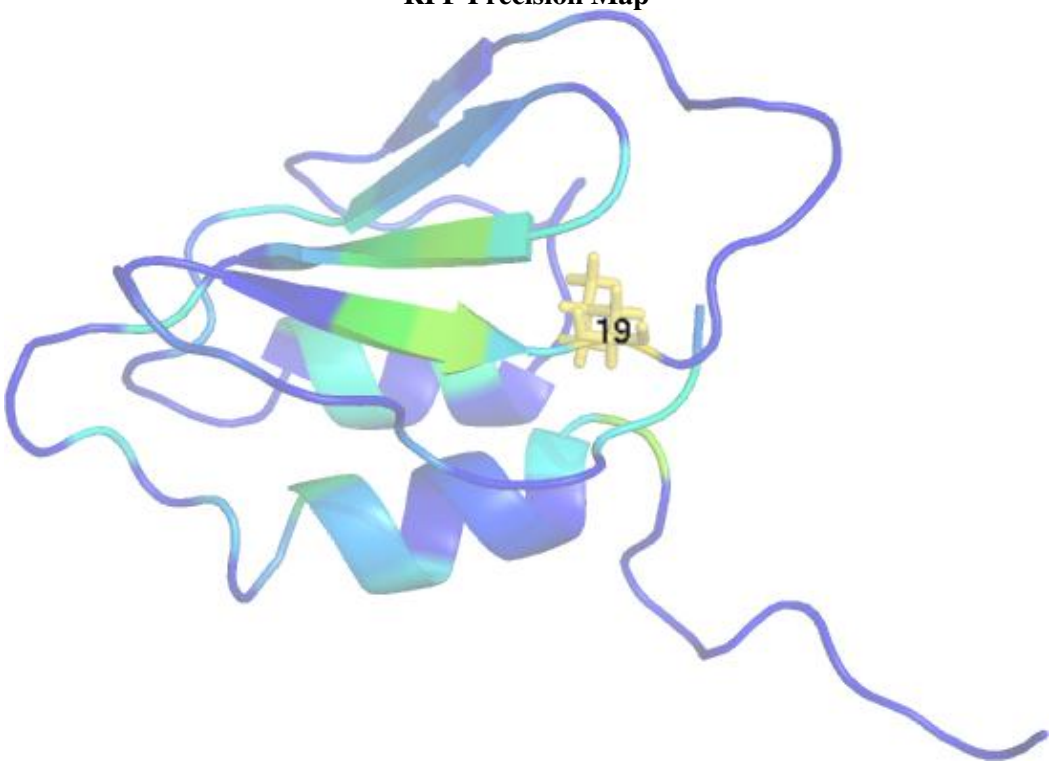
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 14A-18A,28A-32A,38A-50A,53A-68A,71A-82A
[3]Selected residues: 14A-18A,28A-32A,38A-50A,53A-67A,70A-82A


Inter-residue distance constraints per residue
Inter-residue distance constraints
0
5
10
15
20
25
30
35
40
10
20
30
40
50
60
70
80
90
Residue number

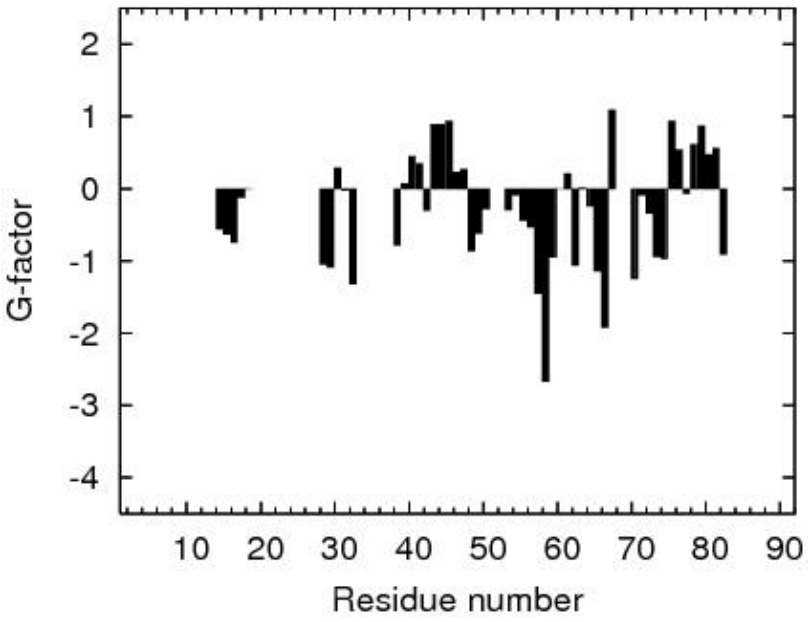

S(phi) v/s Residue number
S(phi)
0
0.2
0.4
0.6
0.8
1
10
20
30
40
50
60
70
80
90
Residue number



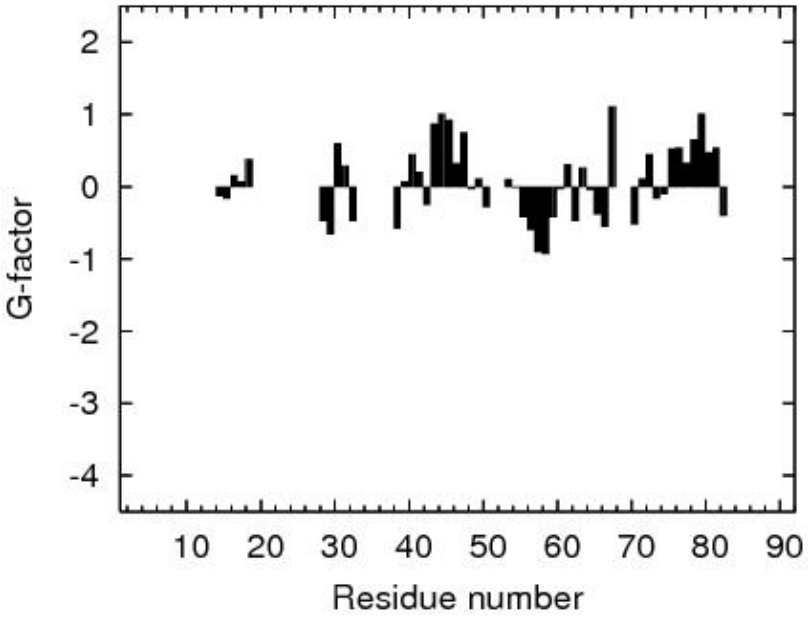
RPF Precision Map

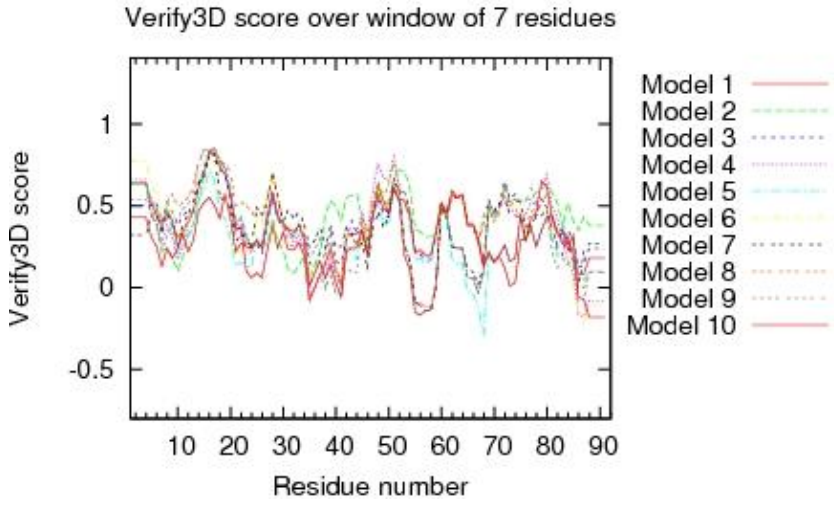


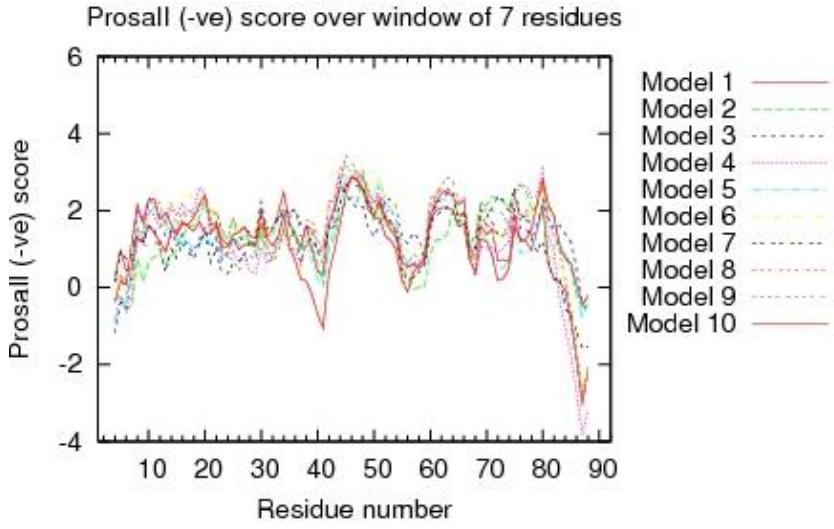
Procheck G-factor for phi-psi

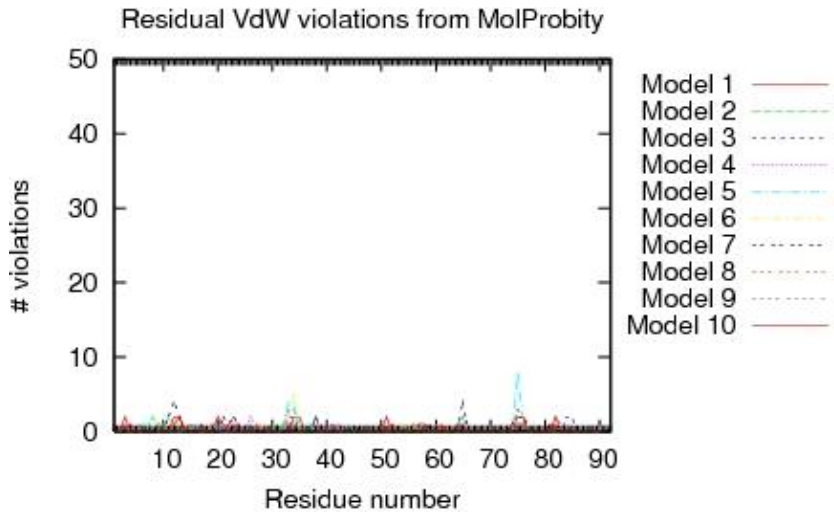


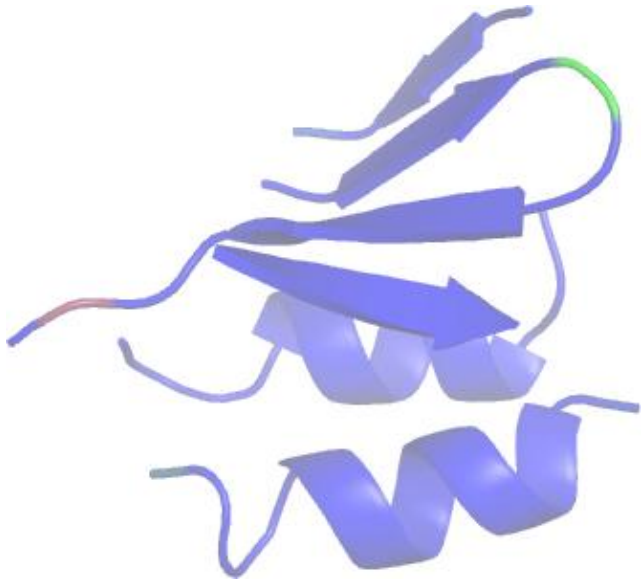
Procheck G-factor for all dihedral angles




Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
10 20 30 40 50 60 70 80 90
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
10 20 30 40 50 60 70 80 90
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
10 20 30 40 50 60 70 80 90
Residue number
Model 1
Model 2
Model 3
Model 4
Model 5
Model 6
Model 7
Model 8
Model 9
Model 10



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
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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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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.

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
```