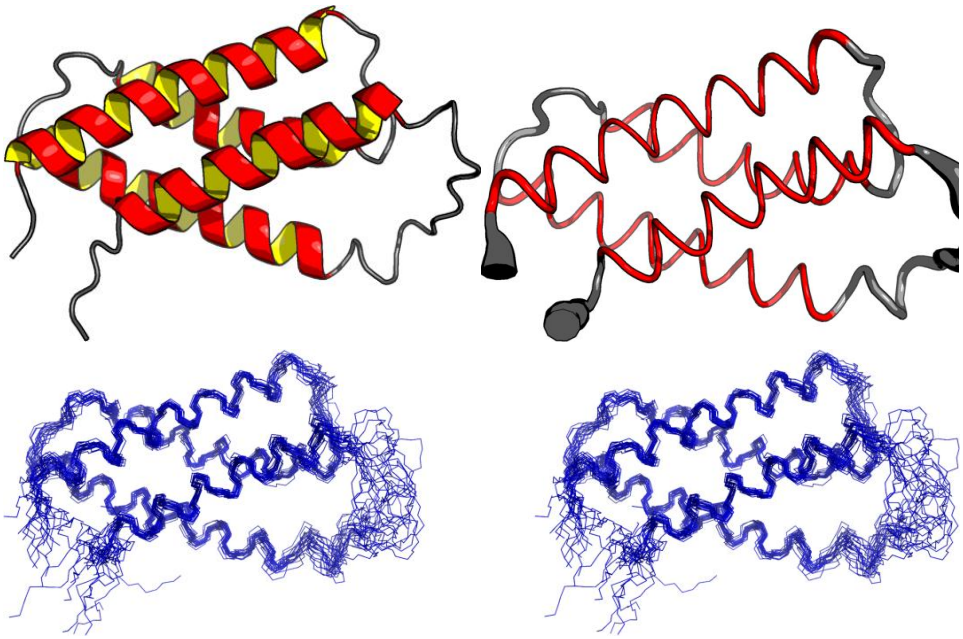
Structure Quality Analysis for NAME

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.):	123
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	monomer
Molecular weight:	14459



Secondary Structure Elements:
alpha helices: 5A-26A, 40A-64A, 72A-91A, 97A-120A
beta strands:

Total number of restricting constraints per restrained residue:	21.2
Restricting long range constraints per restrained residue:	4.4

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

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
7.3	3.5	0

Dihedral angle violations per model

1 - 10 °	> 10 °
1.1	0

FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score
0.963	0.897	0.929	0.76

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	1.7 Å	0.6 Å	0.6 Å
All heavy atoms	2.2 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*
98.1%	1.9%	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
99.3%	0.7%	0.1%		

Global quality scores

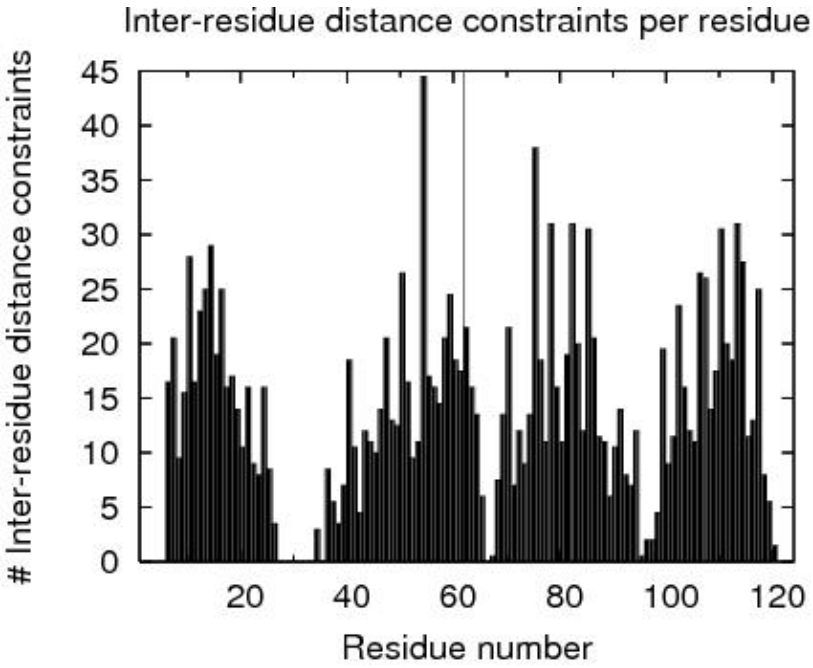
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.35	0.88	0.63	0.34	21.27
Z-score[1]	-1.77	0.95	2.79	2.01	-2.12

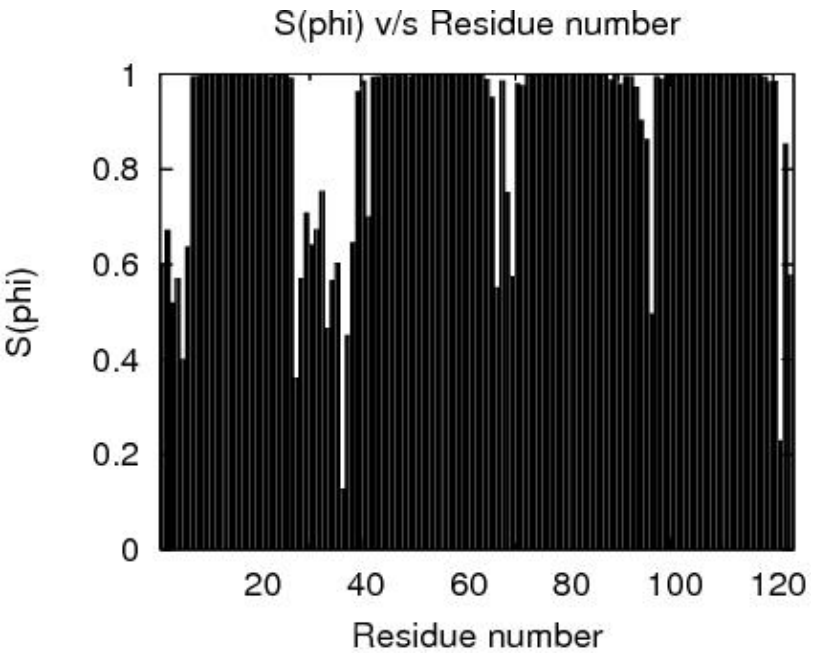
Generalized linear model RMSD prediction: 0.96

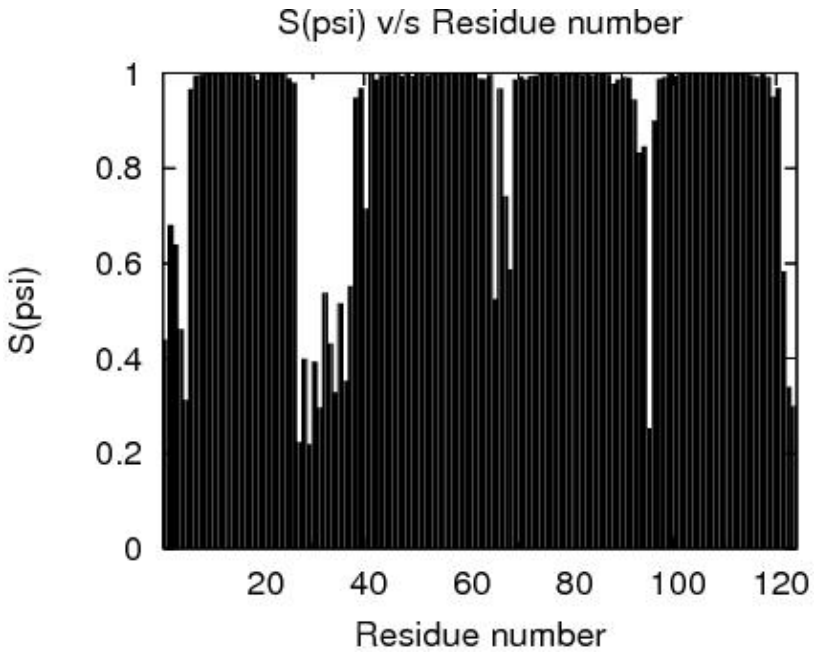
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	45
RMS deviation for bond angles:	0.6 °
RMS deviation for bond lengths:	0.004 Å

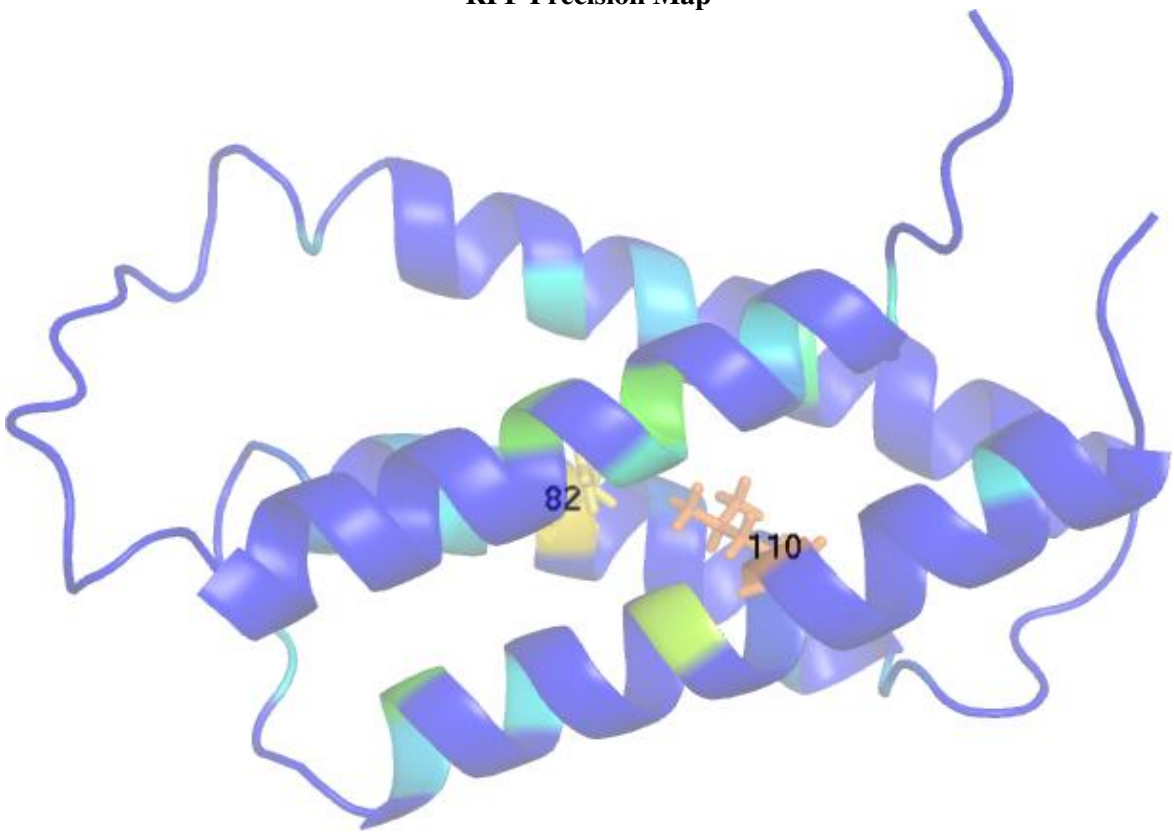
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 7A-26A,42A-64A,70A-93A,97A-120A
[3]Selected residues: 7A-26A,42A-64A,70A-93A,97A-120A


Inter-residue distance constraints per residue
Inter-residue distance constraints
45
40
35
30
25
20
15
10
5
0
20
40
60
80
100
120
Residue number

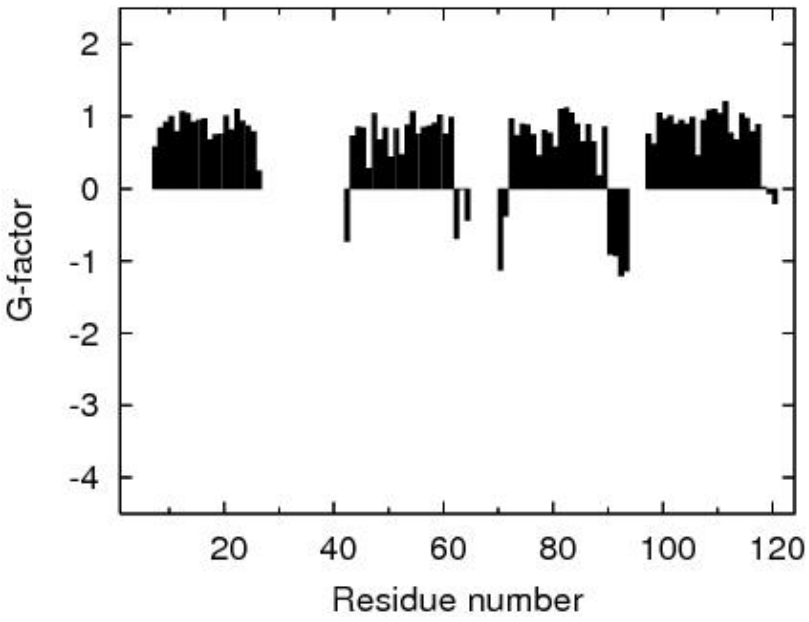

S(phi) v/s Residue number
S(phi)
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
120
Residue number



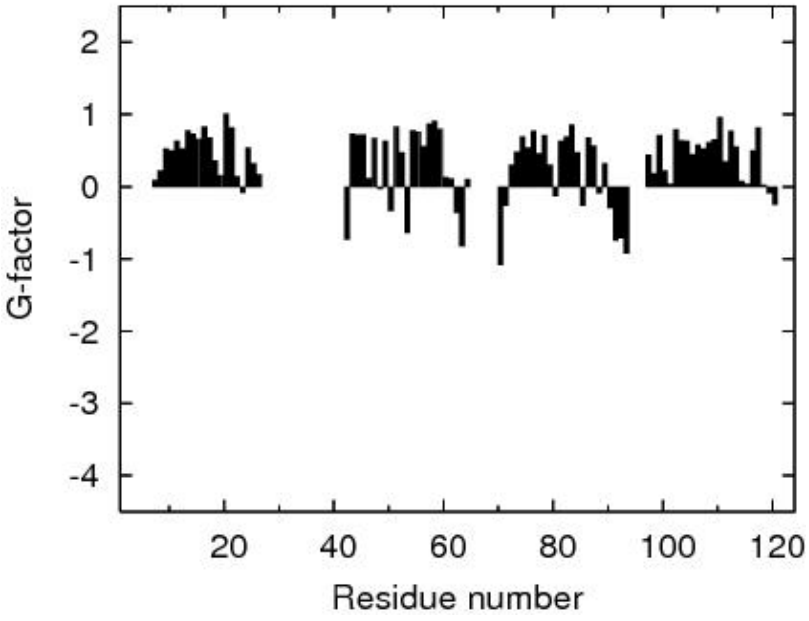
RPF Precision Map

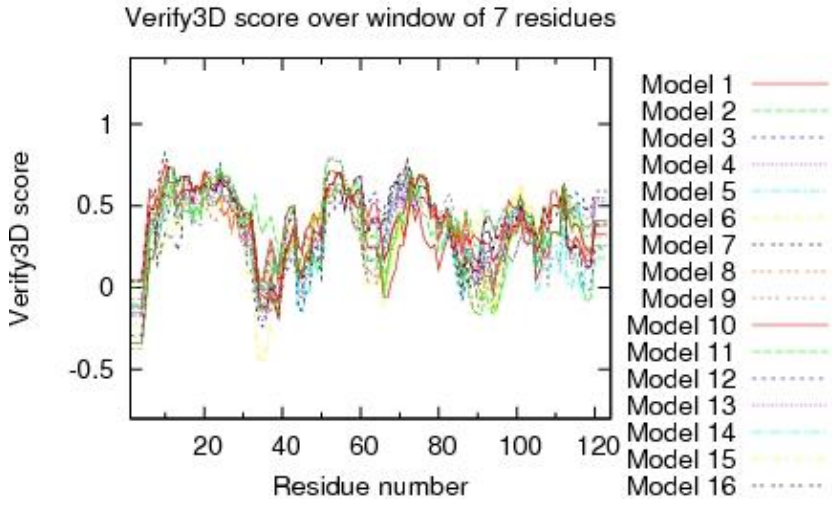


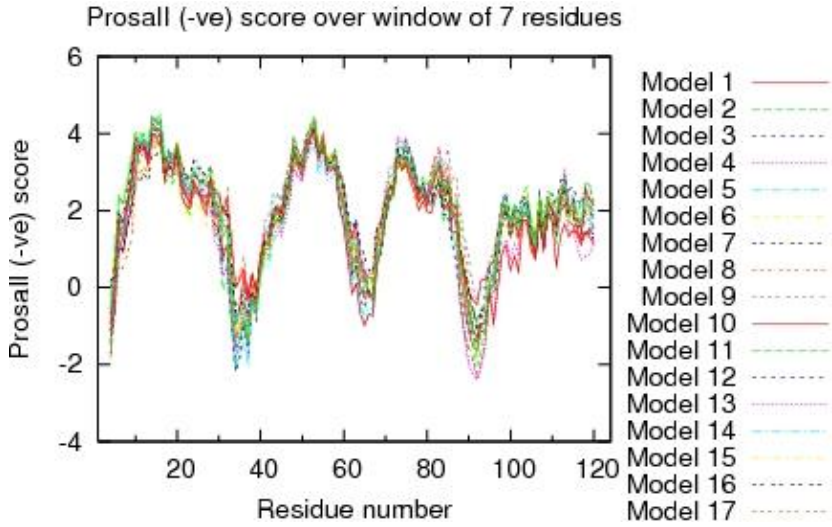
Procheck G-factor for phi-psi

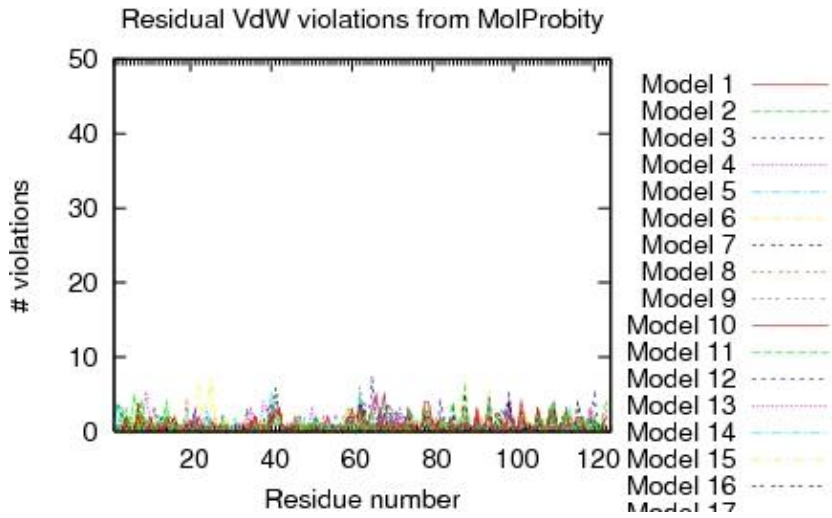


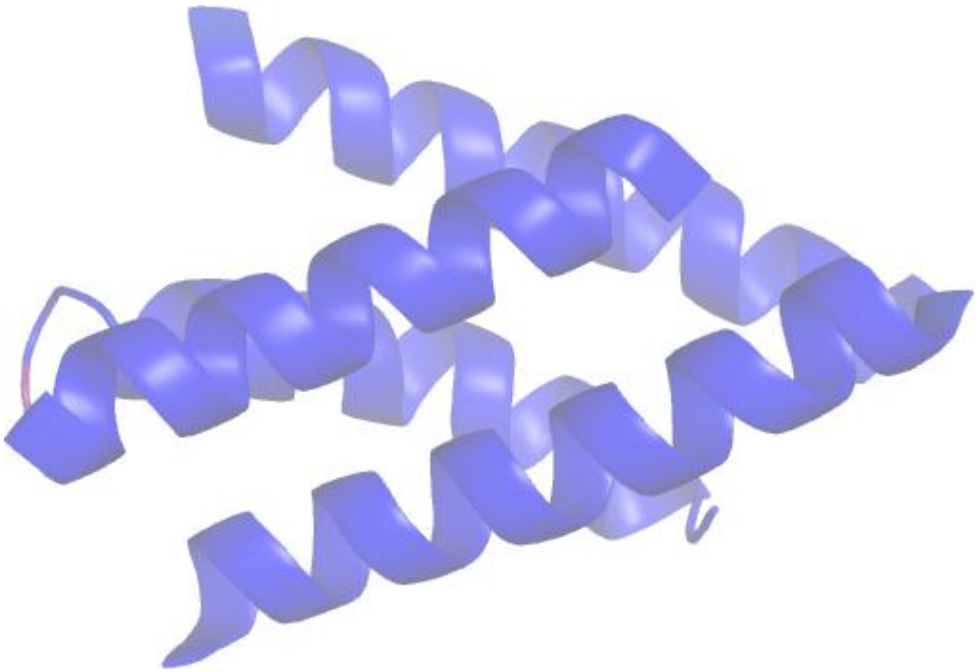
Procheck G-factor for all dihedral angles




Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
20
40
60
80
100
120
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
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
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
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12. Richardson D C, Richardson J S, "The kinemage: a tool for scientific communication", Prot Sci 1(1) (1992): 3-9
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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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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

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
```