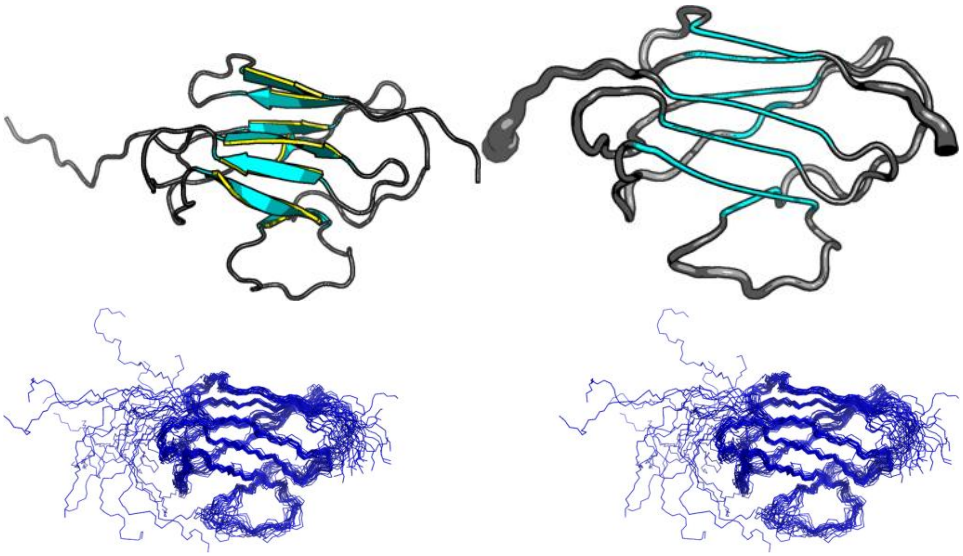
Structure Quality Analysis for NAME

Analyses performed for user defined residues.
The constraints analysis is based on the following files: NOE distance 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.):	122
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	monomer
Molecular weight:	13652



Secondary Structure Elements:
alpha helices:
beta strands: 15L-20L, 26E-31E, 68R-73R, 86U-88U, 37N-38N, 62L-63L, 51R-56R, 43U-48U, 101S-105S, 111U-116U

Total number of restricting constraints per restrained residue:	13.0
Restricting long range constraints per restrained residue:	5.7

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

0.1 - 0.2 Å	0.2 - 0.5 Å	> 0.5 Å
0.45	0	0.05

FIDs deposited in the BMRB? no

RPF Scores

Recall	Precision	F-measure	DP-score
0.965	0.929	0.947	0.815

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	3.4 Å	0.8 Å	0.8 Å
All heavy atoms	3.7 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*
88.3%	11.7%	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
98.9%	1.1%	0%		

Global quality scores

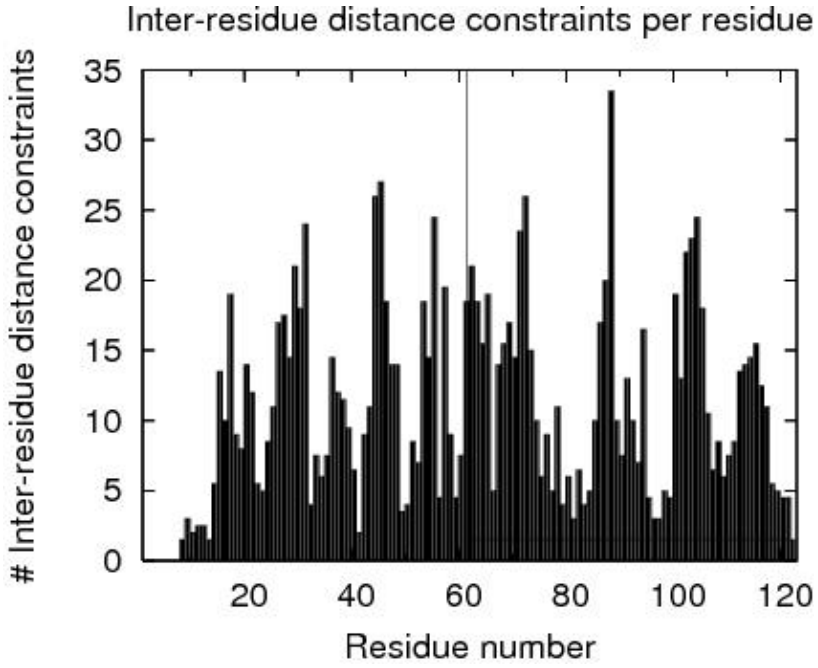
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)[3]*	*Procheck (all)[3]*	*MolProbity Clashscore*
-Raw score	0.39	0.49	-0.53	-0.09	4.49
Z-score[1]	-1.12	-0.66	-1.77	-0.53	0.76

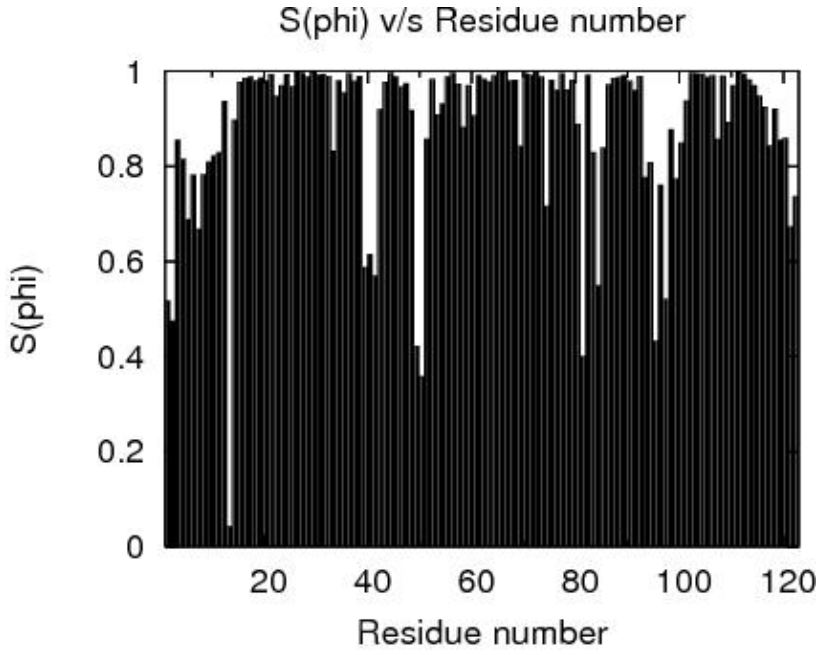
Generalized linear model RMSD prediction: 1.83

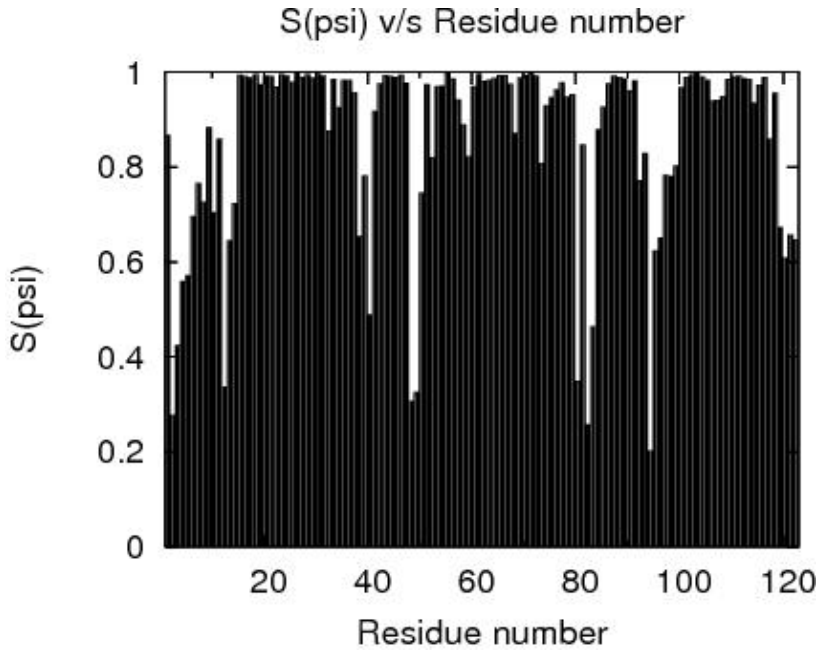
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

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:	0.011 Å

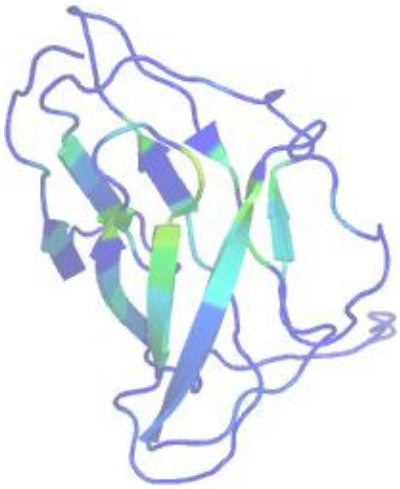
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 15A-37A,42A-47A,51A-57A,60A-72A,75A-79A,86A-91A,100A-106A,108A-116A
[3]Selected residues: 15A-32A,34A-37A,42A-47A,53A-72A,75A-79A,85A-91A,101A-106A,110A-116A

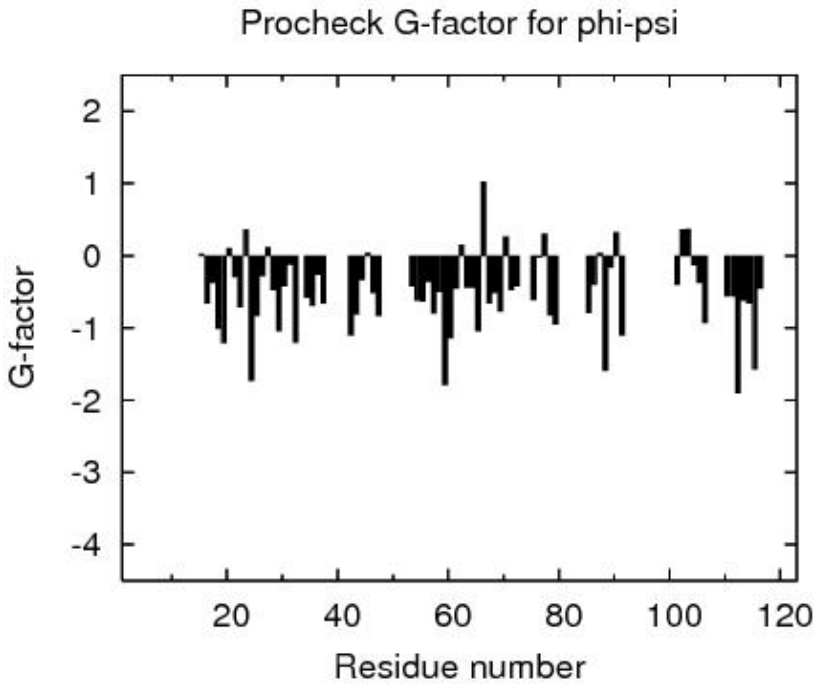


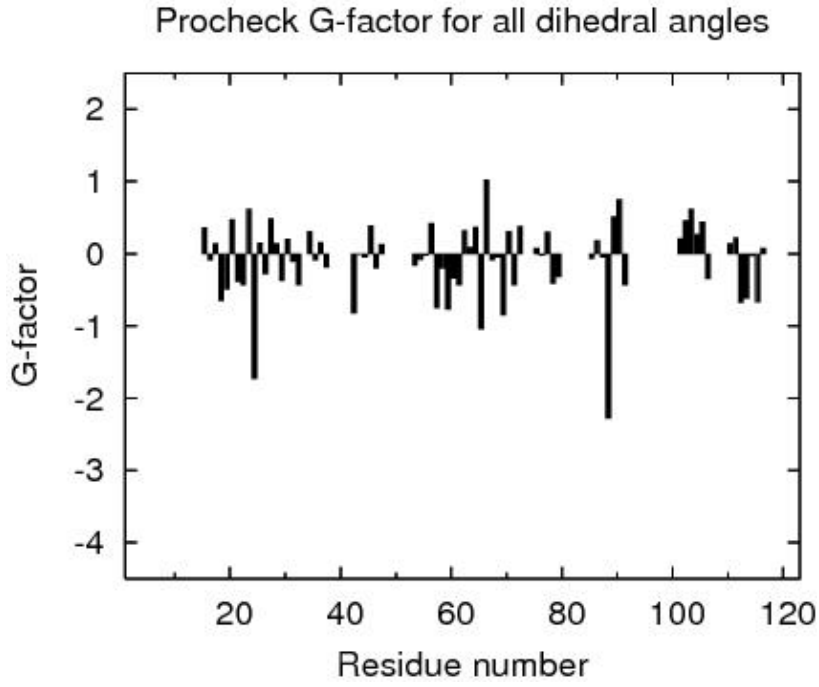


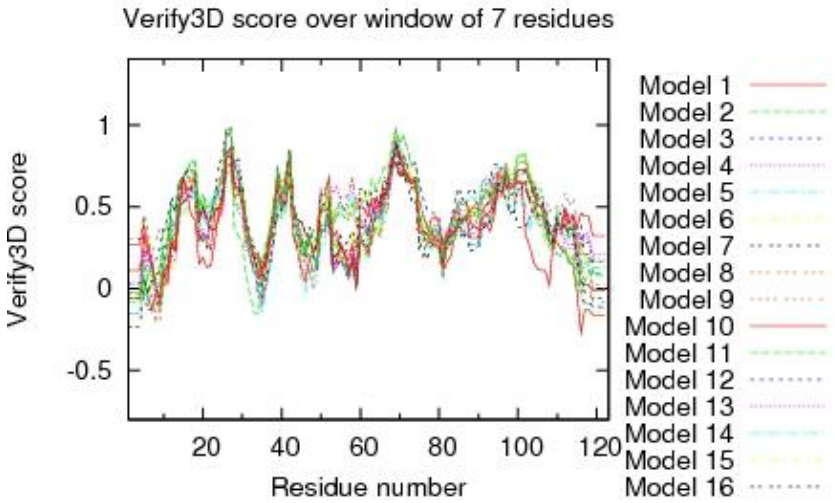


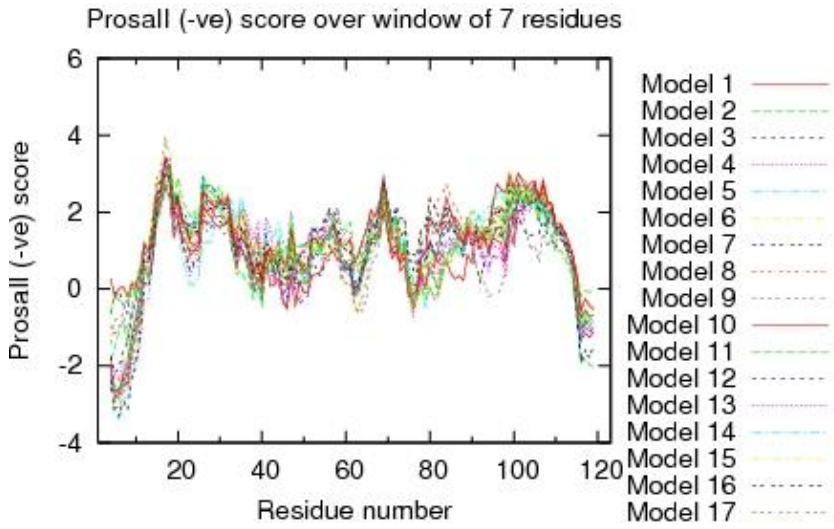
RPF Precision Map

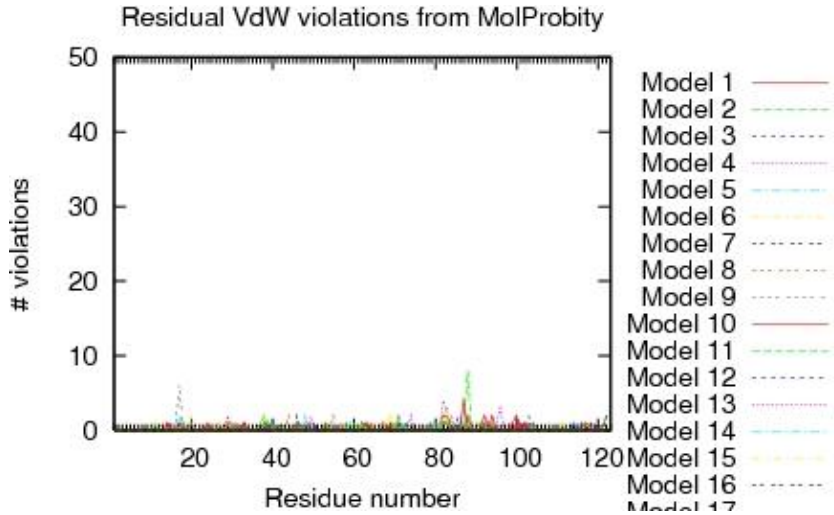


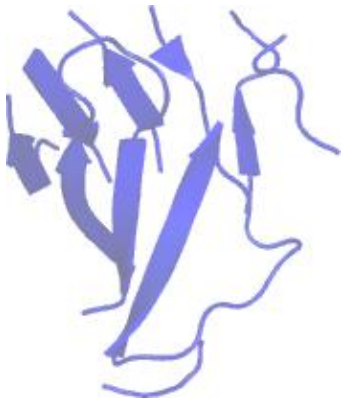

Procheck G-factor for phi-psi
G-factor
2
1
0
-1
-2
-3
-4
20
40
60
80
100
120
Residue number


Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
20
40
60
80
100
120
Residue number


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







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

References:

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Nature 356 (1992): 83-85
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3. Sippl M J, "Recognition of Errors in Three-Dimensional Structures of Proteins", Proteins 17 (1993): 355-362
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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