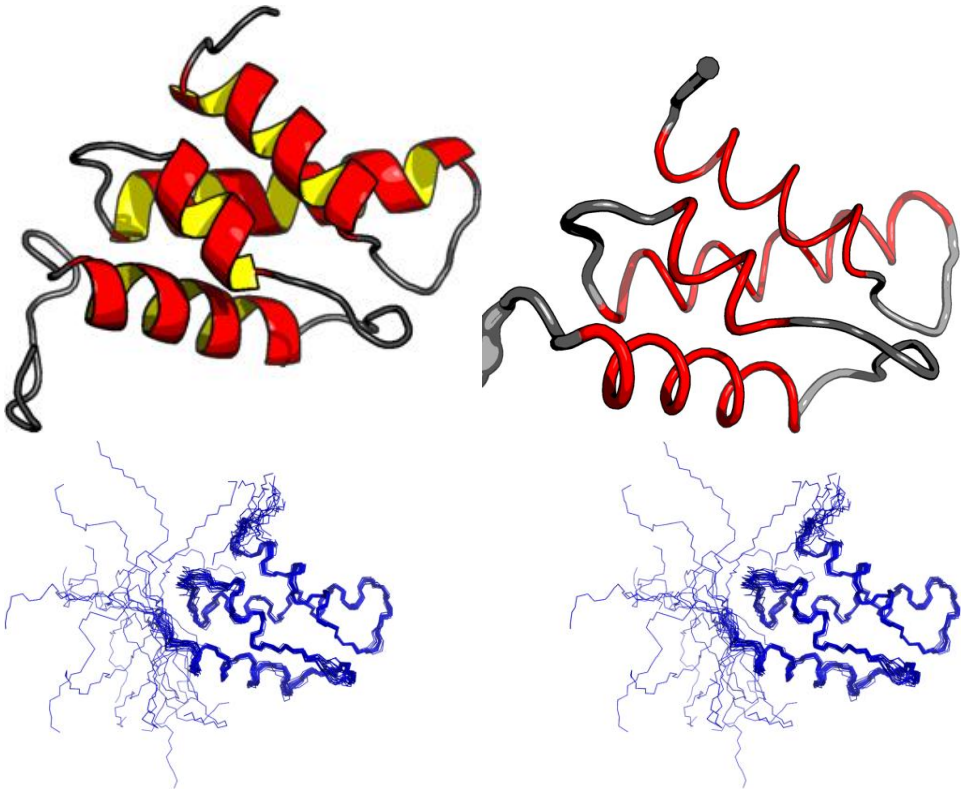
Structure Quality Analysis for NAME

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.):	86
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	monomer
Molecular weight:	9775



Secondary Structure Elements:
alpha helices: 13A-24A, 35A-40A, 47A-63A, 71A-81A
beta strands:

Total number of restricting constraints per restrained residue:	31.6
Restricting long range constraints per restrained residue:	8.1

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	2.25	0.15

Dihedral angle violations per model

1 - 10 °	> 10 °
0.05	0

FIDs deposited in the BMRB? no

RMSD	*All residues*	*Ordered residues*[2]	*Selected residues*[3]
All backbone atoms	3.3 Å	0.4 Å	0.4 Å
All heavy atoms	3.6 Å	0.7 Å	0.7 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
94.2%	5.8%	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
99.4%	0.6%	0%		

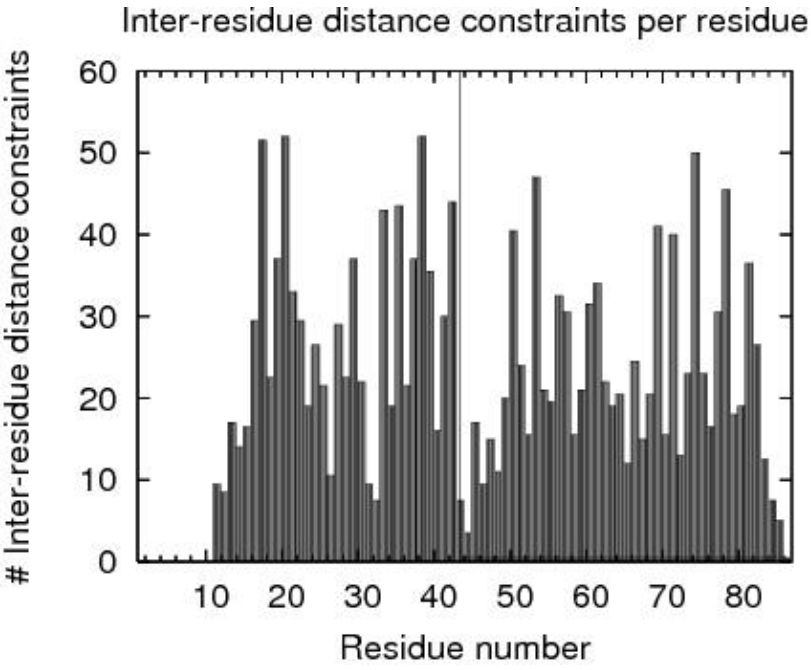
Global quality scores

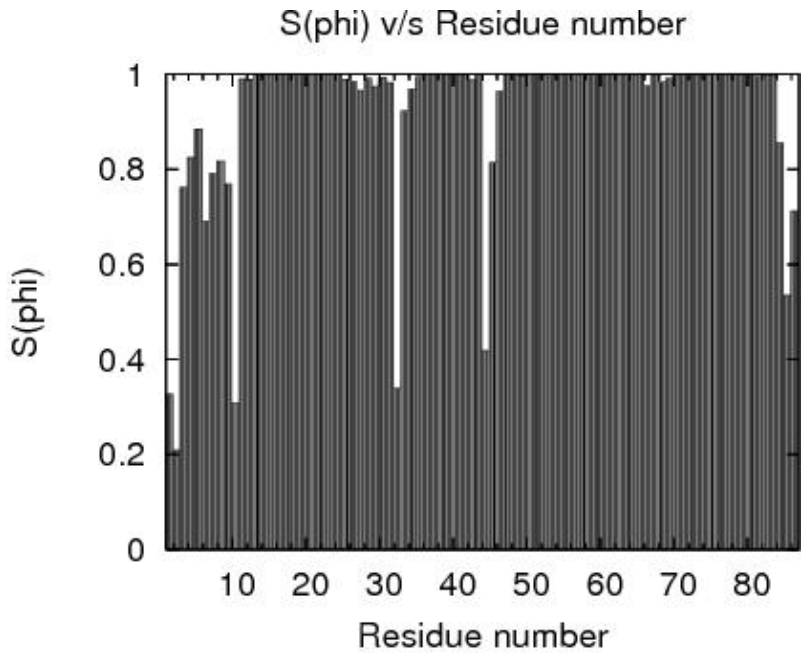
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
-Raw score	0.38	0.80	0.42	0.51	1.73
Z-score[1]	-1.28	0.62	1.97	3.02	1.23

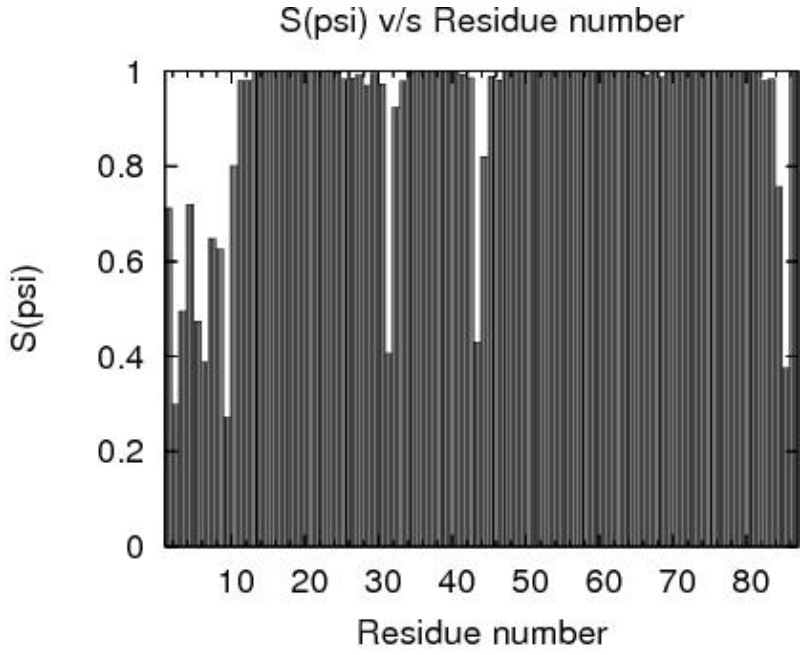
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

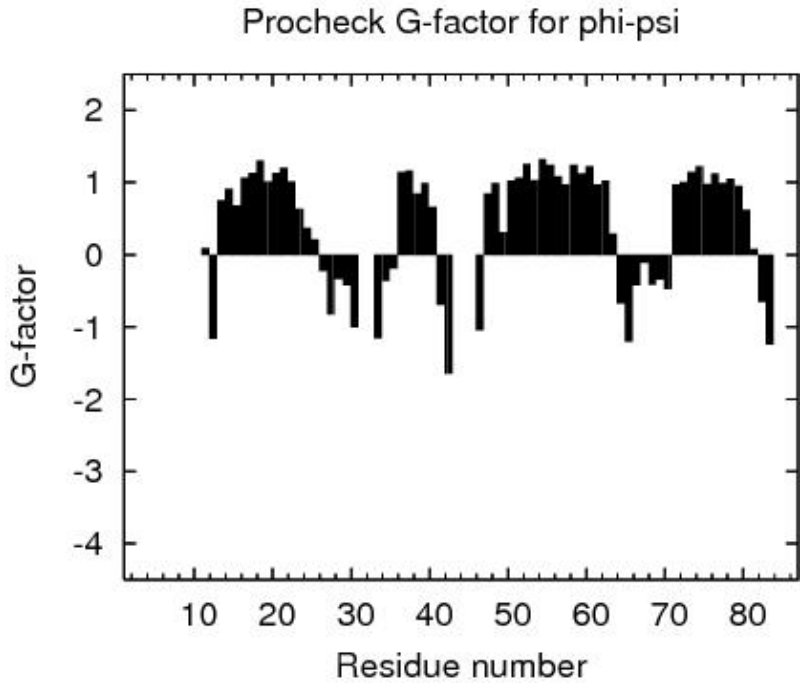
Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	0
RMS deviation for bond angles:	0.7 °
RMS deviation for bond lengths:	0.011 Å

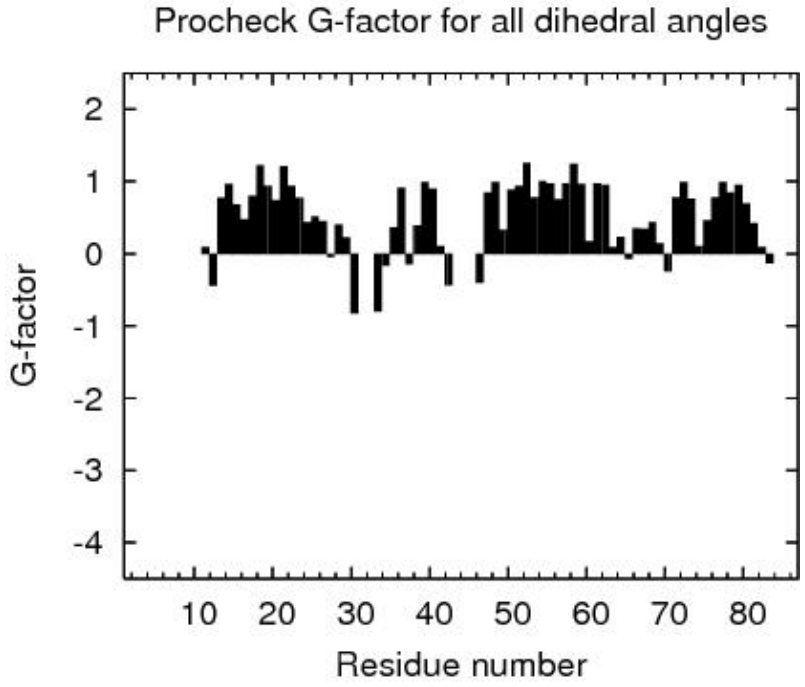
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 11A-30A,33A-42A,45A-83A
[3]Selected residues: 11A-30A,33A-42A,46A-83A

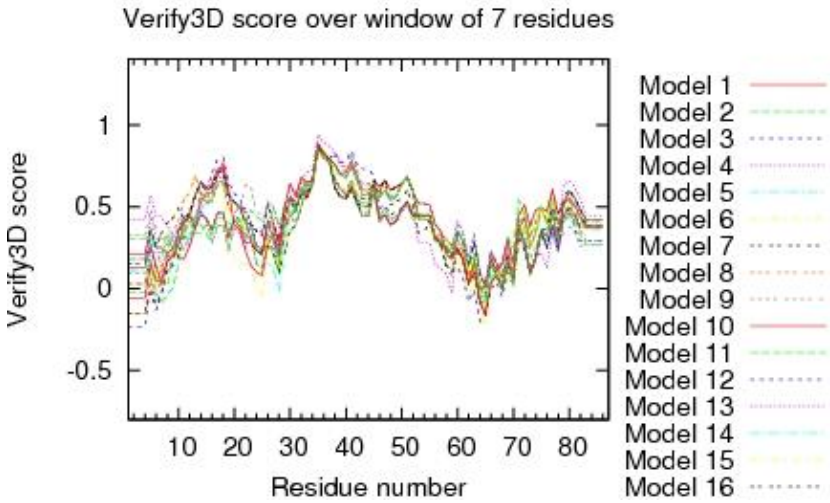

Inter-residue distance constraints per residue
Inter-residue distance constraints
0
10
20
30
40
50
60
10
20
30
40
50
60
70
80
Residue number

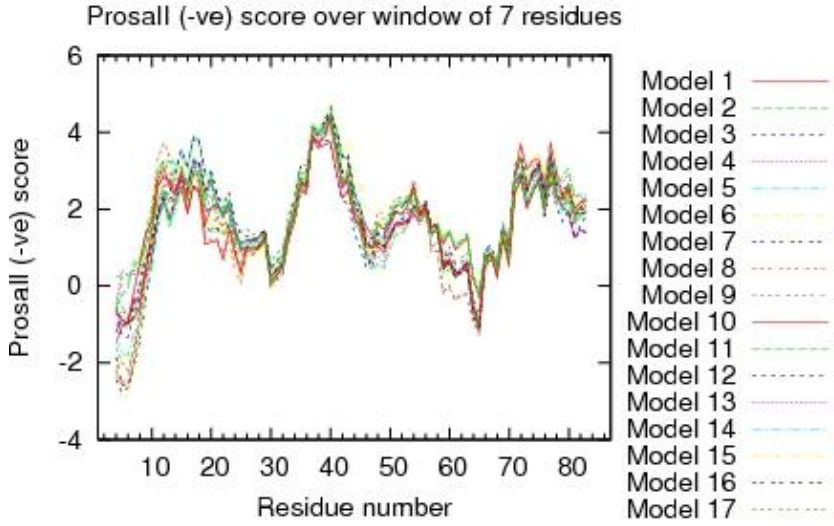

S(phi) v/s Residue number
S(phi)
0
0.2
0.4
0.6
0.8
1
10
20
30
40
50
60
70
80
Residue number

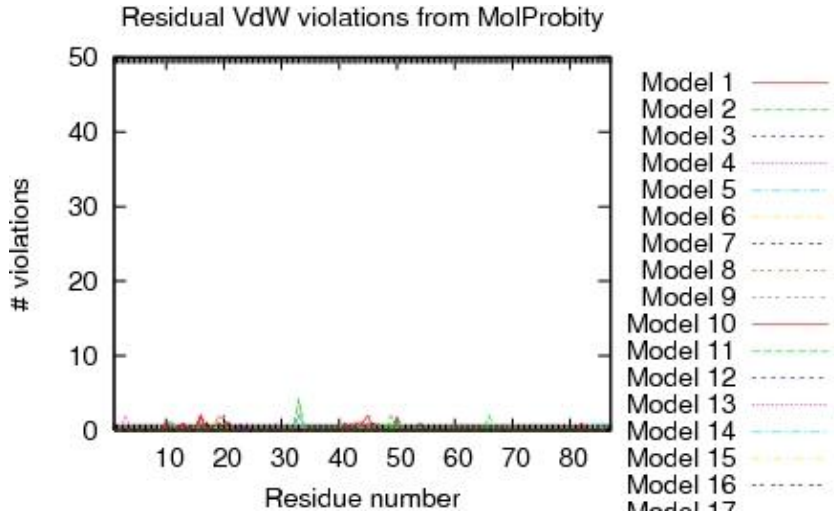

S(psi) v/s Residue number
S(psi)
1
0.8
0.6
0.4
0.2
0
10
20
30
40
50
60
70
80
Residue number

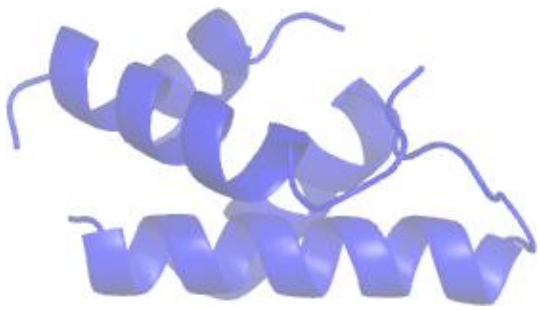

Procheck G-factor for phi-psi
G-factor
2
1
0
-1
-2
-3
-4
10
20
30
40
50
60
70
80
Residue number


Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
10
20
30
40
50
60
70
80
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
10
20
30
40
50
60
70
80
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

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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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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
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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
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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
```