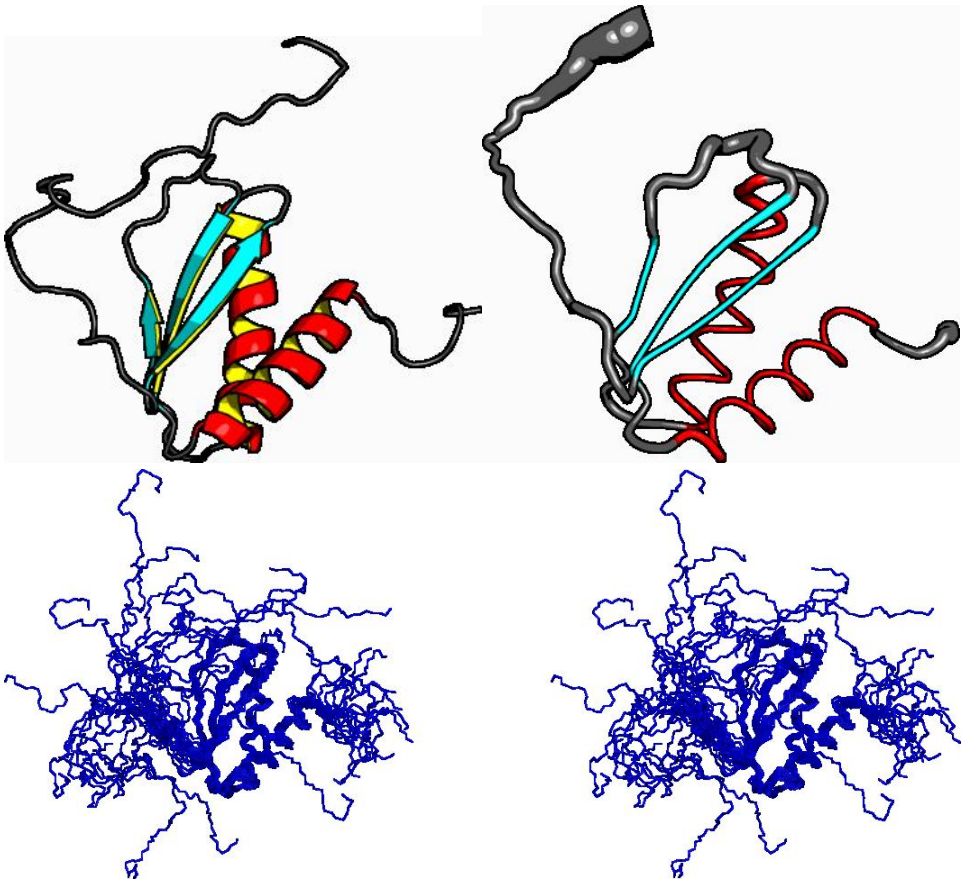
Structure Quality Analysis for NAME

Analyses performed for DAOP well-defined residues.

Procheck analysis, RMSD calculation and structure superimposition are based on DAOP with S(phi)+S(psi)>=1.8 : 31A-38A, 40A-59A, 62A-69A, 75A-81A, 84A-100A

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	108
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	monomer
Molecular weight:	12037



Secondary Structure Elements:
alpha helices: 41A-58A, 85A-100A
beta strands: 31A-37A, 75A-81A, 63A-66A

FIDs deposited in the BMRB? no

Comparison of core atoms:

DAOP > 1.8 Å :	A:31..A:38, A:40..A:58, A:62..A:69, A:75..A:81, A:84..A:100
FindCore2 :	A:25, A:30..A:101
CYRANGE :	30..97

RMSD	*All residues*	*Ordered residues[2]*	*Selected residues[3]*

All backbone atoms	8.9 Å	0.6 Å	0.6 Å
All heavy atoms	8.5 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*
99.3%	0.6%	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
99.3%	0.7%	0%		

Global quality scores

Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)[3]*	*Procheck (all)[3]*	*MolProbity Clashscore*
Raw score	0.10	-0.02	0.39	0.28	20.53
Z-score[1]	-5.78	-2.77	1.85	1.66	-2.00

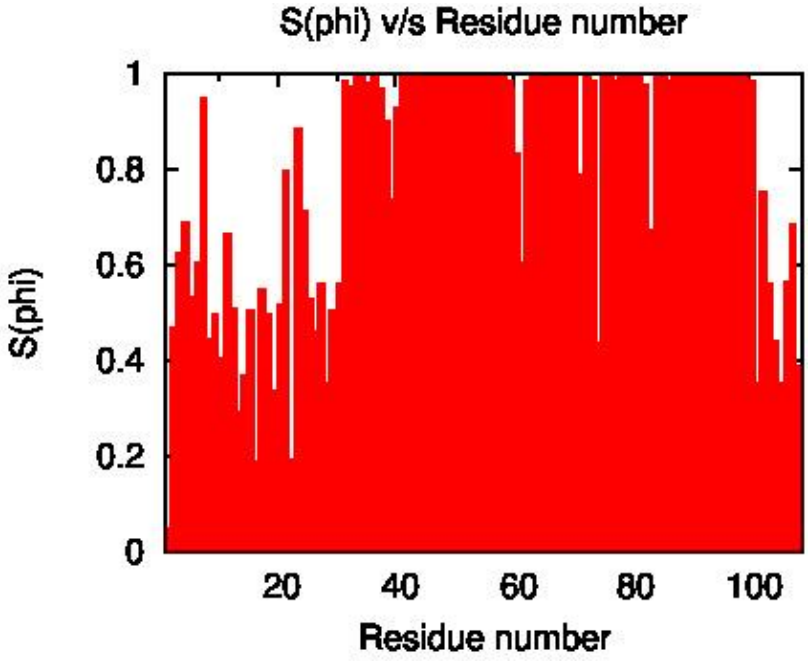
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

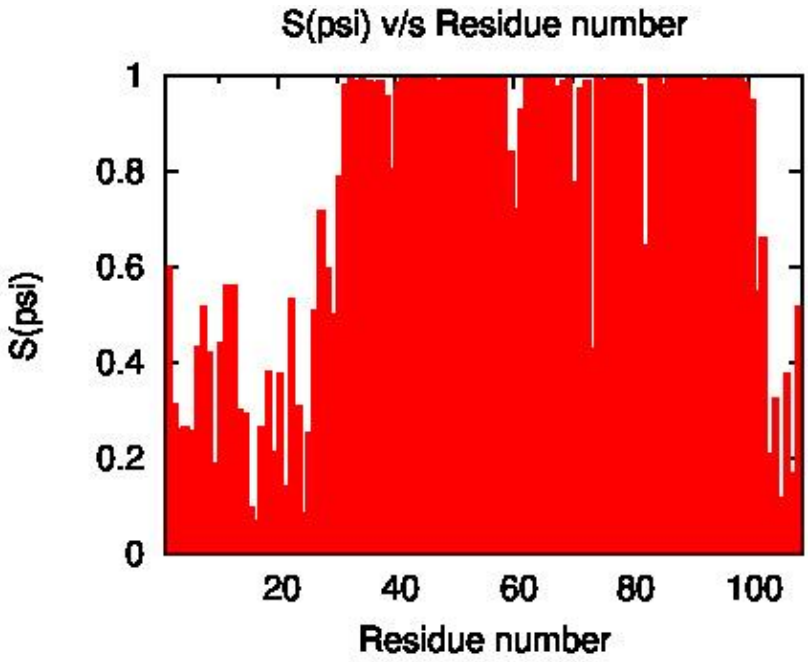
Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	3
RMS deviation for bond angles:	1.7 °
RMS deviation for bond lengths:	0.019 Å

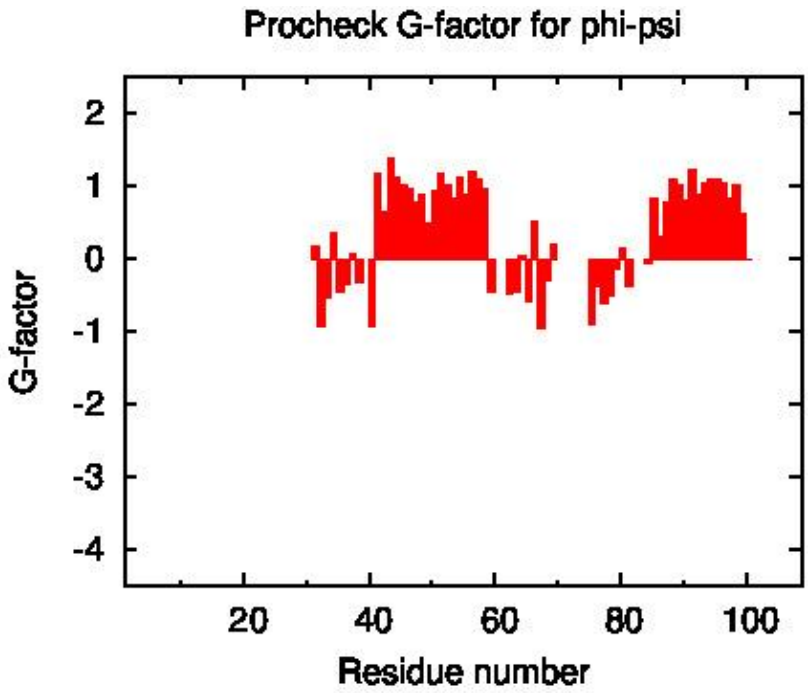
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

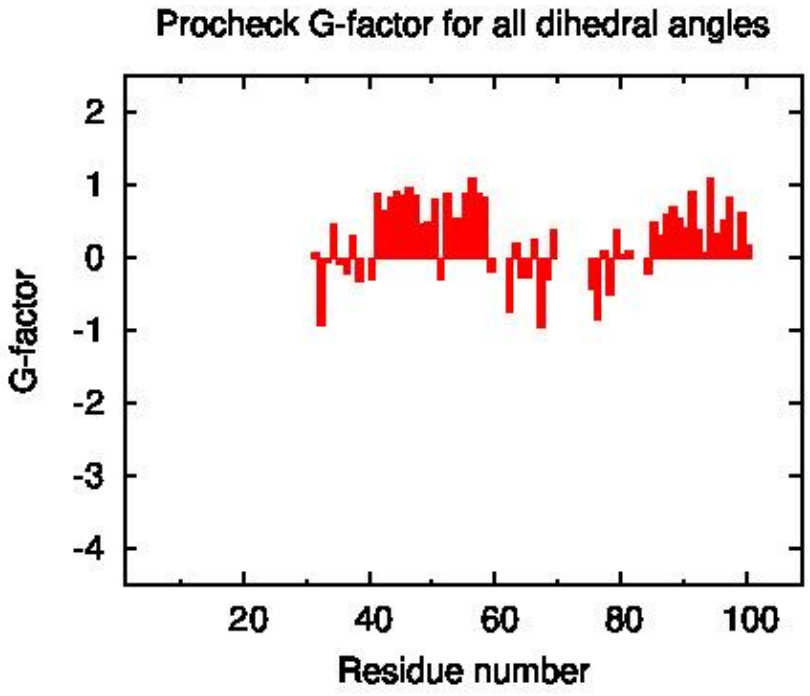
[2] Ordered residues (DAOP): 31A-38A, 40A-59A, 62A-69A, 75A-81A, 84A-100A

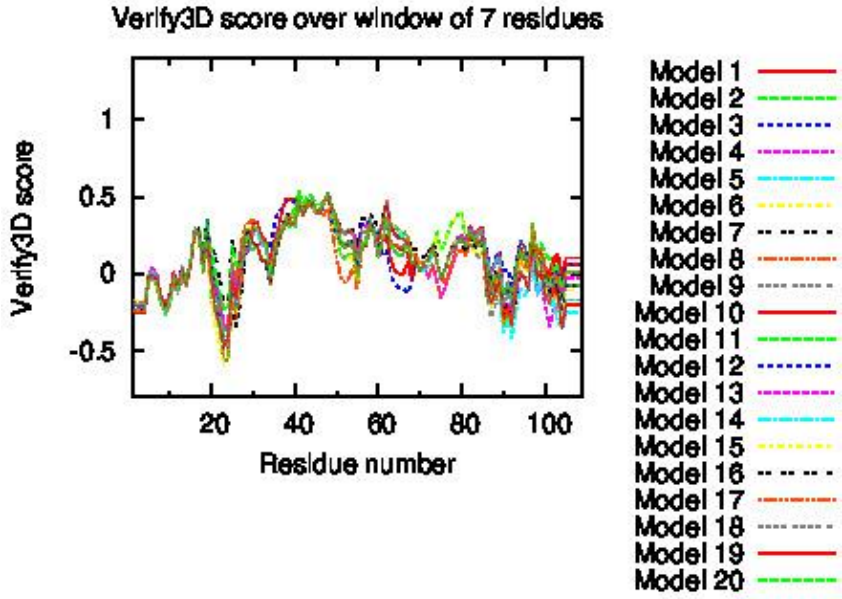
[3] Selected residues DAOP with S(phi)+S(psi)>=1.8 : 31A-38A, 40A-59A, 62A-69A, 75A-81A, 84A-100A

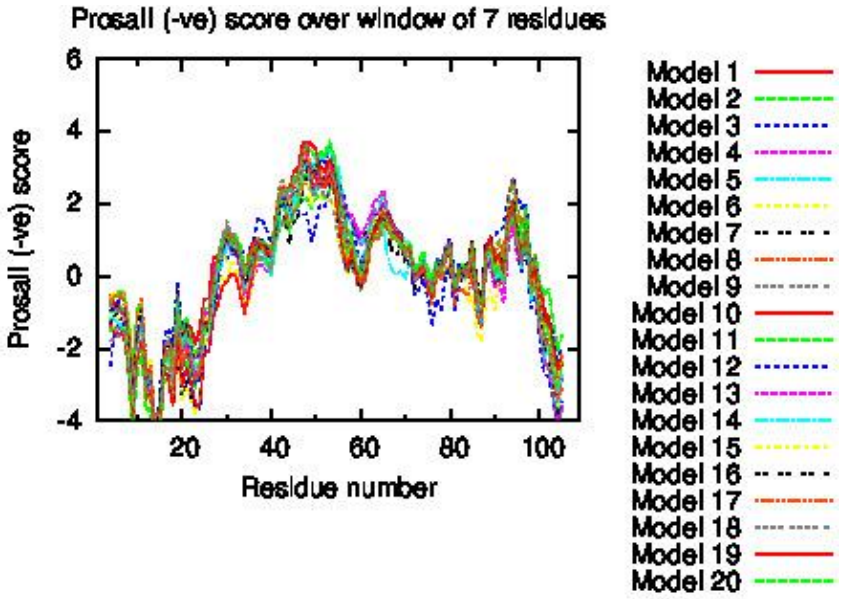


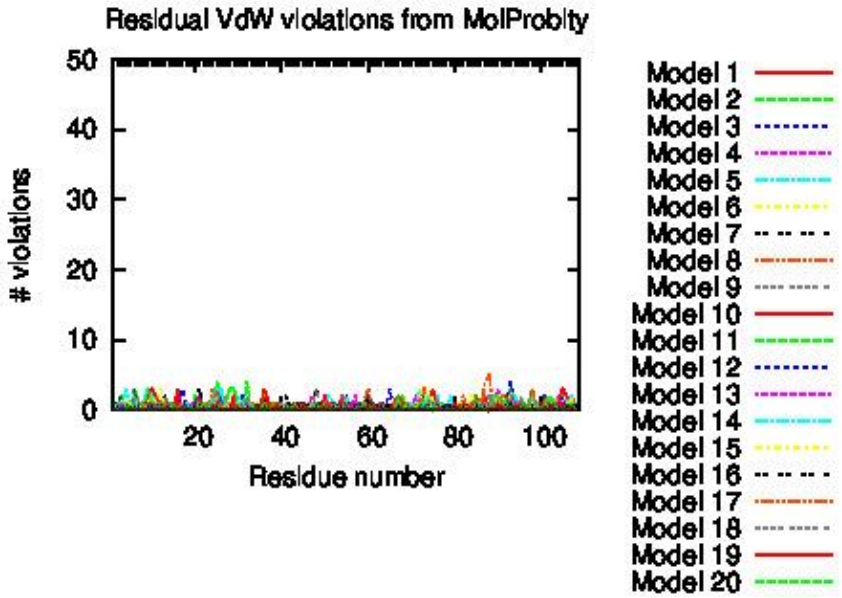

S(psi) v/s Residue number
S(psi)
Residue number
0
0.2
0.4
0.6
0.8
1
20
40
60
80
100

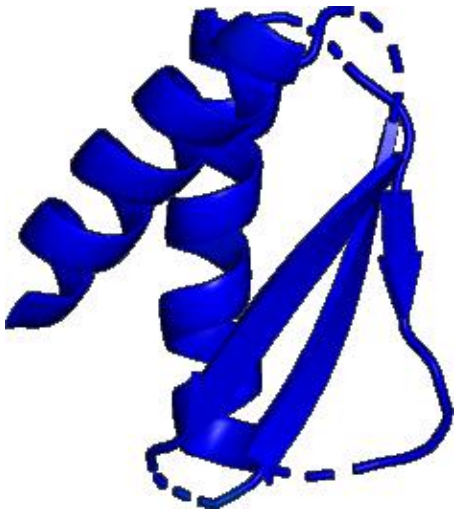

Procheck G-factor for phi-psi
G-factor
Residue number
2
1
0
-1
-2
-3
-4
20
40
60
80
100


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


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
20
40
60
80
100
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
Model 18
Model 19
Model 20







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

References:
1. Bhattacharya A, Tejero R and Montelione GT, "Evaluating protein structures determined by structural genomics consortia". Proteins 2007, 66:778-795
2. Tejero R, Snyder D, Mao B, Aramini JM and Montelione GT, "PDBStat: a universal restraint converter and restraint analysis software package for protein NMR". J Biomol NMR 2013, 56:337-351
3. Luthy R, Bowie JU and Eisenberg D, "Assessment of protein models with three-dimensional profiles". Nature 1992, 356:83-85
4. Bowie JU, Luthy R and Eisenberg D, "A Method to identify protein sequences that fold into a known three-dimensional structure". Science 1991, 253:164-169
5. Sippl MJ, "Recognition of errors in three-dimensional structures of proteins". Proteins 1993, 17:355-362
6. Sippl MJ, "Calculation of conformation ensembles from potentials of mean force". J Mol Biol 1990, 213:859-883
7. Laskowski RA et al, "AQUA and PROCHECK_NMR: programs for checking the quality of proteins structures solved by NMR". J Biomolec NMR 1996, 8:477-486
8. Laskowski RA et al "PROCHECK: a program to check the stereochemical quality of protein structures". J Appl Cryst 1993, 26:283-291
9. Word JM et al, "Exploring steric constrains on protein mutations using MAGE / PROBE". Prot Sci 2000, 9:2251-2259
10. Word JM et al, "Asparagine and glutamine: using hydrogen atom contacts in the choice of side-chain amide orientation". J Mol Biol 1999, 285:1735-1747
11. Word JM et al, "Visualizing and quantifying molecular goodness-of-fit: small-probe contact dots with explicit hydrogens". J Mol Biol 1999, 285:1711-1733
12. Luthy R, McLachlan AD and Eisenberg D, "Secondary structure-based profiles: use of structure-conserving scoring tables in searching protein sequence databases for structural similarities". Proteins 1991, 18:229-239
13. Richardson DC, Richardson J S, "The kinemage: a tool for scientific communication". Prot Sci 1992, 1(1):3-9
14. Guntërt P, Mumenthaler, C & Wüthrich, K "Torsion angle dynamics for NMR structure calculation with the new program DYANA". J. Mol. Biol 1997, 273:283-298
15. Lovell SC 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 YJ, Montelione, GT, and Guntert, P "Protein structure validation by generalized linear model root-mean-square deviation prediction". Protein Sci 2012) 21:229-238.

Software Environment

Software for structure quality evaluation:

DSSP	DsspCMBI-April-2000
pdbstat	PdbStat-5.20.8 Version
AutoAssign	Version 2.4.0 (uses only AVS scripts)
RPF analysis	ASDP-2.3
PDB validation	Version 8.061
Verify3D	Version 1.0 corrected by Aneerban
ProsaII	Prosa2003
PROCHECK	Version 3.5.4

MolProbity programs:

cluster	1999
clashlistcluster	1999 (corrected by Aneerban)
mage	Version 6.35.040409
prekin	Version 6.35.040406
reduce	Version 2.14

```
prope              Version 2.6
```

Other Software:

```
 PERL              Version 5.16.3
 convert           ImageMagick 6.7.8
 ps2pdf            Ghostscript 9.25
 htmldoc           v1.8.28
 gnuplot           Version 4.6.2
 jpegtopnm         netpbm-progs 10.79.00
 pnmcrop           netpbm-progs 10.79.00
 pnmtojpeg         netpbm-progs 10.79.00

Information updated on October, 2021. RTT
```