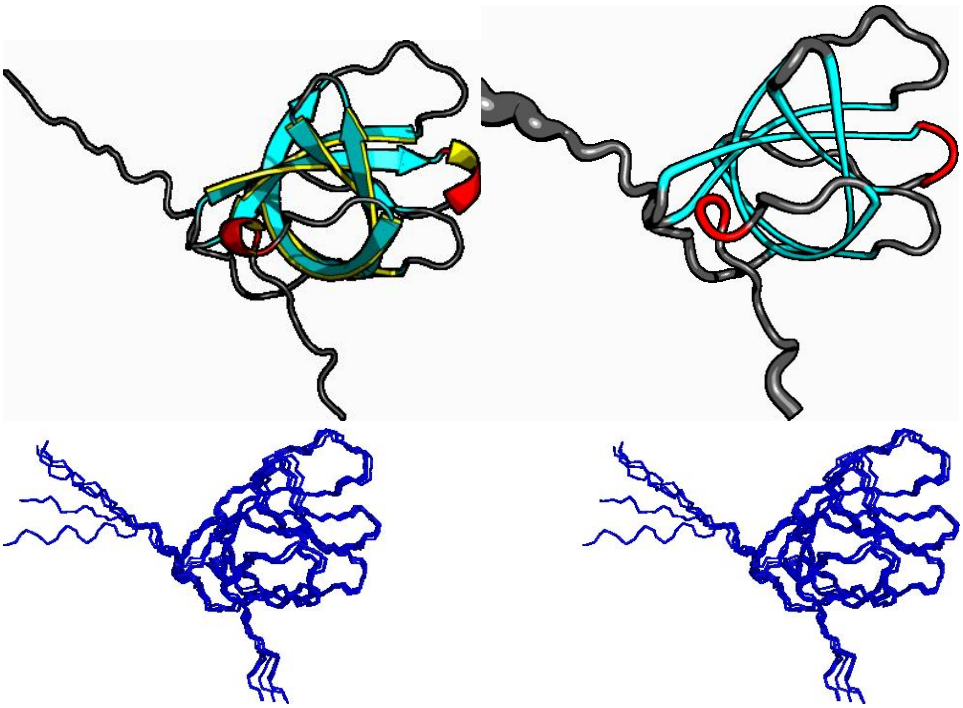
Structure Quality Analysis for NAME

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 : 2A-107A

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	109
Organism:	
SwissProt / TrEMBL ID:	
# models:	5
Oligomerization:	monomer
Molecular weight:	12503



Secondary Structure Elements:
alpha helices:
beta strands: 19A-19A, 17A-18A, 66A-77A, 20A-28A, 35A-43A, 46A-53A, 80A-85A, 90A-93A

FIDs deposited in the BMRB? no

Comparison of core atoms:

DAOP > 1.8 Å : A:2..A:101, A:103..A:107
FindCore2 : A:1..A:102
CYRANGE : 5..28, 33..100

RMSD	***All residues***	***Ordered residues[2]***	***Selected residues[3]***
All backbone atoms	1.1 Å	0.8 Å	0.8 Å
All heavy atoms	1.4 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*
88.1%	11.9%	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
94.2%	5.3%	0.6%		

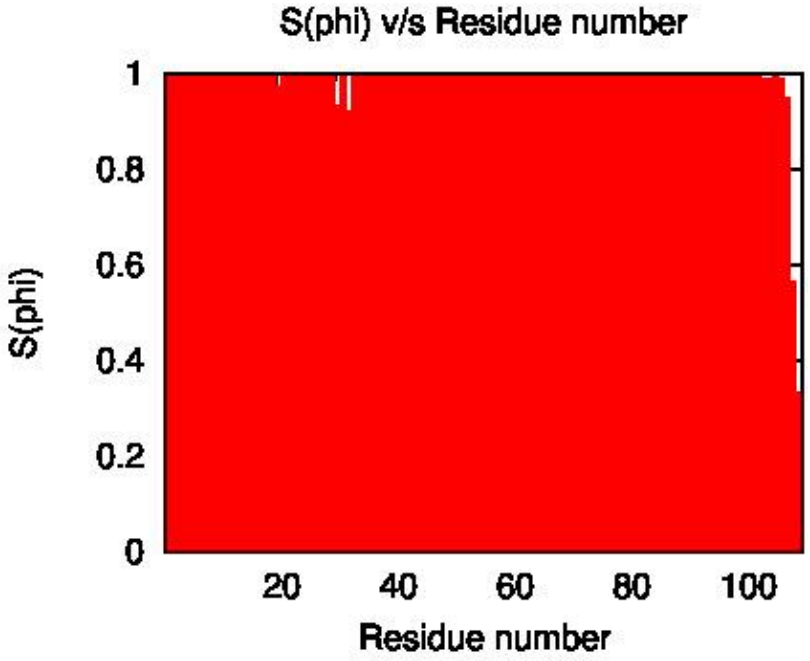
Global quality scores

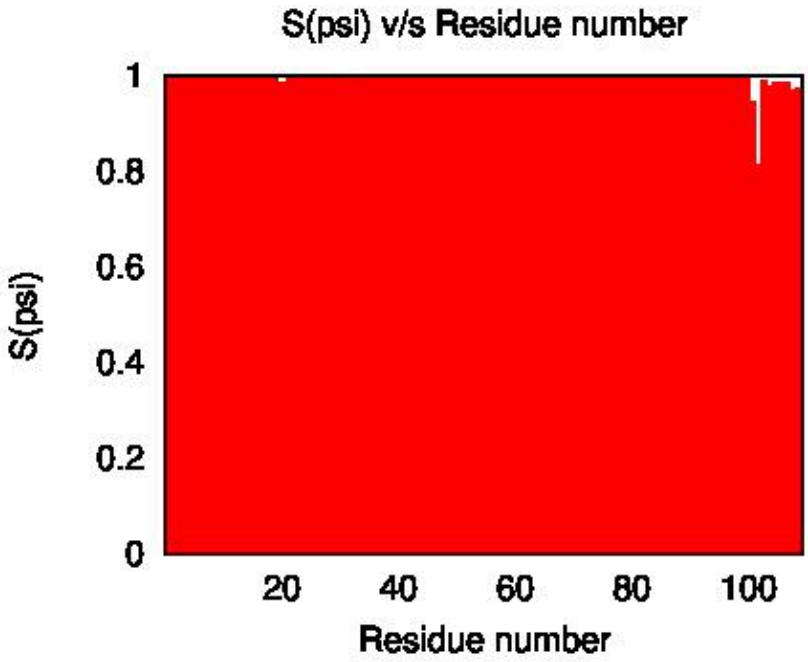
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)[3]*	*Procheck (all)[3]*	*MolProbity Clashscore*
Raw score	0.19	N/A	-0.48	-0.16	0.00
Z-score[1]	-4.33	N/A	-1.57	-0.95	1.53

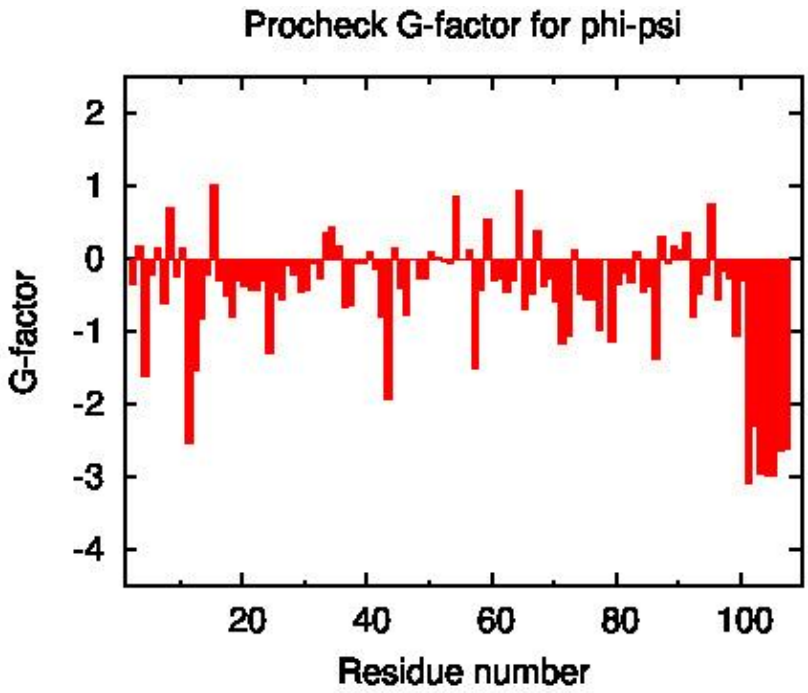
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	0
RMS deviation for bond angles:	1.9 °
RMS deviation for bond lengths:	0.011 Å

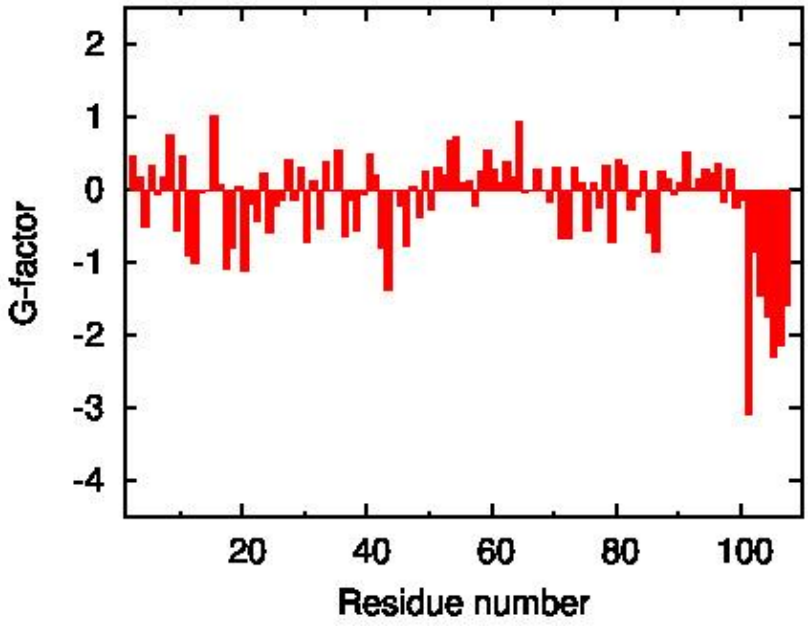
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2] Ordered residues (DAOP): 2A-107A
[3] Selected residues DAOP with S(phi)+S(psi)>=1.8 : 2A-107A



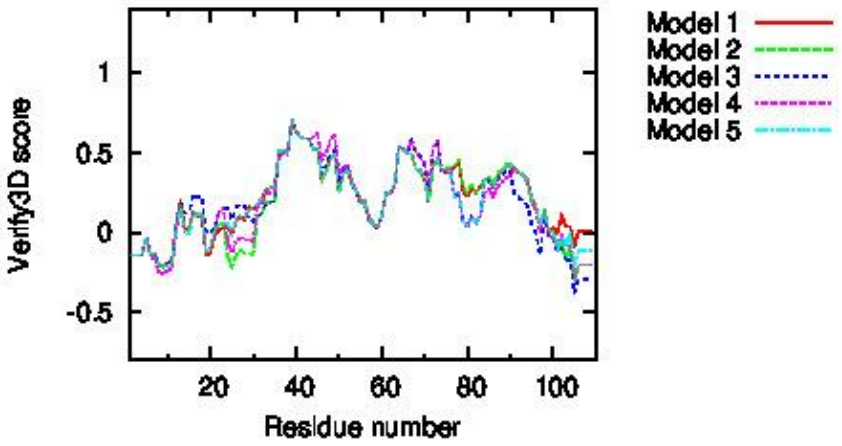

S(psi) v/s Residue number
S(psi)
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
Residue number


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

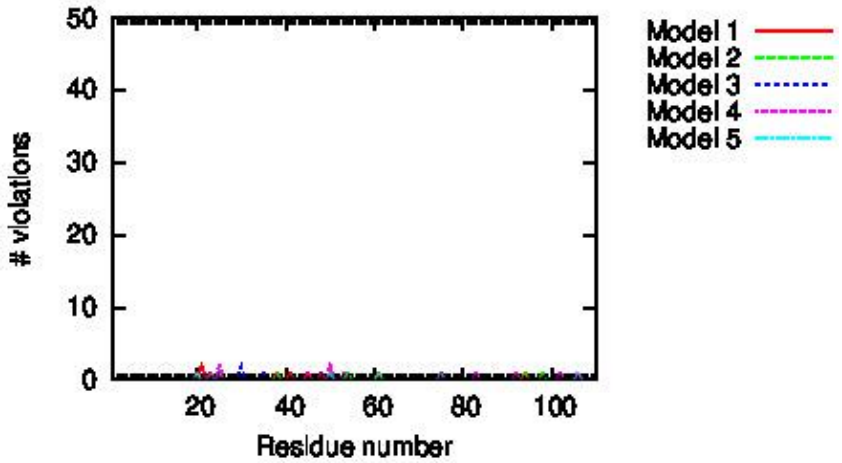
Procheck G-factor for all dihedral angles

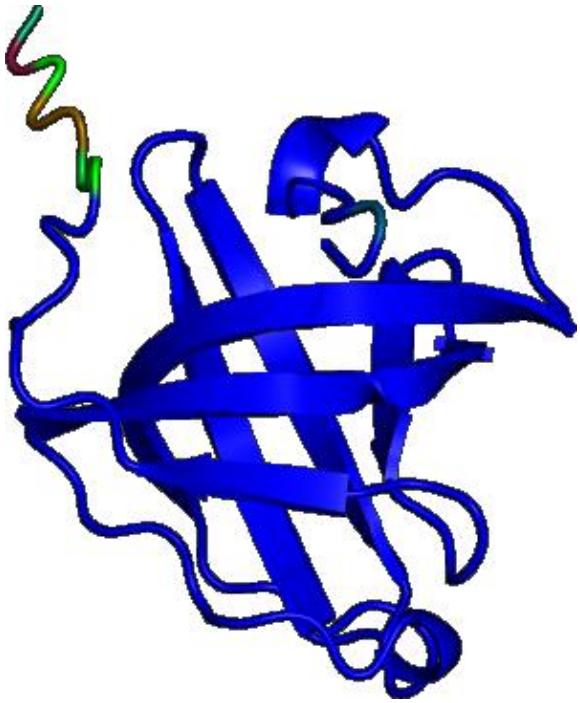


Verify3D score over window of 7 residues



Residual VdW violations from MolProbity





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.

Protein Structure Validation Suite (PSVS)

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
probe	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

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