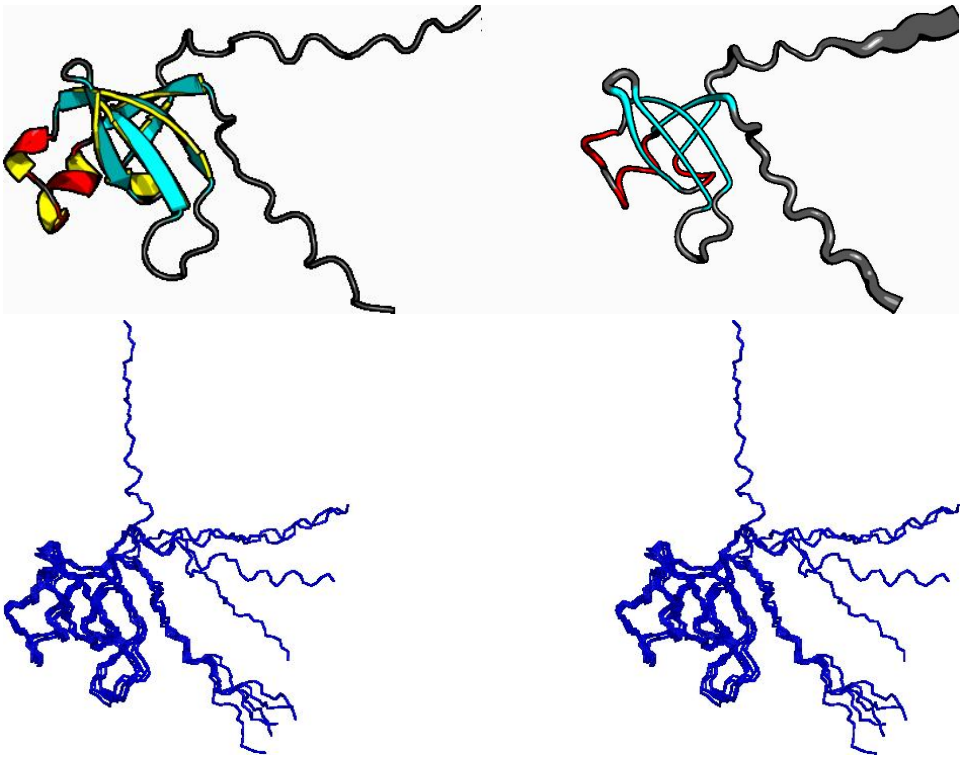
Structure Quality Analysis for NAME

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 : 3A-69A

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	84
Organism:	
SwissProt / TrEMBL ID:	
# models:	5
Oligomerization:	monomer
Molecular weight:	9542



Secondary Structure Elements:
alpha helices:
beta strands: 58A-61A, 49A-53A, 35A-41A, 17A-20A, 66A-68A

FIDs deposited in the BMRB? no

Comparison of core atoms:

DAOP > 1.8 Å :	A:3..A:69, A:72..A:73
FindCore2 :	A:8..A:71
CYRANGE :	11..69 , 71..84

RMSD	***All residues***	***Ordered residues[2]***	***Selected residues[3]***
All backbone atoms	3.6 Å	0.9 Å	0.9 Å
All heavy atoms	4.1 Å	1.0 Å	1.0 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

	Additionally allowed regions	*Generously allowed regions*	*Disallowed regions*

Most favoured regions			
89.3%	10.4%	0.4%	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
93.7%	5.1%	1.2%		

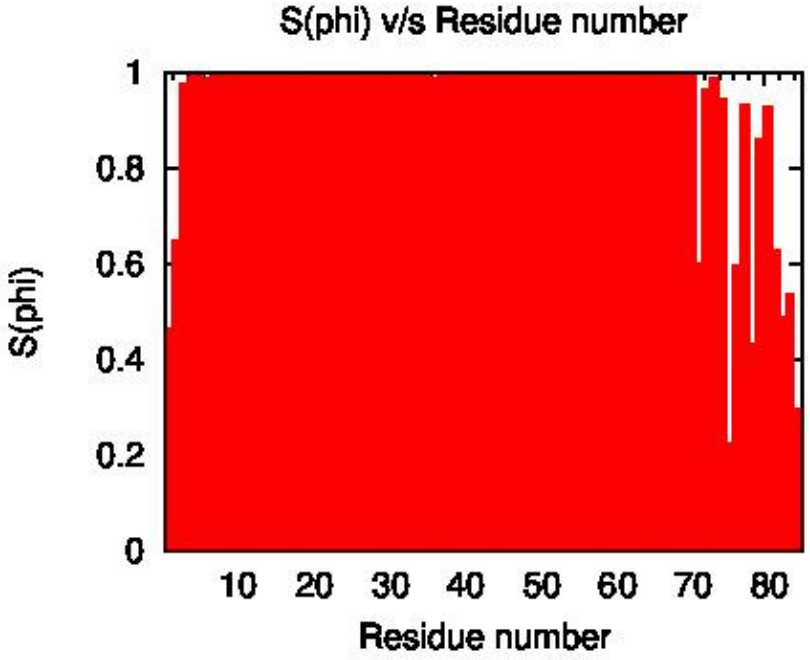
Global quality scores

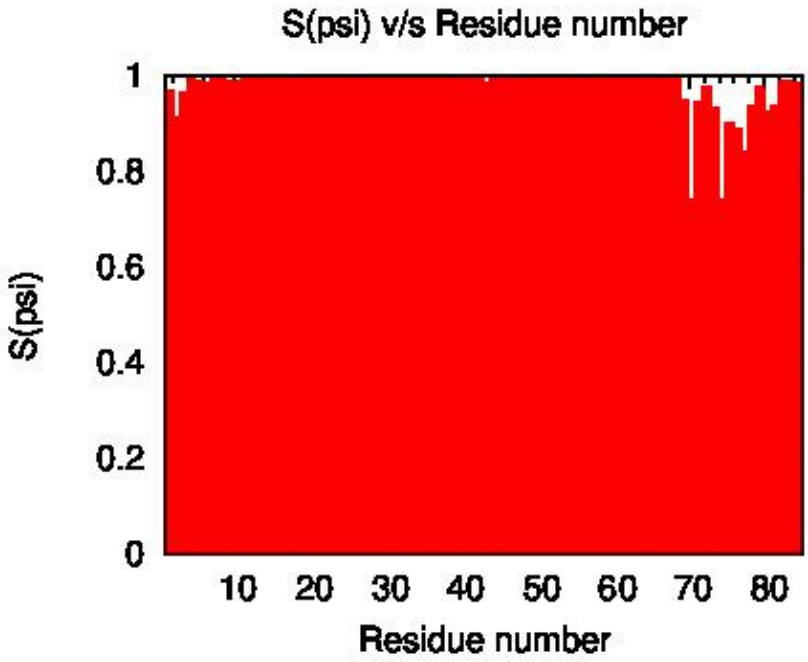
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)[3]*	*Procheck (all)[3]*	*MolProbity Clashscore*
Raw score	0.15	N/A	-0.54	-0.31	5.21
Z-score[1]	-4.98	N/A	-1.81	-1.83	0.63

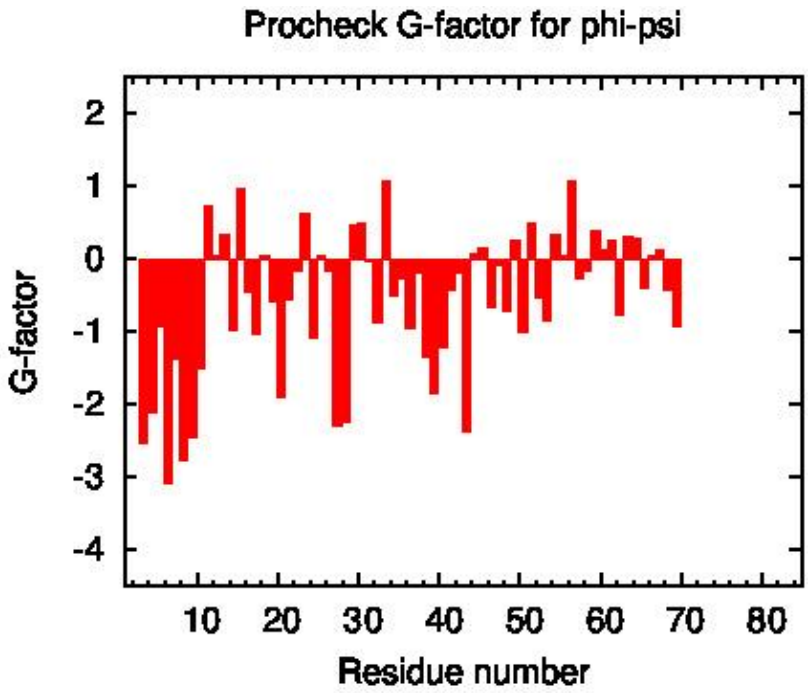
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	2
RMS deviation for bond angles:	2.0 °
RMS deviation for bond lengths:	0.013 Å

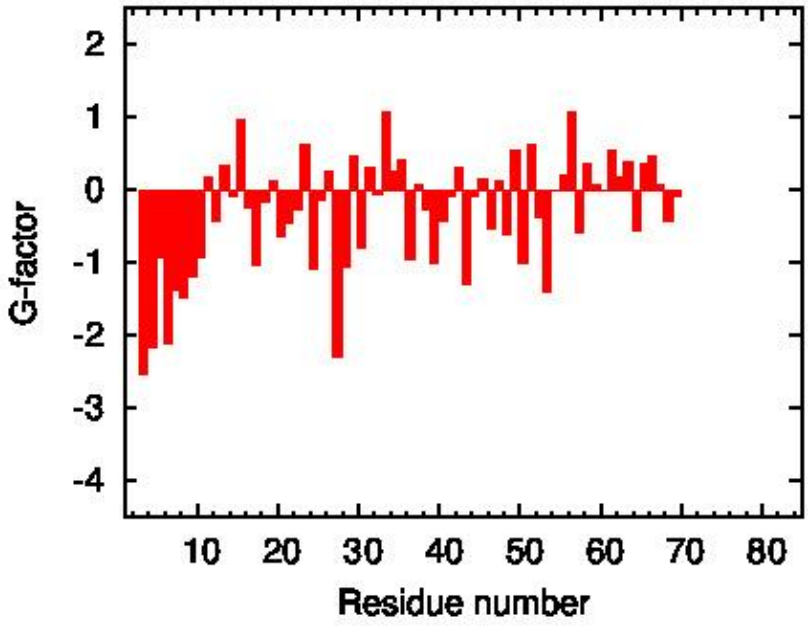
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2] Ordered residues (DAOP): 3A-69A
[3] Selected residues DAOP with S(phi)+S(psi)>=1.8 : 3A-69A



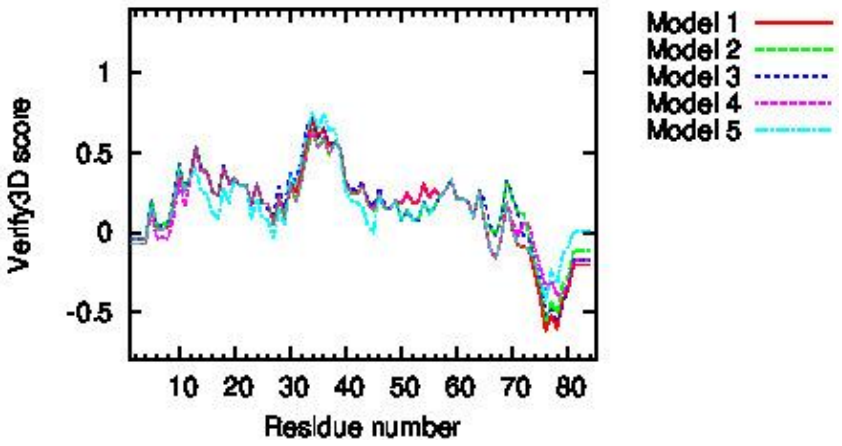

S(psi) v/s Residue number
S(psi)
1
0.8
0.6
0.4
0.2
0
10
20
30
40
50
60
70
80
Residue number


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

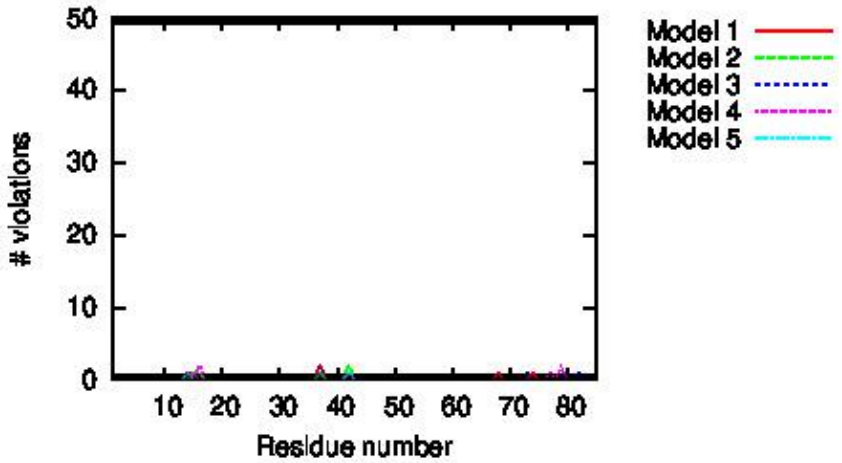
Procheck G-factor for all dihedral angles



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:
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9. Word JM et al, "Exploring steric constrains on protein mutations using MAGE / PROBE". Prot Sci 2000, 9:2251-2259
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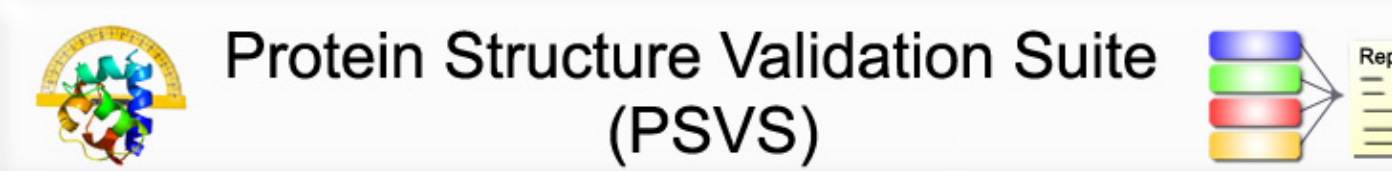
17. Bagaria A, Jaravine, V, Huang YJ, Montelione, GT, and Guntert, P "Protein structure validation by generalized linear model root-mean-square deviation prediction". Protein Sci 2012) 21:229-238.



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
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

Information updated on October, 2021. RTT