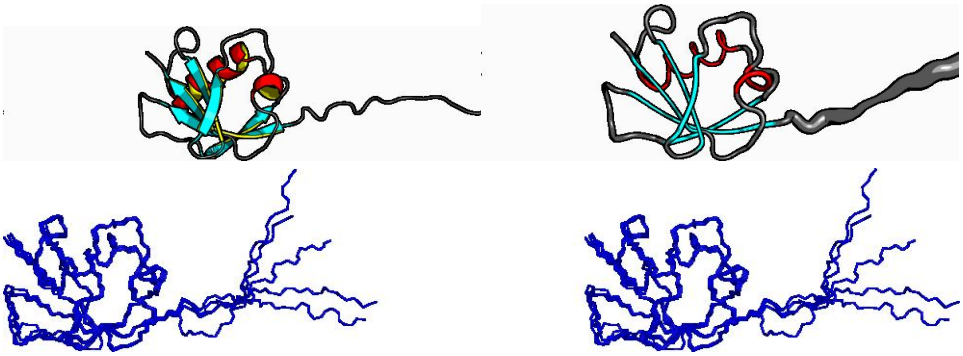
Structure Quality Analysis for NAME

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 : 15A-26A, 28A-30A, 32A-94A

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	95
Organism:	
SwissProt / TrEMBL ID:	
# models:	5
Oligomerization:	monomer
Molecular weight:	10342



Secondary Structure Elements:
alpha helices: 40A-51A, 79A-82A
beta strands: 29A-35A, 15A-22A, 88A-93A, 59A-64A, 67A-72A

FIDs deposited in the BMRB? no

Comparison of core atoms:

DAOP > 1.8 Å :	A:15..A:24, A:28..A:30, A:32..A:94
FindCore2 :	A:14..A:26, A:28..A:95
CYRANGE :	3..16 , 17..23, 32..94

RMSD	***All residues***	***Ordered residues[2]***	***Selected residues[3]***
All backbone atoms	2.3 Å	0.3 Å	0.3 Å
All heavy atoms	2.7 Å	0.6 Å	0.6 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
93.9%	6.1%	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
98.2%	1.8%	0%		

Global quality scores

Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
Raw score	0.15	N/A	-0.12	0.03	0.00
Z-score[1]	-4.98	N/A	-0.16	0.18	1.53

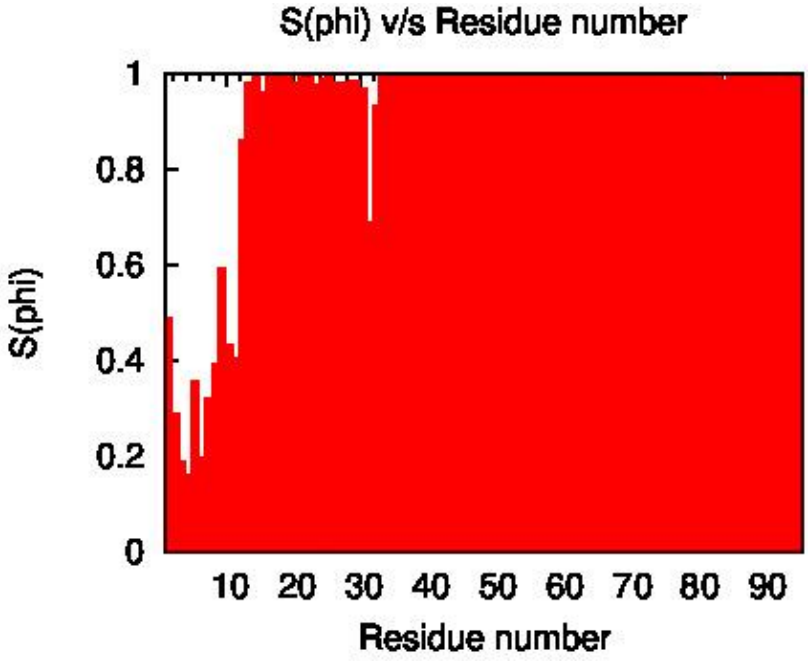
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

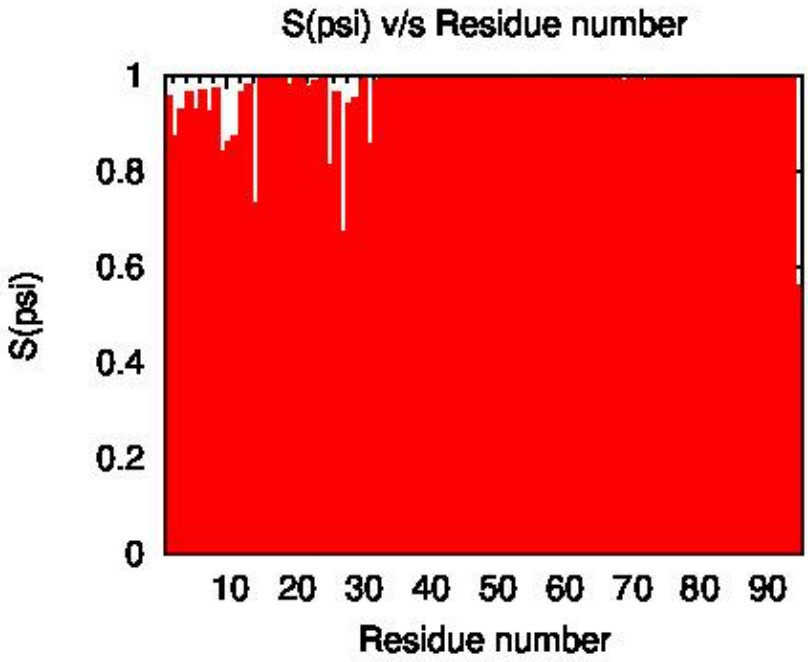
Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	0
RMS deviation for bond angles:	2.0 °
RMS deviation for bond lengths:	0.011 Å

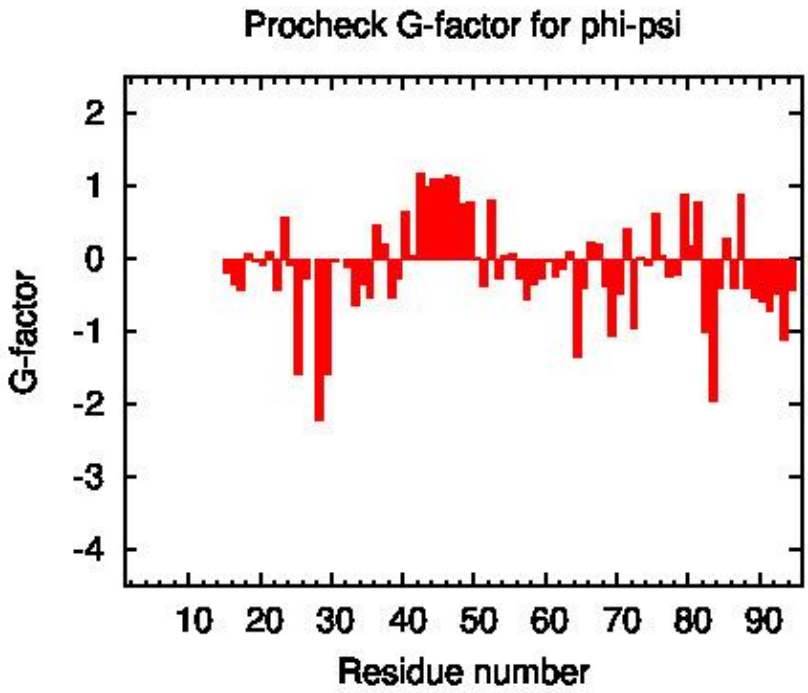
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

[2] Ordered residues (DAOP): 15A-26A, 28A-30A, 32A-94A

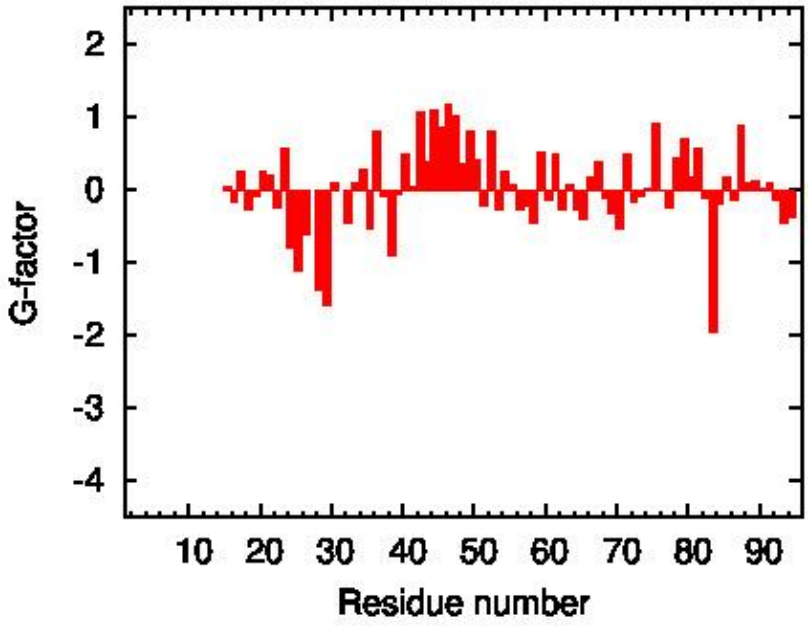
[3] Selected residues DAOP with S(phi)+S(psi)>=1.8 : 15A-26A, 28A-30A, 32A-94A



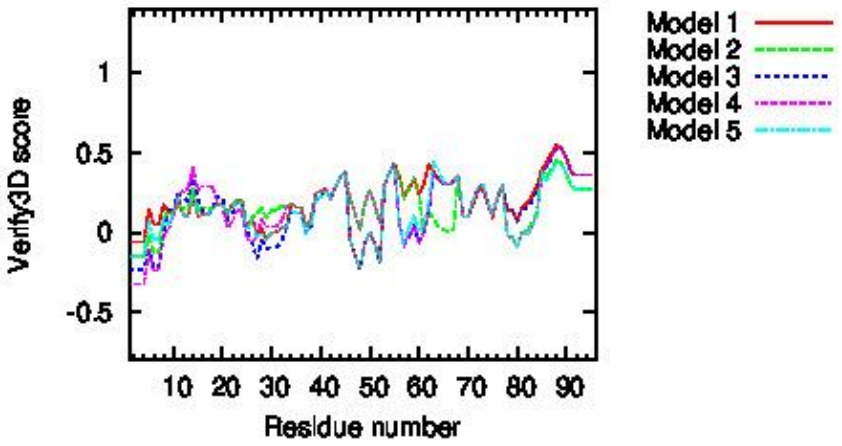

S(psi) v/s Residue number
S(psi)
1
0.8
0.6
0.4
0.2
0
10 20 30 40 50 60 70 80 90
Residue number


Procheck G-factor for phi-psi
G-factor
2
1
0
-1
-2
-3
-4
10 20 30 40 50 60 70 80 90
Residue number

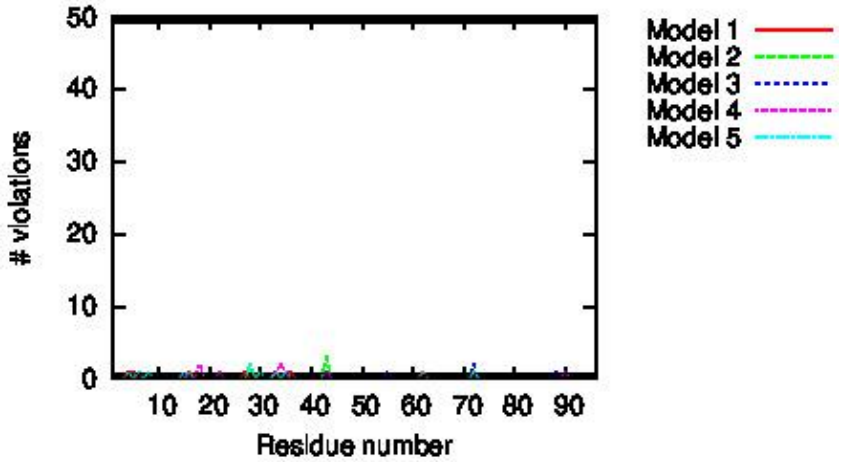
Procheck G-factor for all dihedral angles

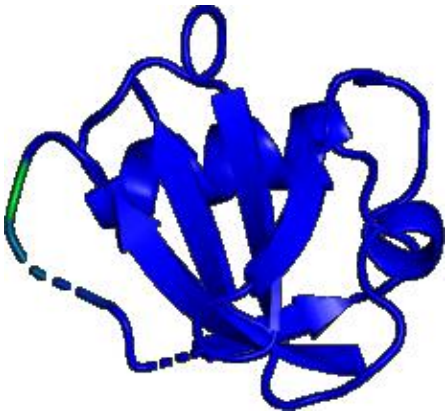


Verify3D score over window of 7 residues



Residual VdW violations from MolProbity





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

References:
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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
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5. Sippl MJ, "Recognition of errors in three-dimensional structures of proteins". Proteins 1993, 17:355-362
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16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features". Biopolymers 1983, 22:2577-2637
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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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