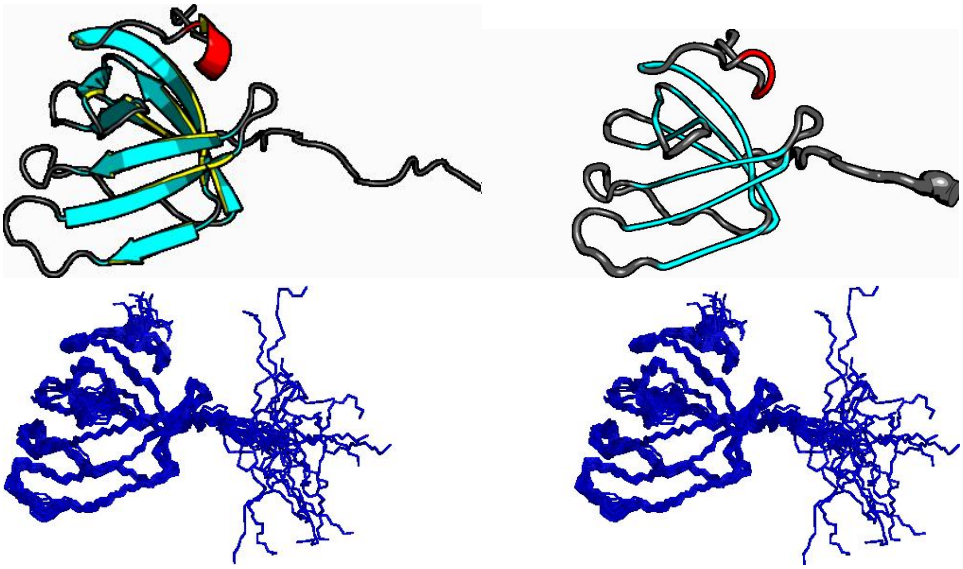
Structure Quality Analysis for NAME

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-14A, 17A-29A, 35A-55A, 58A-77A, 81A-86A, 89A-98A

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	109
Organism:	
SwissProt / TrEMBL ID:	
# models:	20
Oligomerization:	monomer
Molecular weight:	12503



Secondary Structure Elements:
alpha helices:
beta strands: 19A-19A, 17A-18A, 66A-77A, 20A-29A, 35A-42A, 48A-53A, 80A-85A, 90A-93A

FIDs deposited in the BMRB? no

Comparison of core atoms:

DAOP > 1.8 Å :	A:3..A:14, A:17..A:29, A:35..A:53, A:58..A:77, A:81..A:86, A:89..A:97
FindCore2 :	A:2..A:30, A:32..A:101
CYRANGE :	3..29, 34..54, 58..98

RMSD	***All residues***	***Ordered residues[2]***	***Selected residues[3]***
All backbone atoms	2.2 Å	0.4 Å	0.4 Å
All heavy atoms	2.8 Å	0.9 Å	0.9 Å

Ramachandran Plot Summary for selected residues[3] from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
88.0%	11.6%	0.2%	0.1%

Ramachandran Plot Summary for selected residues[3] from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
95.5%	4.4%	0.1%		

Global quality scores

Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*[3]	*Procheck (all)*[3]	*MolProbity Clashscore*
Raw score	0.17	0.18	-0.45	-0.24	19.53
Z-score[1]	-4.65	-1.94	-1.46	-1.42	-1.83

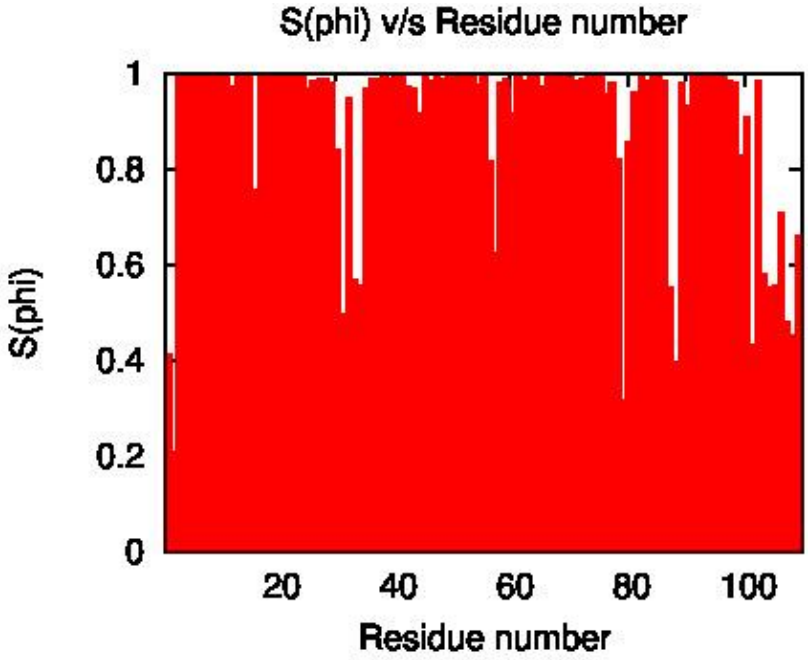
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

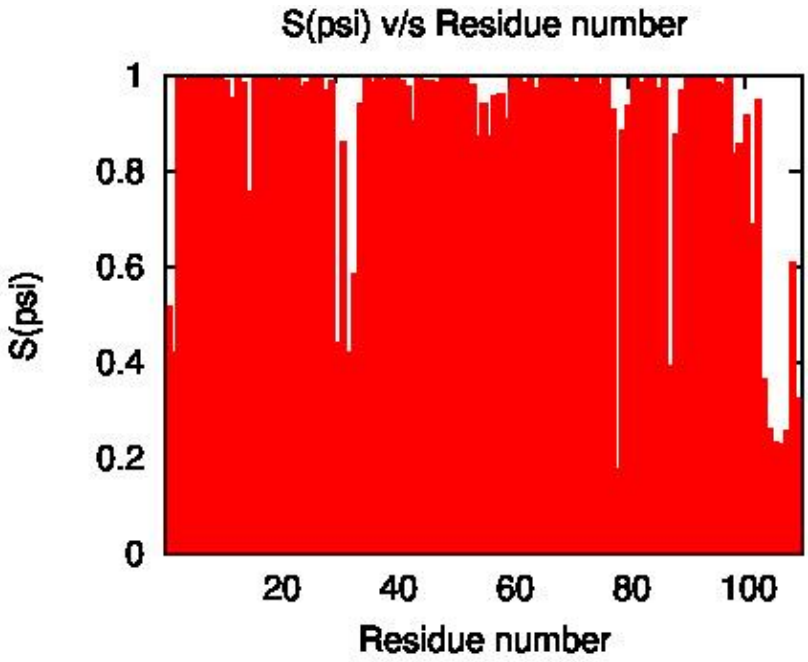
Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms):	11
RMS deviation for bond angles:	1.7 °
RMS deviation for bond lengths:	0.019 Å

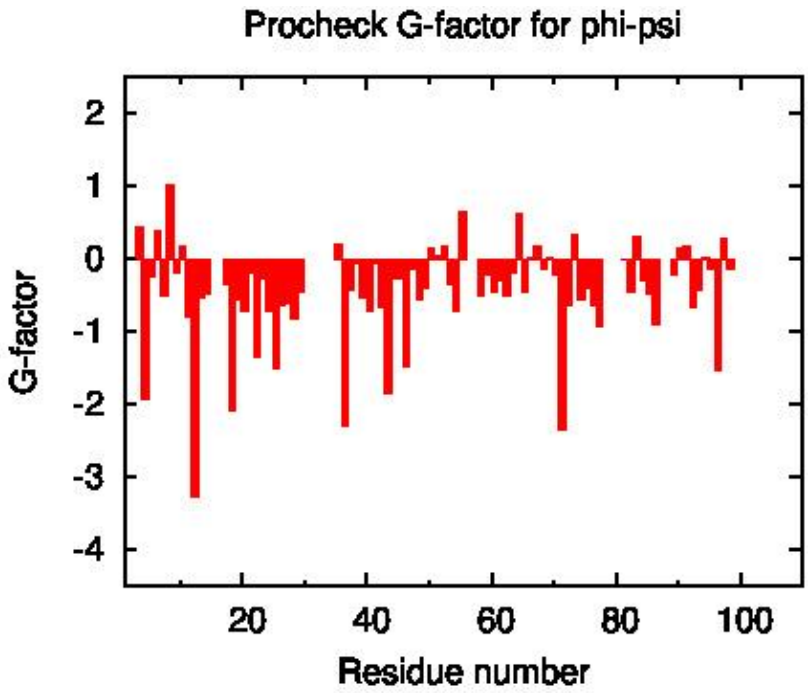
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

[2] Ordered residues (DAOP): 3A-14A, 17A-29A, 35A-55A, 58A-77A, 81A-86A, 89A-98A

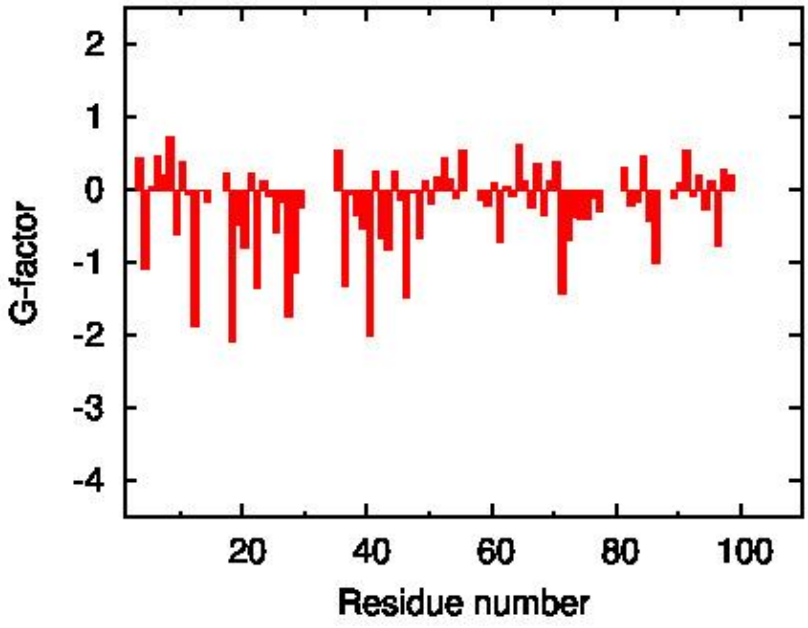
[3] Selected residues DAOP with S(phi)+S(psi)>=1.8 : 3A-14A, 17A-29A, 35A-55A, 58A-77A, 81A-86A, 89A-98A

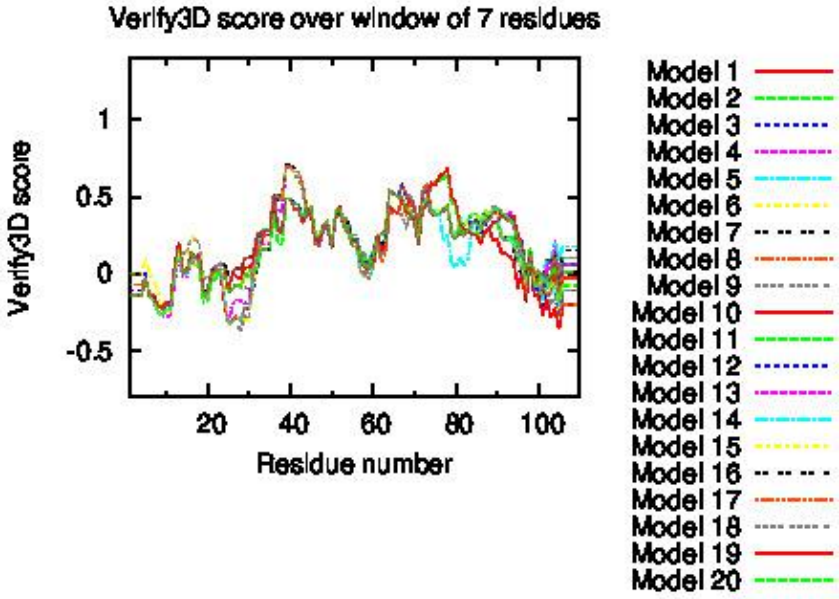


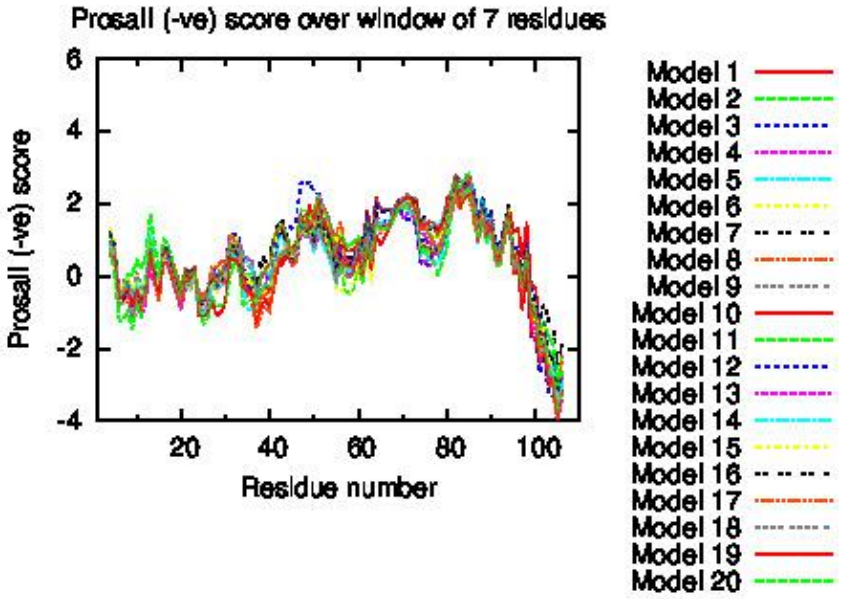

S(psi) v/s Residue number
S(psi)
Residue number
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100

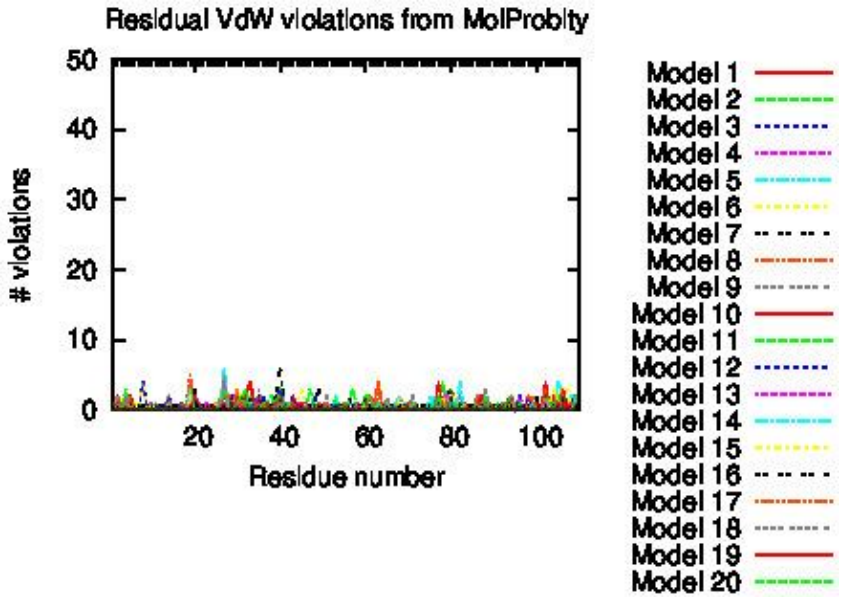

Procheck G-factor for phi-psi
G-factor
Residue number
2
1
0
-1
-2
-3
-4
20
40
60
80
100

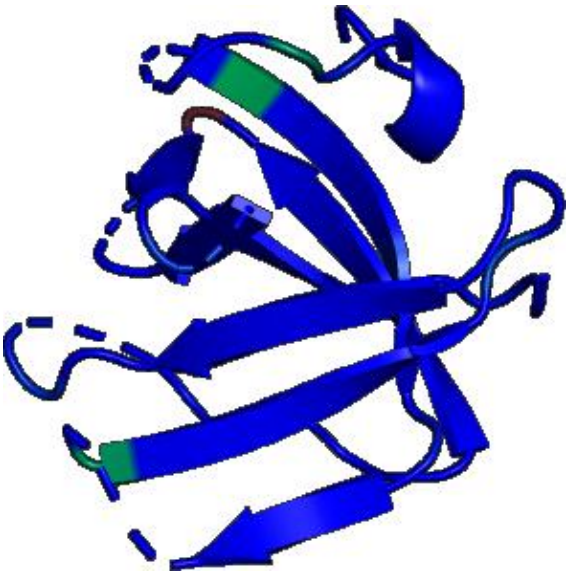
Procheck G-factor for all dihedral angles






Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
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


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
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:

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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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