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-20A, 23A-81A

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	92
Organism:	
SwissProt / TrEMBL ID:	
# models:	5
Oligomerization:	monomer
Molecular weight:	10580
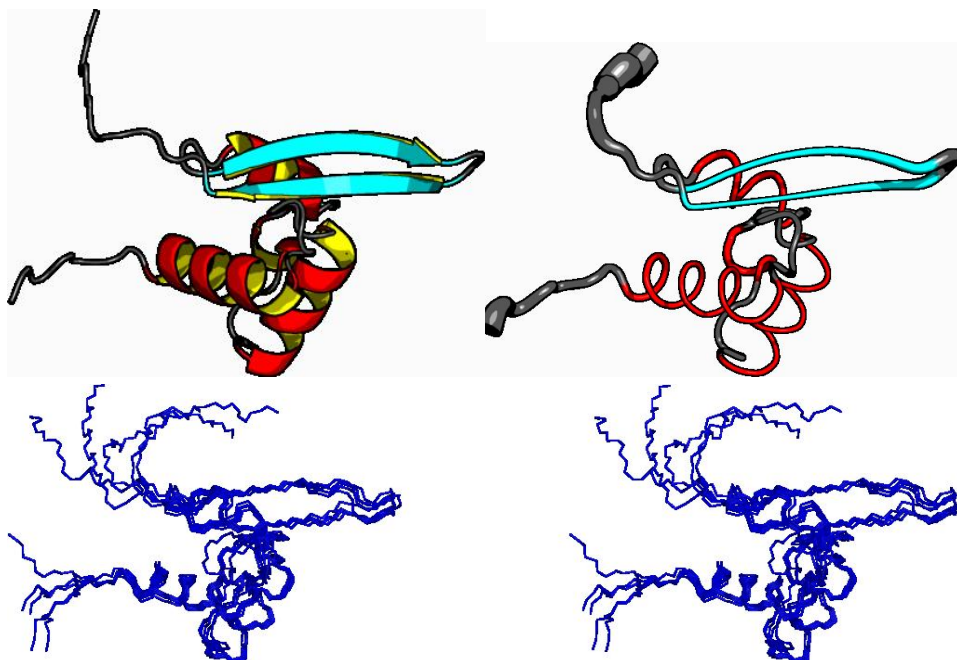
Secondary Structure Elements:
alpha helices: 8A-20A, 29A-39A, 53A-57A
beta strands: 27A-28A, 73A-80A, 63A-70A

FIDs deposited in the BMRB? no

Comparison of core atoms:

DAOP > 1.8 Å : A:4..A:20, A:23..A:81
FindCore2 : A:4..A:45, A:47..A:48, A:50..A:83
CYRANGE : 8..20, 26..38, 57..66, 76..80 , 67..75

RMSD	*All residues*	*Ordered residues[2]*	*Selected residues[3]*
All backbone atoms	2.2 Å	0.7 Å	0.7 Å
All heavy atoms	2.7 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*
91.3%	8.1%	0.6%	0.0%

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

Most favoured regions	*Allowed regions*	*Disallowed regions*	<u>View plot</u> <u>View model summary</u>
95.6%	2.6%	1.8%	

Global quality scores

Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)[3]*	*Procheck (all)[3]*	*MolProbity Clashscore*
Raw score	0.17	N/A	-0.12	0.01	1.60
Z-score[1]	-4.65	N/A	-0.16	0.06	1.25

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: 2.1 °

RMS deviation for bond lengths: 0.012 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
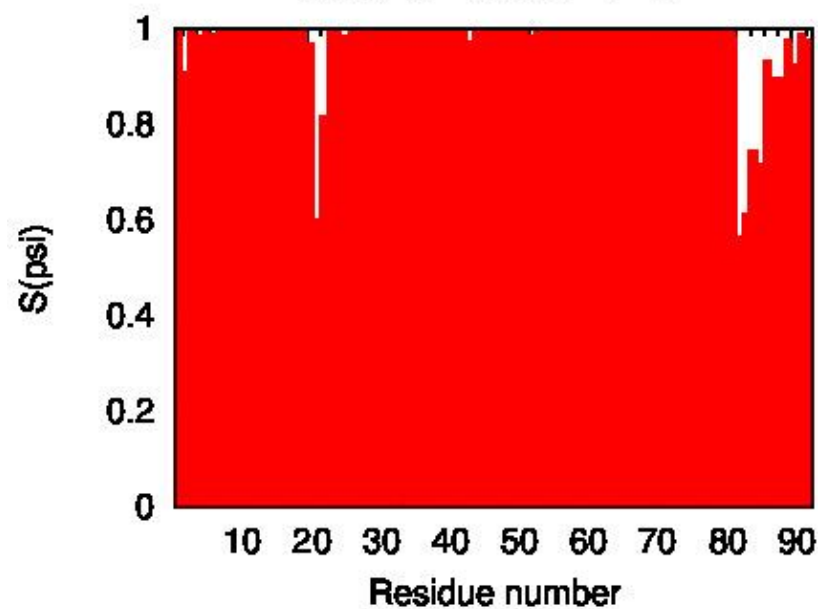
[2] Ordered residues (DAOP): 2A-20A, 23A-81A

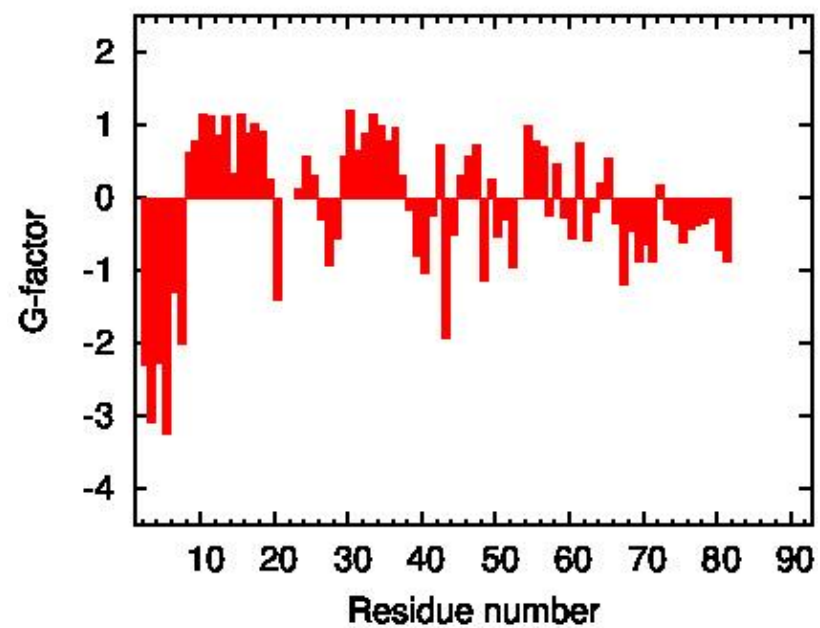[3] Selected residues DAOP with S(phi)+S(psi)>=1.8 : 2A-20A, 23A-81A
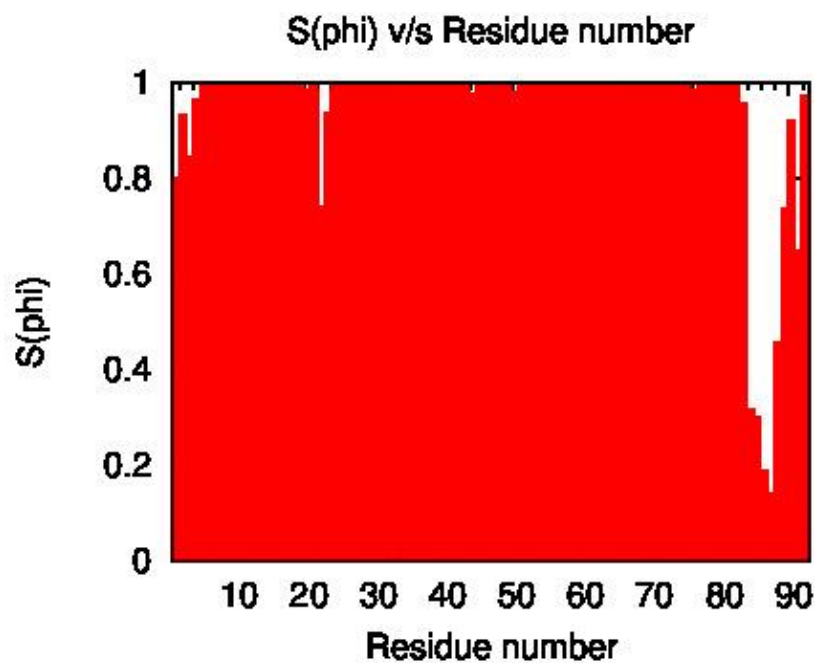
S(phi) v/s Residue number
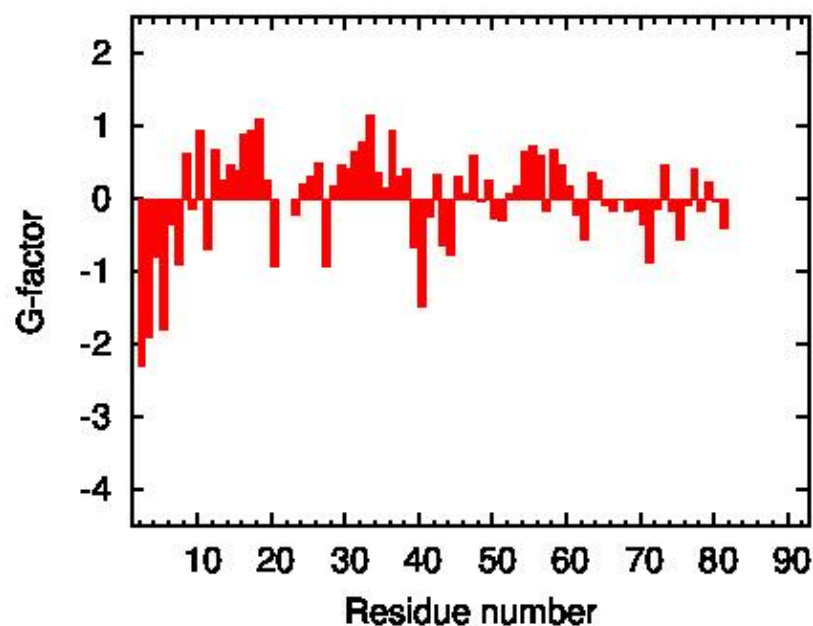
S(psi) v/s Residue number

Procheck G-factor for phi-psi

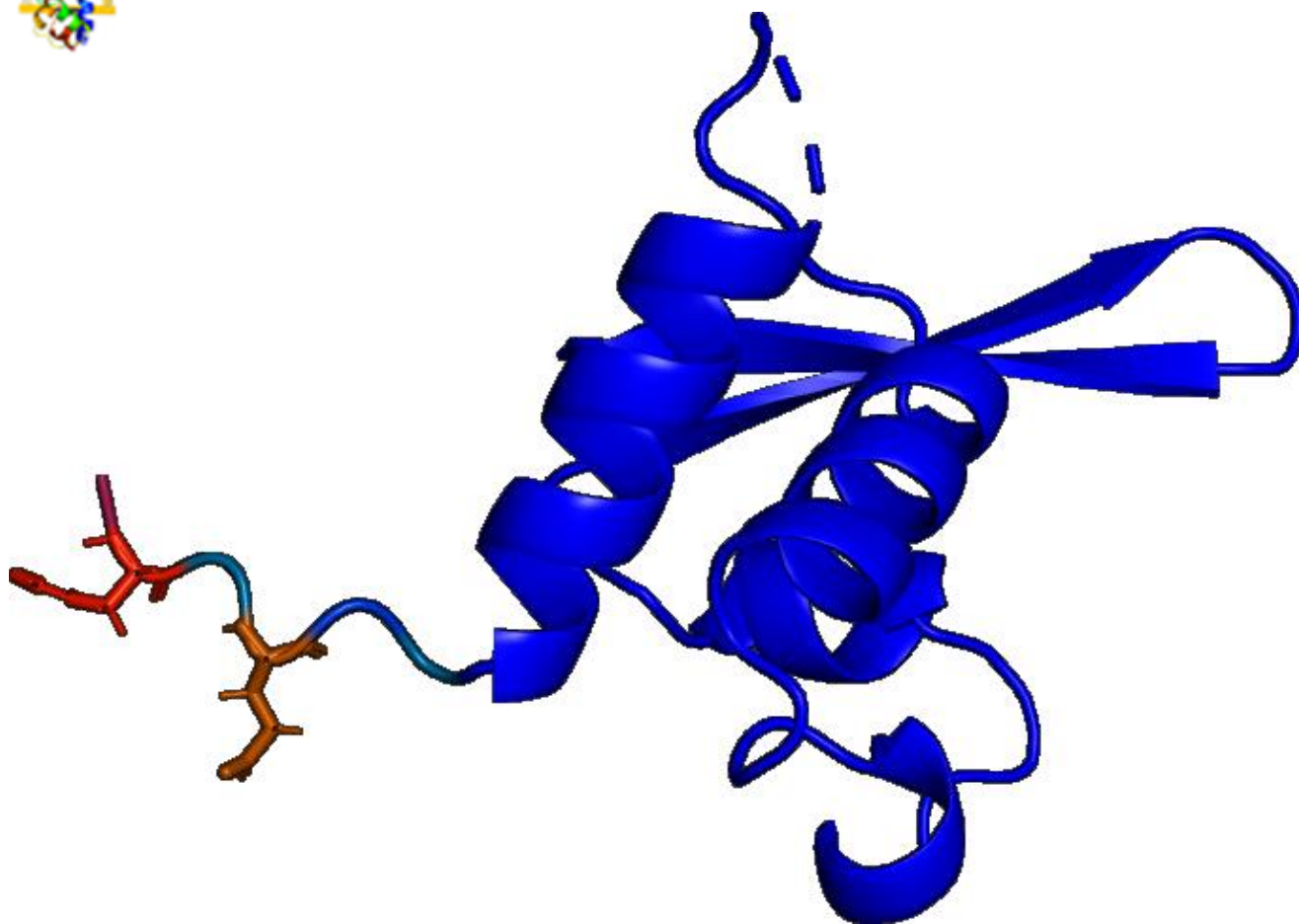## Procheck G-factor for all dihedral angles

Verify3D score over window of 7 residues

Model 1
Model 2
Model 3
Model 4
Model 5
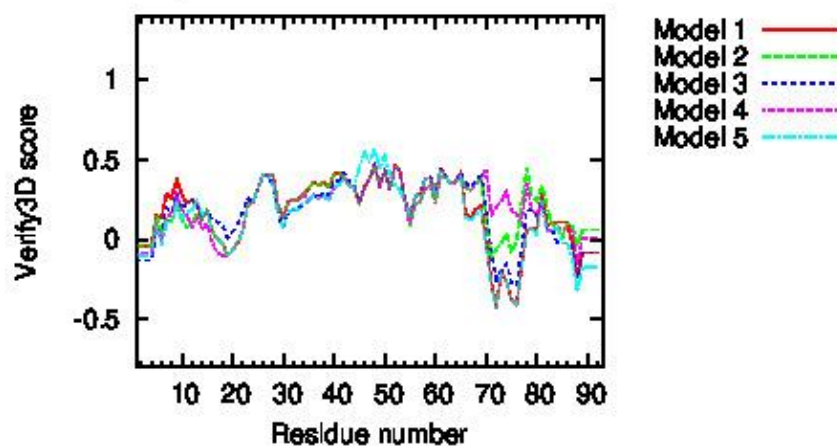
Residual VdW violations from MolProbity

Model 1
Model 2
Model 3
Model 4
Model 5
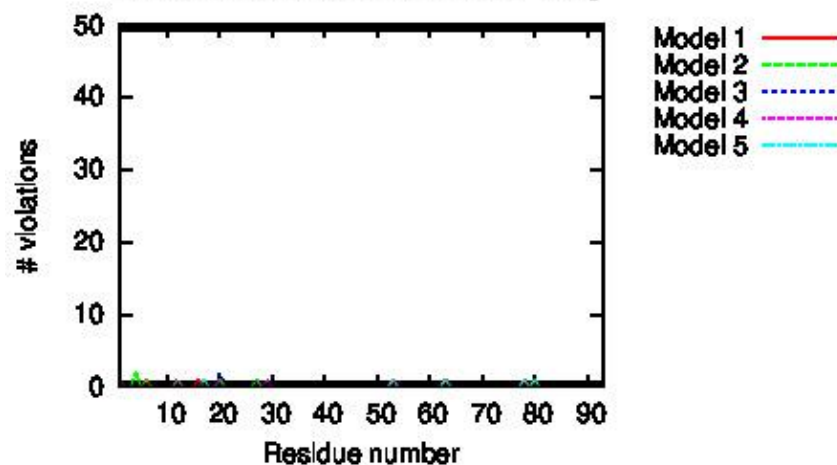
**Residue Plot of Ramachandran anlysis(based on data from Richardson Lab's Molprobity)**

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
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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
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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
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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

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.
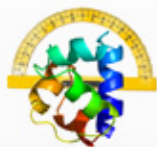
Protein Structure Validation Suite (PSVS)

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

Information updated on October, 2021. RTT
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