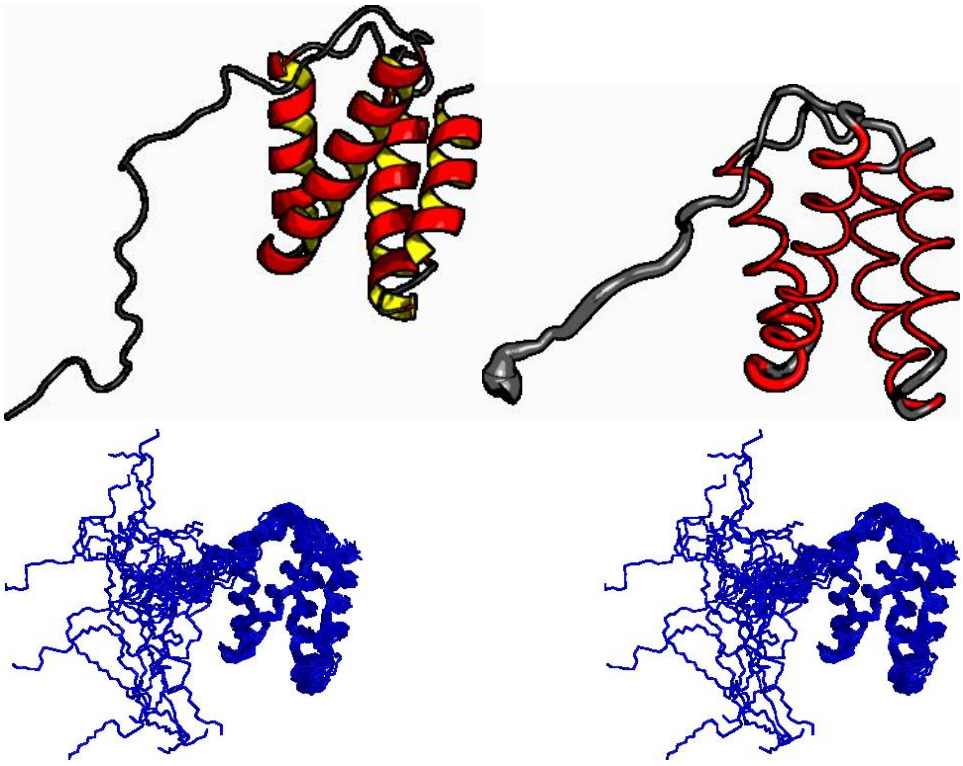
# Structure Quality Analysis for NAME

## 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 : 65A-77A, 81A-148A

| | |
|---|---|
| **NESG ID:** | NAME |
| **PDB ID:** | |
| **Deposition date:** | |
| **Common Name:** | |
| **Class:** | |
| **Length (a.a.):** | 111 |
| **Organism:** | |
| **SwissProt / TrEMBL ID:** | |
| # models: | 20 |
| **Oligomerization:** | monomer |
| **Molecular weight:** | 13095 |



**Secondary Structure Elements:**
**alpha helices**: 65A-76A, 82A-98A, 109A-120A, 125A-144A
**beta strands**:

**FIDs deposited in the BMRB?** no

**Comparison of core atoms:**

**DAOP > 1.8 Å :** A:65..A:77, A:81..A:147
**FindCore2 :** A:64..A:78, A:80..A:154, A:156
**CYRANGE :** 65..152

| **RMSD** | ***All residues*** | ***Ordered residues[2]*** | ***Selected residues[3]*** |
|---|---|---|---|
| *All backbone atoms* | 5.4 Å | 0.7 Å | 0.7 Å |
| *All heavy atoms* | 6.1 Å | 1.2 Å | 1.2 Å |

**Ramachandran Plot Summary for selected residues[3] from Procheck**

| *Most favoured* | *Additionally allowed regions* | *Generously allowed regions* | *Disallowed regions* |
|---|---|---|---|

| *regions* | | | |
|---|---|---|---|
| 97.3% | 2.6% | 0.1% | 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 |
|---|---|---|---|---|
| 98.8% | 1% | 0.1% | | |

**Global quality scores**

| Program | *Verify3D* | *ProsaII (-ve)* | *Procheck (phi-psi)[3]* | *Procheck (all)[3]* | *MolProbity Clashscore* |
|---|---|---|---|---|---|
| *Raw score* | 0.07 | 0.50 | 0.63 | 0.46 | 17.45 |
| *Z-score[1]* | -6.26 | -0.62 | 2.79 | 2.72 | -1.47 |

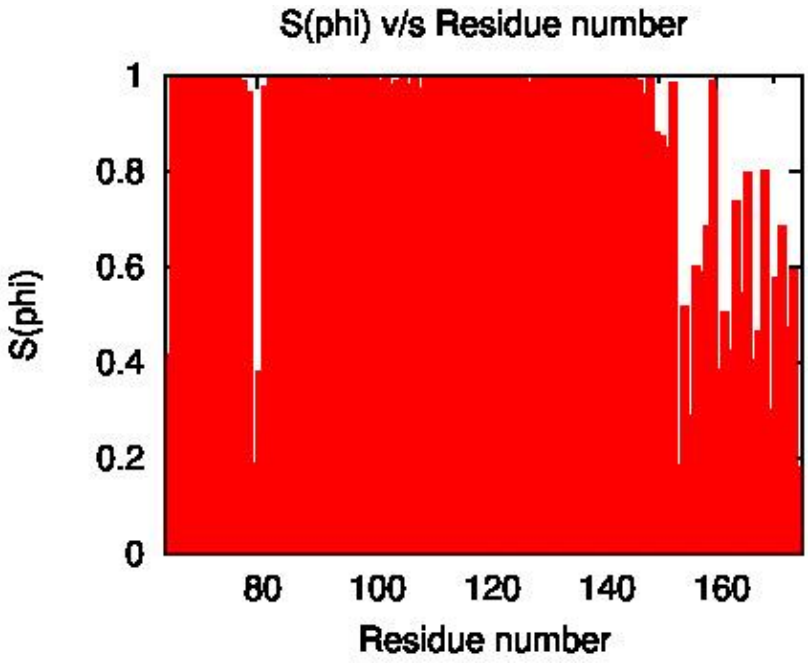
**Close Contacts and Deviations from Ideal Geometry (from PDB validation software)**

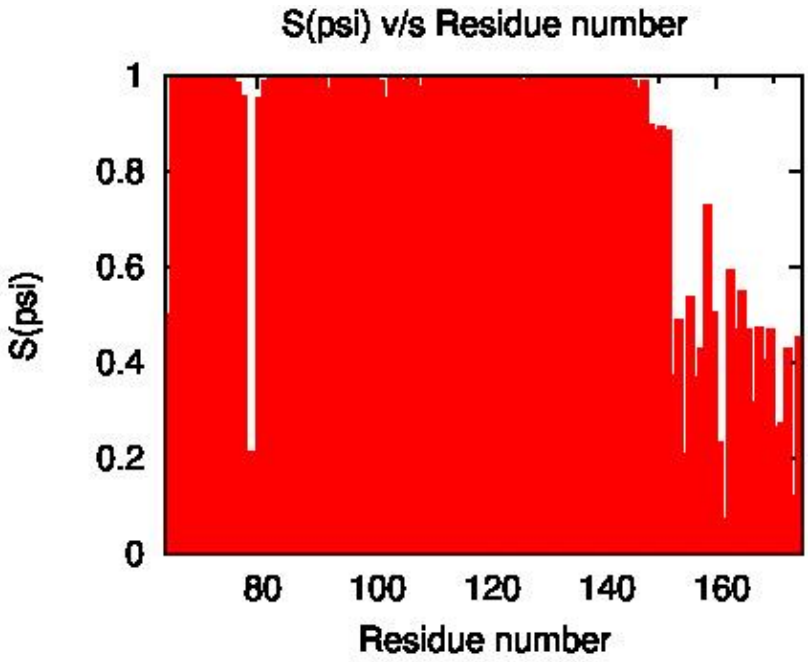
| | |
|---|---|
| Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms): | 11 |
| RMS deviation for bond angles: | 1.7 ° |
| RMS deviation for bond lengths: | 0.019 Å |

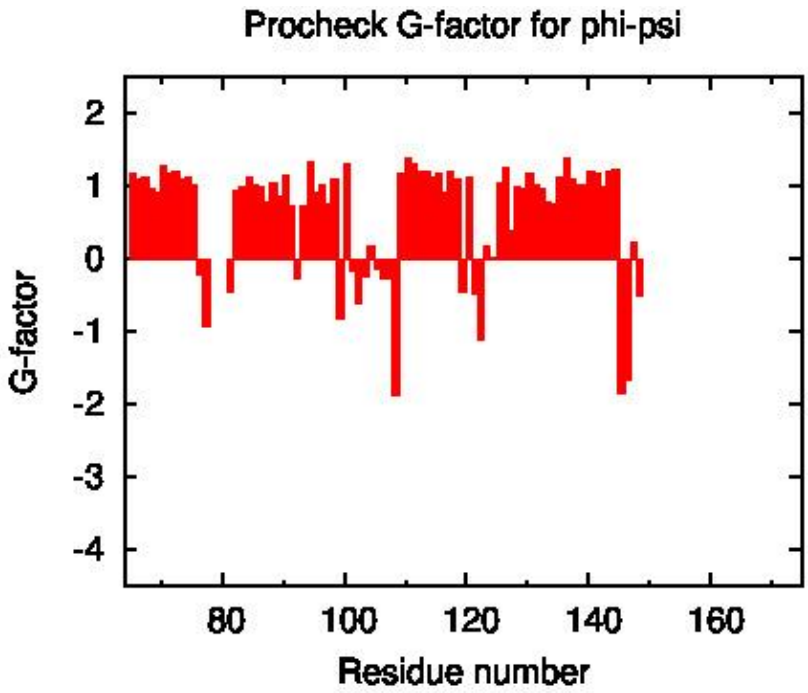
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

[2] Ordered residues (DAOP): 65A-77A, 81A-148A

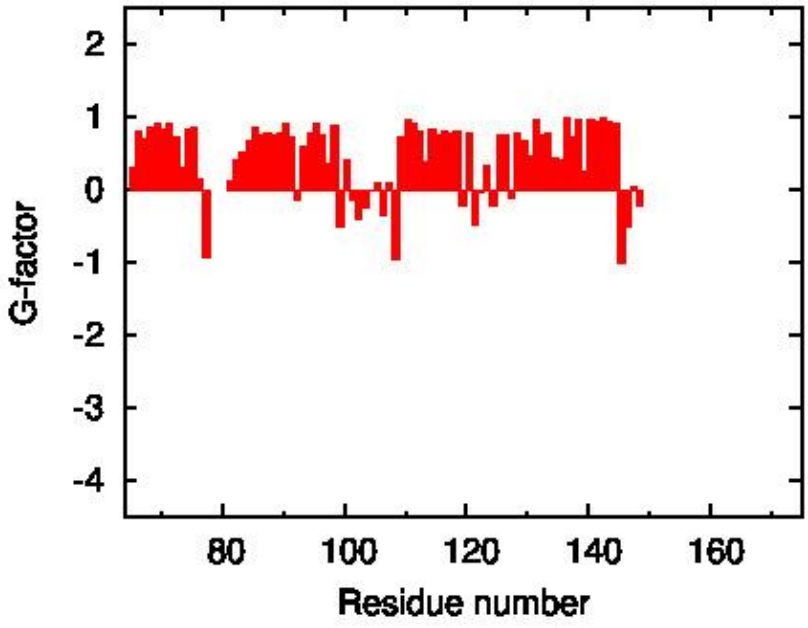
[3] Selected residues DAOP with S(phi)+S(psi)>=1.8 : 65A-77A, 81A-148A



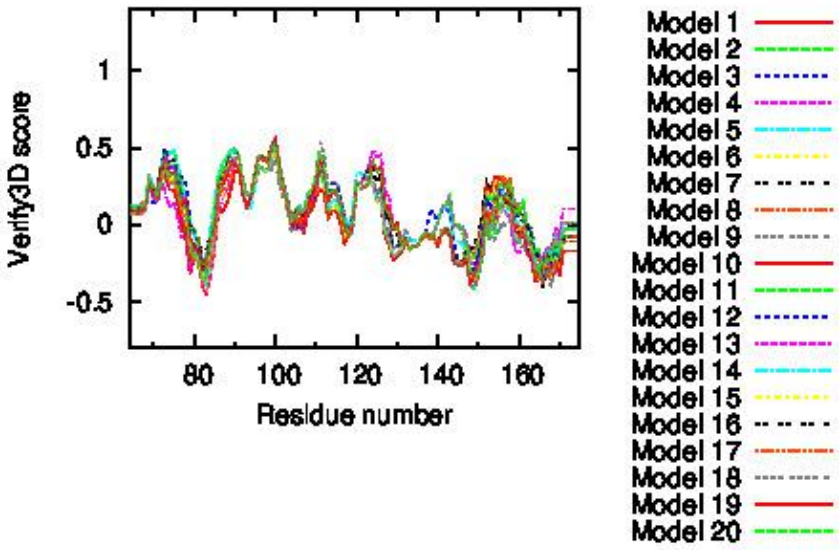

S(psi) v/s Residue number
S(psi)
1
0.8
0.6
0.4
0.2
0
80
100
120
140
160
Residue number

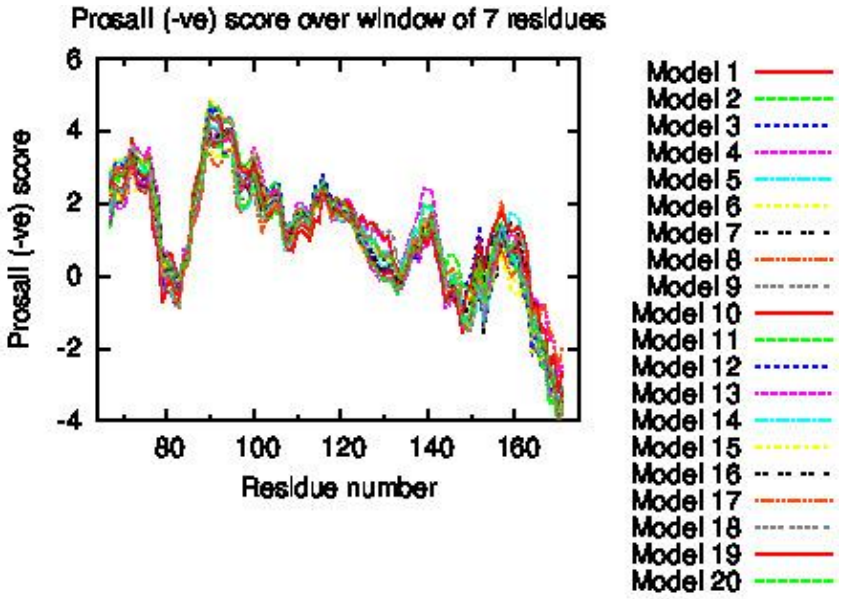

Procheck G-factor for phi-psi
G-factor
2
1
0
-1
-2
-3
-4
80
100
120
140
160
Residue number

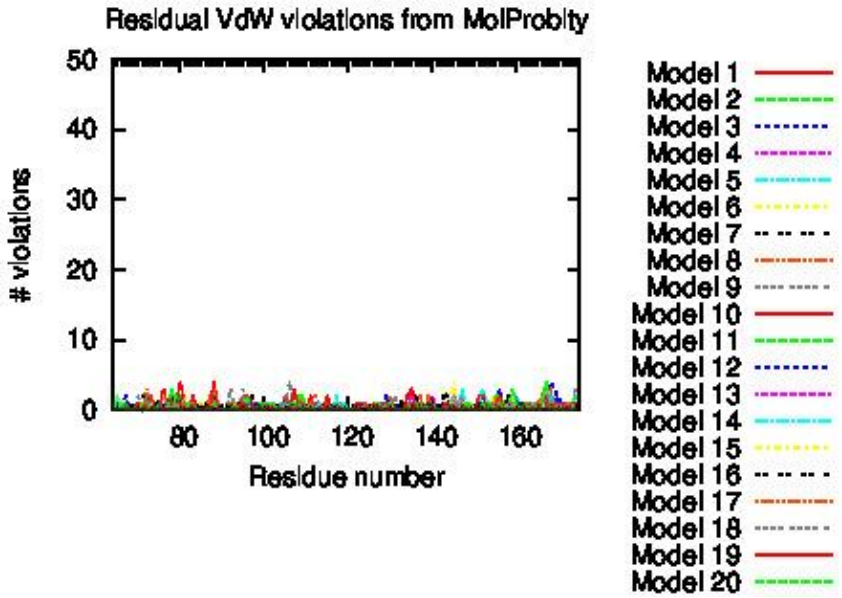
Procheck G-factor for all dihedral angles

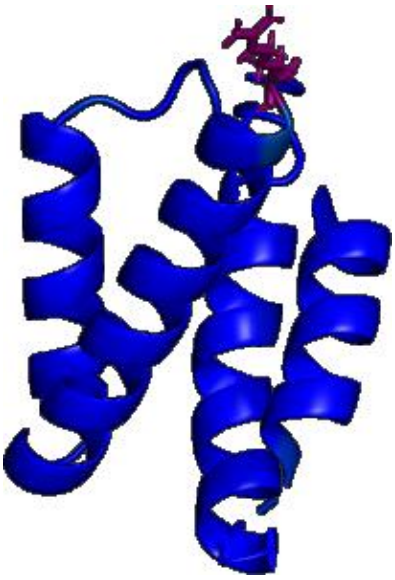



Verify3D score over window of 7 residues




Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
80
100
120
140
160
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
80
100
120
140
160
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:***
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.

# 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