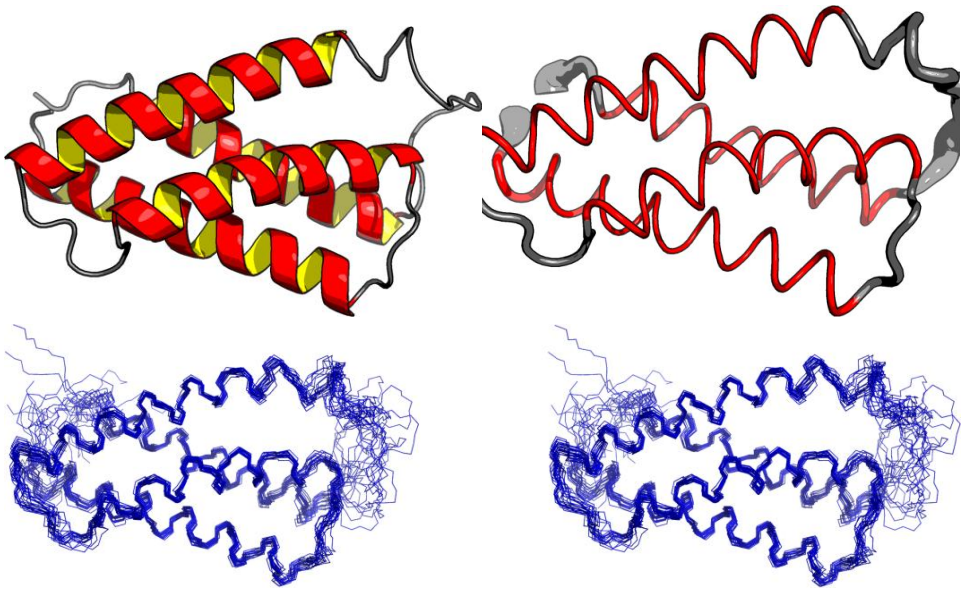
# Structure Quality Analysis for NAME

Analyses performed for user defined residues.
The constraints analysis is based on the following files: NOE distance constraints file. Angular constraints file. H-bond constraints file.
Procheck analysis,RMSD calculation and structure superimposition are based on: User defined residues

| | |
|---|---|
| NESG ID: | NAME |
| PDB ID: | |
| Deposition date: | |
| Common Name: | |
| Class: | |
| Length (a.a.): | 123 |
| Organism: | |
| SwissProt / TrEMBL ID: | |
| # models: | 20 |
| Oligomerization: | monomer |
| Molecular weight: | 14459 |



Secondary Structure Elements:
alpha helices: 6A-26A, 42A-64A, 72A-91A, 96A-120A
beta strands:

| | |
|---|---|
| Total number of restricting constraints per restrained residue: | 21.2 |
| Restricting long range constraints per restrained residue: | 4.4 |

Distance violations per model
Calculated using sum over r^-6

| 0.1 - 0.2 Å | 0.2 - 0.5 Å | > 0.5 Å |
|---|---|---|
| 12.75 | 11.25 | 1.65 |

Dihedral angle violations per model

| 1 - 10 ° | > 10 ° |
|---|---|
| 0.05 | 0 |

FIDs deposited in the BMRB? no

RPF Scores

| Recall | Precision | F-measure | DP-score |
|---|---|---|---|

0.964 0.892 0.926 0.747

| RMSD | *All residues* | *Ordered residues*[2] | *Selected residues*[3] |
|---|---|---|---|
| *All backbone atoms* | 1.7 Å | 0.5 Å | 0.5 Å |
| *All heavy atoms* | 2.2 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* |
|---|---|---|---|
| 98.9% | 1.1% | 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 |
|---|---|---|---|---|
| 99.5% | 0.4% | 0.1% | | |

**Global quality scores**

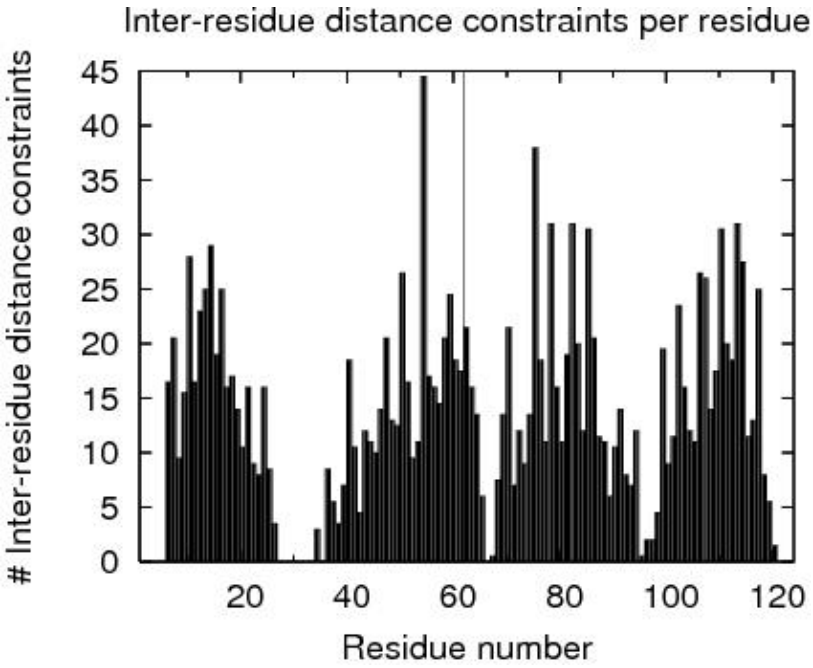
| Program | *Verify3D* | *ProsaII (-ve)* | *Procheck (phi-psi)*[3] | *Procheck (all)*[3] | *MolProbity Clashscore* |
|---|---|---|---|---|---|
| *-Raw score* | 0.36 | 0.99 | 0.81 | 0.73 | 5.00 |
| *Z-score*[1] | -1.61 | 1.41 | 3.50 | 4.32 | 0.67 |

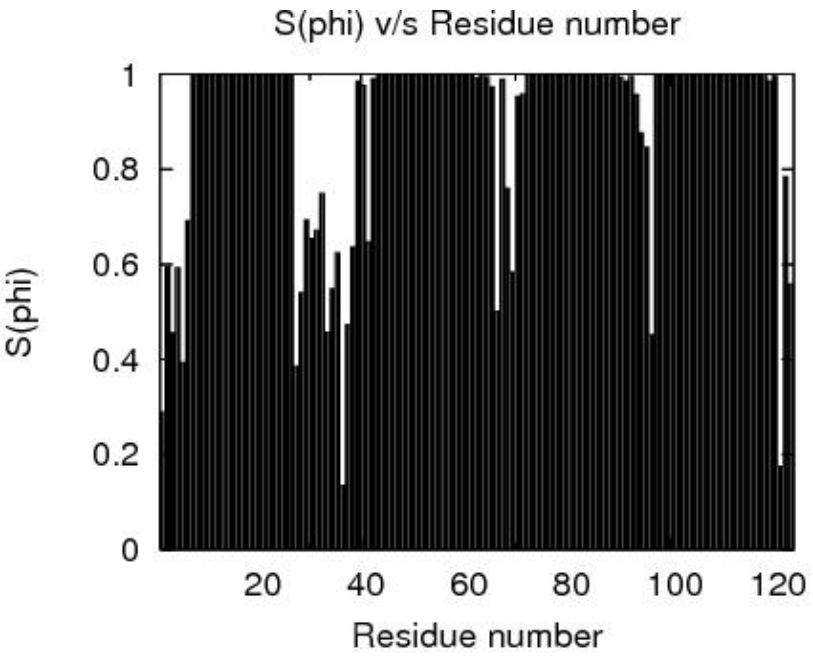
**Generalized linear model RMSD prediction: 0.78**

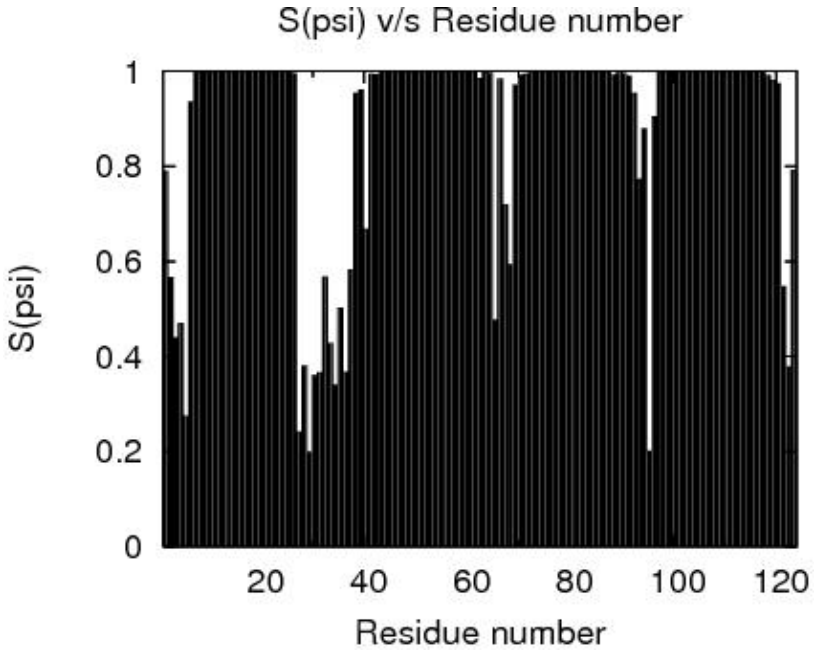
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

| | |
|---|---|
| Number of close contacts (within 1.6 &Aring for H atoms, 2.2 &Aring for heavy atoms): | 1 |
| RMS deviation for bond angles: | 0.6 ° |
| RMS deviation for bond lengths: | 0.010 Å |

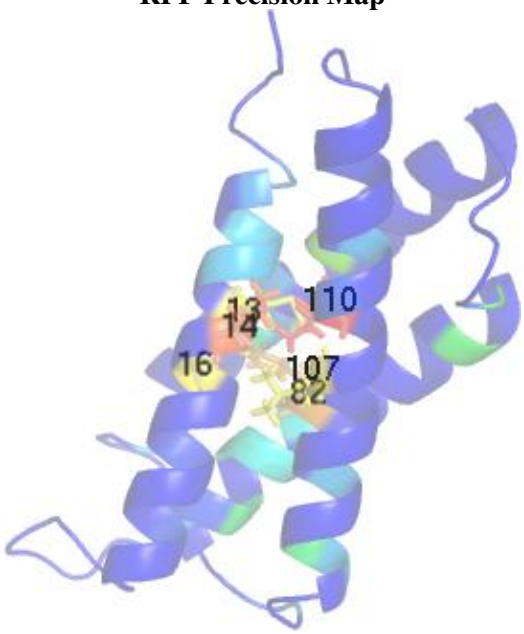
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score
[2]Order residues: 7A-26A,42A-64A,70A-92A,97A-120A
[3]Selected residues: 7A-26A,42A-64A,70A-93A,97A-120A

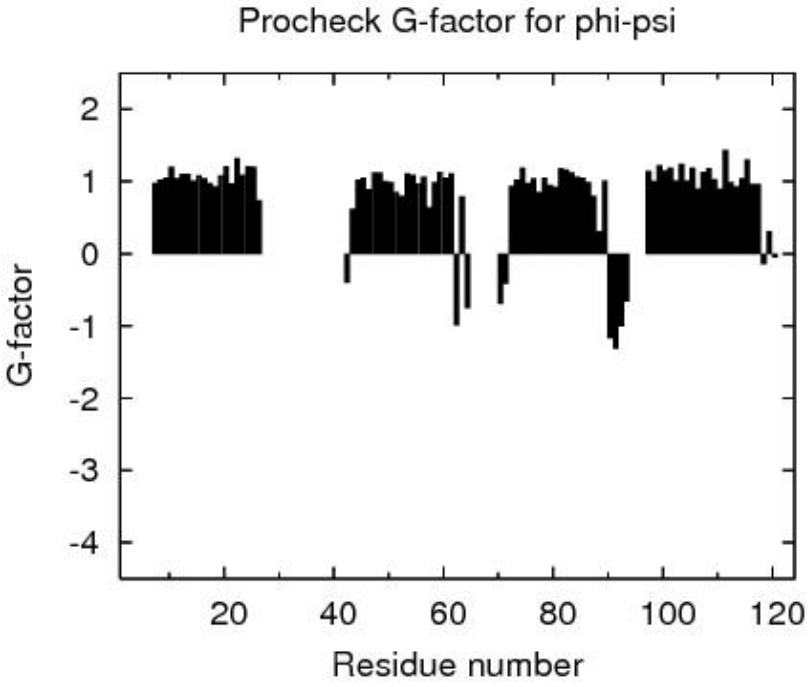

Inter-residue distance constraints per residue
# Inter-residue distance constraints
45
40
35
30
25
20
15
10
5
0
20
40
60
80
100
120
Residue number

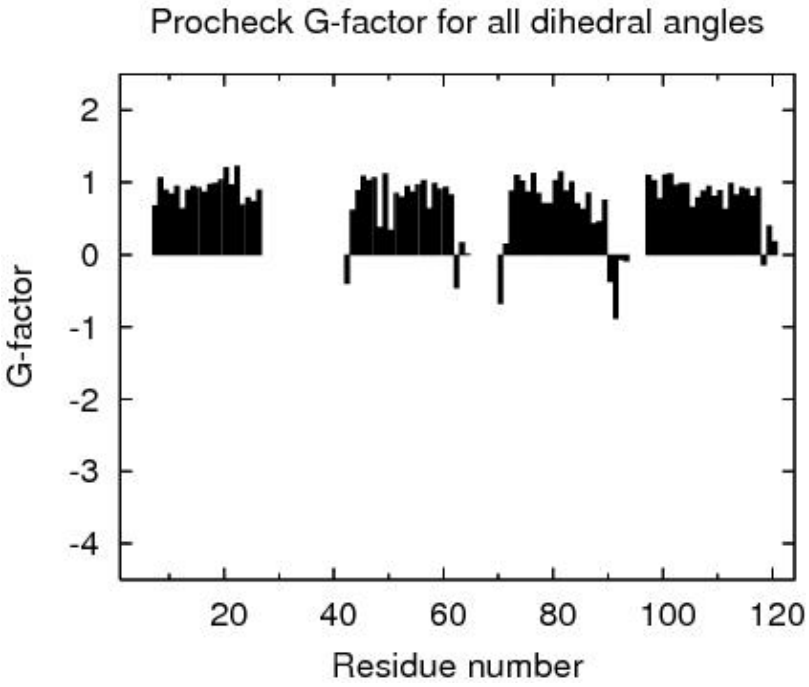

S(phi) v/s Residue number
S(phi)
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
120
Residue number

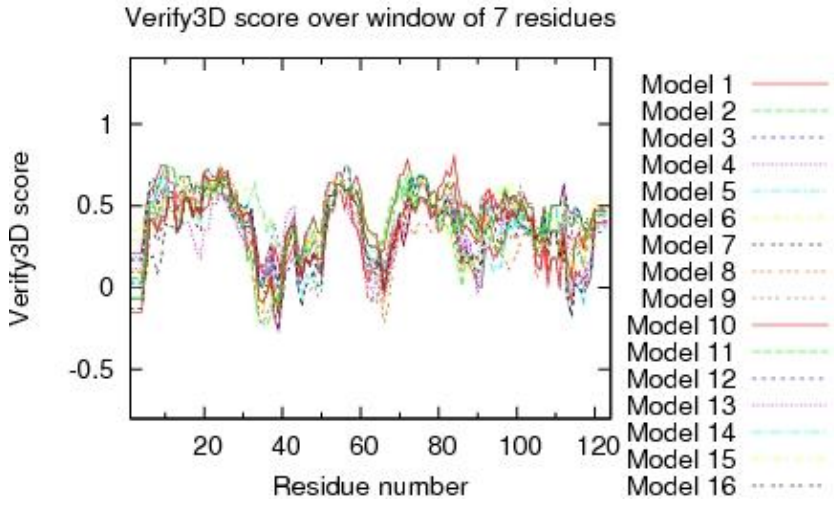


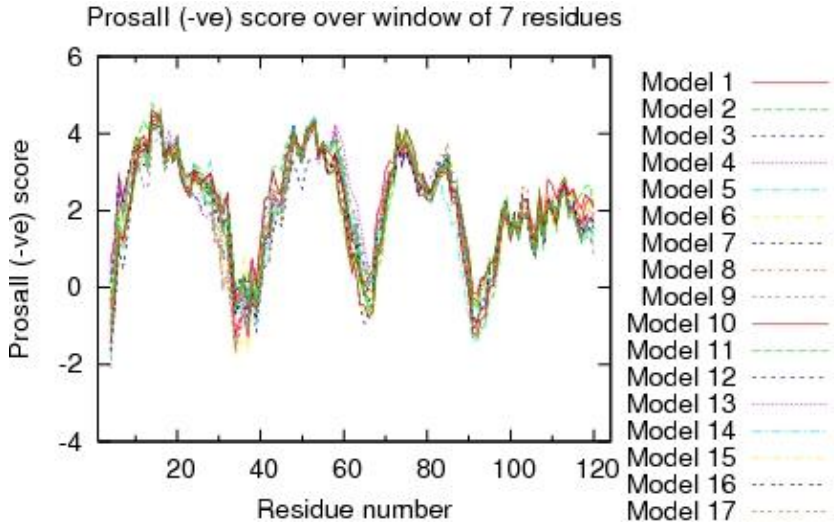

**RPF Precision Map**

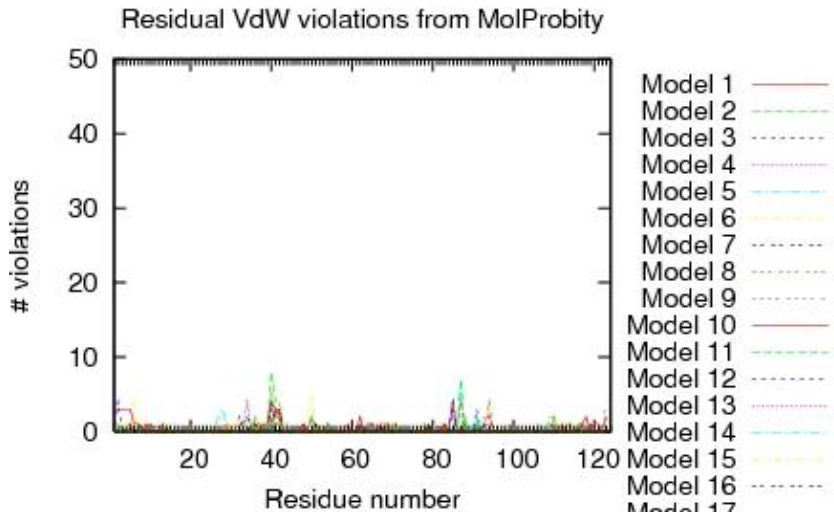


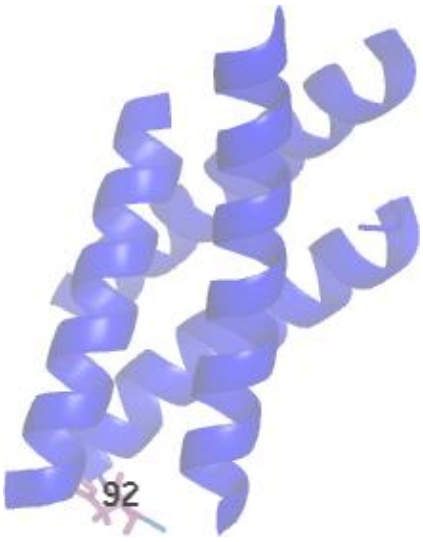

Procheck G-factor for phi-psi
G-factor
2
1
0
-1
-2
-3
-4
20
40
60
80
100
120
Residue number


Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
20
40
60
80
100
120
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
20
40
60
80
100
120
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


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
20
40
60
80
100
120
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


Residual VdW violations from MolProbity
# violations
50
40
30
20
10
0
20
40
60
80
100
120
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




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

***References:***

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5. Laskowski R Ai et al, "AQUA and PROCHECK_NMR: Programs for checking the quality of proteins structures solved by NMR", J Biomolec NMR 8 (1996): 477-486
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7. Word J M et al, "Exploring steric constrains on protein mutations using MAGE / PROBE", Prot Sci 9 (2000): 2251-2259
8. Word J M et al, "Asparagine and Glutamine: Using Hydrogen Atom Contacts in the Choice of Side-chain Amide Orientation", J Mol Biol 285 (1999): 1735-1747
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12. Richardson D C, Richardson J S, "The kinemage: a tool for scientific communication", Prot Sci 1(1) (1992): 3-9
13. Koradi, R, et al, "MOLMOL: a program for display and analysis of macromolecular structures ", J Mol Graphics 14 (1996): 51-55.
14. Güntert, P, Mumenthaler, C & Wüthrich, K "Torsion angle dynamics for NMR structure calculation with the new program DYANA", J. Mol. Biol 273 (1997): 283-298

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17. Bagaria, A., Jaravine, V., Huang, Y.J., Montelione, G.T., and Guntert, P. "Protein structure validation by generalized linear model root-mean-square deviation prediction". Protein Sci 21(2012), 229-238.

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# Software Environment

## Software for structure quality evaluation:

| | |
|---|---|
| DSSP | DsspCMBI-April-2000 |
| pdbstat | PdbStat-5.4 Version |
| AutoAssign | Version 2.4.0 (uses only AVS scripts) |
| RPF analysis | ASDP-1.0 |
| PDB validation | Version 8.061 |
| Verify3D | Version 1.0 corrected by Aneerban |
| ProsaII | Prosa2003 |
| PROCHECK | Version 3.5.4 |
| MolMol | Version 2K.2 |

## 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 5.8.0 |
| convert | ImageMagick 5.5.6 |
| ps2pdf | Ghostscript 7.05 |
| htmldoc | v1.9 |
| gnuplot | Version 3.7 patchlevel 3 |
| jpegtopnm | year 2000 |

```
pnmcrop         year 2000
pnmtojpeg       year 2000
```