



# 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.): 143

Organism:

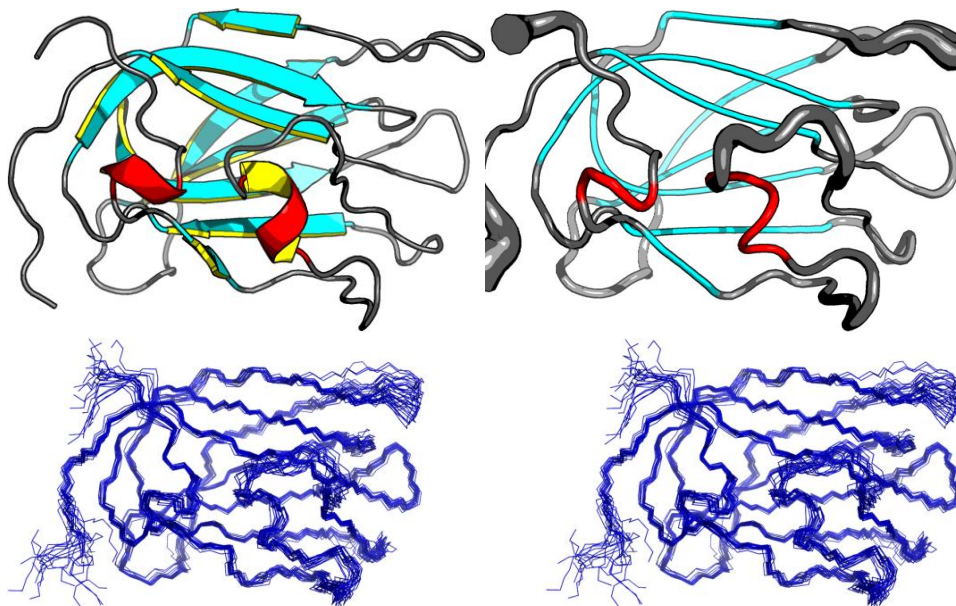
SwissProt /

TrEMBL ID:

# models: 20

Oligomerization: monomer

Molecular weight: 16182



Secondary Structure Elements:

alpha helices:

beta strands: 4E-5E, 109Y-139Y, 47N-77N, 101N-105N, 14U-18U, 39P-40P, 86U-92U

Total number of restricting constraints per restrained residue: 8.3

Restricting long range constraints per restrained residue: 5.0

Distance violations per model

Calculated using sum over  $r^{-6}$

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

1.6 2.05 1.9

Dihedral angle violations per model

1 - 10° > 10°

1.05 0.8

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score



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0.901157 0.882805 0.892 0.834437

RMSD *All residues* *Ordered residues*<sup>2</sup> *Selected residues*<sup>3</sup>

*All backbone atoms* 0.9 Å 0.5 Å 0.5 Å

*All heavy atoms* 1.2 Å 0.9 Å 0.9 Å

Ramachandran Plot Summary for selected residues<sup>3</sup> from Procheck

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

90.8% 8.8% 0.3% 0.1%

Ramachandran Plot Summary for selected residues<sup>3</sup> from Richardson Lab's Molprobit

*Most favoured regions* *Allowed regions* *Disallowed regions* [View plot](#) [View model summary](#)

97.6% 2.2% 0.2%

### Global quality scores

Program *Verify3D* *ProsaII (-ve)* *Procheck (phi-psi)*<sup>3</sup> *Procheck (all)*<sup>3</sup> *MolProbit Clashscore*

*-Raw score* 0.43 0.29 -0.36 -0.00 5.26

*Z-score*<sup>1</sup> -0.48 -1.49 -1.10 -0.00 0.62

**Generalized linear model RMSD prediction: 1.82**

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

Number of close contacts (within 1.6 Å for H atoms, 2.2 Å for heavy atoms): 0

RMS deviation for bond angles: 0.7 °

RMS deviation for bond lengths: 0.010 Å

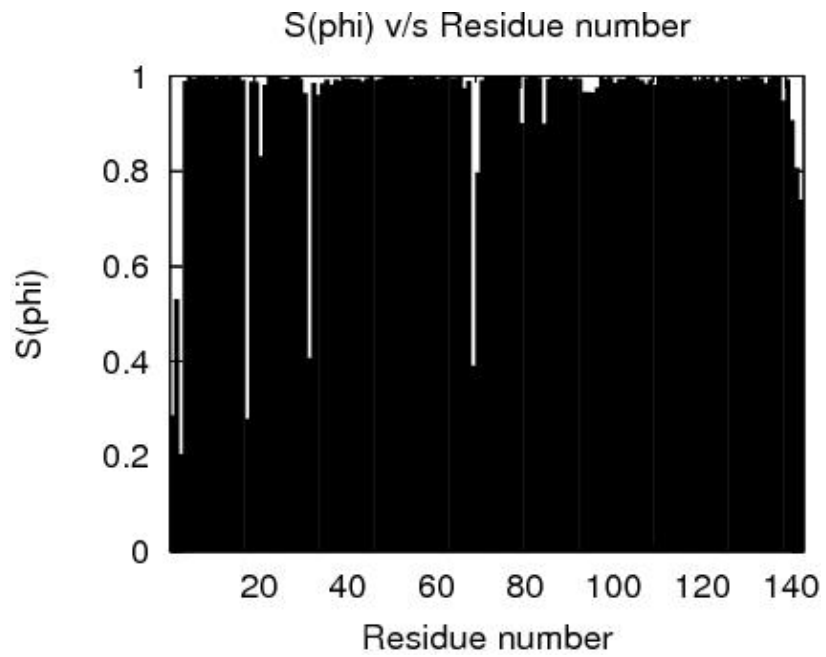
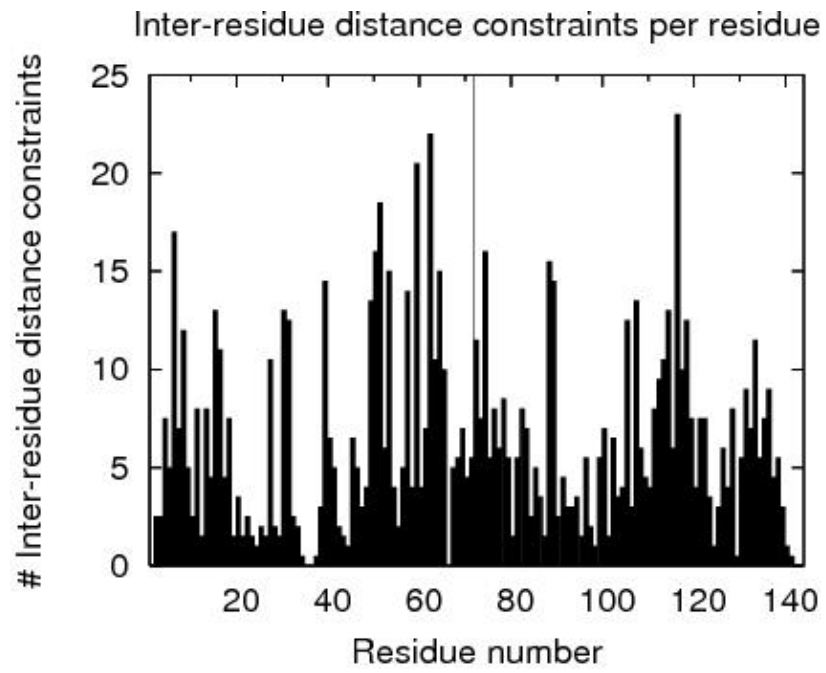
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

<sup>2</sup>Order residues: 4A-16A,22A-30A,33A-67A,71A-139A

<sup>3</sup>Selected residues: 4A-16A,19A-30A,33A-67A,70A-139A

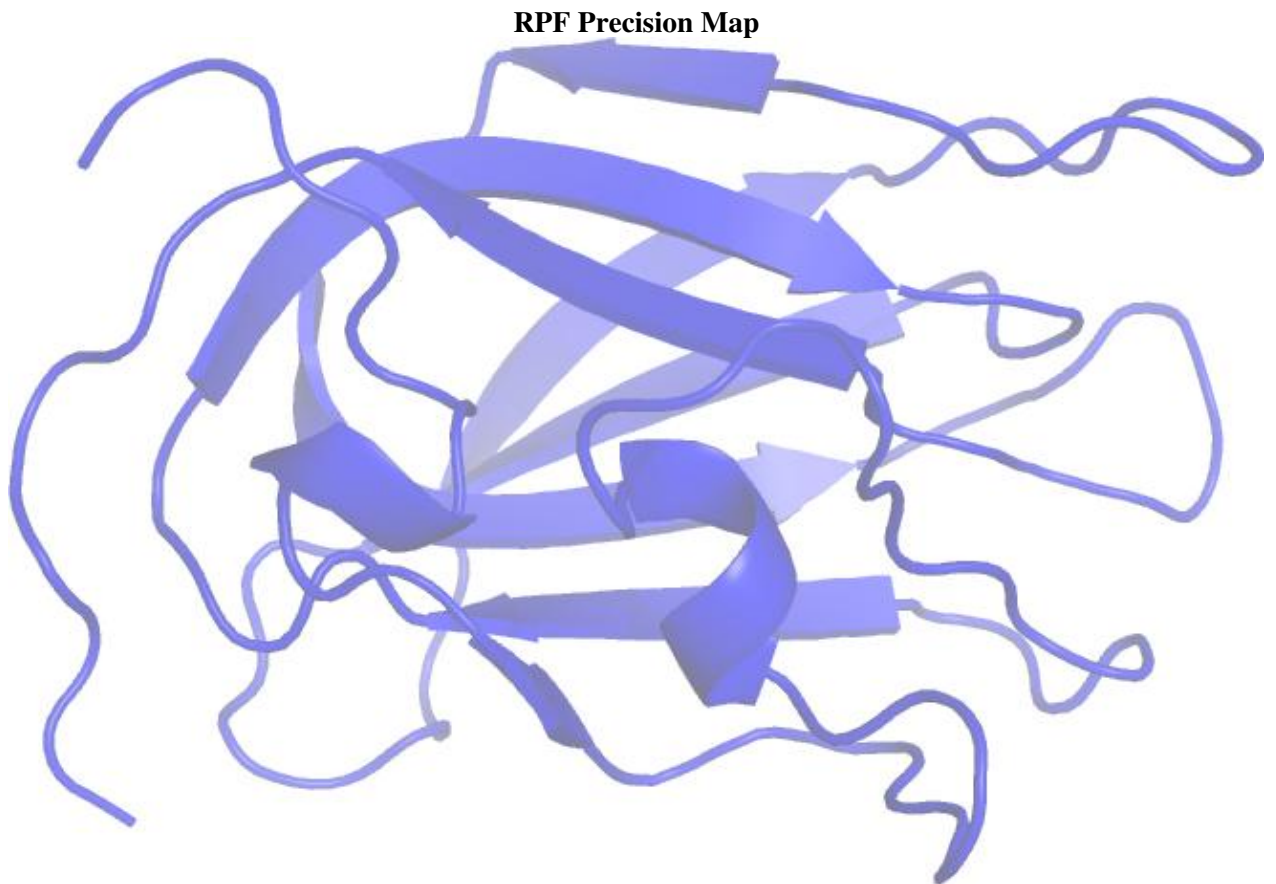
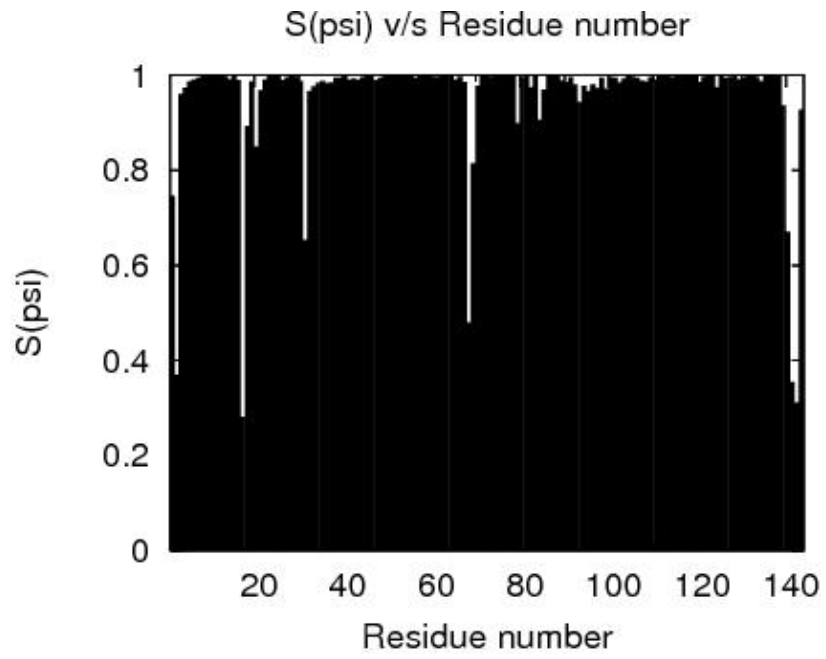


# Structure Quality Analysis for NAME





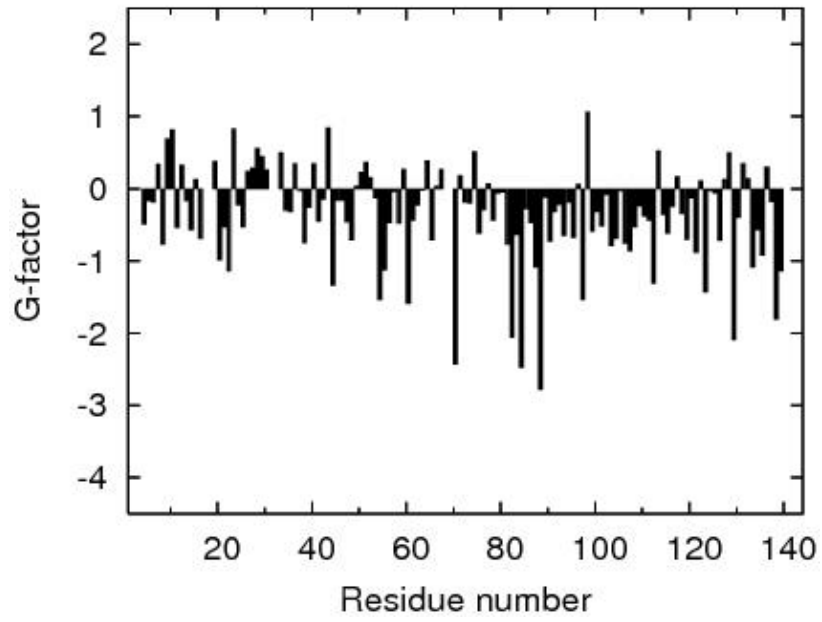
# Structure Quality Analysis for NAME



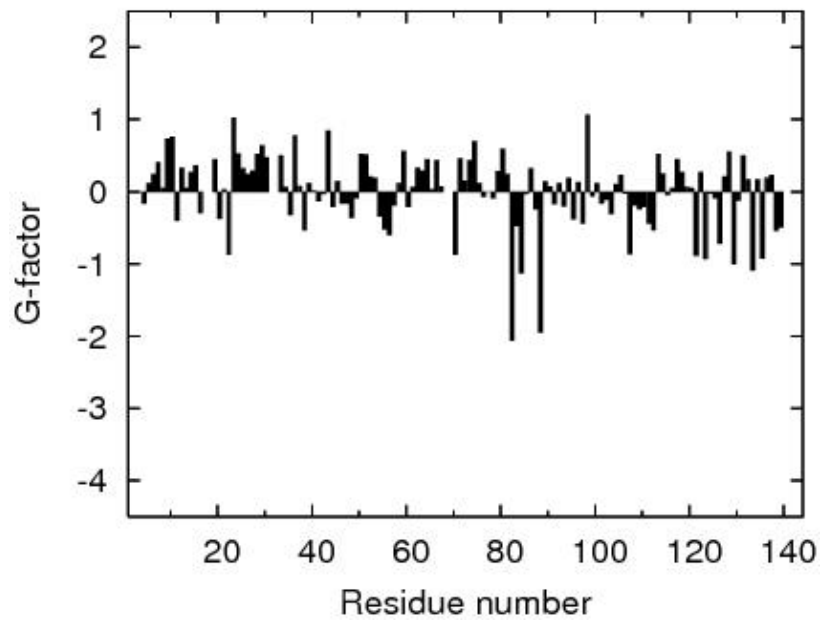


# Structure Quality Analysis for NAME

## Procheck G-factor for phi-psi

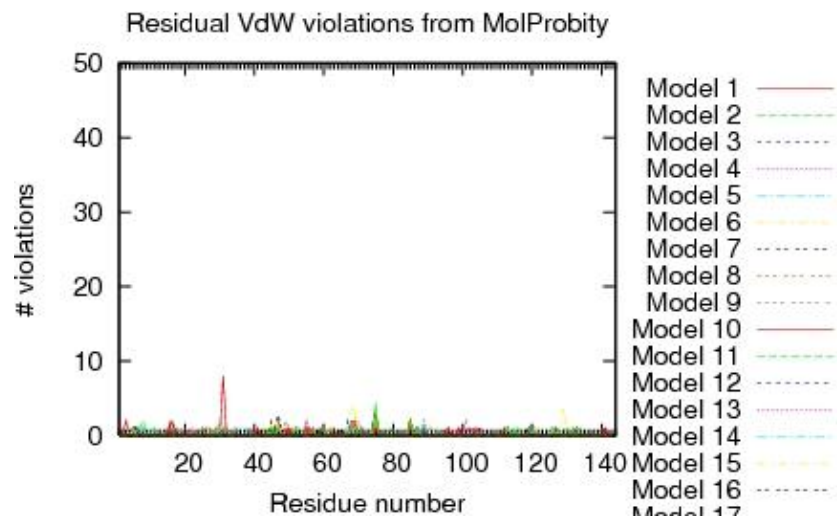
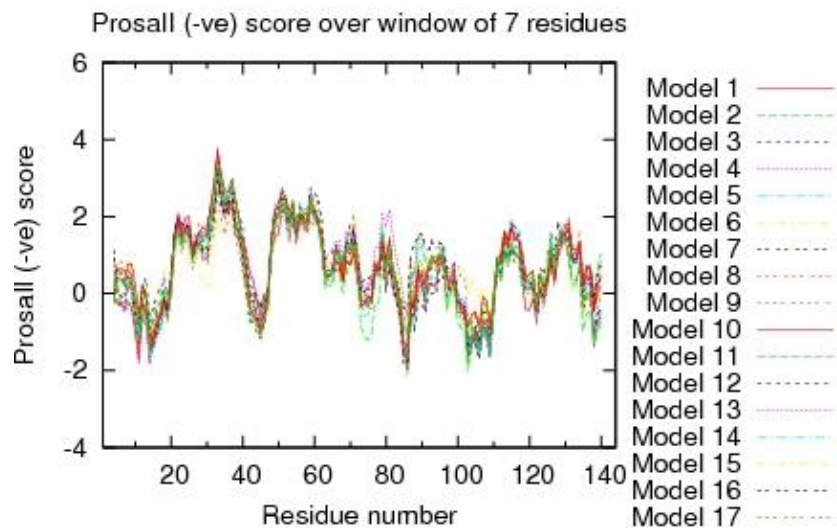
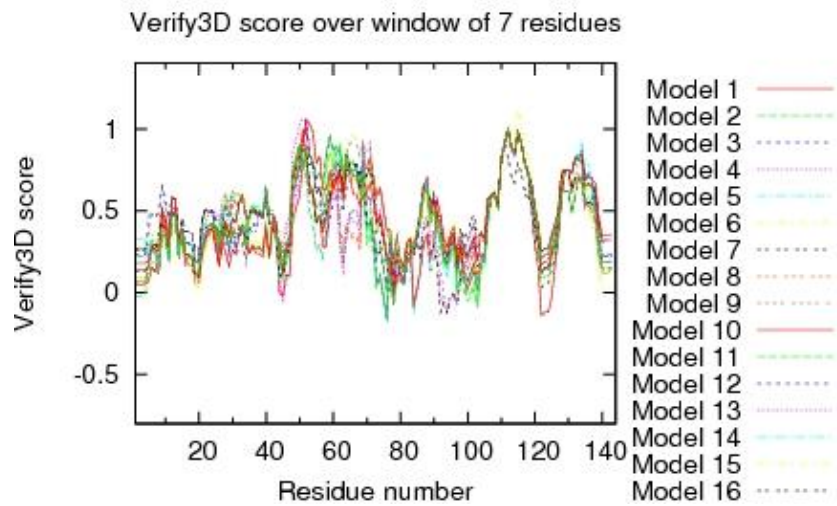


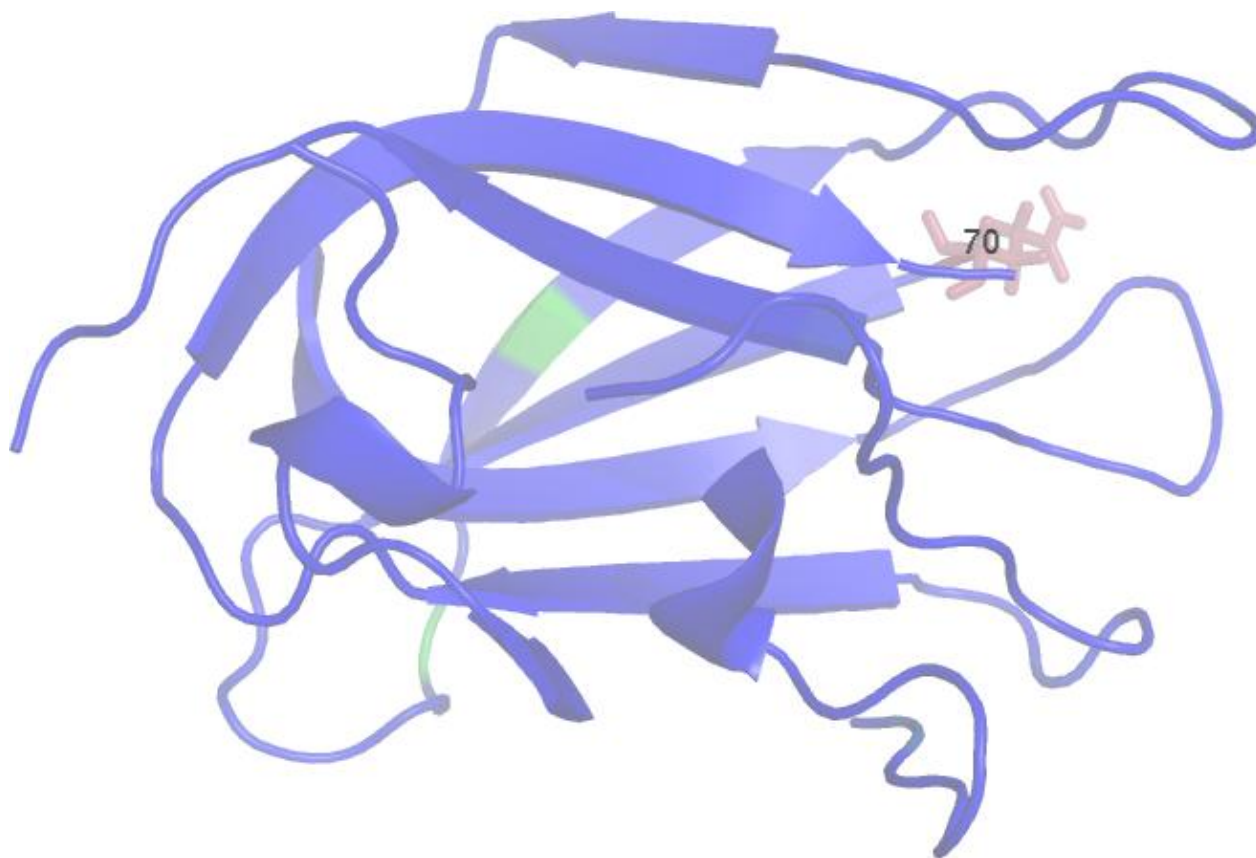
## Procheck G-factor for all dihedral angles





# Structure Quality Analysis for NAME





**Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobit)**

**References:**

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3. Sippl M J, "Recognition of Errors in Three-Dimensional Structures of Proteins", Proteins 17 (1993): 355-362
4. Sippl M J, "Calculation of Conformation Ensembles from Potentials of Mean Force", J Mol Biol 213 (1990): 859-883
5. Laskowski R A 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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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.

Analysed by on May-10-2013 using PSVS 1.3



## 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