



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.): 166

Organism:

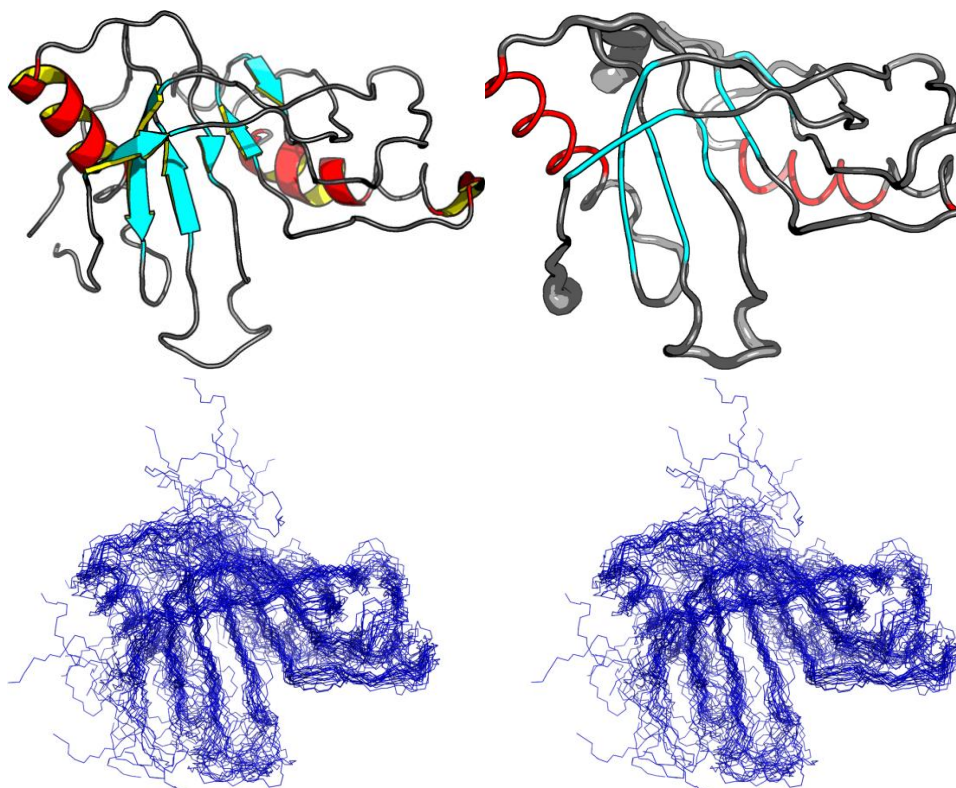
SwissProt /

TrEMBL ID:

models: 20

Oligomerization: monomer

Molecular weight: 18119



Secondary Structure Elements:

alpha helices: 30A-47A, 109A-123A

beta strands: 6N-14N, 95Y-103Y, 148G-152G, 131A-135A, 58E-61E, 70U-72U, 23G-25G, 75E-76E, 18O-22O, 87L-91L

Total number of restricting constraints per restrained residue: 11.4

Restricting long range constraints per restrained residue: 2.6

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å

11.5 15.9 29.65

Dihedral angle violations per model

1 - 10 ° > 10 °



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19.5 22.75

FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score

0.957 0.945 0.951 0.71

RMSD *All residues* *Ordered residues*² *Selected residues*³

All backbone atoms 3.8 Å 1.6 Å 1.7 Å

All heavy atoms 4.4 Å 2.0 Å 2.1 Å

Ramachandran Plot Summary for selected residues³ from Procheck

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

92.3% 7.1% 0.0% 0.6%

Ramachandran Plot Summary for selected residues³ from Richardson Lab's Molprobrity

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

98.1% 1.9% 0%

Global quality scores

Program *Verify3D* *ProsaII (-ve)* *Procheck (phi-psi)*³ *Procheck (all)*³ *MolProbrity Clashscore*

-Raw score 0.43 0.40 -0.29 -0.06 5.93

*Z-score*¹ -0.48 -1.03 -0.83 -0.35 0.51

Generalized linear model RMSD prediction: 2.42

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

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

RMS deviation for bond angles: 0.7 °

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

²Order residues:

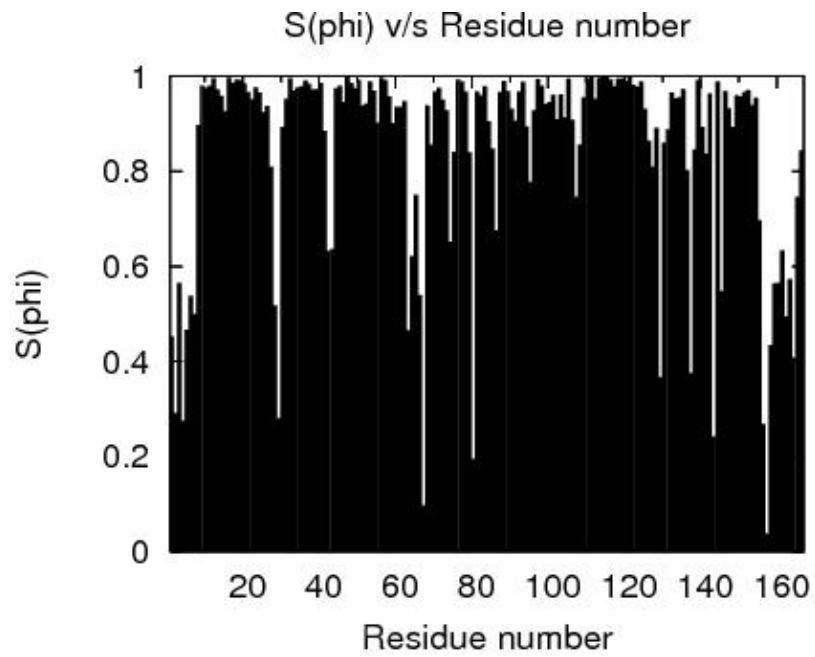
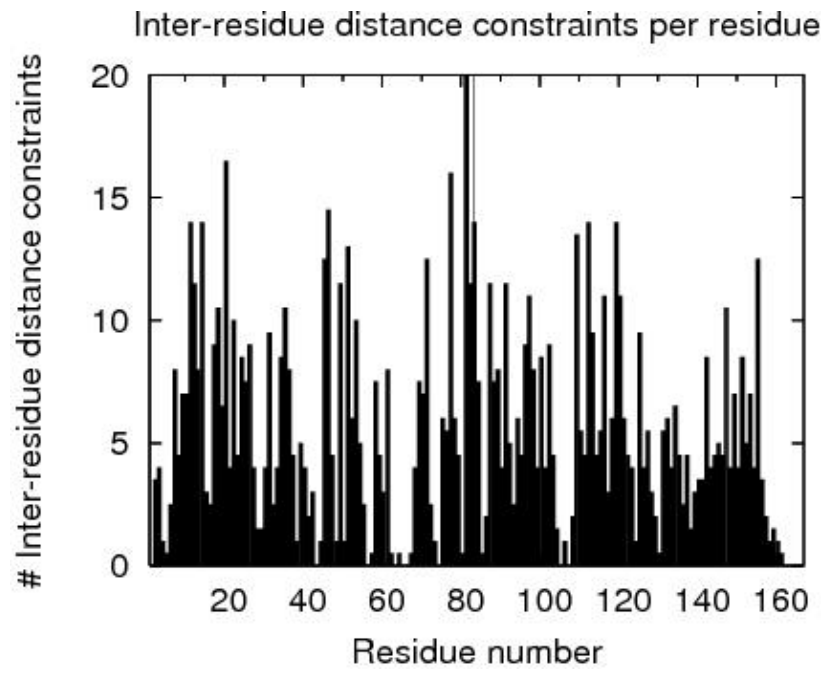
8A-26A,31A-40A,44A-62A,70A-72A,75A-78A,81A-83A,87A-94A,96A-106A,109A-125A,130A-134A,146A-153A

³Selected residues:

8A-27A,31A-40A,44A-62A,68A-73A,75A-78A,81A-83A,87A-106A,109A-126A,130A-134A,138A-140A,146A-153A

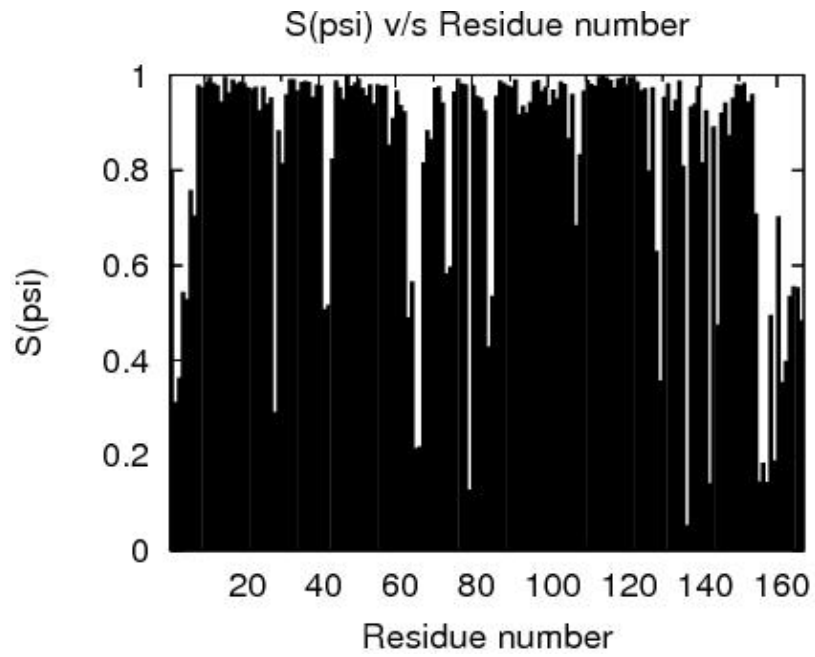


Structure Quality Analysis for NAME

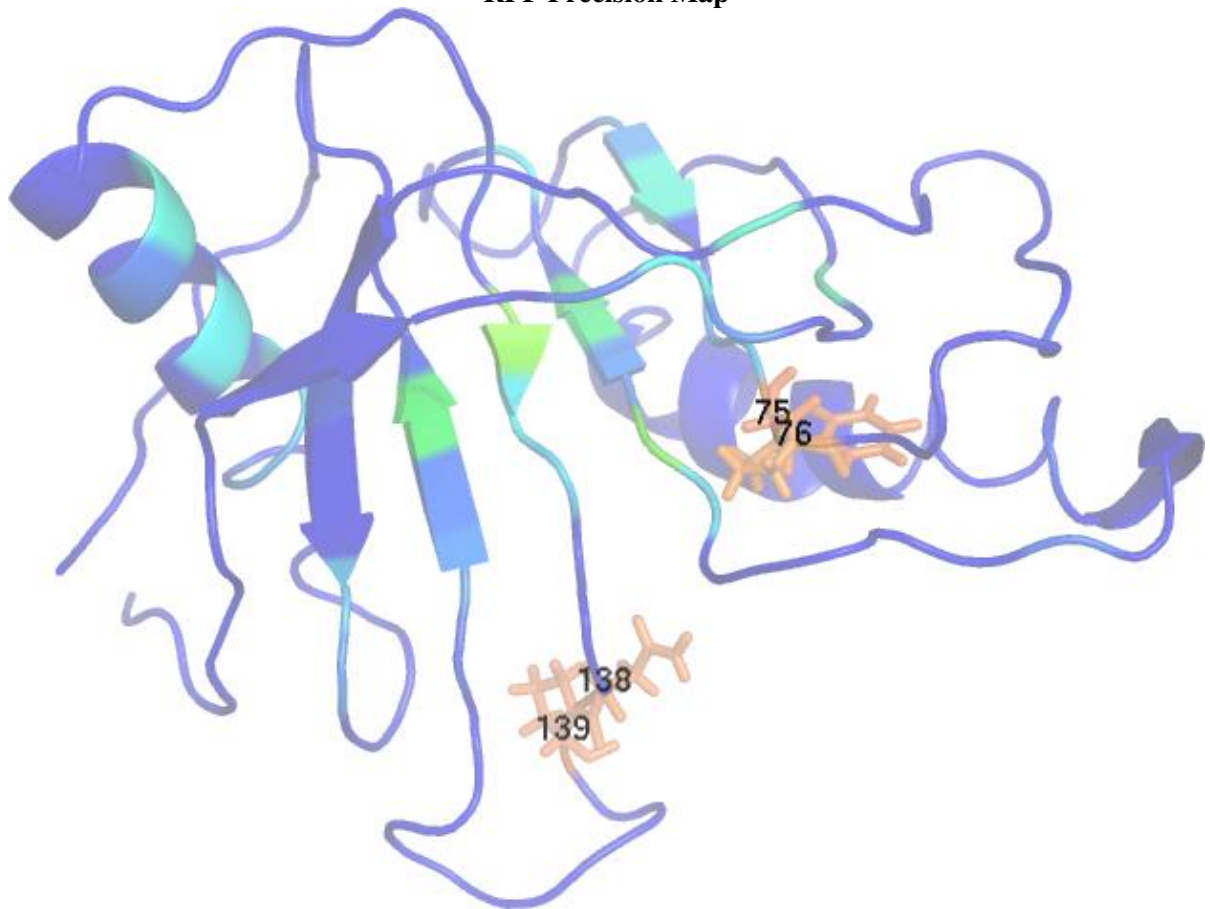




Structure Quality Analysis for NAME



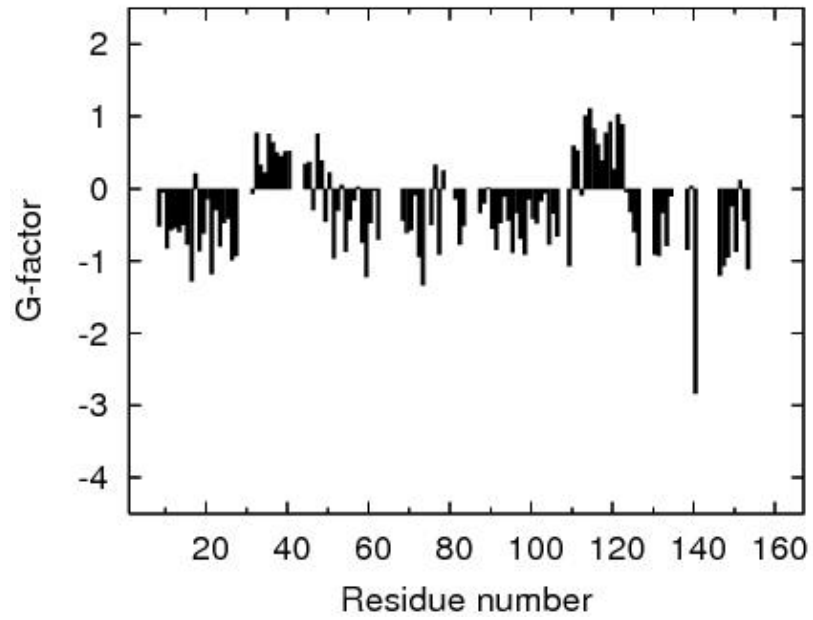
RPF Precision Map



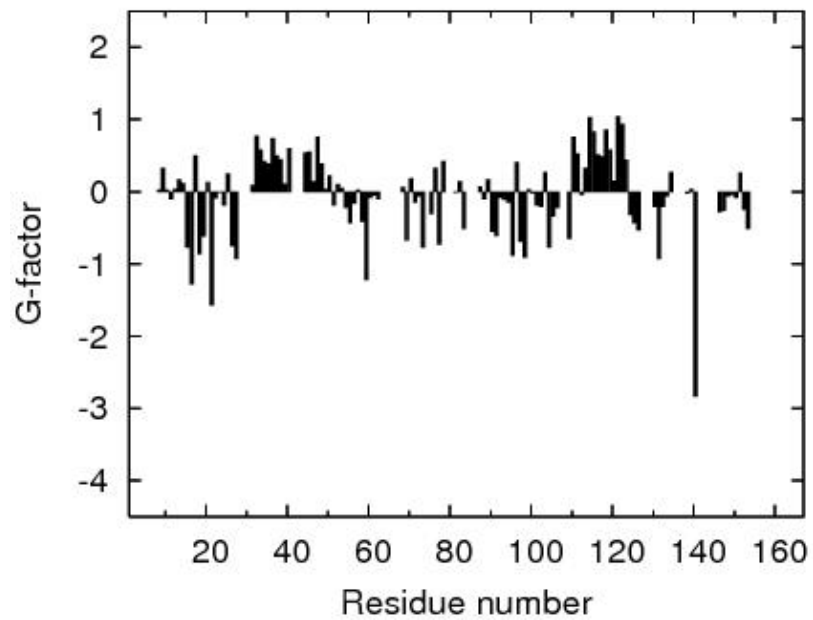


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi

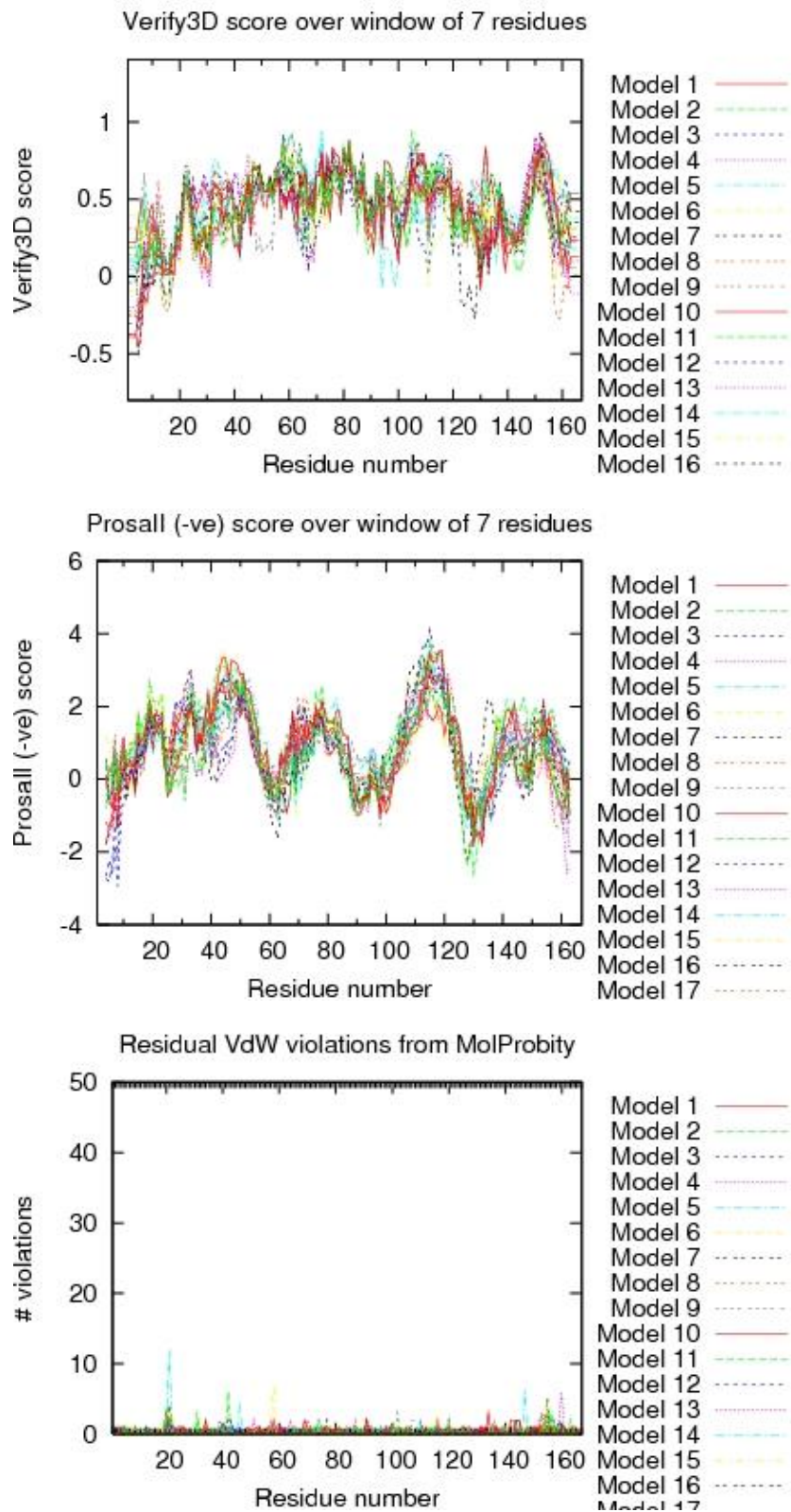


Procheck G-factor for all dihedral angles





Structure Quality Analysis for NAME





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

References:

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2. Bowie J U, Luthy R and Eisenberg D, "A Method to Identify Protein Sequences that Fold into a Known Three-Dimensional Structure", Science 253 (1991): 164-169
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 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
9. Word J M et al, "Visualizing and Quantifying Molecular Goodness-of-Fit: Small-probe Contact Dots with Explicit Hydrogens", J Mol Biol 285 (1999): 1711-1733
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11. Luthy R, McLachlan A D and Eisenberg D, "Secondary Structure-Based Profiles: Use of Structure-Conserving Scoring Tables in Searching Protein Sequence Databases for Structural Similarities",



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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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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, 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-9-2013 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