



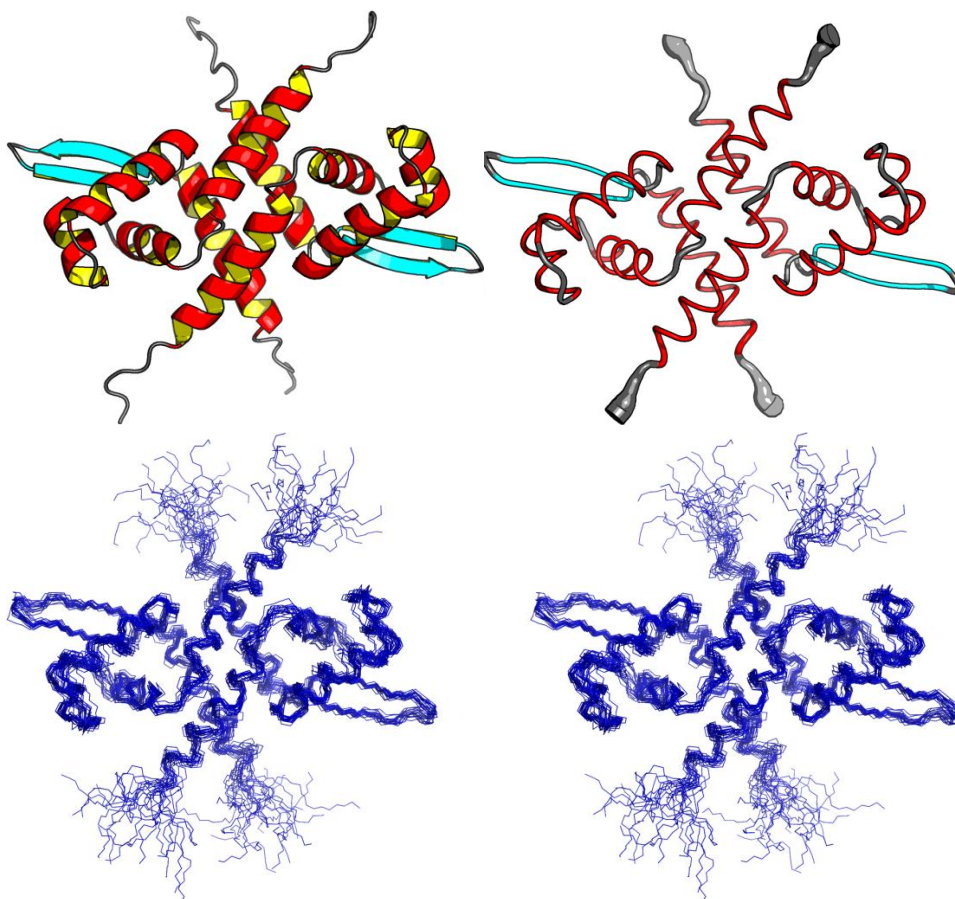
Structure Quality Analysis for NAME

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.): 216
Organism:
SwissProt /
TrEMBL ID:
models: 20
Oligomerization: dimer
Molecular
weight: 23434



Secondary Structure Elements:

Inter-chain break(s) between 108 & 119

alpha helices: 8A-22A, 28A-34A, 41A-48A, 52A-65A, 84A-101A, 8B-22B, 25B-34B, 41B-48B, 52B-65B, 84B-100B

beta strands: 39G-40G, 76G-81G, 68L-73L, 39G-40G, 76G-81G, 68L-73L

Total number of restricting constraints per restrained residue: 29.2

Restricting long range constraints per restrained residue: 6.6

Distance violations per model

Calculated using sum over r^{-6}

0.1 - 0.2 Å 0.2 - 0.5 Å > 0.5 Å



Structure Quality Analysis for NAME

2.65 0.35 0
Dihedral angle violations per model

1 - 10 ° > 10 °

2.2 0
FIDs deposited in the BMRB? no

RPF Scores

Recall Precision F-measure DP-score
0.949 0.855 0.899 0.785

RMSD	All residues	Ordered residues ²	Selected residues ³
All backbone atoms	2.3 Å	0.8 Å	0.8 Å
All heavy atoms	2.9 Å	1.2 Å	1.2 Å

Ramachandran Plot Summary for selected residues³ from Procheck

Most favoured regions	Additionally allowed regions	Generously allowed regions	Disallowed regions
98.5%	1.5%	0.0%	0.0%

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

Most favoured regions	Allowed regions	Disallowed regions	View plot	View model summary
99.3%	0.7%	0%		

Global quality scores

Program	Verify3D	ProsaII (-ve)	Procheck (phi-psi) ³	Procheck (all) ³	MolProbability Clashscore
-Raw score	0.37	0.86	0.30	0.19	17.67
Z-score ¹	-1.44	0.87	1.49	1.12	-1.51

Generalized linear model RMSD prediction: 2.16

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):	35
RMS deviation for bond angles:	0.5 °
RMS deviation for bond lengths:	0.003 Å

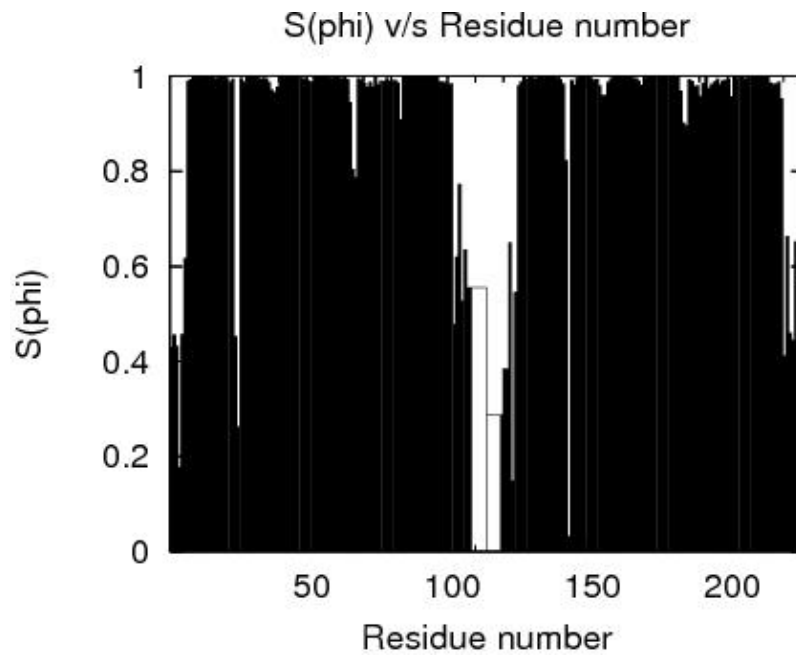
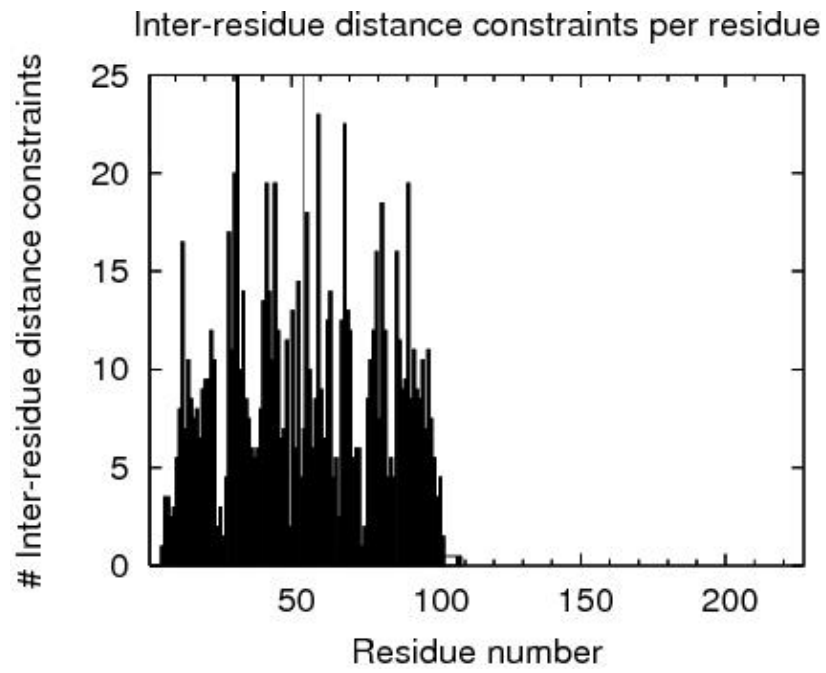
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

²Order residues: 7A-22A,26A-65A,68A-101A,7B-22B,26B-100B

³Selected residues: 7A-22A,26A-65A,68A-101A,7B-22B,26B-100B

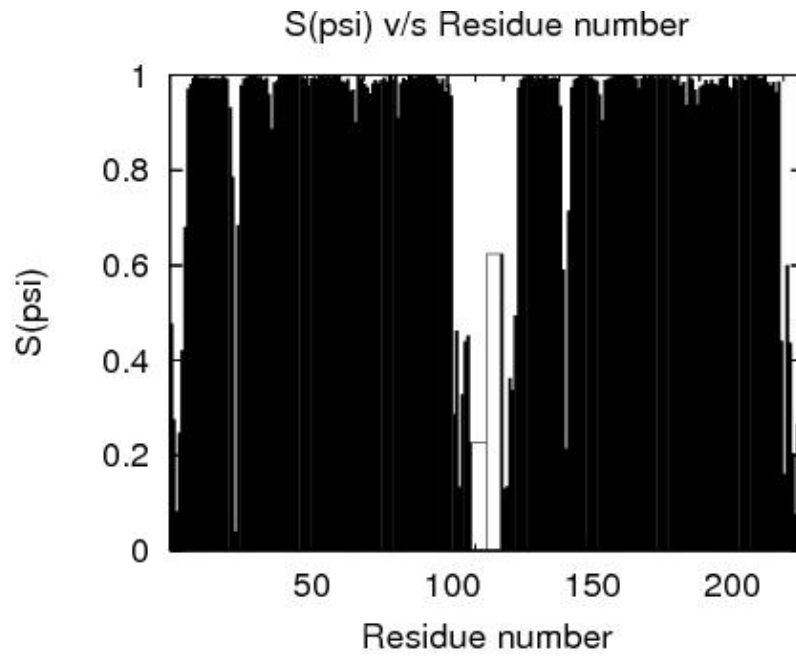


Structure Quality Analysis for NAME





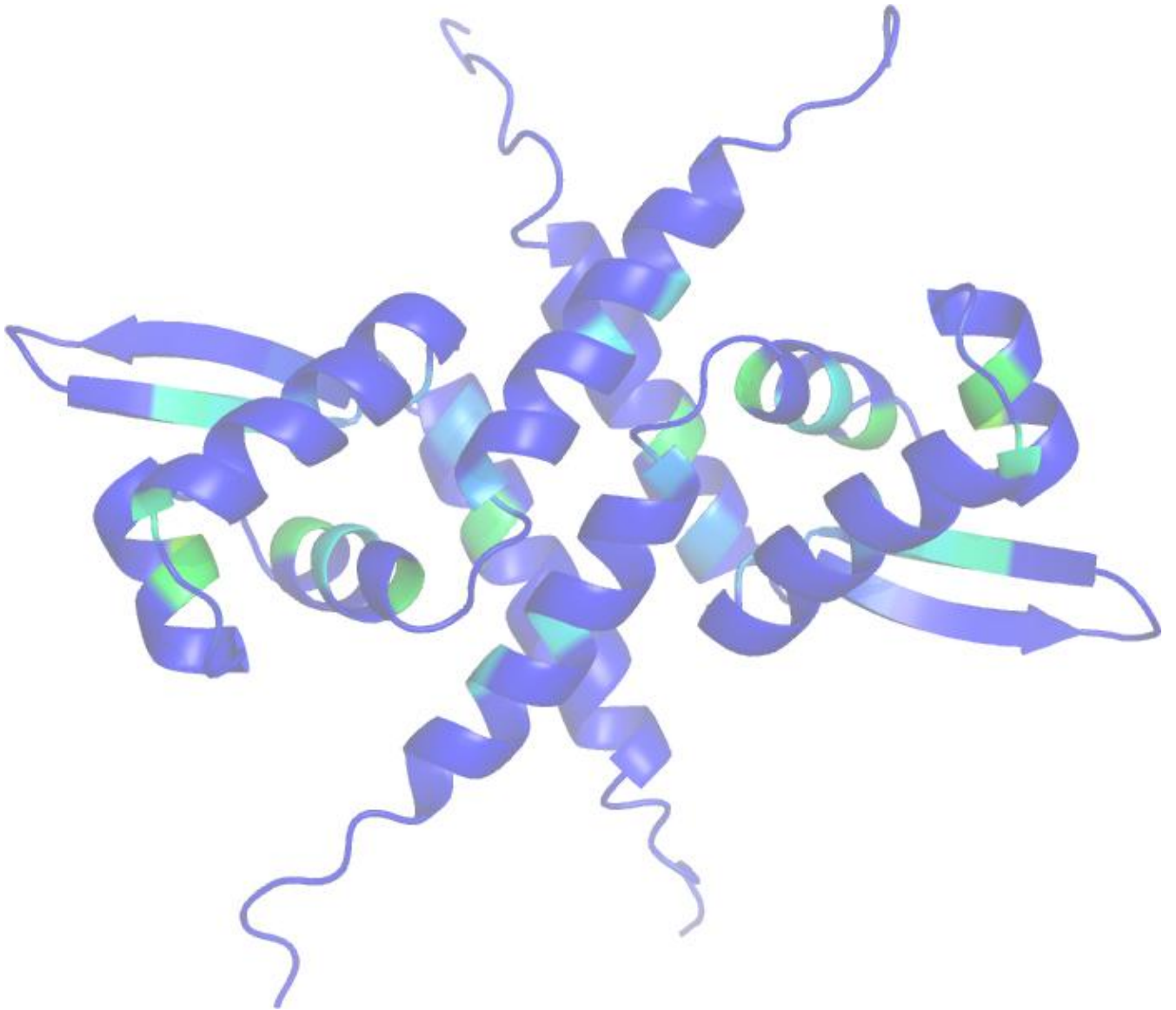
Structure Quality Analysis for NAME



RPF Precision Map



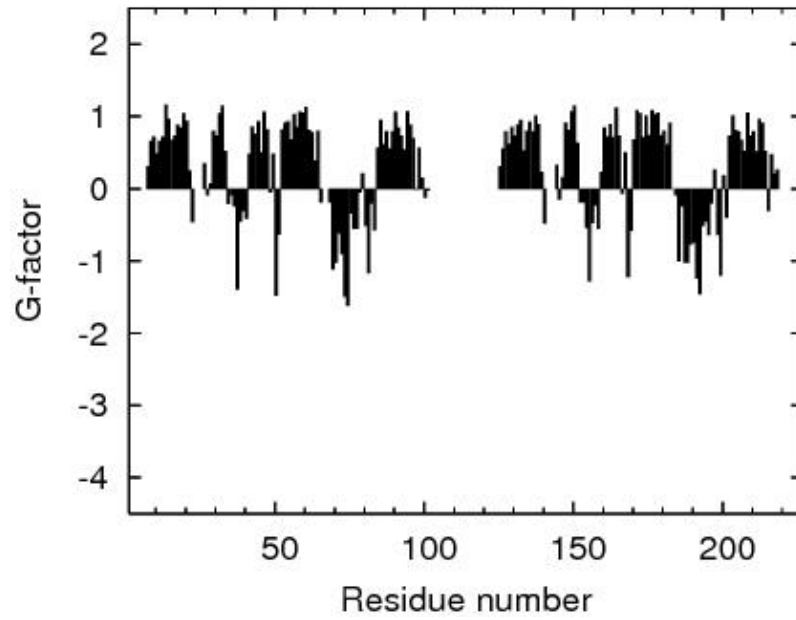
Structure Quality Analysis for NAME



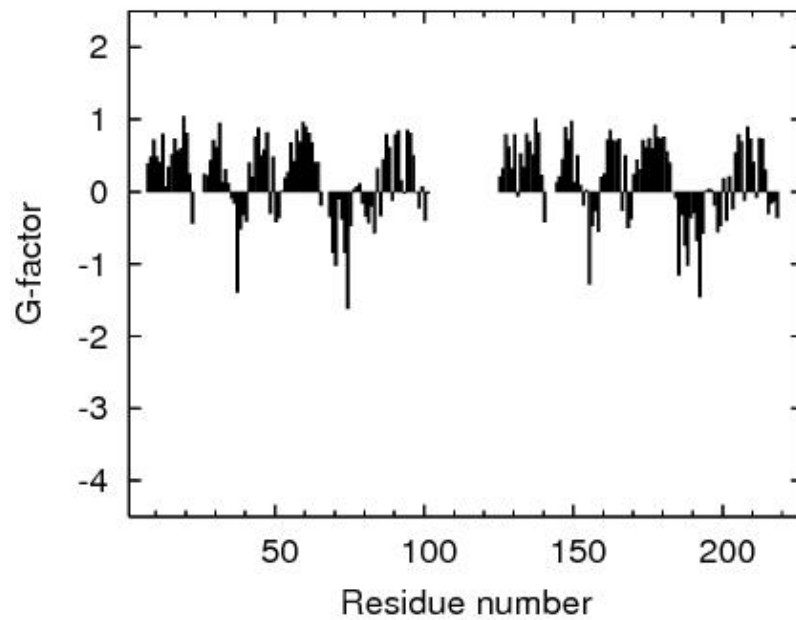


Structure Quality Analysis for NAME

Procheck G-factor for phi-psi



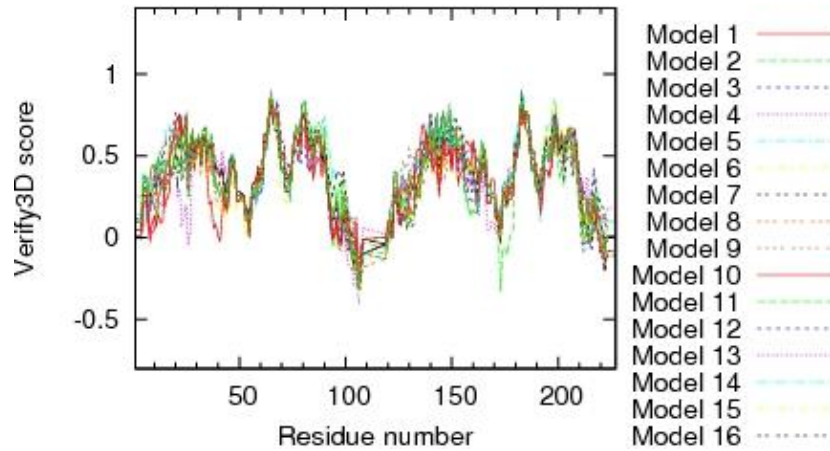
Procheck G-factor for all dihedral angles



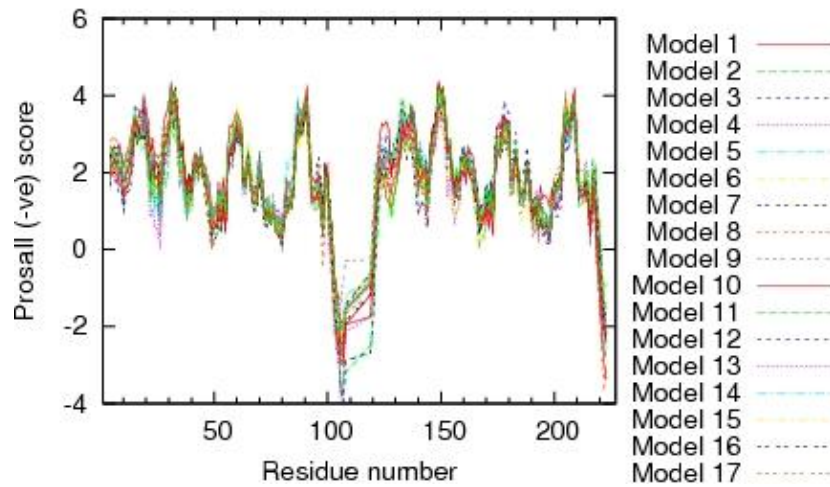


Structure Quality Analysis for NAME

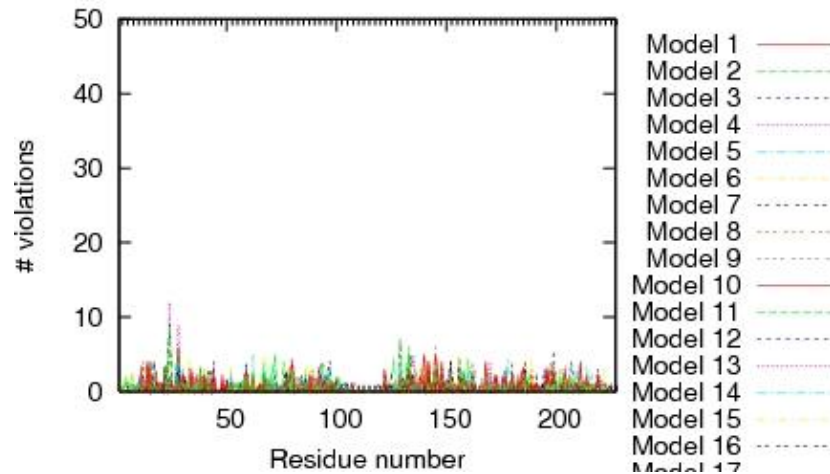
Verify3D score over window of 7 residues

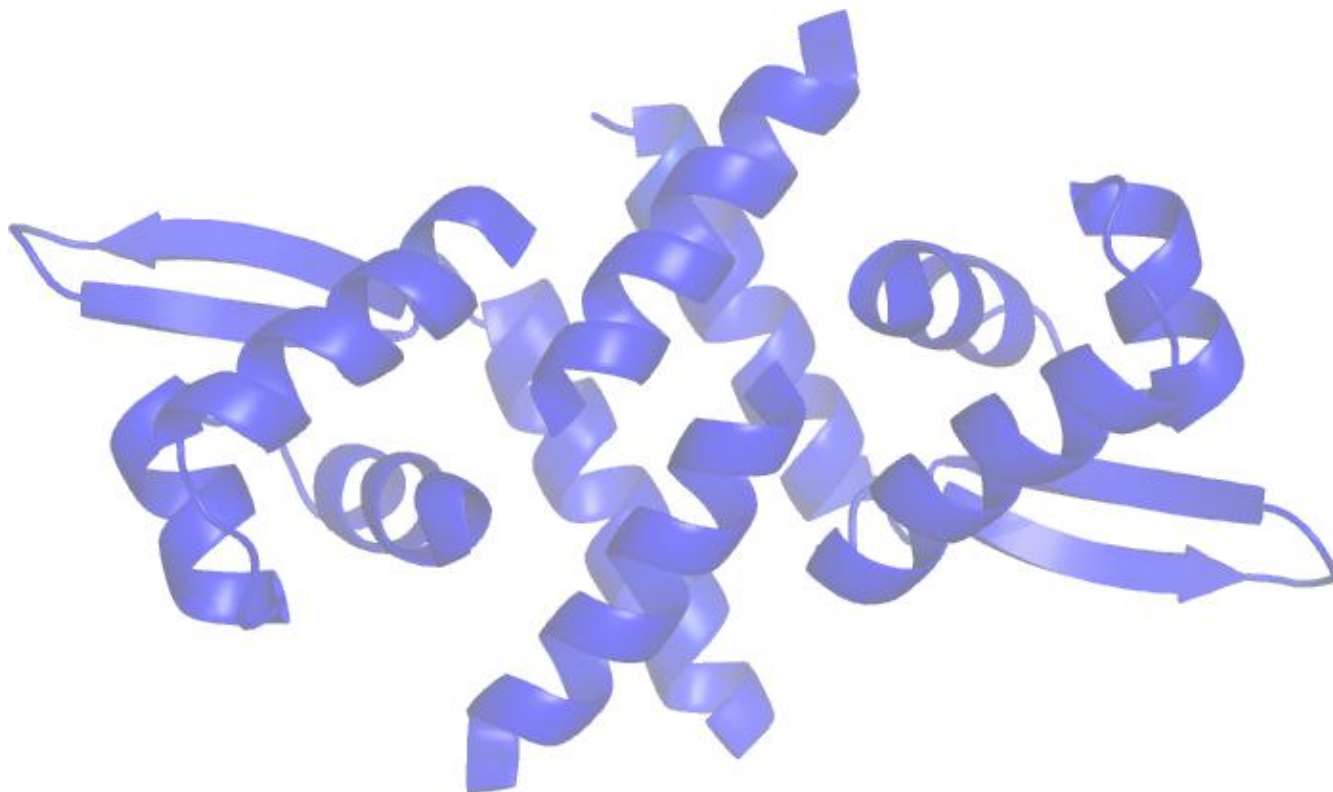


ProsaII (-ve) score over window of 7 residues



Residual VdW violations from MolProbity





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

References:

1. Luthy R, Bowie J U and Eisenberg D, "Assessment of protein models with three-dimensional profiles", Nature 356 (1992): 83-85
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 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
6. Laskowski R A et al "PROCHECK: a program to check the stereochemical quality of protein structures" J Appl Cryst, 26 (1993): 283-291
7. Word J M et al, "Exploring steric constraints 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
10. Tejero R and Montelione G T, "PDBStat", unpublished
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", Proteins 10 (1991): 229-239

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

15. Lovell S C 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, 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