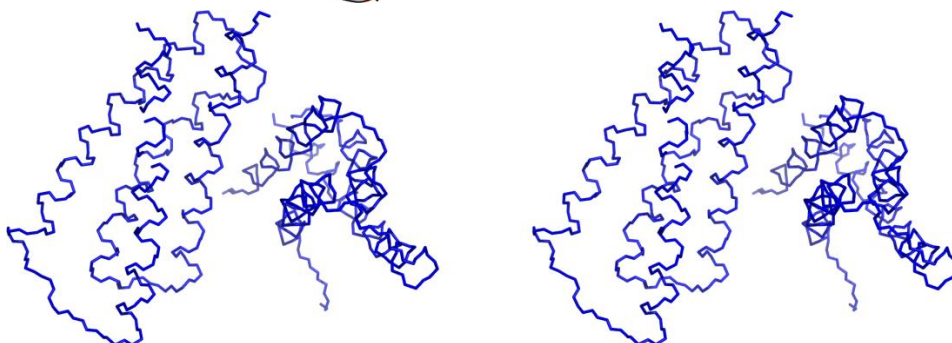
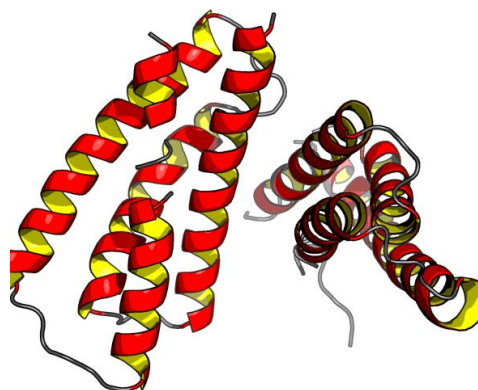




Structure Quality Analysis for NAME

Procheck analysis, RMSD calculation and structure superimposition are based on: all residues

NESG ID: NAME
PDB ID:
Deposition date:
Common Name:
Class:
Length (a.a.): 239
Organism:
SwissProt /
TrEMBL ID:
Oligomerization: dimer
Molecular weight: 28022



Secondary Structure Elements:

Inter-chain break(s) between 123 & 134

alpha helices: 3A-29A, 40A-64A, 72A-91A, 96A-121A, 6B-30B, 40B-64B, 75B-91B, 96B-116B

beta strands:

Resolution: 2.000 Å R-factor: 0.236 R-free: 0.257

Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

<i>Most favoured regions</i>	<i>Additionally allowed regions</i>	<i>Generously allowed regions</i>	<i>Disallowed regions</i>
92.9%	6.7%	0.5%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	View plot	View model summary
96.1%	3.9%	0%		

Global quality scores

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



Structure Quality Analysis for NAME

-Raw score 0.30 0.97 0.33 0.31 18.40
Z-score¹ -2.57 1.32 1.61 1.83 -1.63

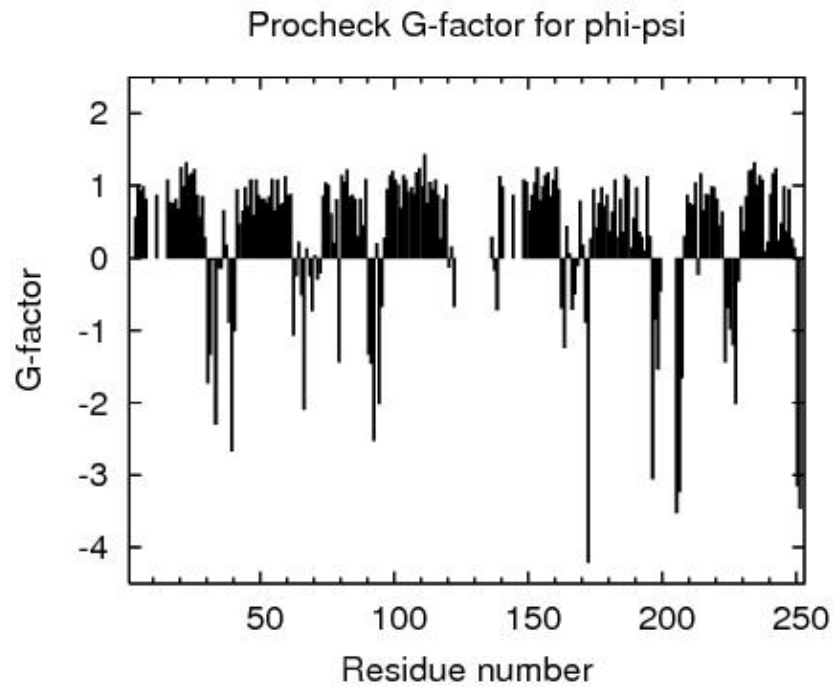
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.0 °

RMS deviation for bond lengths: 0.005 Å

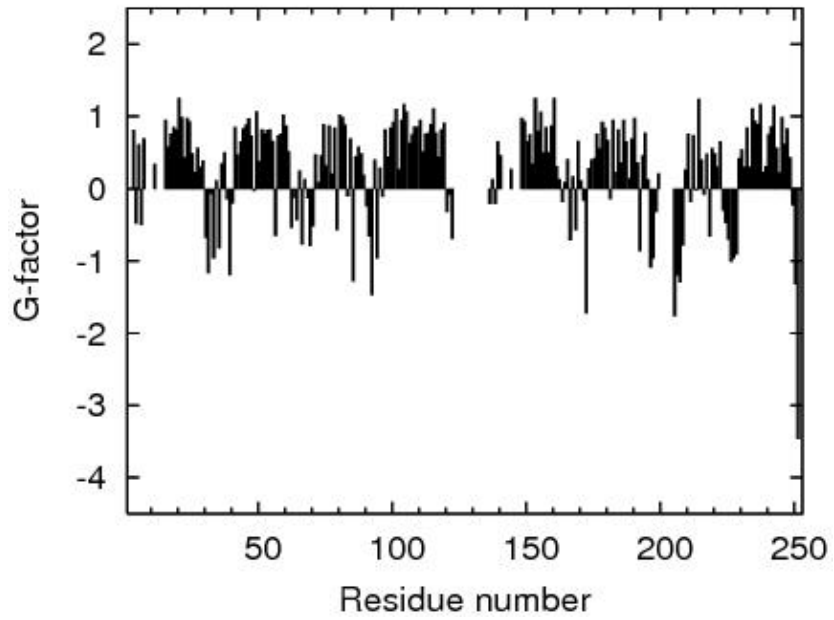
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score



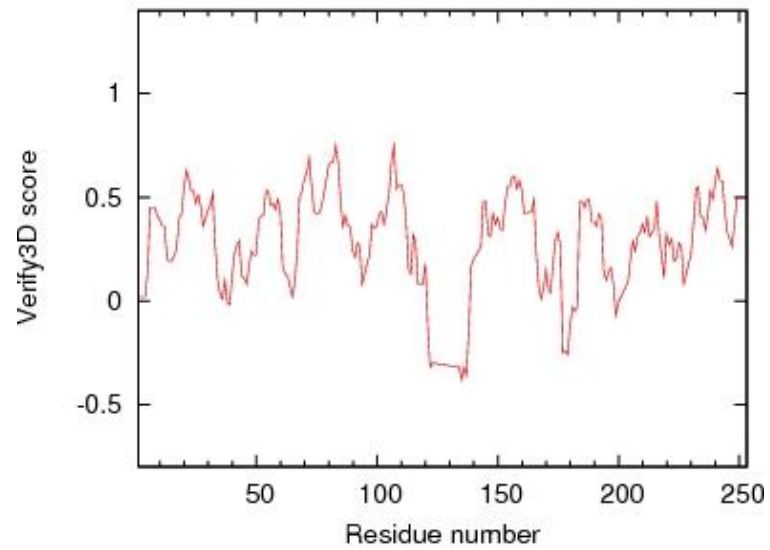


Structure Quality Analysis for NAME

Procheck G-factor for all dihedral angles

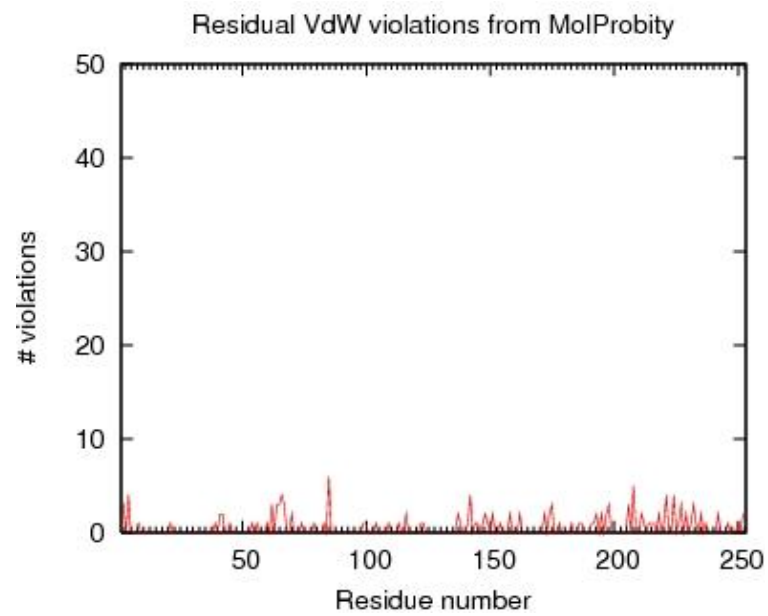
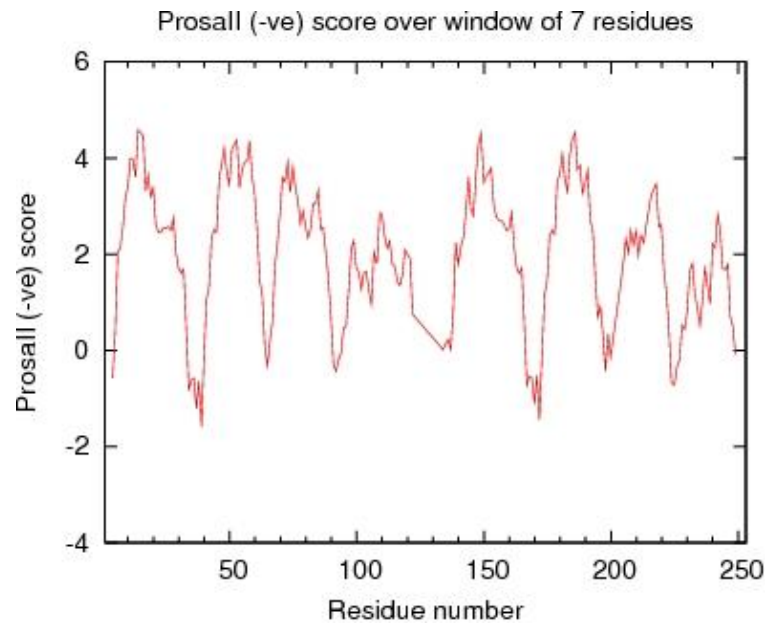


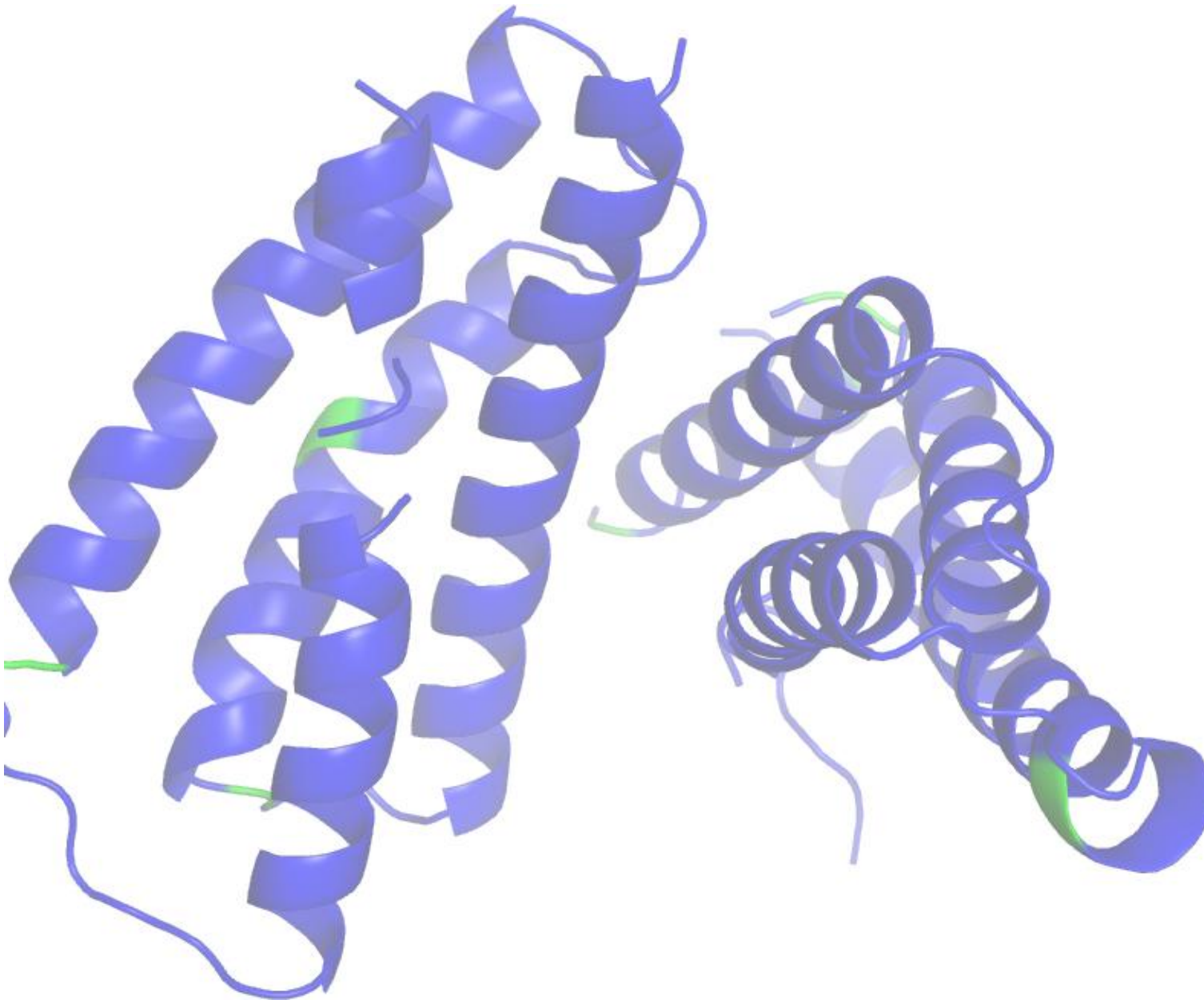
Verify3D score over window of 7 residues





Structure Quality Analysis for NAME





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 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
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