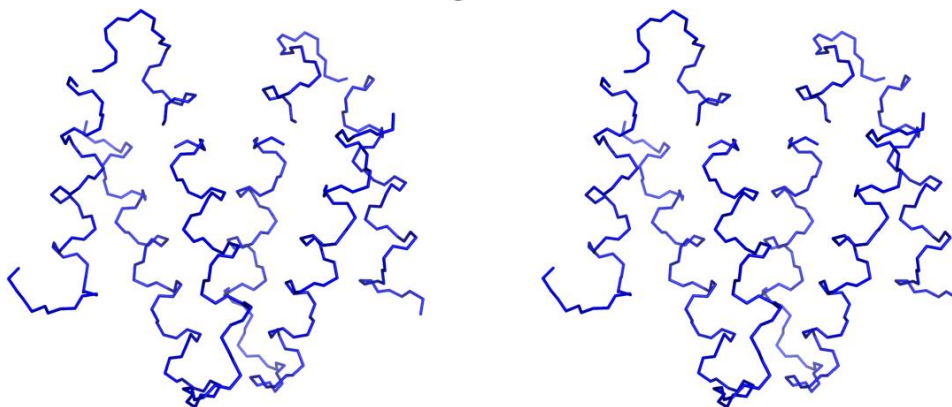
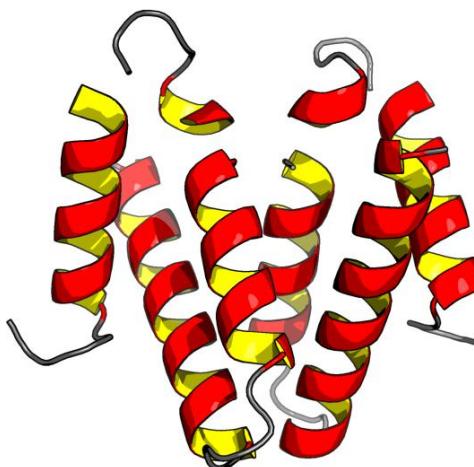




Structure Quality Analysis for NAME

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.): 135
Organism:
SwissProt /
TrEMBL ID:
Oligomerization: dimer
Molecular
weight: 15887



Secondary Structure Elements:

Inter-chain break(s) between 69 & 80

alpha helices: 7A-20A, 26A-43A, 49A-68A, 7B-20B, 26B-42B, 49B-68B

beta strands:

Resolution: 1.900 Å R-factor: 0.229 R-free: 0.264

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>
94.0%	6.0%	0.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobit

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



Structure Quality Analysis for NAME

97.7% 2.3% 0%

Global quality scores

Program	<i>Verify3D</i>	<i>ProsaII (-ve)</i>	<i>Procheck (phi-psi)</i>	<i>Procheck (all)</i>	<i>MolProbity Clashscore</i>
-Raw score	0.38	0.51	0.46	0.28	20.60
Z-score ¹	-1.28	-0.58	2.12	1.66	-2.01

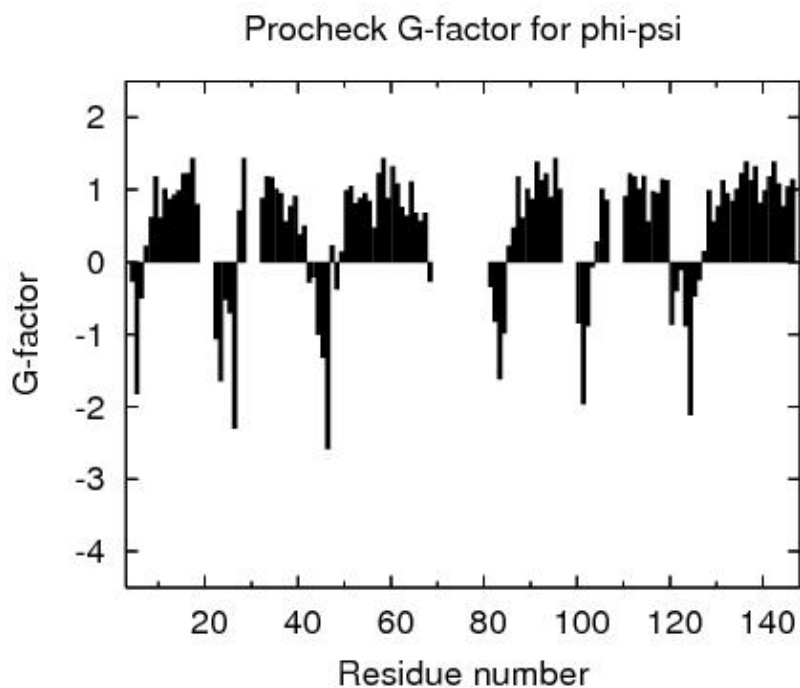
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 0.9 °

RMS deviation for bond lengths: 0.005 Å

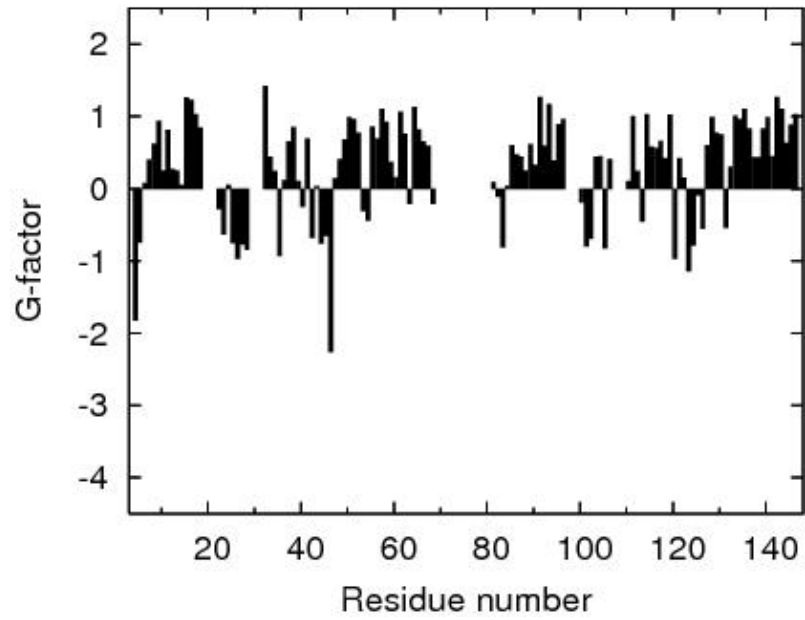
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score



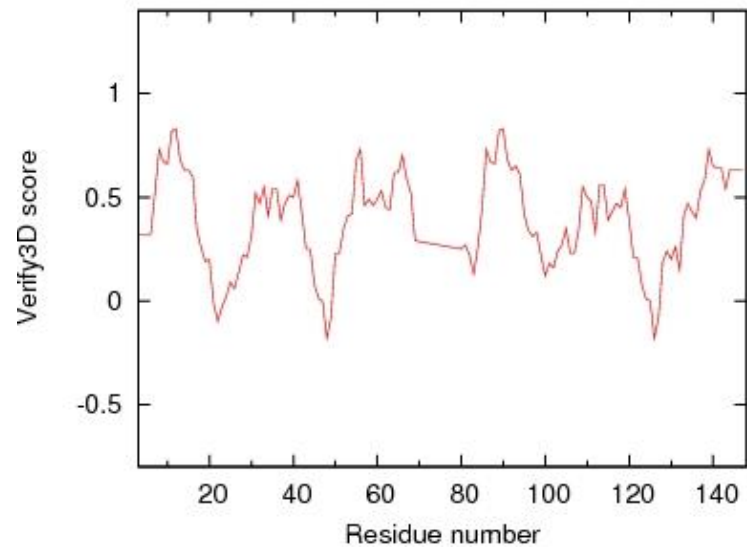


Structure Quality Analysis for NAME

Procheck G-factor for all dihedral angles

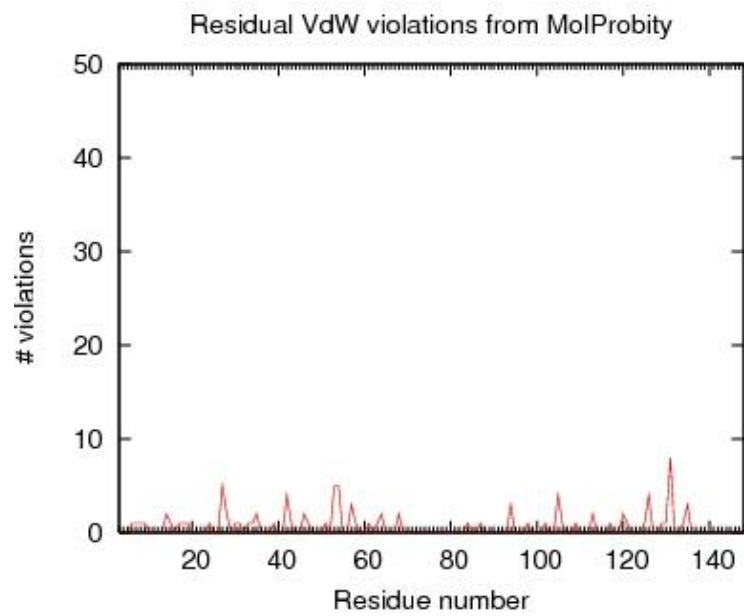
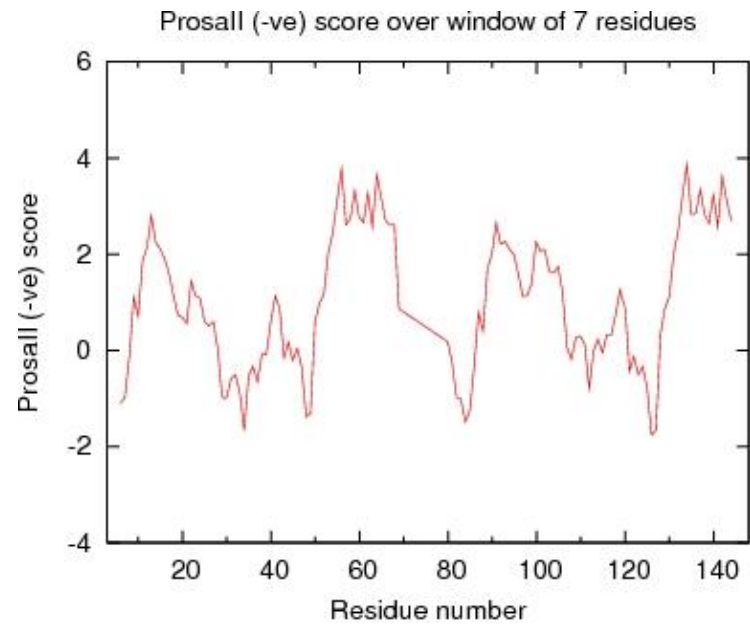


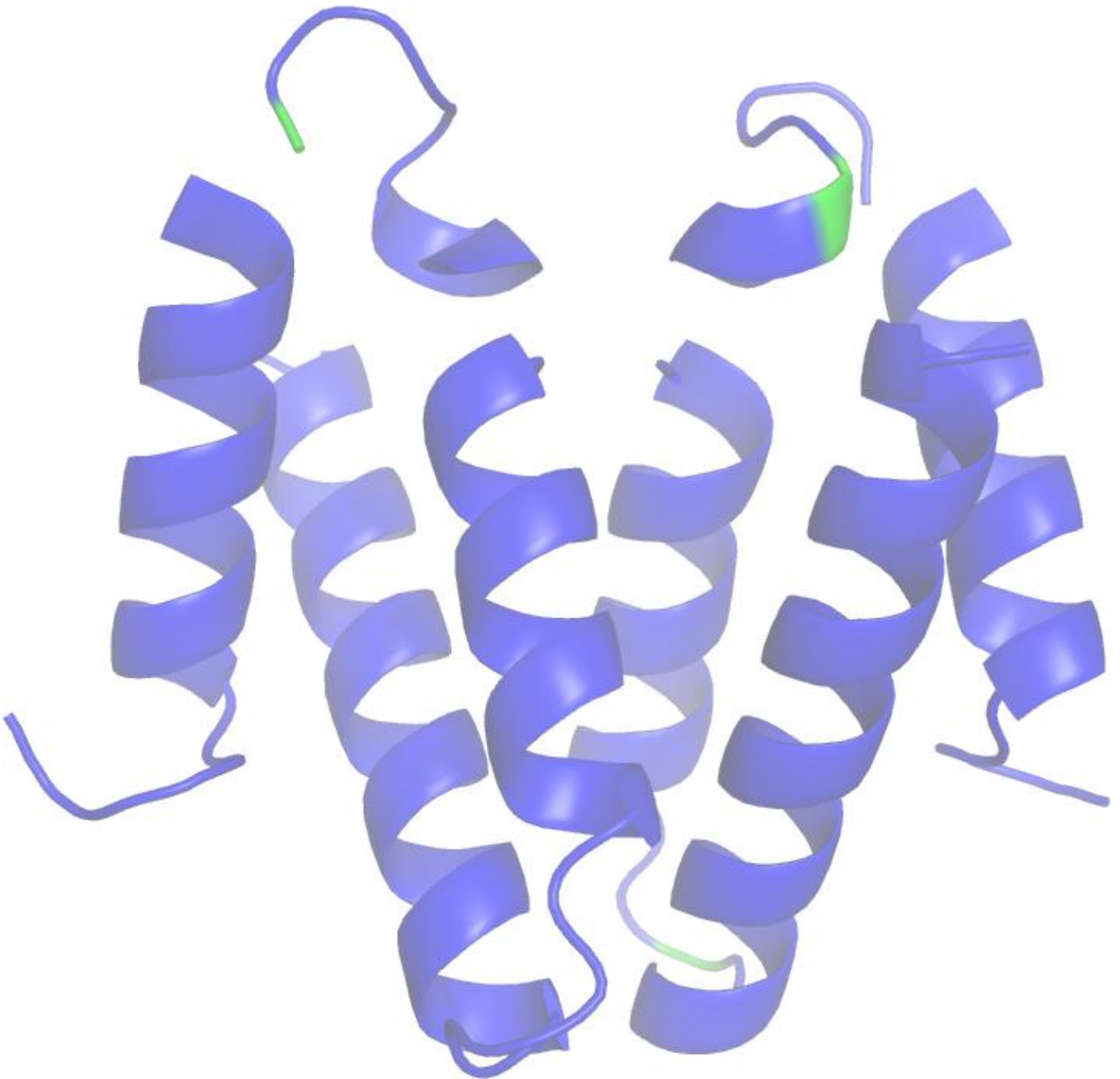
Verify3D score over window of 7 residues





Structure Quality Analysis for NAME





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

References:

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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
pdbstat

DsspCMBI-April-2000
PdbStat-5.4 Version



Structure Quality Analysis for NAME

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

MolProbit 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