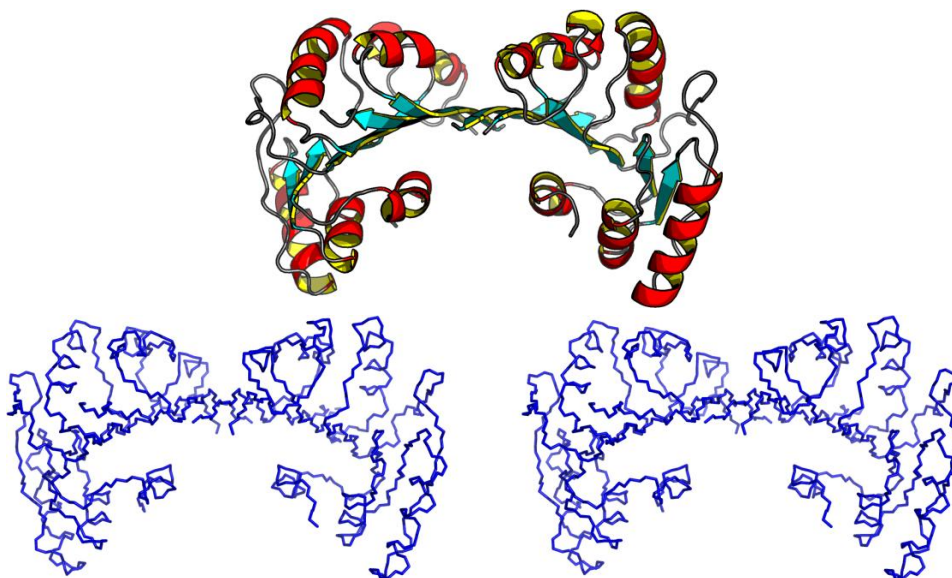




Structure Quality Analysis for NAME

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.): 346
 Organism:
 SwissProt /
 TrEMBL ID:
 Oligomerization: dimer
 Molecular weight: 37669



Secondary Structure Elements:

Inter-chain break(s) between 197 & 208

alpha helices: 19A-24A, 42A-48A, 61A-74A, 107A-120A, 153A-157A, 19B-24B, 42B-48B, 61B-74B, 107B-120B, 153B-157B

beta strands: 53U-57U, 32S-36S, 95P-101P, 121U-132U, 185A-194A, 163U-173U, 53U-57U, 32S-36S, 95P-101P, 121U-132U, 185A-194A, 163U-173U

Resolution: 2.200 Å R-factor: 0.224 R-free: 0.249
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>
87.0%	12.3%	0.7%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobit

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	View plot	View model summary
93.5%	4.7%	1.8%		

Global quality scores

Program	<i>Verify3D</i>	<i>ProsaII (-ve)</i>	<i>Procheck (phi-psi)</i>	<i>Procheck (all)</i>	<i>MolProbit</i>	<i>Clashscore</i>
-Raw score	0.44	0.55	-0.45	-0.39	30.14	
Z-score ¹	-0.32	-0.41	-1.46	-2.31	-3.65	



Structure Quality Analysis for NAME

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

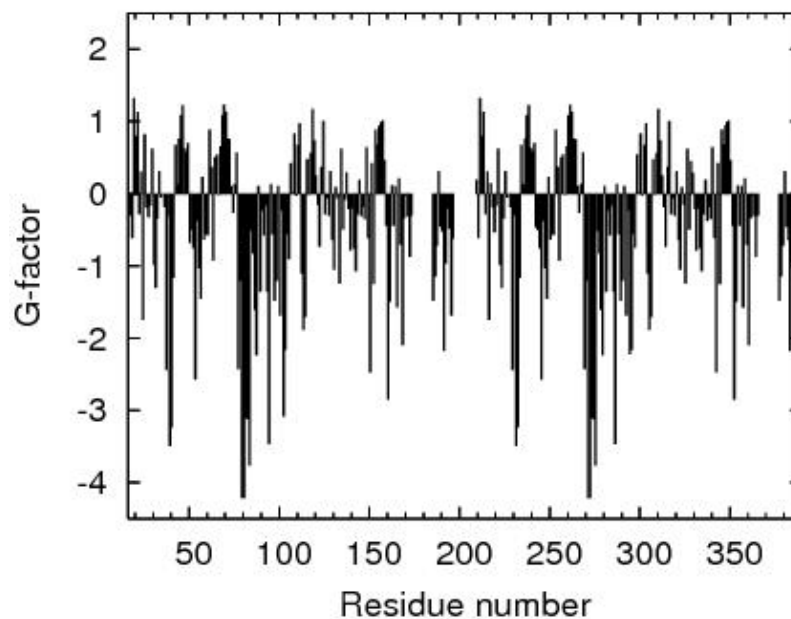
Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.3 °

RMS deviation for bond lengths: 0.007 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

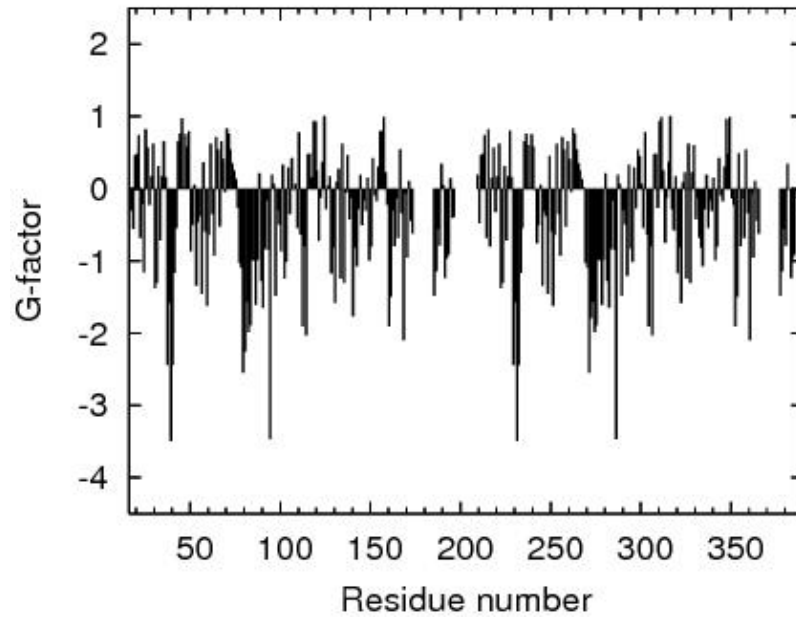
Procheck G-factor for phi-psi



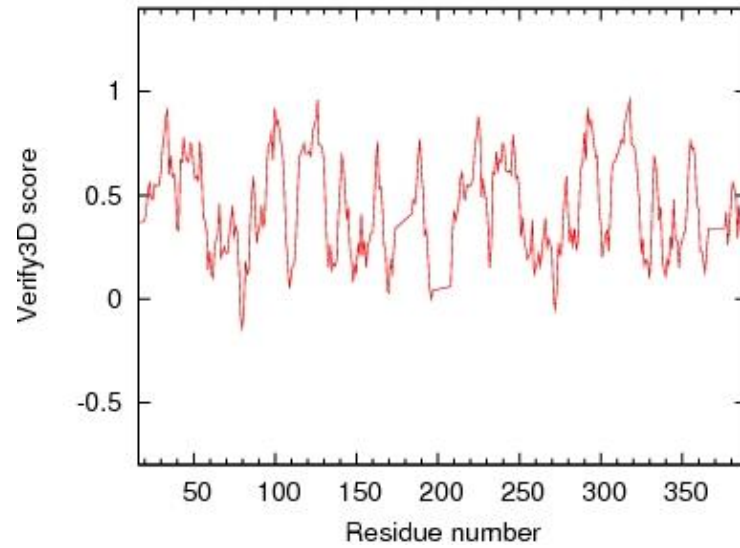


Structure Quality Analysis for NAME

Procheck G-factor for all dihedral angles

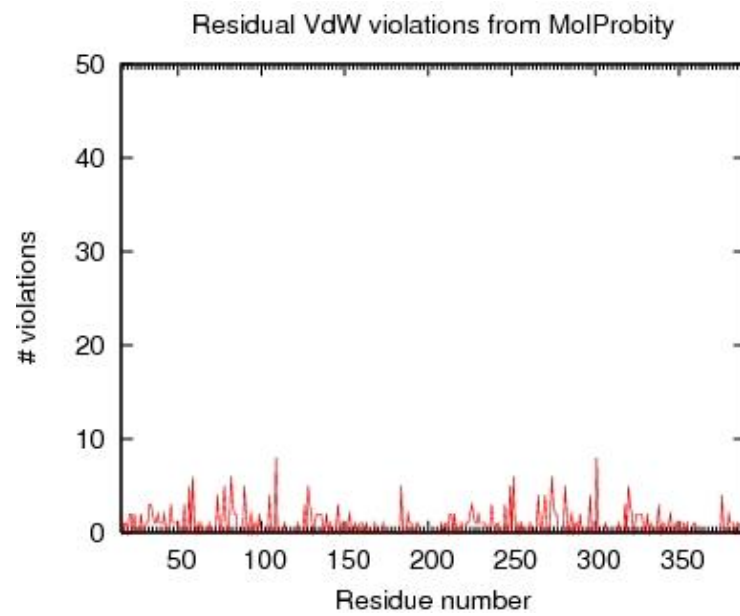
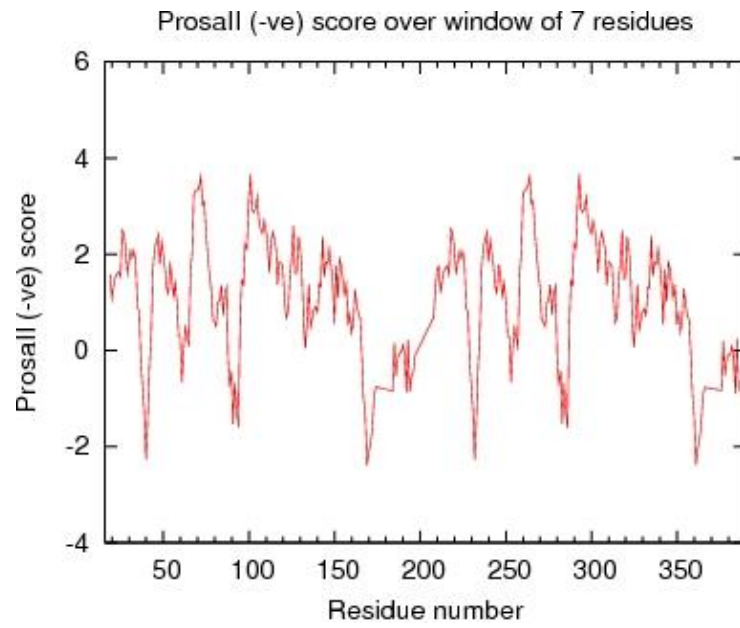


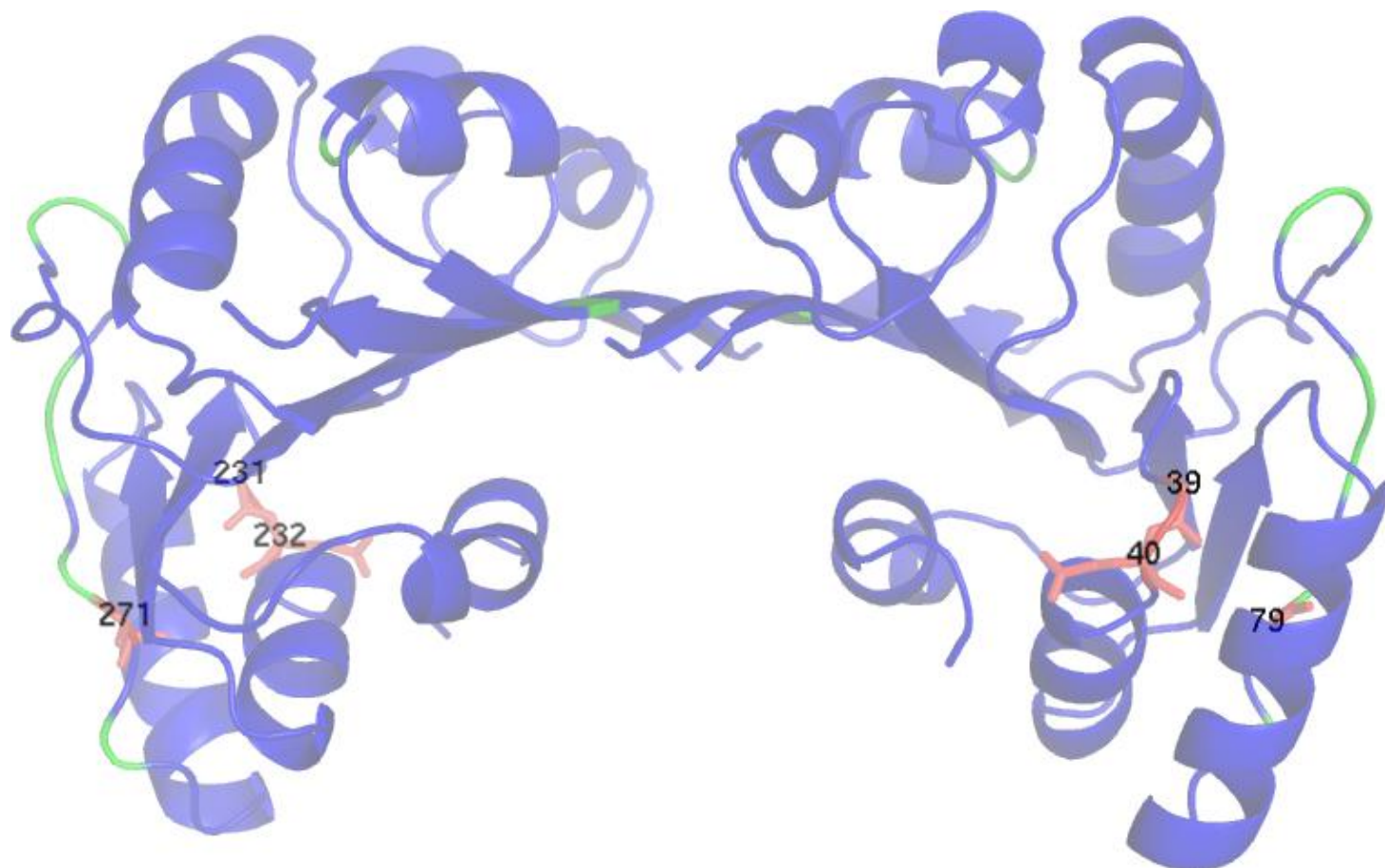
Verify3D score over window of 7 residues





Structure Quality Analysis for NAME





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

References:

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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

MolProbit programs:

cluster	1999
clashlistcluster	1999 (corrected by Aneerban)
mage	Version 6.35.040409



Structure Quality Analysis for NAME

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