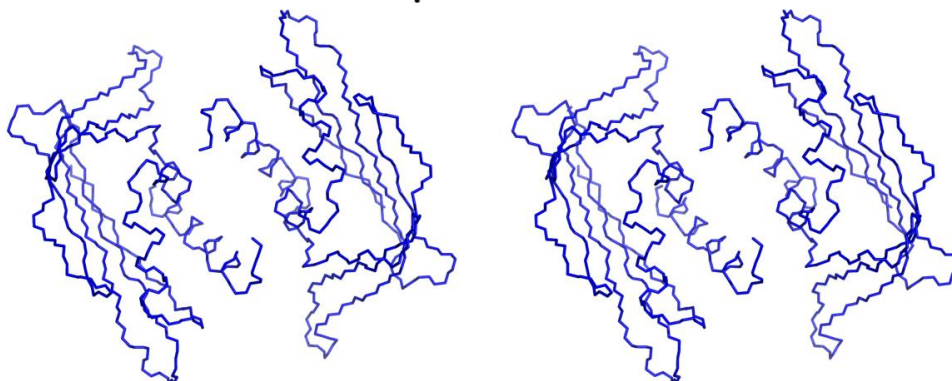
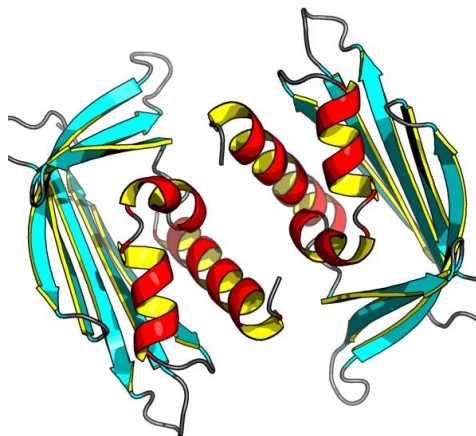




Structure Quality Analysis for NAME

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.): 260
Organism:
SwissProt /
TrEMBL ID:
Oligomerization: dimer
Molecular
weight: 29291



Secondary Structure Elements:

Inter-chain break(s) between 147 & 158

alpha helices: 15A-23A, 28A-31A, 128A-145A, 15B-23B, 28B-31B, 129B-145B

beta strands: 4L-11L, 101R-109R, 86N-94N, 73G-78G, 58R-69R, 45G-51G, 37R-40R, 3R-11R, 101R-110R, 85U-94U, 73G-78G, 58R-69R, 45G-51G, 35U-40U

Resolution: 2.000 Å R-factor: 0.242 R-free: 0.274

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>
89.7%	9.3%	0.9%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobit

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	<u>View plot</u>	<u>View model summary</u>
93.3%	6%	0.8%		



Structure Quality Analysis for NAME

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	0.35	0.60	-0.34	-0.23	21.38
Z-score ¹	-1.77	-0.21	-1.02	-1.36	-2.14

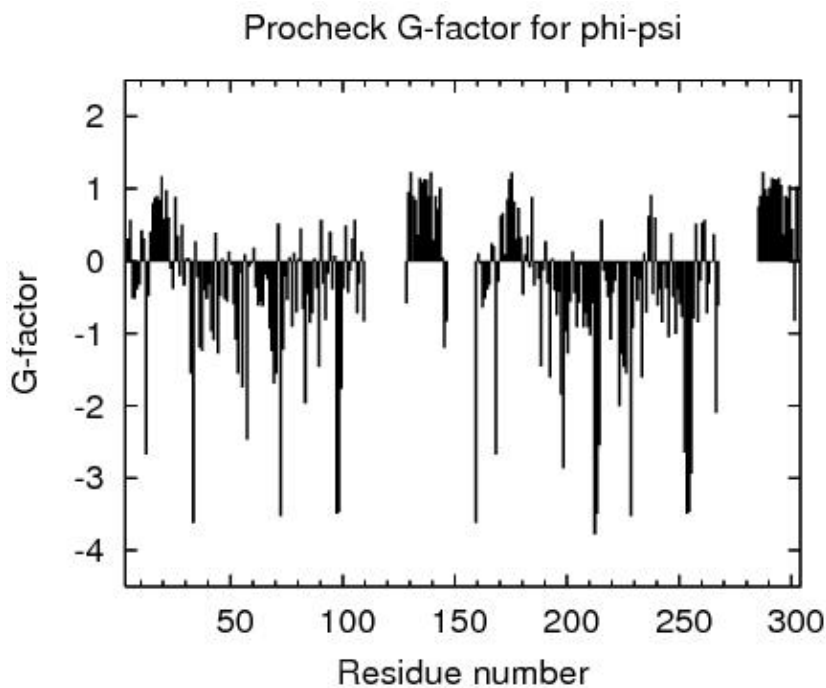
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.3 °

RMS deviation for bond lengths: 0.009 Å

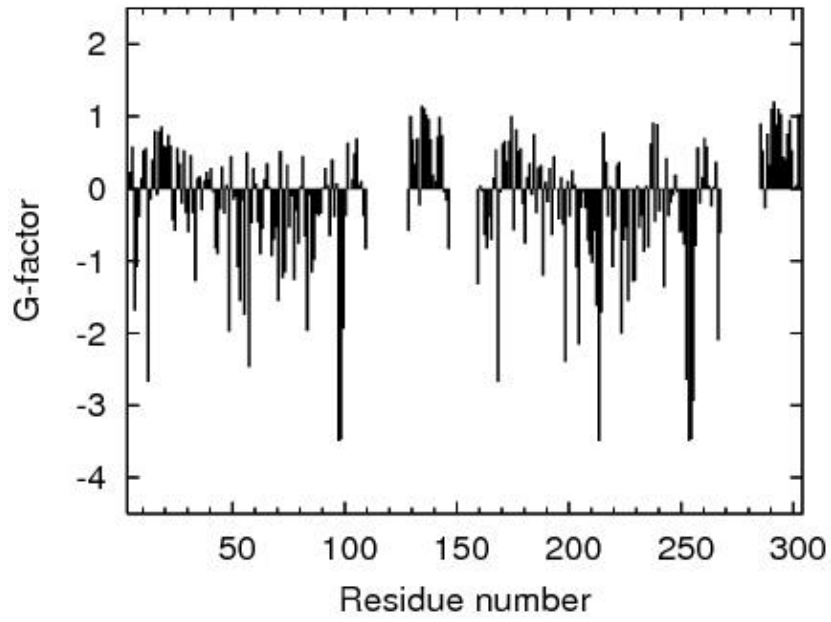
¹ With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score



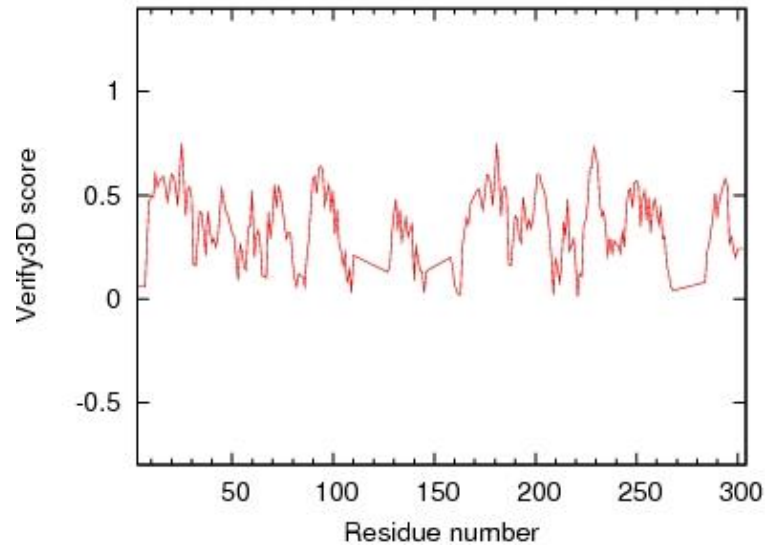


Structure Quality Analysis for NAME

Procheck G-factor for all dihedral angles

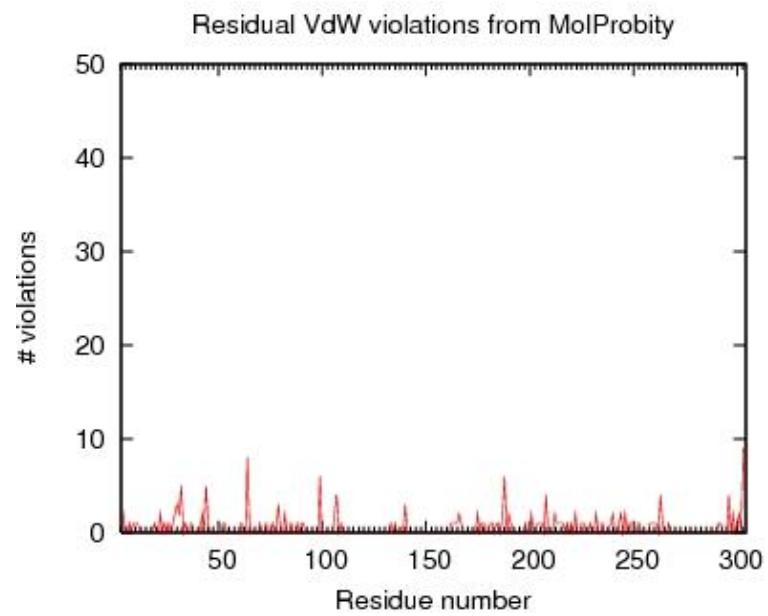
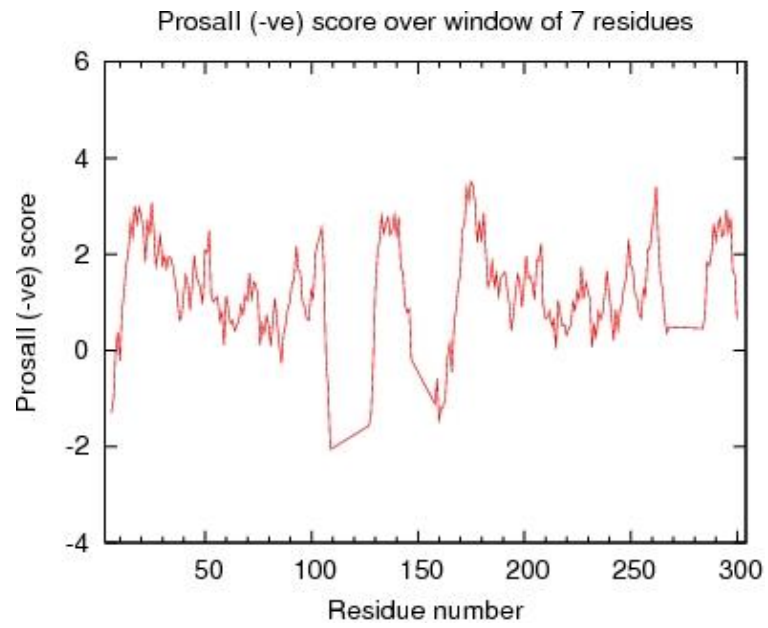


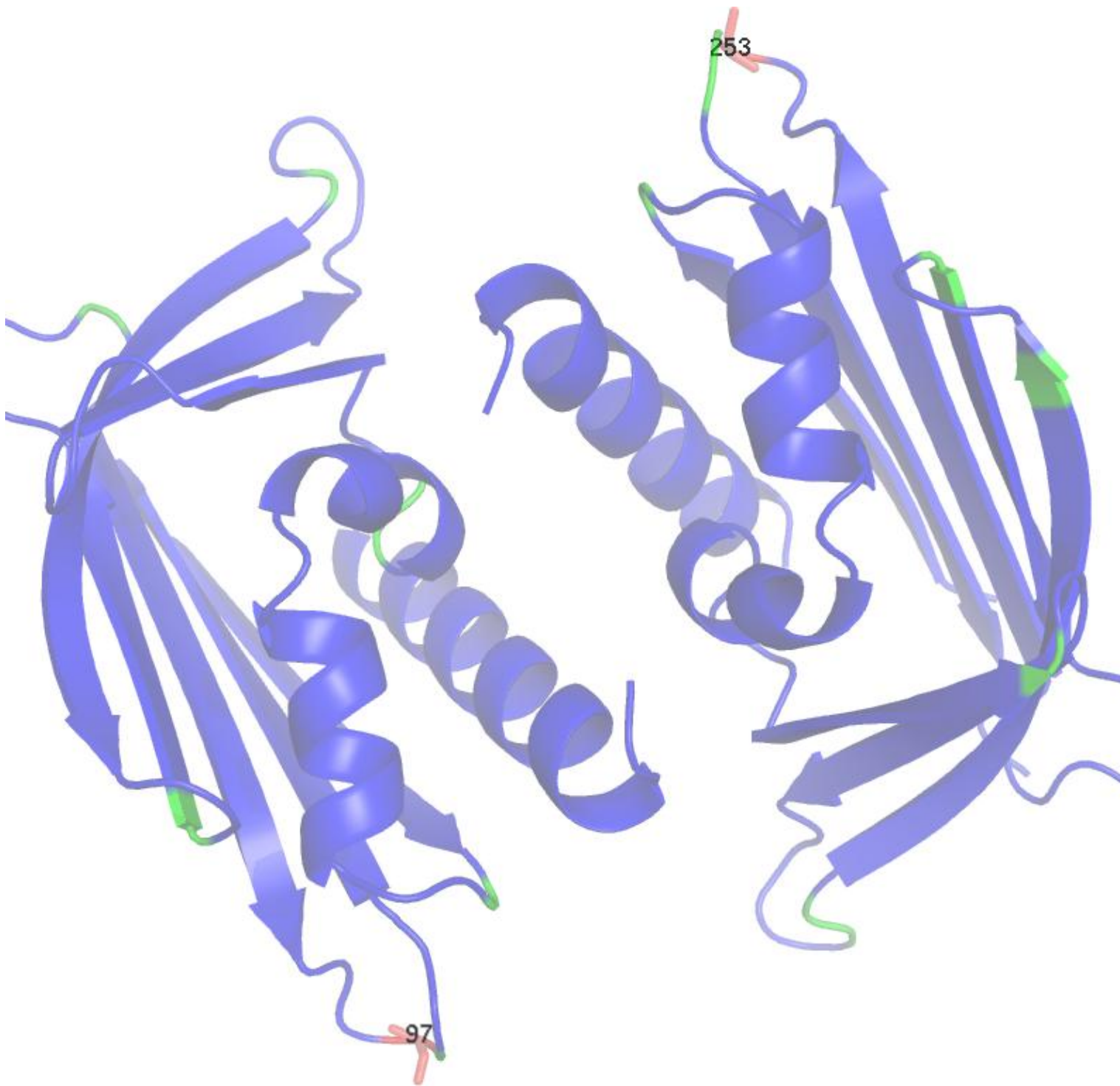
Verify3D score over window of 7 residues





Structure Quality Analysis for NAME





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

References:

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Structure Quality Analysis for NAME

Nature 356 (1992): 83-85

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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
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