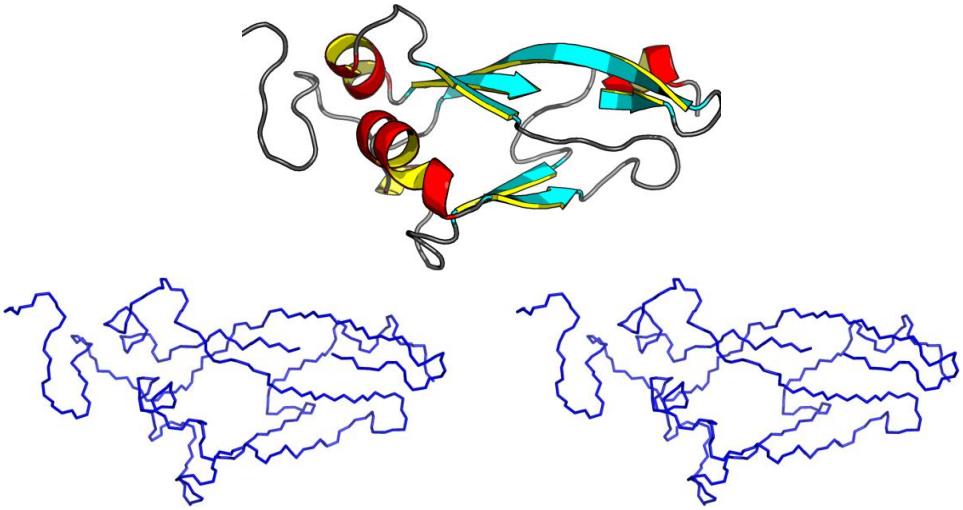
Structure Quality Analysis for NAME

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.):	118
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	monomer
Molecular weight:	13676



Secondary Structure Elements:
alpha helices: 135A-138A, 165A-171A, 201A-207A
beta strands: 148E-152E, 176E-180E, 187U-195U, 210U-218U, 224L-231L

Resolution: 2.494 Å R-factor: 0.213 R-free: 0.248
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
85.1%	14.9%	0.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
94.9%	5.1%	0%		

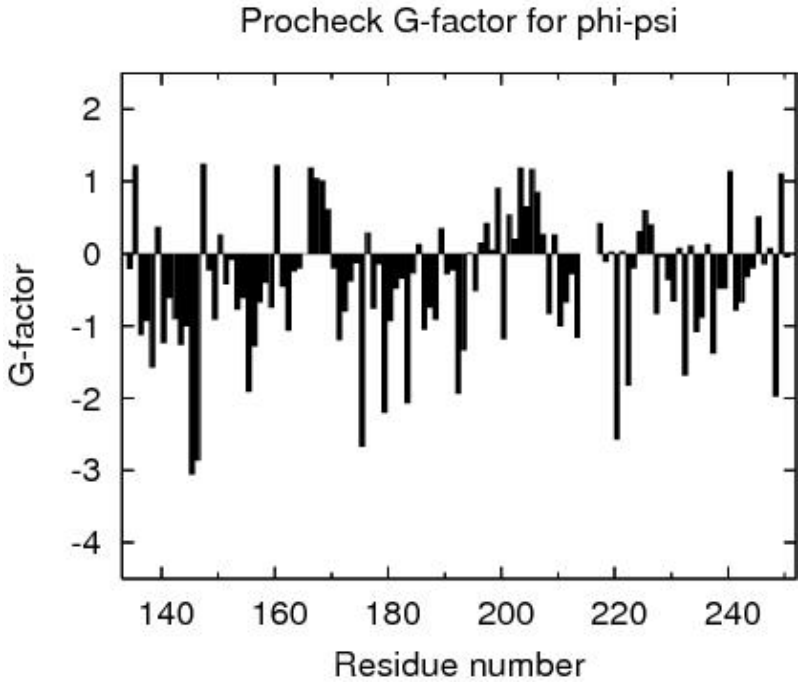
Global quality scores

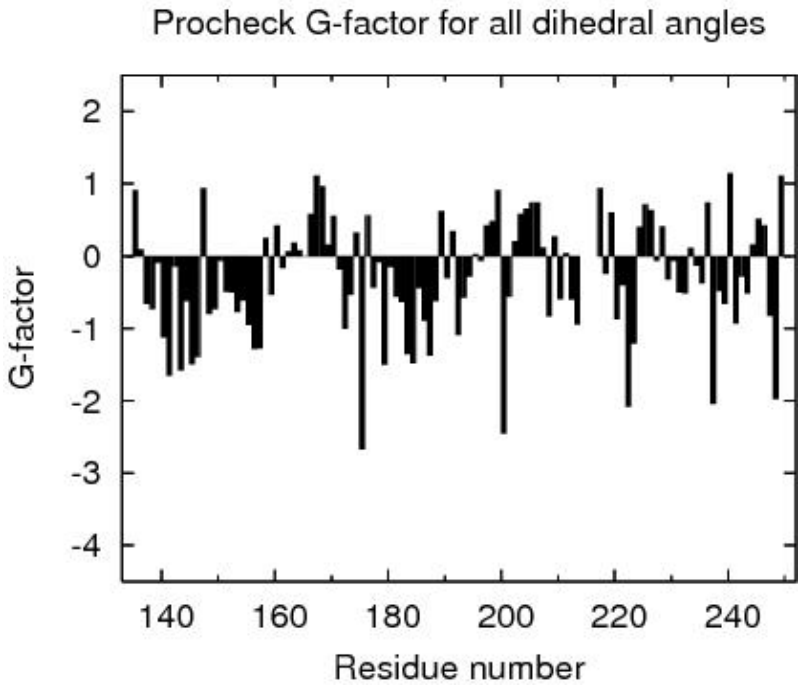
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*
-Raw score	0.39	0.42	-0.40	-0.28	14.08
Z-score[1]	-1.12	-0.95	-1.26	-1.66	-0.89

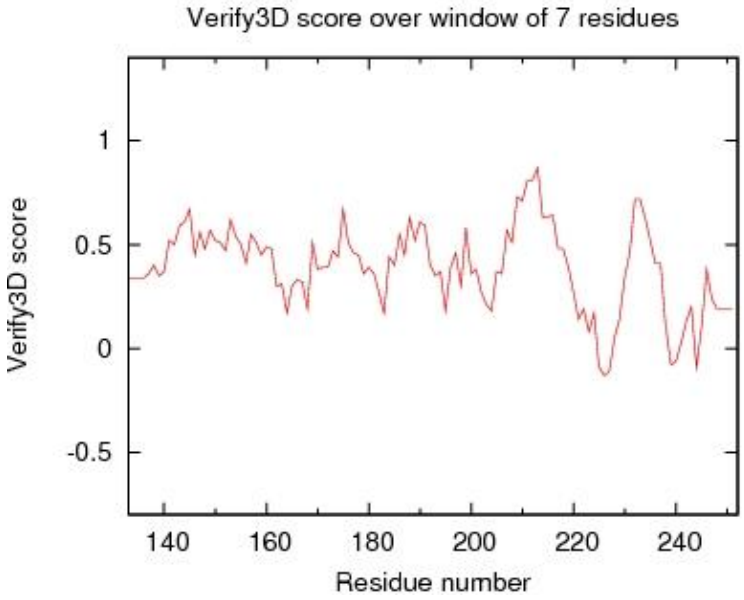
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

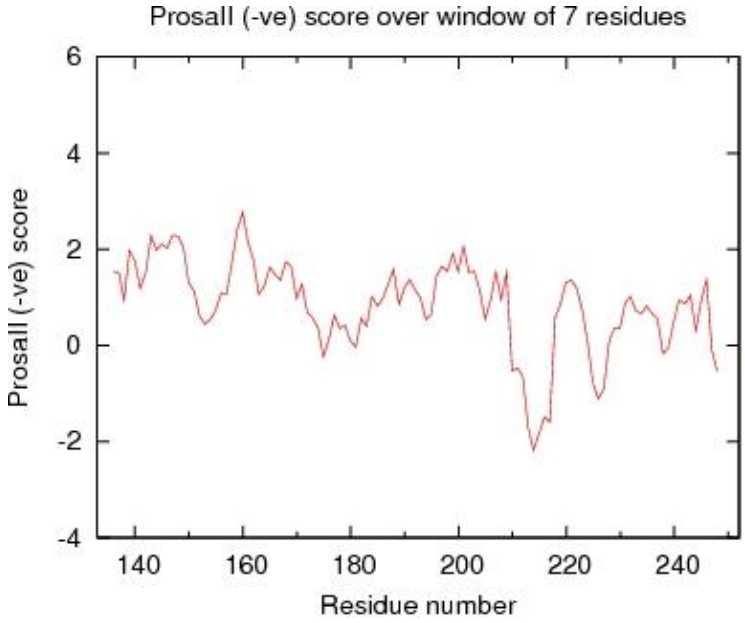
Number of close contacts (within 2.2 Å):	0
RMS deviation for bond angles:	1.6 °
RMS deviation for bond lengths:	0.008 Å

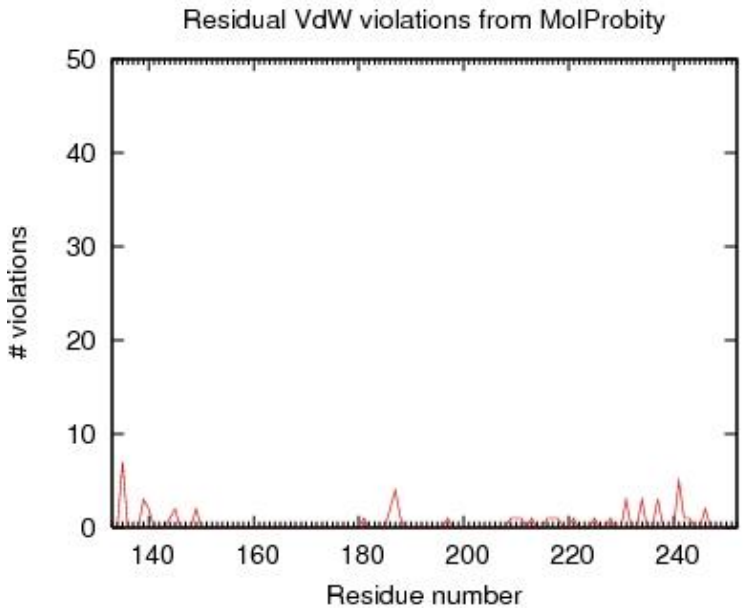
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score






Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
140
160
180
200
220
240
Residue number


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
140
160
180
200
220
240
Residue number



Residue Plot of Ramachandran anlysis(based on data from Richardson Lab's Molprobity)

References:

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Analysed by on May-11-2013 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