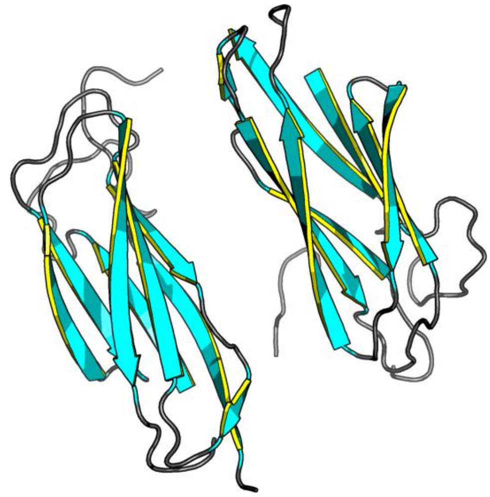
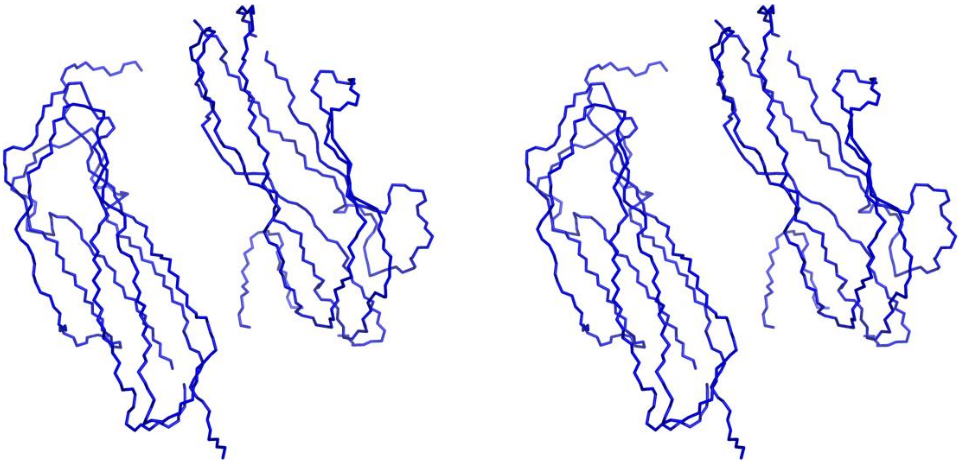
Structure Quality Analysis for NAME

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.):	226
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	dimer
Molecular weight:	25238



Secondary Structure Elements:
Inter-chain break(s) between 540 & 551
alpha helices:
beta strands: 440U-445U, 456A-464A, 496U-503U, 449L-450L, 532L-539L, 509Y-517Y, 470L-479L, 482R-491R, 440U-445U, 456A-464A, 495U-503U, 449L-451L, 532L-540L, 509Y-517Y, 470L-479L, 482R-491R

Resolution: 1.700 Å R-factor: 0.190 R-free: 0.212
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
91.1%	8.4%	0.5%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
99.1%	0.5%	0.5%		

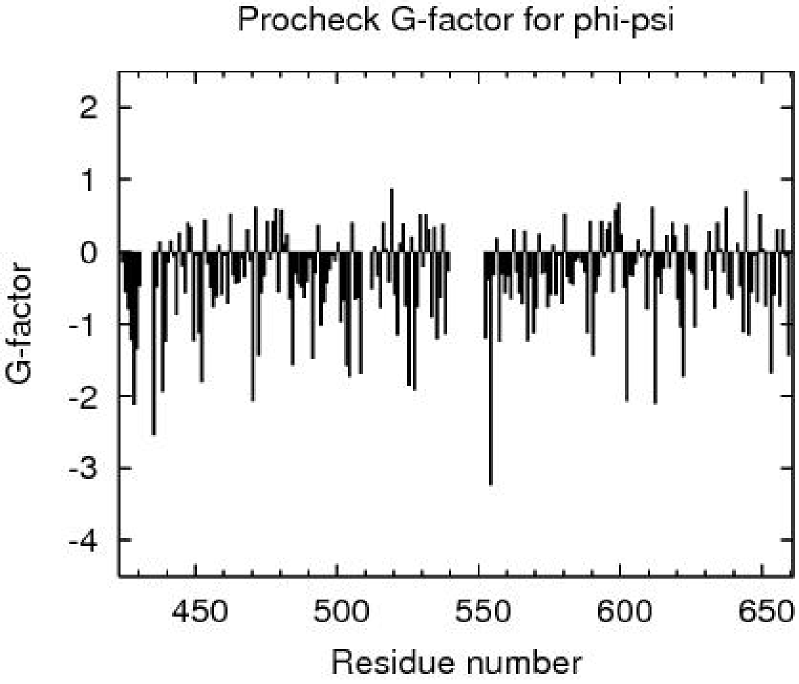
Global quality scores

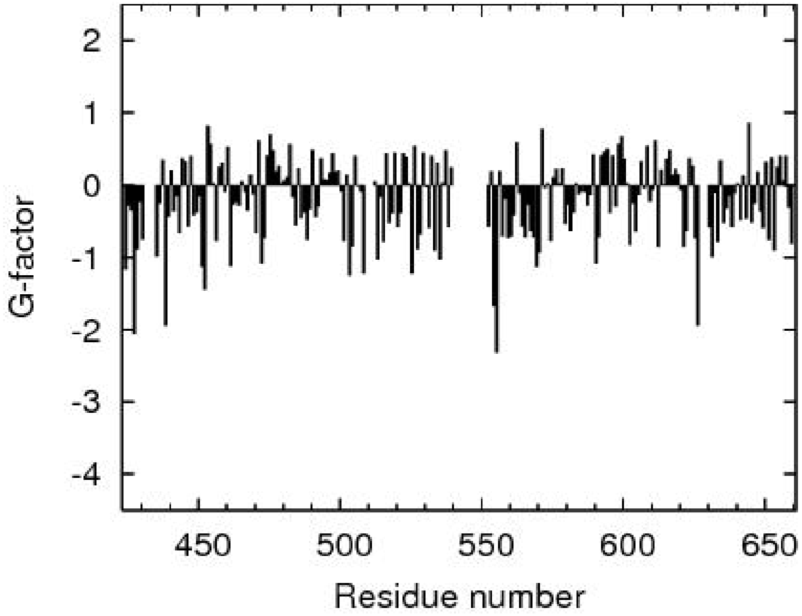
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*
-Raw score	0.34	0.17	-0.40	-0.21	15.58
Z-score[1]	-1.93	-1.99	-1.26	-1.24	-1.15

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

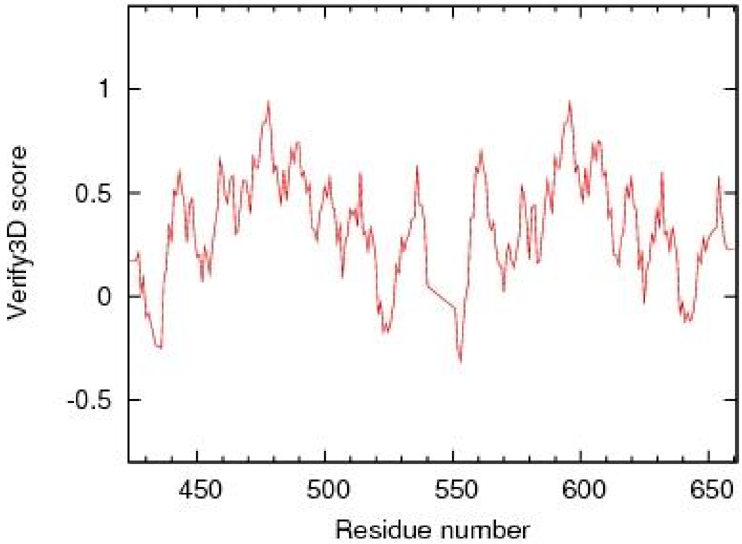
Number of close contacts (within 2.2 Å): 0
RMS deviation for bond angles: 1.2 °
RMS deviation for bond lengths: 0.005 Å

[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

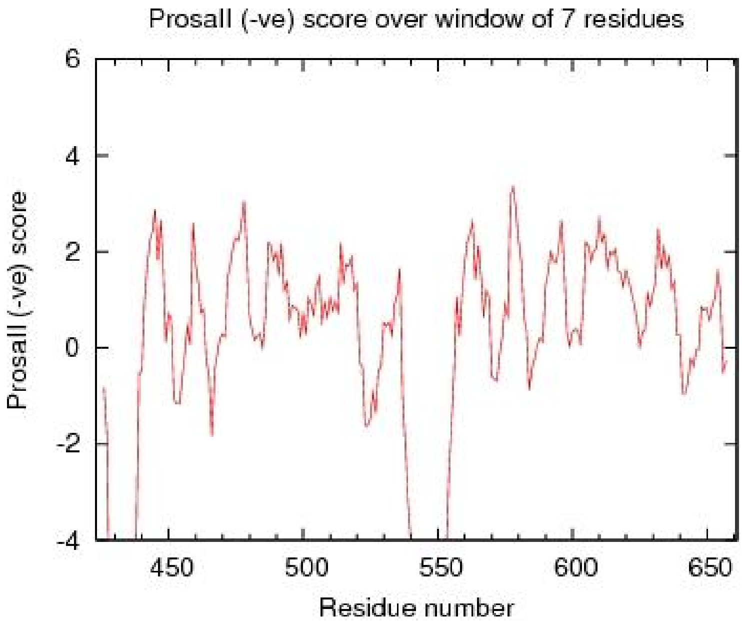


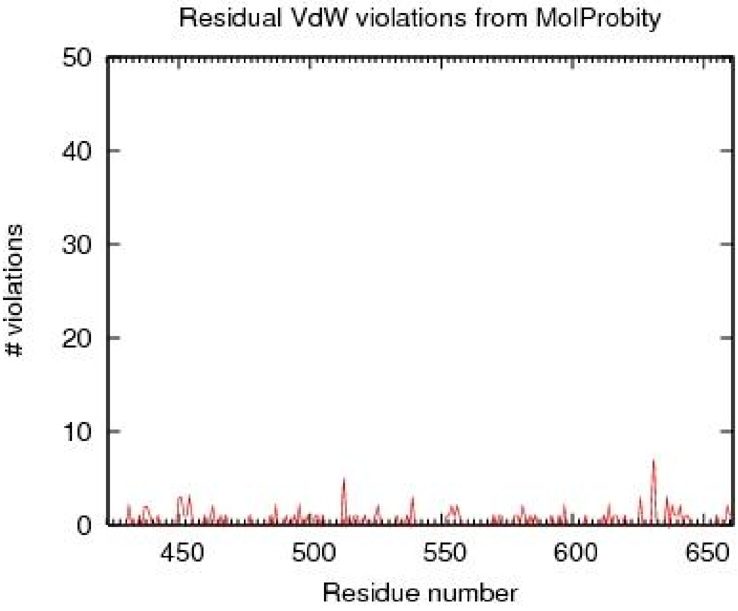


Procheck G-factor for all dihedral angles



Verify3D score over window of 7 residues


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
450
500
550
600
650
Residue number


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
450
500
550
600
650
Residue number

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

References:

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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
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4. Sippl M J, "Calculation of Conformation Ensembles from Potentials of Mean Force", J Mol Biol 213 (1990): 859-883
5. Laskowski R Ai et al, "AQUA and PROCHECK_NMR: Programs for checking the quality of proteins structures solved by NMR", J Biomolec NMR 8 (1996): 477-486
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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

Protein Structure Validation Suite (PSVS)

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