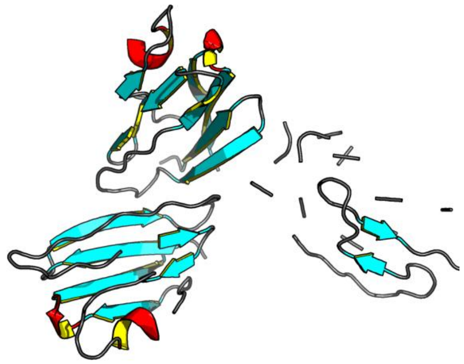
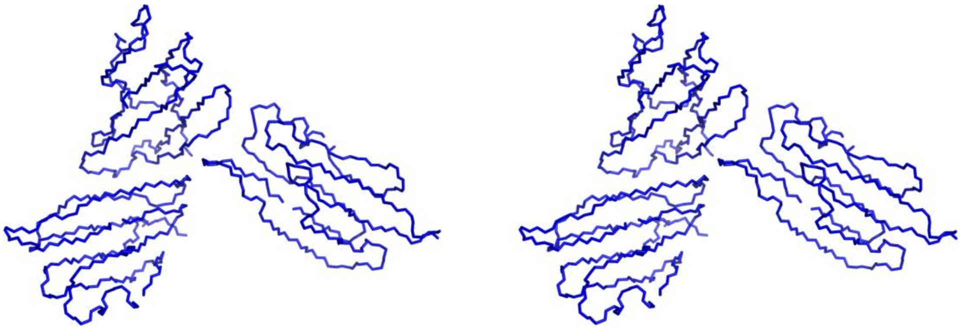
Structure Quality Analysis for NAME

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.):	261
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	trimer
Molecular weight:	28840



Secondary Structure Elements:
Inter-chain break(s) between 125 & 136, 222 & 233
alpha helices: 97A-101A, 97B-101B, 97C-101C
beta strands: 51S-57S, 42L-48L, 118L-124L, 110R-113R, 64N-70N, 76R-82R, 85G-91G, 51S-57S, 42L-48L, 118L-124L, 110R-113R, 64N-70N, 76R-82R, 85G-91G, 51S-57S, 42L-48L, 118L-124L, 110R-113R, 64N-70N, 76R-82R, 85G-91G

Resolution: 1.550 Å R-factor: 0.165 R-free: 0.194
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
95.1%	4.9%	0.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
98.8%	1.2%	0%		

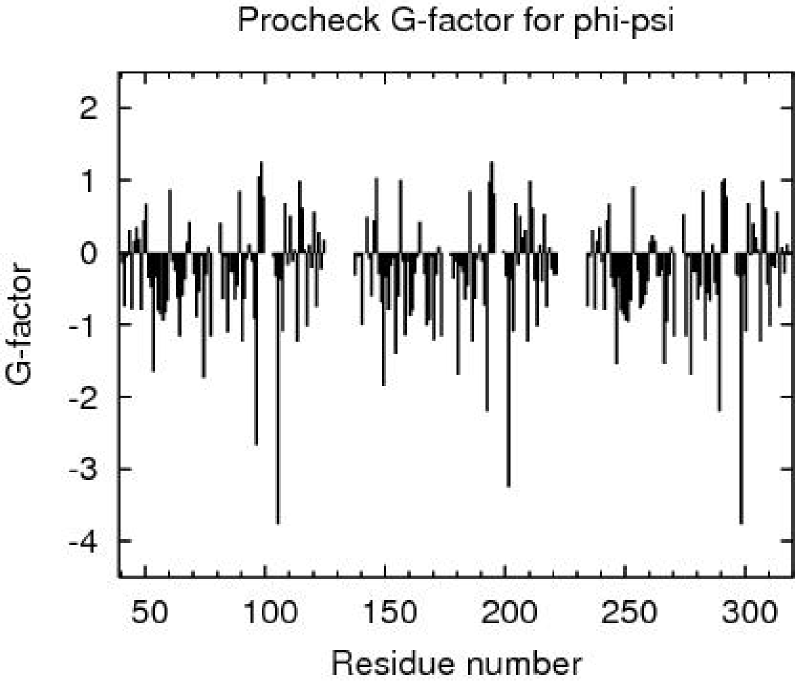
Global quality scores

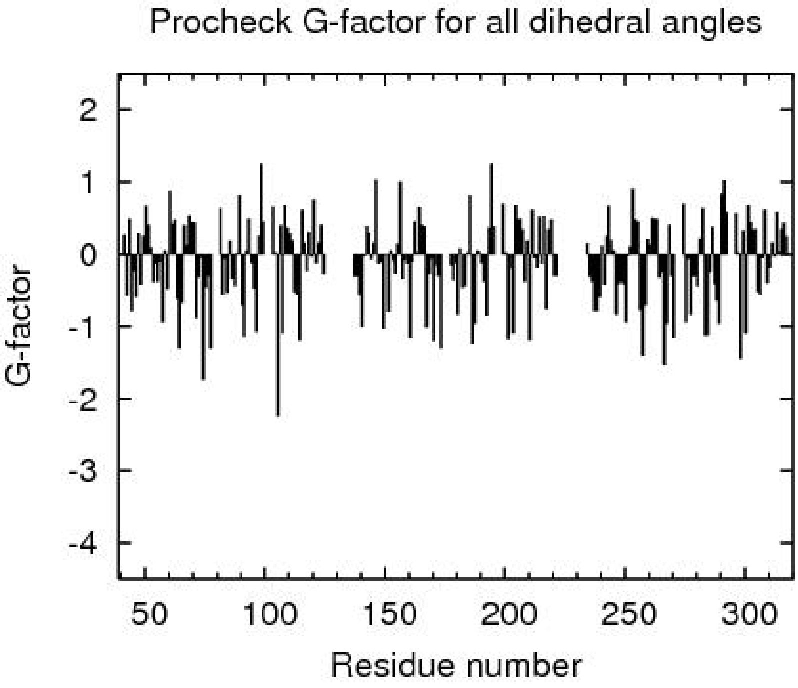
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*
-Raw score	0.34	0.61	-0.31	-0.09	7.40
Z-score[1]	-1.93	-0.17	-0.90	-0.53	0.26

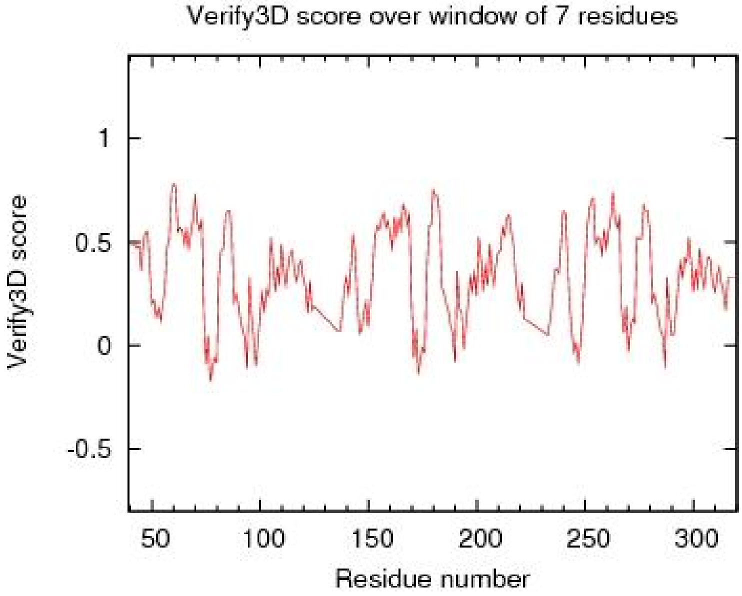
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

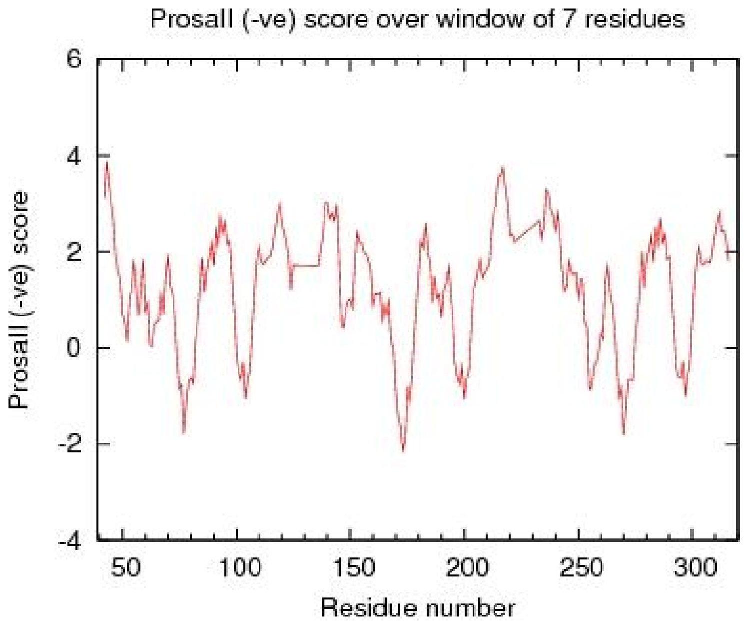
Number of close contacts (within 2.2 Å):	0
RMS deviation for bond angles:	1.2 °
RMS deviation for bond lengths:	0.009 Å

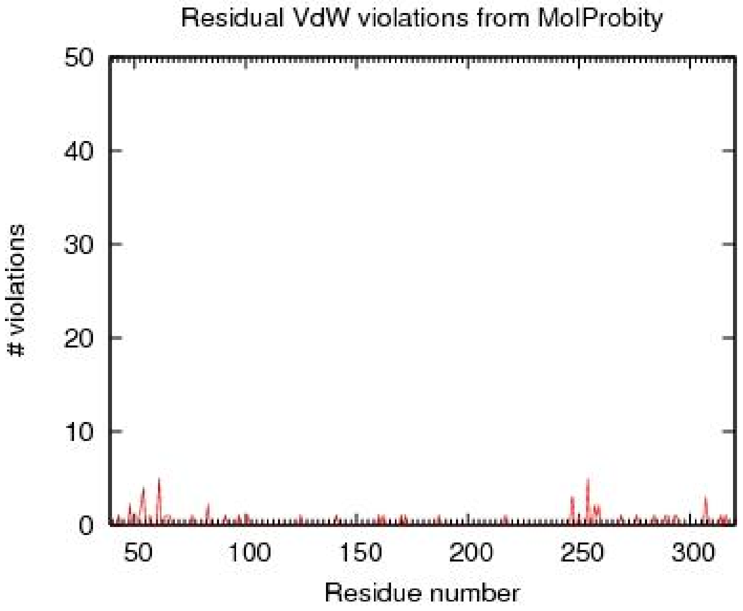
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

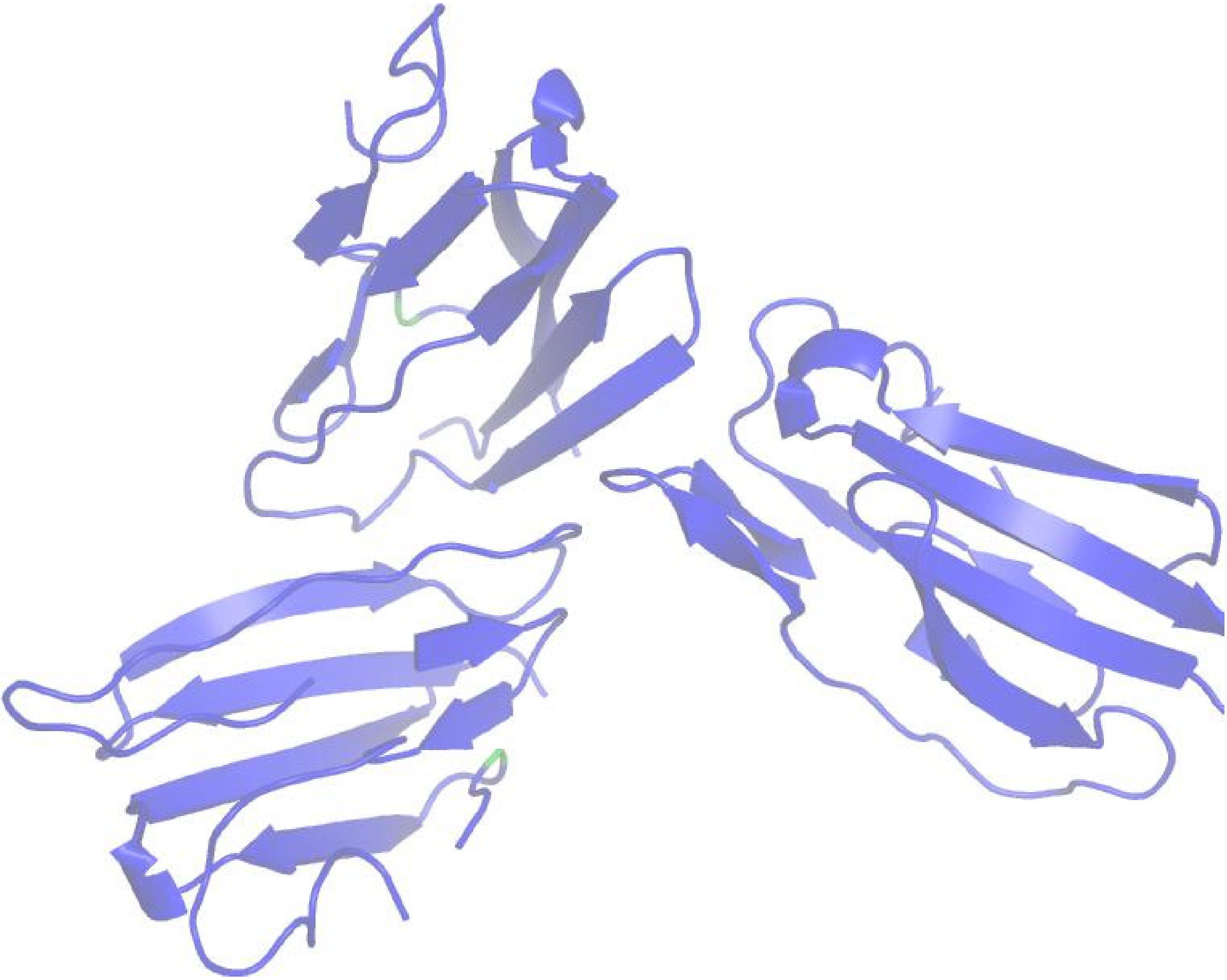



Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
50
100
150
200
250
300
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
50
100
150
200
250
300
Residue number


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
50
100
150
200
250
300
Residue number


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
50
100
150
200
250
300
Residue number



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

References:

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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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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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14. Güntert, P, Mumenthaler, C & Wüthrich, K "Torsion angle dynamics for NMR structure calculation with the new program DYANA", J. Mol. Biol 273 (1997): 283-298
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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