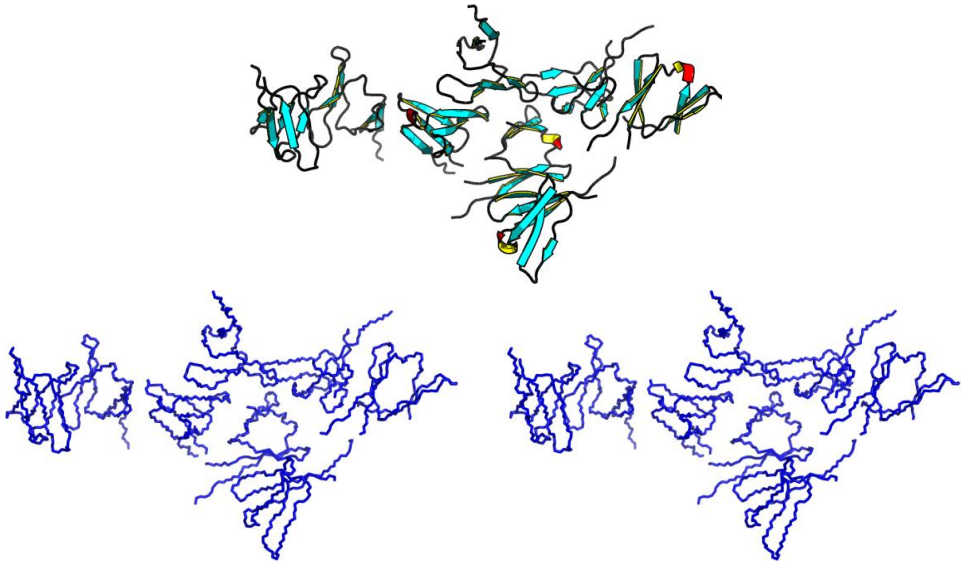
Structure Quality Analysis for NAME

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.):	452
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	9 mer
Molecular weight:	50935



Secondary Structure Elements:
Inter-chain break(s) between 57 & 68, 123 & 134, 190 & 201, 257 & 268, 323 & 334, 389 & 400, 456 & 467, 522 & 533
alpha helices:
beta strands: 14T-16T, 4P-9P, 47L-53L, 22U-24U, 29U-33U, 39A-43A, 14T-16T, 4P-9P, 47L-53L, 22U-24U, 29U-33U, 39A-43A, 15E-16E, 4P-9P, 47L-53L, 18P-24P, 29U-33U, 39A-43A, 14T-16T, 4P-9P, 47L-53L, 22U-24U, 29U-33U, 39A-43A, 14T-17T, 4P-9P, 47L-53L, 22U-24U, 29U-32U, 40T-43T, 14T-17T, 5R-9R, 47L-52L, 22U-24U, 29U-33U, 39A-43A, 14T-17T, 4P-9P, 47L-53L, 22U-24U, 29U-33U, 39A-43A, 13G-17G, 4P-9P, 47L-53L, 22U-24U, 29U-32U, 40T-43T

Resolution: 2.700 Å R-factor: 0.238 R-free: 0.253
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
88.9%	10.6%	0.5%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
93.7%	4.9%	1.4%		

Global quality scores

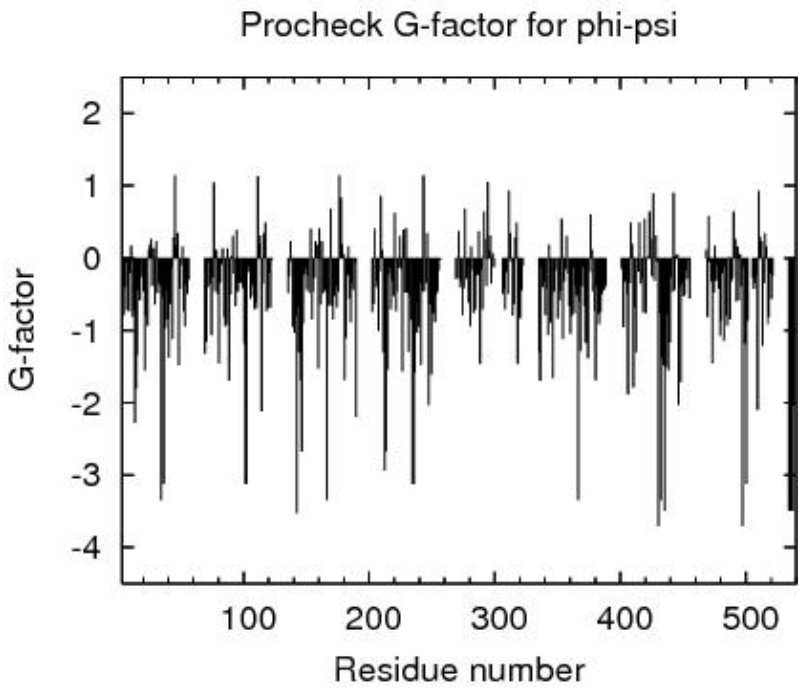
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*

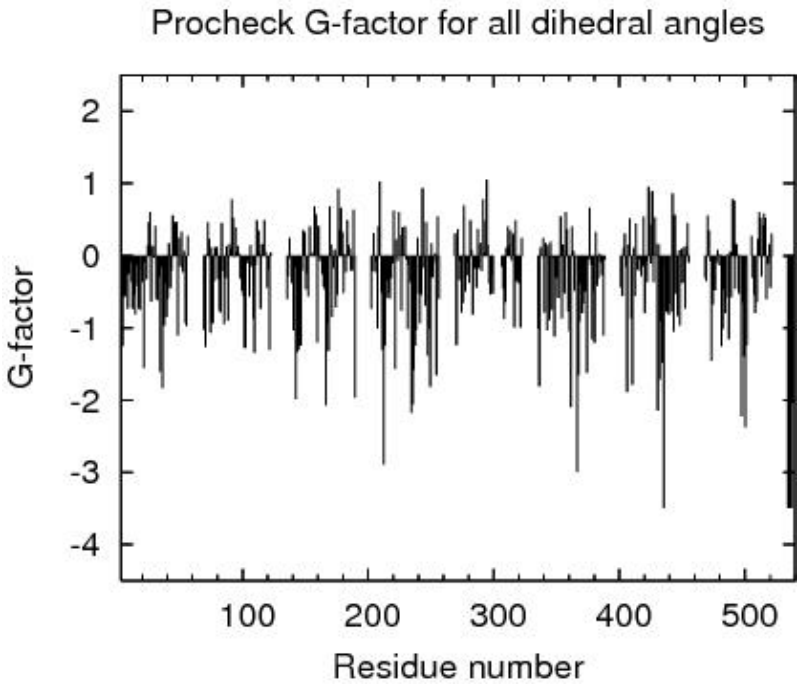
-Raw score	0.36	0.28	-0.56	-0.37	18.76
Z-score[1]	-1.61	-1.53	-1.89	-2.19	-1.69

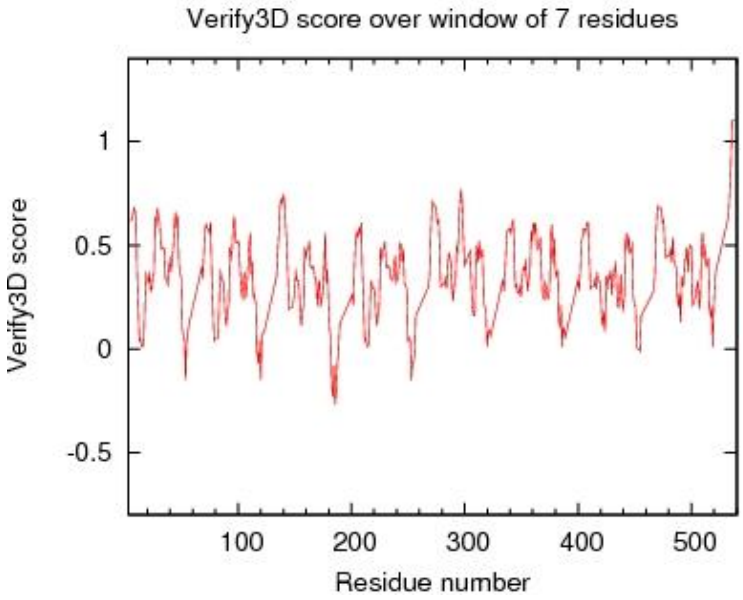
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

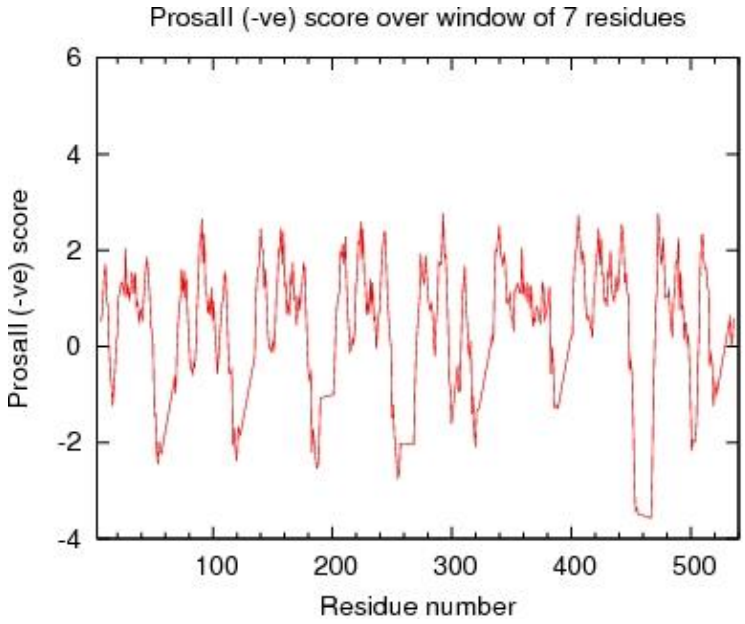
Number of close contacts (within 2.2 Å):	0
RMS deviation for bond angles:	1.2 °
RMS deviation for bond lengths:	0.007 Å

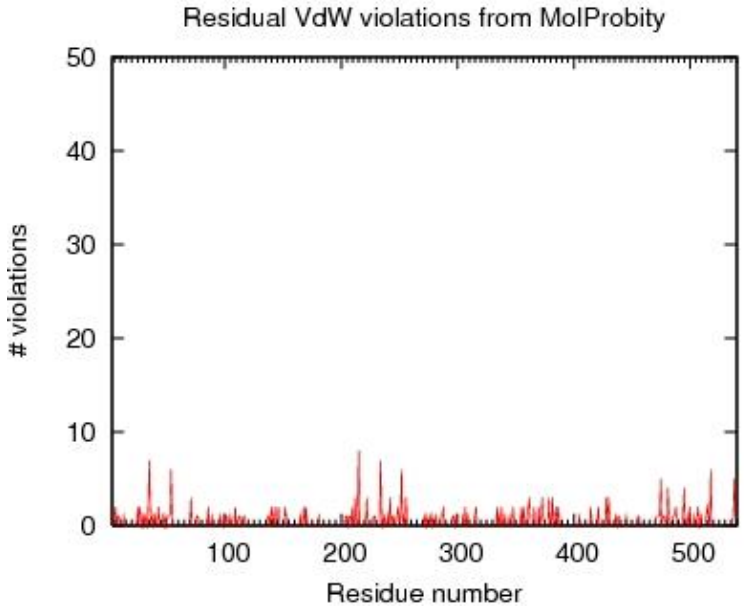
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

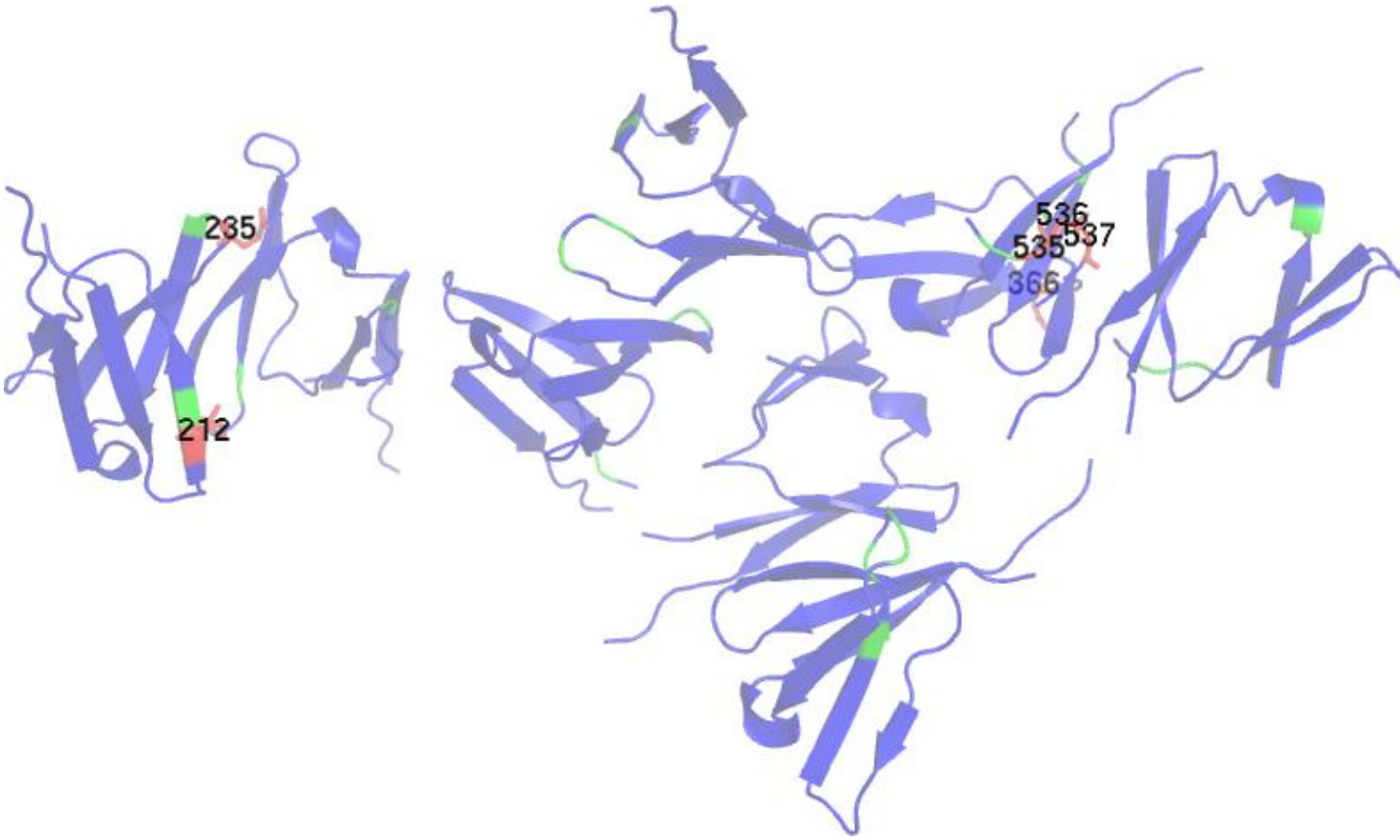



Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
100
200
300
400
500
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
100
200
300
400
500
Residue number


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
100
200
300
400
500
Residue number


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
100
200
300
400
500
Residue number



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

References:

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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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8. Word J M et al, "Asparagine and Glutamine: Using Hydrogen Atom Contacts in the Choice of Side-chain Amide Orientation", J Mol Biol 285 (1999): 1735-1747
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Explicit Hydrogens", J Mol Biol 285 (1999): 1711-1733
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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

MolProbity programs:

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

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prekin            Version 6.35.040406
reduce            Version 2.14
probe             Version 2.6
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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
```