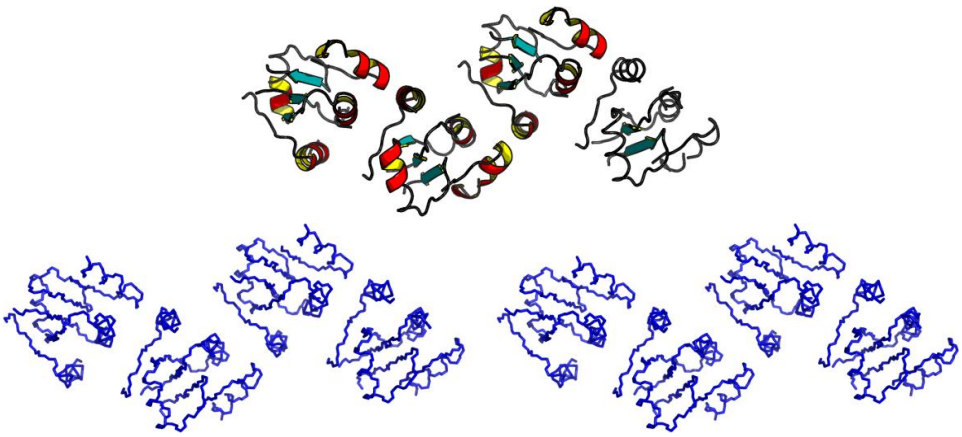
Structure Quality Analysis for NAME

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.):	412
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	tetramer
Molecular weight:	46386



Secondary Structure Elements:
Inter-chain break(s) between 125 & 136, 254 & 265, 383 & 394
alpha helices: 8A-15A, 54A-63A, 77A-85A, 113A-124A, 8B-15B, 54B-63B, 77B-85B, 113B-124B, 8C-15C, 54C-63C, 77C-85C, 113C-124C, 8D-15D, 54D-63D, 77D-85D, 113D-124D
beta strands: 20N-21N, 71N-75N, 37Y-41Y, 94A-98A, 107U-108U, 20N-21N, 71N-75N, 36P-41P, 94A-99A, 107U-108U, 20N-21N, 71N-75N, 36P-41P, 94A-99A, 107U-108U, 20N-21N, 71N-75N, 36P-41P, 94A-99A, 107U-108U

Resolution: 2.800 Å R-factor: 0.285 R-free: 0.338
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
85.6%	13.1%	1.3%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
90%	8.7%	1.3%		

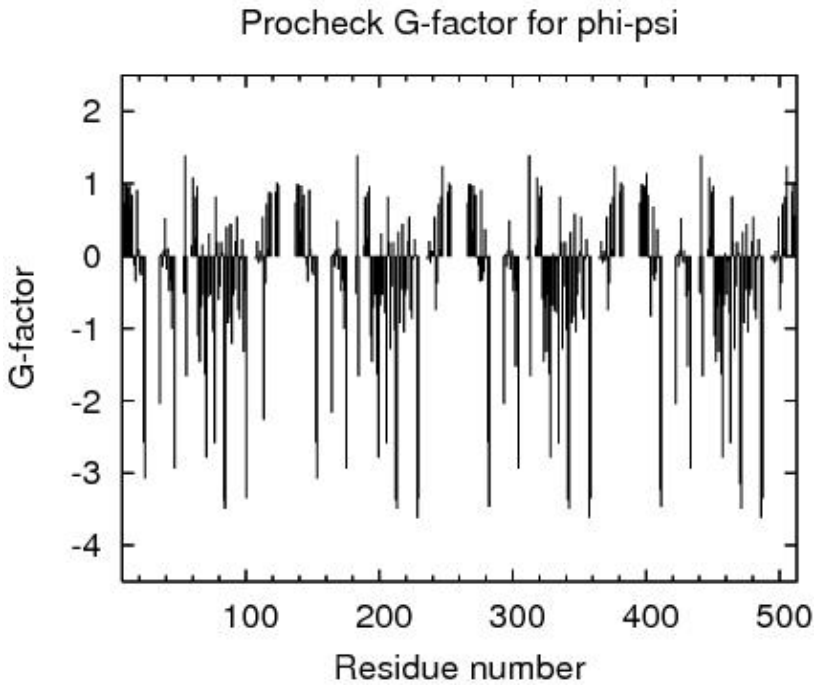
Global quality scores

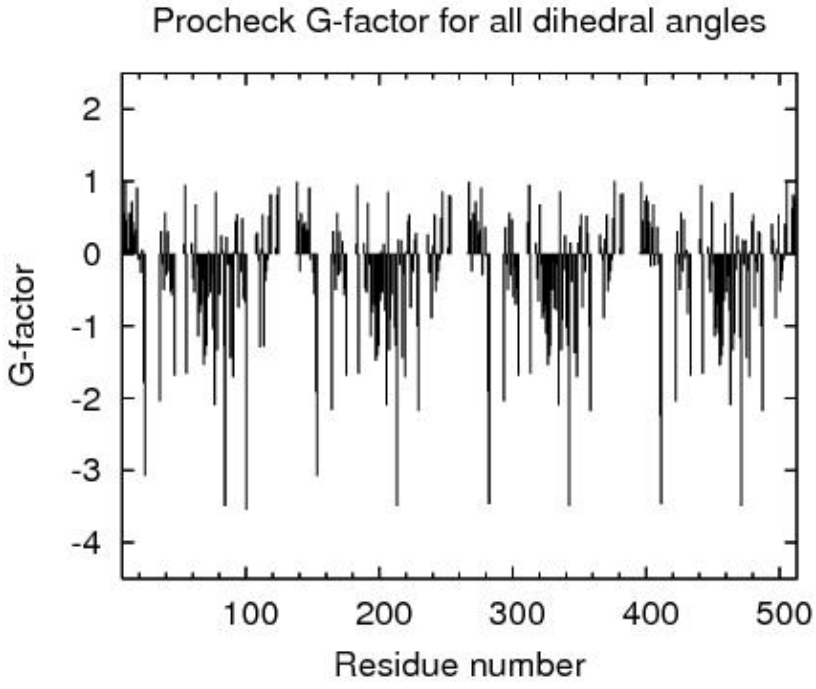
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*
-Raw score	0.43	0.37	-0.35	-0.30	37.44
Z-score[1]	-0.48	-1.16	-1.06	-1.77	-4.90

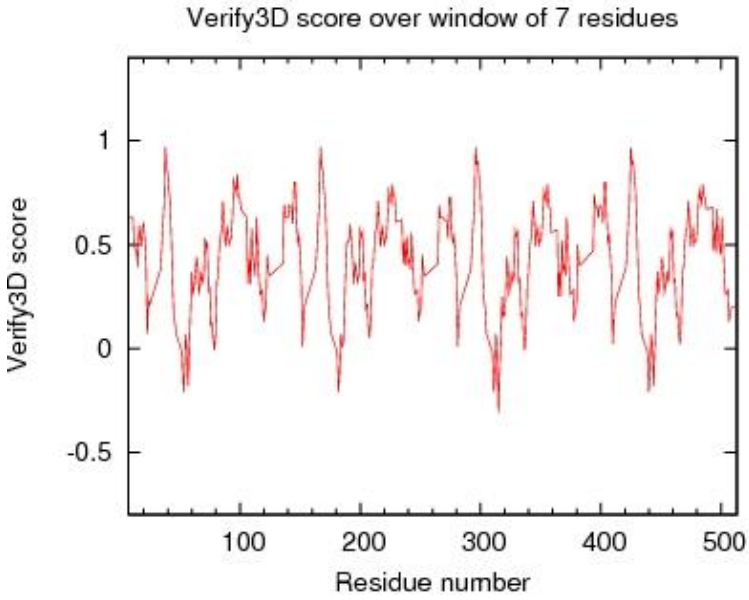
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

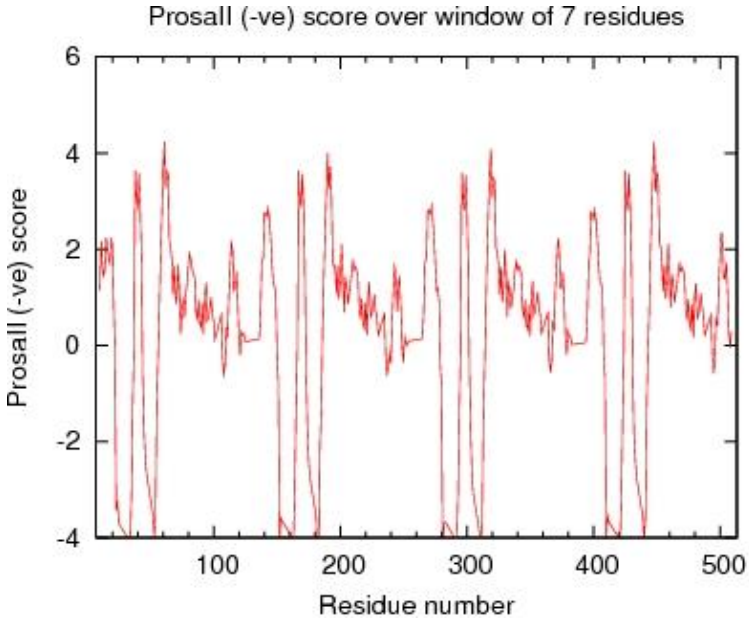
Number of close contacts (within 2.2 Å): 0
RMS deviation for bond angles: 2.4 °
RMS deviation for bond lengths: 0.016 Å

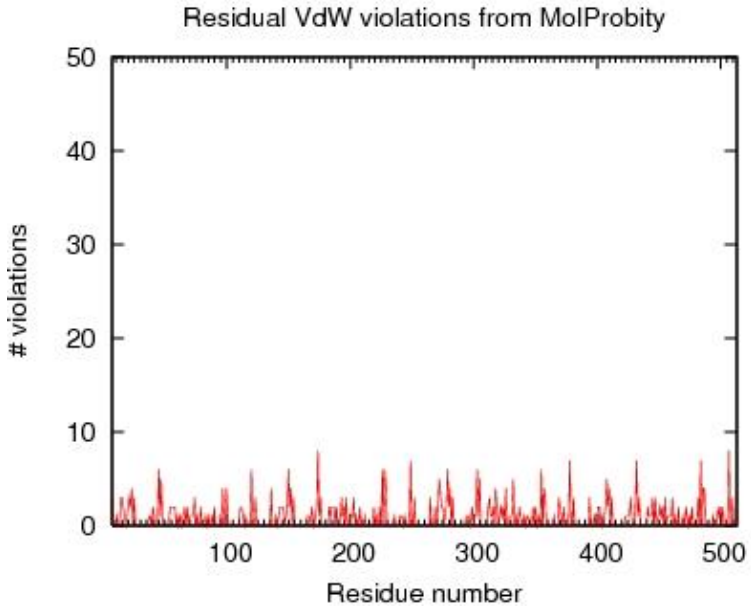
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

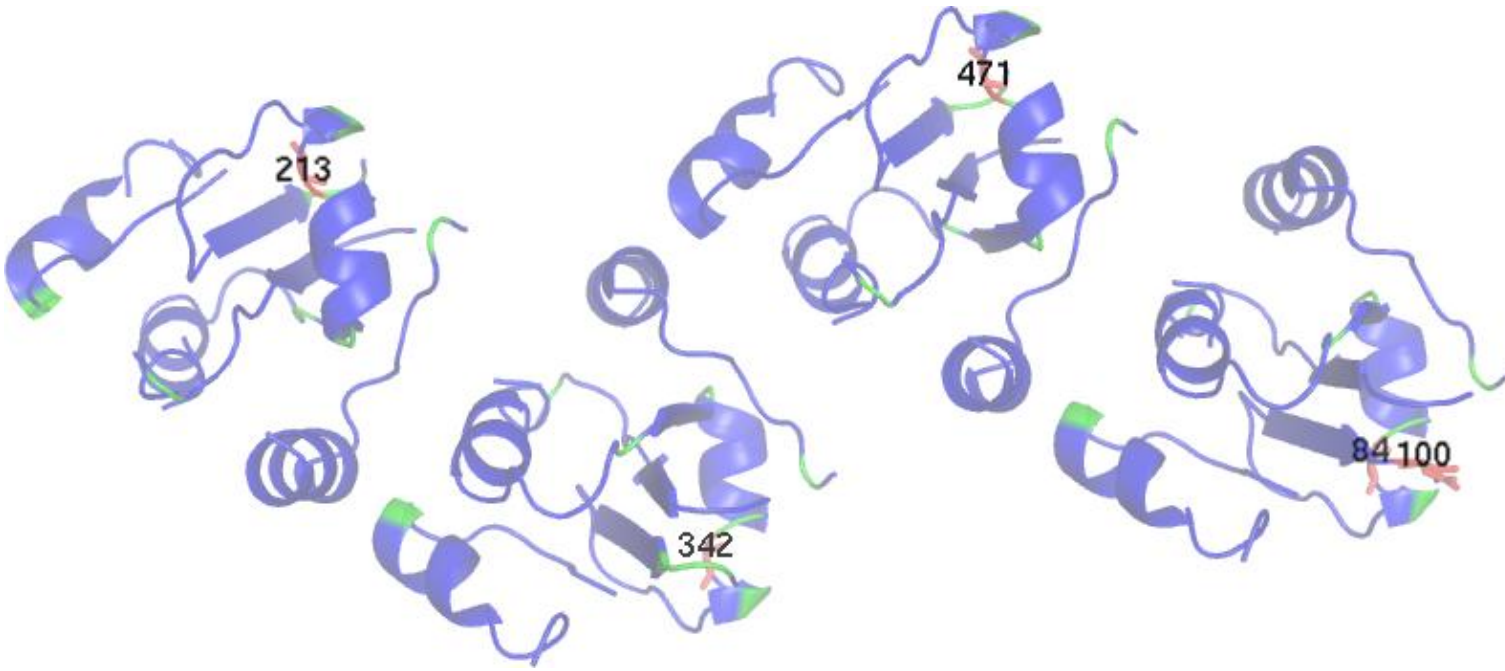





Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
100
200
300
400
500
Residue number


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





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

References:

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3. Sippl M J, "Recognition of Errors in Three-Dimensional Structures of Proteins", Proteins 17 (1993):

355-362
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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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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11. Luthy R, McLachlan A D and Eisenberg D, "Secondary Structure-Based Profiles: Use of Structure-Conserving Scoring Tables in Searching Protein Sequence Databases for Structural Similarities", Proteins 10 (1991): 229-239
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13. Koradi, R, et al, "MOLMOL: a program for display and analysis of macromolecular structures ", J Mol Graphics 14 (1996): 51-55.
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-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
```