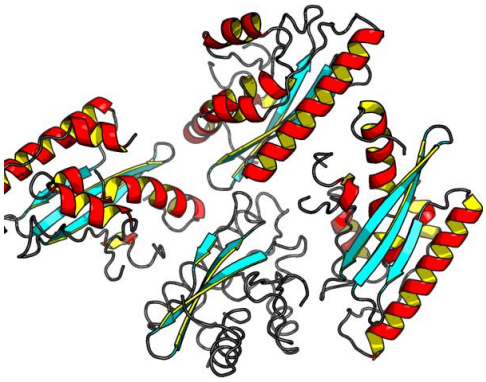
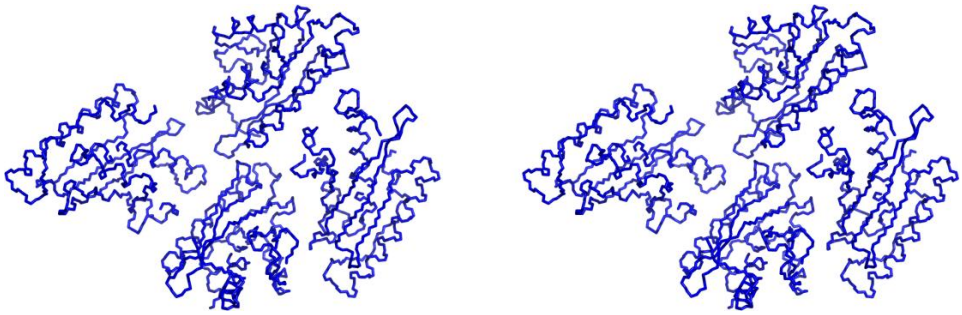
Structure Quality Analysis for NAME

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.):	632
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	tetramer
Molecular weight:	73582





Secondary Structure Elements:
Inter-chain break(s) between 162 & 173, 330 & 341, 498 & 509
alpha helices: 6A-12A, 25A-48A, 121A-126A, 134A-140A, 142A-155A, 6B-12B, 25B-48B, 121B-126B, 134B-140B, 142B-155B, 6C-12C, 25C-48C, 121C-126C, 134C-140C, 142C-155C, 6D-12D, 25D-48D, 121D-126D, 134D-140D, 142D-155D
beta strands: 54E-58E, 64G-73G, 76U-85U, 54E-58E, 64G-73G, 76U-85U, 54E-58E, 64G-73G, 76U-85U, 54E-58E, 64G-73G, 76U-85U

Resolution: 2.540 Å R-factor: 0.233 R-free: 0.279
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
86.7%	11.7%	0.8%	0.8%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
92.1%	7.2%	0.6%		

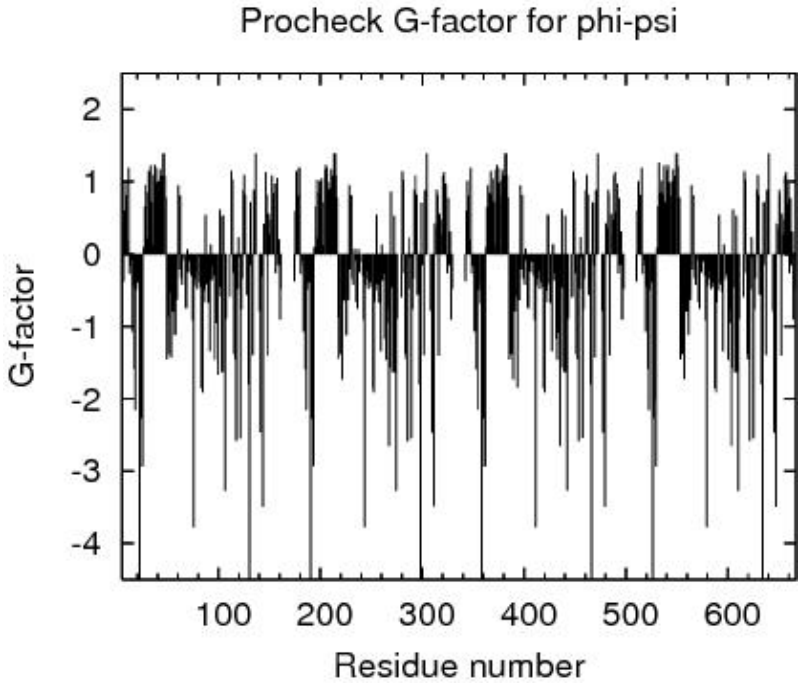
Global quality scores

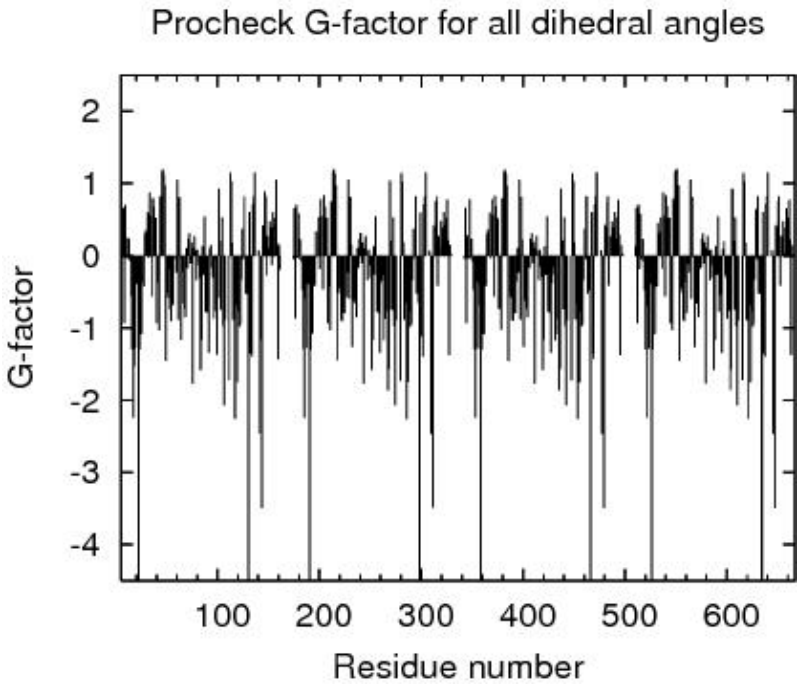
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*
-Raw score	0.39	0.48	-0.32	-0.30	33.35
Z-score[1]	-1.12	-0.70	-0.94	-1.77	-4.20

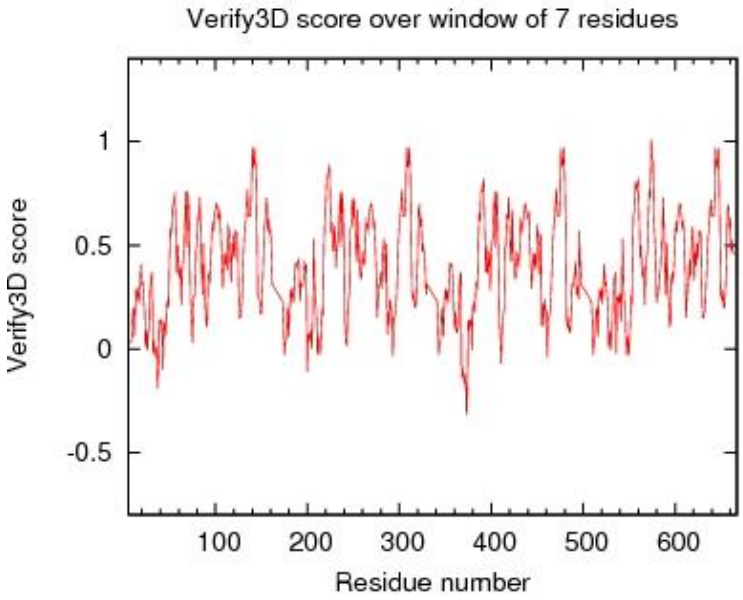
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

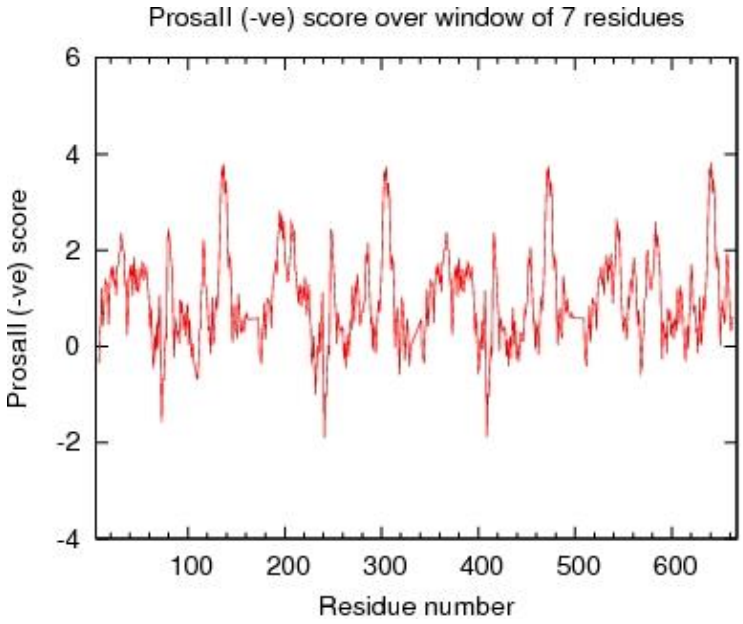
Number of close contacts (within 2.2 Å):	0
RMS deviation for bond angles:	1.2 °
RMS deviation for bond lengths:	0.008 Å

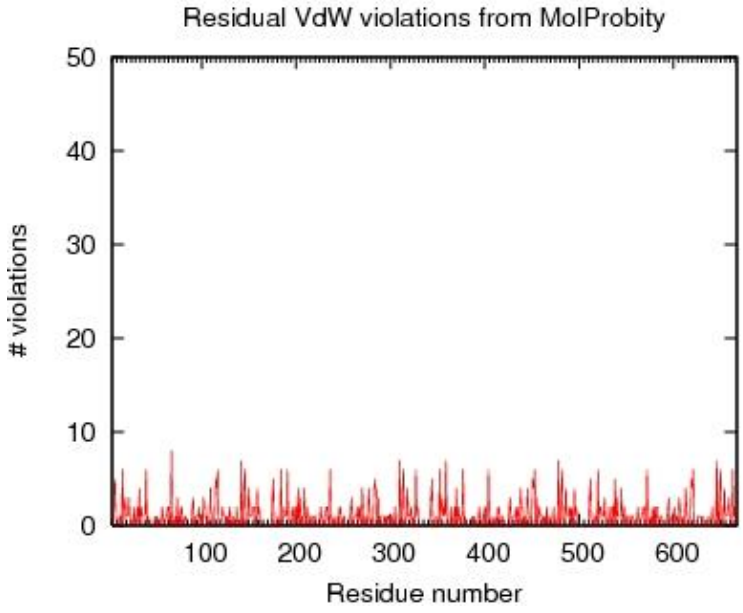
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

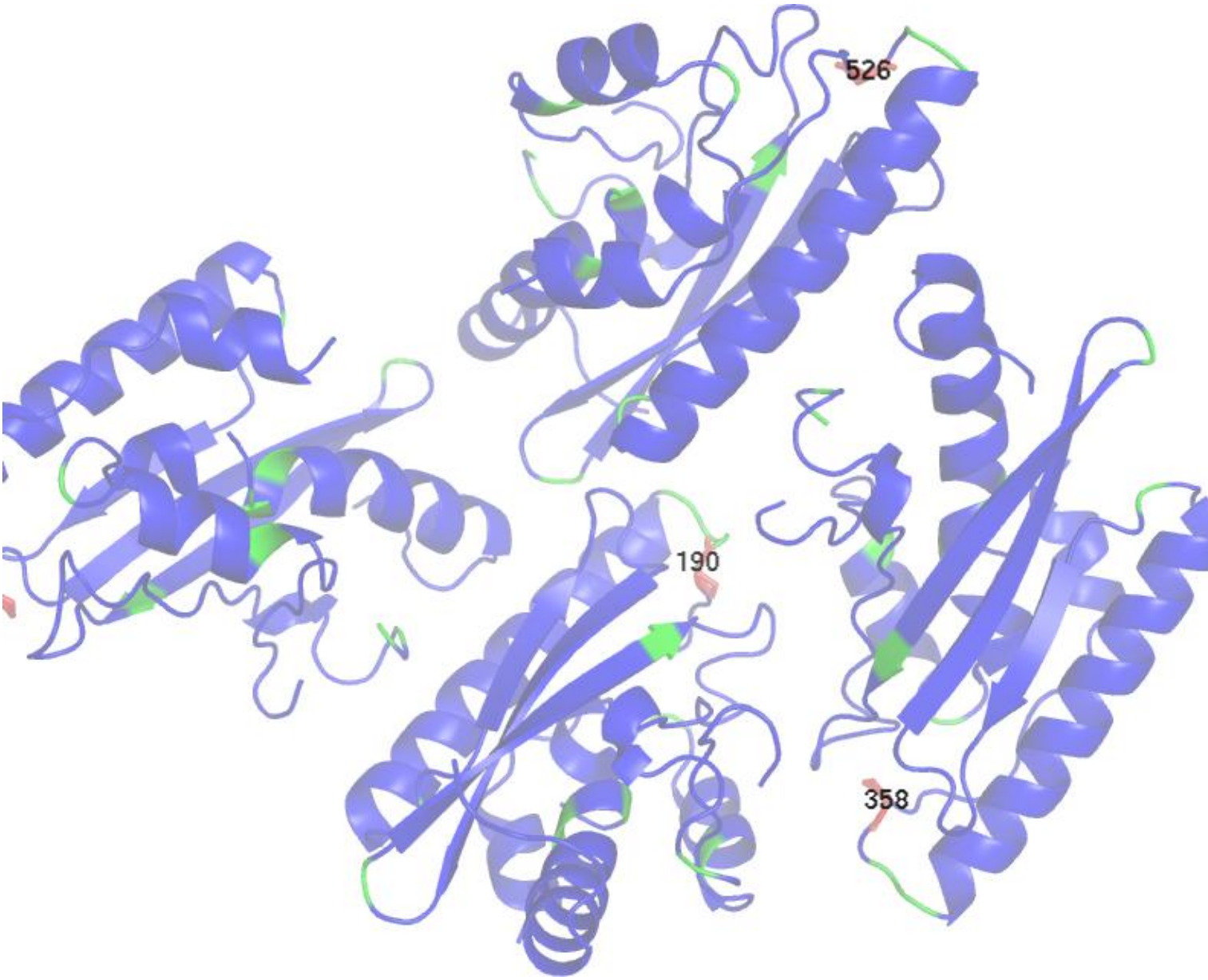



Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
100
200
300
400
500
600
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
100
200
300
400
500
600
Residue number


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
100
200
300
400
500
600
Residue number


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
100
200
300
400
500
600
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
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
9. Word J M et al, "Visualizing and Quantifying Molecular Goodness-of-Fit: Small-probe Contact Dots with Explicit Hydrogens", J Mol Biol 285 (1999): 1711-1733
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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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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

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
```