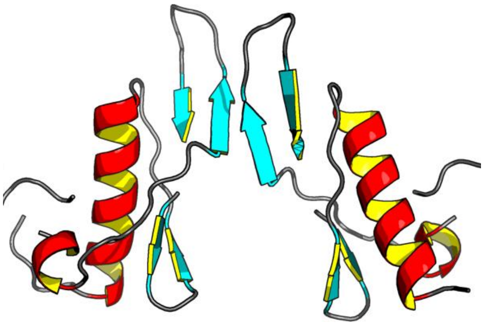
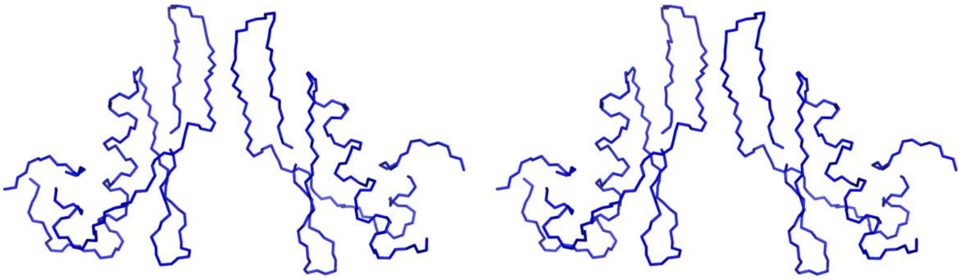
Structure Quality Analysis for NAME

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.):	136
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	dimer
Molecular weight:	14971





Secondary Structure Elements:
Inter-chain break(s) between 594 & 605
alpha helices: 528A-535A, 573A-588A, 528B-533B, 573B-588B
beta strands: 541R-547R, 554G-561G, 564N-570N, 541R-547R, 554G-561G, 564N-570N

Resolution: 2.300 Å R-factor: 0.213 R-free: 0.250
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
86.5%	11.5%	1.9%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
95.5%	3%	1.5%		

Global quality scores

Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*
-Raw score	0.29	0.93	-0.25	-0.04	14.16
Z-score[1]	-2.73	1.16	-0.67	-0.24	-0.90

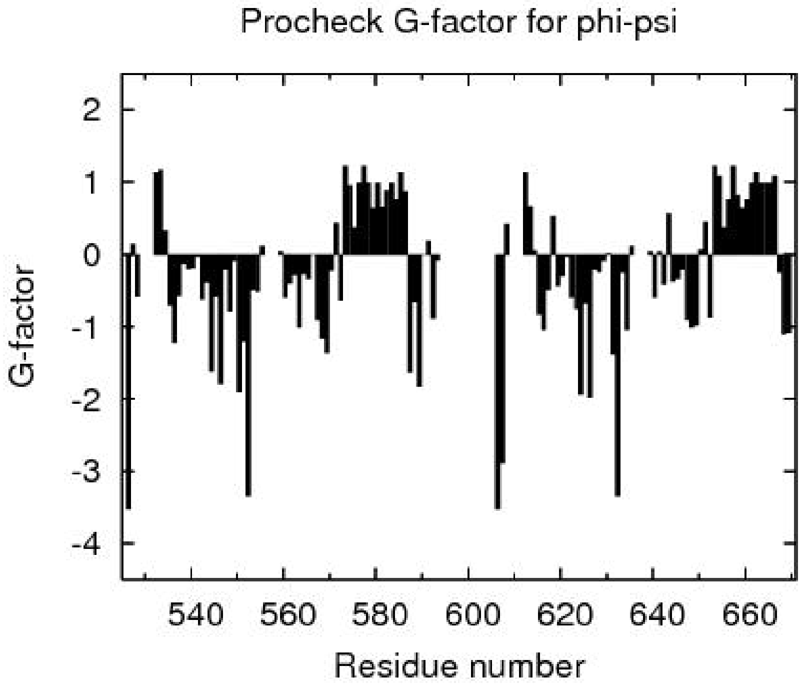
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

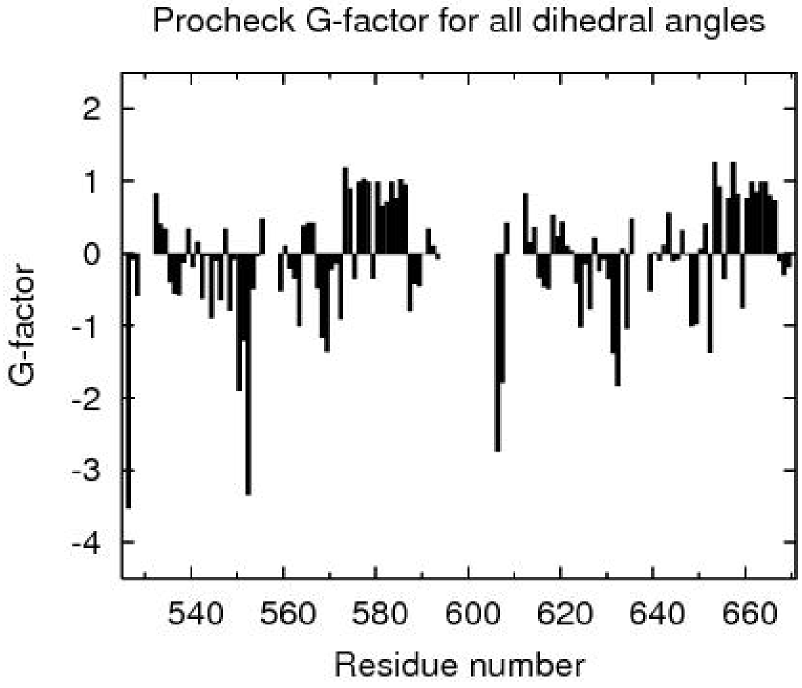
Number of close contacts (within 2.2 Å): 0

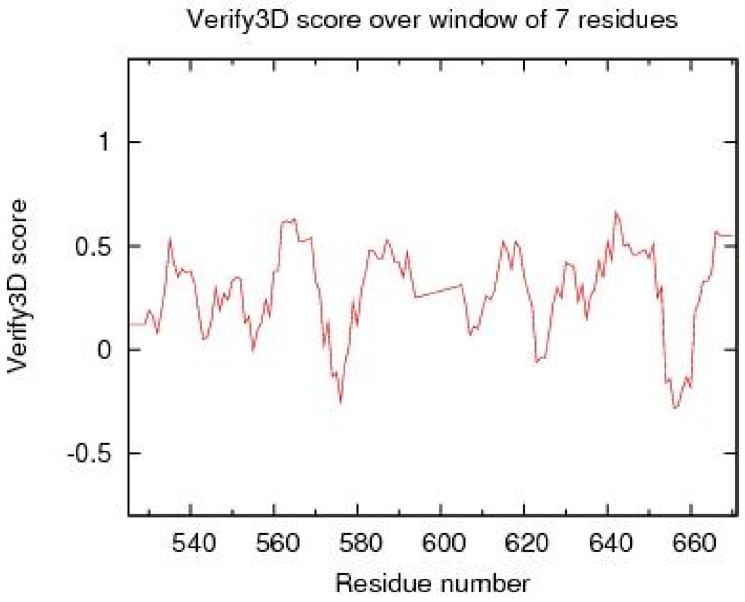
RMS deviation for bond angles: 1.1 °

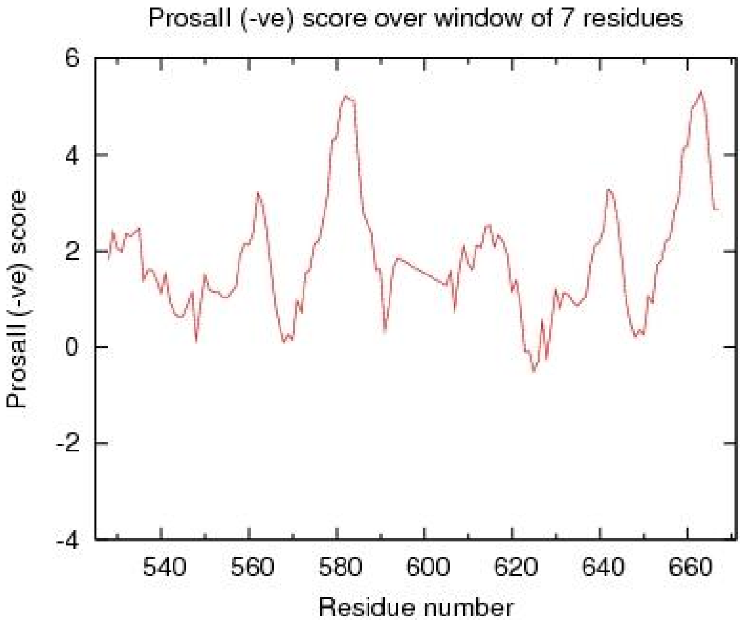
RMS deviation for bond lengths: 0.005 Å

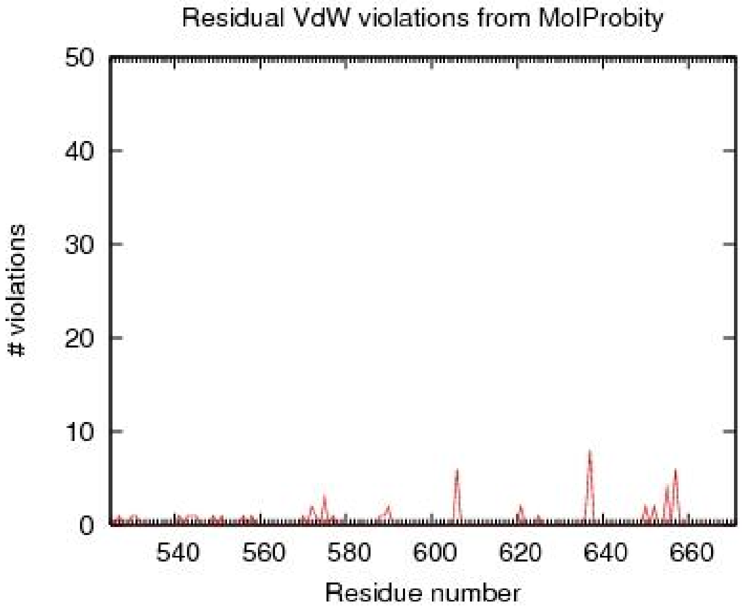
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

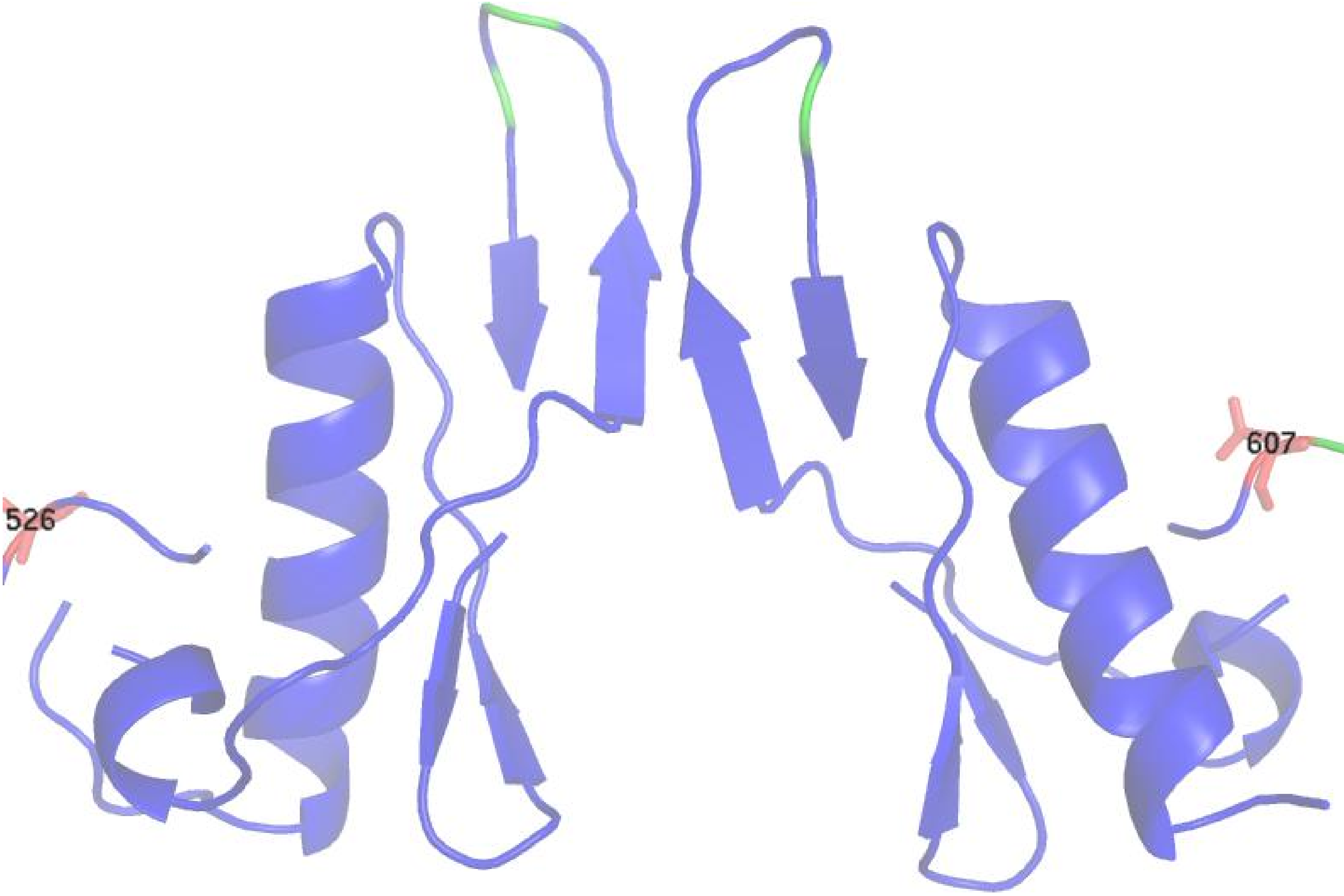





Verify3D score over window of 7 residues


ProsaII (-ve) score over window of 7 residues


Residual VdW violations from MolProbity
violations
0
10
20
30
40
50
540
560
580
600
620
640
660
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
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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
12. Richardson D C, Richardson J S, "The kinemage: a tool for scientific communication", Prot Sci 1(1) (1992): 3-9
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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16. Kabsch W, Sander C, "Dictionary of protein secondary structure: pattern recognition of hydrogen-bonded and geometrical features", Biopolymers (1983) 22: 2577-2637
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
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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