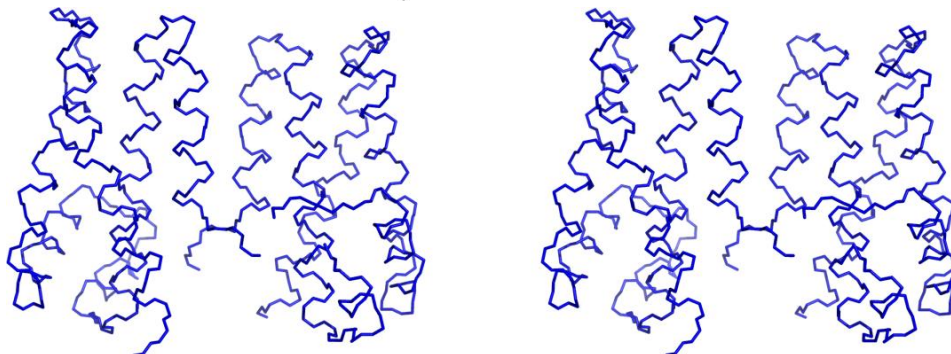
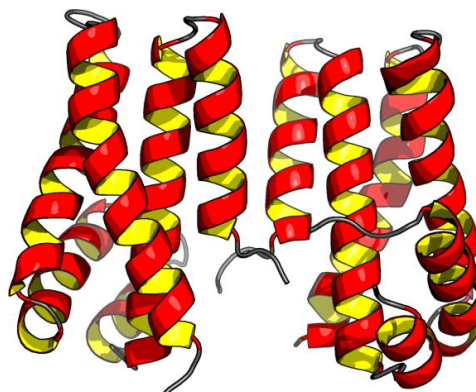




# Structure Quality Analysis for NAME

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.): 242  
Organism:  
SwissProt /  
TrEMBL ID:  
Oligomerization: dimer  
Molecular  
weight: 27996



## Secondary Structure Elements:

*Inter-chain break(s) between 123 & 134*

alpha helices: 6A-19A, 23A-45A, 48A-52A, 62A-71A, 79A-91A, 101A-122A, 6B-19B, 23B-44B, 48B-54B, 62B-71B, 79B-94B, 101B-121B

beta strands:

Resolution: 2.400 Å R-factor: 0.225 R-free: 0.265

Structure Factors deposited in the PDB? no

## Ramachandran Plot Summary from Procheck

<i>Most favoured regions</i>	<i>Additionally allowed regions</i>	<i>Generously allowed regions</i>	<i>Disallowed regions</i>
91.7%	8.3%	0.0%	0.0%

## Ramachandran Plot Summary from Richardson Lab's Molprobit

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	<a href="#">View plot</a>	<a href="#">View model summary</a>
94.9%	5.1%	0%		

## Global quality scores



## Structure Quality Analysis for NAME

Program	<i>Verify3D</i>	<i>ProsaII</i> (-ve)	<i>Procheck</i> (phi-psi)	<i>Procheck</i> (all)	<i>MolProbity</i>	<i>Clashscore</i>
-Raw score	0.26	0.83	0.32	0.16	16.90	
Z-score <sup>1</sup>	-3.21	0.74	1.57	0.95	-1.37	

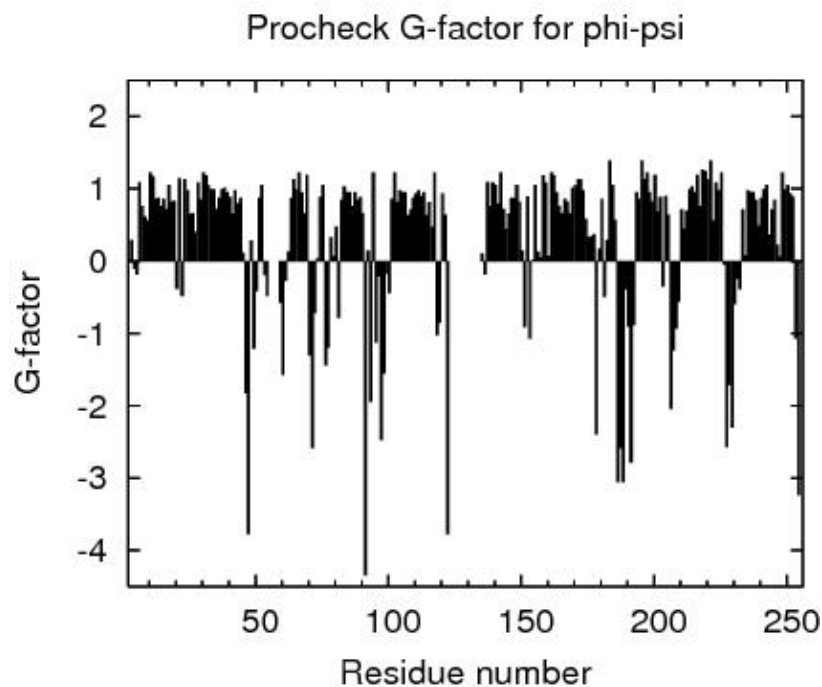
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.1 °

RMS deviation for bond lengths: 0.008 Å

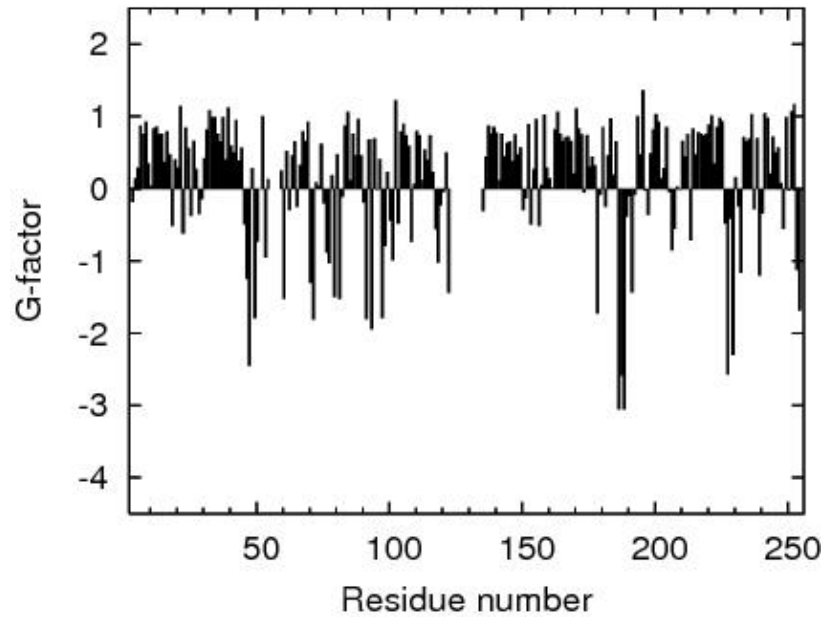
<sup>1</sup> With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution ≤ 1.80 Å, R-factor ≤ 0.25 and R-free ≤ 0.28; a positive value indicates a 'better' score



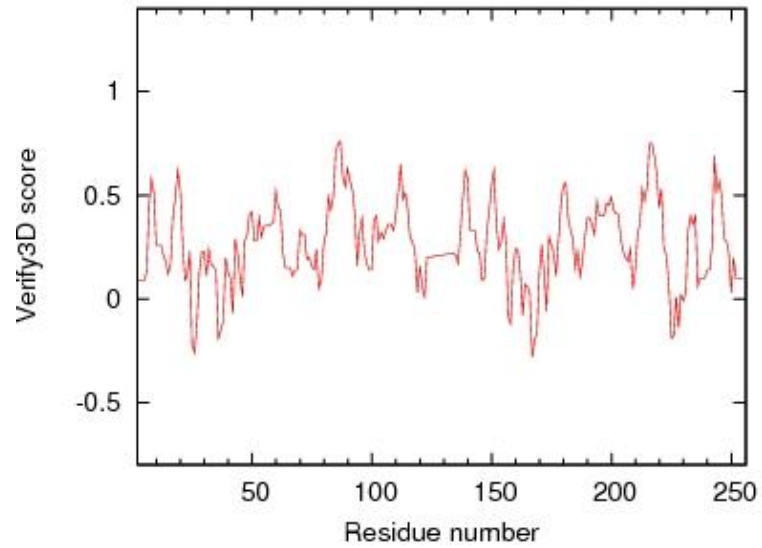


# Structure Quality Analysis for NAME

## Procheck G-factor for all dihedral angles

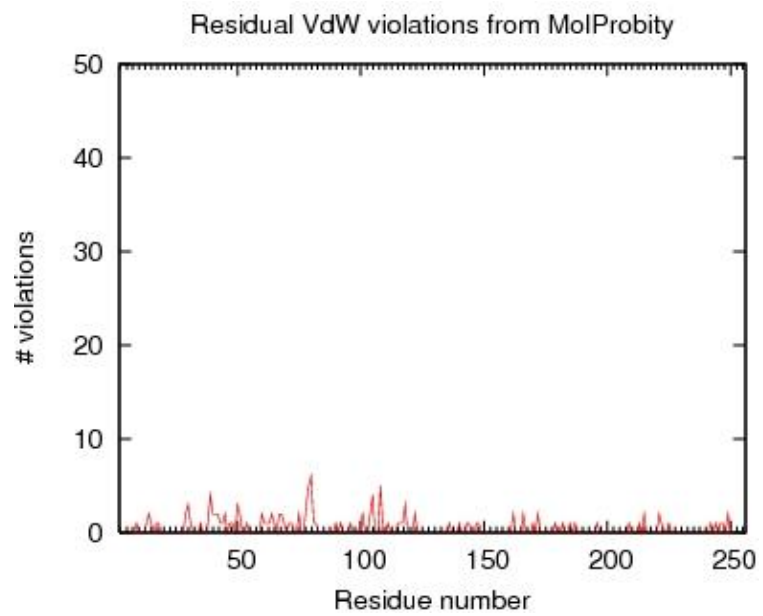
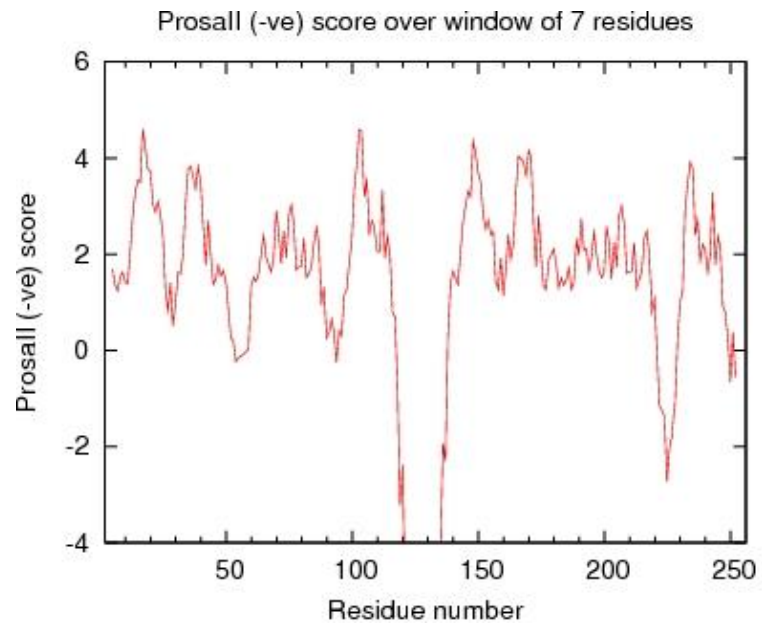


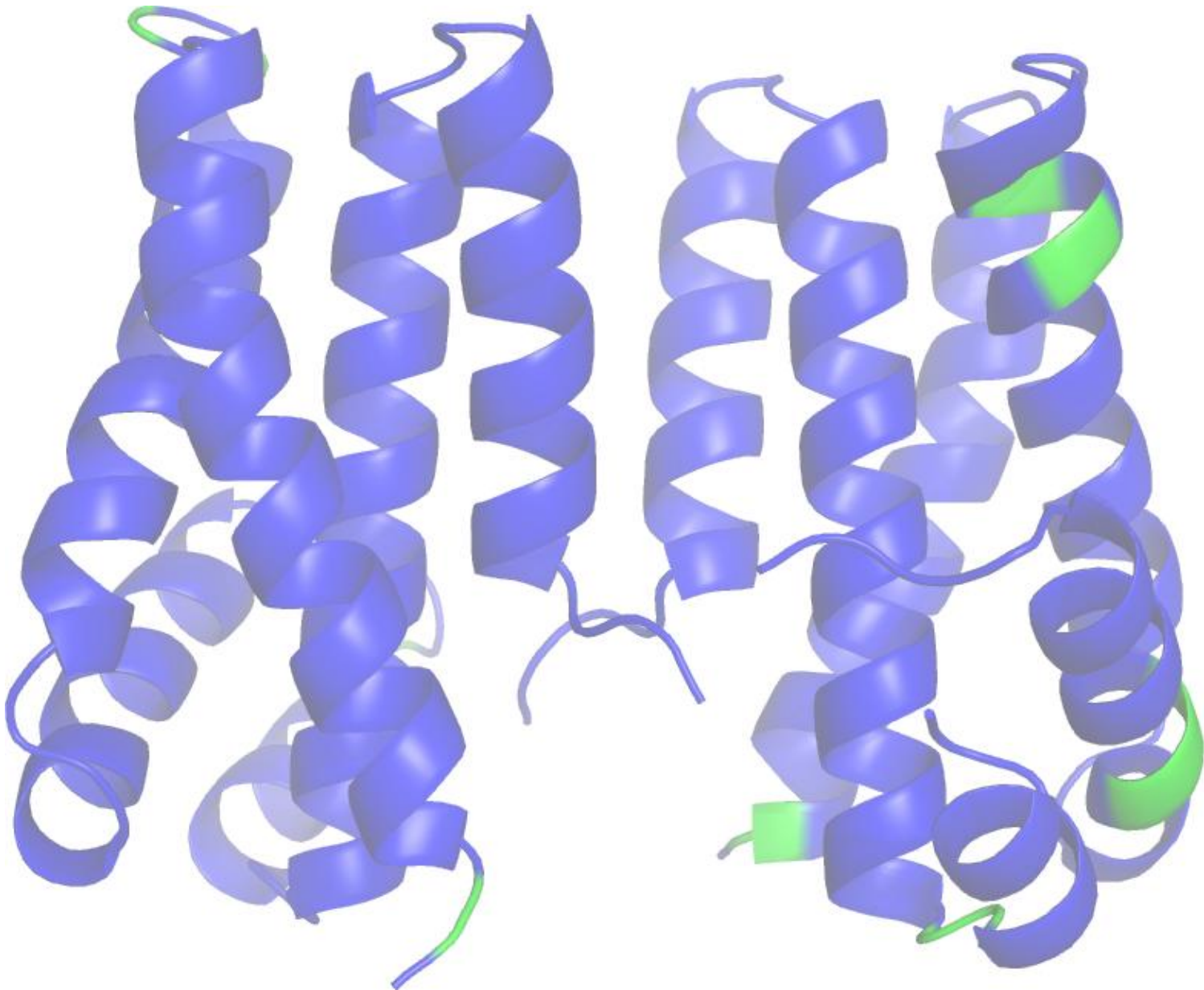
## Verify3D score over window of 7 residues





## Structure Quality Analysis for NAME





**Residue Plot of Ramachandran analysis(based on data from Richardson Lab's Molprobit)**

***References:***

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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