



# 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.): 538

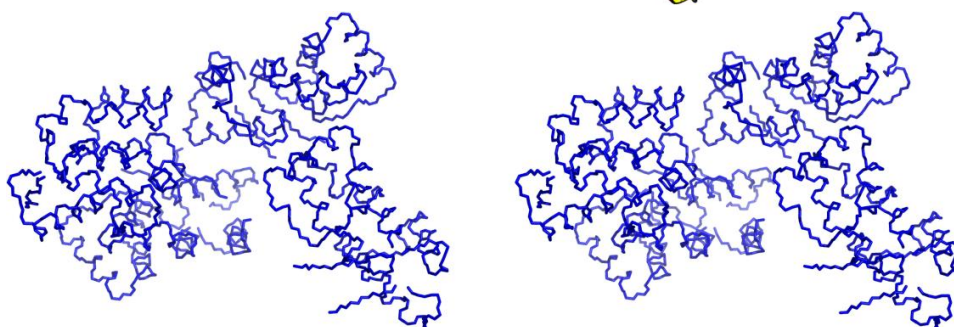
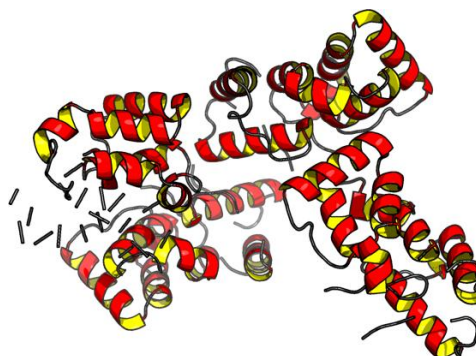
Organism:

SwissProt /

TrEMBL ID:

Oligomerization: tetramer

Molecular weight: 61731



## Secondary Structure Elements:

*Inter-chain break(s) between 399 & 410, 545 & 556, 690 & 701*

alpha helices: 275A-290A, 300A-311A, 316A-325A, 327A-333A, 339A-351A, 358A-382A, 384A-389A, 275B-290B, 300B-310B, 316B-325B, 327B-333B, 339B-351B, 358B-381B, 384B-389B, 275C-290C, 300C-311C, 316C-325C, 327C-333C, 339C-351C, 358C-381C, 384C-389C, 275D-290D, 300D-311D, 316D-323D, 327D-333D, 339D-351D, 358D-381D, 384D-389D

beta strands:

Resolution: 2.230 Å R-factor: 0.162 R-free: 0.228

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>
94.5%	5.5%	0.0%	0.0%

## Ramachandran Plot Summary from Richardson Lab's Molprobrity

<i>Most favoured regions</i>	<i>Allowed regions</i>	<i>Disallowed regions</i>	<a href="#">View plot</a>	<a href="#">View model summary</a>
98.3%	1.5%	0.2%		

## 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	0.44	0.96	0.21	0.13	17.86	
Z-score <sup>1</sup>	-0.32	1.28	1.14	0.77	-1.54	

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

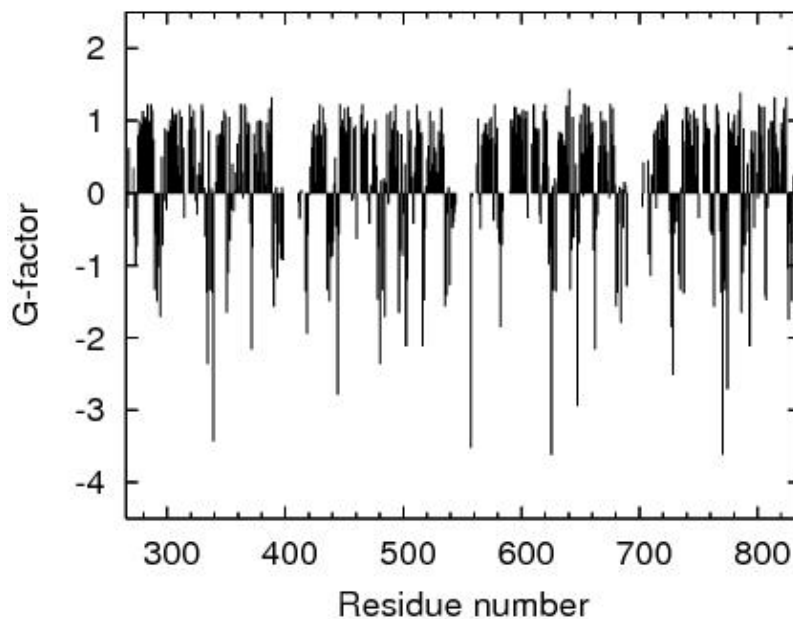
Number of close contacts (within 2.2 Å): 0

RMS deviation for bond angles: 1.0 °

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

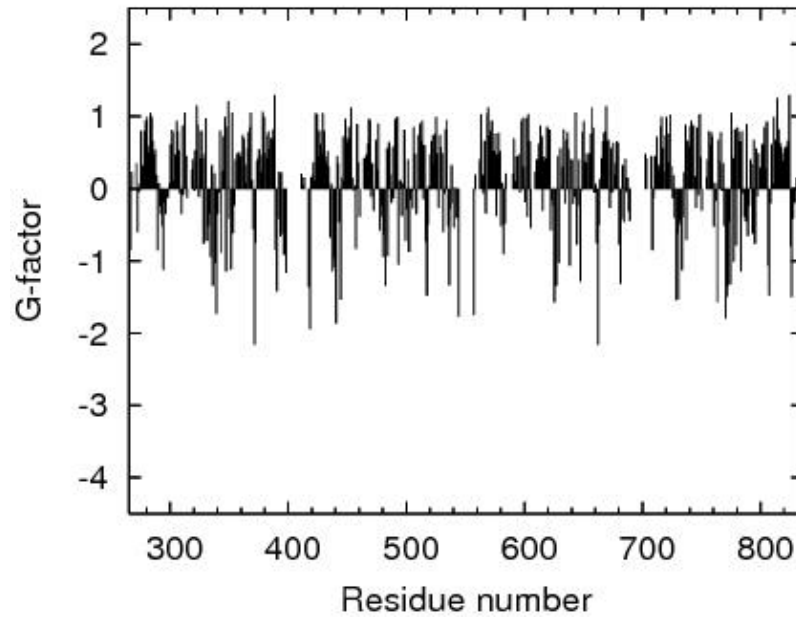
Procheck G-factor for phi-psi



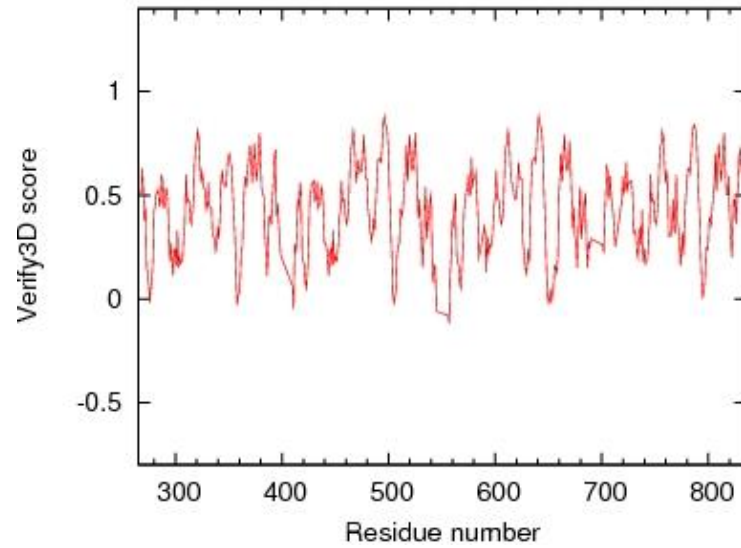


## Structure Quality Analysis for NAME

Procheck G-factor for all dihedral angles

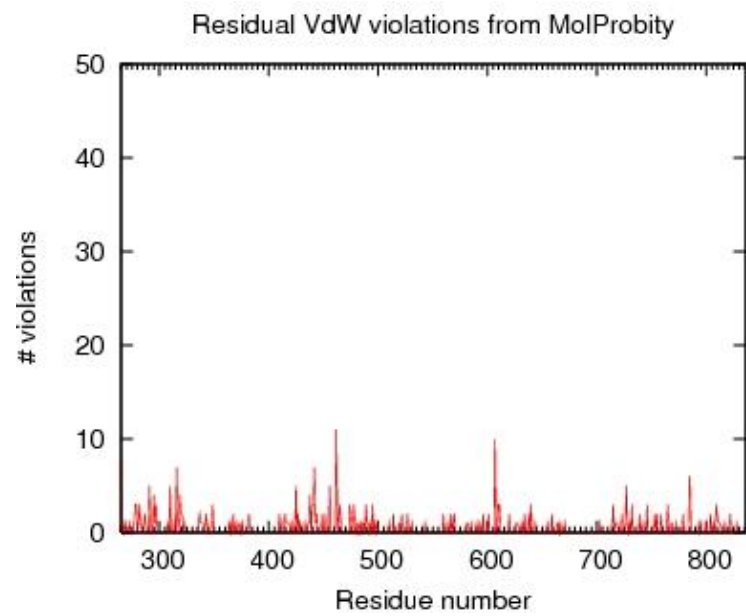
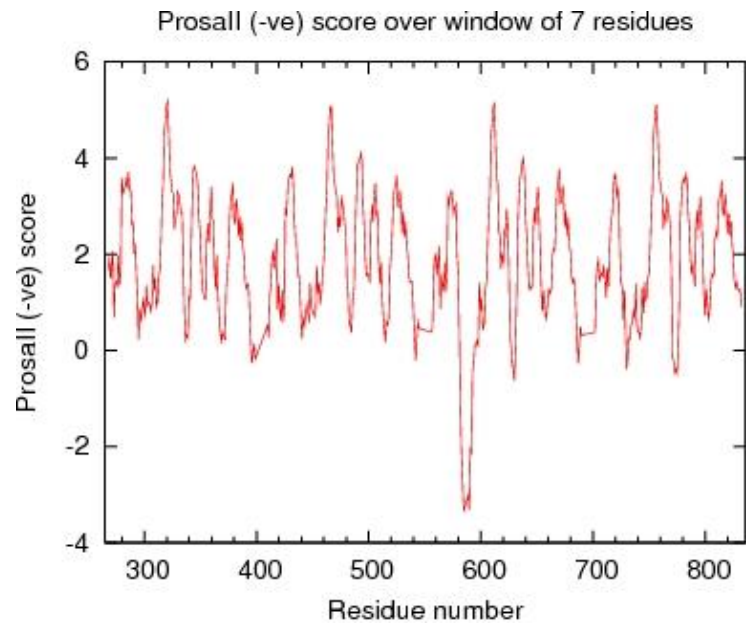


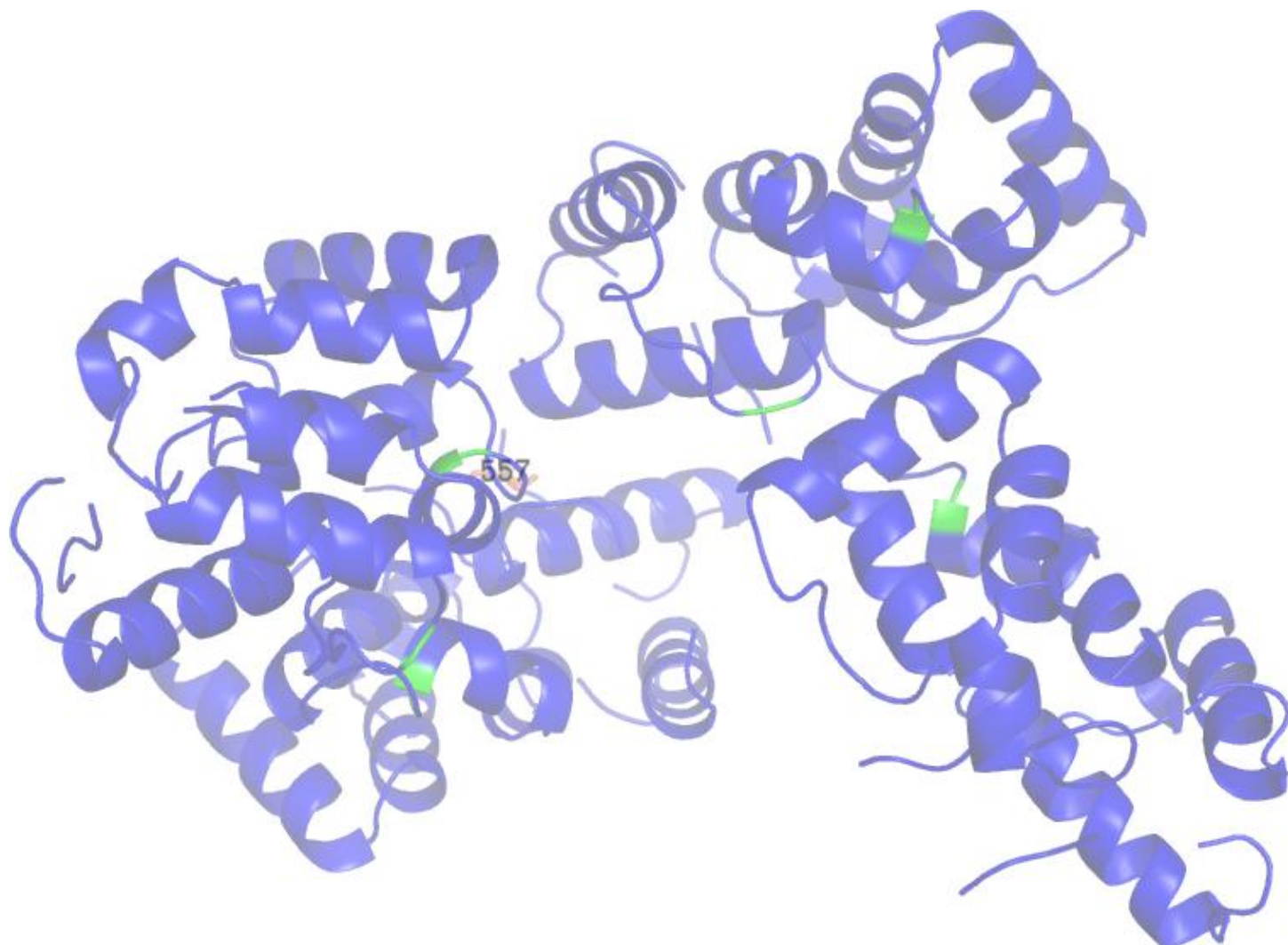
Verify3D score over window of 7 residues





## Structure Quality Analysis for NAME





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

**References:**

1. Luthy R, Bowie J U and Eisenberg D, "Assessment of protein models with three-dimensional profiles", Nature 356 (1992): 83-85
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 A et al, "AQUA and PROCHECK\_NMR: Programs for checking the quality of proteins structures solved by NMR", J Biomolec NMR 8 (1996): 477-486
6. Laskowski R A et al "PROCHECK: a program to check the stereochemical quality of protein structures" J Appl Cryst, 26 (1993): 283-291
7. Word J M et al, "Exploring steric constraints on protein mutations using MAGE / PROBE", Prot Sci 9



(2000): 2251-2259

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

10. Tejero R and Montelione G T, "PDBStat", unpublished

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

15. Lovell S C et al, "Structure validation by Calpha geometry: phi,psi and Cbeta deviation" Proteins (2003) 50: 437-450

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



## 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