Supplementary File S2

Wild-type S protein

saves

Plot statistics

Residues in most favoured regions [A,B,L]	150	89.3%
Residues in additional allowed regions [a,b,l,p]	18	10.7%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	0	0.0%
	----	------
Number of non-glycine and non-proline residues	168	100.0%
Number of end-residues (excl. Gly and Pro)	1	
Number of glycine residues (shown as triangles)	15	
Number of proline residues	10	

Total number of residues	194	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms
and R-factor no greater than 20%, a good quality model would be expected
to have over 90% in the most favoured regions.

saves_01.ps

N439K S protein

saves



Plot statistics

|		
Residues in most favoured regions [A,B,L]	152	90.5%
Residues in additional allowed regions [a,b,l,p]	16	9.5%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	0	0.0%
	----	------
Number of non-glycine and non-proline residues	168	100.0%
Number of end-residues (excl. Gly and Pro)	1	
Number of glycine residues (shown as triangles)	15	
Number of proline residues	10	

Total number of residues	194	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms
and R-factor no greater than 20%, a good quality model would be expected
to have over 90% in the most favoured regions.

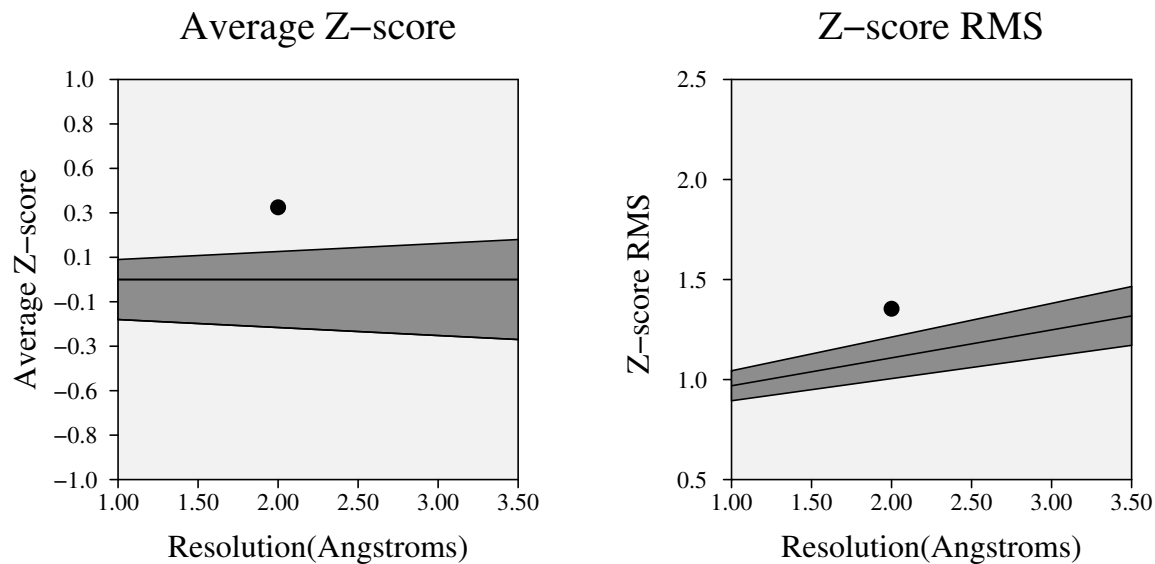**A** ANOLEA results of wild-type Spike protein
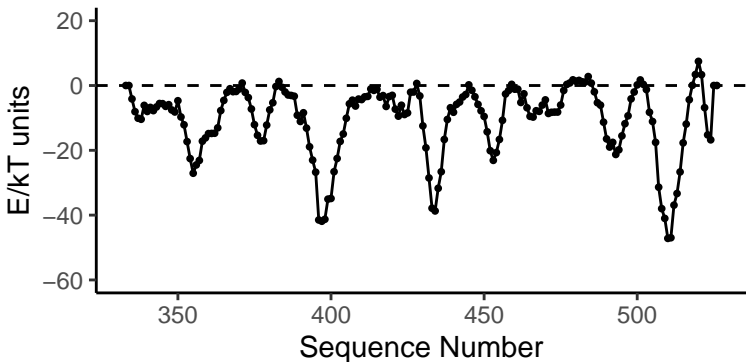
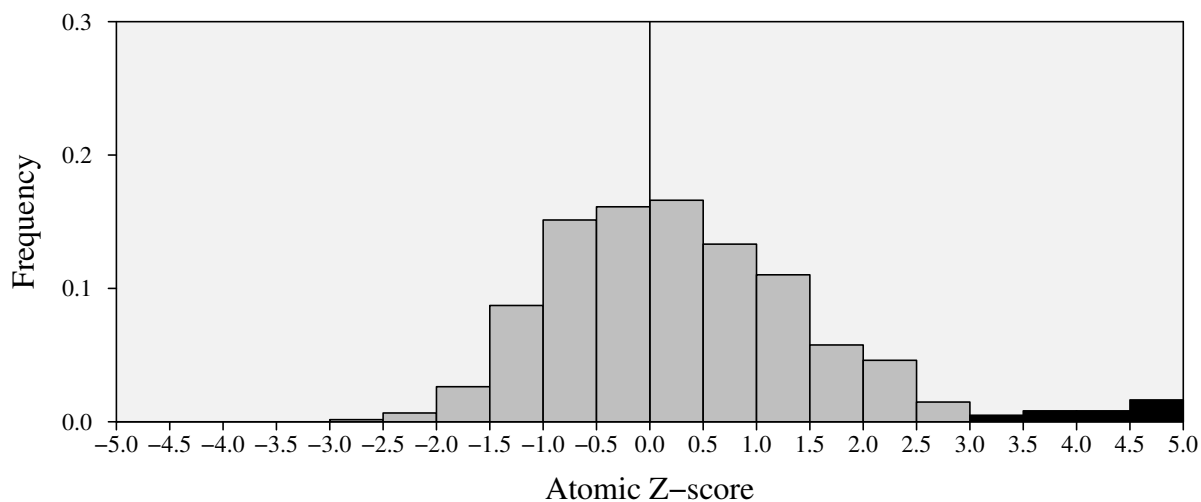**B** ANOLEA results of N439K Spike protein
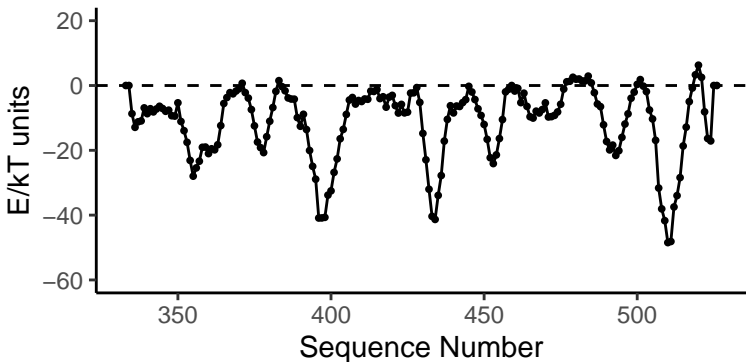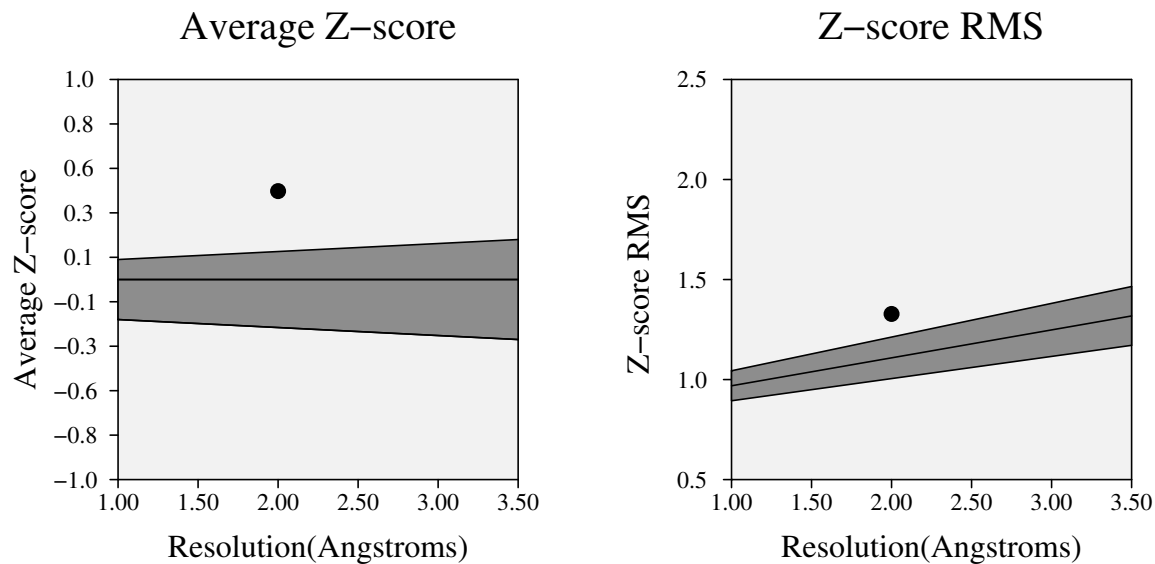
Wild-type S protein

Analysis of entire structure

Average Z−score

Z−score RMS

Distribution of atomic Z−scores

Z−score mean	0.361
Z−score stddev	1.306
Z−score RMS	1.354
# scored atoms	680
# outliers	25
% outliers	3.700

Pontius et al. (1996) J. Mol. Biol. 264, 121–136

N439K S protein

Analysis of entire structure

Average Z−score

Z−score RMS

Distribution of atomic Z−scores
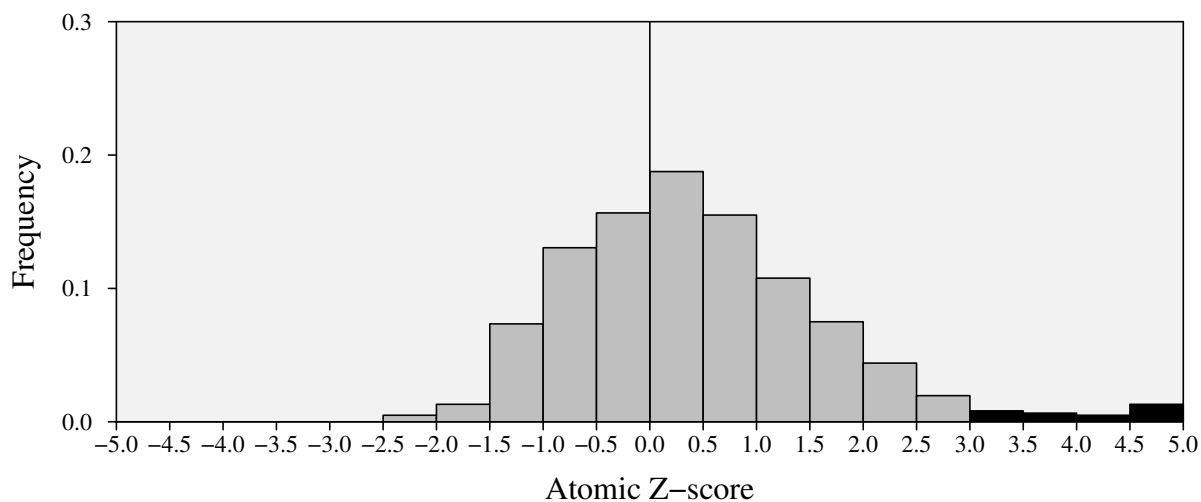
Z−score mean	0.442
Z−score stddev	1.254
Z−score RMS	1.328
# scored atoms	686
# outliers	23
% outliers	3.400

A   Verify 3D plot of wild-type S protein
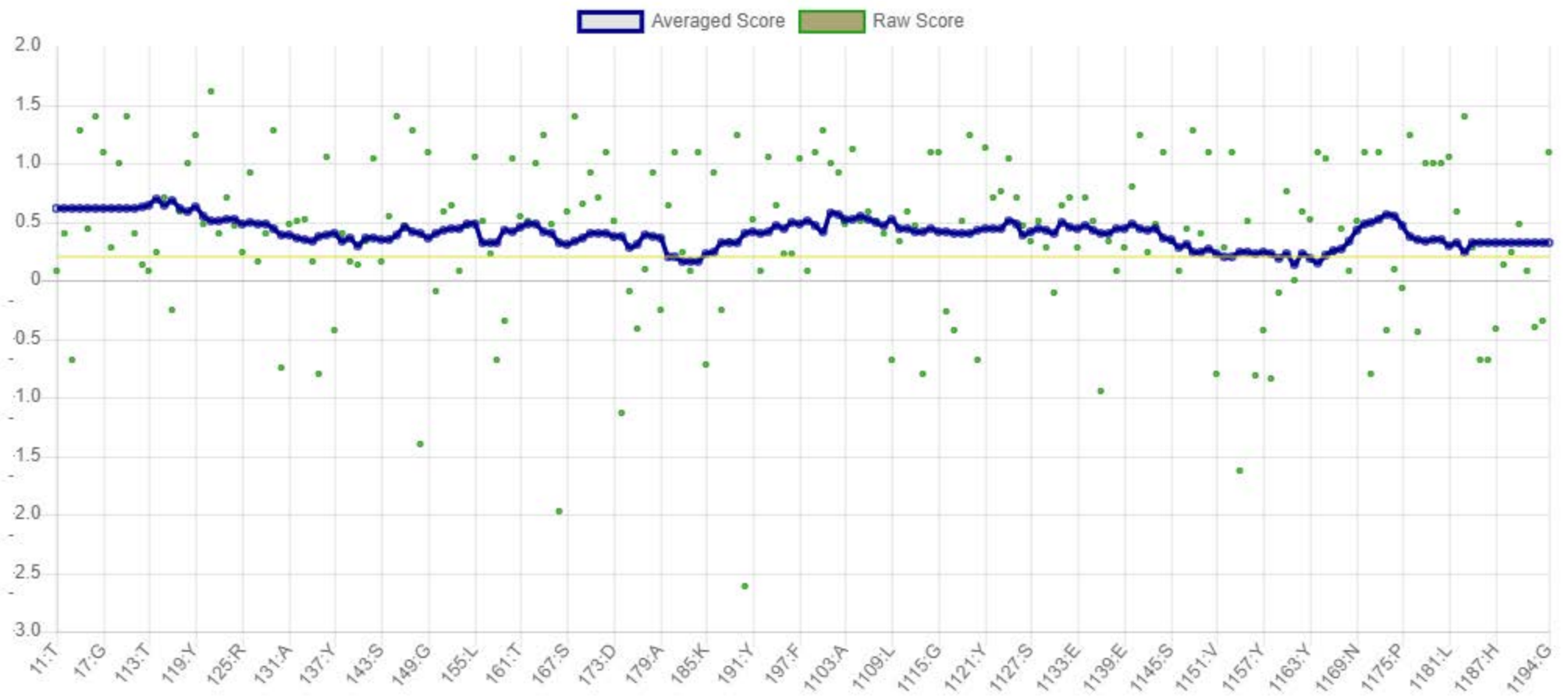
B Verify 3D plot of N439K S protein
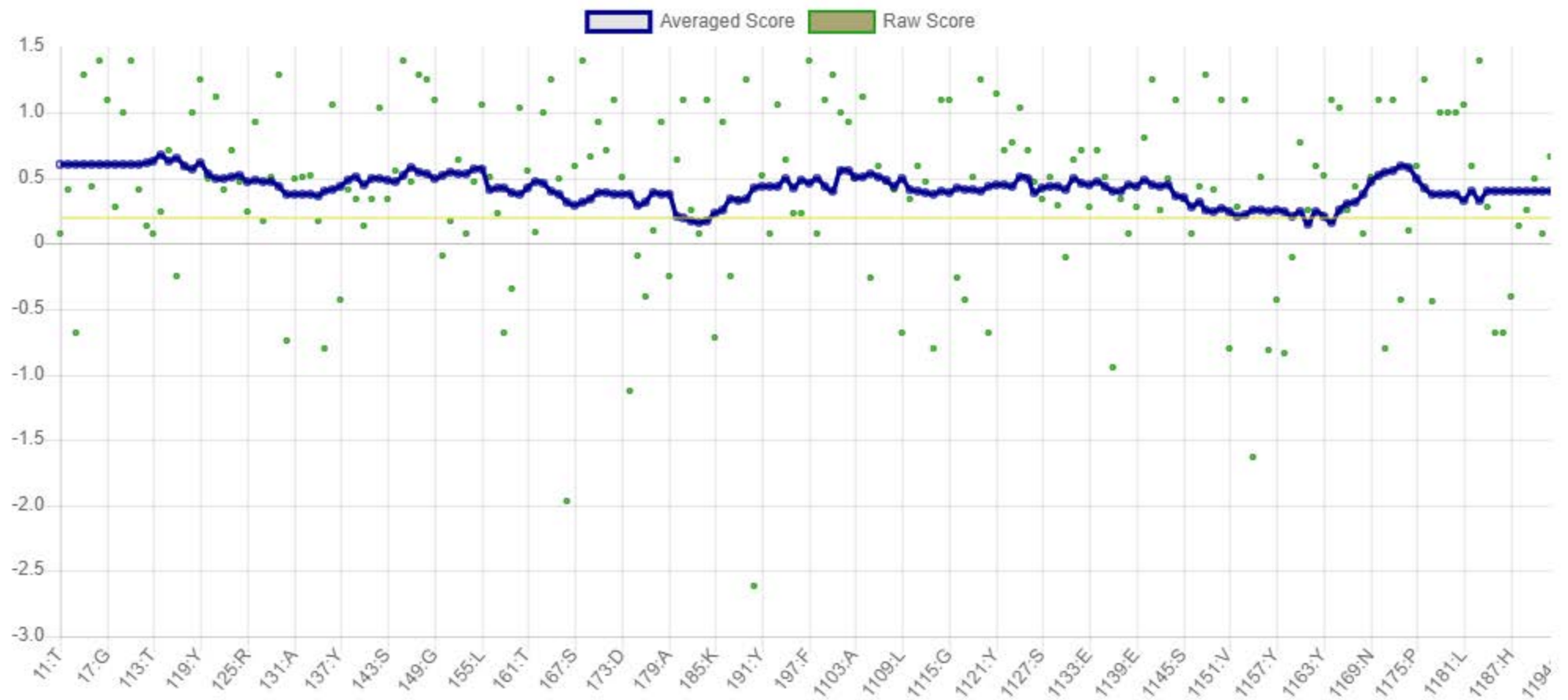
The PROCHECK of wild-type S protein

Summary	
Ramachandran plot	**Warning**
All Ramachandrans	**Warning**
Chi1-chi2 plots	**Pass**
Main-chain params	
Side-chain params	**Warning**
Residue properties	**Pass**
Bond len/angle	**Pass**
M/c bond lengths	
M/c bond angles	
Planar groups	**Pass**
Program output	

```
+----------<<<  P R O C H E C K    S U M M A R Y  >>>----------+
|                                                              |
| /var/www/SAVES/Jobs/638906/saves.pdb   1.5        194 residues |
|                                                              |
+| Ramachandran plot:   89.3% core   10.7% allow   0.0% gener   0.0% disall |
|                                                              |
+| All Ramachandrans:    2 labelled residues (out of 192)       |
+| Chi1-chi2 plots:      2 labelled residues (out of 115)       |
|  Side-chain params:    5 better     0 inside      0 worse     |
|                                                              |
+| Residue properties: Max.deviation:     4.4        Bad contacts:    0 |
|                      Bond len/angle:    2.2    Morris et al class:  1  2  2 |
|                                                              |
|  G-factors          Dihedrals:  -0.27 Covalent:   0.52   Overall:   0.05 |
|                                                              |
|  Planar groups:   100.0% within limits   0.0% highlighted    |
|                                                              |
+--------------------------------------------------------------+
   + May be worth investigating further.  * Worth investigating further.
```

Summary file

The PROCHECK of N439K S protein

Summary	
Ramachandran plot	**Warning**
All Ramachandrans	**Warning**
Chi1-chi2 plots	**Pass**
Main-chain params	
Side-chain params	**Warning**
Residue properties	**Warning**
Bond len/angle	**Warning**
M/c bond lengths	
M/c bond angles	
Planar groups	**Warning**
Program output	

```
+----------<<< P R O C H E C K   S U M M A R Y >>>----------+
|                                                                     |
| /var/www/SAVES/Jobs/638912/saves.pdb   1.5           194 residues   |
|                                                                     |
| Ramachandran plot:   90.5% core    9.5% allow    0.0% gener    0.0% disall |
|                                                                     |
+| All Ramachandrans:    3 labelled residues (out of 192)            |
+| Chi1-chi2 plots:      2 labelled residues (out of 115)            |
| Side-chain params:    5 better     0 inside      0 worse          |
|                                                                     |
+| Residue properties: Max.deviation:    4.5           Bad contacts:    0 |
+|                     Bond len/angle:   4.3    Morris et al class:  1  2  2 |
|                                                                     |
| G-factors          Dihedrals:  -0.25  Covalent:  -0.04   Overall:  -0.16 |
|                                                                     |
+| Planar groups:    96.2% within limits   3.8% highlighted     1 off graph |
|                                                                     |
+---------------------------------------------------------------------+
  + May be worth investigating further.  * Worth investigating further.
```

Summary file

QMEAN of N439K_S_Protein

Model Results ❓

Order by: GMQE ▼

Oligo-State	**Ligands**
Monomer	None

GMQE 0.87

QMEAN -1.66 👍

Global Quality Estimate
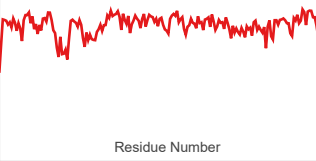
QMEAN		-1.66
Cβ		0.17
All Atom		-1.59
solvation		-1.92
torsion		-0.90
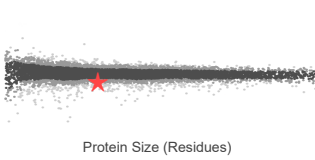
Local Quality Estimate

Residue Number

Comparison

Protein Size (Residues)

Template	**Seq Identity**	**Coverage**	**Description**
template_upload.1.A	99.48%		Polypeptide

Model 01 ▼

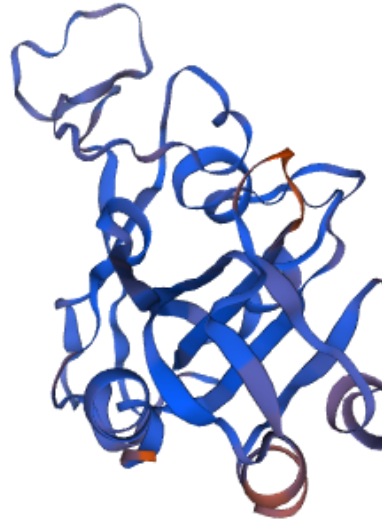Structure Assessment

Model-Template Alignment

```
       Model_01  TNLCPFGEVFNATRFASVYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKL   55
template_upload.1.A  TNLCPFGEVFNATRFASVYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKL   55

       Model_01  NDLCFTNVYADSFVIRGDEVRQIAPGQTGKIADYNYKLPDDFTGCVIAWNSKNLD  110
template_upload.1.A  NDLCFTNVYADSFVIRGDEVRQIAPGQTGKIADYNYKLPDDFTGCVIAWNSNNLD  110

       Model_01  SKVGGNYNYLYRLFRKSNLKPFERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGF  165
template_upload.1.A  SKVGGNYNYLYRLFRKSNLKPFERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGF  165

       Model_01  QPTNGVGYQPYRVVVLSFELLHAPATVCG  194
template_upload.1.A  QPTNGVGYQPYRVVVLSFELLHAPATVCG  194
```

⚙ Cartoon ▲ 📷▲ ▶ ⏏ ↻

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