



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:43 PM UTC

PDB ID : 6ACG / pdb_00006acg
EMDB ID : EMD-9591
Title : Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-bound conformation 1
Authors : Gui, M.; Song, W.
Deposited on : 2018-07-26
Resolution : 5.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

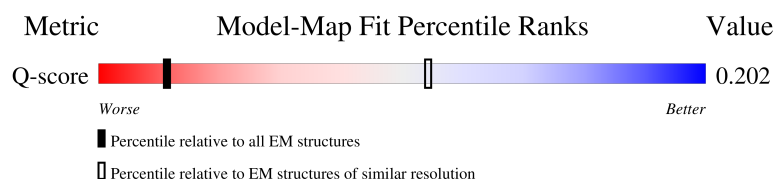
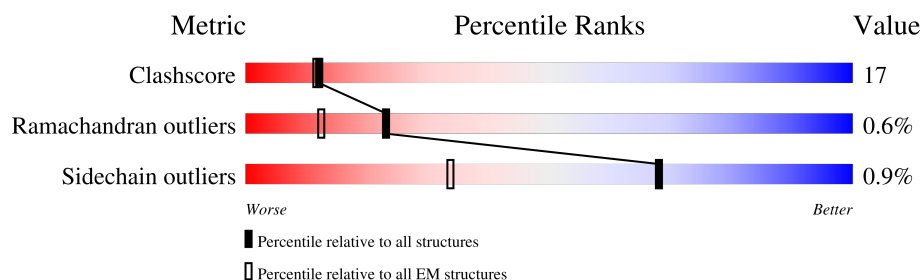
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	538 (4.90 - 5.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1203	43% 51% 37% 11%
1	B	1203	37% 51% 36% 11%
1	C	1203	45% 52% 34% 12%
2	D	603	99% 75% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29715 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	B	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	C	1057	Total	C	N	O	S	0	0
			8241	5264	1364	1568	45		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1197	SER	-	expression tag	UNP P59594
A	1198	HIS	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	GLN	-	expression tag	UNP P59594
A	1201	PHE	-	expression tag	UNP P59594
A	1202	GLU	-	expression tag	UNP P59594
A	1203	LYS	-	expression tag	UNP P59594
B	1197	SER	-	expression tag	UNP P59594
B	1198	HIS	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	GLN	-	expression tag	UNP P59594
B	1201	PHE	-	expression tag	UNP P59594
B	1202	GLU	-	expression tag	UNP P59594
B	1203	LYS	-	expression tag	UNP P59594
C	1197	SER	-	expression tag	UNP P59594
C	1198	HIS	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	GLN	-	expression tag	UNP P59594
C	1201	PHE	-	expression tag	UNP P59594
C	1202	GLU	-	expression tag	UNP P59594
C	1203	LYS	-	expression tag	UNP P59594

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

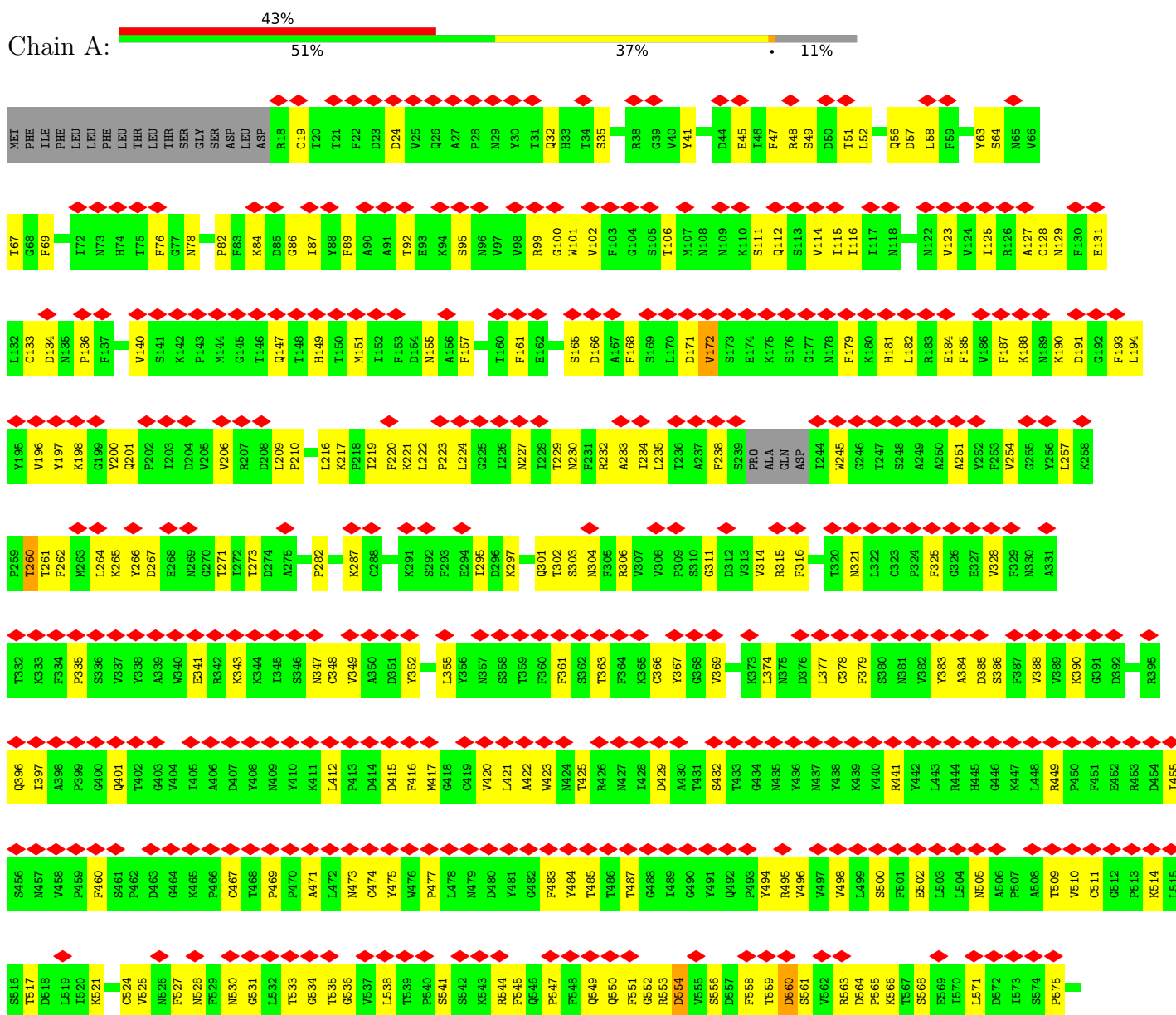
There are 6 discrepancies between the modelled and reference sequences:

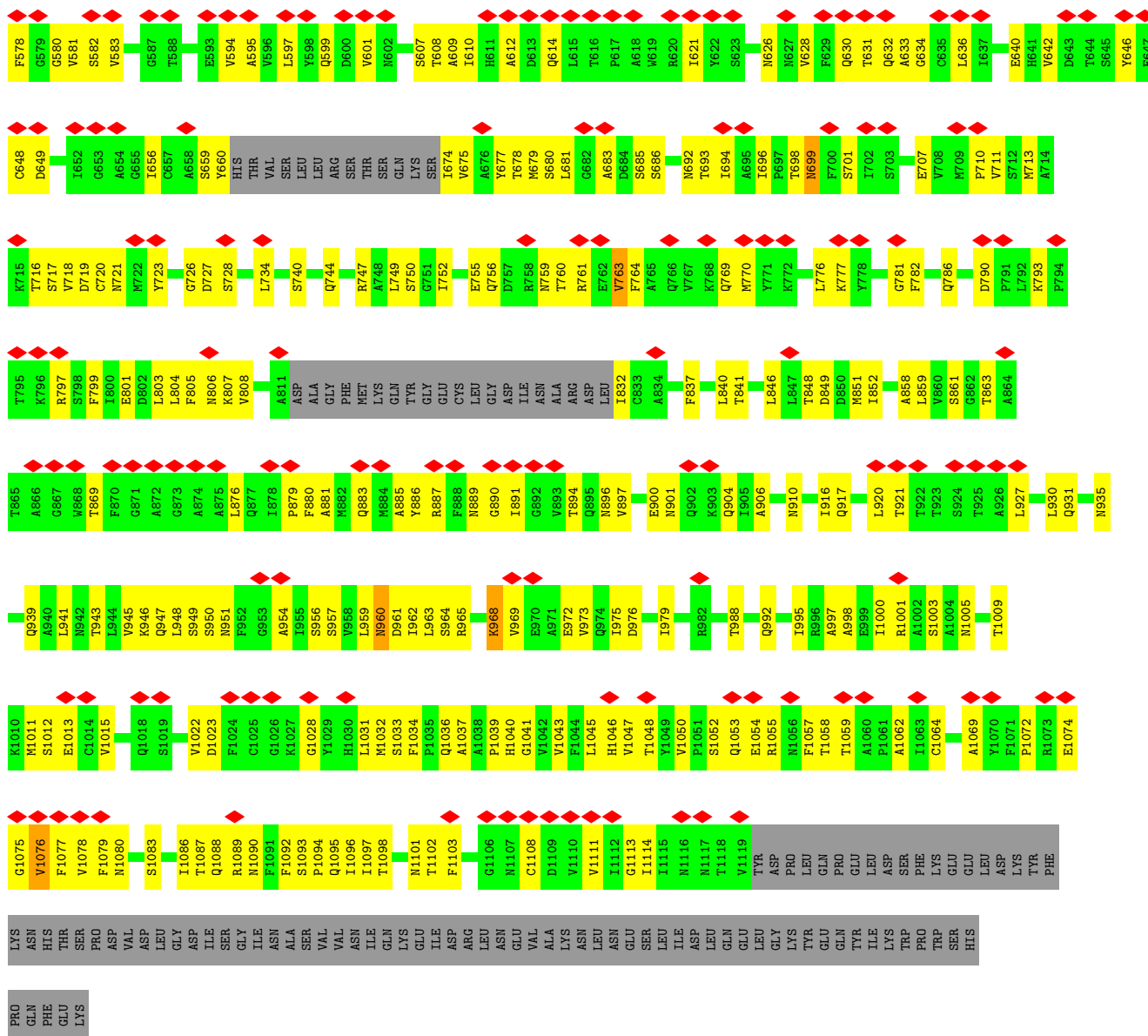
Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1

3 Residue-property plots

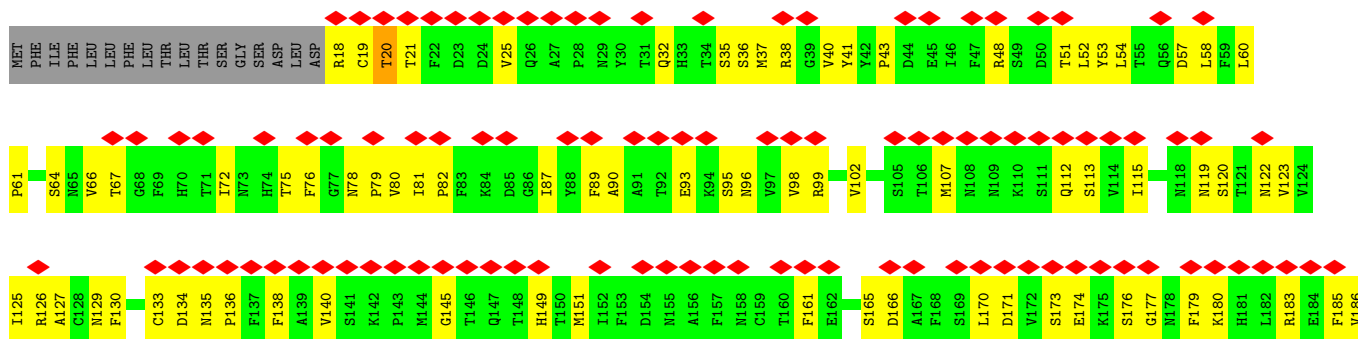
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

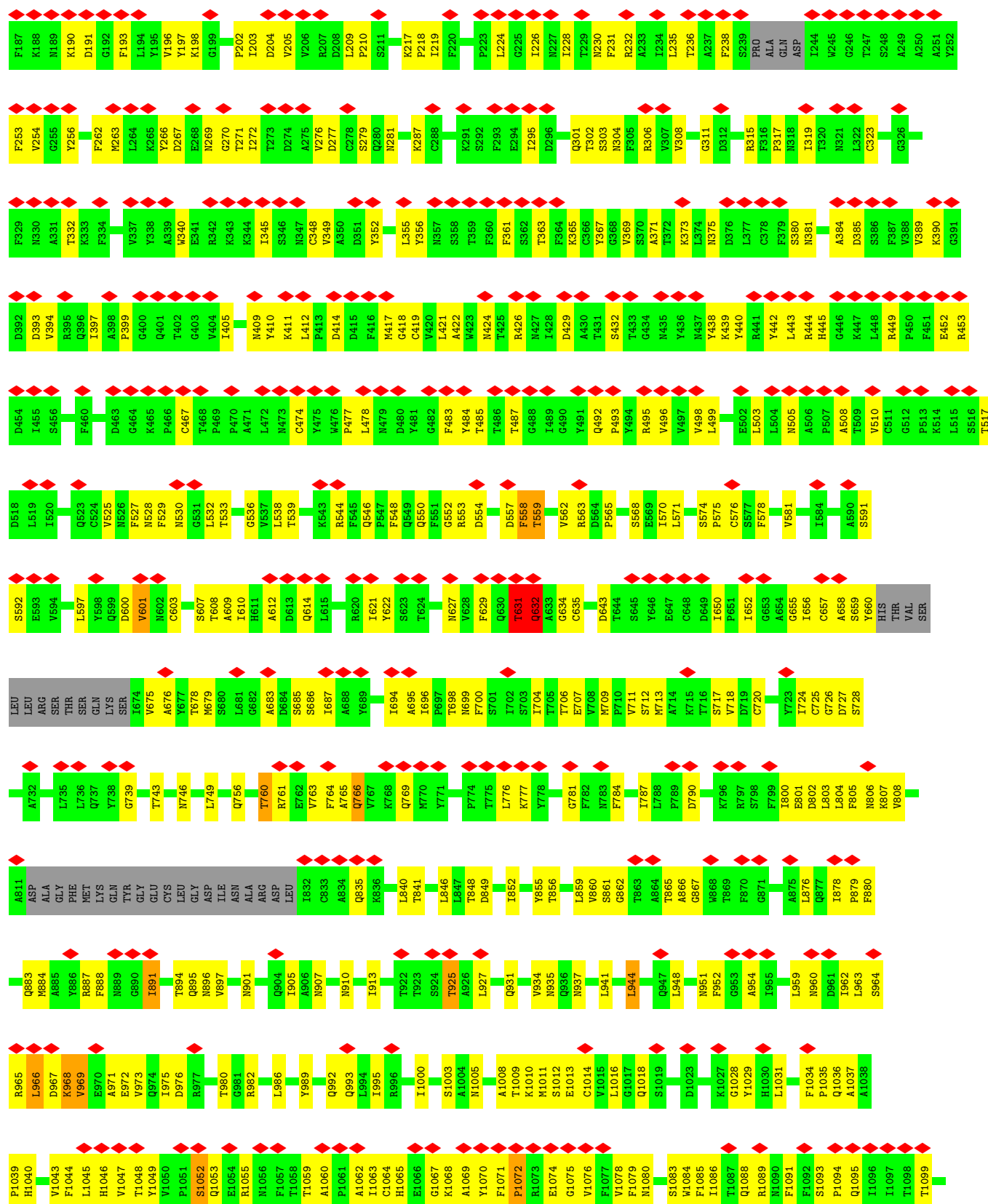
• Molecule 1: Spike glycoprotein

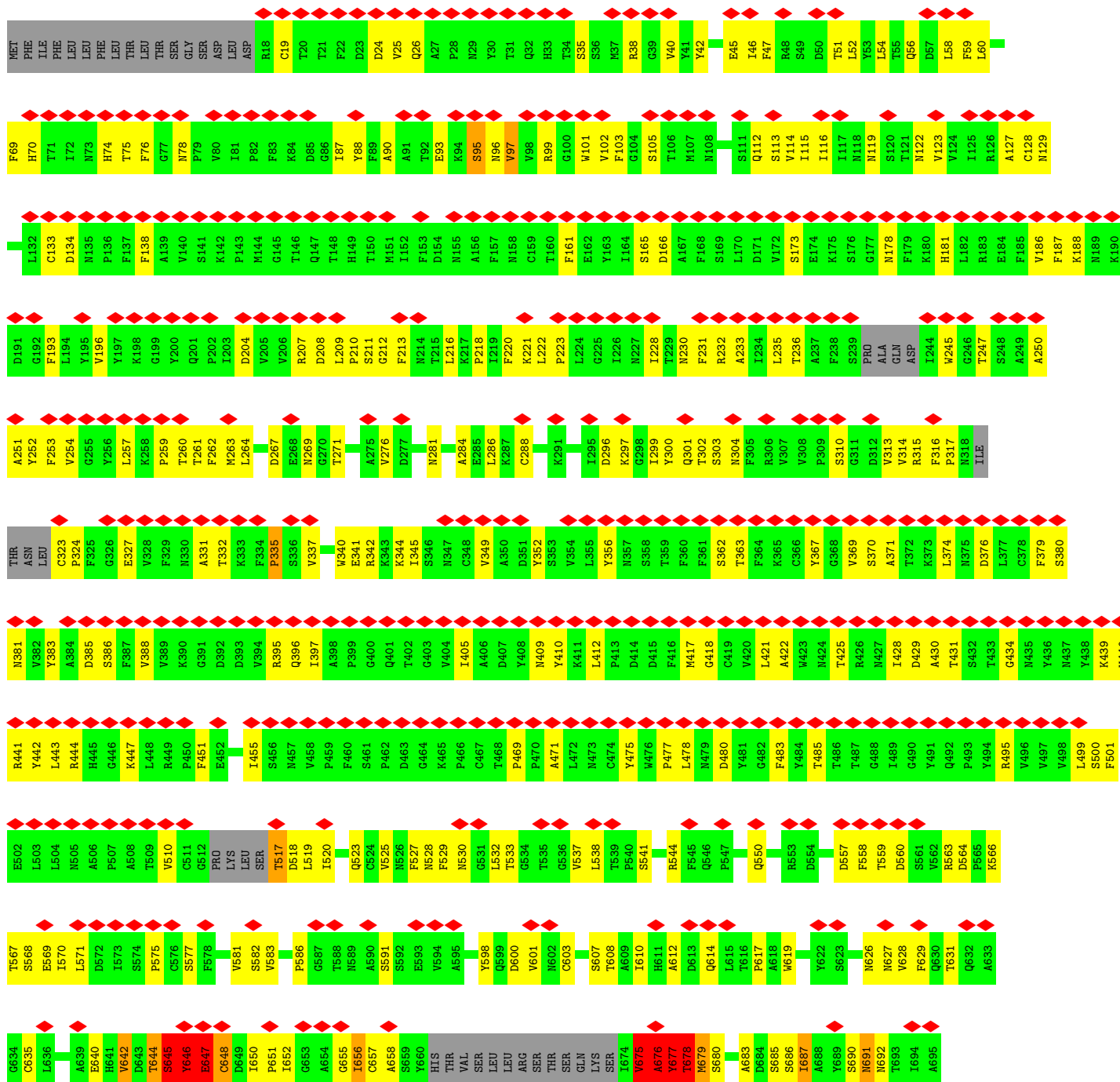




• Molecule 1: Spike glycoprotein







HIS	R559	G319	L379	L439	D499	G319
HIS	L560	L320	Q380	L440	P500	L320
HIS	G561	P321	Y381	K441	A501	P321
	K562	N322	D382	Q442	S502	N322
	S563	M323	M383	A443	L503	M323
	E564	T324	A384	L444	F504	T324
	P565	Q325	Y385	T445	H505	Q325
	W566	G326	A386	I446	V506	G326
	T567	F327	A387	V447	S507	F327
	L568	W328	Q388	G448	N508	W328
	A569	E329	P389	T449	D509	E329
	L570	N330	F390	L450	Y510	N330
	E571	S331	L391	P451	S511	S331
	N572	M332	L392	F452	F512	M332
	V573	L333	R393	T453	I513	L333
	V574	T334	N394	Y454	R514	T334
	G575	D335	G395	M455	Y515	D335
	A576	P336	A396	L456	Y516	P336
	K577	G337	N397	E457	T517	G337
	N578	N338	E398	K458	R518	N338
	W579	V339	G399	W459	T519	W579
	N580	Q340	F400	L460	L520	N580
	V581	K341	H401	W461	Y521	V581
	R582	A342	E402	M462	Q522	R582
	F583	V343	A403	V463	F523	F583
	L584	C344	V404	F464	Q524	L584
	L585	H345	G405	K465	F525	L585
	N586	P346	E406	G466	Q526	N586
	Y587	T347	I407	E467	E527	Y587
	F588	A348	M408	I468	A528	F588
	E589	W349	S409	P469	L529	E589
	P590	D350	L410	K470	C530	P590
	L591	L351	S411	D471	Q531	L591
	F592	G352	A412	Q472	A532	F592
	T593	K353	A413	W473	A533	T593
	N594	G354	T414	M474	K534	N594
	L595	D355	P415	K475	H535	L595
	K596	F356	K416	K476	E536	K596
	D597	R357	H417	W477	G537	D597
	Q598	I358	L418	W478	P538	Q598
	N599	L359	K419	E479	L539	N599
	K600	M360	S420	M480	H540	K600
	M601	C361	I421	K481	K541	M601
	S602	T362	G422	R482	C542	S602
	F603	K363	L423	E483	D543	F603
	V604	V364	L424	I484	I544	V604
	G605	T365	S425	V485	S545	G605
	W606	M366	P426	G486	N546	W606
	S607	D367	D427	V487	S547	S607
	T608	D368	D428	V488	T548	T608
	D609	F369	Q429	E489	E549	D609
	W610	L370	E430	P490	A550	W610
	S611	T371	D431	V491	G551	S611
	P612	A372	N432	P492	Q552	P612
	Y613	H373	E433	H493	K553	Y613
	A614	H374	T434	D494	L554	A614
	D615	E375	E435	E495	F555	D615
	HIS	M376	I436	T496	N556	HIS
	HIS	G377	N437	Y497	M557	HIS
	HIS	H378	F438	C498	L558	HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53189	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.981	Depositor
Minimum map value	-13.647	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.921	Depositor
Recommended contour level	8	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/8499	0.86	14/11568 (0.1%)
1	B	0.56	0/8499	0.88	10/11568 (0.1%)
1	C	0.60	7/8435 (0.1%)	0.94	20/11477 (0.2%)
2	D	0.29	0/5007	0.65	0/6803
All	All	0.53	7/30440 (0.0%)	0.86	44/41416 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	B	0	17
1	C	0	19
2	D	0	2
All	All	0	55

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	676	ALA	C-O	-9.44	1.12	1.24
1	C	675	VAL	CA-CB	-7.00	1.45	1.54
1	C	677	TYR	C-O	-6.40	1.16	1.24
1	C	677	TYR	CA-CB	-6.36	1.42	1.53
1	C	676	ALA	N-CA	6.20	1.54	1.46

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	646	TYR	N-CA-C	11.87	122.15	108.49
1	A	1114	ILE	N-CA-C	-9.63	103.57	112.43
1	C	787	ILE	N-CA-C	-8.41	102.51	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	646	TYR	N-CA-CB	-8.40	100.94	109.51
1	A	556	SER	CA-C-N	7.86	134.05	122.74

There are no chirality outliers.

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	VAL	Peptide
1	A	206	VAL	Peptide
1	A	415	ASP	Peptide
1	A	416	PHE	Peptide
1	A	558	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8302	0	8082	304	0
1	B	8302	0	8082	310	0
1	C	8241	0	8011	345	0
2	D	4870	0	4643	90	0
All	All	29715	0	28818	1008	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 1008 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ILE:CG1	1:C:677:TYR:O	1.89	1.21
1:C:678:THR:O	1:C:679:MET:HB2	1.43	1.18
1:C:656:ILE:HG12	1:C:677:TYR:O	1.00	1.17
1:C:647:GLU:O	1:C:648:CYS:CB	1.91	1.14
1:C:646:TYR:C	1:C:680:SER:OG	1.94	1.11

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1057/1203 (88%)	850 (80%)	203 (19%)	4 (0%)	30	67
1	B	1057/1203 (88%)	836 (79%)	213 (20%)	8 (1%)	16	53
1	C	1045/1203 (87%)	834 (80%)	201 (19%)	10 (1%)	12	47
2	D	595/603 (99%)	565 (95%)	30 (5%)	0	100	100
All	All	3754/4212 (89%)	3085 (82%)	647 (17%)	22 (1%)	23	59

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	645	SER
1	C	648	CYS
1	C	675	VAL
1	C	676	ALA
1	C	679	MET

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	922/1048 (88%)	918 (100%)	4 (0%)	84	83
1	B	922/1048 (88%)	913 (99%)	9 (1%)	68	76
1	C	914/1048 (87%)	899 (98%)	15 (2%)	55	69
2	D	527/533 (99%)	524 (99%)	3 (1%)	78	81
All	All	3285/3677 (89%)	3254 (99%)	31 (1%)	68	77

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	642	VAL
1	C	1097	ILE
1	C	647	GLU
2	D	436	ILE
1	C	720	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	546	GLN
1	C	987	GLN
1	C	699	ASN
1	C	896	ASN
2	D	24	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

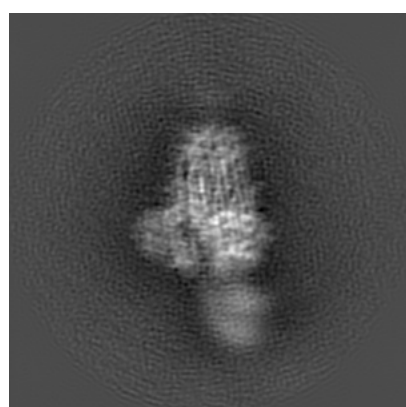
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9591. These allow visual inspection of the internal detail of the map and identification of artifacts.

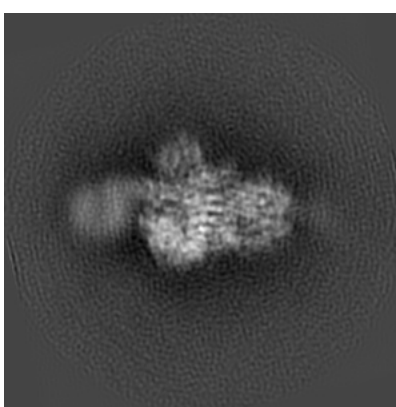
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

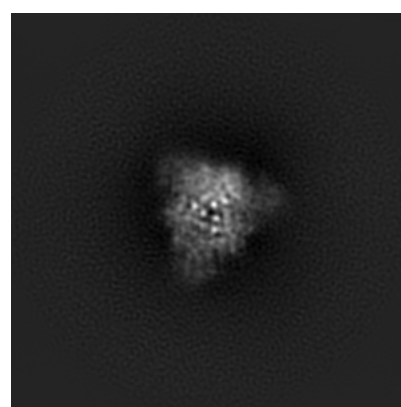
6.1.1 Primary map



X



Y

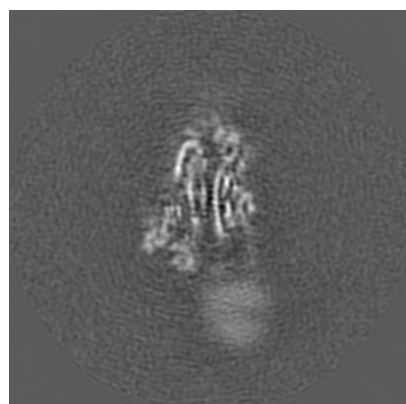


Z

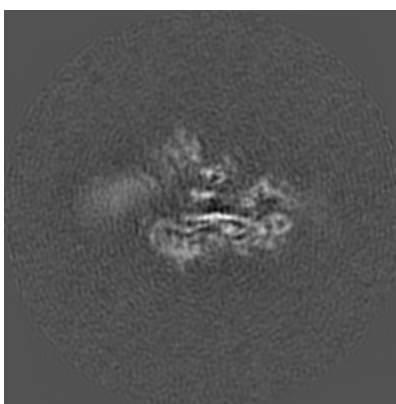
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

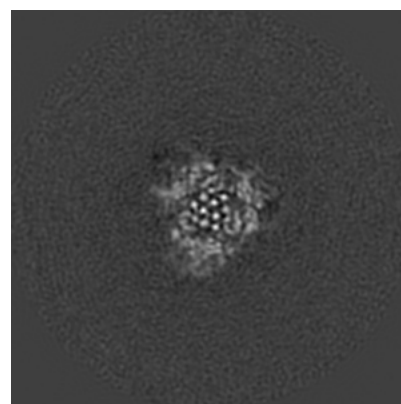
6.2.1 Primary map



X Index: 144



Y Index: 144

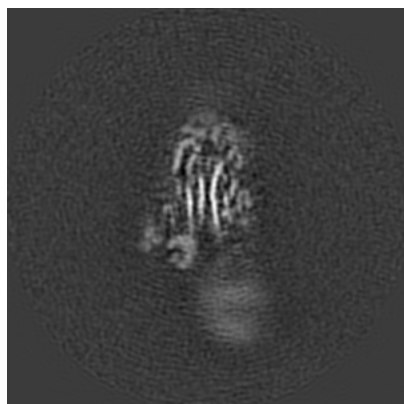


Z Index: 144

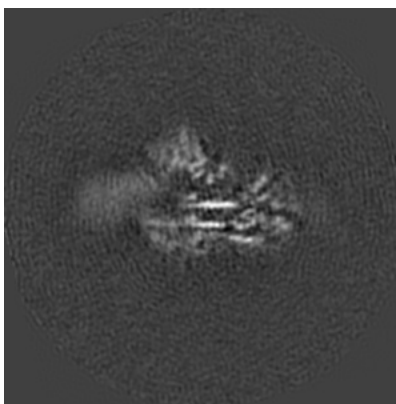
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

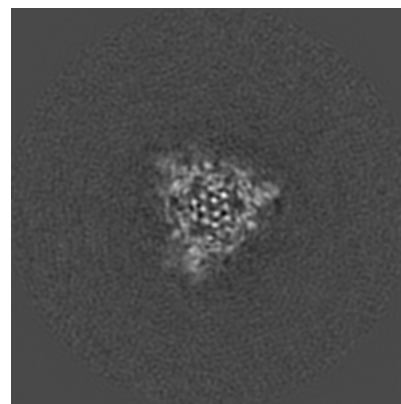
6.3.1 Primary map



X Index: 146



Y Index: 148

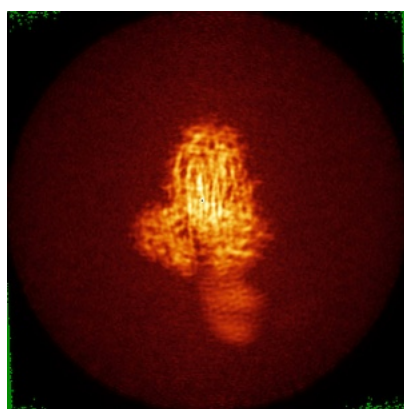


Z Index: 142

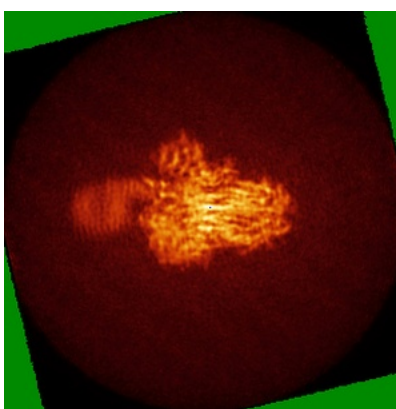
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

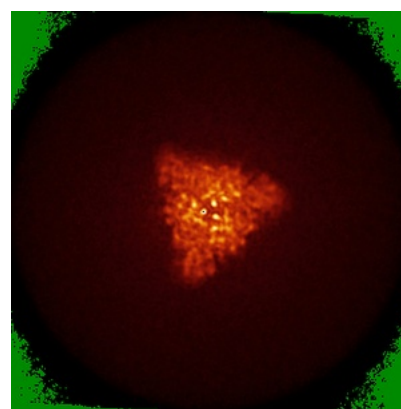
6.4.1 Primary map



X



Y



Z

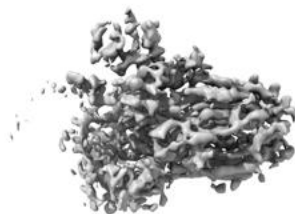
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

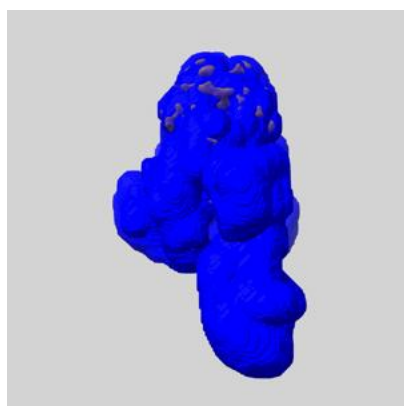
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

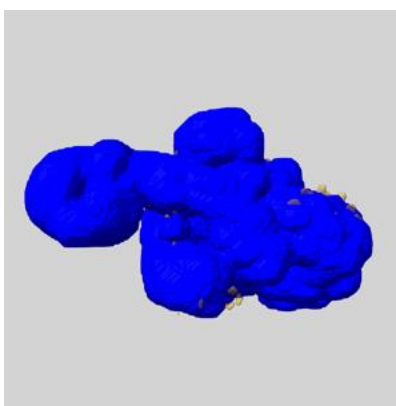
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

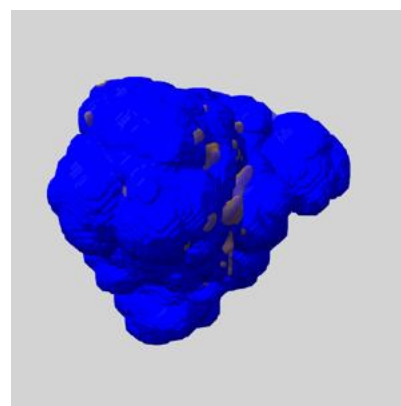
6.6.1 emd_9591_msk_1.map [i](#)



X



Y

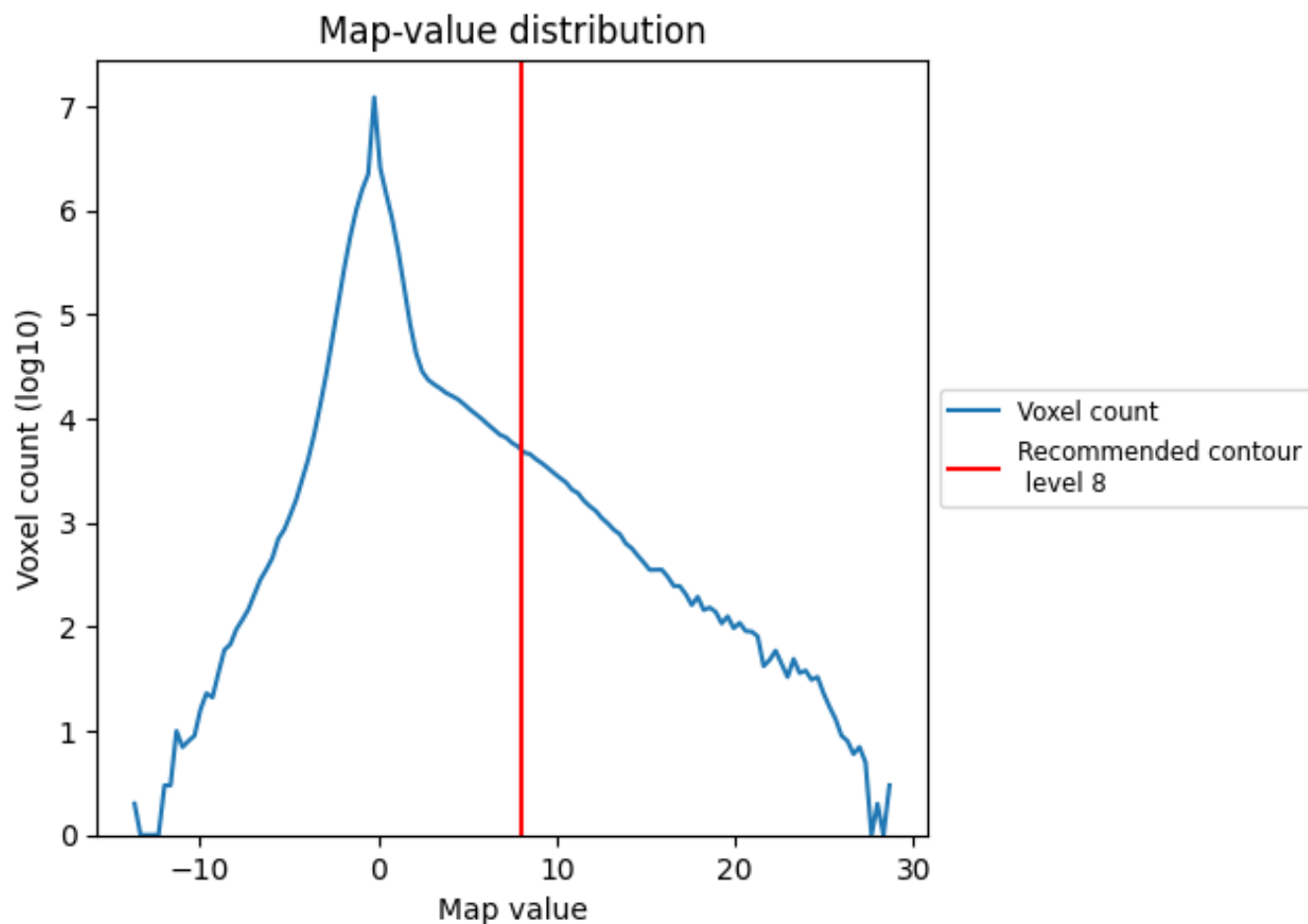


Z

7 Map analysis [i](#)

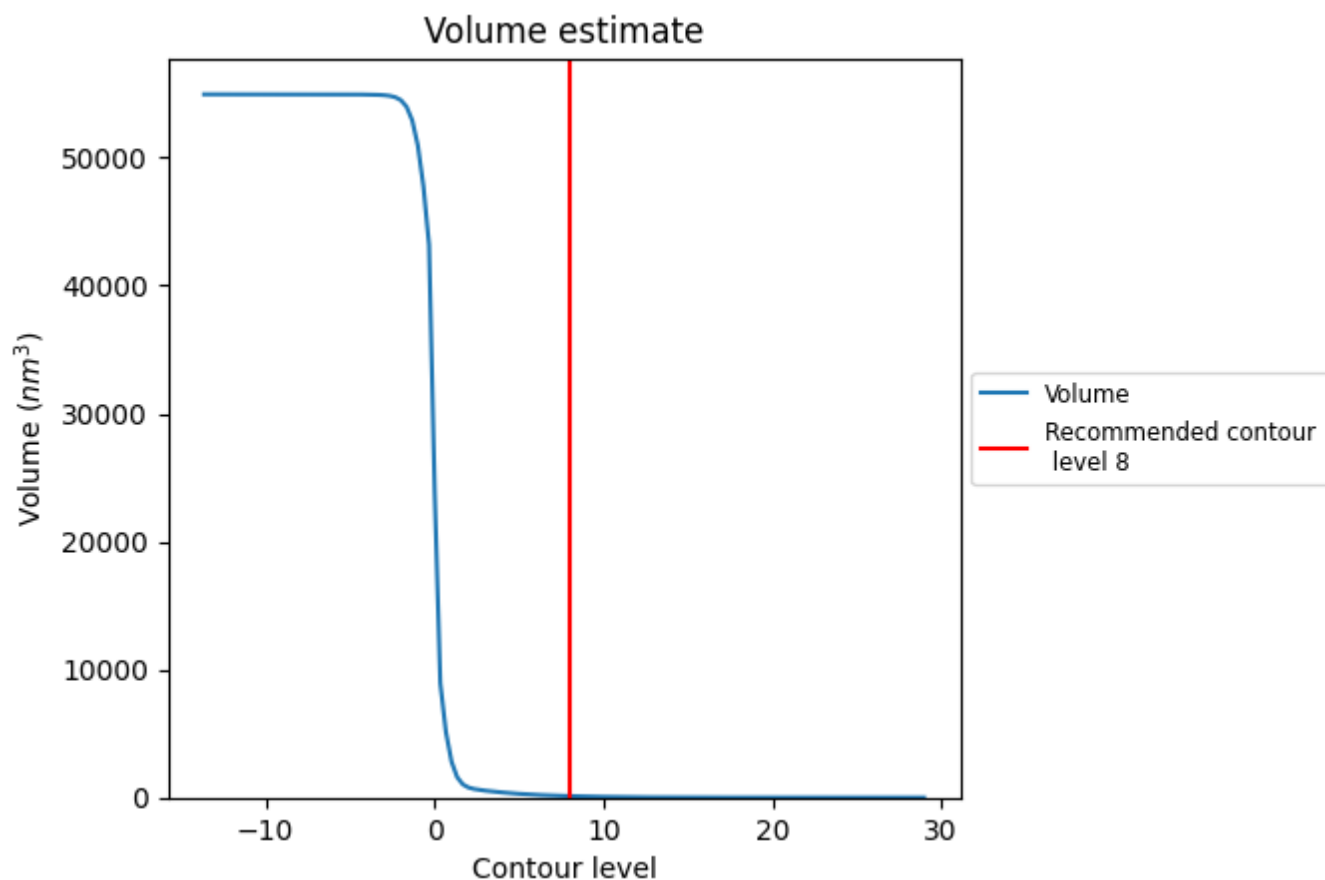
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

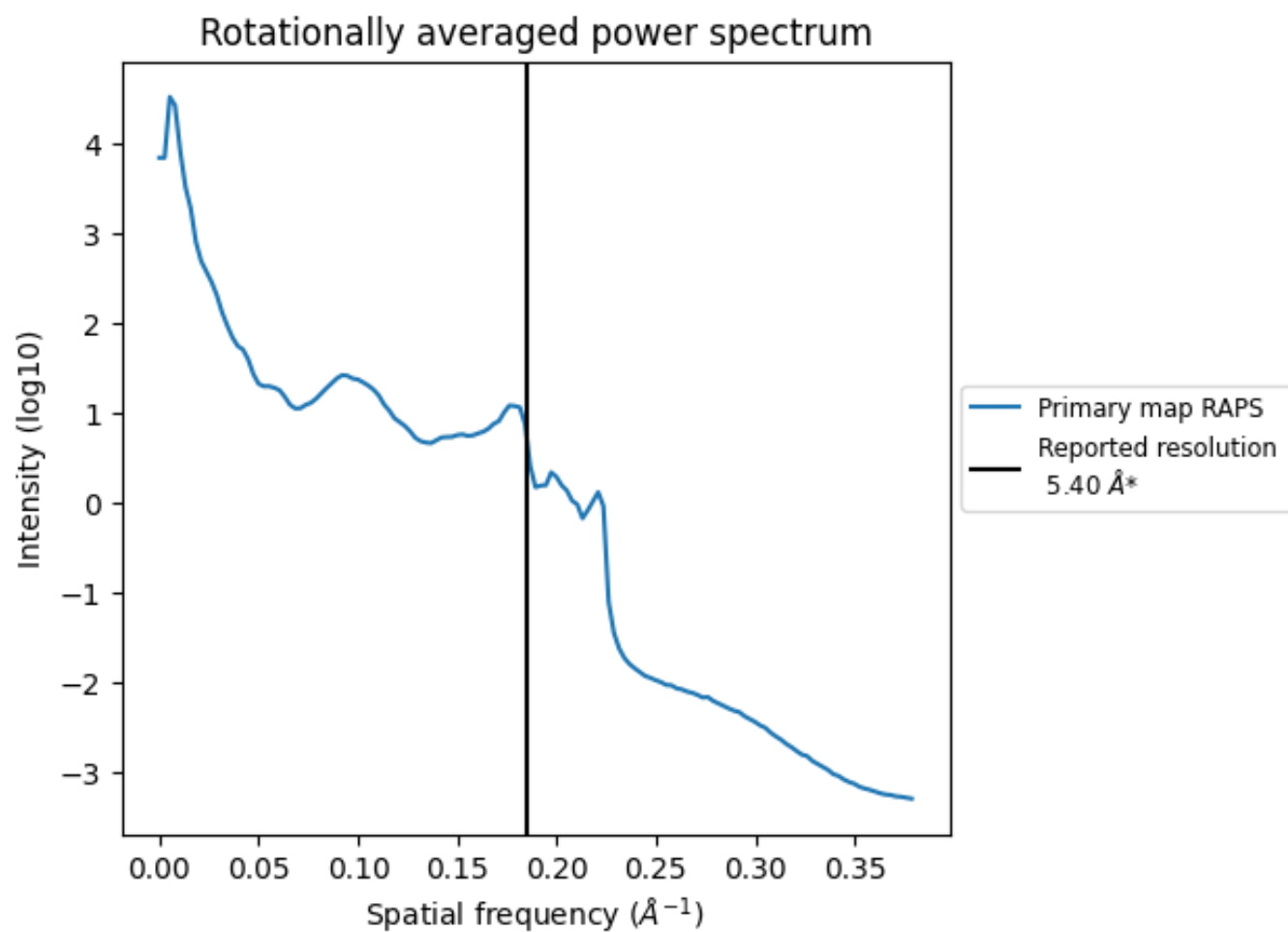
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

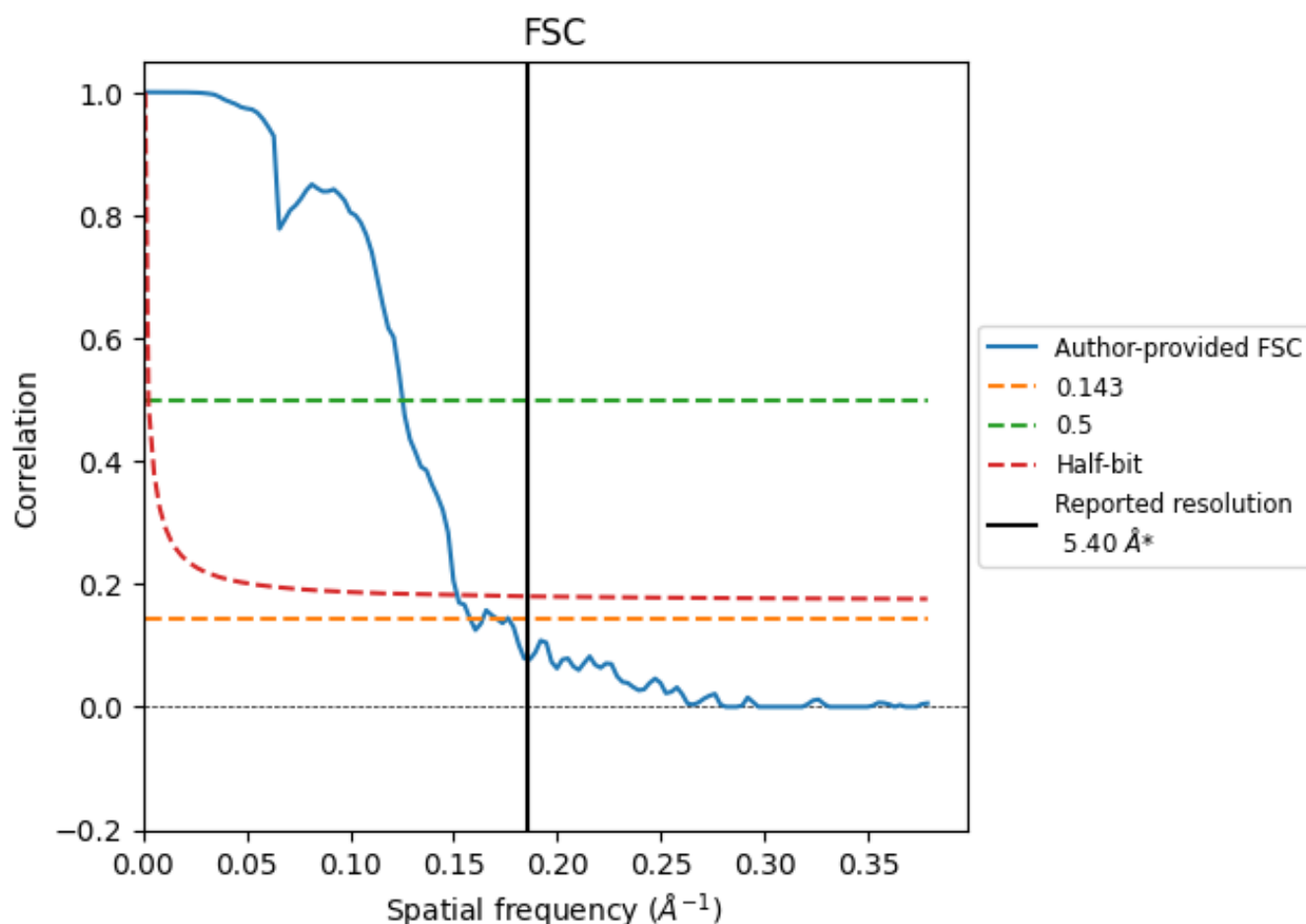


*Reported resolution corresponds to spatial frequency of 0.185 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.185 Å⁻¹

8.2 Resolution estimates [i](#)

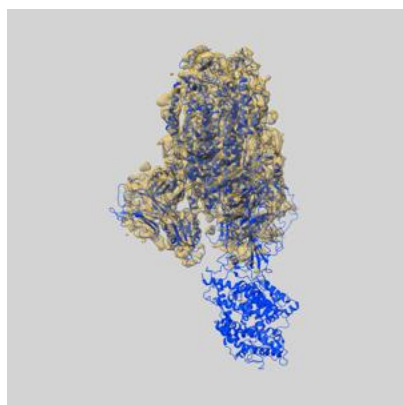
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	6.33	7.98	6.59
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.33 differs from the reported value 5.4 by more than 10 %

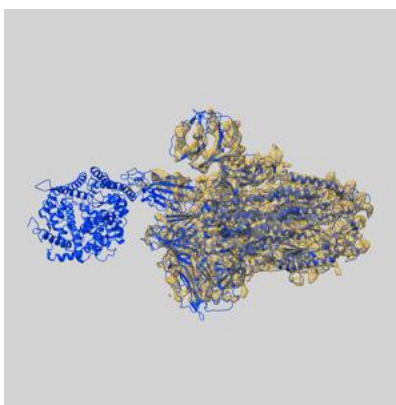
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9591 and PDB model 6ACG. Per-residue inclusion information can be found in section [3](#) on page [5](#).

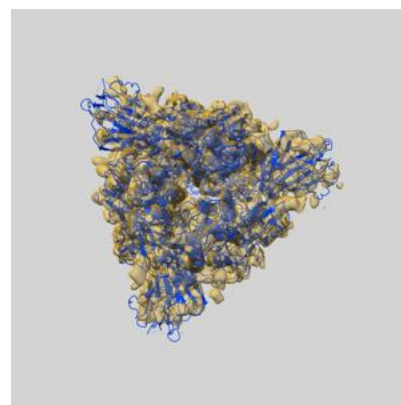
9.1 Map-model overlay [i](#)



X



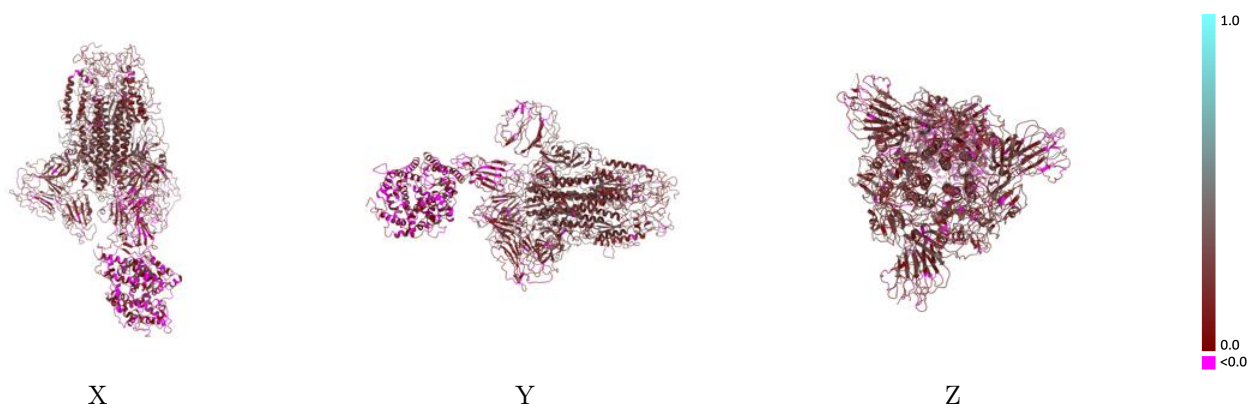
Y



Z

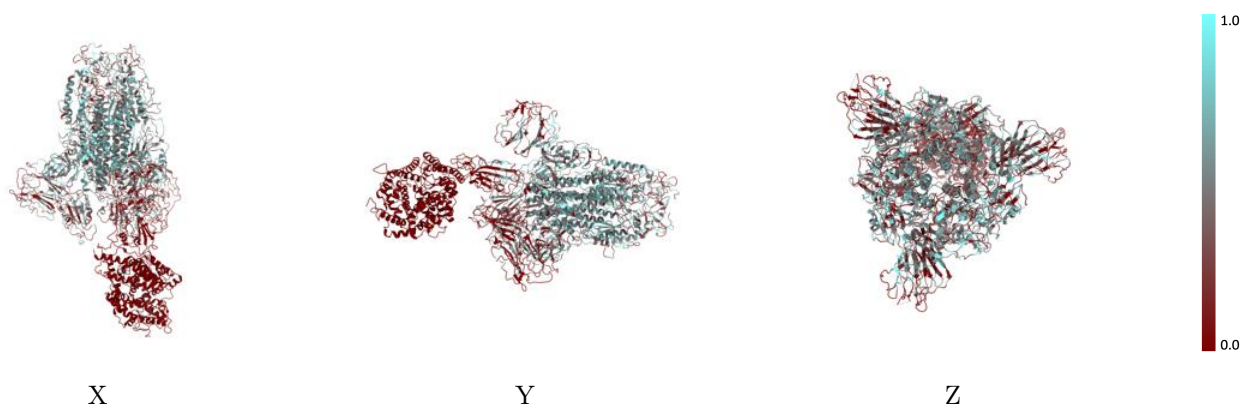
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



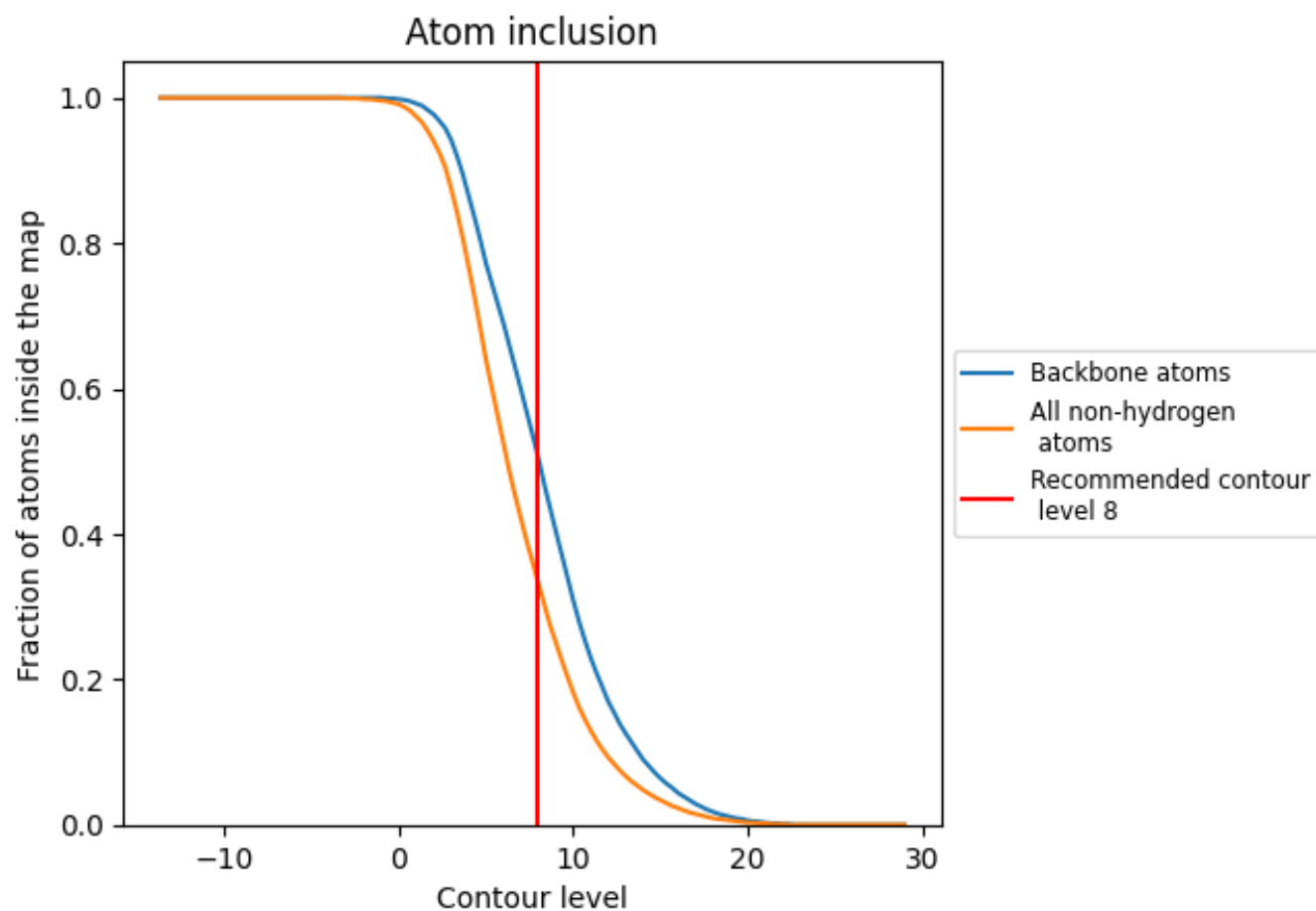
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 33% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3320	0.2020
A	0.3870	0.2280
B	0.4300	0.2360
C	0.3730	0.2150
D	0.0000	0.0800

