



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 07:44 PM EST

PDB ID : 7JWB  
EMDB ID : EMD-22514  
Title : SARS CoV2 Spike ectodomain with engineered trimerized VH binder  
Authors : QCRG Structural Biology Consortium  
Deposited on : 2020-08-25  
Resolution : 6.00 Å(reported)  
Based on initial models : 6X2B, 4G80

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

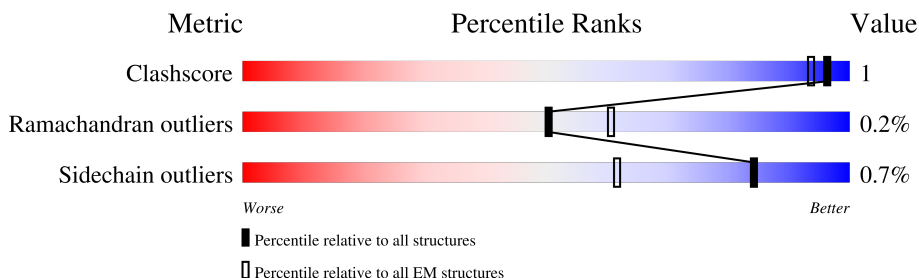
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 6.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	D	421	
2	A	1208	
2	B	1208	
2	C	1208	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25654 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 autonomous human heavy chain variable domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	366	2818	1785	474	550	9	0	0

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	991	7738	4946	1283	1474	35	0	0
2	B	986	7705	4919	1278	1473	35	0	0
2	C	946	7393	4721	1228	1411	33	0	0

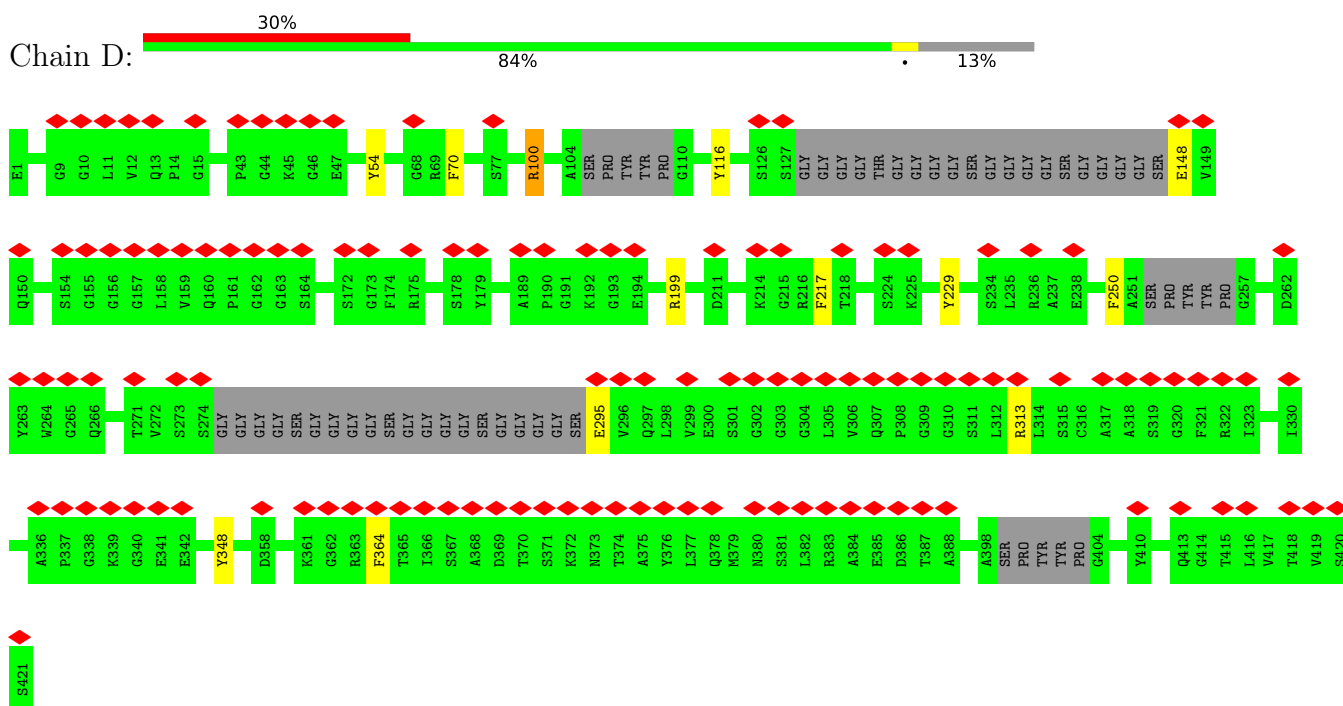
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

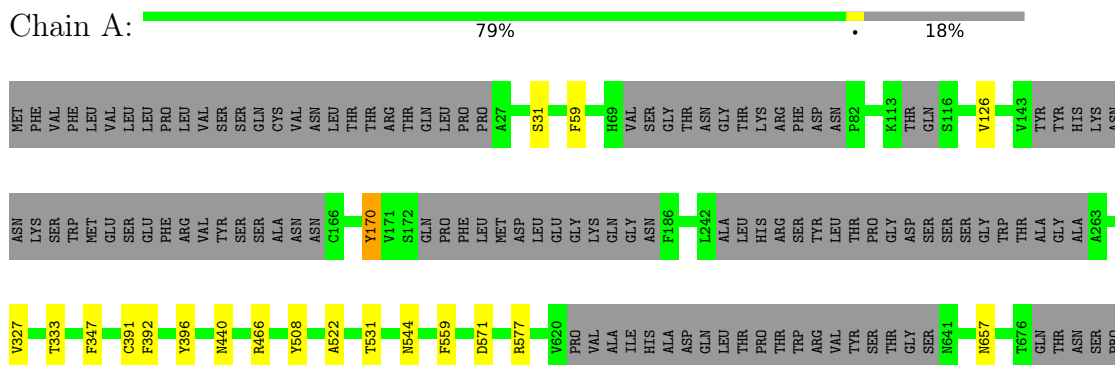
### 3 Residue-property plots

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: autonomous human heavy chain variable domain



- Molecule 2: Spike glycoprotein





R816	PHE
D820	LYS
7827	ASN
	HIS
	THR
	SER
	LEU
	ALA
	ASP
	VAL
	GLY
	PHE
	LEU
	ILE
	LYS
	GLN
	TYR
	GLY
	ILE
	ASP
	CYS
	ASN
	ALA
	LEU
	GLY
	SER
	VAL
	ASP
	VAL
	ILE
	ASN
	ALA
	ILE
	ALA
	GLN
	ARG
	LYS
	ASP
	LEU
	ILE
	ILE
	ASP
	CYS
	ARG
	ALA
	LEU
	ASN
R853	GLN
D867	ASN
G908	GLU
K1028	VAL
K1038	ALA
R1039	LYS
F1042	ASN
D1084	LEU
Q1142	LEU
P1143	GLN
E1144	GLU
	LEU
	LYS
	TYR
	ASP
	SER
	GLU
	PHE
	LYS
	GLU
	LEU
	ASP
	LYS
	TYR
	GLN

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	21000, 21000	Depositor
Resolution determination method	OTHER, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	78	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.641	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	D	0.93	0/2884	0.93	8/3906 (0.2%)
2	A	0.94	0/7910	0.91	8/10759 (0.1%)
2	B	0.93	0/7875	0.90	9/10710 (0.1%)
2	C	0.92	0/7552	0.91	6/10265 (0.1%)
All	All	0.93	0/26221	0.91	31/35640 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	815	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	199	ARG	NE-CZ-NH2	-5.87	117.36	120.30
2	A	577	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	C	577	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	466	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	364	PHE	CB-CG-CD1	5.68	124.78	120.80
2	C	646	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	70	PHE	CB-CG-CD1	5.67	124.77	120.80
2	B	421	TYR	CB-CG-CD1	-5.65	117.61	121.00
2	B	91	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	D	54	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	D	199	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	B	363	ALA	N-CA-CB	-5.56	102.32	110.10
2	C	44	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	217	PHE	CB-CG-CD2	5.50	124.65	120.80
2	C	194	PHE	CB-CG-CD1	5.47	124.63	120.80
2	B	377	PHE	CB-CG-CD2	5.46	124.62	120.80
2	A	170	TYR	CB-CG-CD1	-5.45	117.73	121.00
2	C	423	TYR	CB-CG-CD1	-5.44	117.74	121.00
2	A	559	PHE	CB-CG-CD1	5.41	124.58	120.80
2	B	237	ARG	NE-CZ-NH2	-5.41	117.60	120.30
2	B	347	PHE	CB-CG-CD1	5.39	124.57	120.80
2	A	466	ARG	NE-CZ-NH2	-5.27	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	59	PHE	CB-CG-CD1	5.25	124.47	120.80
2	A	396	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	D	229	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	D	348	TYR	CB-CG-CD1	5.14	124.08	121.00
2	A	508	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	B	365	TYR	CB-CG-CD1	-5.06	117.97	121.00
2	B	508	TYR	CB-CG-CD2	-5.06	117.97	121.00
2	A	347	PHE	CB-CG-CD1	5.01	124.31	120.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	D	2818	0	2676	2	0
2	A	7738	0	7562	13	0
2	B	7705	0	7514	13	0
2	C	7393	0	7219	13	0
All	All	25654	0	24971	39	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 1.

All (39) 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)
2:B:332:ILE:HB	2:B:362:VAL:HG21	1.66	0.78
1:D:100:ARG:HB3	1:D:116:TYR:HB2	1.75	0.68
2:B:332:ILE:HG21	2:B:527:PRO:HA	1.77	0.65
2:A:954:GLN:HB3	2:A:1014:ARG:HE	1.69	0.56
2:C:215:ASP:N	2:C:266:TYR:HH	2.04	0.55
2:C:811:LYS:NZ	2:C:820:ASP:OD2	2.39	0.55
2:B:389:ASP:OD1	2:B:529:LYS:NZ	2.40	0.55
2:A:1083:HIS:HB2	2:A:1137:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:522:ALA:H	2:A:544:ASN:HD21	1.55	0.54
2:B:811:LYS:NZ	2:B:820:ASP:OD2	2.40	0.48
2:C:574:ASP:OD1	2:C:575:ALA:N	2.47	0.47
2:A:571:ASP:OD2	2:B:964:LYS:NZ	2.46	0.47
2:C:92:PHE:HB2	2:C:192:PHE:HB2	1.96	0.47
2:A:1084:ASP:OD1	2:A:1084:ASP:N	2.47	0.47
2:B:577:ARG:HH11	2:B:582:LEU:HB3	1.80	0.47
2:A:126:VAL:HB	2:A:170:TYR:HB2	1.96	0.47
2:A:811:LYS:NZ	2:A:820:ASP:OD2	2.40	0.46
2:C:1028:LYS:NZ	2:C:1042:PHE:O	2.50	0.45
2:B:1084:ASP:N	2:B:1084:ASP:OD1	2.47	0.44
2:C:1142:GLN:N	2:C:1143:PRO:CD	2.80	0.44
2:A:657:ASN:OD1	2:A:657:ASN:N	2.52	0.43
2:A:327:VAL:H	2:A:531:THR:HG22	1.84	0.42
2:B:908:GLY:O	2:B:1038:LYS:NZ	2.53	0.42
2:C:186:PHE:HB3	2:C:187:LYS:H	1.60	0.42
1:D:250:PHE:CZ	2:B:455:LEU:HB3	2.55	0.42
2:A:391:CYS:O	2:A:392:PHE:HB2	2.20	0.42
2:A:1098:ASN:OD1	2:A:1098:ASN:N	2.53	0.42
2:C:908:GLY:O	2:C:1038:LYS:NZ	2.52	0.42
2:C:867:ASP:OD1	2:C:867:ASP:N	2.52	0.42
2:A:440:ASN:OD1	2:A:440:ASN:N	2.53	0.41
2:C:395:VAL:HG22	2:C:515:PHE:HD2	1.85	0.41
2:C:1039:ARG:HB2	2:C:1042:PHE:HB2	2.03	0.41
2:A:917:TYR:HA	2:A:920:GLN:HG3	2.02	0.41
2:B:1098:ASN:N	2:B:1098:ASN:OD1	2.53	0.41
2:C:528:LYS:NZ	2:C:544:ASN:O	2.54	0.41
2:B:200:TYR:CG	2:B:230:PRO:HA	2.56	0.41
2:B:440:ASN:OD1	2:B:440:ASN:N	2.54	0.40
2:C:1084:ASP:N	2:C:1084:ASP:OD1	2.47	0.40
2:B:344:ALA:O	2:B:509:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	D	354/421 (84%)	354 (100%)	0	0	100	100
2	A	971/1208 (80%)	948 (98%)	21 (2%)	2 (0%)	47	81
2	B	964/1208 (80%)	946 (98%)	16 (2%)	2 (0%)	47	81
2	C	918/1208 (76%)	897 (98%)	20 (2%)	1 (0%)	51	85
All	All	3207/4045 (79%)	3145 (98%)	57 (2%)	5 (0%)	50	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	32	PHE
2	A	333	THR
2	A	1112	PRO
2	B	1036	GLN
2	C	32	PHE

### 5.3.2 Protein sidechains [i](#)

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	D	288/311 (93%)	284 (99%)	4 (1%)	67	80
2	A	866/1053 (82%)	863 (100%)	3 (0%)	92	94
2	B	864/1053 (82%)	856 (99%)	8 (1%)	78	88
2	C	829/1053 (79%)	825 (100%)	4 (0%)	88	93
All	All	2847/3470 (82%)	2828 (99%)	19 (1%)	84	90

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	100	ARG
1	D	148	GLU
1	D	295	GLU

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Mol	Chain	Res	Type
1	D	313	ARG
2	A	31	SER
2	A	855	PHE
2	A	1014	ARG
2	B	34	ARG
2	B	140	PHE
2	B	324	GLU
2	B	332	ILE
2	B	334	ASN
2	B	335	LEU
2	B	815	ARG
2	B	1107	ARG
2	C	140	PHE
2	C	186	PHE
2	C	382	VAL
2	C	1039	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	641	ASN
2	C	655	HIS

### 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 monosaccharides 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 [i](#)

There are no chain breaks in this entry.

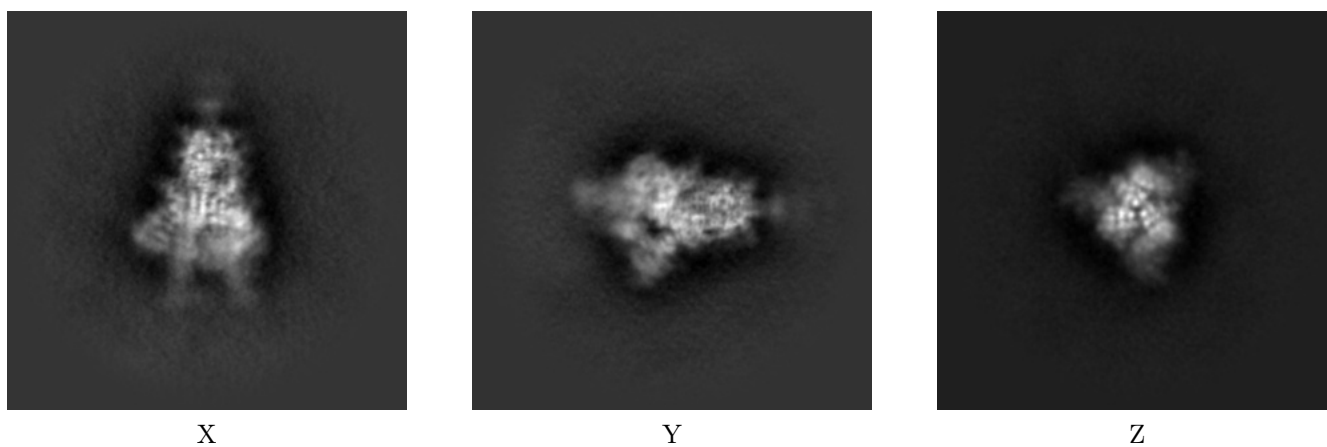
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22514. 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](#)

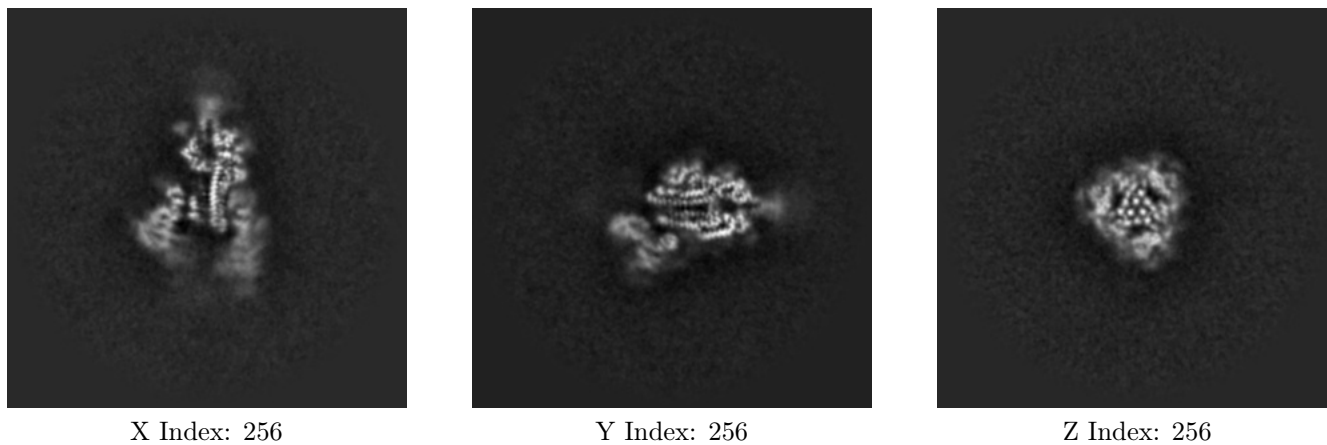
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

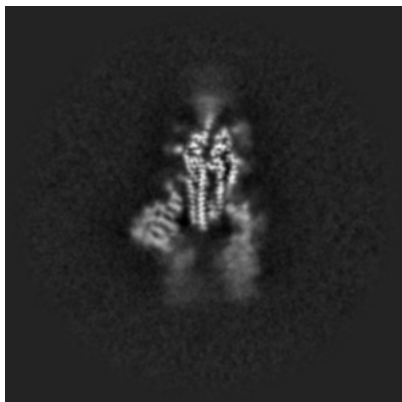
#### 6.2.1 Primary map



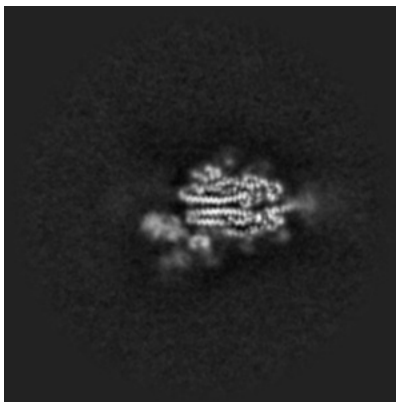
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

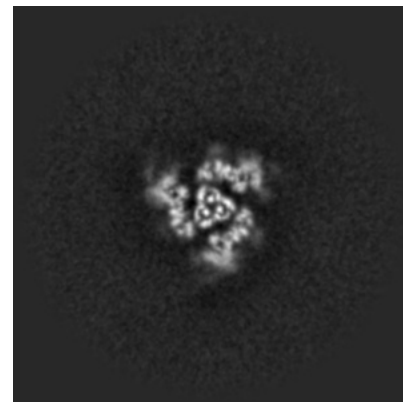
### 6.3.1 Primary map



X Index: 265



Y Index: 251



Z Index: 242

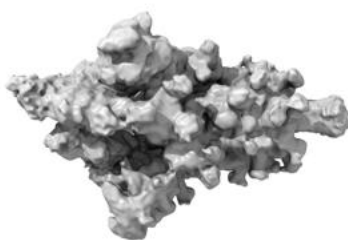
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

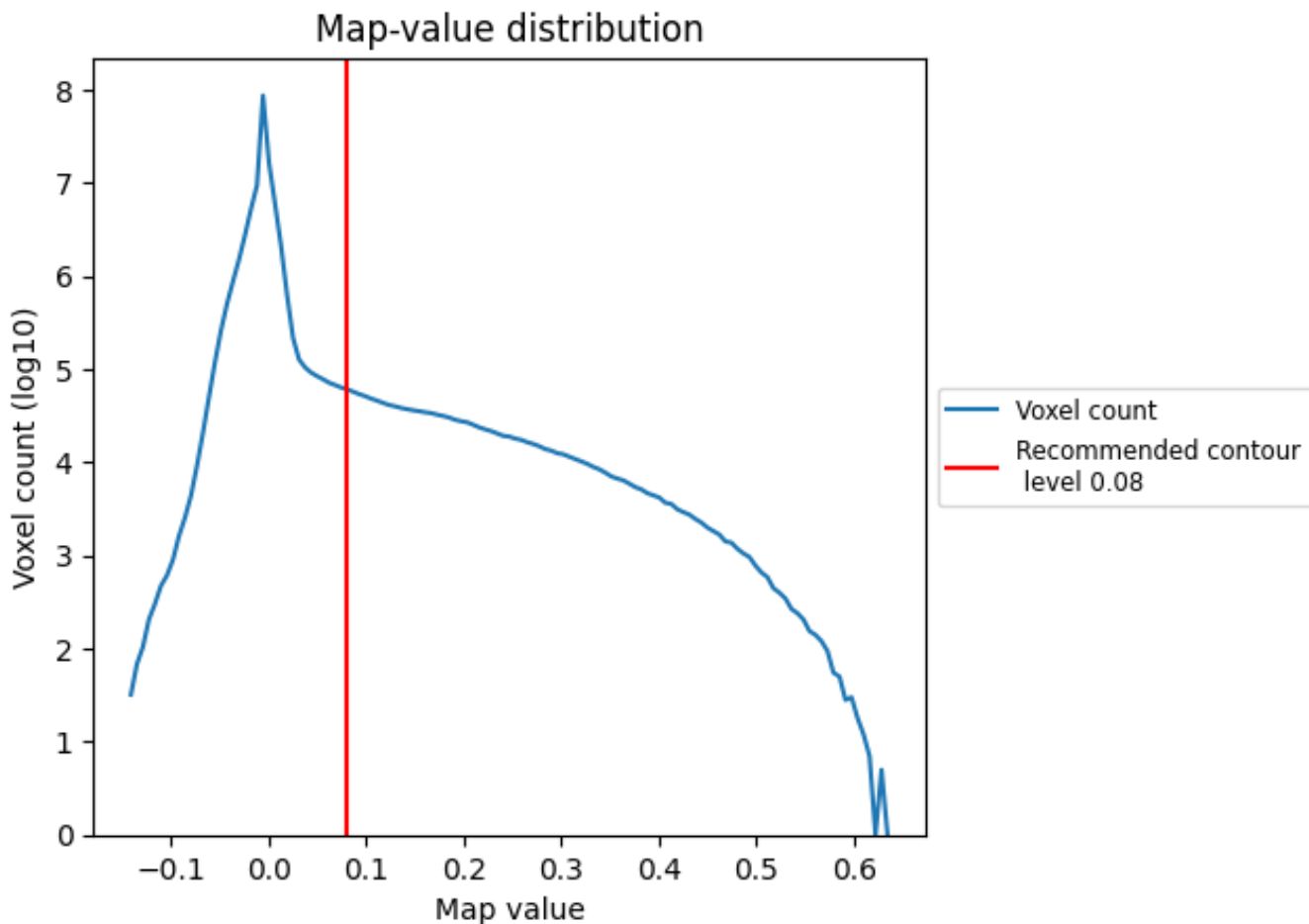
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

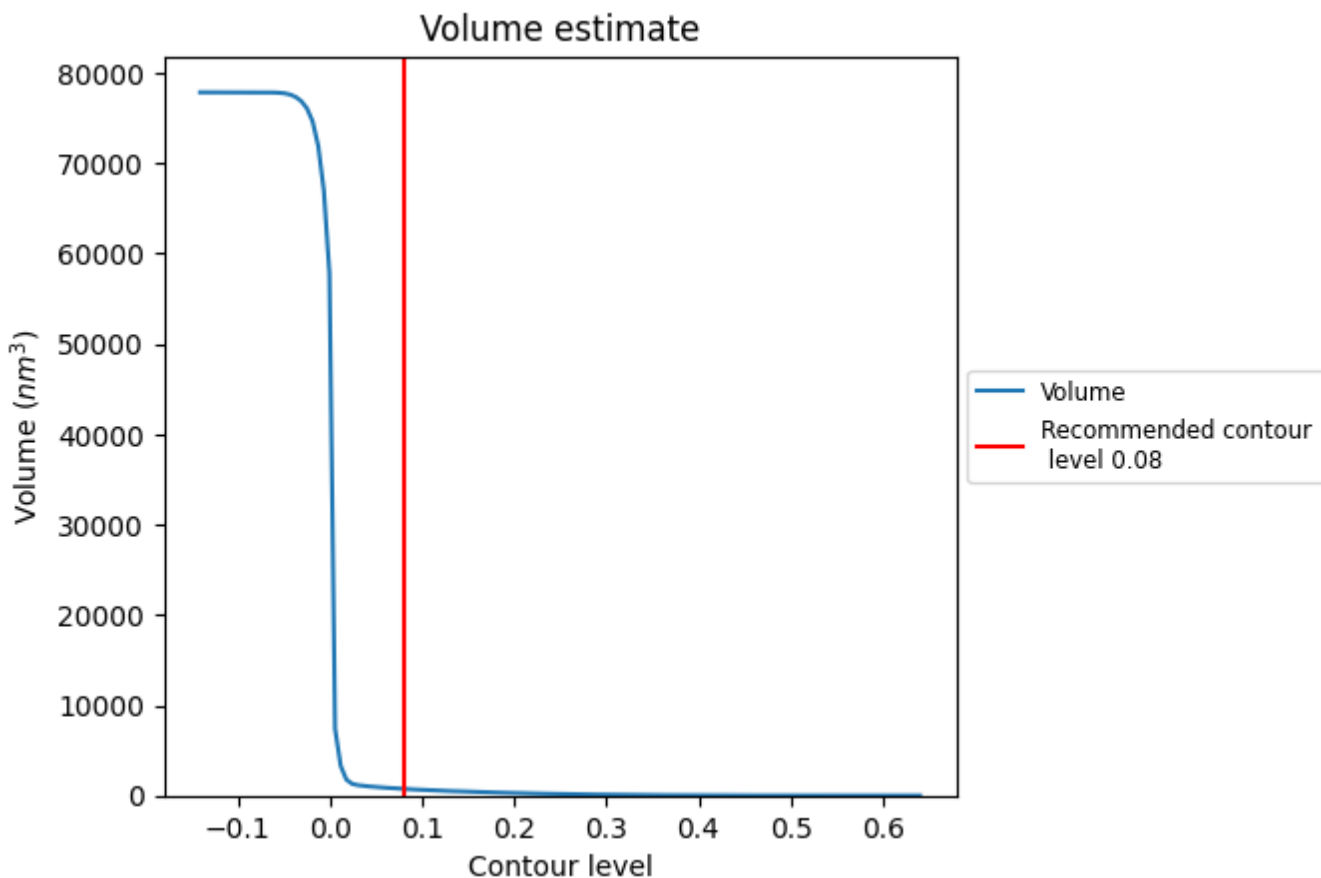
This section contains the results of statistical analysis of the map.

### 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.

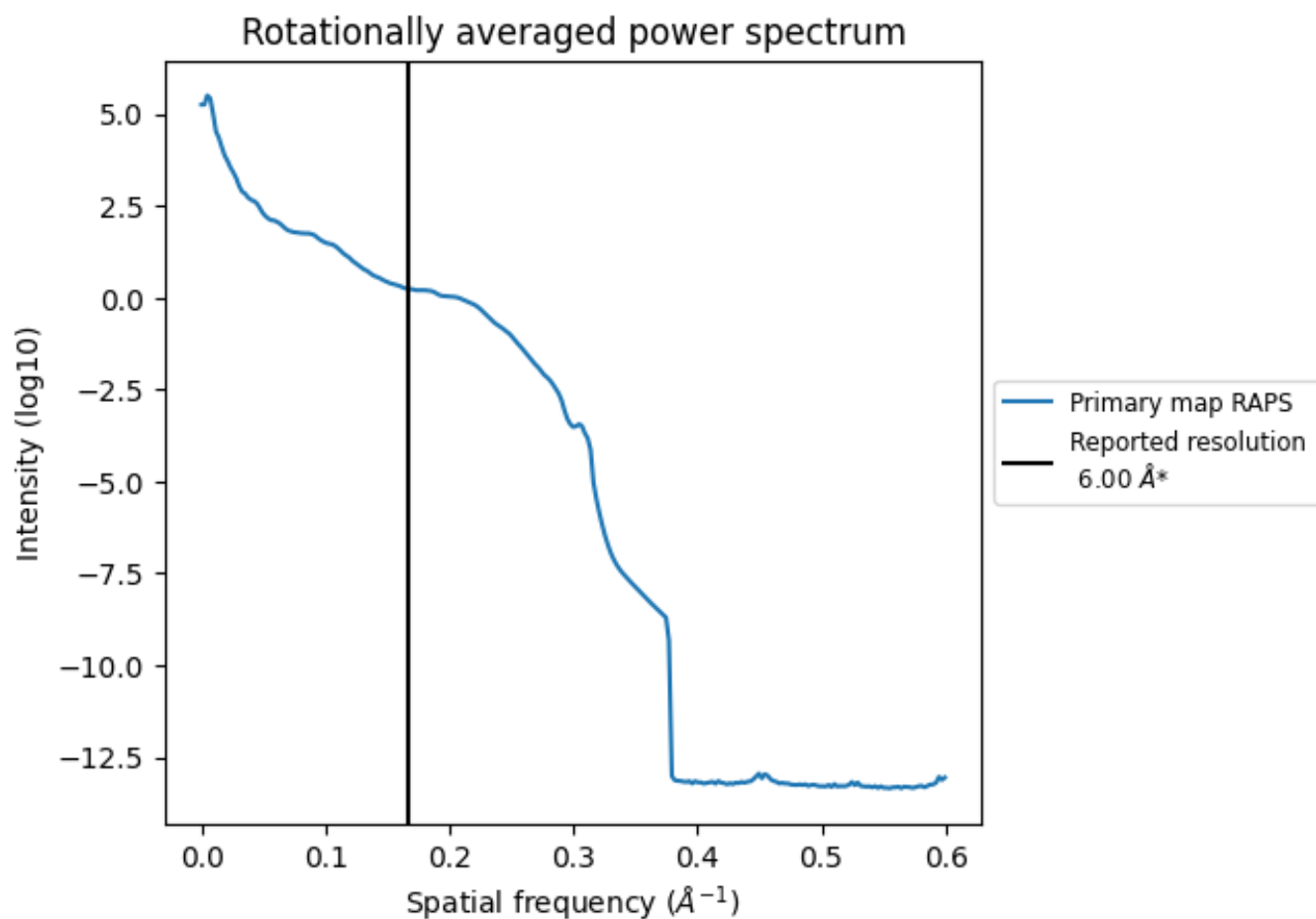
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 739  $\text{nm}^3$ ; this corresponds to an approximate mass of 668 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 [i](#)

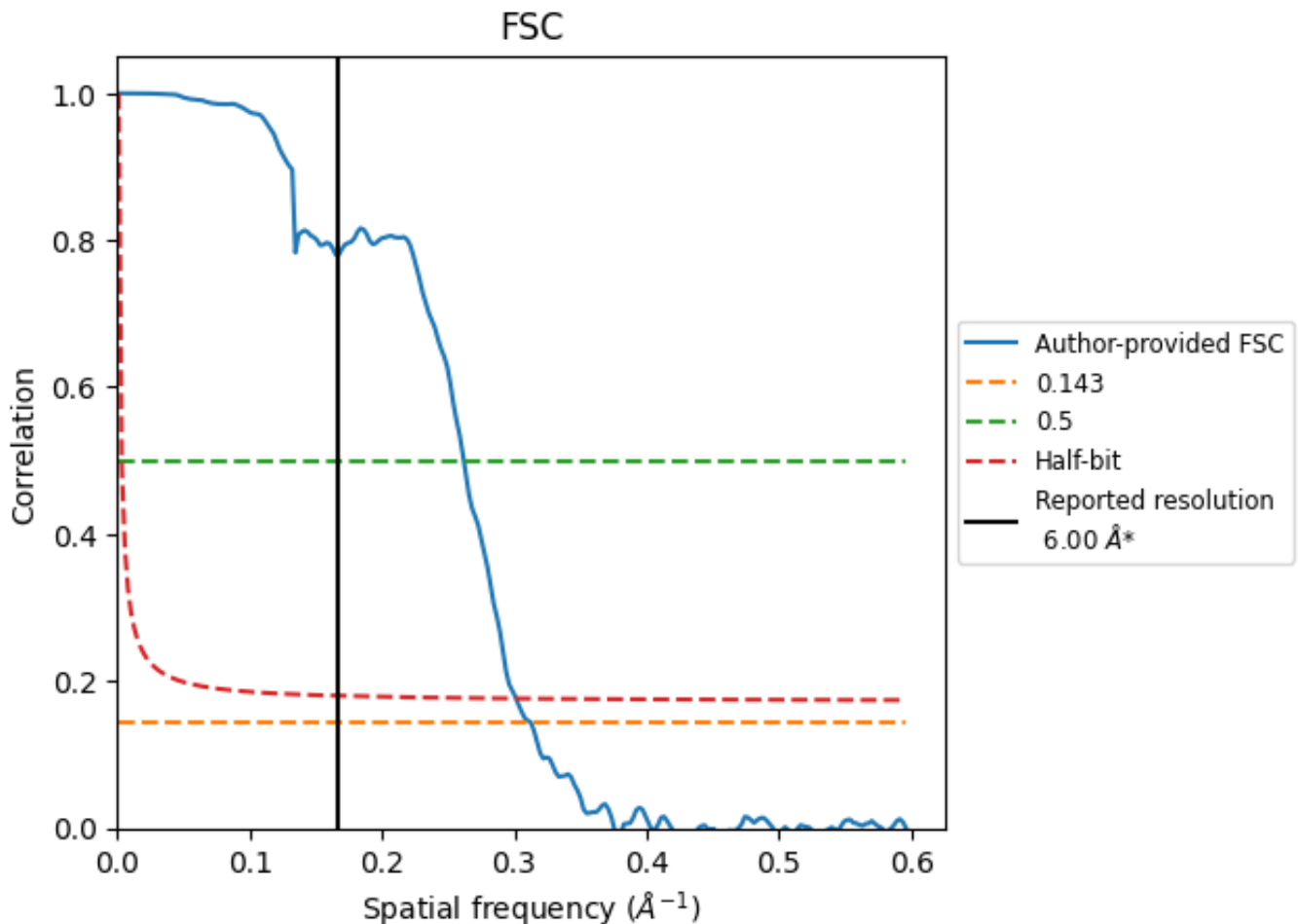


\*Reported resolution corresponds to spatial frequency of 0.167 Å<sup>-1</sup>

## 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 0.167 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

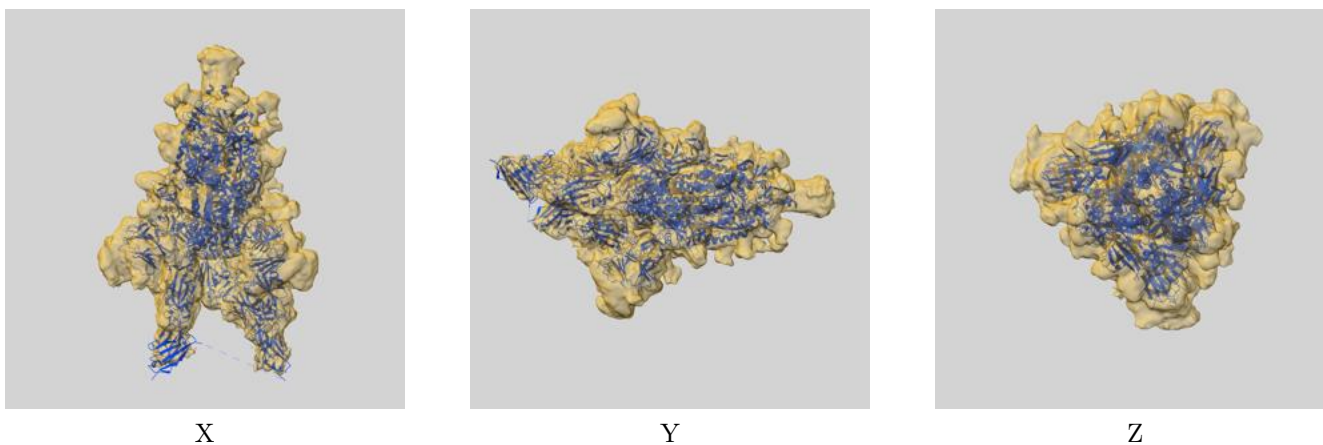
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.20	3.82	3.32
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

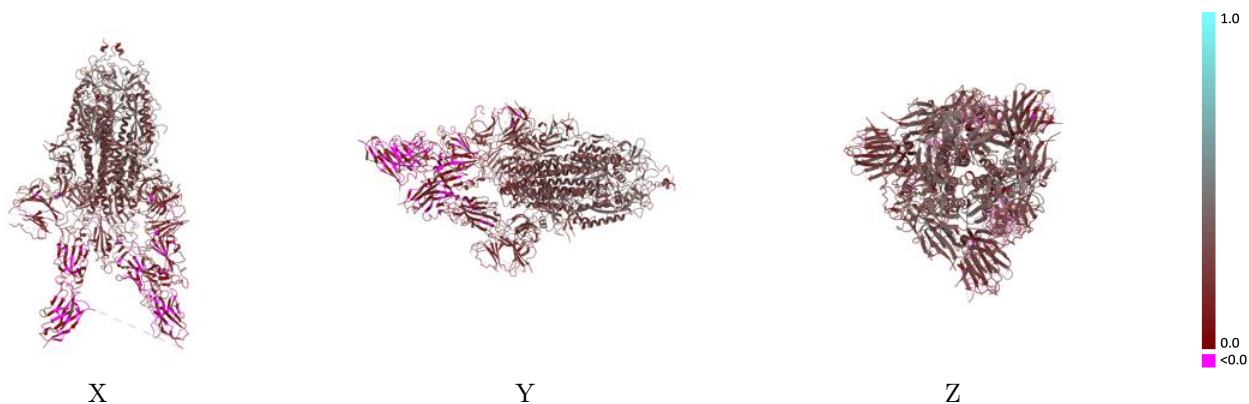
This section contains information regarding the fit between EMDB map EMD-22514 and PDB model 7JWB. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 9.1 Map-model overlay [i](#)



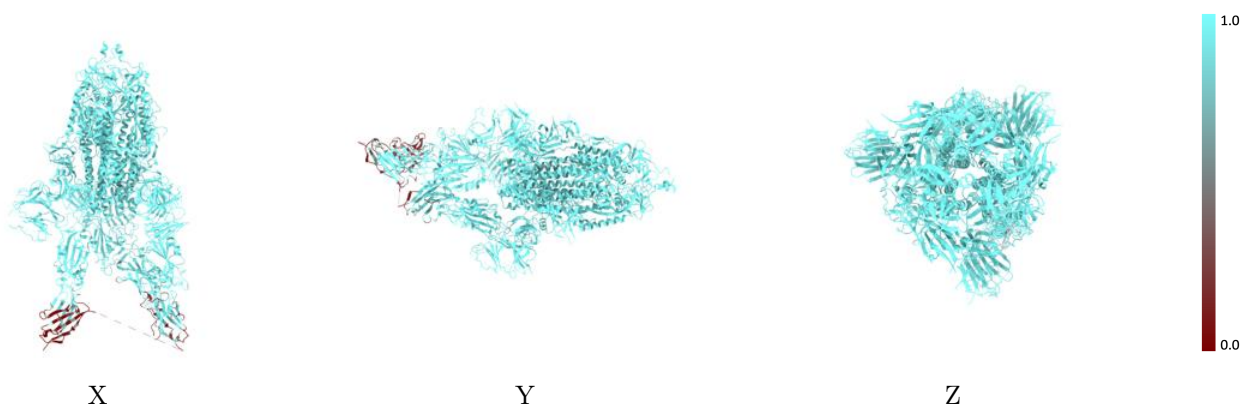
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



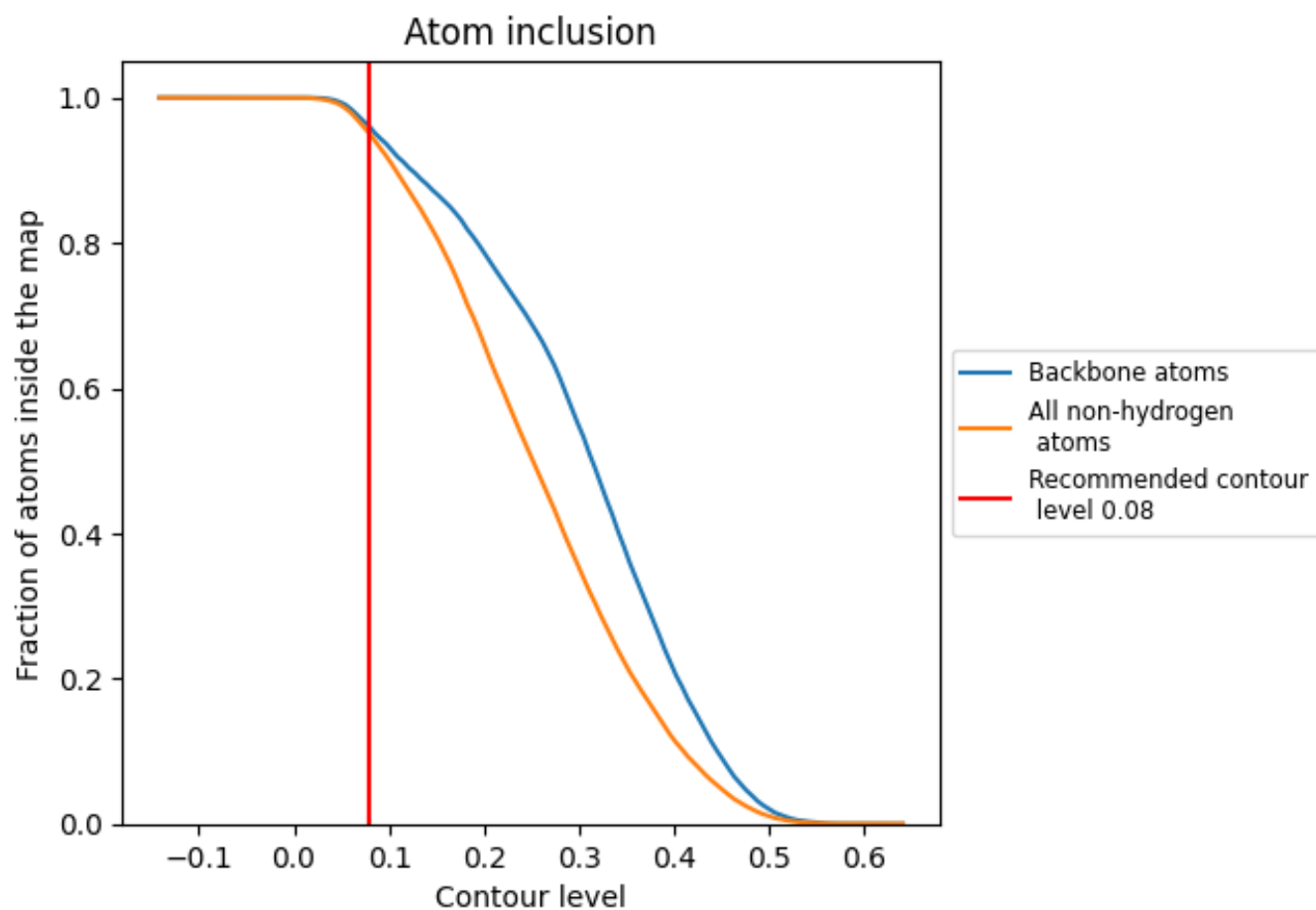
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

## 9.4 Atom inclusion [i](#)












At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9498	 0.2320
A	 0.9898	 0.2560
B	 0.9825	 0.2520
C	 0.9896	 0.2500
D	 0.6407	 0.0650

