



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 11:11 PM EDT

PDB ID : 5UJA  
EMDB ID : EMD-8560  
Title : Cryo-EM structure of bovine multidrug resistance protein 1 (MRP1) bound to leukotriene C4  
Authors : Johnson, Z.L.; Chen, J.  
Deposited on : 2017-01-17  
Resolution : 3.34 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](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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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

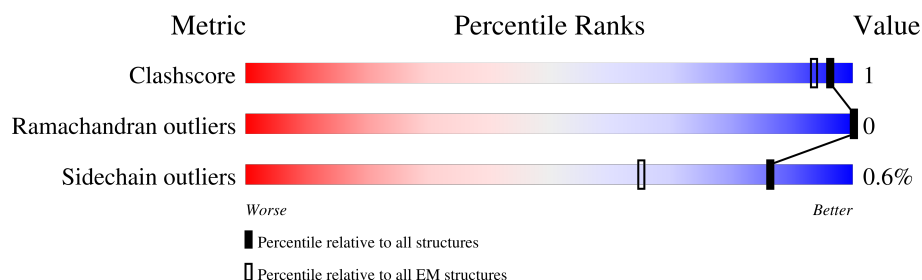
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.34 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	A	1460	<div> <div>23%</div> <div>86%</div> <div>11%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9900 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.

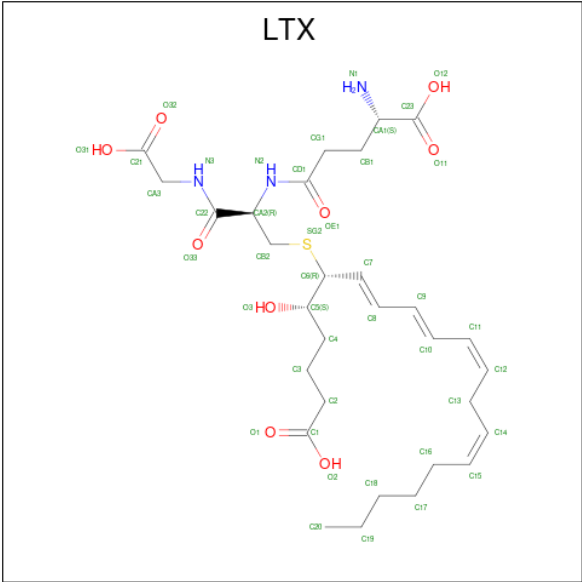
- Molecule 1 is a protein called bovine multidrug resistance protein 1 (MRP1), Multidrug resistance-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1295	9857	6345	1672	1794	46	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1531	SER	-	expression tag	UNP Q8HXQ5
A	1532	ASN	-	expression tag	UNP Q8HXQ5
A	1533	SER	-	expression tag	UNP Q8HXQ5
A	1534	LEU	-	expression tag	UNP Q8HXQ5
A	1535	GLU	-	expression tag	UNP Q8HXQ5
A	1536	VAL	-	expression tag	UNP Q8HXQ5
A	1537	LEU	-	expression tag	UNP Q8HXQ5
A	1538	PHE	-	expression tag	UNP Q8HXQ5
A	1539	GLN	-	expression tag	UNP Q8HXQ5

- Molecule 2 is (5 {S},6 {R},7 {E},9 {E},11 {Z},14 {Z})-6-[(2 {R})-2-[(4 {S})-4-azanyl-5-oxidanyl-5-oxidanylidene-pentanoyl]amino]-3-(2-hydroxy-2-oxoethylamino)-3-oxidanylidene-propyl]sulfanyl-5-oxidanyl-icosa-7,9,11,14-tetraenoic acid (three-letter code: LTX) (formula: C<sub>30</sub>H<sub>47</sub>N<sub>3</sub>O<sub>9</sub>S).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			43	30	3	9	1	



L1307	V1308	H1311	T1315	I1316	D1317	G1318	G1319	E1320	K1321	V1322	G1326	R1327	T1328	G1329	A1330	L1337	K1343	A1346	E1347	G1348	E1349	I1350	I1351	I1352	D1353	D1354	I1355	N1356	K1359	I1360	R1366	Q1374	D1375	P1376	V1377	L1383	R1384	M1385	N1386	L1387	F1390	S1391	Q1392	Y1393	S1394	D1395	E1396						
E1403	H1406	L1407	K1408	G1409	F1410	V1411	S1412	A1413	L1414	P1415	D1416	K1417	L1418	N1419	A1423	E1424	G1425	G1426	E1427	N1428	L1429	G1432	Q1433	R1434	Q1435	L1436	V1437	C1438	L1439	L1443	L1444	R1445	K1446	D1453	E1454	A1455	T1456	A1457	A1458	V1459	D1460	L1461	E1462	T1463	D1464	D1465	L1466	I1467	Q1468	I1471	R1472	T1473	Q1474
F1475	D1476	D1477	C1478	I1483	A1484	M1488	M1491	D1492	Y1493	T1494	R1495	L1499	D1500	K1501	G1502	E1503	I1504	W1507	G1508	S1509	P1510	S1511	D1512	L1513	L1514	Q1515	Q1516	ARG	GLY	LEU	PHE	TYR	SER	MET	ALA	LYS	ASP	SER	GLY	LEU	VAL	SER	ASN	SER	LEU	GLU	VAL	LEU	PHE	GLN			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	203732	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 ( $e^-/\text{\AA}^2$ )	84	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	37000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.214	Depositor
Minimum map value	-4.154	Depositor
Average map value	0.212	Depositor
Map value standard deviation	0.618	Depositor
Recommended contour level	1.6	Depositor
Map size (Å)	146.00064, 98.99904, 107.001595	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.38021, 0.25781, 0.27865	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LTX

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	0.39	0/9422	0.55	0/12780

There are no bond length outliers.

There are no bond angle outliers.

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	A	9857	0	9587	16	0
2	A	43	0	0	0	0
All	All	9900	0	9587	16	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.

The worst 5 of 16 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:A:209:PRO:O	1:A:213:ALA:N	2.32	0.62
1:A:1299:LEU:HA	1:A:1346:ALA:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:HG22	1:A:379:LEU:HD22	1.90	0.52
1:A:257:LEU:HD22	1:A:398:ALA:HB1	1.93	0.51
1:A:1298:GLY:N	1:A:1347:GLU:O	2.44	0.51

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	A	1162/1460 (80%)	1116 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	1021/1159 (88%)	1015 (99%)	6 (1%)	86	92

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	628	ASP
1	A	787	ASP
1	A	1393	TYR

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Mol	Chain	Res	Type
1	A	389	PHE
1	A	384	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LTX	A	1601	-	38,42,42	2.03	6 (15%)	42,50,50	1.41	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LTX	A	1601	-	-	16/51/51/51	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	LTX	CD1-N2	6.54	1.48	1.34
2	A	1601	LTX	C22-N3	6.39	1.47	1.33
2	A	1601	LTX	C11-C10	4.19	1.56	1.44
2	A	1601	LTX	C9-C8	3.83	1.55	1.44
2	A	1601	LTX	O33-C22	-2.32	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	LTX	CG1-CD1-N2	4.35	123.37	115.83
2	A	1601	LTX	CA2-C22-N3	2.77	122.13	116.54
2	A	1601	LTX	OE1-CD1-N2	-2.62	118.53	122.95
2	A	1601	LTX	O31-C21-CA3	2.35	120.92	112.74
2	A	1601	LTX	OE1-CD1-CG1	-2.14	118.10	122.02

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

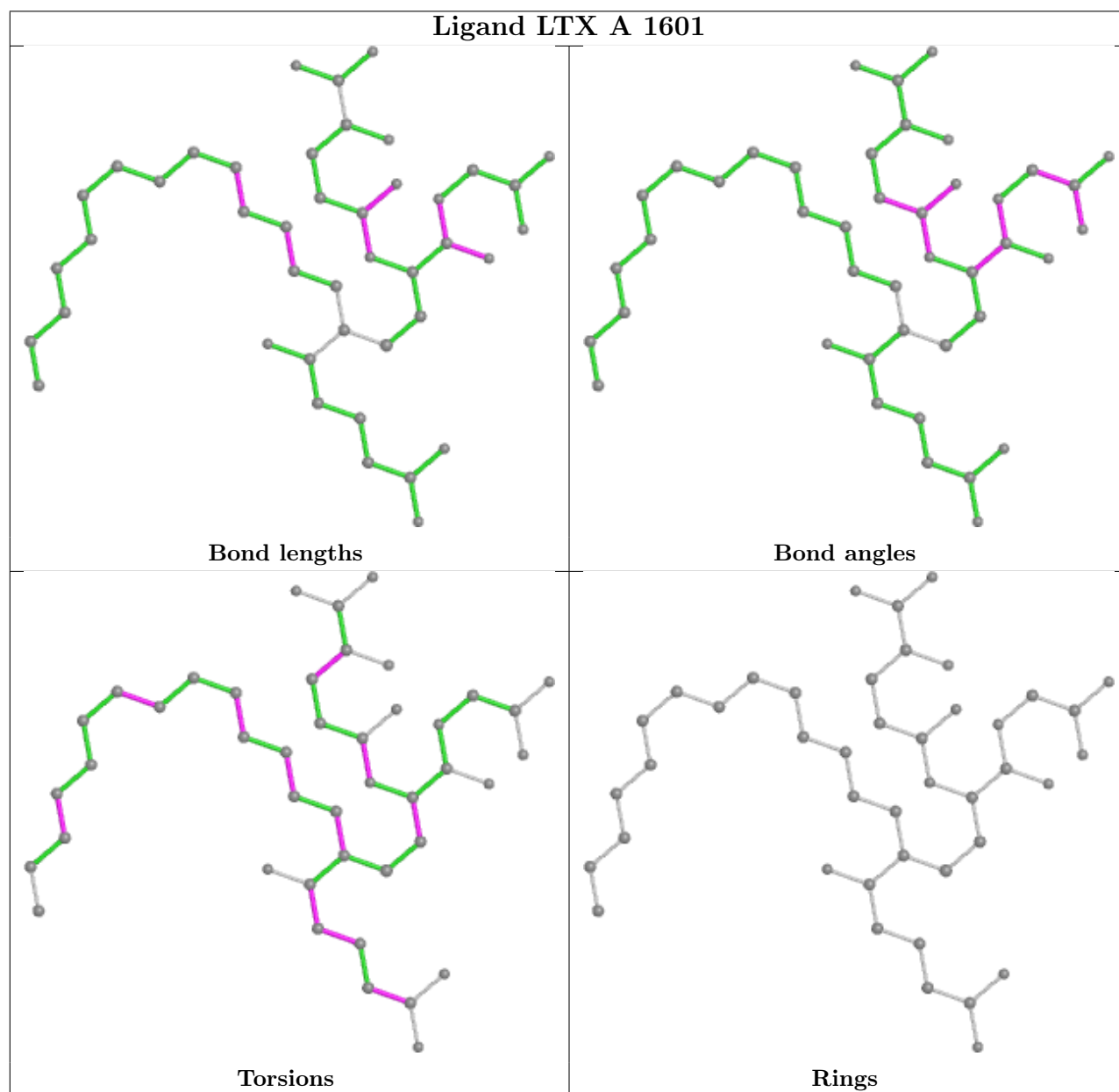
Mol	Chain	Res	Type	Atoms
2	A	1601	LTX	C3-C4-C5-O3
2	A	1601	LTX	C5-C6-C7-C8
2	A	1601	LTX	SG2-C6-C7-C8
2	A	1601	LTX	C7-C8-C9-C10
2	A	1601	LTX	C22-CA2-CB2-SG2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	194:UNK	C	205:PRO	N	23.77
1	A	54:UNK	C	75:UNK	N	21.76
1	A	159:UNK	C	171:UNK	N	16.02
1	A	131:UNK	C	136:UNK	N	13.11
1	A	99:UNK	C	104:UNK	N	9.04

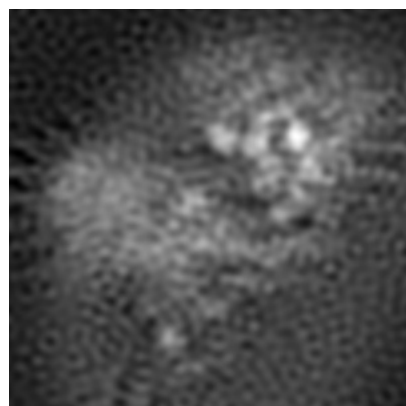
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8560. These allow visual inspection of the internal detail of the map and identification of artifacts.

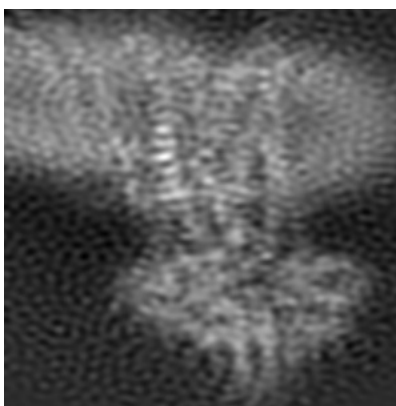
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

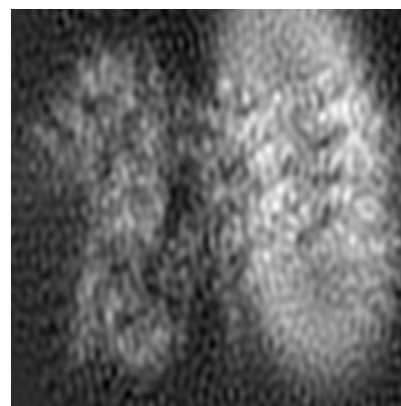
#### 6.1.1 Primary map



X

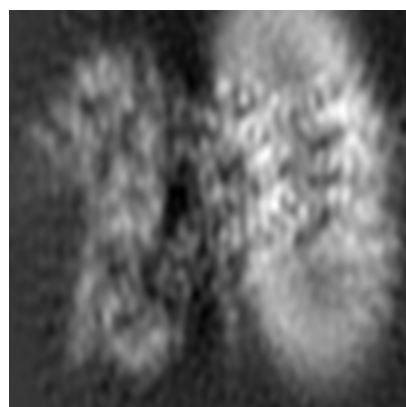


Y

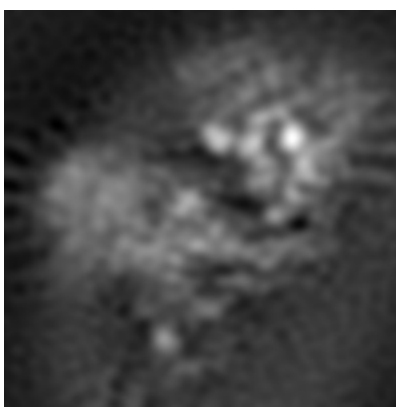


Z

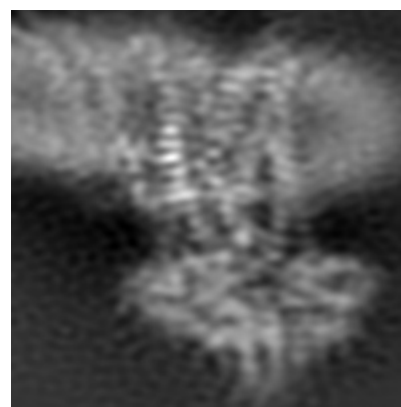
#### 6.1.2 Raw map



X



Y

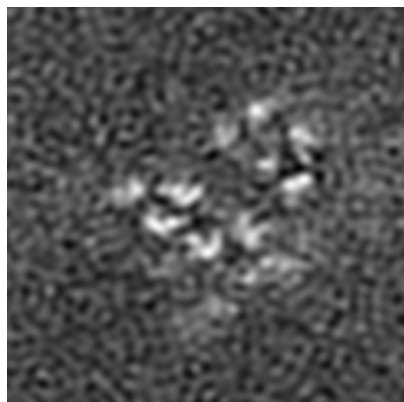


Z

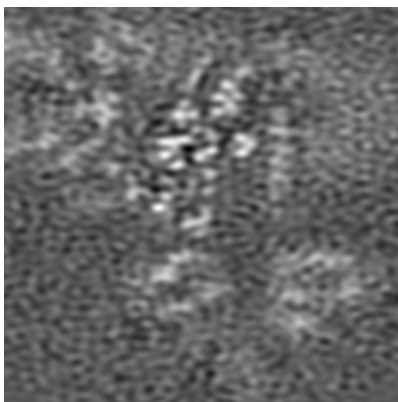
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

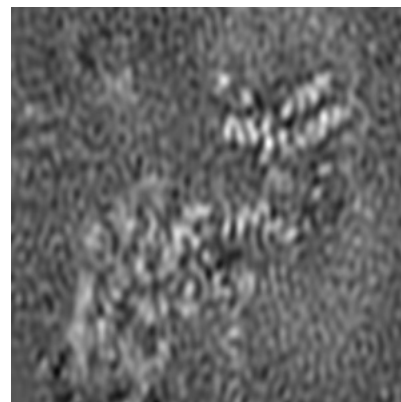
### 6.2.1 Primary map



X Index: 192

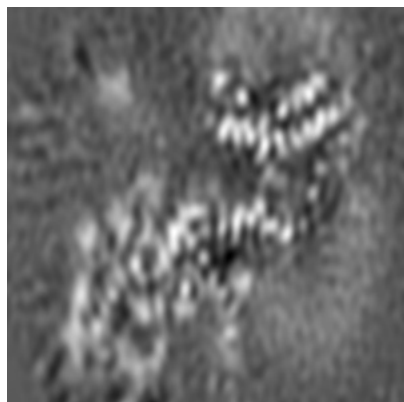


Y Index: 192

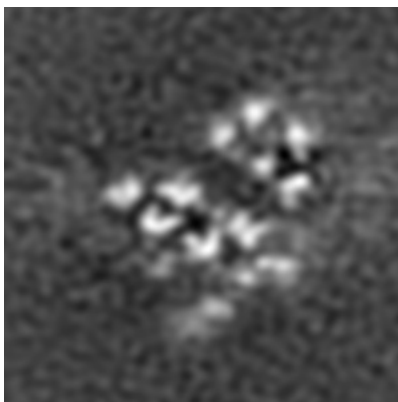


Z Index: 192

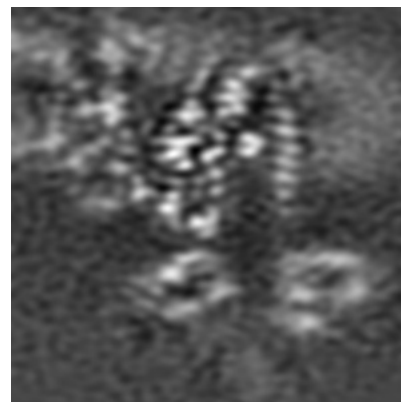
### 6.2.2 Raw map



X Index: 192



Y Index: 192

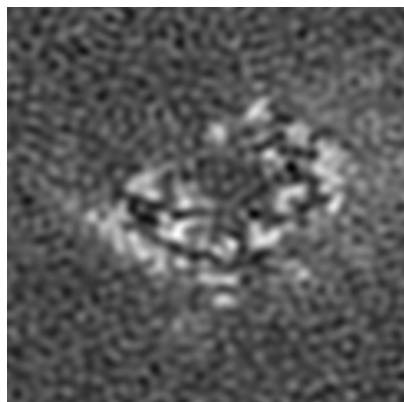


Z Index: 192

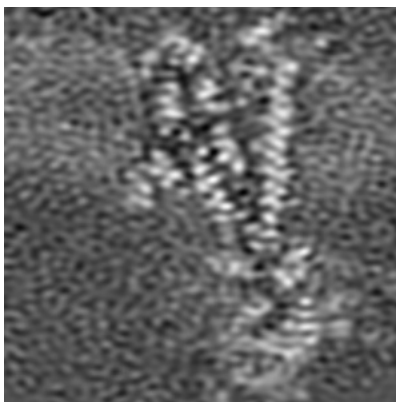
The images above show central slices of the map in three orthogonal directions.

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

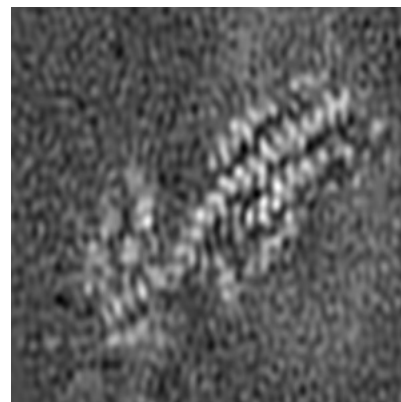
### 6.3.1 Primary map



X Index: 205

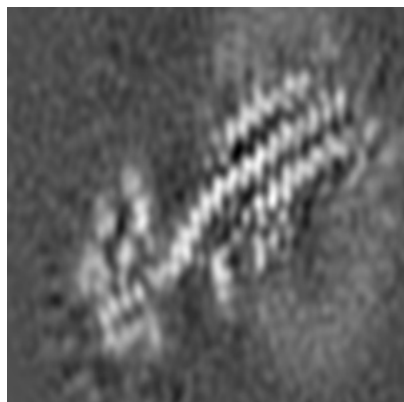


Y Index: 273

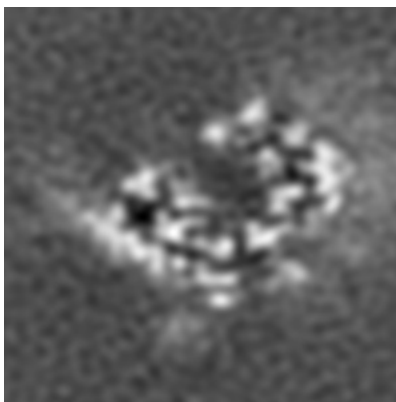


Z Index: 156

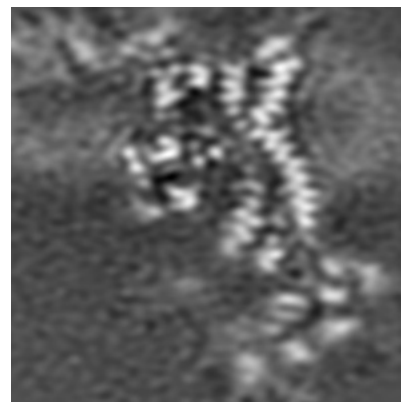
### 6.3.2 Raw map



X Index: 152



Y Index: 205

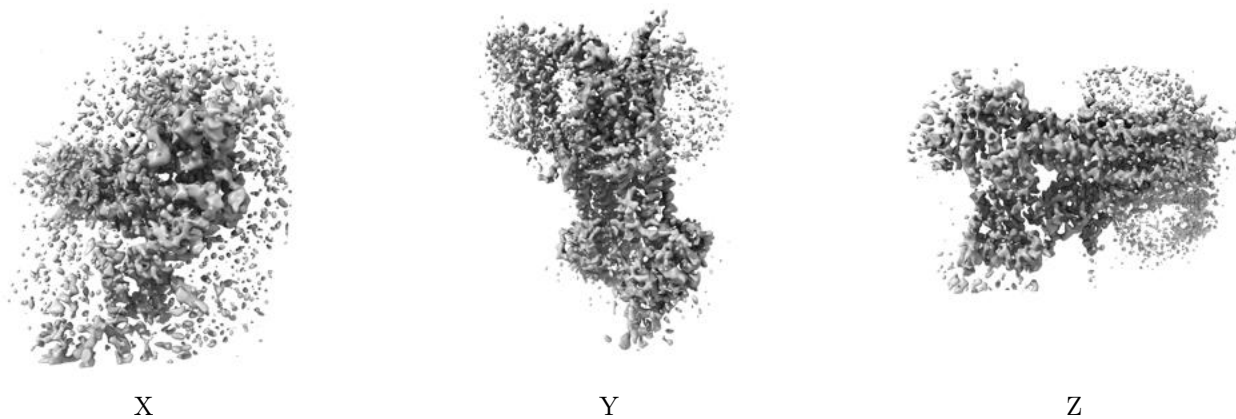


Z Index: 241

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

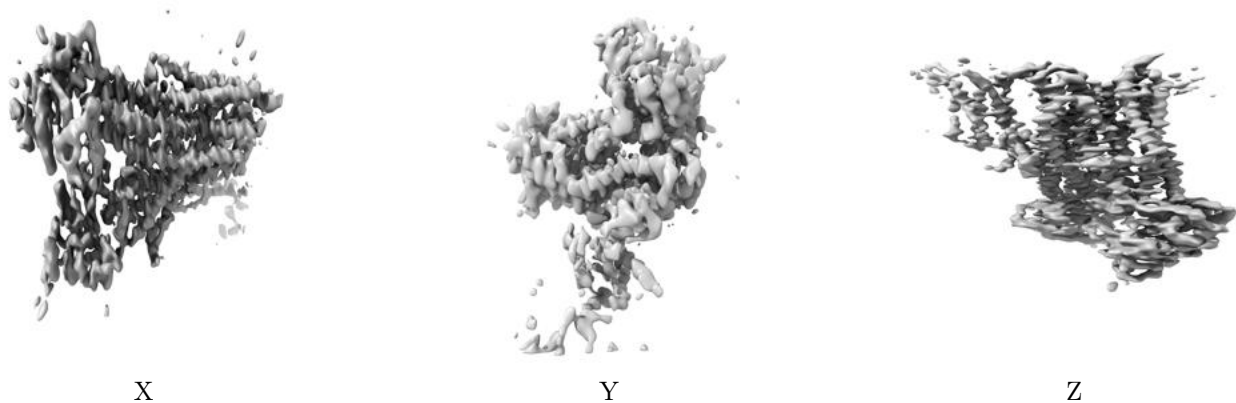
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

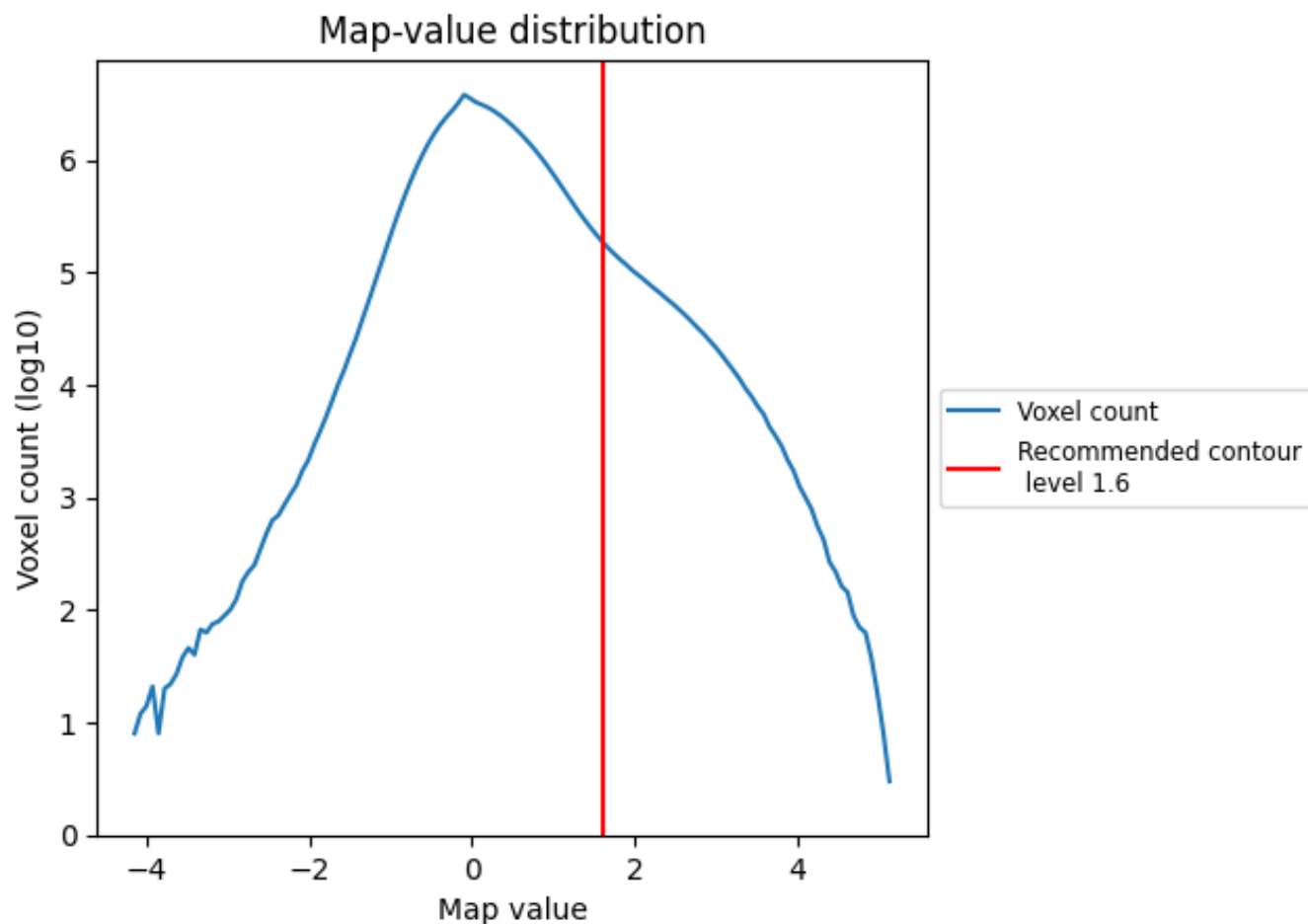
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

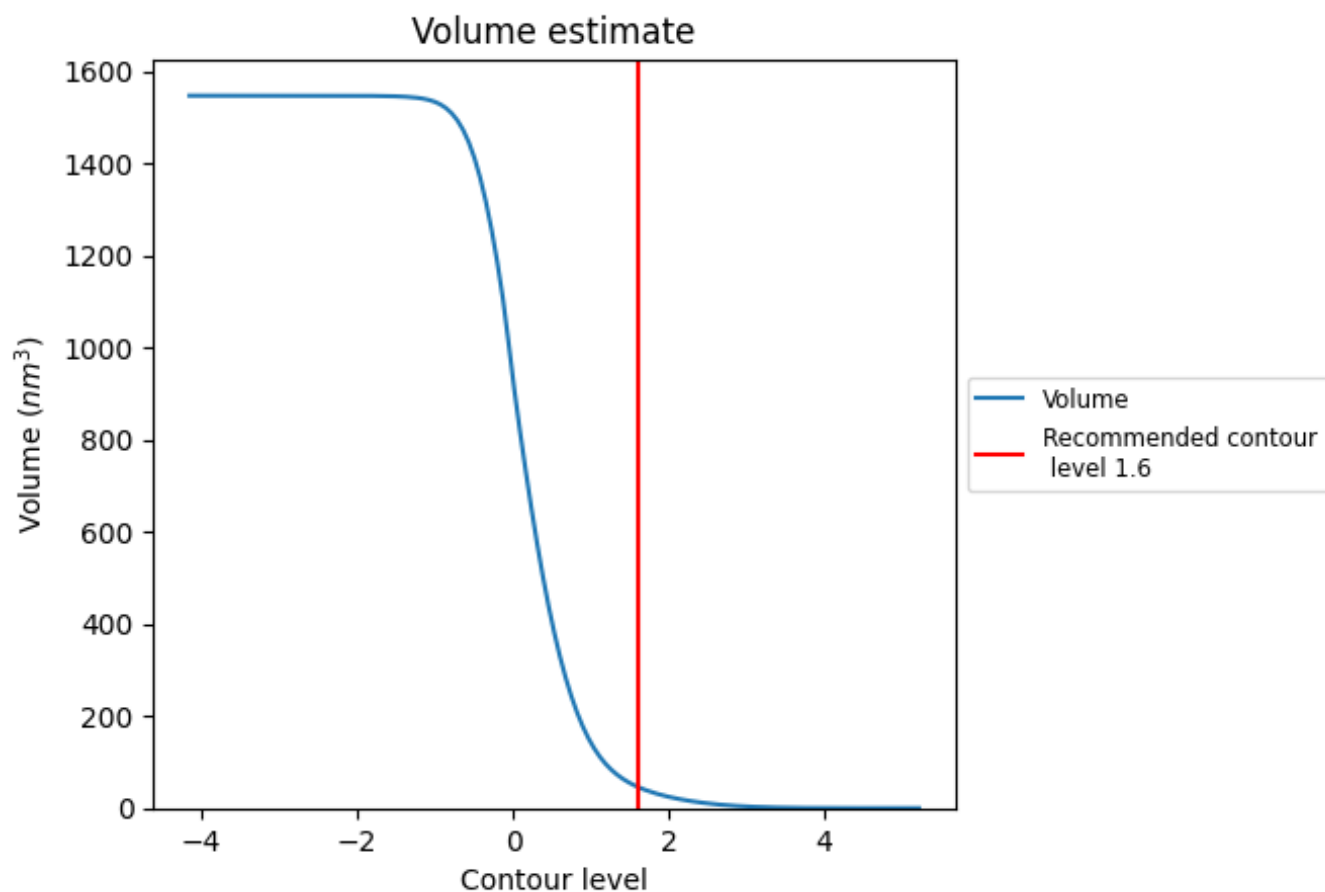
This section contains the results of statistical analysis of the map.

### 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.

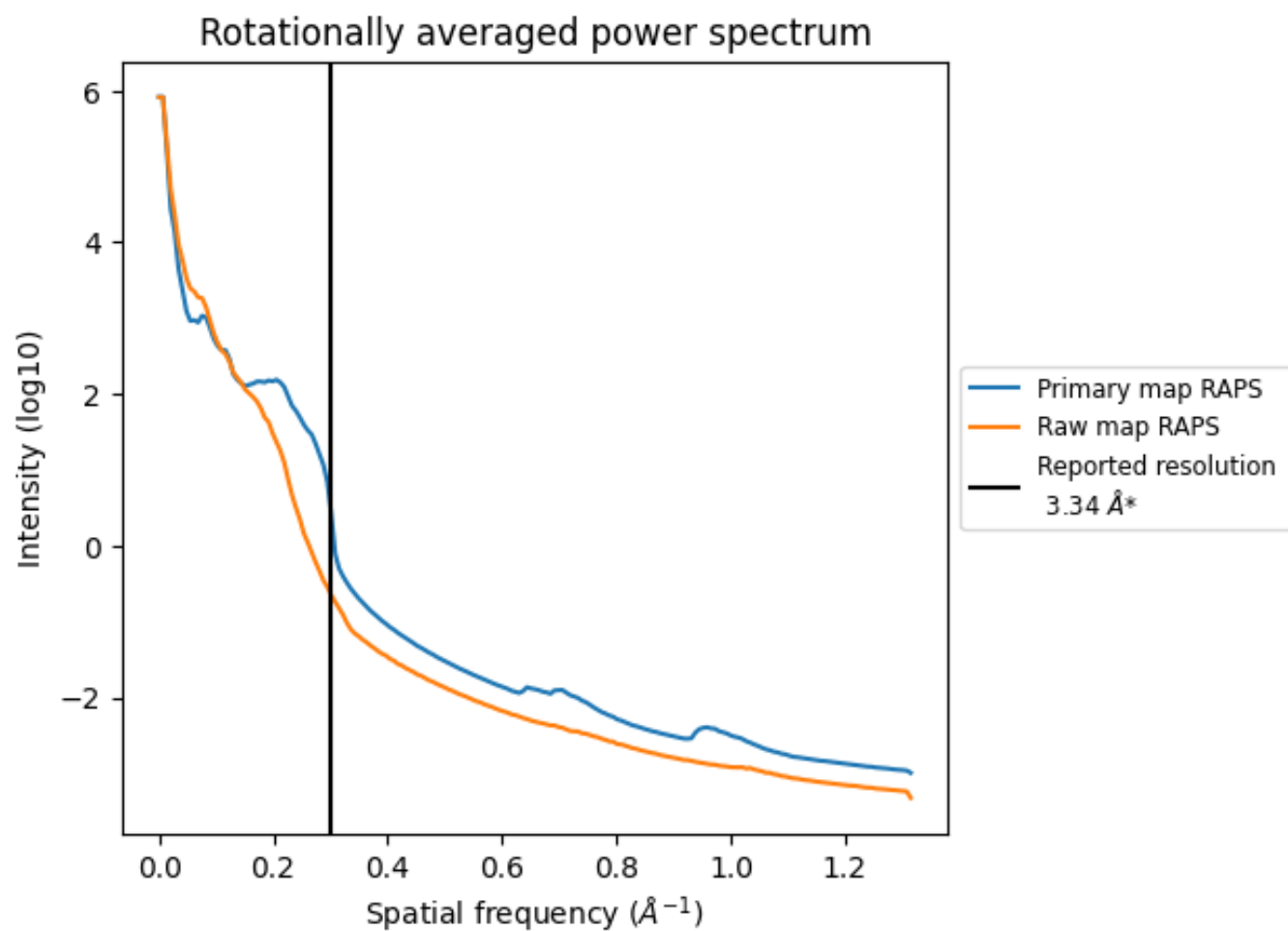
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46  $\text{nm}^3$ ; this corresponds to an approximate mass of 42 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 ⓘ

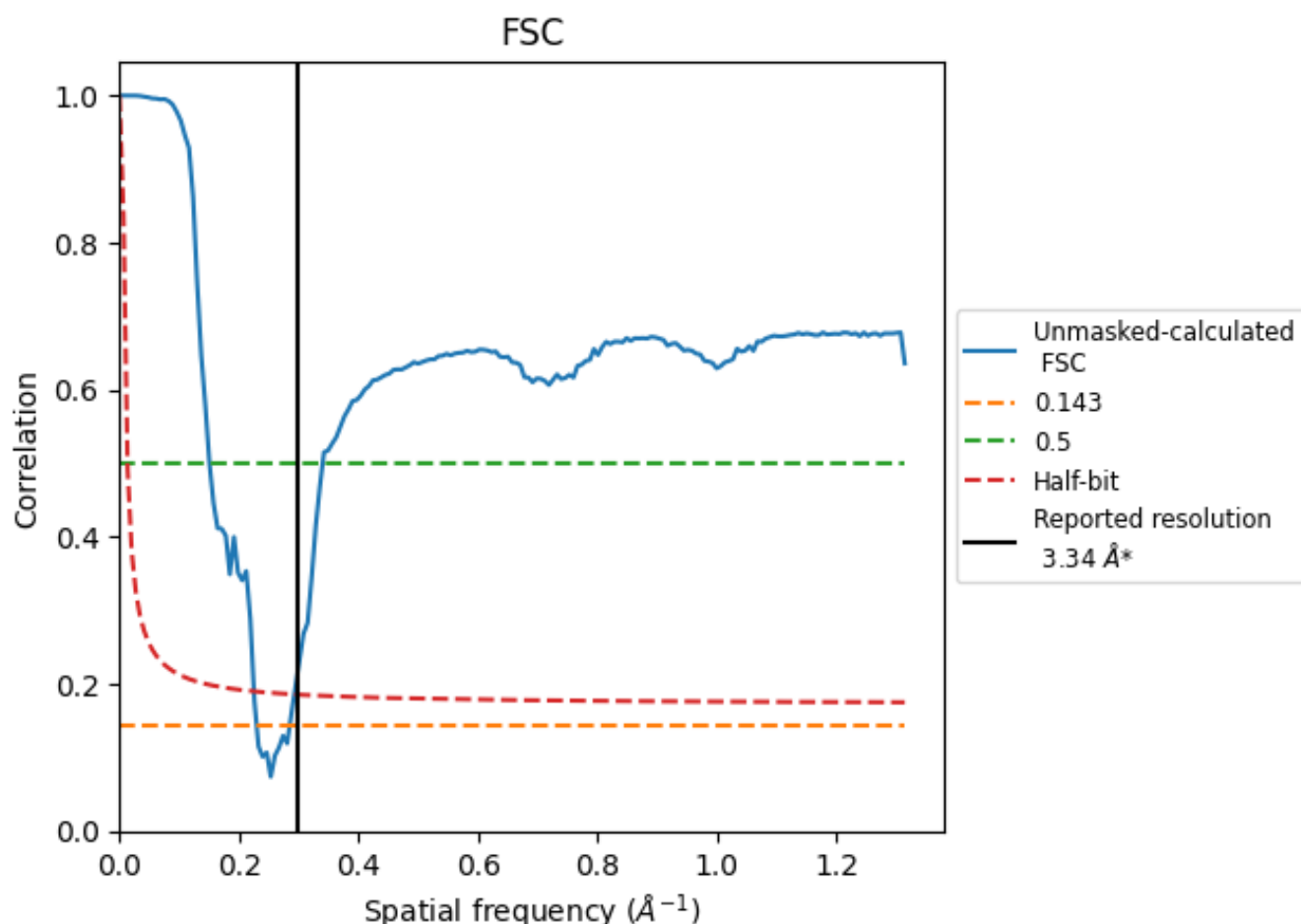


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 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 0.299 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

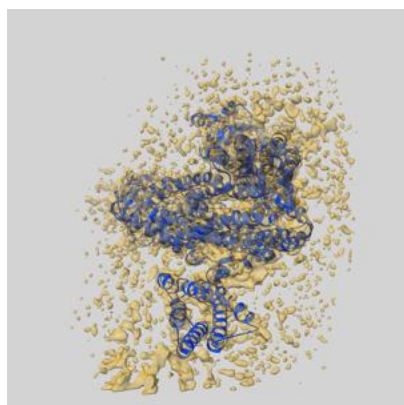
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.35	6.64	4.44

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.34 by more than 10 %

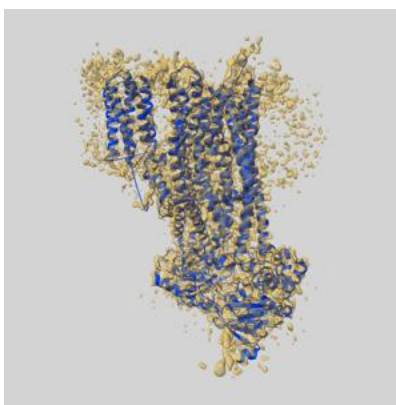
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8560 and PDB model 5UJA. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

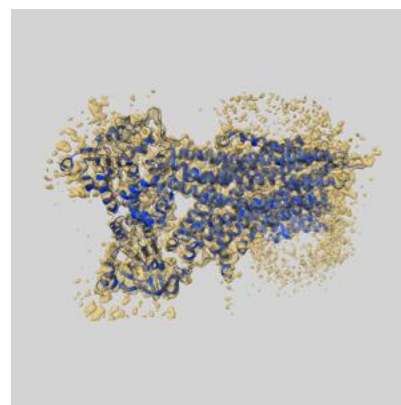
### 9.1 Map-model overlay [i](#)



X



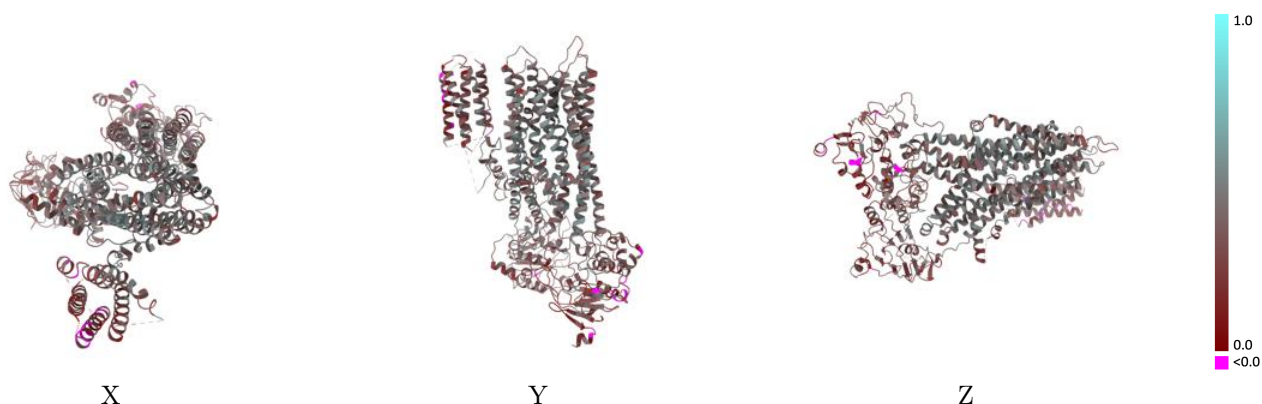
Y



Z

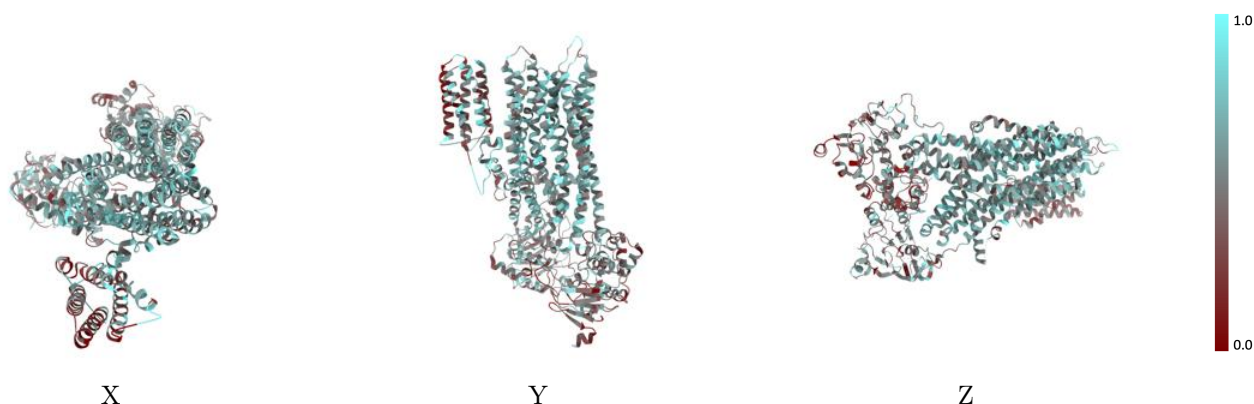
The images above show the 3D surface view of the map at the recommended contour level 1.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



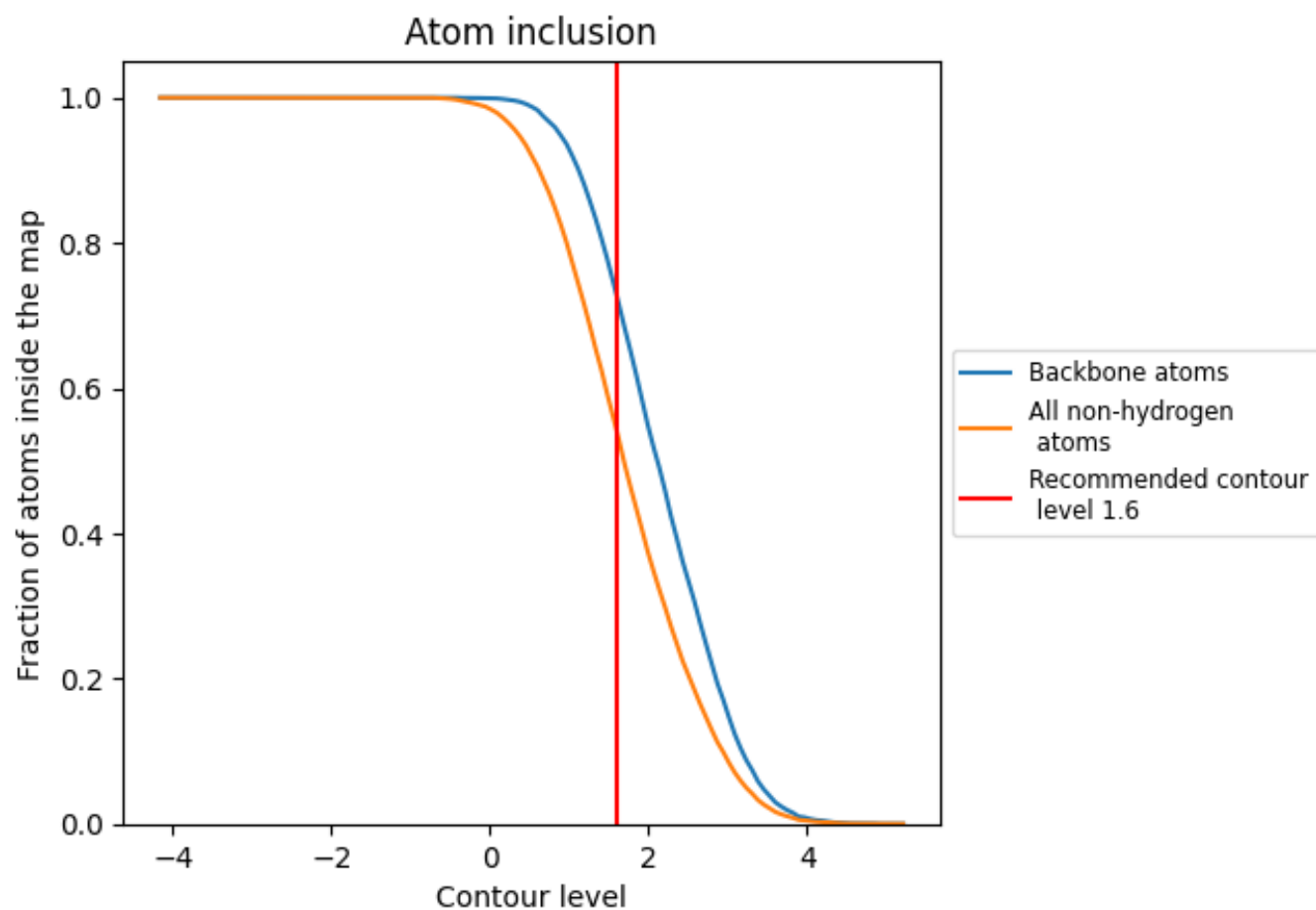
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 54% 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 (1.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5419	<div></div> 0.3720
A	<div></div> 0.5419	<div></div> 0.3720

