



## wwPDB EM Validation Summary Report ⓘ

May 13, 2025 – 12:08 PM EDT

PDB ID : 8TQC / pdb\_00008tqc  
EMDB ID : EMD-41502  
Title : Structure of the human CDK8 kinase module  
Authors : Chen, S.F.; Chao, T.C.; Kim, H.J.; Tang, H.C.; Khadka, S.; Li, T.; Murakami, K.; Boyer, T.G.; Tsai, K.L.  
Deposited on : 2023-08-06  
Resolution : 3.80 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

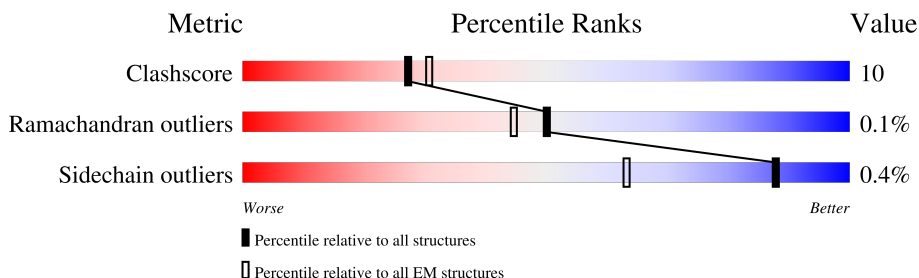
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	2177	<div> <div>37%</div> <div>52%</div> <div>12%</div> <div>36%</div> </div>
2	D	2174	<div> <div>37%</div> <div>8%</div> <div>55%</div> </div>
3	A	464	<div> <div>57%</div> <div>10%</div> <div>33%</div> </div>
4	B	283	<div> <div>72%</div> <div>21%</div> <div>7%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23620 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 Mediator of RNA polymerase II transcription subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1400	Total	C	N	O	S	0	0
			11147	7063	1947	2065	72		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	969	Total	C	N	O	S	0	0
			7714	4945	1310	1393	66		

- Molecule 3 is a protein called Cyclin-dependent kinase 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	313	Total	C	N	O	S	0	0
			2561	1663	439	442	17		

- Molecule 4 is a protein called Cyclin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	262	Total	C	N	O	S	1	0
			2196	1442	358	379	17		

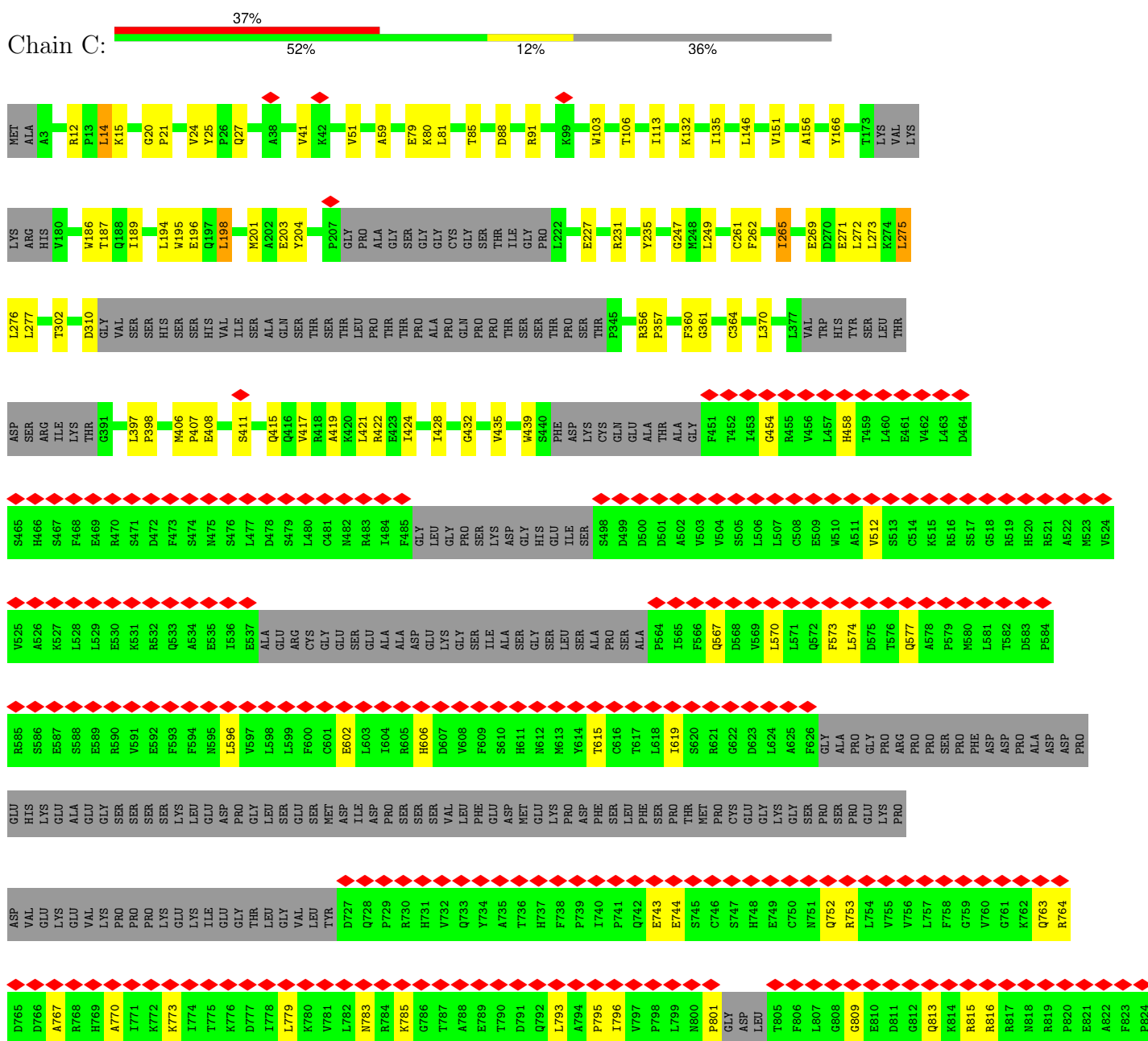
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	

### 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.

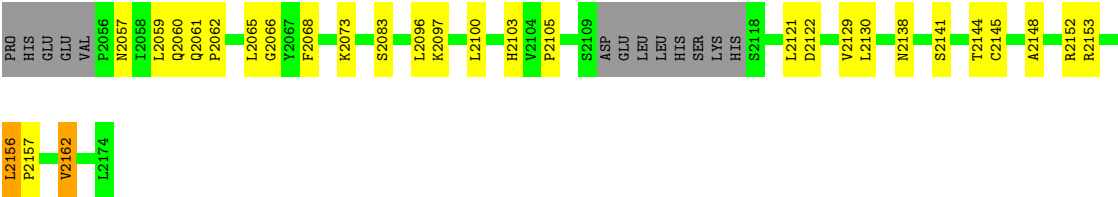
- Molecule 1: Mediator of RNA polymerase II transcription subunit 12



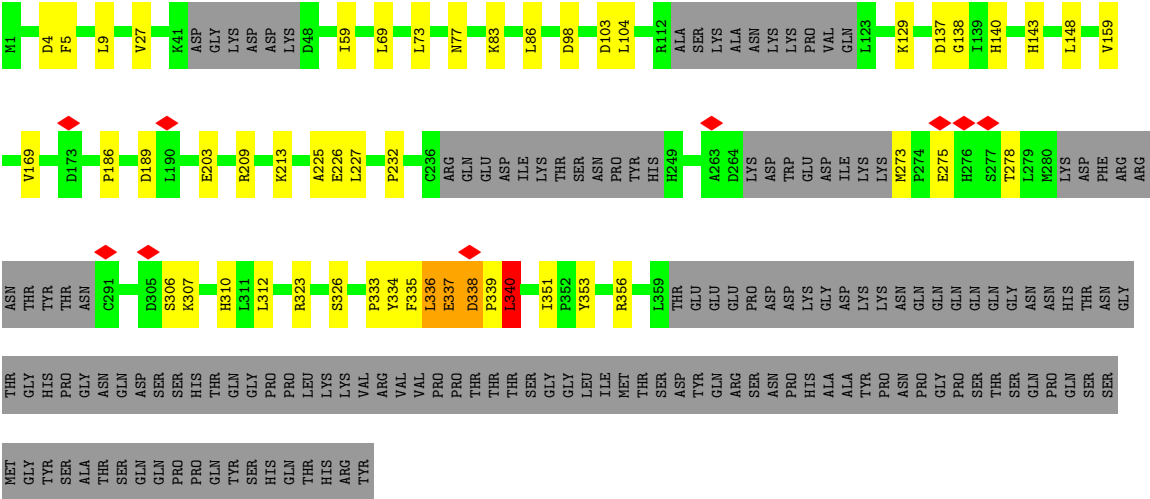
L1583	L1584	M1585	L1586	S1587	V1588	L1589	L1590	M1591	G1592	L1593	L1594	A1595	ALA	ASP	MET	SER	SER	ILE	SER	GLN	GLY	MET	GLU	GLU	G1596	G1597	G1598	G1599	G1600	Y1613		L1616	K1619	L1620	Q1621	Q1622	E1623	L1624	GLY	GLU	ARG	GLN	SER	D1630		K1634	V1635	Q1637	L1638	L1639		Q1644	C1651	E1652	P1653	T1580	T1581	V1582																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
Q1509		M1512	M1513	TRP	ARG	ASP	ASP	L1591	T1592	L1593	ASP	ASP	CYS	LYS	P1595	E1531				K1534		L1537	M1538	L1539	V1540	G1541	G1542	G1543	F1544	D1545	R1546	K1547	S1548	S1550	T1551	Q1552	Q1553		E1556	L1560	L1561	E1562	I1564	L1565	S1566	L1567	V1570	D1571	M1572	Q1573	S1574	M1575	M1576	E1577	L1578	T1579	T1580	T1581	V1582																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
K1434	L1435	P1436	T1437	S1438	V1439	Q1440	G1441	H1442	L1443	L1444		E1449	E1450	L1451	E1452	K1453	G1454	Q1455	H1456	L1457	G1458	S1459	S1460	S1461	R1462	K1463	E1464	R1465	D1466	R1467	Q1468	K1469	Q1470	K1471	S1472	M1473	S1474	L1475	L1476	S1477	Q1478		L1484	V1485	C1488	L1489	K1490	G1491	Q1492	L1500	L1503	Y1504	S1505	Q1506	V1507	H1508																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
L1365	M1366	I1367	K1368	Q1369	T1370	P1371	M1372	M1373	E1374	M1375	M1376	S1377	L1378	L1379			E1388	V1389	F1390	Q1391	Q1392	S1393	A1394	E1395	T1396	GLY	SER	SER	SER	GLY	SER	MET	PRO	SER	SER	SER	LYS	L1419	L1420	E1421	R1422	S1423	G1424	V1425	W1426	L1427	V1428	A1429	P1430																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								







● Molecule 3: Cyclin-dependent kinase 8



● Molecule 4: Cyclin-C





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122015	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	376.67517, 376.67517, 376.67517	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0701, 1.0701, 1.0701	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: ZN

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	C	0.16	0/11361	0.42	2/15364 (0.0%)
2	D	0.13	0/7895	0.34	2/10703 (0.0%)
3	A	0.11	0/2627	0.34	2/3542 (0.1%)
4	B	0.11	0/2253	0.30	0/3051
All	All	0.14	0/24136	0.37	6/32660 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	GLY	CA-C-N	8.33	125.74	119.66
1	C	20	GLY	C-N-CA	8.33	125.74	119.66
3	A	340	LEU	CA-C-N	7.05	127.08	119.89
3	A	340	LEU	C-N-CA	7.05	127.08	119.89
2	D	1365	SER	N-CA-C	6.00	119.84	111.74

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	C	11147	0	11175	252	0
2	D	7714	0	7627	144	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2561	0	2578	51	0
4	B	2196	0	2233	52	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	23620	0	23613	453	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 10.

The worst 5 of 453 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)
3:A:338:ASP:HB3	3:A:339:PRO:CD	1.56	1.34
3:A:333:PRO:HA	3:A:336:LEU:HD23	1.26	1.15
3:A:338:ASP:CB	3:A:339:PRO:HD2	1.74	1.14
3:A:338:ASP:CB	3:A:339:PRO:CD	2.28	1.09
1:C:1616:LEU:O	1:C:1620:LEU:HG	1.55	1.07

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	C	1366/2177 (63%)	1320 (97%)	46 (3%)	0	100	100
2	D	923/2174 (42%)	884 (96%)	38 (4%)	1 (0%)	48	79
3	A	301/464 (65%)	294 (98%)	6 (2%)	1 (0%)	37	69
4	B	261/283 (92%)	258 (99%)	3 (1%)	0	100	100
All	All	2851/5098 (56%)	2756 (97%)	93 (3%)	2 (0%)	50	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	338	ASP
2	D	2156	LEU

### 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	C	1247/1916 (65%)	1242 (100%)	5 (0%)	89	91
2	D	869/1918 (45%)	867 (100%)	2 (0%)	92	94
3	A	277/412 (67%)	274 (99%)	3 (1%)	70	79
4	B	241/258 (93%)	241 (100%)	0	100	100
All	All	2634/4504 (58%)	2624 (100%)	10 (0%)	88	91

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	336	LEU
3	A	337	GLU
3	A	340	LEU
1	C	275	LEU
1	C	1585	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1575	ASN
4	B	49	GLN
1	C	1729	HIS
2	D	2138	ASN
1	C	1644	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

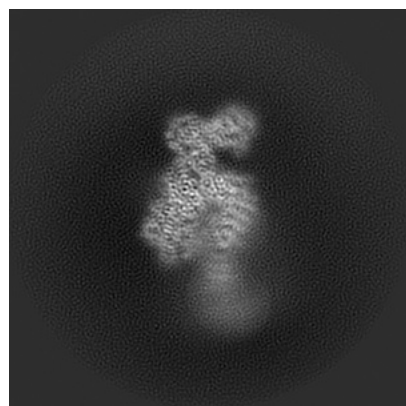
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41502. These allow visual inspection of the internal detail of the map and identification of artifacts.

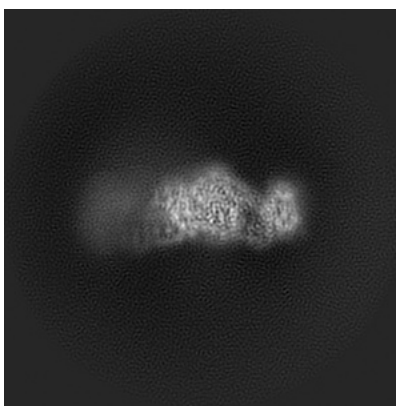
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

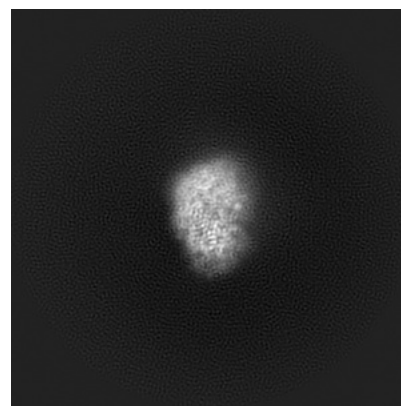
#### 6.1.1 Primary map



X

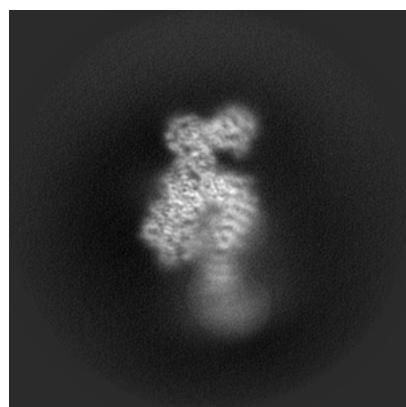


Y

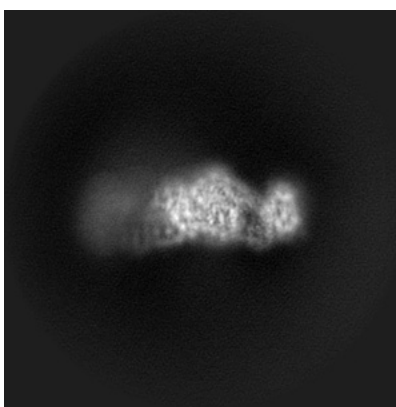


Z

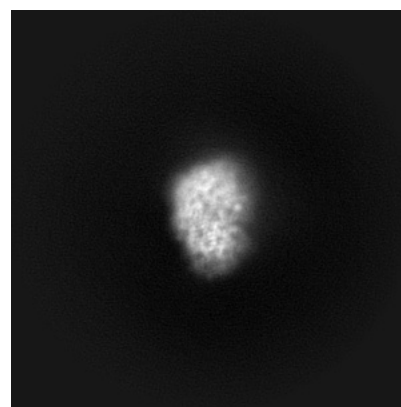
#### 6.1.2 Raw map



X



Y

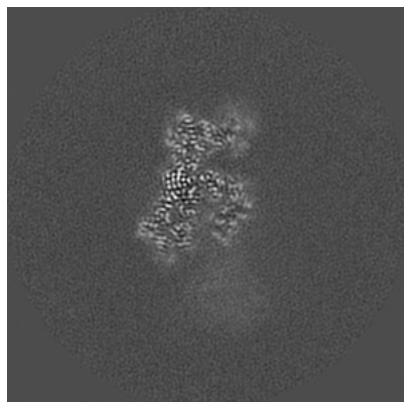


Z

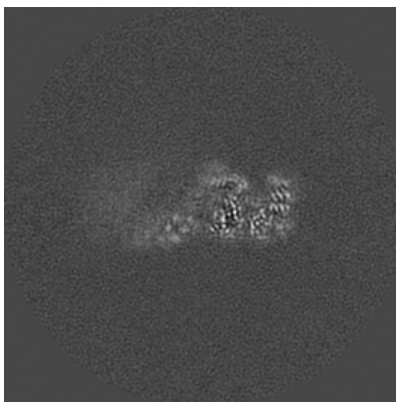
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

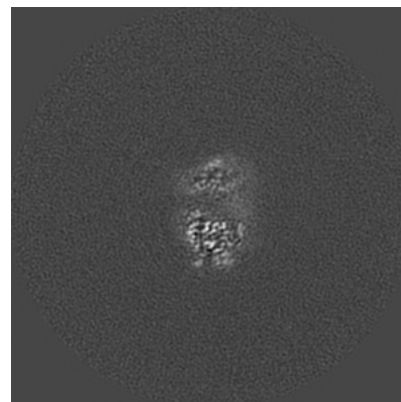
### 6.2.1 Primary map



X Index: 176

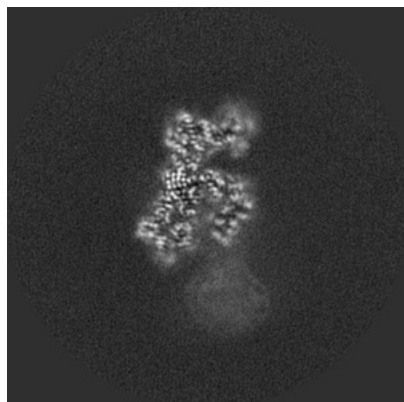


Y Index: 176

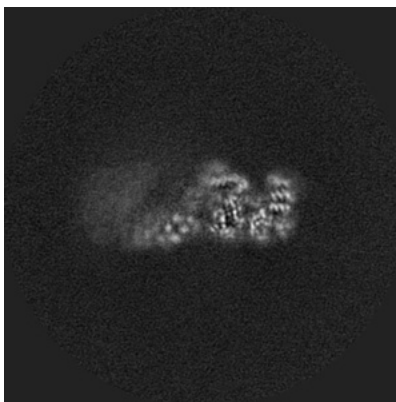


Z Index: 176

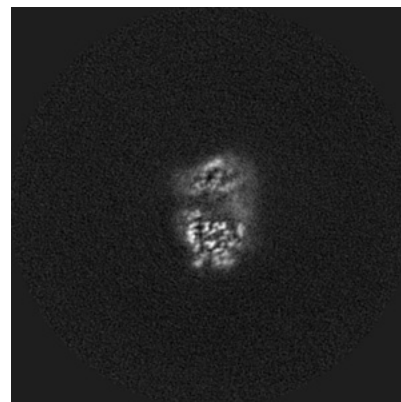
### 6.2.2 Raw map



X Index: 176



Y Index: 176



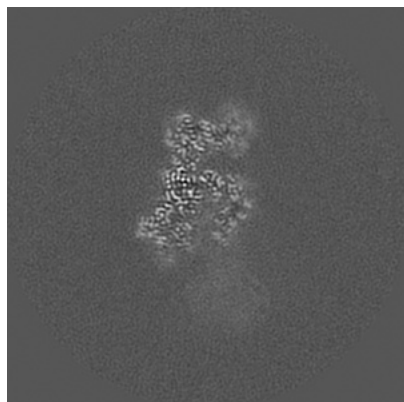
Z Index: 176

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

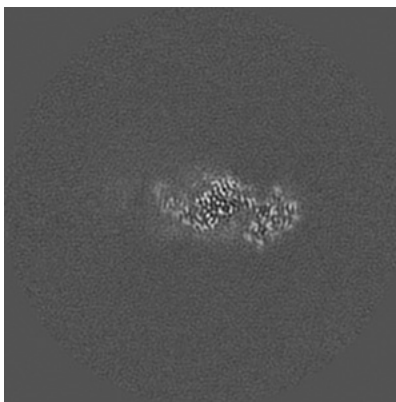


## 6.3 Largest variance slices [i](#)

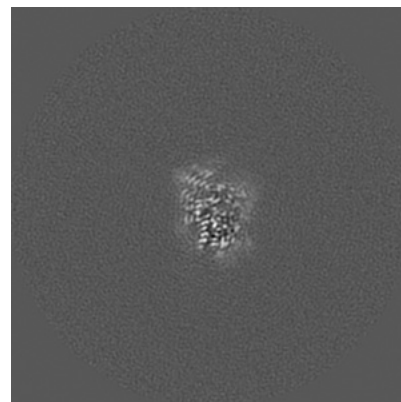
### 6.3.1 Primary map



X Index: 175



Y Index: 158

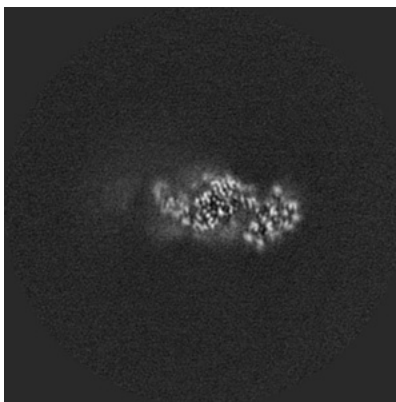


Z Index: 192

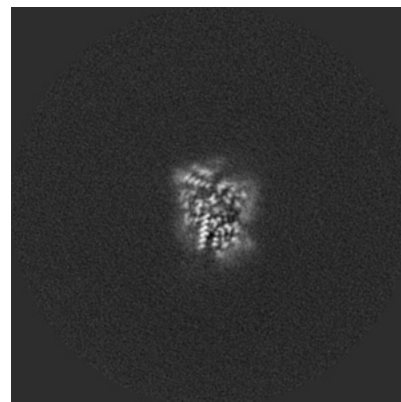
### 6.3.2 Raw map



X Index: 171



Y Index: 158



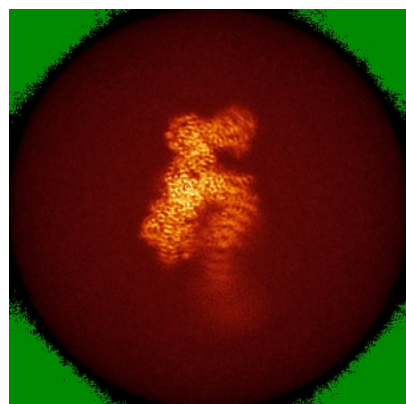
Z Index: 191

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

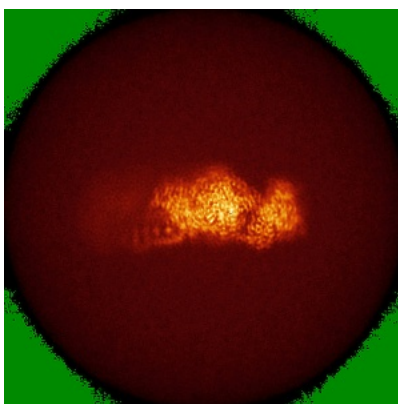


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

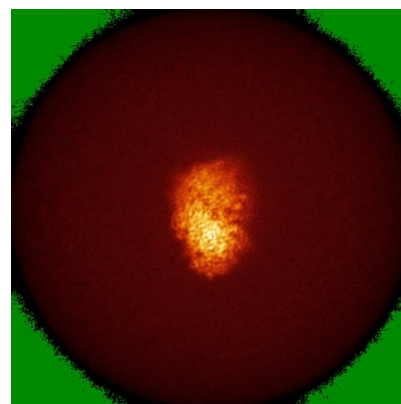
### 6.4.1 Primary map



X

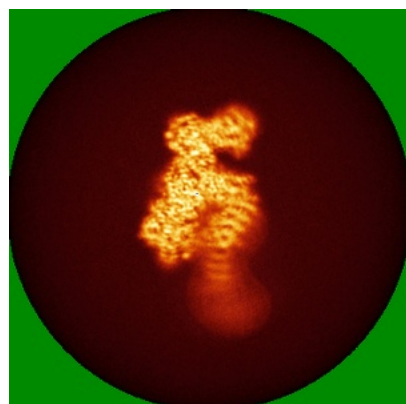


Y

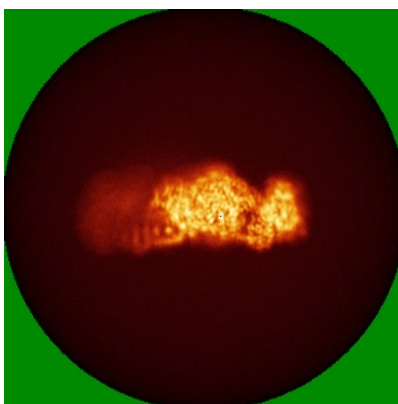


Z

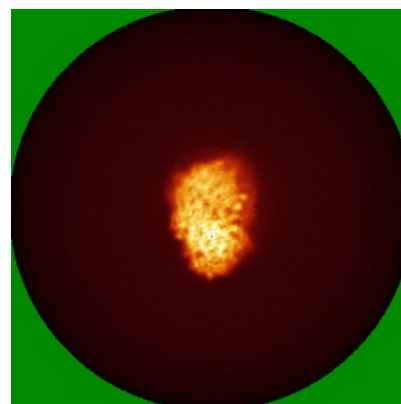
### 6.4.2 Raw map



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



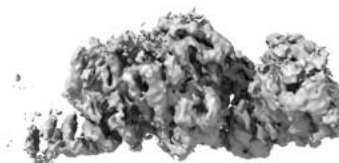
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

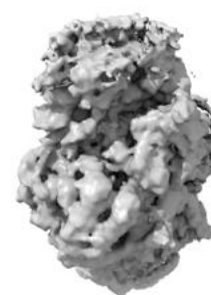
### 6.5.2 Raw map



X



Y



Z

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.

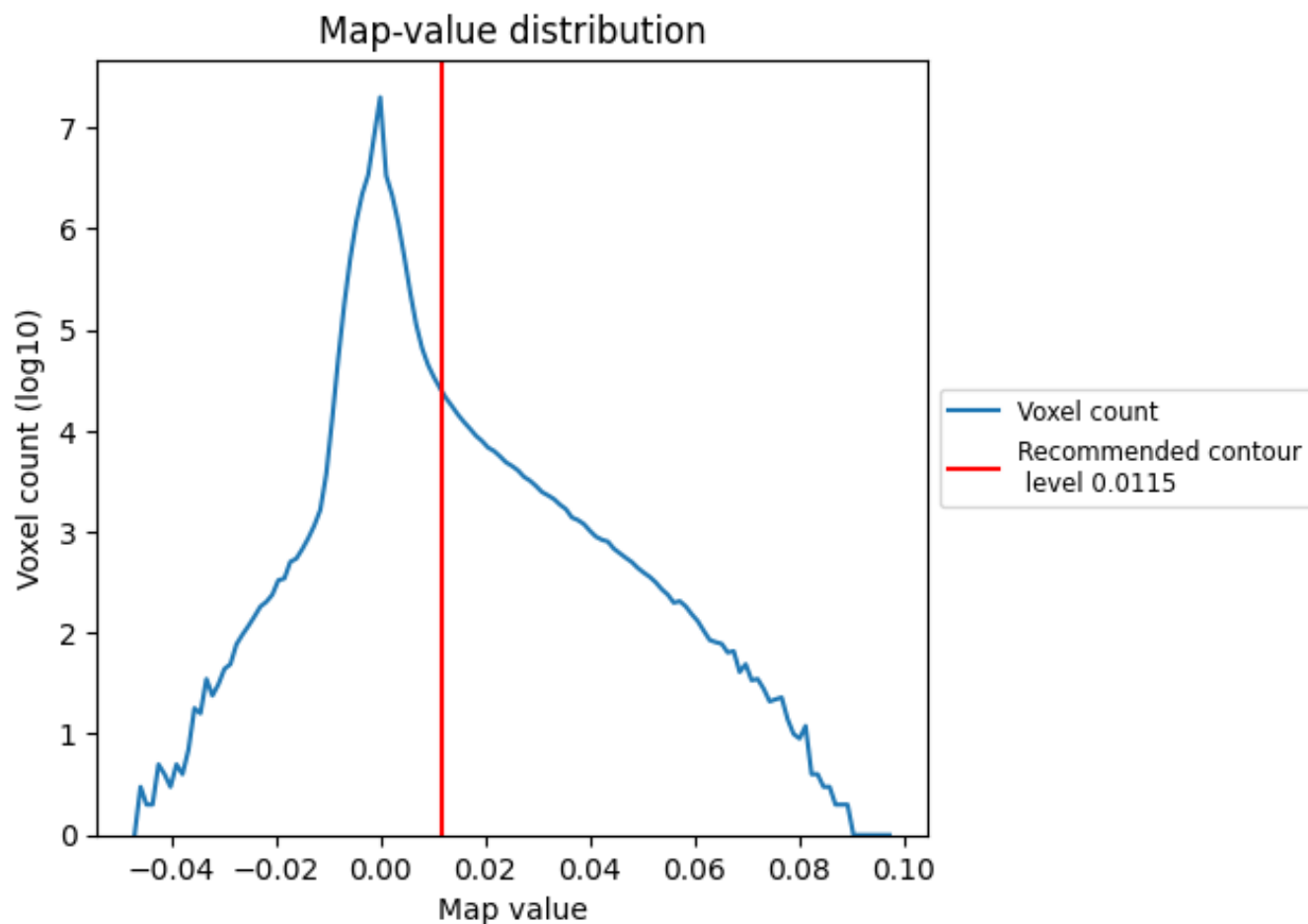
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

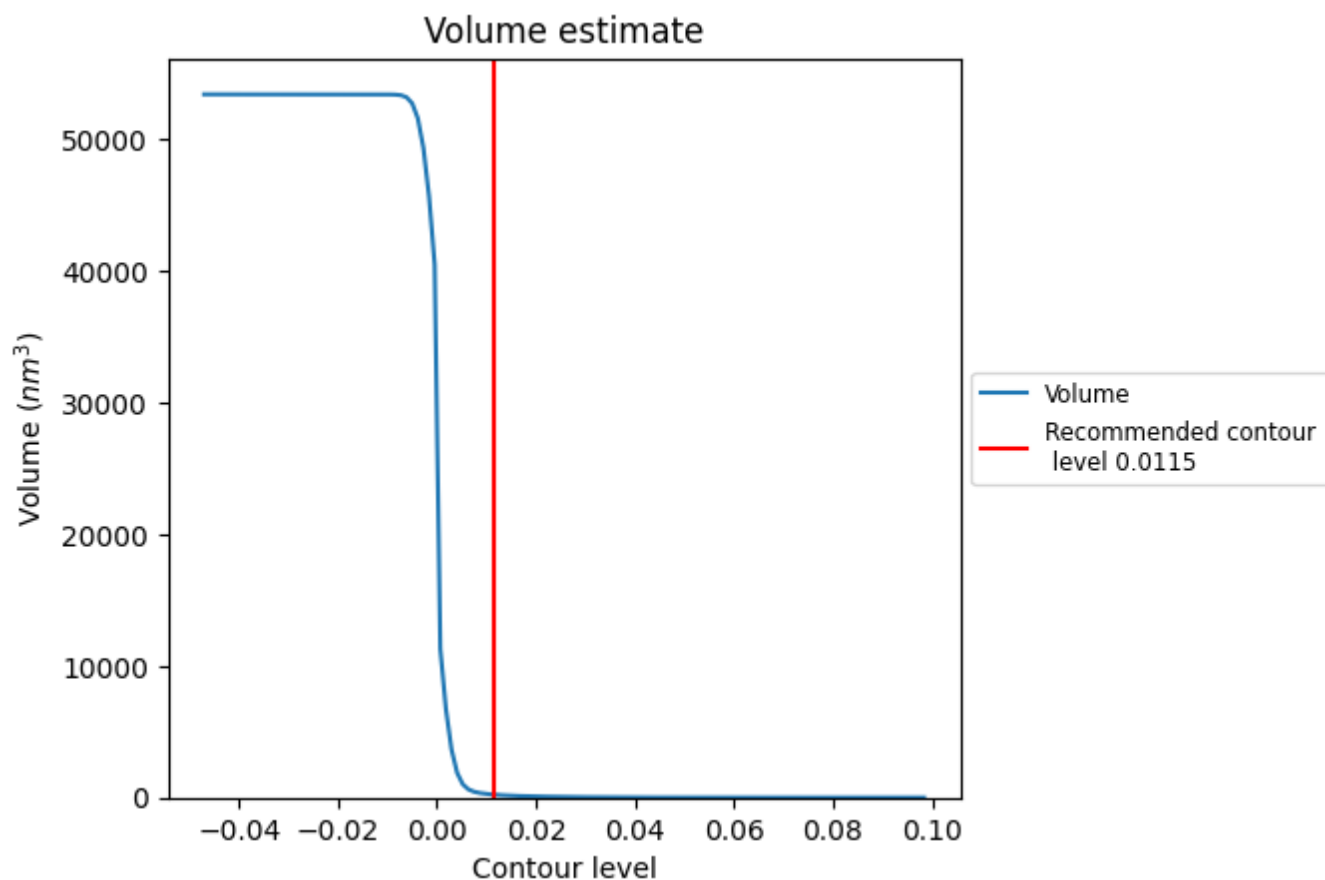
This section contains the results of statistical analysis of the map.

### 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.

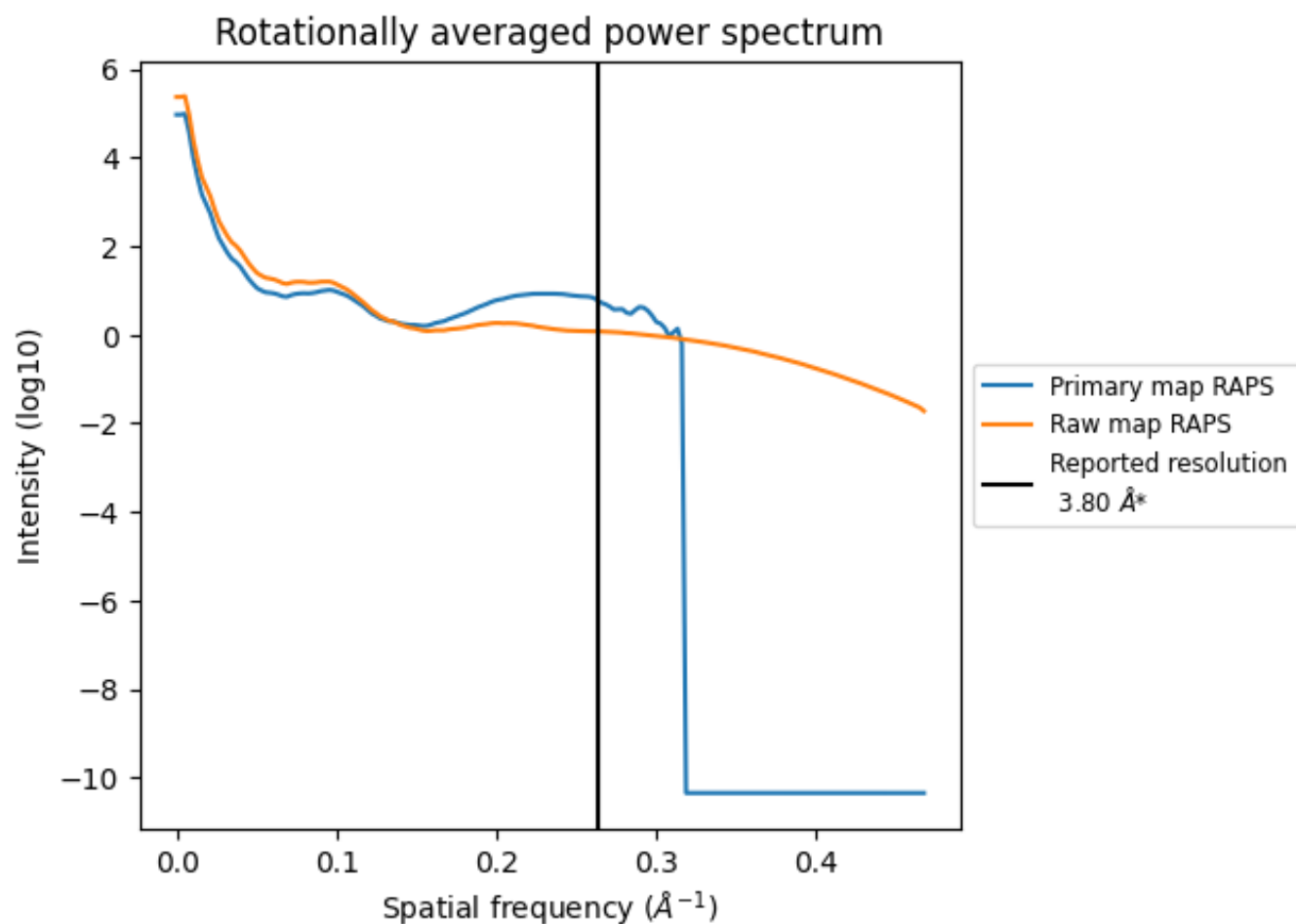
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222  $\text{nm}^3$ ; this corresponds to an approximate mass of 201 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 ⓘ

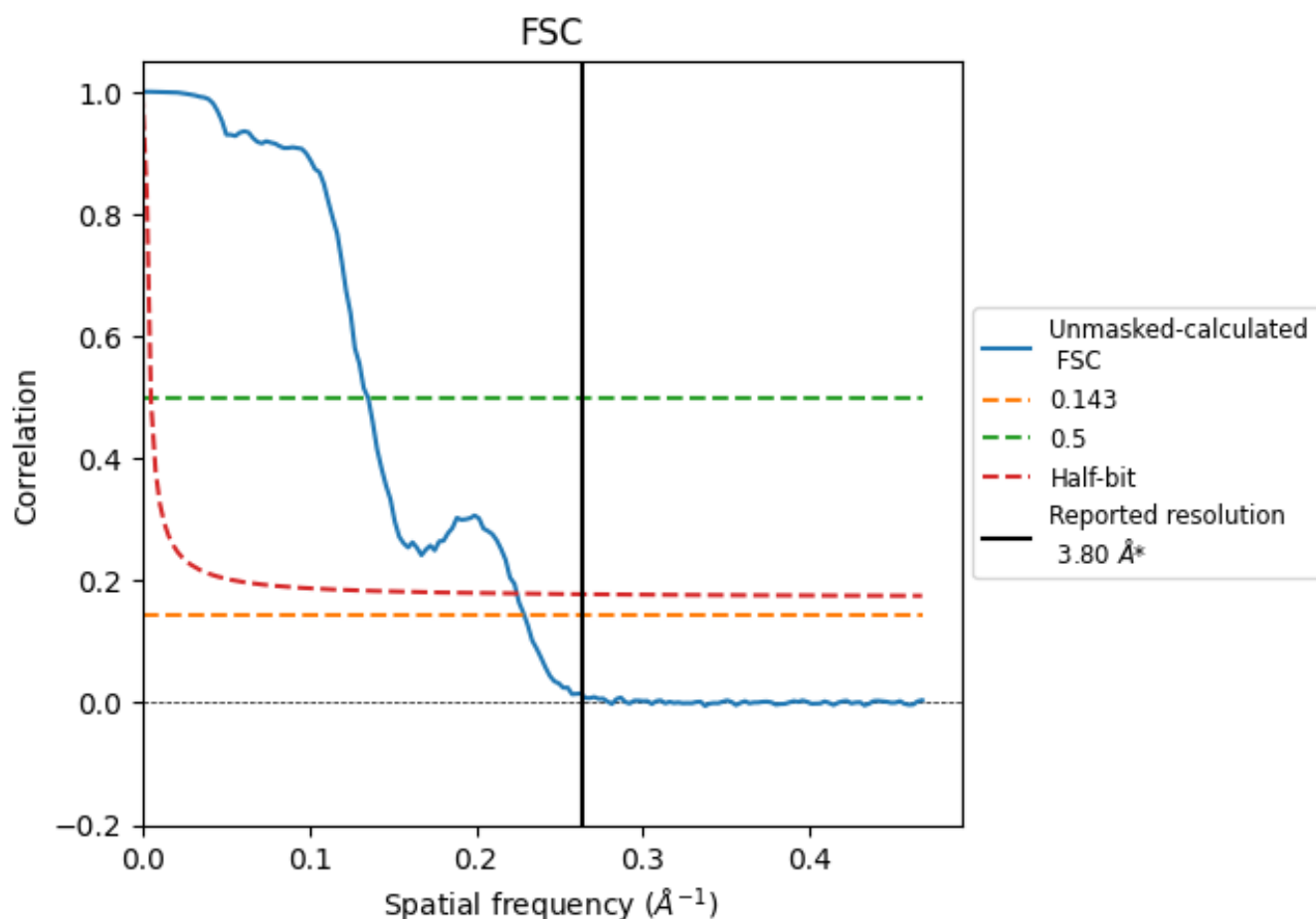


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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  $0.263 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

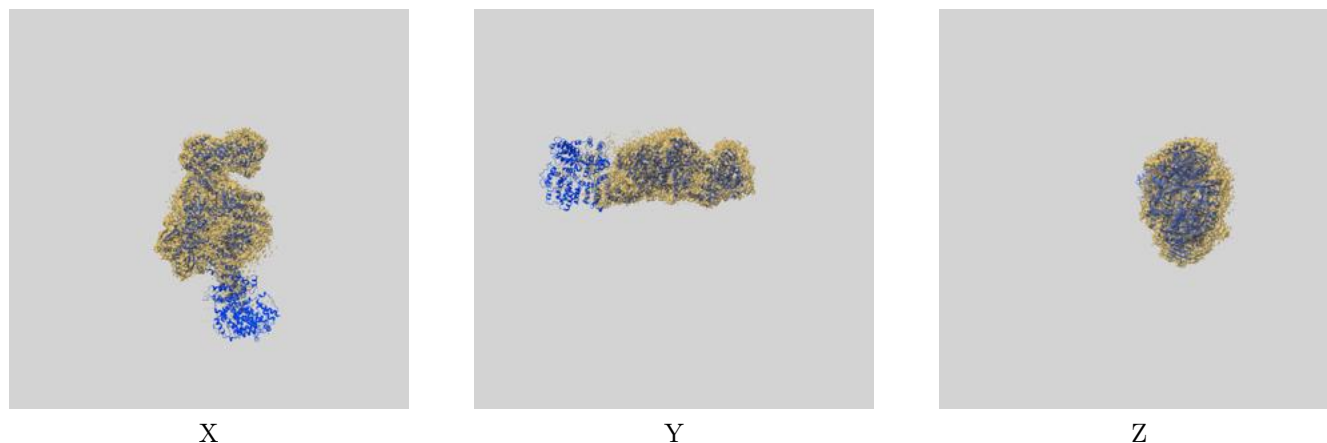
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	7.40	4.46

\*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 4.37 differs from the reported value 3.8 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-41502 and PDB model 8TQC. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

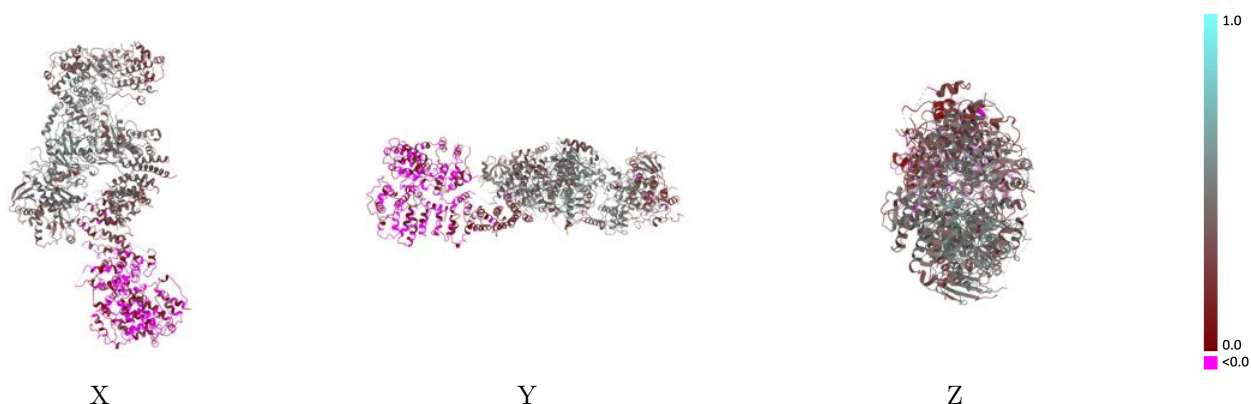
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0115 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.

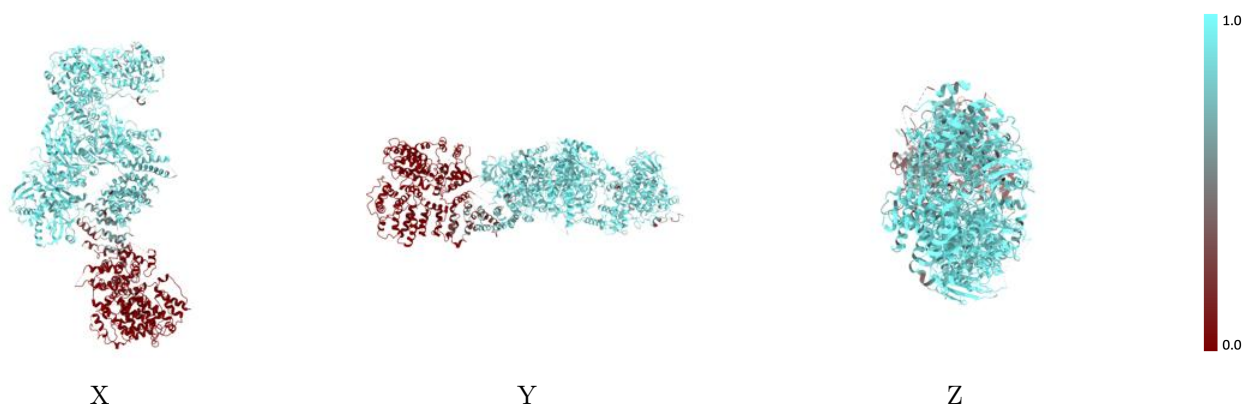


## 9.2 Q-score mapped to coordinate model [i](#)



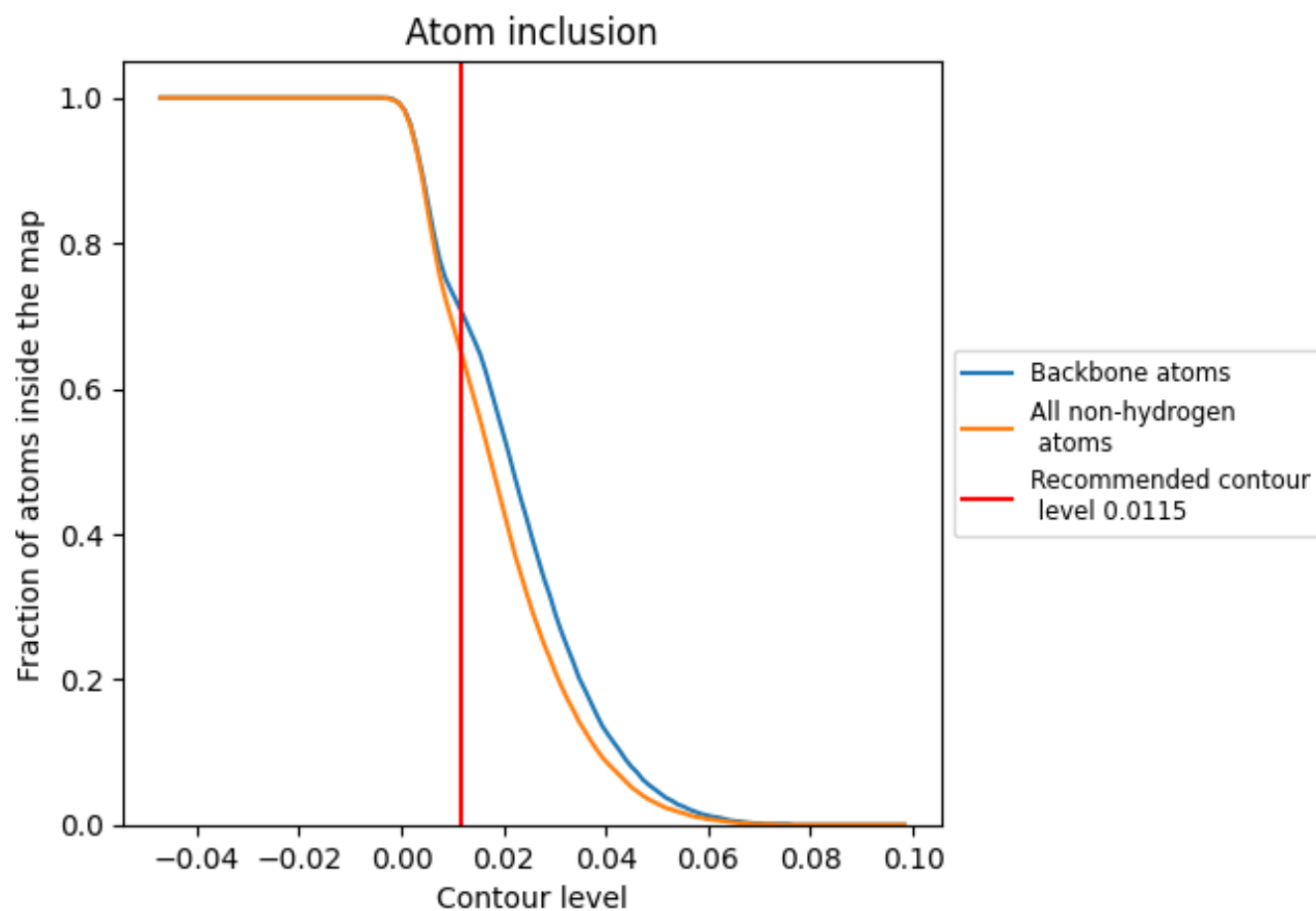
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0115).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6540	<div></div> 0.3020
A	<div></div> 0.8470	<div></div> 0.3370
B	<div></div> 0.8980	<div></div> 0.4320
C	<div></div> 0.3800	<div></div> 0.1570
D	<div></div> 0.9170	<div></div> 0.4620

