



## Full wwPDB EM Validation Report ⓘ

Aug 11, 2025 – 03:24 PM EDT

PDB ID : 9D4C / pdb\_00009d4c  
EMDB ID : EMD-46559  
Title : Proteasome core particle assembly intermediate Blm10:alpha-ring purified from *Saccharomyces cerevisiae*.  
Authors : Chen, X.; Kaur, M.; Roelofs, J.; Walters, K.J.  
Deposited on : 2024-08-12  
Resolution : 2.75 Å (reported)  
Based on initial models : 4V7O, 7LSX

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.dev126  
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) : 2.45.1

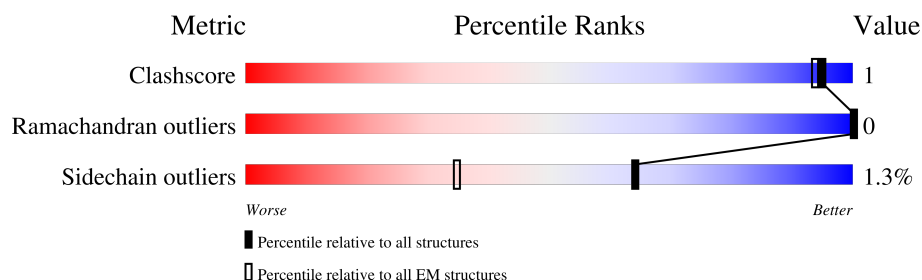
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

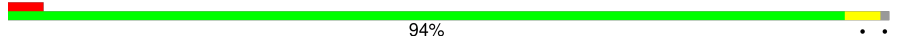


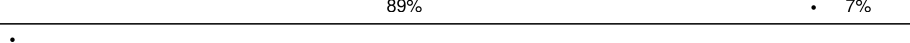
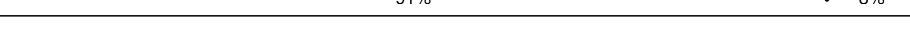



The reported resolution of this entry is 2.75 Å.

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	A	252	
2	B	250	
3	C	258	
4	D	254	
5	E	260	
6	F	234	
7	G	288	
8	I	261	

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Mol	Chain	Length	Quality of chain
9	O	2143	 A horizontal bar chart showing the quality of chain O. The bar is primarily green, representing 86% of the chain. A small yellow segment at the end represents 11%. A red dot is visible at the very beginning of the bar. The background of the bar is grey.

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 59192 atoms, of which 29612 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	249	Total	C	H	N	O	S	0	0
			3894	1239	1942	328	377	8		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	234	Total	C	H	N	O	S	0	0
			3602	1140	1812	296	351	3		

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	225	Total	C	H	N	O	S	0	0
			3494	1103	1749	290	349	3		

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	235	Total	C	H	N	O	S	0	0
			3684	1150	1849	319	362	4		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	240	Total	C	H	N	O	S	0	0
			3701	1167	1841	312	374	7		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	234	Total	C	H	N	O	S	0	0
			3613	1134	1810	313	351	5		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	243	Total	C	H	N	O	S	0	0
			3772	1202	1883	329	354	4		

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	165	Total	C	H	N	O	S	0	0
			2483	788	1244	210	236	5		

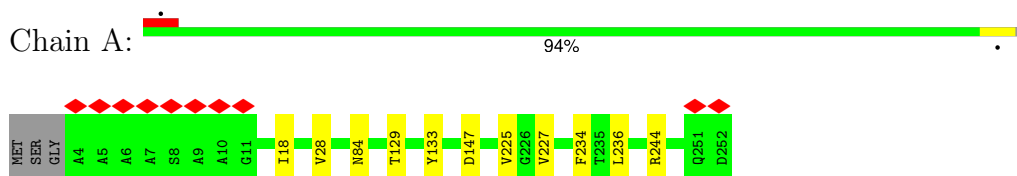
- Molecule 9 is a protein called Proteasome activator BLM10.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	O	1906	Total	C	H	N	O	S	0	0
			30949	9964	15482	2563	2869	71		

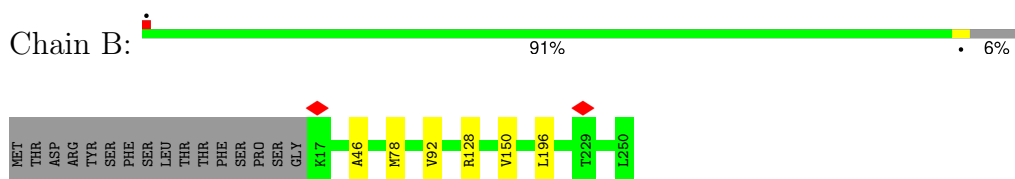
### 3 Residue-property plots

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.

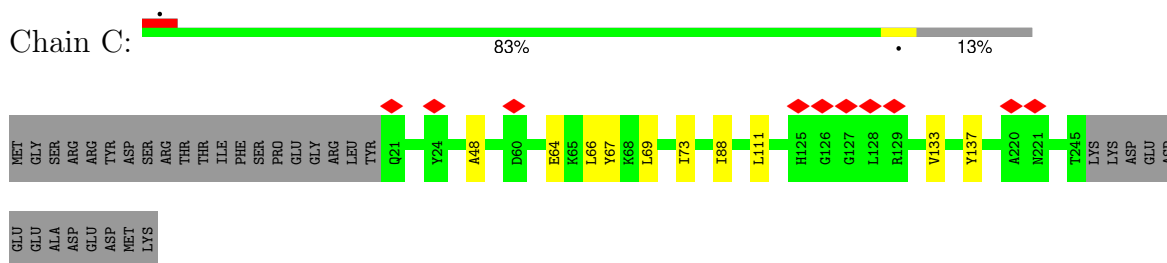
- Molecule 1: Proteasome subunit alpha type-1



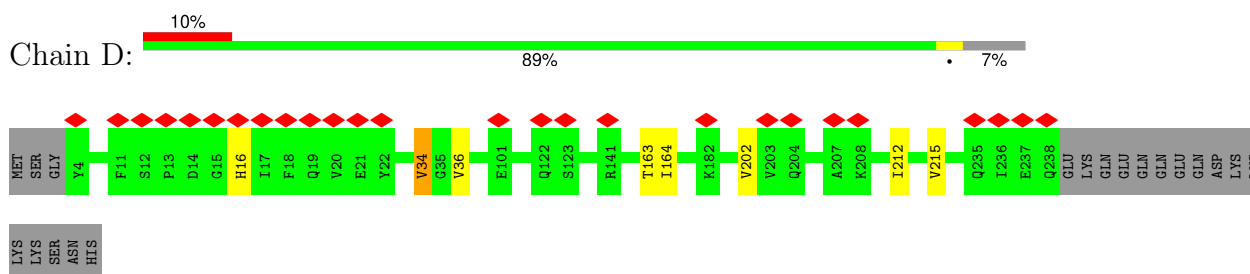
- Molecule 2: Proteasome subunit alpha type-2



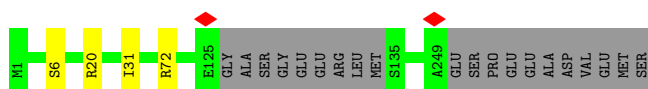
- Molecule 3: Proteasome subunit alpha type-3



- Molecule 4: Proteasome subunit alpha type-4




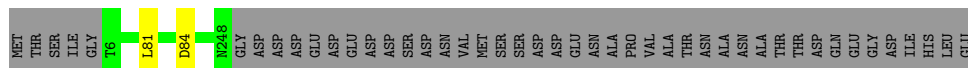
- Molecule 5: Proteasome subunit alpha type-5



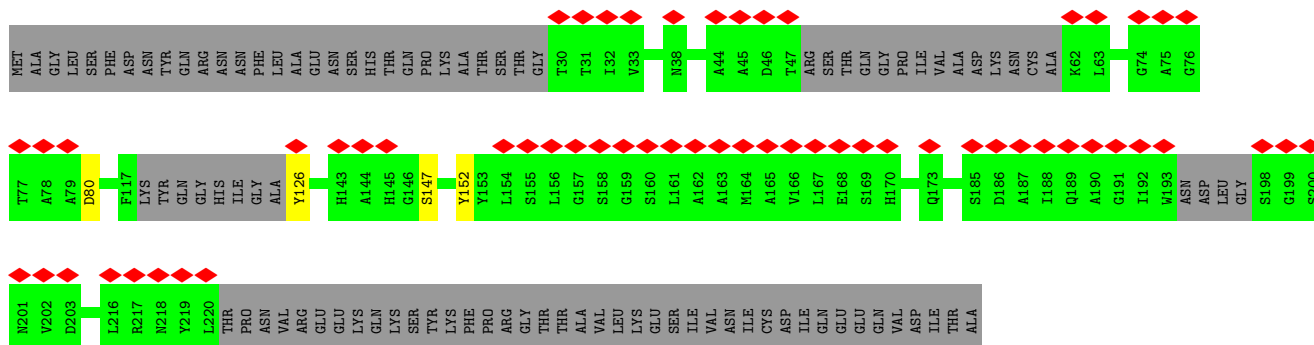
- Chain F:  96%



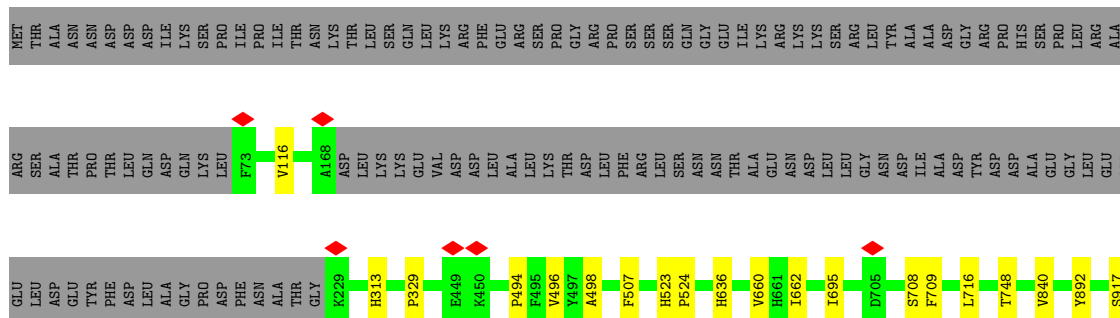
- Chain G:  84% • 16%

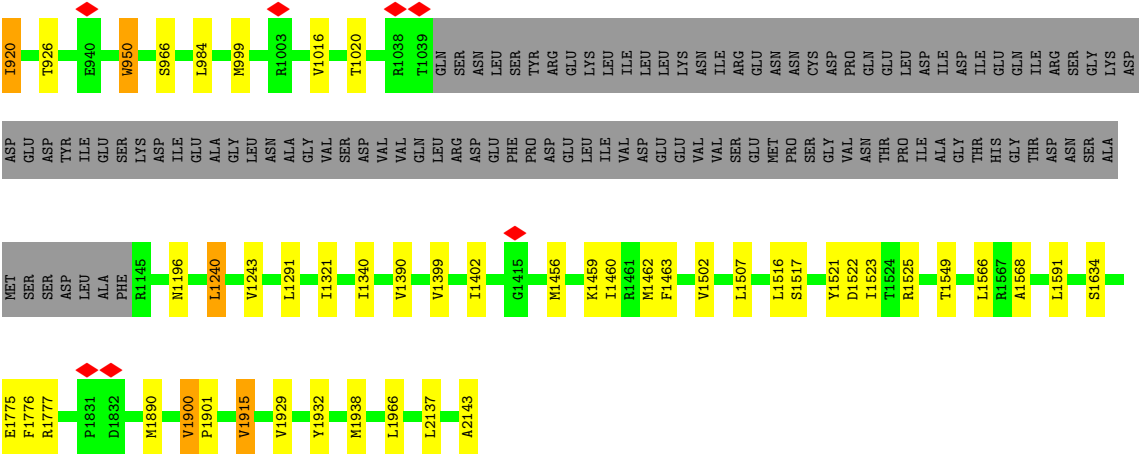


- Chain I:  23% 62% 15%



- Chain 0:  86% 11%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	414121	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	17.746	Depositor
Minimum map value	-0.268	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.513	Depositor
Recommended contour level	3	Depositor
Map size (Å)	363.12, 363.12, 363.12	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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	A	0.78	0/1990	1.31	0/2695
2	B	0.71	0/1823	1.30	0/2467
3	C	0.76	0/1771	1.27	0/2399
4	D	0.76	0/1864	1.35	0/2527
5	E	0.73	0/1886	1.28	0/2541
6	F	0.77	0/1831	1.30	0/2473
7	G	0.71	0/1929	1.29	0/2605
8	I	0.74	0/1259	1.32	0/1706
9	O	0.77	0/15814	1.35	0/21427
All	All	0.76	0/30167	1.33	0/40840

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	1952	1942	1940	4	0
2	B	1790	1812	1811	2	0
3	C	1745	1749	1748	7	0
4	D	1835	1849	1845	2	0
5	E	1860	1841	1840	1	0
6	F	1803	1810	1809	7	0
7	G	1889	1883	1881	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	1239	1244	1235	0	0
9	O	15467	15482	15465	41	0
All	All	29580	29612	29574	61	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 (61) 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)
9:O:748:THR:HG22	9:O:950:TRP:CH2	2.29	0.68
3:C:69:LEU:HD13	3:C:111:LEU:HD21	1.77	0.67
3:C:69:LEU:HD12	3:C:73:ILE:CG2	2.26	0.65
9:O:1915:VAL:HG21	9:O:1966:LEU:CD2	2.30	0.61
9:O:1775:GLU:O	9:O:1777:ARG:HG3	2.01	0.60
9:O:1016:VAL:O	9:O:1020:THR:HG23	2.01	0.60
9:O:1568:ALA:HB3	9:O:1776:PHE:CZ	2.38	0.59
9:O:840:VAL:HG11	9:O:892:TYR:CZ	2.37	0.59
1:A:28:VAL:HG21	1:A:129:THR:HG23	1.85	0.58
3:C:69:LEU:HD12	3:C:73:ILE:HG22	1.85	0.58
9:O:1390:VAL:HG21	9:O:1462:MET:HG2	1.85	0.58
9:O:1775:GLU:O	9:O:1776:PHE:CD2	2.58	0.57
9:O:1900:VAL:HG23	9:O:1938:MET:HE3	1.87	0.57
9:O:662:ILE:HG21	9:O:695:ILE:CD1	2.36	0.55
6:F:78:ALA:HB2	9:O:2143:ALA:HB2	1.86	0.55
9:O:840:VAL:HG11	9:O:892:TYR:CE1	2.41	0.55
9:O:1776:PHE:CD1	9:O:1776:PHE:O	2.61	0.54
3:C:69:LEU:HD12	3:C:73:ILE:HG21	1.91	0.52
9:O:1507:LEU:HD21	9:O:1634:SER:HB3	1.91	0.52
2:B:78:MET:HE1	2:B:128:ARG:NH1	2.25	0.52
9:O:1776:PHE:O	9:O:1776:PHE:CG	2.63	0.50
6:F:78:ALA:HB2	9:O:2143:ALA:CB	2.41	0.50
6:F:105:VAL:HG11	6:F:143:HIS:HB2	1.93	0.50
4:D:34:VAL:HB	4:D:163:THR:HG23	1.93	0.50
9:O:1399:VAL:CG1	9:O:1523:ILE:HG23	2.42	0.49
9:O:1915:VAL:HG21	9:O:1966:LEU:HD22	1.94	0.49
9:O:1568:ALA:CB	9:O:1776:PHE:CZ	2.96	0.48
9:O:1291:LEU:H	9:O:1291:LEU:HD23	1.78	0.48
6:F:3:ARG:O	6:F:3:ARG:HG2	2.15	0.47
9:O:660:VAL:HG11	9:O:716:LEU:HD22	1.96	0.46
9:O:1568:ALA:CB	9:O:1776:PHE:HZ	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:523:HIS:ND1	9:O:524:PRO:HD2	2.31	0.46
9:O:1775:GLU:C	9:O:1776:PHE:CD2	2.94	0.45
2:B:46:ALA:HB1	2:B:196:LEU:HD11	1.99	0.44
4:D:164:ILE:HG23	4:D:164:ILE:O	2.17	0.43
6:F:81:ALA:HB2	6:F:130:VAL:HG21	2.00	0.43
9:O:1516:LEU:HD22	9:O:1521:TYR:CD1	2.53	0.43
9:O:1240:LEU:HD23	9:O:1243:VAL:HG21	2.01	0.43
3:C:69:LEU:HD13	3:C:111:LEU:CD2	2.47	0.42
9:O:1932:TYR:CD2	9:O:1966:LEU:HG	2.54	0.42
6:F:3:ARG:HB3	9:O:636:HIS:CD2	2.54	0.42
6:F:179:PHE:HA	6:F:182:ILE:CD1	2.49	0.42
9:O:917:SER:O	9:O:920:ILE:HD12	2.20	0.42
9:O:329:PRO:HD3	9:O:1566:LEU:HD11	2.01	0.42
9:O:708:SER:O	9:O:709:PHE:C	2.63	0.42
9:O:950:TRP:CE3	9:O:950:TRP:HA	2.54	0.42
5:E:20:ARG:CD	9:O:2137:LEU:HD22	2.50	0.42
9:O:1456:MET:SD	9:O:1460:ILE:HG22	2.60	0.42
1:A:225:VAL:HG11	1:A:236:LEU:HD12	2.02	0.41
9:O:1522:ASP:HB3	9:O:1525:ARG:HD2	2.02	0.41
7:G:81:LEU:HD12	7:G:84:ASP:OD2	2.20	0.41
9:O:494:PRO:O	9:O:498:ALA:HB2	2.20	0.41
9:O:1517:SER:HB3	9:O:1591:LEU:HD21	2.01	0.41
3:C:48:ALA:HB3	3:C:66:LEU:CD1	2.51	0.41
9:O:507:PHE:CD1	9:O:507:PHE:C	2.99	0.41
9:O:1321:ILE:HG23	9:O:1340:ILE:HG23	2.03	0.41
1:A:227:VAL:HB	1:A:234:PHE:CE2	2.56	0.41
9:O:496:VAL:HG12	9:O:496:VAL:O	2.21	0.41
9:O:1900:VAL:N	9:O:1901:PRO:CD	2.84	0.40
1:A:225:VAL:HG11	1:A:236:LEU:CD1	2.51	0.40
3:C:67:TYR:CG	3:C:88:ILE:HD13	2.55	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	A	247/252 (98%)	241 (98%)	6 (2%)	0	100	100
2	B	232/250 (93%)	228 (98%)	4 (2%)	0	100	100
3	C	223/258 (86%)	213 (96%)	10 (4%)	0	100	100
4	D	233/254 (92%)	220 (94%)	13 (6%)	0	100	100
5	E	236/260 (91%)	229 (97%)	7 (3%)	0	100	100
6	F	232/234 (99%)	222 (96%)	10 (4%)	0	100	100
7	G	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
8	I	157/261 (60%)	148 (94%)	9 (6%)	0	100	100
9	O	1900/2143 (89%)	1812 (95%)	88 (5%)	0	100	100
All	All	3701/4200 (88%)	3550 (96%)	151 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	208/210 (99%)	203 (98%)	5 (2%)	44	65
2	B	194/209 (93%)	192 (99%)	2 (1%)	73	84
3	C	186/216 (86%)	183 (98%)	3 (2%)	58	75
4	D	207/226 (92%)	201 (97%)	6 (3%)	37	59
5	E	199/215 (93%)	196 (98%)	3 (2%)	60	76
6	F	193/193 (100%)	191 (99%)	2 (1%)	73	84
7	G	200/239 (84%)	200 (100%)	0	100	100
8	I	131/214 (61%)	127 (97%)	4 (3%)	35	56
9	O	1750/1963 (89%)	1731 (99%)	19 (1%)	70	83
All	All	3268/3685 (89%)	3224 (99%)	44 (1%)	64	80

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	84	ASN
1	A	133	TYR
1	A	147	ASP
1	A	244	ARG
2	B	92	VAL
2	B	150	VAL
3	C	64	GLU
3	C	133	VAL
3	C	137	TYR
4	D	16	HIS
4	D	34	VAL
4	D	36	VAL
4	D	202	VAL
4	D	212	ILE
4	D	215	VAL
5	E	6	SER
5	E	31	ILE
5	E	72	ARG
6	F	74	LEU
6	F	208	VAL
8	I	80	ASP
8	I	126	TYR
8	I	147	SER
8	I	152	TYR
9	O	116	VAL
9	O	313	HIS
9	O	920	ILE
9	O	926	THR
9	O	950	TRP
9	O	966	SER
9	O	984	LEU
9	O	999	MET
9	O	1196	ASN
9	O	1240	LEU
9	O	1402	ILE
9	O	1459	LYS
9	O	1463	PHE
9	O	1502	VAL
9	O	1549	THR
9	O	1890	MET
9	O	1900	VAL

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Mol	Chain	Res	Type
9	O	1915	VAL
9	O	1929	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	55	GLN
5	E	154	GLN
6	F	166	GLN
7	G	64	ASN
8	I	110	GLN
9	O	314	GLN
9	O	440	HIS
9	O	441	ASN
9	O	484	GLN
9	O	562	ASN
9	O	571	HIS
9	O	683	ASN
9	O	850	GLN
9	O	866	GLN
9	O	993	ASN
9	O	1013	GLN
9	O	1035	ASN
9	O	1158	ASN
9	O	1278	ASN
9	O	1342	ASN
9	O	1420	GLN
9	O	1490	GLN
9	O	1511	ASN
9	O	1532	ASN
9	O	1811	ASN
9	O	1870	GLN
9	O	1973	HIS
9	O	2088	ASN

### 5.3.3 RNA ⓘ

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 [i](#)

There are no chain breaks in this entry.



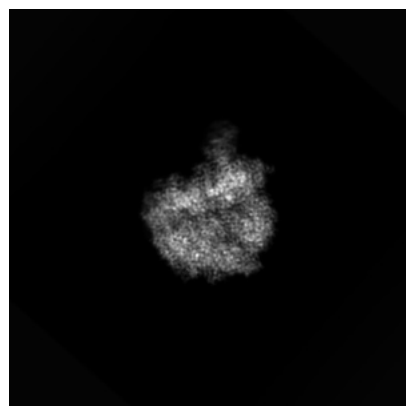
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46559. These allow visual inspection of the internal detail of the map and identification of artifacts.

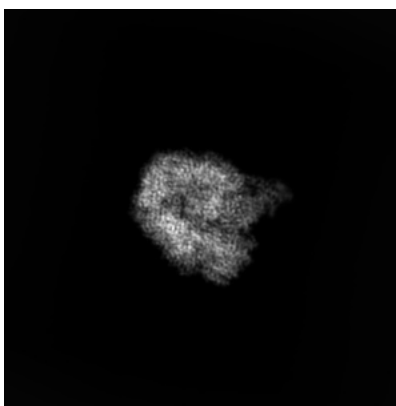
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

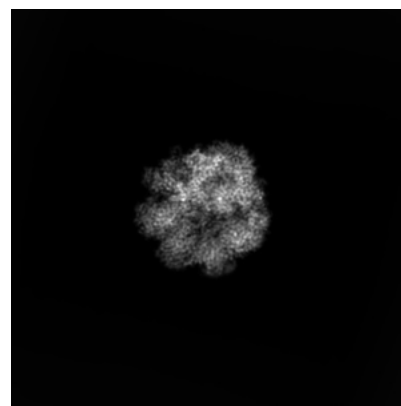
#### 6.1.1 Primary map



X

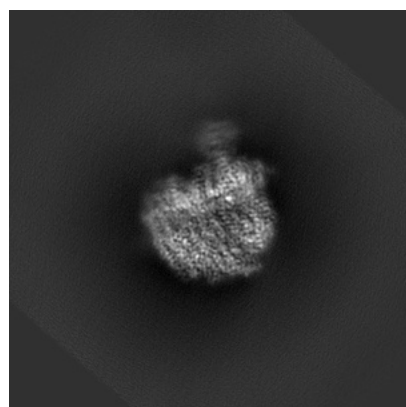


Y

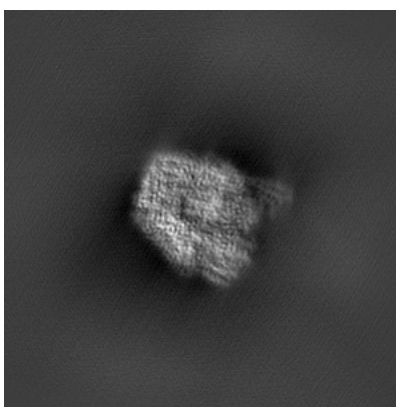


Z

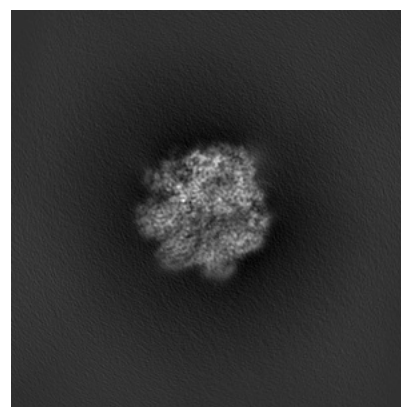
#### 6.1.2 Raw map



X



Y

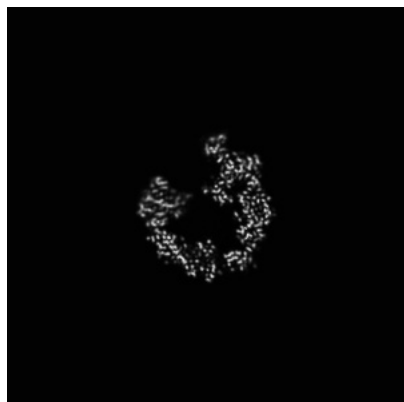


Z

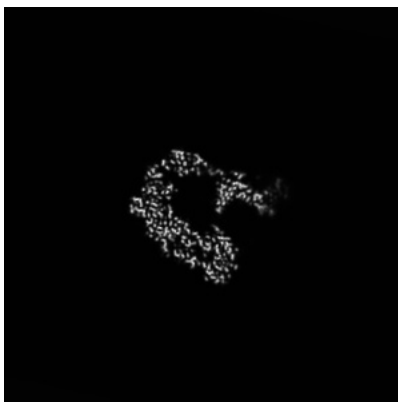
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

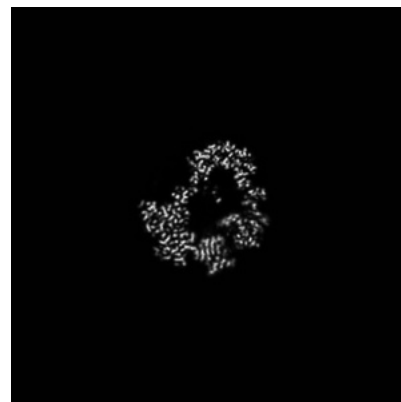
### 6.2.1 Primary map



X Index: 170

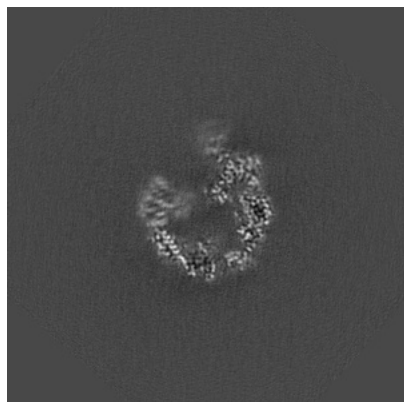


Y Index: 170

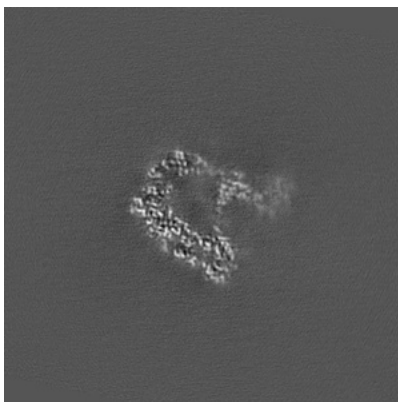


Z Index: 170

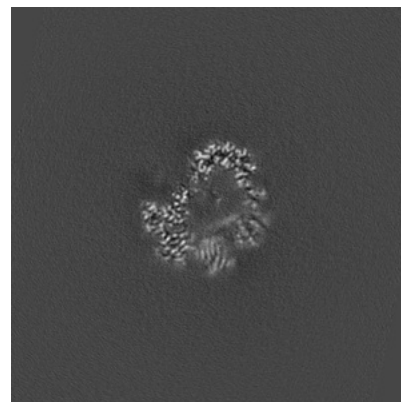
### 6.2.2 Raw map



X Index: 170



Y Index: 170

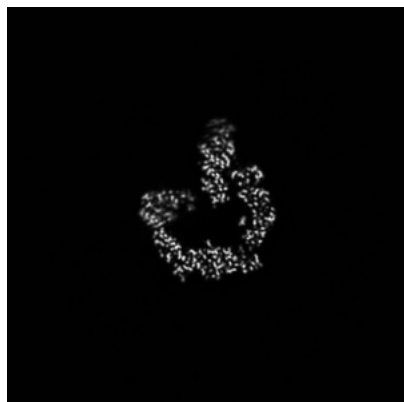


Z Index: 170

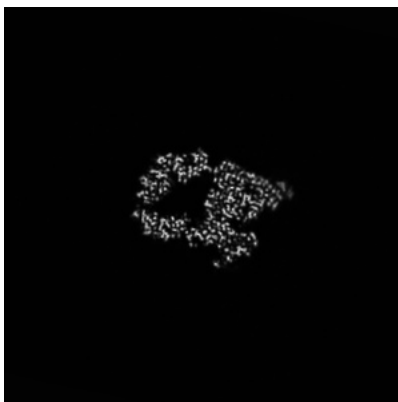
The images above show central slices of the map in three orthogonal directions.

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

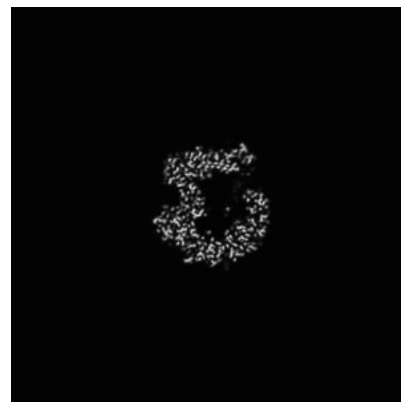
### 6.3.1 Primary map



X Index: 178

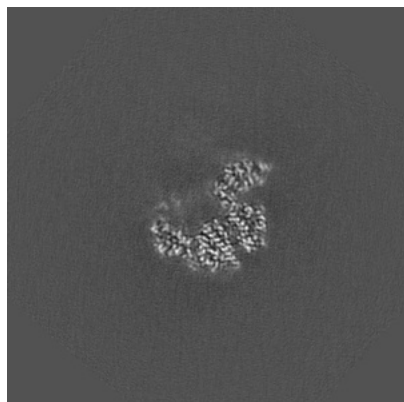


Y Index: 182

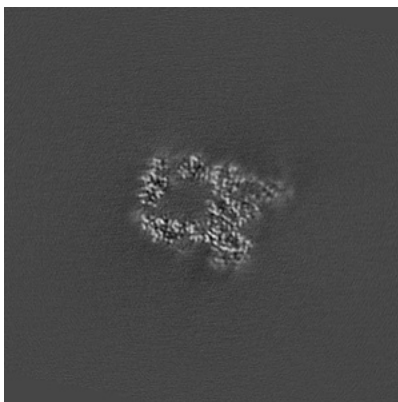


Z Index: 144

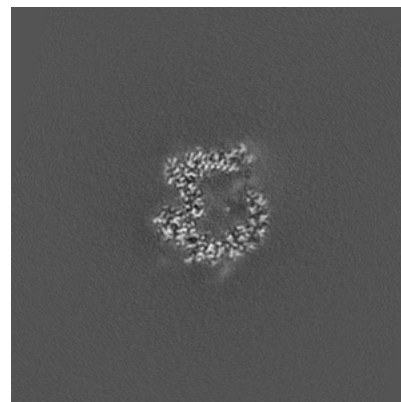
### 6.3.2 Raw map



X Index: 156



Y Index: 186

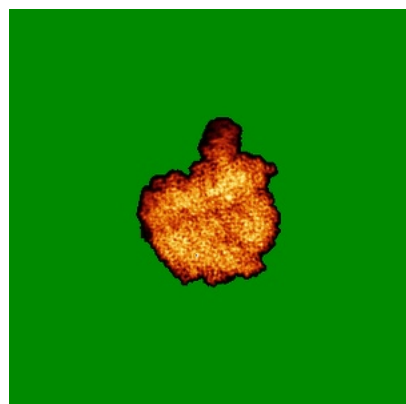


Z Index: 144

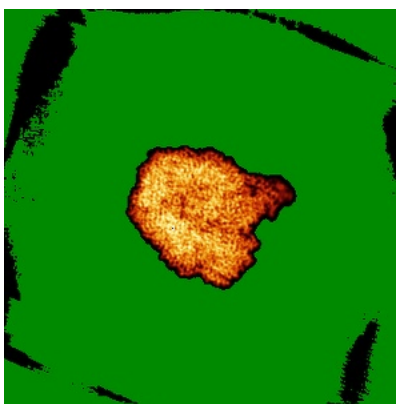
The images above show the largest variance slices of the map in three orthogonal directions.

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

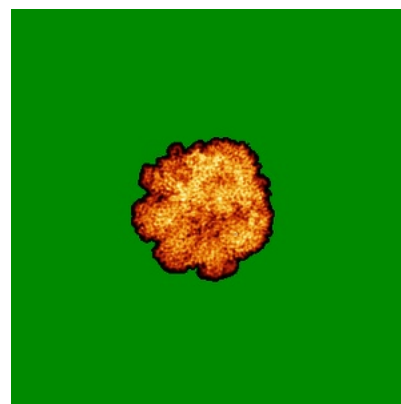
### 6.4.1 Primary map



X

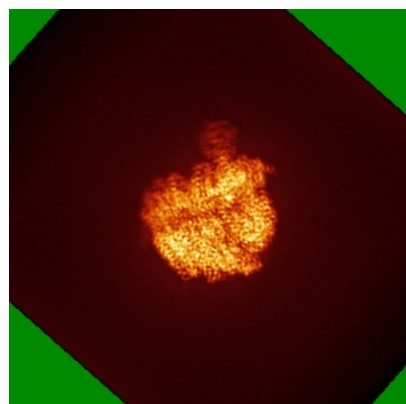


Y

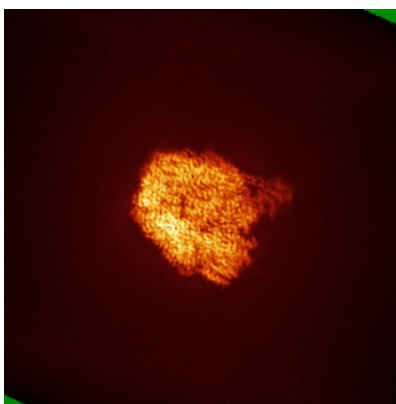


Z

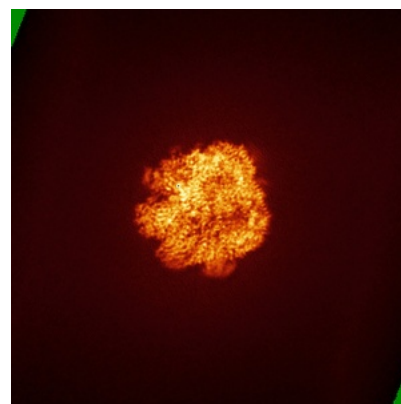
### 6.4.2 Raw map



X



Y

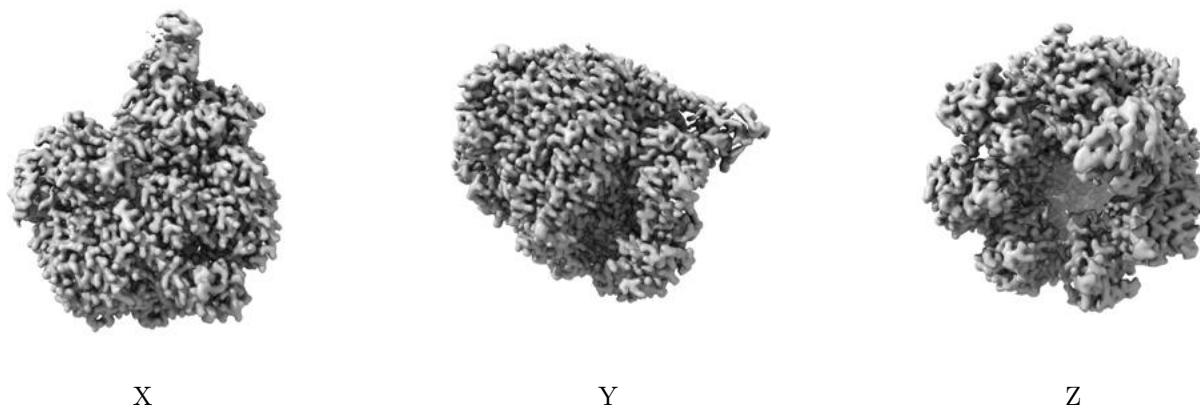


Z

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.

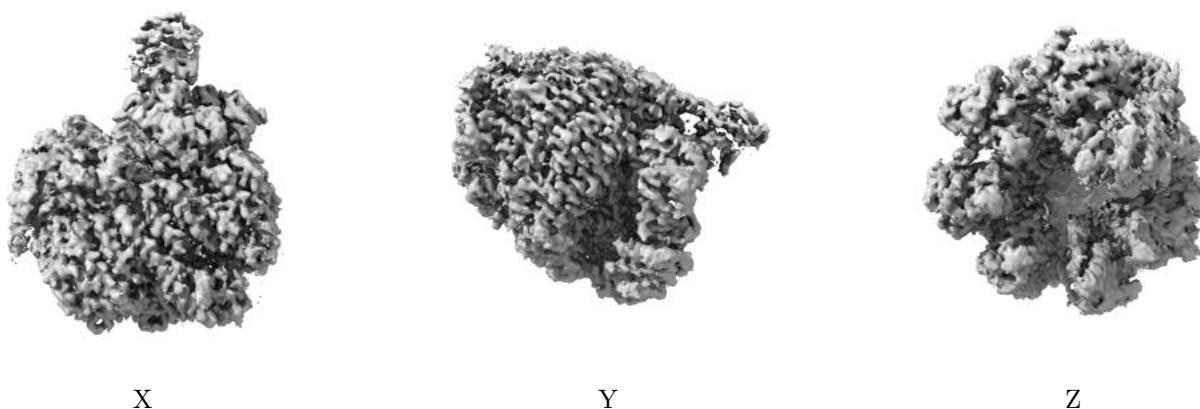
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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



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.

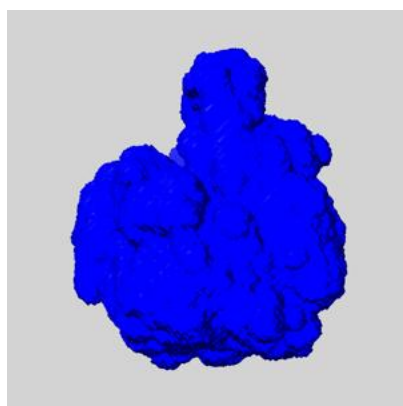
## 6.6 Mask visualisation [i](#)

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

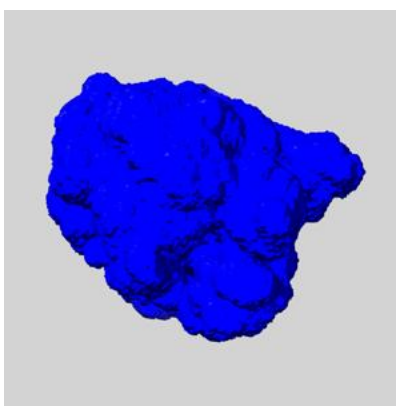
A mask typically either:

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

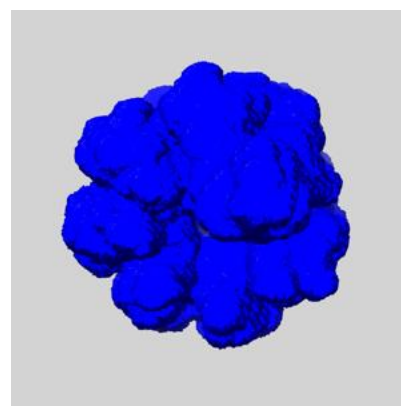
### 6.6.1 emd\_46559\_msk\_1.map [i](#)



X



Y

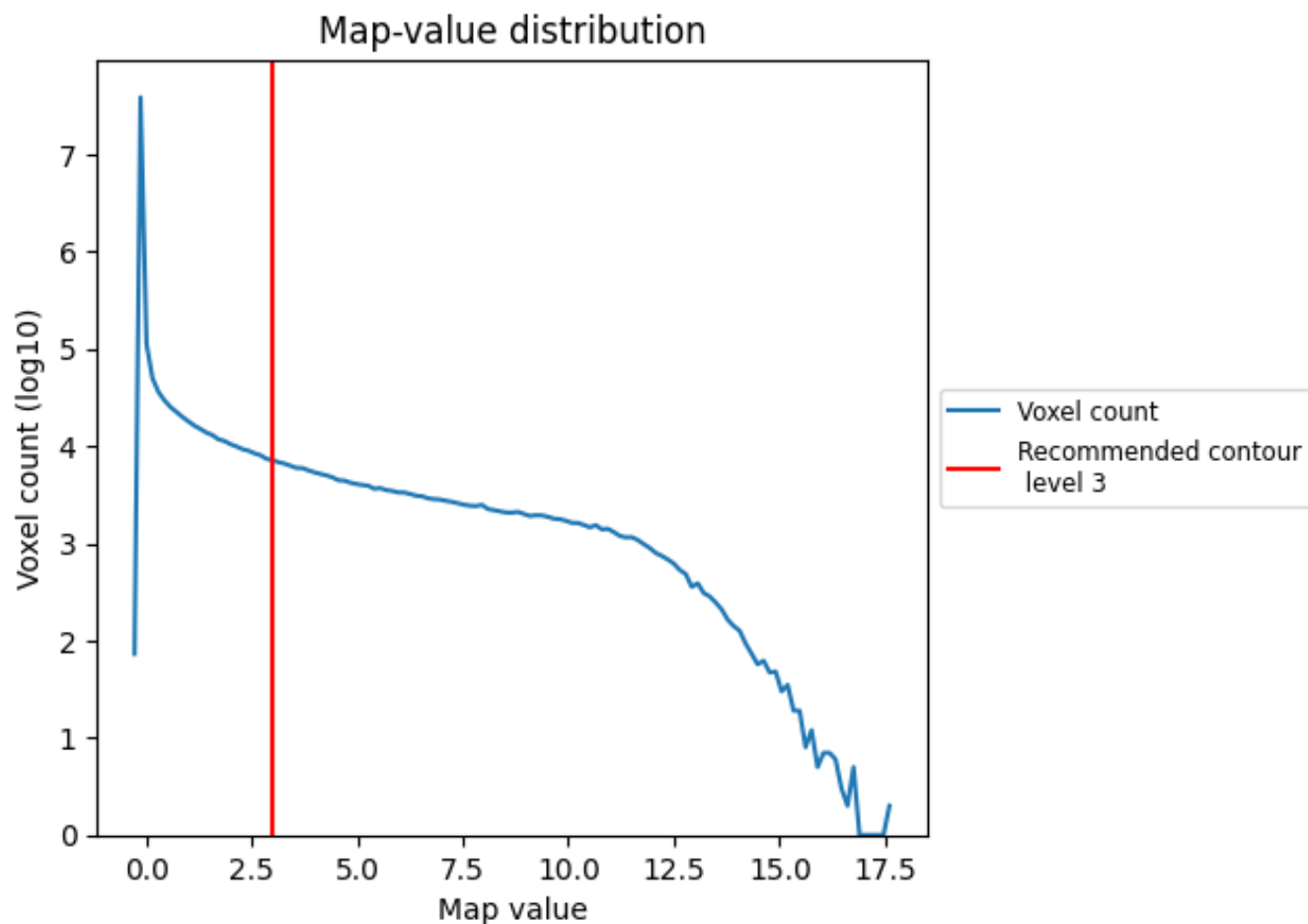


Z

## 7 Map analysis [i](#)

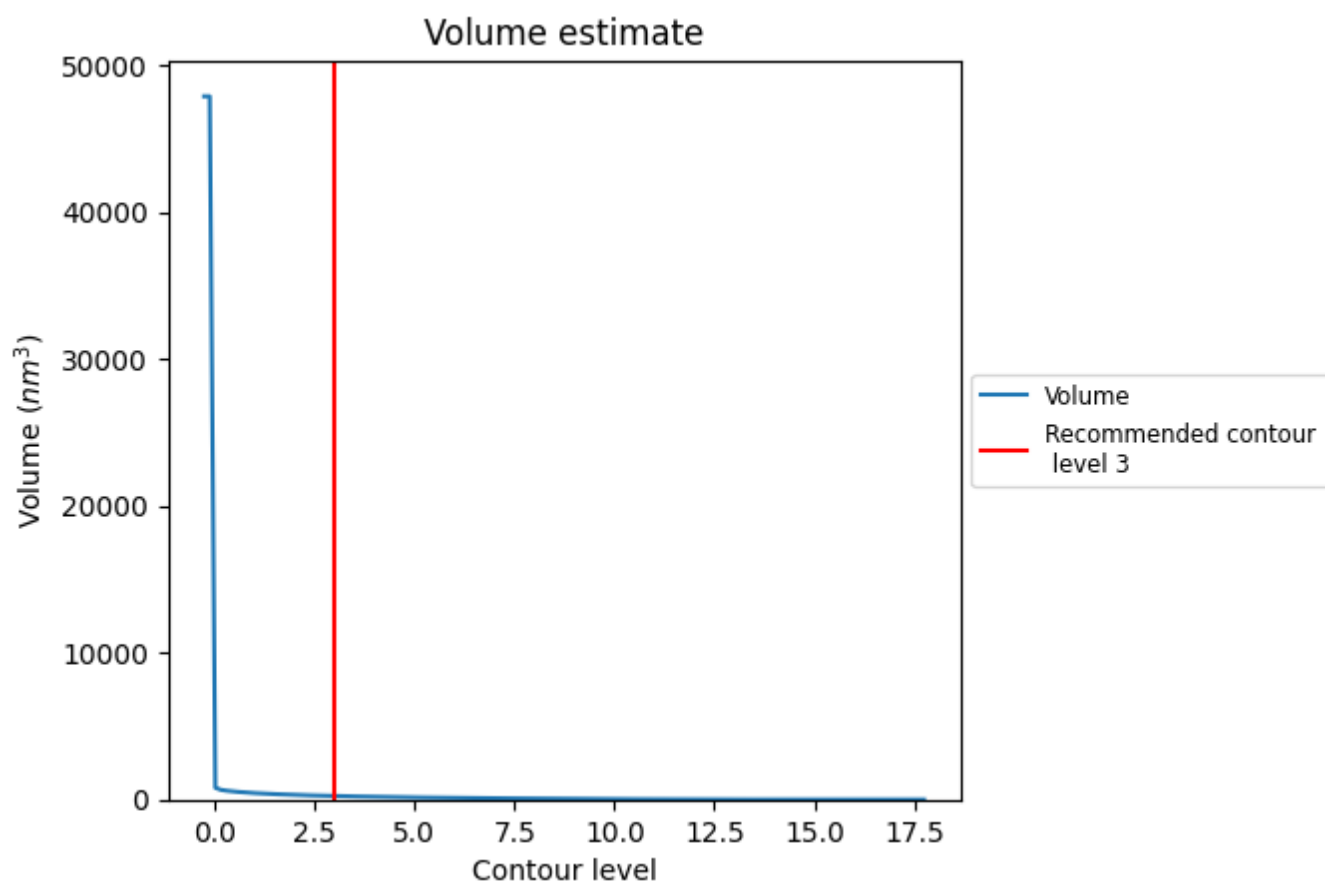
This section contains the results of statistical analysis of the map.

### 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](#)

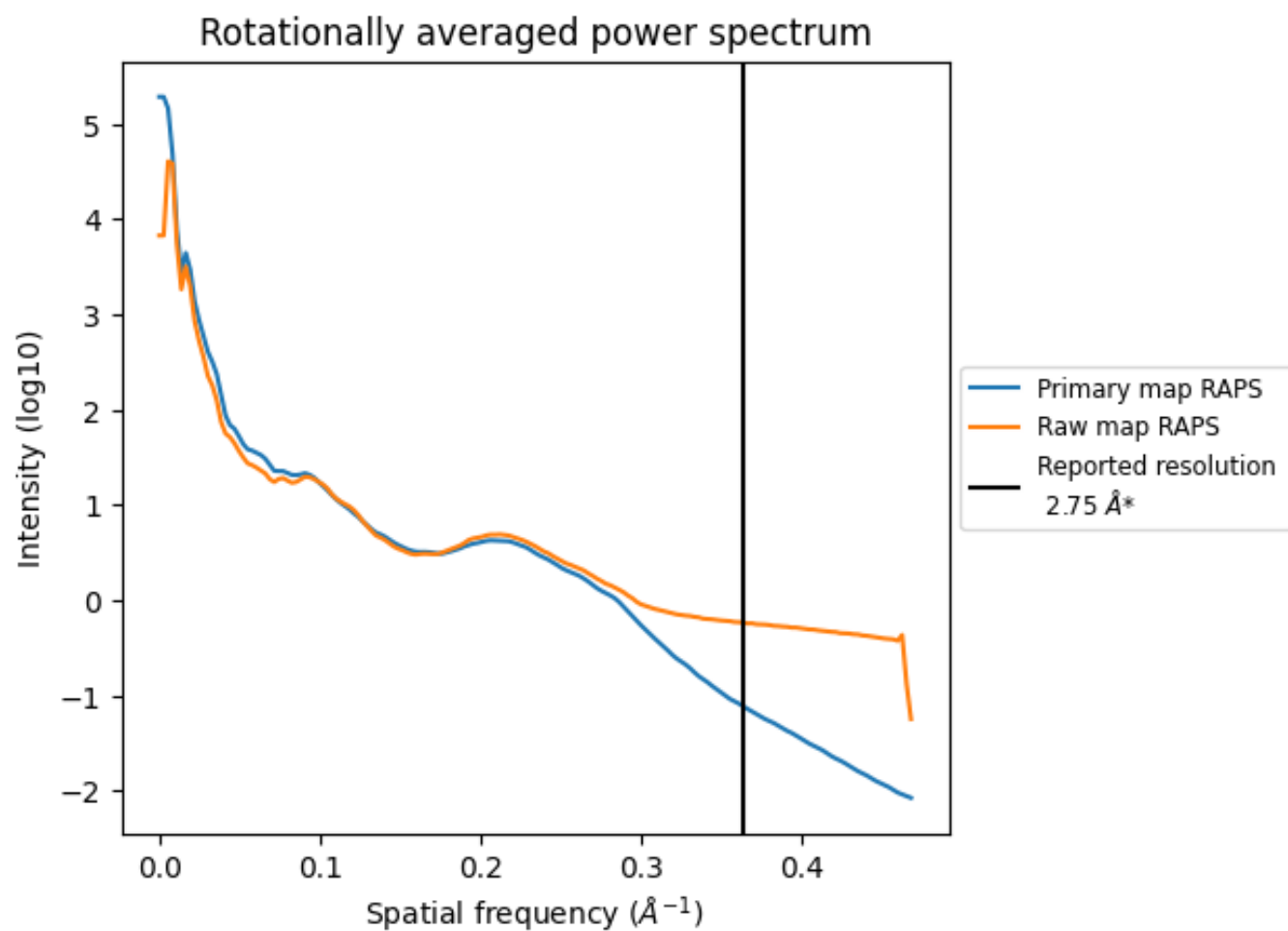


The volume at the recommended contour level is 242 nm<sup>3</sup>; this corresponds to an approximate mass of 219 kDa.

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 ⓘ

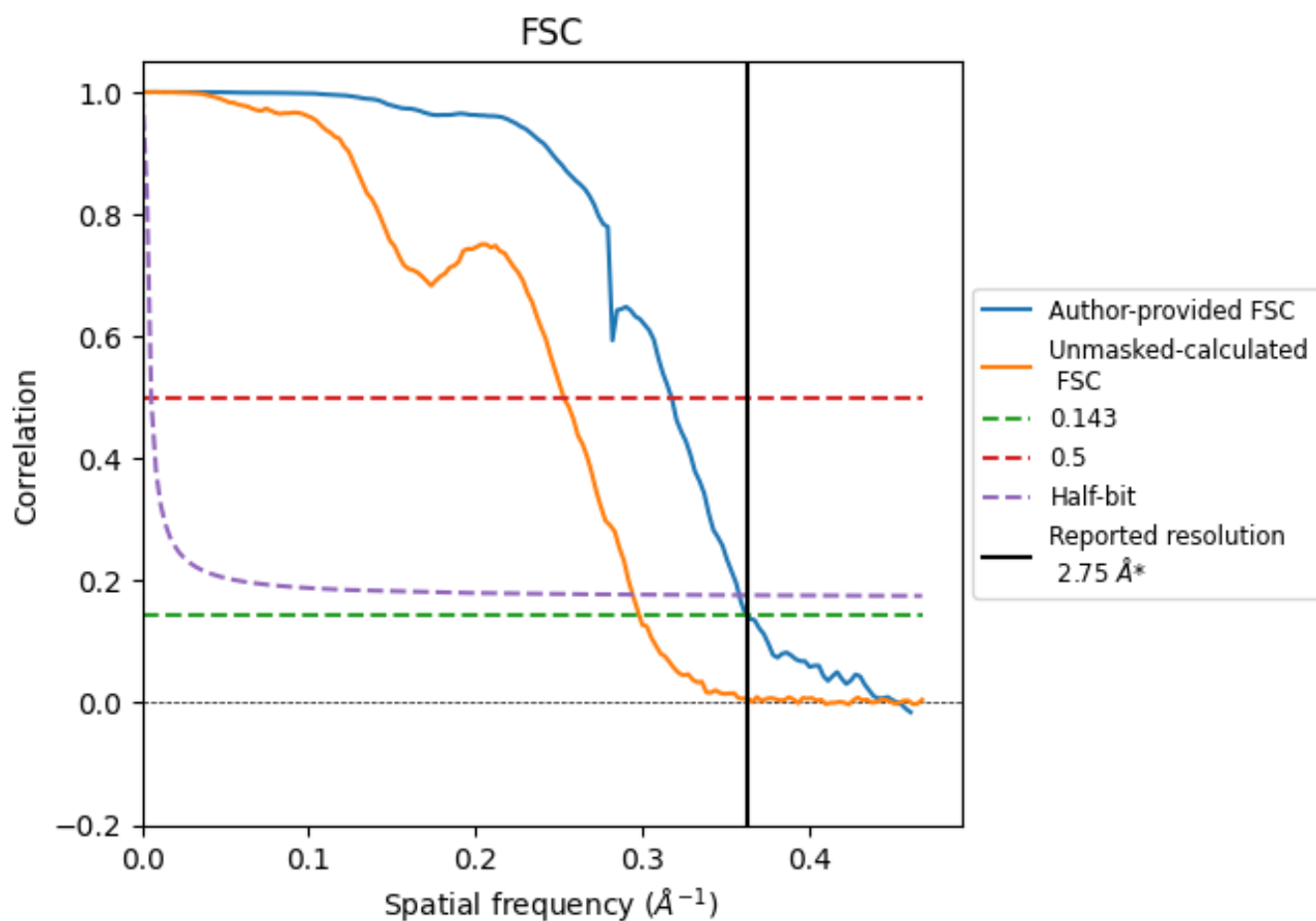


\*Reported resolution corresponds to spatial frequency of 0.364 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

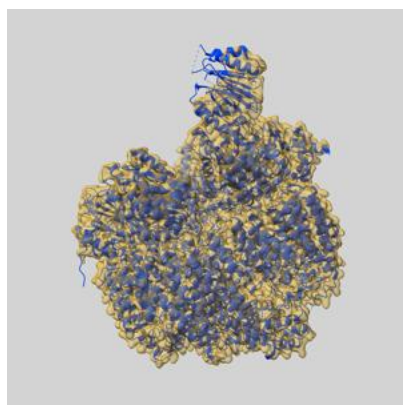
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.75	3.15	2.79
Unmasked-calculated*	3.35	3.95	3.40

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

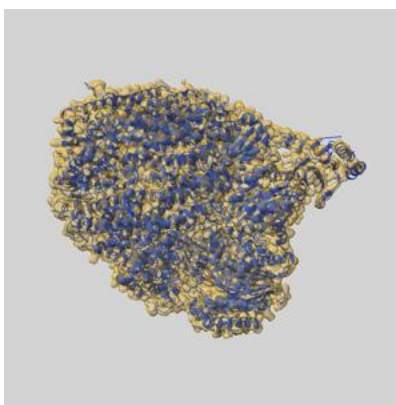
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46559 and PDB model 9D4C. Per-residue inclusion information can be found in section [3](#) on page [6](#).

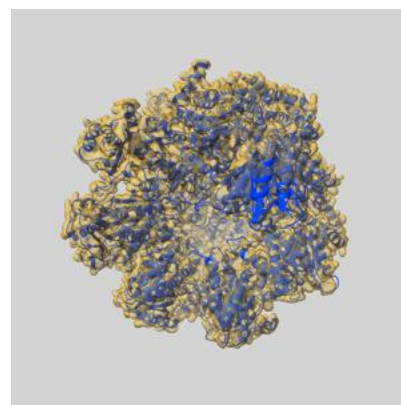
### 9.1 Map-model overlay [i](#)



X



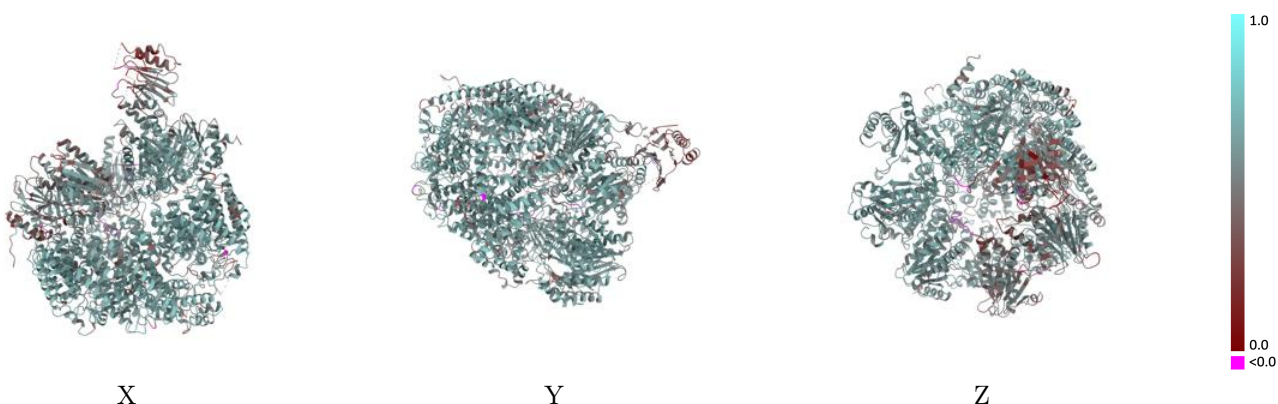
Y



Z

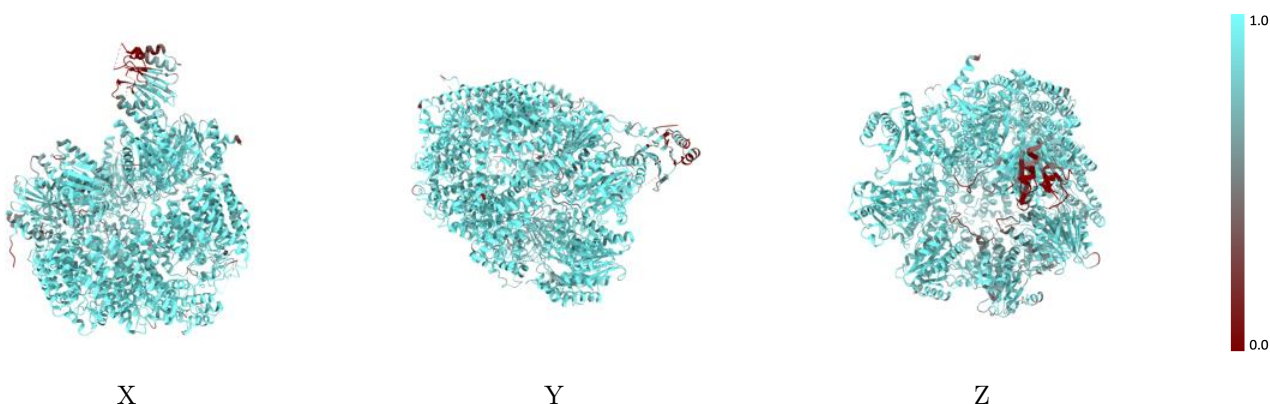
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



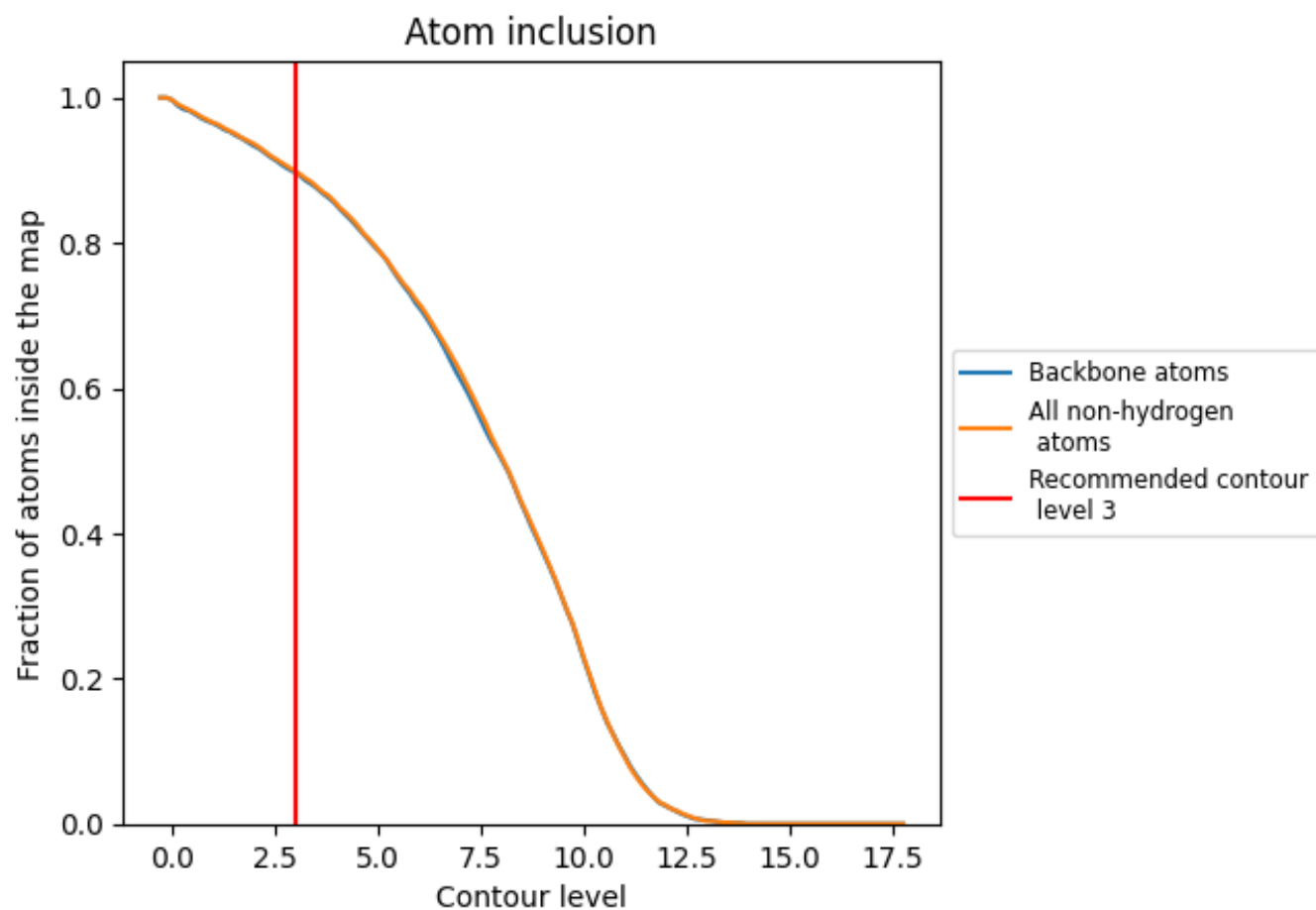
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8990</div>	<div><div></div>0.5660</div>
A	<div><div></div>0.9180</div>	<div><div></div>0.5700</div>
B	<div><div></div>0.9220</div>	<div><div></div>0.5820</div>
C	<div><div></div>0.8170</div>	<div><div></div>0.4790</div>
D	<div><div></div>0.7240</div>	<div><div></div>0.4030</div>
E	<div><div></div>0.9050</div>	<div><div></div>0.5660</div>
F	<div><div></div>0.9500</div>	<div><div></div>0.5950</div>
G	<div><div></div>0.9360</div>	<div><div></div>0.5980</div>
I	<div><div></div>0.5720</div>	<div><div></div>0.3810</div>
O	<div><div></div>0.9500</div>	<div><div></div>0.6000</div>

1.0

0.0

<0.0