



## Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 02:19 PM EDT

PDB ID : 9Y0L / pdb\_00009y0l  
EMDB ID : EMD-72395  
Title : Incorrectly assembled half-Pf20S  
Authors : Zhang, H.; Zhao, J.; Fajtova, P.; O'Donoghue, A.J.  
Deposited on : 2025-08-28  
Resolution : 3.00 Å(reported)

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:

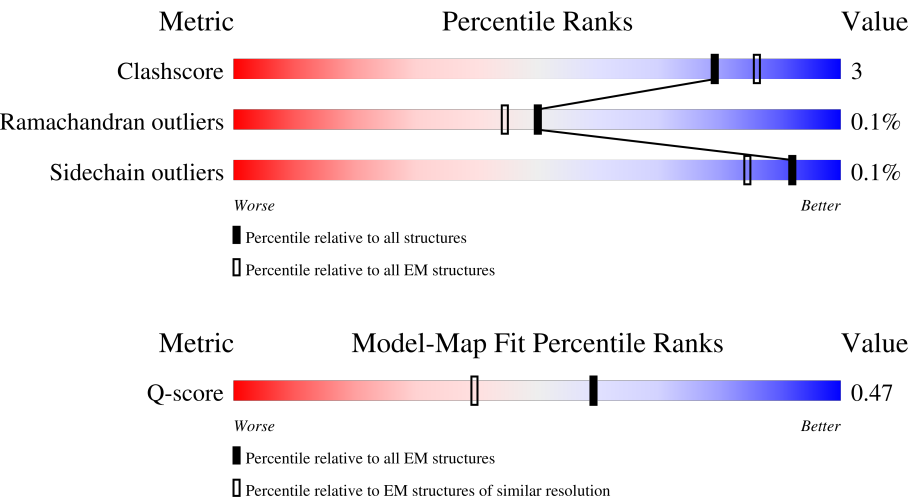
EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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	260	
2	B	235	
3	C	246	
4	D	241	

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Mol	Chain	Length	Quality of chain
5	E	256	
6	F	254	
7	G	252	
8	H	282	
9	I	270	
10	J	218	
11	K	195	
12	L	271	
13	M	240	
14	N	302	
15	e	124	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 24452 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 Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	246	Total	C	N	O	S	0	0
			1852	1170	312	358	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	227	Total	C	N	O	S	0	0
			1696	1102	278	310	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	240	Total	C	N	O	S	0	0
			1789	1151	296	339	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total	C	N	O	S	0	0
			1777	1141	307	321	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	231	Total	C	N	O	S	0	0
			1722	1087	288	338	9		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	232	Total	C	N	O	S	0	0
			1743	1122	288	323	10		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	245	Total	C	N	O	S	0	0
			1945	1242	328	364	11		

- Molecule 8 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	191	Total	C	N	O	S	0	0
			1480	952	254	265	9		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	216	Total	C	N	O	S	0	0
			1575	1002	275	285	13		

- Molecule 10 is a protein called Proteasome subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	193	Total	C	N	O	S	0	0
			1433	925	233	266	9		

- Molecule 11 is a protein called Proteasome subunit beta-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	186	Total	C	N	O	S	0	0
			1494	966	246	276	6		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	223	Total	C	N	O	S	0	0
			1670	1078	274	311	7		

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	196	Total	C	N	O	S	0	0
			1497	961	247	283	6		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	228	Total	C	N	O	S	0	0
			1838	1181	316	334	7		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	266	GLU	-	expression tag	UNP A0A0L7LW03
N	267	ASN	-	expression tag	UNP A0A0L7LW03
N	268	LEU	-	expression tag	UNP A0A0L7LW03
N	269	TYR	-	expression tag	UNP A0A0L7LW03
N	270	PHE	-	expression tag	UNP A0A0L7LW03
N	271	GLN	-	expression tag	UNP A0A0L7LW03
N	272	SER	-	expression tag	UNP A0A0L7LW03
N	273	SER	-	expression tag	UNP A0A0L7LW03
N	274	ALA	-	expression tag	UNP A0A0L7LW03
N	275	TRP	-	expression tag	UNP A0A0L7LW03
N	276	SER	-	expression tag	UNP A0A0L7LW03
N	277	HIS	-	expression tag	UNP A0A0L7LW03
N	278	PRO	-	expression tag	UNP A0A0L7LW03
N	279	GLN	-	expression tag	UNP A0A0L7LW03
N	280	PHE	-	expression tag	UNP A0A0L7LW03
N	281	GLU	-	expression tag	UNP A0A0L7LW03
N	282	LYS	-	expression tag	UNP A0A0L7LW03
N	283	GLY	-	expression tag	UNP A0A0L7LW03
N	284	GLY	-	expression tag	UNP A0A0L7LW03
N	285	GLY	-	expression tag	UNP A0A0L7LW03
N	286	SER	-	expression tag	UNP A0A0L7LW03
N	287	GLY	-	expression tag	UNP A0A0L7LW03
N	288	GLY	-	expression tag	UNP A0A0L7LW03
N	289	GLY	-	expression tag	UNP A0A0L7LW03
N	290	SER	-	expression tag	UNP A0A0L7LW03
N	291	GLY	-	expression tag	UNP A0A0L7LW03
N	292	GLY	-	expression tag	UNP A0A0L7LW03
N	293	SER	-	expression tag	UNP A0A0L7LW03
N	294	ALA	-	expression tag	UNP A0A0L7LW03
N	295	TRP	-	expression tag	UNP A0A0L7LW03
N	296	SER	-	expression tag	UNP A0A0L7LW03
N	297	HIS	-	expression tag	UNP A0A0L7LW03
N	298	PRO	-	expression tag	UNP A0A0L7LW03
N	299	GLN	-	expression tag	UNP A0A0L7LW03
N	300	PHE	-	expression tag	UNP A0A0L7LW03
N	301	GLU	-	expression tag	UNP A0A0L7LW03
N	302	LYS	-	expression tag	UNP A0A0L7LW03

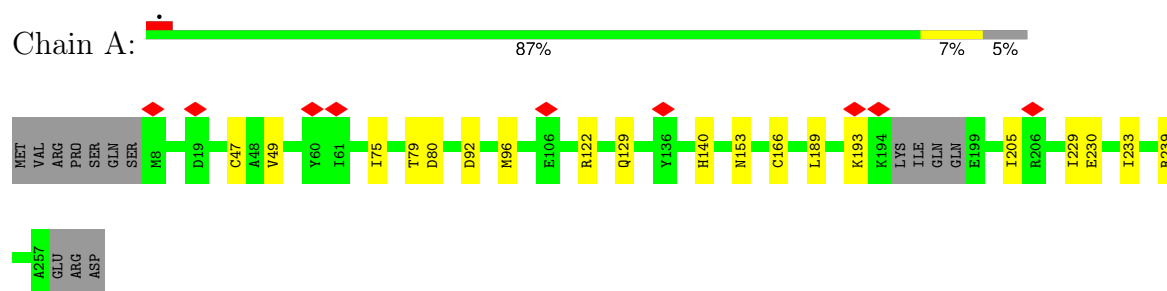
- Molecule 15 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	e	119	941	605	159	175	2	0	0

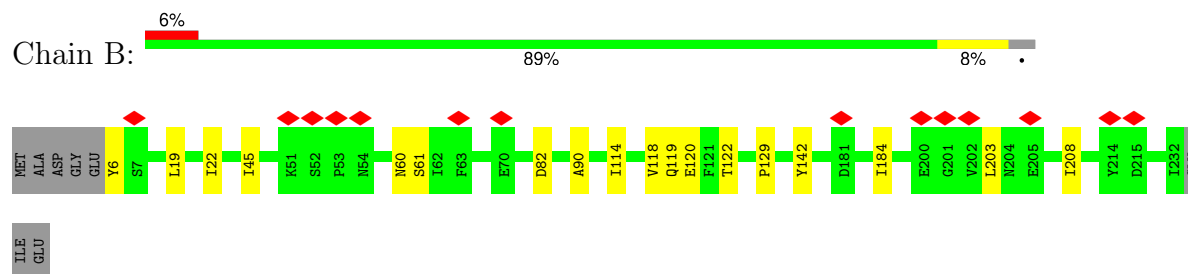
### 3 Residue-property plots [i](#)

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.

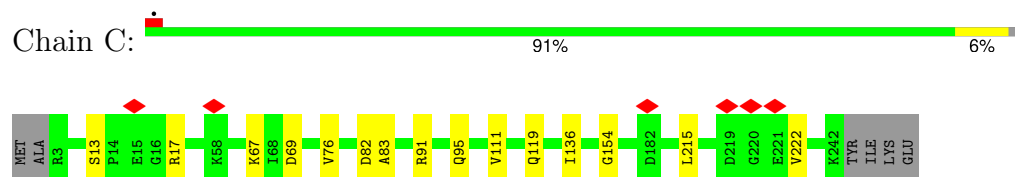
- Molecule 1: Proteasome subunit alpha type-6



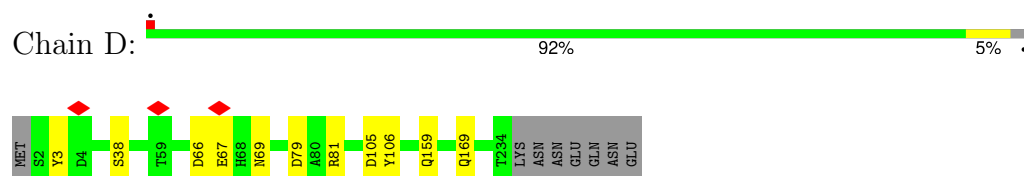
- Molecule 2: Proteasome subunit alpha type-2



- Molecule 3: Proteasome subunit alpha type-3



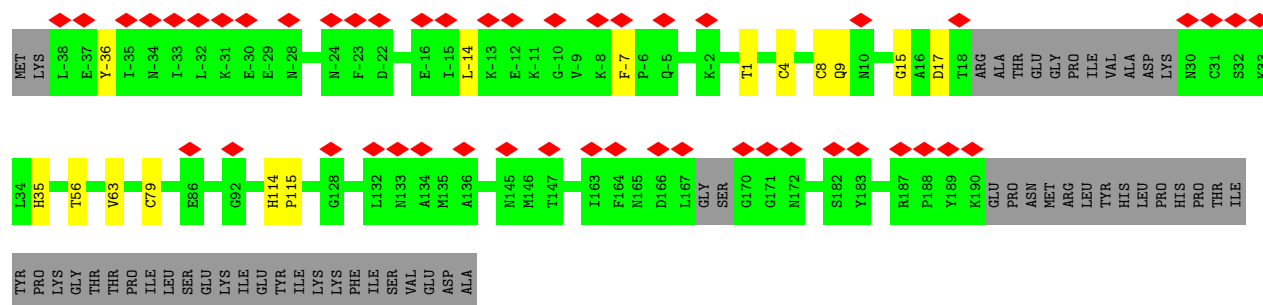
- Molecule 4: Proteasome subunit alpha type-4



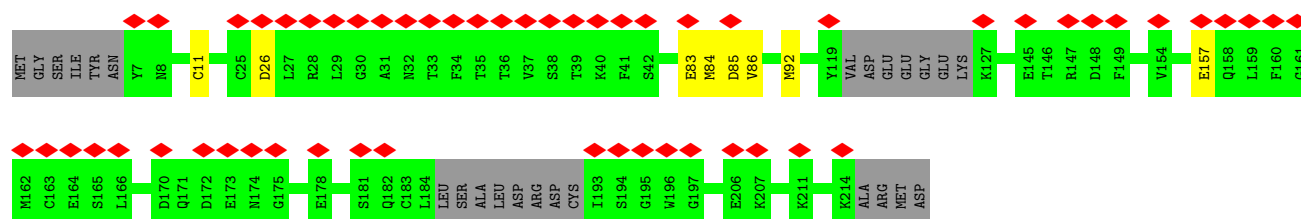
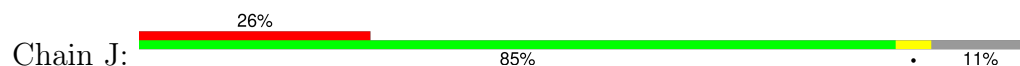
- Molecule 5: Proteasome subunit alpha type-5



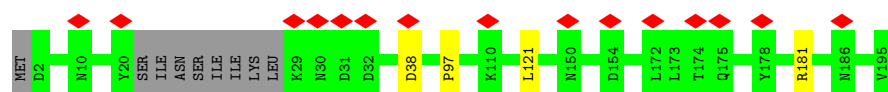




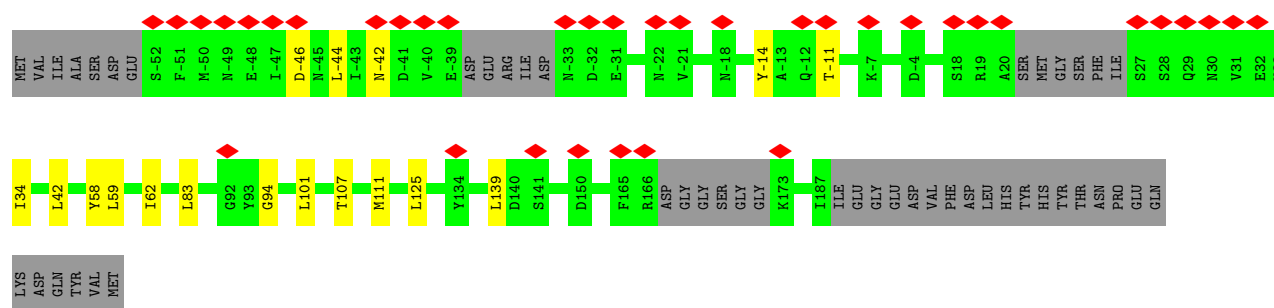
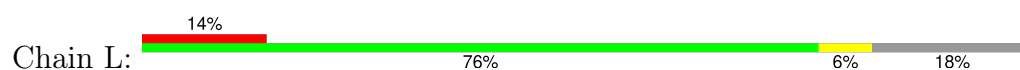
• Molecule 10: Proteasome subunit beta-3



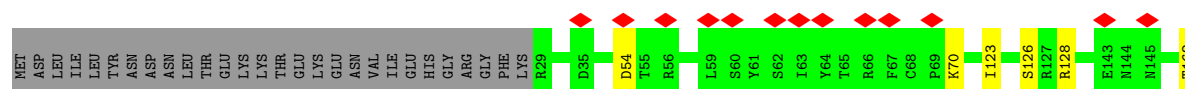
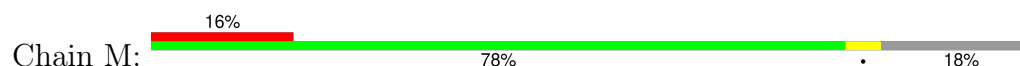
• Molecule 11: Proteasome subunit beta-4

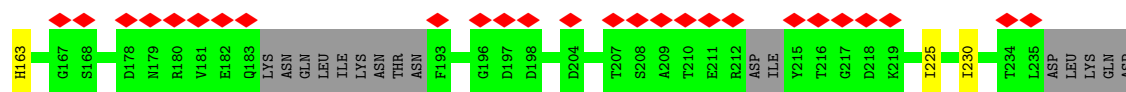


• Molecule 12: Proteasome subunit beta

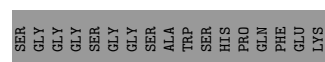
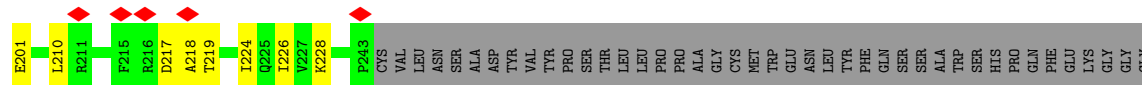
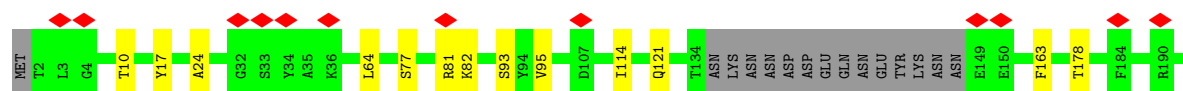


• Molecule 13: Proteasome subunit beta

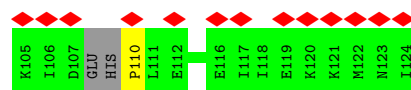
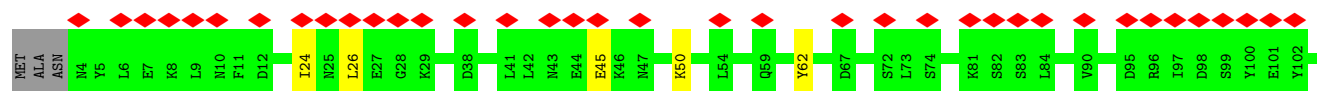
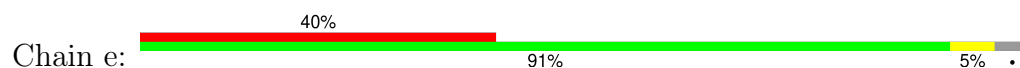




• Molecule 14: Proteasome subunit beta



• Molecule 15: Proteasome maturation factor UMP1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	456152	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	51.733	Depositor
Minimum map value	-32.734	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	10	Depositor
Map size (Å)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/1878	0.46	0/2550
2	B	0.29	1/1730 (0.1%)	0.50	3/2356 (0.1%)
3	C	0.23	0/1824	0.44	0/2496
4	D	0.26	0/1807	0.49	0/2447
5	E	0.26	0/1745	0.48	0/2368
6	F	0.29	0/1775	0.50	0/2406
7	G	0.28	0/1989	0.50	0/2702
8	H	0.28	0/1504	0.51	0/2026
9	I	0.27	0/1603	0.47	0/2179
10	J	0.24	0/1457	0.50	0/1979
11	K	0.29	0/1527	0.50	0/2064
12	L	0.26	0/1701	0.47	0/2306
13	M	0.25	0/1525	0.46	0/2074
14	N	0.25	0/1877	0.46	0/2537
15	e	0.32	0/952	0.53	0/1283
All	All	0.27	1/24894 (0.0%)	0.49	3/33773 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	120	GLU	C-O	-5.79	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	GLU	CA-C-O	-5.62	115.10	121.00
2	B	120	GLU	N-CA-CB	5.29	117.63	109.91
2	B	120	GLU	N-CA-C	-5.17	105.33	110.97

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1852	0	1765	14	0
2	B	1696	0	1633	12	0
3	C	1789	0	1656	10	0
4	D	1777	0	1773	7	0
5	E	1722	0	1657	11	0
6	F	1743	0	1672	15	0
7	G	1945	0	1833	13	0
8	H	1480	0	1429	12	0
9	I	1575	0	1513	10	0
10	J	1433	0	1363	5	0
11	K	1494	0	1407	3	0
12	L	1670	0	1559	13	0
13	M	1497	0	1454	6	0
14	N	1838	0	1797	13	0
15	e	941	0	945	4	0
All	All	24452	0	23456	126	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 3.

All (126) 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)
14:N:210:LEU:HD13	14:N:224:ILE:HD12	1.65	0.78
12:L:-14:TYR:O	12:L:-11:THR:OG1	2.09	0.70
7:G:131:MET:SD	15:e:62:TYR:OH	2.50	0.69
12:L:107:THR:HG22	12:L:107:THR:O	1.92	0.69
6:F:117:GLN:OE1	6:F:118:LYS:NZ	2.26	0.68
2:B:45:ILE:HD11	2:B:184:ILE:HD12	1.75	0.68
12:L:-44:LEU:O	15:e:50:LYS:NZ	2.27	0.67
14:N:24:ALA:HB2	14:N:226:ILE:HD13	1.77	0.66
2:B:119:GLN:NE2	3:C:82:ASP:OD1	2.29	0.65
1:A:96:MET:SD	1:A:140:HIS:ND1	2.68	0.65
1:A:129:GLN:NE2	2:B:82:ASP:OD1	2.29	0.65
4:D:66:ASP:OD1	4:D:69:ASN:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:201:LEU:HD21	5:E:240:ILE:HD12	1.81	0.62
12:L:125:LEU:HD11	12:L:139:LEU:HD13	1.81	0.62
1:A:75:ILE:HD12	1:A:230:GLU:HG3	1.82	0.62
6:F:117:GLN:NE2	6:F:121:GLN:OE1	2.34	0.61
8:H:152:ILE:HD11	8:H:180:ALA:HB1	1.82	0.61
10:J:11:CYS:N	10:J:26:ASP:OD2	2.34	0.61
1:A:92:ASP:OD1	7:G:123:HIS:NE2	2.34	0.60
12:L:-46:ASP:OD1	12:L:-42:ASN:ND2	2.35	0.60
3:C:154:GLY:O	4:D:81:ARG:NH2	2.35	0.60
3:C:76:VAL:HG11	3:C:83:ALA:HB1	1.83	0.59
7:G:95:ARG:NH2	14:N:77:SER:O	2.36	0.59
12:L:94:GLY:O	13:M:128:ARG:NH1	2.35	0.59
1:A:229:ILE:O	8:H:75:ARG:NH2	2.35	0.59
5:E:42:VAL:HG11	5:E:196:ALA:HB2	1.84	0.59
7:G:104:ASN:OD1	8:H:138:LYS:NZ	2.29	0.59
11:K:38:ASP:OD1	11:K:181:ARG:NH1	2.36	0.58
2:B:6:TYR:N	4:D:3:TYR:O	2.36	0.58
5:E:73:HIS:NE2	5:E:107:ILE:O	2.30	0.58
6:F:185:GLU:O	6:F:189:HIS:ND1	2.29	0.57
14:N:82:LYS:O	14:N:121:GLN:NE2	2.38	0.56
3:C:215:LEU:HD21	3:C:222:VAL:HG13	1.89	0.55
8:H:233:ILE:HA	8:H:238:VAL:HG22	1.88	0.55
13:M:123:ILE:O	13:M:126:SER:OG	2.24	0.55
5:E:65:GLU:N	5:E:65:GLU:OE1	2.40	0.54
14:N:17:TYR:OH	14:N:228:LYS:NZ	2.40	0.54
1:A:153:ASN:OD1	1:A:239:ARG:NH1	2.40	0.54
6:F:105:ILE:HD11	6:F:134:ILE:HG22	1.90	0.54
11:K:97:PRO:HD2	15:e:24:ILE:HD13	1.90	0.54
8:H:38:ASN:ND2	8:H:40:ASN:OD1	2.40	0.53
12:L:83:LEU:HD23	12:L:101:LEU:HD11	1.90	0.53
1:A:205:ILE:HG23	1:A:233:ILE:HD13	1.91	0.53
2:B:118:VAL:O	2:B:122:THR:HG23	2.07	0.53
13:M:162:THR:HG23	13:M:163:HIS:ND1	2.23	0.53
3:C:69:ASP:OD1	3:C:95:GLN:NE2	2.43	0.52
6:F:7:ASP:O	6:F:21:GLN:NE2	2.42	0.52
14:N:163:PHE:HE1	14:N:178:THR:HG22	1.73	0.52
2:B:122:THR:HG22	2:B:129:PRO:HB3	1.92	0.52
3:C:13:SER:N	3:C:17:ARG:O	2.41	0.52
14:N:64:LEU:HD11	14:N:95:VAL:HG22	1.93	0.51
13:M:225:ILE:HG13	13:M:230:ILE:HG22	1.91	0.51
13:M:225:ILE:CG1	13:M:230:ILE:HG22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:O	8:H:68:ASN:ND2	2.44	0.50
12:L:34:ILE:CG2	12:L:42:LEU:HD22	2.42	0.50
12:L:58:TYR:CE2	12:L:62:ILE:HD11	2.47	0.50
10:J:157:GLU:OE1	10:J:157:GLU:N	2.45	0.49
4:D:159:GLN:NE2	4:D:169:GLN:OE1	2.45	0.49
13:M:54:ASP:OD1	13:M:70:LYS:NZ	2.30	0.49
9:I:114:HIS:HB3	9:I:115:PRO:HD2	1.95	0.49
5:E:204:LEU:O	5:E:208:MET:N	2.45	0.48
2:B:203:LEU:HD11	2:B:208:ILE:CG2	2.42	0.48
8:H:152:ILE:HD12	8:H:166:ALA:HA	1.96	0.48
1:A:49:VAL:HG22	1:A:233:ILE:HD12	1.95	0.48
8:H:12:VAL:HG21	8:H:164:LEU:HD13	1.97	0.47
6:F:88:MET:SD	6:F:112:VAL:HG11	2.54	0.47
5:E:69:SER:O	5:E:93:ARG:NH2	2.49	0.47
9:I:-36:TYR:OH	15:e:45:GLU:OE2	2.27	0.47
1:A:122:ARG:NH1	1:A:166:CYS:SG	2.88	0.46
7:G:111:LEU:HD11	7:G:140:ILE:HG22	1.97	0.46
7:G:220:TRP:CD1	7:G:222:CYS:HG	2.32	0.46
5:E:177:GLU:OE1	5:E:177:GLU:N	2.48	0.46
4:D:67:GLU:OE1	4:D:67:GLU:N	2.45	0.46
6:F:150:GLY:O	7:G:85:GLY:N	2.49	0.46
6:F:110:ARG:NH2	7:G:92:ASP:OD1	2.50	0.45
8:H:45:ARG:HD2	8:H:52:SER:HB3	1.98	0.45
9:I:63:VAL:HG21	9:I:79:CYS:SG	2.57	0.45
1:A:189:LEU:O	1:A:193:LYS:N	2.50	0.45
2:B:60:ASN:OD1	2:B:61:SER:N	2.50	0.45
6:F:19:LEU:HD13	6:F:22:VAL:HG21	1.99	0.45
1:A:49:VAL:CG2	1:A:233:ILE:HD12	2.47	0.45
1:A:47:CYS:HB2	1:A:233:ILE:HD11	2.00	0.44
6:F:62:LYS:NZ	6:F:74:MET:O	2.49	0.44
5:E:165:THR:HG21	6:F:53:ILE:HD13	2.00	0.44
12:L:34:ILE:HG22	12:L:42:LEU:HD22	2.00	0.44
7:G:218:PHE:O	7:G:231:ASN:ND2	2.47	0.44
2:B:203:LEU:HD11	2:B:208:ILE:HG23	2.00	0.43
10:J:85:ASP:OD1	10:J:86:VAL:N	2.51	0.43
6:F:98:LEU:O	14:N:93:SER:OG	2.37	0.43
9:I:35:HIS:CB	9:I:56:THR:HG21	2.48	0.43
2:B:90:ALA:HB2	2:B:114:ILE:HD11	2.01	0.43
5:E:191:MET:HE1	5:E:199:LEU:CD2	2.49	0.43
3:C:76:VAL:HG11	3:C:83:ALA:CB	2.47	0.42
8:H:152:ILE:HD11	8:H:180:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:201:GLU:OE1	14:N:201:GLU:N	2.52	0.42
6:F:139:ASN:OD1	14:N:81:ARG:NH1	2.53	0.42
14:N:217:ASP:OD1	14:N:218:ALA:N	2.52	0.42
5:E:76:CYS:SG	5:E:77:ALA:N	2.92	0.42
7:G:86:ASP:OD2	7:G:132:ARG:NH2	2.52	0.42
9:I:4:CYS:O	9:I:15:GLY:N	2.51	0.42
1:A:79:THR:HG23	1:A:80:ASP:H	1.85	0.42
5:E:201:LEU:HB2	5:E:244:LEU:HD21	2.02	0.42
9:I:8:CYS:SG	9:I:9:GLN:N	2.89	0.42
2:B:142:TYR:OH	10:J:83:GLU:O	2.37	0.42
6:F:72:ILE:HG22	6:F:134:ILE:HA	2.02	0.42
8:H:37:ILE:HD11	8:H:56:ILE:HG23	2.01	0.42
12:L:59:LEU:HD22	12:L:83:LEU:HB2	2.01	0.42
14:N:114:ILE:HD11	14:N:178:THR:HG23	2.01	0.42
2:B:19:LEU:CD2	2:B:22:ILE:HD12	2.50	0.42
6:F:44:VAL:HG13	6:F:214:VAL:HG13	2.01	0.42
9:I:-14:LEU:HD21	11:K:121:LEU:HD11	2.02	0.41
10:J:84:MET:HE1	10:J:92:MET:HE3	2.02	0.41
4:D:105:ASP:OD1	4:D:106:TYR:N	2.54	0.41
7:G:111:LEU:HD11	7:G:140:ILE:CG2	2.50	0.41
3:C:111:VAL:HG12	3:C:136:ILE:HD13	2.02	0.41
7:G:56:ASP:OD1	7:G:57:LYS:N	2.54	0.41
9:I:-14:LEU:HD13	9:I:-7:PHE:HZ	1.85	0.41
3:C:67:LYS:O	3:C:91:ARG:NH2	2.54	0.41
9:I:1:THR:OG1	9:I:17:ASP:OD1	2.32	0.40
9:I:35:HIS:HB3	9:I:56:THR:HG21	2.03	0.40
8:H:62:TYR:O	8:H:66:MET:HE3	2.22	0.40
7:G:35:ASN:O	7:G:81:SER:OG	2.27	0.40
12:L:59:LEU:HD22	12:L:83:LEU:HD22	2.02	0.40
12:L:111:MET:O	12:L:111:MET:HG3	2.21	0.40
14:N:10:THR:OG1	14:N:219:THR:O	2.39	0.40
3:C:119:GLN:NE2	4:D:79:ASP:OD1	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/260 (93%)	228 (94%)	14 (6%)	0	100	100
2	B	225/235 (96%)	218 (97%)	7 (3%)	0	100	100
3	C	238/246 (97%)	230 (97%)	8 (3%)	0	100	100
4	D	231/241 (96%)	224 (97%)	6 (3%)	1 (0%)	30	66
5	E	227/256 (89%)	218 (96%)	9 (4%)	0	100	100
6	F	228/254 (90%)	215 (94%)	13 (6%)	0	100	100
7	G	243/252 (96%)	228 (94%)	15 (6%)	0	100	100
8	H	183/282 (65%)	170 (93%)	13 (7%)	0	100	100
9	I	210/270 (78%)	200 (95%)	10 (5%)	0	100	100
10	J	187/218 (86%)	173 (92%)	14 (8%)	0	100	100
11	K	182/195 (93%)	178 (98%)	4 (2%)	0	100	100
12	L	215/271 (79%)	208 (97%)	7 (3%)	0	100	100
13	M	190/240 (79%)	178 (94%)	12 (6%)	0	100	100
14	N	224/302 (74%)	215 (96%)	9 (4%)	0	100	100
15	e	115/124 (93%)	105 (91%)	9 (8%)	1 (1%)	14	49
All	All	3140/3646 (86%)	2988 (95%)	150 (5%)	2 (0%)	50	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	e	26	LEU
4	D	38	SER

### 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	190/231 (82%)	190 (100%)	0	100	100
2	B	168/205 (82%)	168 (100%)	0	100	100
3	C	168/213 (79%)	168 (100%)	0	100	100
4	D	180/207 (87%)	180 (100%)	0	100	100
5	E	178/223 (80%)	178 (100%)	0	100	100
6	F	176/227 (78%)	175 (99%)	1 (1%)	84	93
7	G	205/229 (90%)	205 (100%)	0	100	100
8	H	151/260 (58%)	151 (100%)	0	100	100
9	I	158/231 (68%)	158 (100%)	0	100	100
10	J	144/191 (75%)	144 (100%)	0	100	100
11	K	152/174 (87%)	152 (100%)	0	100	100
12	L	161/232 (69%)	161 (100%)	0	100	100
13	M	161/216 (74%)	161 (100%)	0	100	100
14	N	193/266 (73%)	193 (100%)	0	100	100
15	e	102/119 (86%)	101 (99%)	1 (1%)	73	88
All	All	2487/3224 (77%)	2485 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	44	VAL
15	e	110	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	176	ASN
1	A	238	ASN
3	C	167	ASN
4	D	92	GLN
4	D	175	ASN
6	F	89	GLN
6	F	218	HIS
7	G	73	ASN
7	G	206	HIS
9	I	109	GLN

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Mol	Chain	Res	Type
10	J	171	GLN
11	K	96	ASN
12	L	-2	HIS
12	L	124	ASN
14	N	19	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 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.

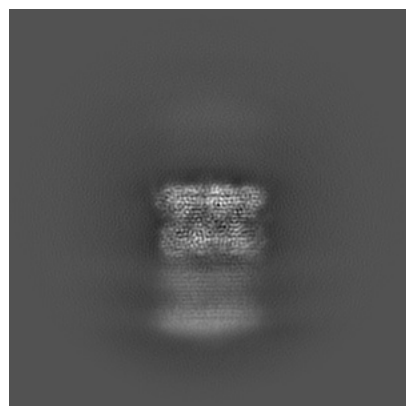
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72395. These allow visual inspection of the internal detail of the map and identification of artifacts.

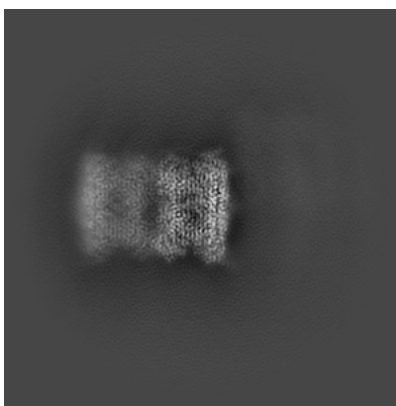
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

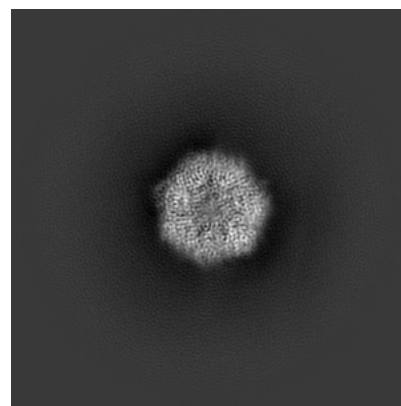
#### 6.1.1 Primary map



X

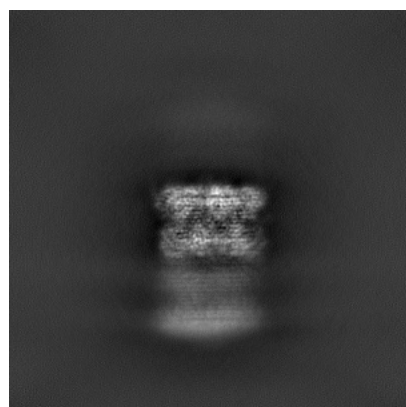


Y

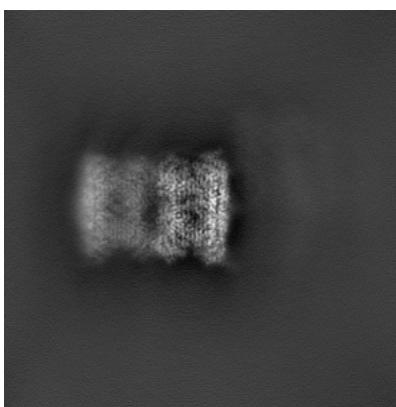


Z

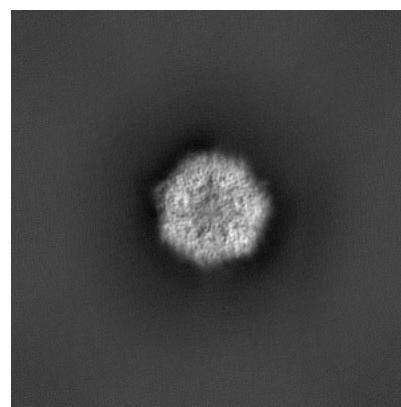
#### 6.1.2 Raw map



X



Y

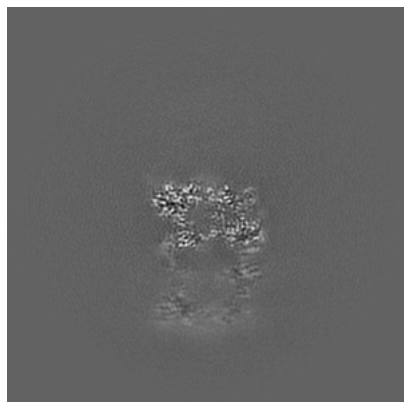


Z

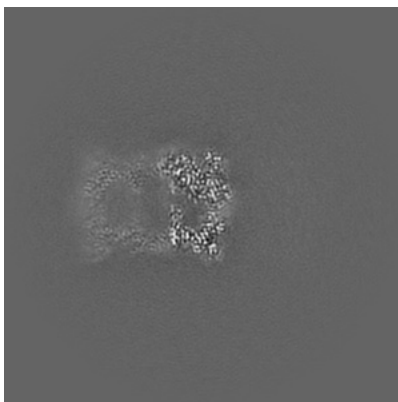
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

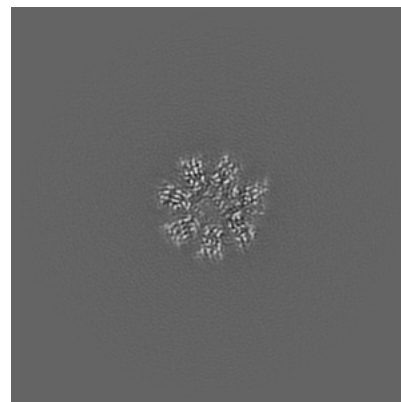
### 6.2.1 Primary map



X Index: 200

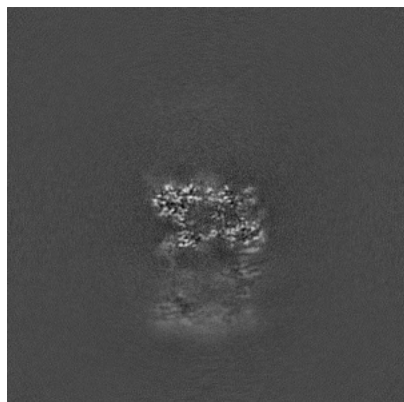


Y Index: 200

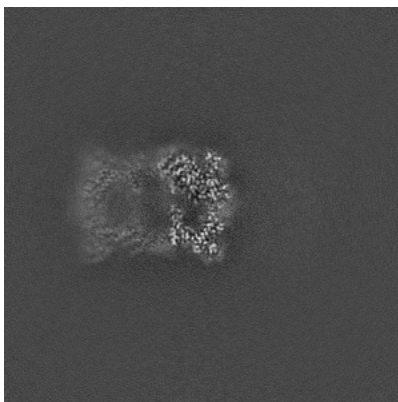


Z Index: 200

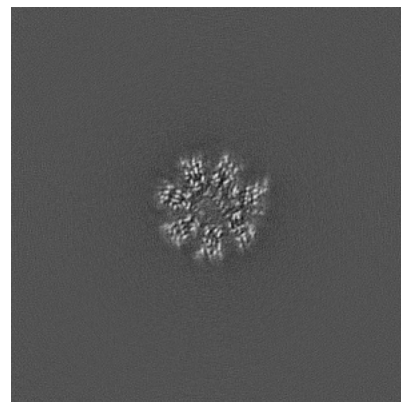
### 6.2.2 Raw map



X Index: 200



Y Index: 200

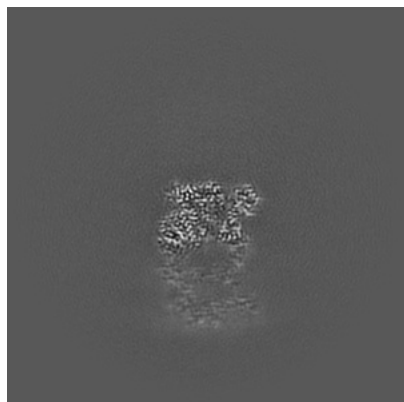


Z Index: 200

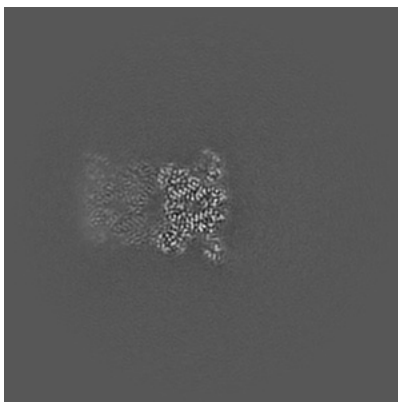
The images above show central slices of the map in three orthogonal directions.

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

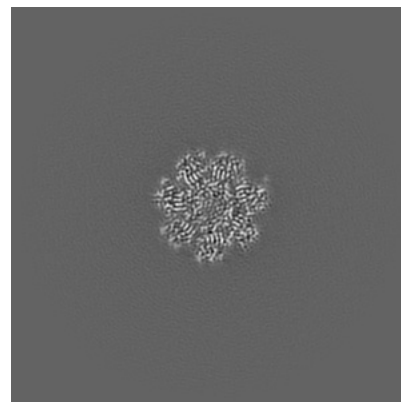
### 6.3.1 Primary map



X Index: 220



Y Index: 225

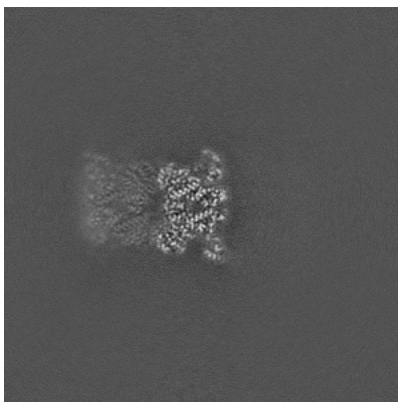


Z Index: 206

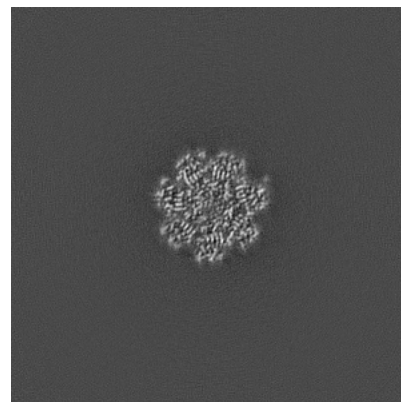
### 6.3.2 Raw map



X Index: 220



Y Index: 225



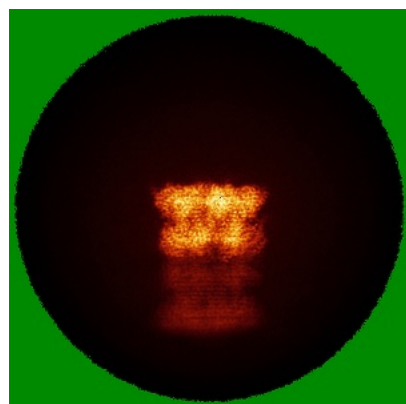
Z Index: 206

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

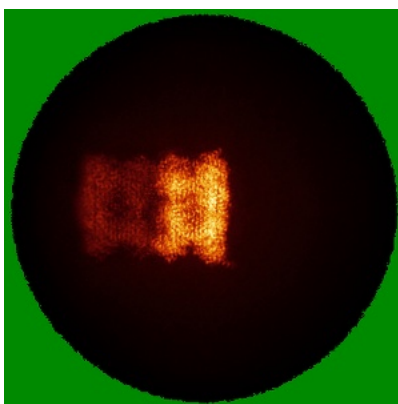


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

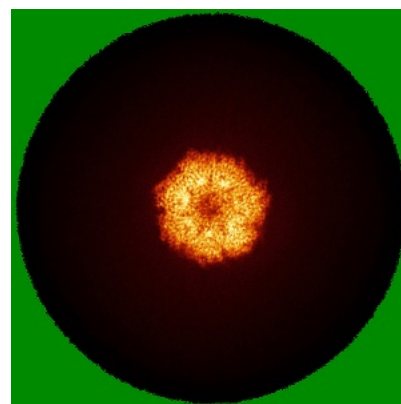
### 6.4.1 Primary map



X

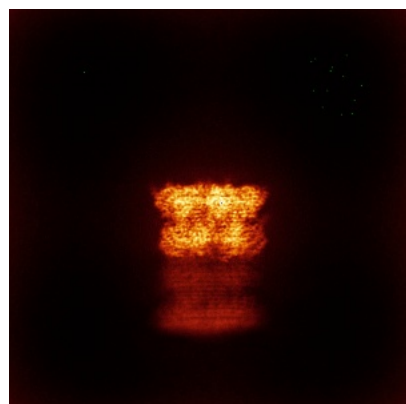


Y

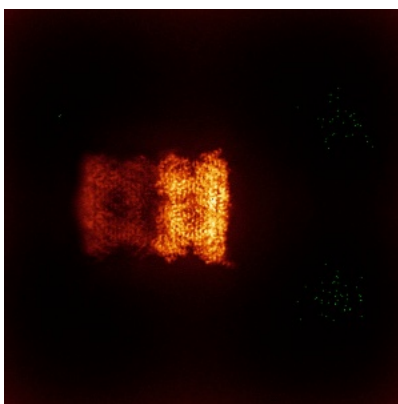


Z

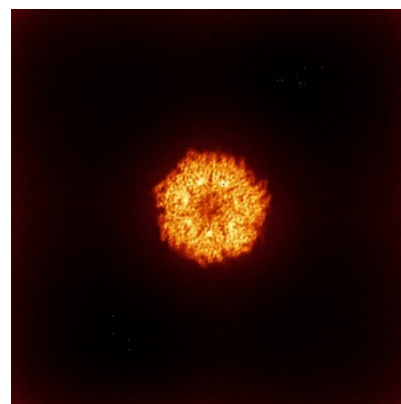
### 6.4.2 Raw map



X



Y



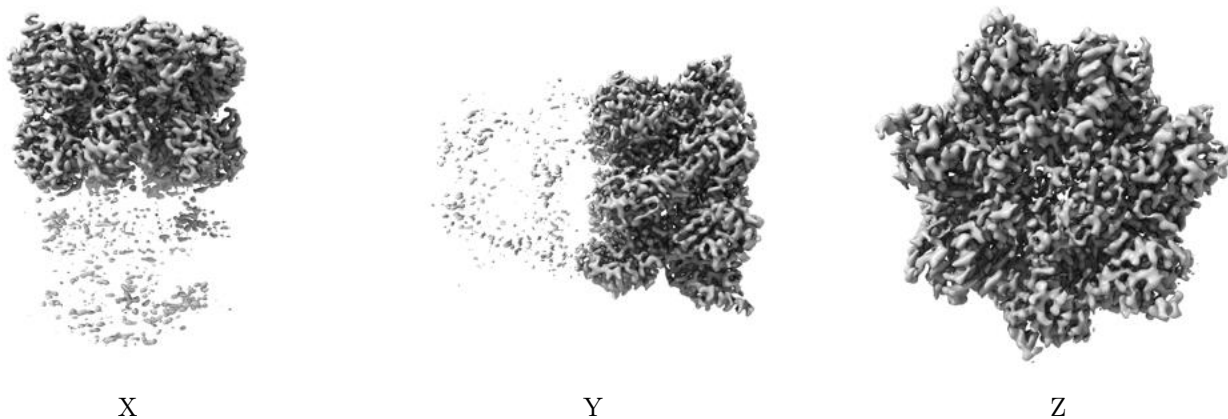
Z

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.



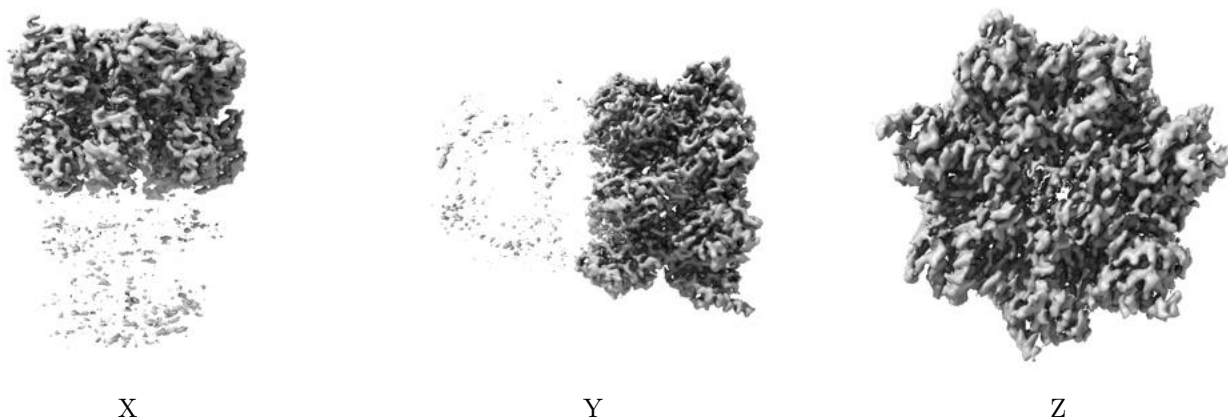
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.0. 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.

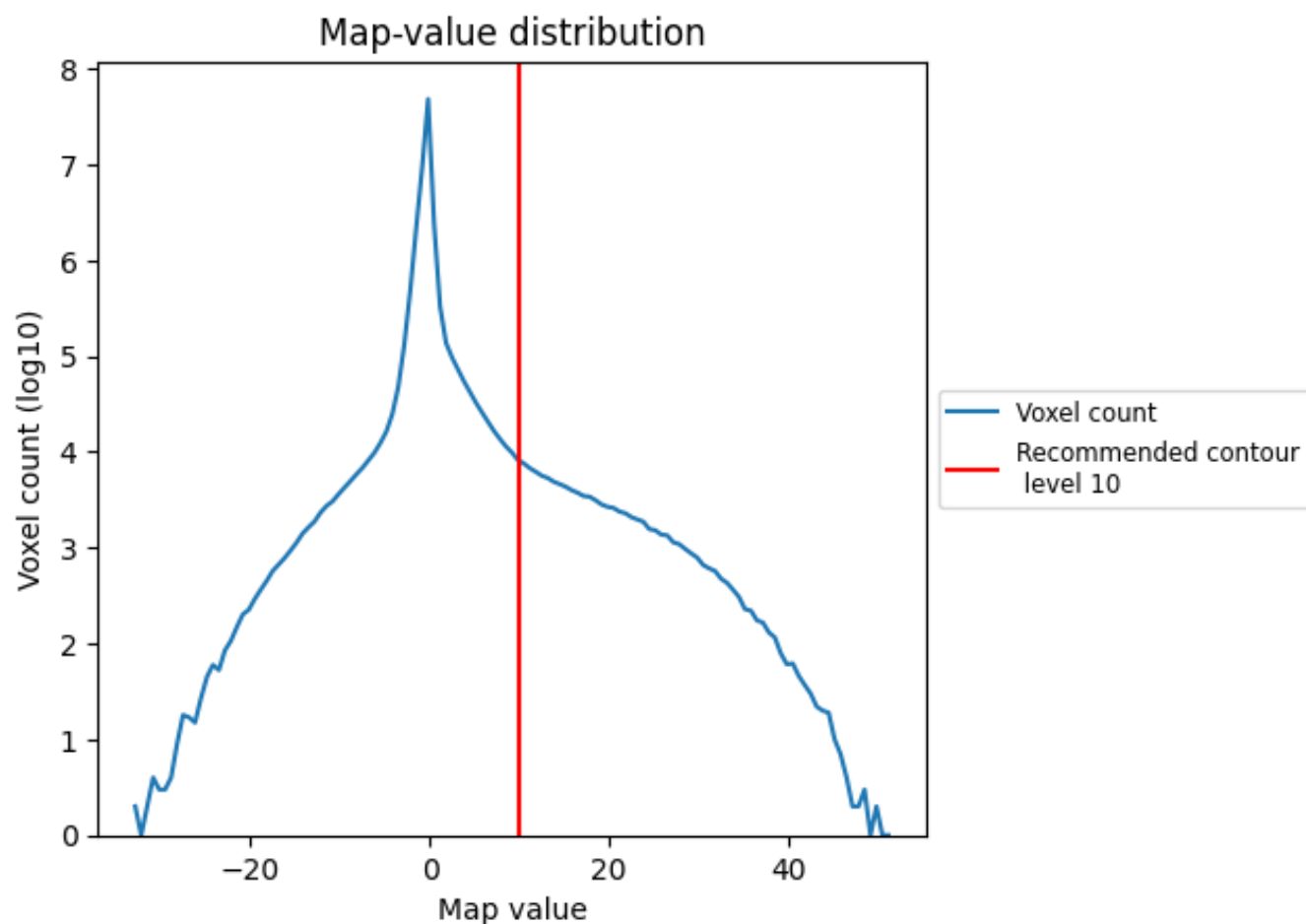
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

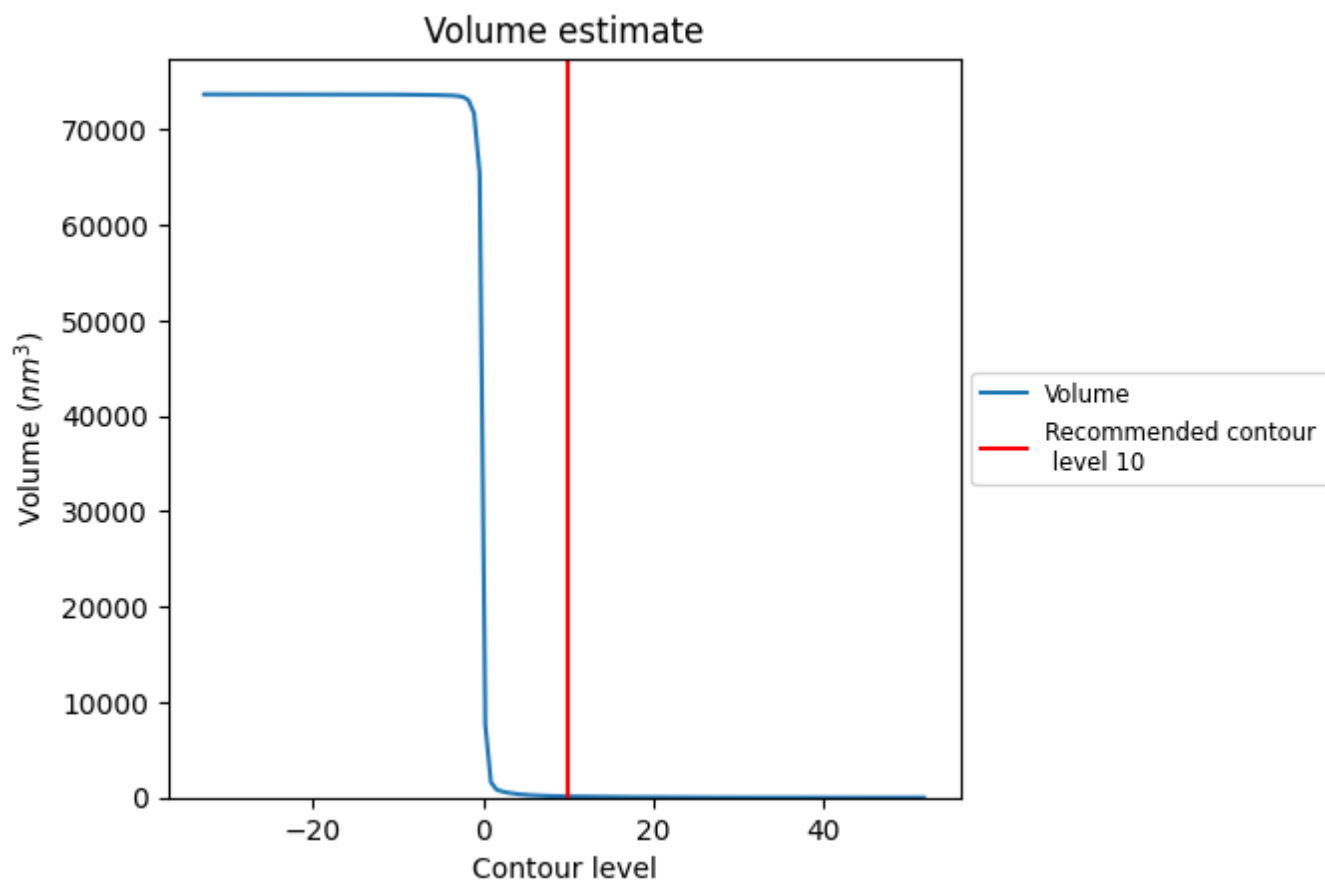
This section contains the results of statistical analysis of the map.

### 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.

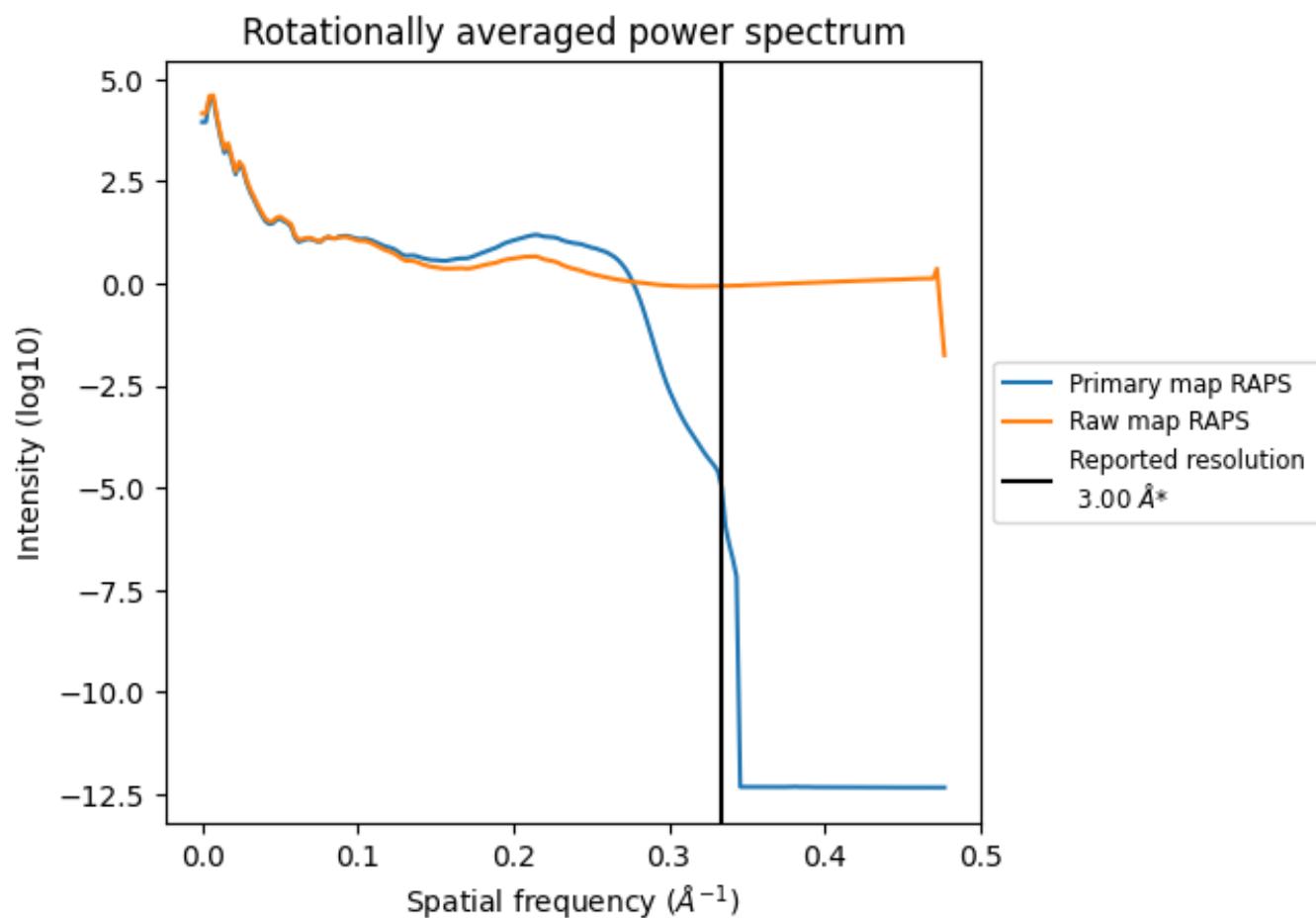
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm<sup>3</sup>; this corresponds to an approximate mass of 108 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 ⓘ

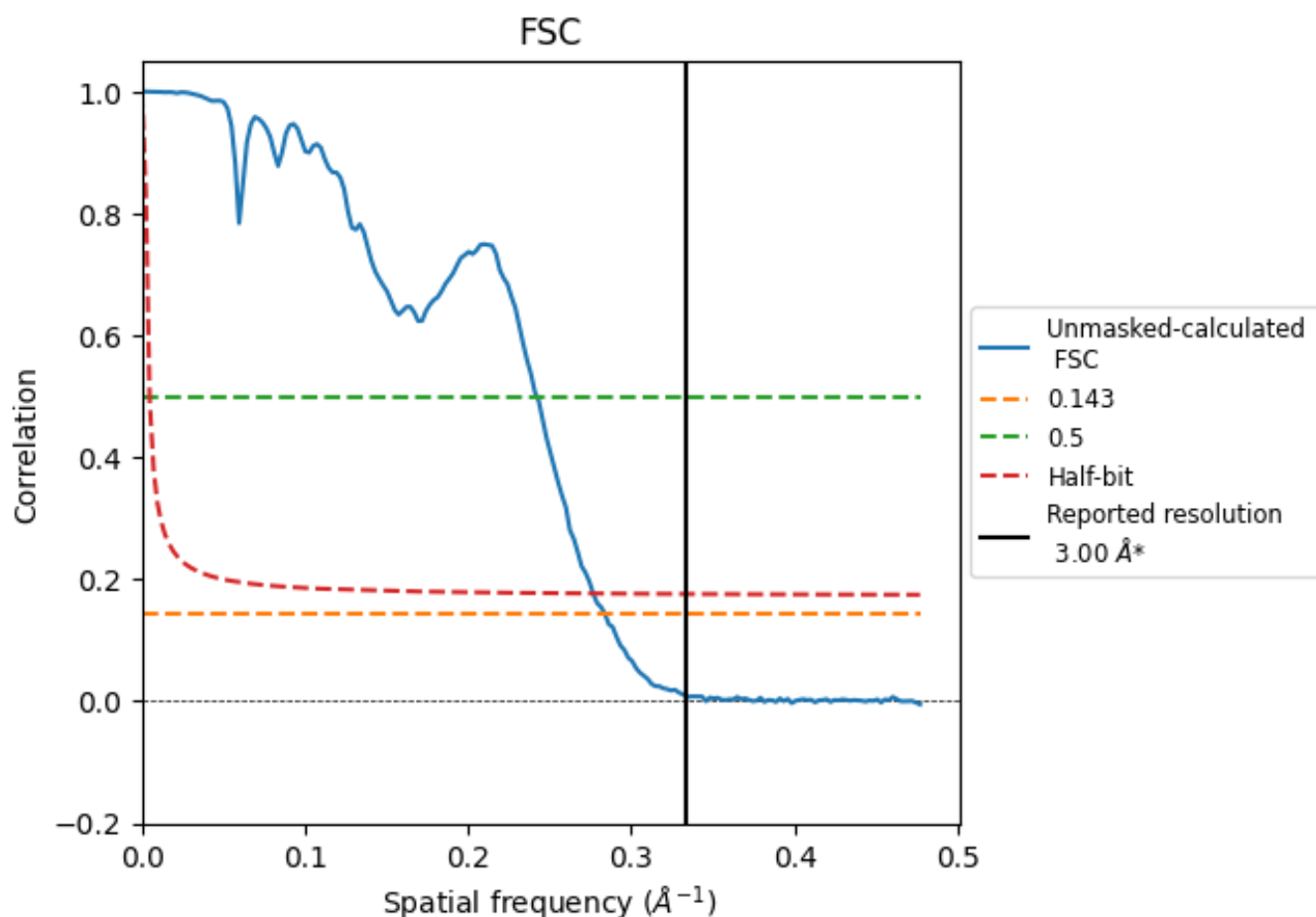


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 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  $0.333 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

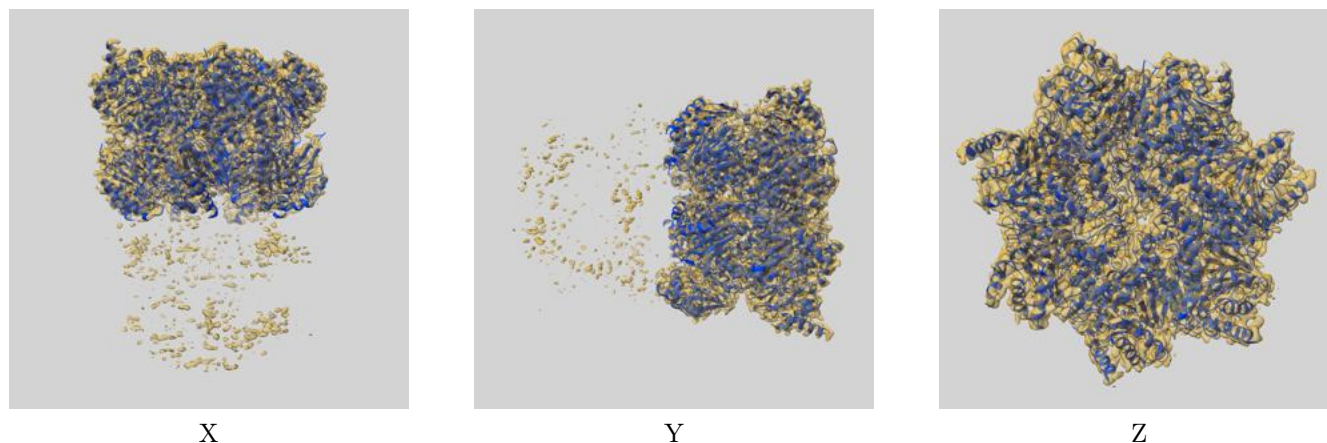
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.52	4.13	3.61

\*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 3.52 differs from the reported value 3.0 by more than 10 %

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

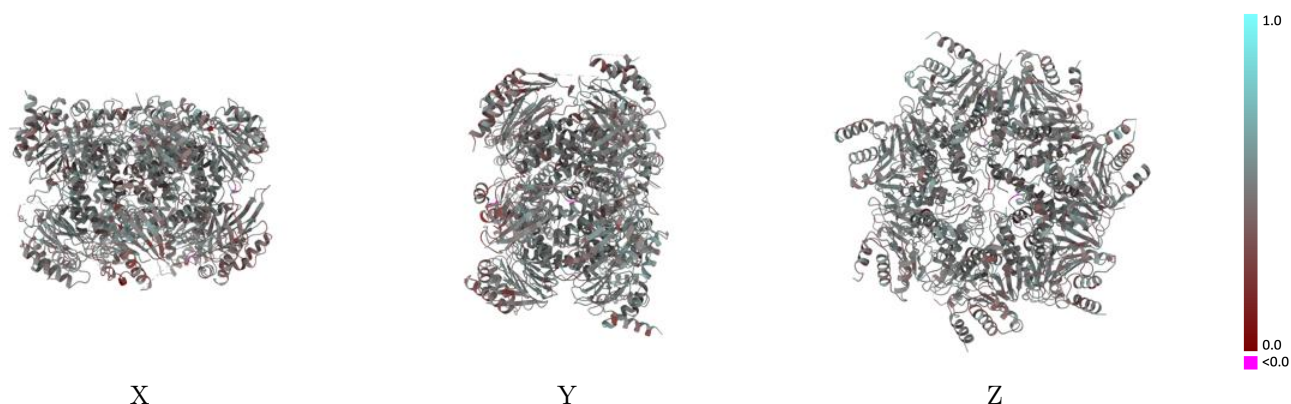
This section contains information regarding the fit between EMDB map EMD-72395 and PDB model 9Y0L. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



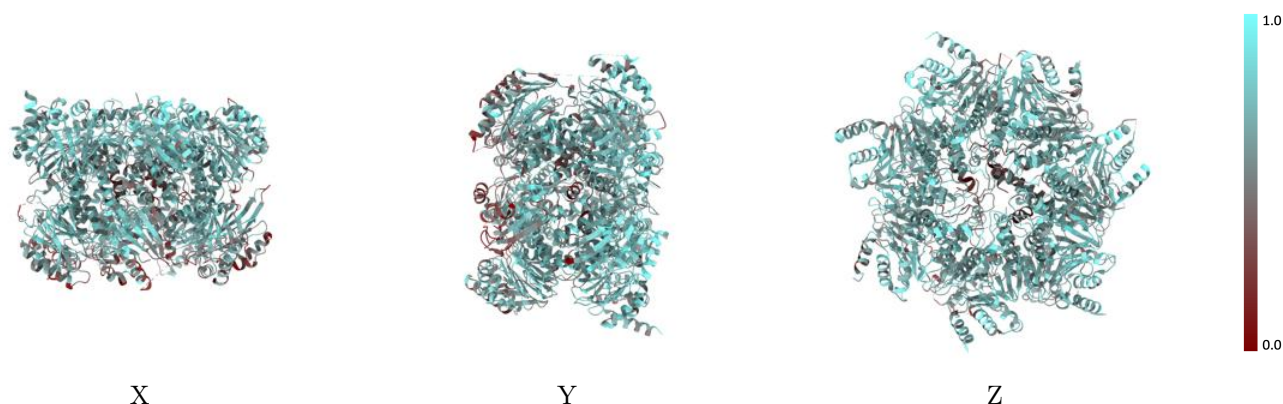
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

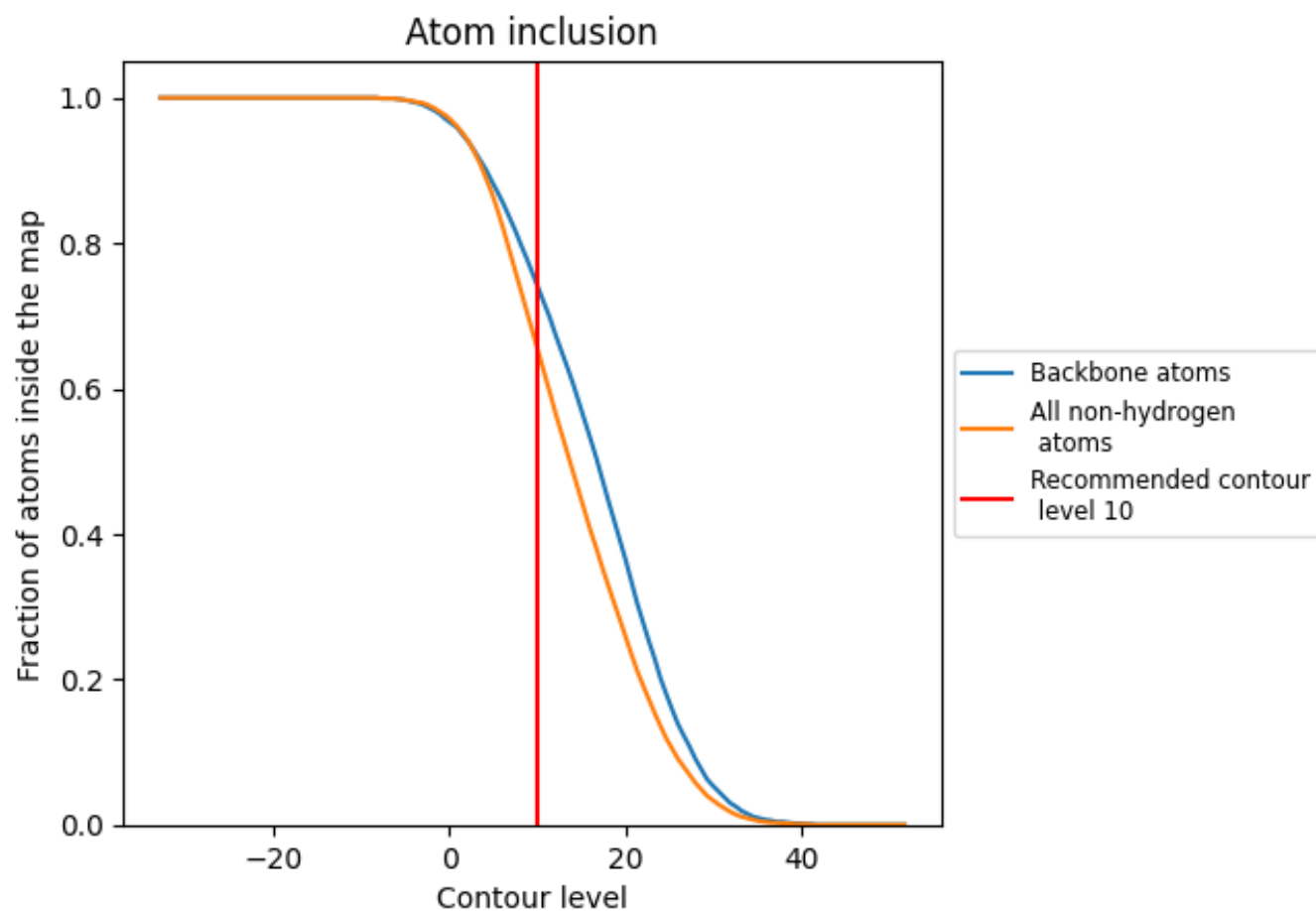
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (10).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 66% 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 (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6570	 0.4700
A	 0.7130	 0.4760
B	 0.7020	 0.4820
C	 0.7490	 0.4930
D	 0.7160	 0.4910
E	 0.6720	 0.4730
F	 0.7090	 0.4630
G	 0.7350	 0.4740
H	 0.5950	 0.4390
I	 0.5720	 0.4510
J	 0.5490	 0.4360
K	 0.6800	 0.4690
L	 0.6080	 0.4740
M	 0.5970	 0.4610
N	 0.6540	 0.4820
e	 0.4530	 0.4570

