



## Full wwPDB EM Validation Report ⓘ

Apr 11, 2024 – 04:33 pm BST

PDB ID : 8QYN  
EMDB ID : EMD-18759  
Title : Human 20S proteasome assembly intermediate structure 5  
Authors : Schulman, B.A.; Hanna, J.W.; Harper, J.W.; Adolf, F.; Du, J.; Rawson, S.D.;  
Walsh Jr, R.M.; Goodall, E.A.  
Deposited on : 2023-10-26  
Resolution : 2.88 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:

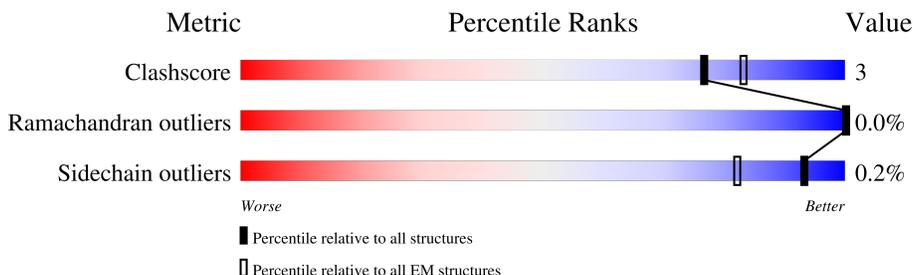
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	93% 6% .
2	B	261	87% 8% 5%
3	C	248	88% 6% 6%
4	D	242	94% 6%
5	E	264	85% 6% 9%
6	F	255	90% 5% 5%
7	G	246	93% 6% .
8	H	142	80% 10% 10%

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Mol	Chain	Length	Quality of chain
9	I	288	<p>5% 90% 5% 5%</p>
10	J	265	<p>86% 8% 6%</p>
11	K	332	<p>64% 5% 31%</p>
12	L	205	<p>84% 12%</p>
13	M	202	<p>7% 83% 14%</p>
14	N	264	<p>5% 77% 6% 18%</p>
15	O	241	<p>6% 71% 11% 18%</p>
16	P	264	<p>70% 5% 25%</p>
17	Q	239	<p>6% 78% 6% 15%</p>

## 2 Entry composition i

There are 17 unique types of molecules in this entry. The entry contains 29115 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-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	232	1805	1155	307	337	6	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	247	1937	1225	332	370	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	233	1826	1149	326	346	5	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	242	1840	1159	305	364	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ACE	-	acetylation	UNP P28066

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	241	1889	1185	340	352	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ACE	-	acetylation	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	242	1885	1197	323	354	11	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	243	1892	1200	316	363	13	0	0

- Molecule 8 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	128	1008	639	170	193	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ACE	-	acetylation	UNP Q9Y244

- Molecule 9 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	273	2180	1392	365	405	18	0	0

- Molecule 10 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	250	1952	1259	321	357	15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ACE	-	acetylation	UNP Q969U7

- Molecule 11 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	230	1696	1074	292	320	10	0	0

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	238O	GLU	-	expression tag	UNP Q99436
K	238P	ASP	-	expression tag	UNP Q99436
K	238Q	LEU	-	expression tag	UNP Q99436
K	238R	TYR	-	expression tag	UNP Q99436
K	238S	PHE	-	expression tag	UNP Q99436
K	238T	GLN	-	expression tag	UNP Q99436
K	238U	SER	-	expression tag	UNP Q99436
K	238V	VAL	-	expression tag	UNP Q99436
K	238W	ASP	-	expression tag	UNP Q99436
K	238X	SER	-	expression tag	UNP Q99436
K	238Y	ALA	-	expression tag	UNP Q99436
K	238Z	TRP	-	expression tag	UNP Q99436
K	239A	SER	-	expression tag	UNP Q99436
K	239B	HIS	-	expression tag	UNP Q99436
K	239C	PRO	-	expression tag	UNP Q99436
K	239D	GLN	-	expression tag	UNP Q99436
K	239E	PHE	-	expression tag	UNP Q99436
K	239F	GLU	-	expression tag	UNP Q99436
K	239G	LYS	-	expression tag	UNP Q99436
K	239H	GLY	-	expression tag	UNP Q99436
K	239I	GLY	-	expression tag	UNP Q99436
K	239J	GLY	-	expression tag	UNP Q99436
K	239K	SER	-	expression tag	UNP Q99436
K	239L	GLY	-	expression tag	UNP Q99436
K	239M	GLY	-	expression tag	UNP Q99436
K	239N	GLY	-	expression tag	UNP Q99436
K	239O	SER	-	expression tag	UNP Q99436
K	239P	GLY	-	expression tag	UNP Q99436
K	239Q	GLY	-	expression tag	UNP Q99436
K	239R	SER	-	expression tag	UNP Q99436
K	239S	ALA	-	expression tag	UNP Q99436
K	239T	TRP	-	expression tag	UNP Q99436
K	239U	SER	-	expression tag	UNP Q99436
K	239V	HIS	-	expression tag	UNP Q99436
K	239W	PRO	-	expression tag	UNP Q99436
K	239X	GLN	-	expression tag	UNP Q99436

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Chain	Residue	Modelled	Actual	Comment	Reference
K	239Y	PHE	-	expression tag	UNP Q99436
K	239Z	GLU	-	expression tag	UNP Q99436
K	240A	LYS	-	expression tag	UNP Q99436
K	247	UNK	-	expression tag	UNP Q99436
K	248	UNK	-	expression tag	UNP Q99436
K	249	UNK	-	expression tag	UNP Q99436
K	250	UNK	-	expression tag	UNP Q99436
K	251	UNK	-	expression tag	UNP Q99436
K	252	UNK	-	expression tag	UNP Q99436
K	253	UNK	-	expression tag	UNP Q99436
K	254	UNK	-	expression tag	UNP Q99436
K	255	UNK	-	expression tag	UNP Q99436
K	256	UNK	-	expression tag	UNP Q99436
K	257	UNK	-	expression tag	UNP Q99436
K	258	UNK	-	expression tag	UNP Q99436
K	259	UNK	-	expression tag	UNP Q99436
K	260	UNK	-	expression tag	UNP Q99436
K	261	UNK	-	expression tag	UNP Q99436
K	262	UNK	-	expression tag	UNP Q99436

- Molecule 12 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	180	1412	905	236	256	15	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	198	1581	1013	268	291	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	ACE	-	acetylation	UNP P49721

- Molecule 14 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	217	1651	1048	290	303	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	0	ACE	-	acetylation	UNP P28074

- Molecule 15 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	197	1509	960	255	285	9	0	0

- Molecule 16 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	198	1537	971	265	290	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	234	THR	ILE	variant	UNP P28070

- Molecule 17 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	202	1515	946	260	297	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	145	GLY	VAL	variant	UNP P28072





• Molecule 6: Proteasome subunit alpha type-3



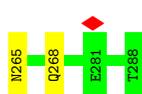
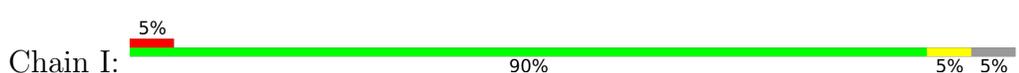
• Molecule 7: Proteasome subunit alpha type-6



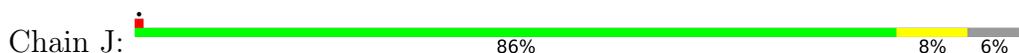
• Molecule 8: Proteasome maturation protein



• Molecule 9: Proteasome assembly chaperone 1

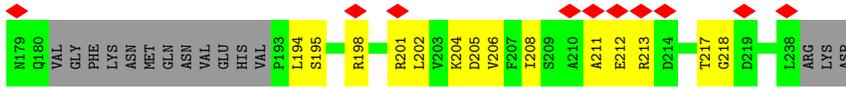


• Molecule 10: Proteasome assembly chaperone 2

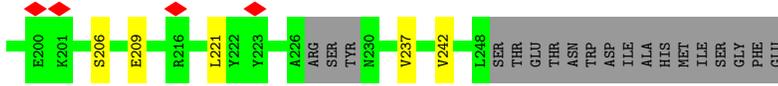


• Molecule 11: Proteasome subunit beta type-7

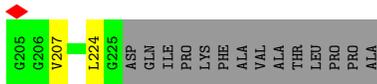
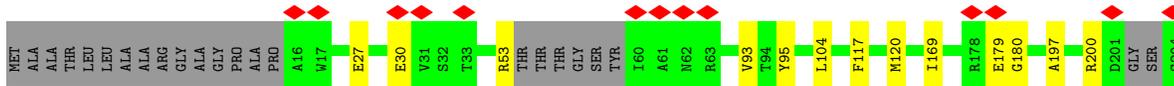
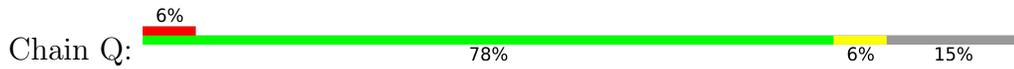




• Molecule 16: Proteasome subunit beta type-4



• Molecule 17: Proteasome subunit beta type-6



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	66.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.532	Depositor
Minimum map value	-1.083	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	255.36, 255.36, 255.36	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8512, 0.8512, 0.8512	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: ACE

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	0.29	0/1844	0.48	0/2498
2	B	0.29	0/1967	0.48	0/2650
3	C	0.27	0/1852	0.50	0/2501
4	D	0.27	0/1867	0.47	0/2523
5	E	0.27	0/1923	0.51	0/2598
6	F	0.29	0/1920	0.48	0/2586
7	G	0.30	0/1926	0.46	0/2603
8	H	0.26	0/1020	0.47	0/1371
9	I	0.26	0/2224	0.48	0/3013
10	J	0.27	0/1992	0.46	0/2696
11	K	0.28	0/1646	0.48	0/2229
12	L	0.27	0/1438	0.50	0/1938
13	M	0.30	0/1612	0.50	0/2182
14	N	0.27	0/1679	0.50	0/2264
15	O	0.27	0/1536	0.51	0/2071
16	P	0.27	0/1565	0.50	0/2115
17	Q	0.27	0/1541	0.51	0/2083
All	All	0.28	0/29552	0.49	0/39921

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	1805	0	1800	12	0
2	B	1937	0	1951	13	0
3	C	1826	0	1854	9	0
4	D	1840	0	1825	10	0
5	E	1889	0	1878	12	0
6	F	1885	0	1874	11	0
7	G	1892	0	1898	12	0
8	H	1008	0	1018	10	0
9	I	2180	0	2198	9	0
10	J	1952	0	1998	12	0
11	K	1696	0	1647	11	0
12	L	1412	0	1429	6	0
13	M	1581	0	1581	19	0
14	N	1651	0	1632	9	0
15	O	1509	0	1508	18	0
16	P	1537	0	1523	8	0
17	Q	1515	0	1460	13	0
All	All	29115	0	29074	172	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 (172) 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)
11:K:61:THR:HG1	11:K:215:ASN:N	1.72	0.87
4:D:127:ASP:HB2	5:E:125:ARG:HH22	1.53	0.74
3:C:39:ASP:OD1	3:C:213:ARG:NH1	2.28	0.67
13:M:168:GLN:HE22	13:M:173:LEU:HA	1.58	0.66
1:A:84:ARG:NH1	7:G:120:ASP:OD1	2.29	0.65
11:K:75:SER:OG	11:K:76:LYS:N	2.30	0.65
10:J:33:ASP:OD1	10:J:89:GLN:NE2	2.31	0.64
1:A:69:THR:HG22	1:A:70:LYS:H	1.62	0.64
4:D:210:LEU:HG	4:D:238:ILE:HD11	1.79	0.64
8:H:90:GLN:NE2	8:H:99:ASN:OD1	2.31	0.63
5:E:164:ARG:NH1	9:I:243:ASP:OD2	2.29	0.63
17:Q:179:GLU:HG3	17:Q:180:GLY:H	1.64	0.63
15:O:205:ASP:HA	15:O:208:ILE:HG12	1.81	0.62
3:C:48:LYS:HG3	3:C:163:ARG:HH21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:ARG:NH1	6:F:147:ALA:O	2.33	0.61
15:O:195:SER:HB2	15:O:198:ARG:HE	1.65	0.61
8:H:37:CYS:SG	8:H:40:ASN:ND2	2.73	0.61
16:P:237:VAL:HG22	16:P:242:VAL:HG22	1.83	0.60
7:G:13:ILE:HG23	7:G:14:THR:HG23	1.82	0.60
13:M:96:THR:HB	13:M:97:PRO:HD3	1.83	0.60
13:M:3:TYR:HD2	13:M:178:PHE:HZ	1.49	0.60
6:F:98:ASN:ND2	14:N:18:PHE:O	2.35	0.59
4:D:85:ALA:HB2	4:D:139:VAL:HG21	1.83	0.59
11:K:78:HIS:HB3	11:K:99:THR:HG21	1.85	0.59
9:I:254:LEU:HD22	9:I:263:VAL:HG11	1.85	0.59
7:G:103:TYR:HB2	17:Q:95:TYR:CD1	2.39	0.58
11:K:165:LEU:HD12	11:K:168:VAL:HG12	1.85	0.58
4:D:186:HIS:NE2	4:D:188:SER:O	2.37	0.57
1:A:119:GLN:HG3	2:B:81:SER:HB3	1.85	0.57
7:G:43:ARG:HG3	7:G:149:PRO:HB2	1.87	0.56
13:M:35:MET:SD	13:M:181:ARG:NH1	2.79	0.56
1:A:119:GLN:OE1	8:H:91:ARG:NH2	2.38	0.56
15:O:63:ILE:O	16:P:196:ARG:NH2	2.40	0.55
15:O:153:ASP:OD1	15:O:157:SER:N	2.39	0.55
5:E:84:LEU:O	5:E:88:MET:HG3	2.07	0.55
1:A:166:ASN:OD1	1:A:169:ASN:ND2	2.41	0.54
3:C:140:GLY:O	3:C:213:ARG:NH2	2.38	0.54
1:A:84:ARG:NH2	7:G:158:GLY:O	2.41	0.54
8:H:128:GLY:H	8:H:133:MET:HE3	1.74	0.53
10:J:18:LEU:HD23	10:J:119:ILE:HB	1.91	0.52
6:F:231:ASP:OD1	6:F:231:ASP:N	2.42	0.52
10:J:95:ILE:HG22	10:J:96:LYS:H	1.73	0.52
8:H:57:LEU:HD21	8:H:61:LYS:HE2	1.90	0.52
5:E:186:GLU:HA	5:E:189:LYS:HB2	1.92	0.52
4:D:195:ILE:HD12	4:D:217:LEU:HD21	1.90	0.52
9:I:175:TYR:OH	9:I:207:GLU:OE1	2.27	0.52
13:M:168:GLN:HE22	13:M:174:ASN:H	1.58	0.52
16:P:206:SER:HB3	16:P:209:GLU:HG3	1.91	0.51
1:A:64:LYS:HG2	1:A:76:TYR:HE1	1.75	0.51
5:E:230:SER:O	5:E:234:GLU:HG2	2.10	0.51
12:L:125:ASP:OD1	12:L:129:CYS:N	2.42	0.51
1:A:143:ARG:NH1	1:A:144:PRO:O	2.43	0.51
17:Q:169:ILE:HD13	17:Q:197:ALA:HB2	1.91	0.51
3:C:97:THR:HG22	8:H:30:LEU:HD13	1.92	0.51
10:J:63:THR:HG23	10:J:64:THR:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:243:ASP:OD1	9:I:244:LEU:N	2.44	0.51
13:M:154:GLU:O	13:M:157:VAL:HG12	2.11	0.50
12:L:159:ASP:N	12:L:159:ASP:OD1	2.42	0.50
15:O:74:LEU:HB2	15:O:78:THR:HG23	1.94	0.50
6:F:216:TRP:HE1	6:F:221:THR:HG23	1.77	0.49
2:B:165:GLY:O	2:B:168:SER:OG	2.27	0.49
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.94	0.49
15:O:56:ARG:HB2	15:O:218:GLY:HA2	1.95	0.49
13:M:143:LEU:O	13:M:147:TYR:HB2	2.13	0.49
2:B:69:ASN:OD1	2:B:70:GLU:N	2.45	0.48
4:D:68:VAL:HG21	4:D:89:ILE:HD13	1.93	0.48
6:F:216:TRP:CE3	6:F:228:VAL:HG22	2.49	0.48
2:B:51:ASN:HB3	2:B:56:LEU:HD13	1.94	0.48
2:B:95:GLN:HG3	12:L:73:LEU:HG	1.96	0.48
1:A:69:THR:HG22	1:A:70:LYS:N	2.29	0.48
17:Q:179:GLU:HG3	17:Q:180:GLY:N	2.28	0.48
15:O:41:LEU:HD11	15:O:177:LEU:HD11	1.95	0.48
16:P:60:LYS:HD3	16:P:180:PRO:HA	1.96	0.48
14:N:238:VAL:HG22	14:N:243:TRP:HB3	1.96	0.47
13:M:169:LYS:HD2	13:M:170:ARG:HG3	1.96	0.47
13:M:192:ASP:N	13:M:192:ASP:OD1	2.48	0.47
14:N:57:LEU:HD23	14:N:60:THR:HG21	1.97	0.47
11:K:40:ARG:NH1	12:L:129:CYS:O	2.48	0.47
11:K:127:LYS:HD3	11:K:162:THR:HG23	1.95	0.47
2:B:240:HIS:NE2	2:B:244:GLU:OE2	2.47	0.47
17:Q:30:GLU:N	17:Q:30:GLU:OE2	2.47	0.47
7:G:184:LYS:HB3	7:G:184:LYS:HE2	1.74	0.47
11:K:76:LYS:HE2	11:K:76:LYS:HB3	1.64	0.46
15:O:103:TYR:CE1	15:O:111:MET:HB3	2.51	0.46
7:G:174:GLU:OE1	7:G:174:GLU:N	2.48	0.46
14:N:96:ILE:HG23	14:N:119:ALA:HB2	1.97	0.46
15:O:201:ARG:O	15:O:201:ARG:NE	2.48	0.46
11:K:35:LYS:HA	11:K:35:LYS:HD2	1.80	0.46
13:M:20:VAL:HB	13:M:176:PRO:HB3	1.97	0.46
5:E:3:ARG:NH2	10:J:256:GLY:HA3	2.31	0.46
10:J:60:PRO:O	10:J:250:SER:OG	2.32	0.46
2:B:199:LYS:HA	2:B:199:LYS:HD2	1.74	0.46
13:M:92:LEU:HD12	13:M:98:TYR:HD2	1.81	0.46
5:E:218:ASP:OD1	5:E:218:ASP:N	2.49	0.45
9:I:72:ILE:HB	9:I:134:LEU:HD23	1.98	0.45
8:H:40:ASN:HD21	13:M:95:ARG:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:HIS:CE1	3:C:156:TRP:HE1	2.35	0.45
3:C:209:ALA:HB1	3:C:217:LEU:HD11	1.99	0.45
2:B:43:VAL:HG12	2:B:216:LEU:HB3	1.97	0.45
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.99	0.45
16:P:194:LEU:O	16:P:197:GLU:HG3	2.16	0.45
15:O:204:LYS:O	15:O:208:ILE:HG23	2.16	0.45
15:O:202:LEU:HA	15:O:205:ASP:OD2	2.16	0.45
15:O:201:ARG:HH21	15:O:205:ASP:N	2.14	0.44
2:B:43:VAL:HG11	2:B:137:ILE:HB	2.00	0.44
2:B:231:LYS:O	2:B:235:GLN:HG3	2.16	0.44
10:J:5:CYS:HB2	10:J:45:GLY:HA2	1.99	0.44
14:N:194:ALA:HB2	14:N:222:ALA:HB2	1.99	0.44
14:N:198:MET:O	14:N:202:TYR:HB2	2.18	0.44
2:B:176:LYS:HG2	3:C:52:LYS:HD3	1.99	0.44
10:J:224:LEU:HD11	10:J:228:LEU:HD12	2.00	0.44
7:G:112:ASP:N	7:G:112:ASP:OD1	2.48	0.44
9:I:265:ASN:HB3	9:I:268:GLN:HG2	2.00	0.44
11:K:45:THR:HA	11:K:171:GLY:HA3	2.00	0.44
6:F:35:SER:HB2	6:F:66:ARG:HH12	1.82	0.43
10:J:133:GLN:NE2	10:J:164:GLU:OE1	2.50	0.43
16:P:77:SER:HB3	17:Q:27:GLU:HB3	1.99	0.43
10:J:149:LYS:HA	10:J:149:LYS:HD3	1.78	0.43
5:E:238:GLU:OE1	5:E:238:GLU:N	2.51	0.43
13:M:164:LEU:O	13:M:168:GLN:HG2	2.18	0.43
1:A:179:ASN:HB3	1:A:182:LEU:HG	2.00	0.43
13:M:138:LEU:HD21	13:M:166:GLU:OE1	2.19	0.43
5:E:176:MET:SD	6:F:58:LEU:HD23	2.58	0.43
10:J:228:LEU:HD23	10:J:228:LEU:HA	1.88	0.43
12:L:122:CYS:SG	12:L:123:SER:N	2.92	0.43
4:D:192:LYS:HE2	4:D:192:LYS:HB2	1.84	0.43
15:O:103:TYR:CD1	15:O:111:MET:HB3	2.53	0.43
6:F:13:SER:HB2	7:G:132:ARG:HB3	2.00	0.43
17:Q:207:VAL:HG22	17:Q:224:LEU:HD13	2.01	0.43
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.87	0.42
1:A:169:ASN:HA	1:A:172:THR:HG22	2.02	0.42
10:J:214:ILE:HB	10:J:215:PRO:HD3	2.01	0.42
8:H:43:LEU:HD23	8:H:43:LEU:HA	1.94	0.42
12:L:161:ASP:O	12:L:165:GLU:OE1	2.38	0.42
7:G:78:CYS:SG	7:G:79:VAL:N	2.93	0.42
17:Q:93:VAL:HG11	17:Q:117:PHE:CE2	2.55	0.42
17:Q:104:LEU:HD23	17:Q:104:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:128:GLY:H	8:H:133:MET:CE	2.32	0.41
11:K:88:GLY:HA3	11:K:95:THR:HG21	2.01	0.41
13:M:11:ASP:N	13:M:11:ASP:OD1	2.52	0.41
5:E:138:ASP:N	5:E:138:ASP:OD1	2.54	0.41
16:P:48:ASN:HB3	16:P:49:PRO:HD3	2.02	0.41
4:D:239:LYS:HE2	4:D:239:LYS:HB3	1.87	0.41
15:O:202:LEU:O	15:O:206:VAL:HG23	2.21	0.41
8:H:92:LEU:HD23	8:H:92:LEU:HA	1.87	0.41
11:K:102:ILE:HD13	11:K:102:ILE:HA	1.89	0.41
4:D:168:ARG:HA	4:D:168:ARG:HD2	1.91	0.41
13:M:43:LEU:HD12	13:M:183:ILE:HD11	2.03	0.41
16:P:221:LEU:HD23	16:P:221:LEU:HA	1.94	0.41
17:Q:53:ARG:HA	17:Q:53:ARG:HD2	1.88	0.41
17:Q:197:ALA:O	17:Q:200:ARG:HG3	2.21	0.41
2:B:178:ASP:OD2	2:B:195:LYS:NZ	2.41	0.41
13:M:168:GLN:NE2	13:M:173:LEU:HA	2.32	0.41
15:O:194:LEU:HD23	15:O:198:ARG:HB3	2.02	0.41
5:E:157:ARG:HG2	6:F:58:LEU:O	2.21	0.40
7:G:103:TYR:HB2	17:Q:95:TYR:HD1	1.85	0.40
9:I:83:LEU:HD23	9:I:83:LEU:HA	1.90	0.40
14:N:21:LEU:HD11	17:Q:120:MET:HG2	2.02	0.40
15:O:36:ASN:ND2	15:O:58:SER:O	2.50	0.40
15:O:212:GLU:HG3	15:O:213:ARG:HG2	2.03	0.40
14:N:188:GLY:N	14:N:191:SER:OG	2.54	0.40
3:C:96:LEU:HD12	3:C:96:LEU:HA	1.96	0.40
6:F:216:TRP:CZ3	6:F:228:VAL:HG13	2.56	0.40
4:D:47:CYS:SG	4:D:195:ILE:HD13	2.61	0.40
7:G:112:ASP:HB3	7:G:152:TYR:CZ	2.56	0.40
9:I:98:CYS:SG	9:I:99:ALA:N	2.95	0.40
13:M:166:GLU:HG2	13:M:169:LYS:HE3	2.03	0.40
15:O:211:ALA:HA	15:O:217:THR:HG21	2.04	0.40
2:B:160:LYS:NZ	2:B:181:GLU:OE1	2.38	0.40
6:F:94:GLU:HG2	14:N:16:ARG:HH11	1.86	0.40
9:I:59:GLU:HG2	9:I:60:VAL:HG23	2.02	0.40
13:M:4:LEU:HB2	13:M:132:HIS:HB2	2.03	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	230/234 (98%)	221 (96%)	9 (4%)	0	100	100
2	B	245/261 (94%)	239 (98%)	6 (2%)	0	100	100
3	C	231/248 (93%)	228 (99%)	3 (1%)	0	100	100
4	D	240/242 (99%)	230 (96%)	10 (4%)	0	100	100
5	E	239/264 (90%)	230 (96%)	9 (4%)	0	100	100
6	F	240/255 (94%)	234 (98%)	6 (2%)	0	100	100
7	G	241/246 (98%)	238 (99%)	3 (1%)	0	100	100
8	H	122/142 (86%)	119 (98%)	3 (2%)	0	100	100
9	I	267/288 (93%)	260 (97%)	7 (3%)	0	100	100
10	J	244/265 (92%)	229 (94%)	15 (6%)	0	100	100
11	K	208/332 (63%)	202 (97%)	6 (3%)	0	100	100
12	L	174/205 (85%)	167 (96%)	7 (4%)	0	100	100
13	M	196/202 (97%)	182 (93%)	13 (7%)	1 (0%)	29	59
14	N	209/264 (79%)	202 (97%)	7 (3%)	0	100	100
15	O	193/241 (80%)	187 (97%)	6 (3%)	0	100	100
16	P	194/264 (74%)	189 (97%)	5 (3%)	0	100	100
17	Q	196/239 (82%)	186 (95%)	10 (5%)	0	100	100
All	All	3669/4192 (88%)	3543 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	1	MET

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/191 (98%)	187 (100%)	1 (0%)	88	96
2	B	205/221 (93%)	205 (100%)	0	100	100
3	C	195/211 (92%)	195 (100%)	0	100	100
4	D	200/203 (98%)	200 (100%)	0	100	100
5	E	204/224 (91%)	204 (100%)	0	100	100
6	F	197/212 (93%)	197 (100%)	0	100	100
7	G	207/210 (99%)	207 (100%)	0	100	100
8	H	116/128 (91%)	114 (98%)	2 (2%)	60	84
9	I	248/262 (95%)	248 (100%)	0	100	100
10	J	222/237 (94%)	221 (100%)	1 (0%)	88	96
11	K	173/257 (67%)	173 (100%)	0	100	100
12	L	152/174 (87%)	152 (100%)	0	100	100
13	M	168/171 (98%)	167 (99%)	1 (1%)	86	95
14	N	165/202 (82%)	165 (100%)	0	100	100
15	O	161/199 (81%)	161 (100%)	0	100	100
16	P	162/215 (75%)	162 (100%)	0	100	100
17	Q	155/180 (86%)	155 (100%)	0	100	100
All	All	3118/3497 (89%)	3113 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ARG
8	H	33	LYS
8	H	68	ARG
10	J	232	LYS
13	M	169	LYS

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

sidechains are listed below:

Mol	Chain	Res	Type
8	H	40	ASN
13	M	168	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

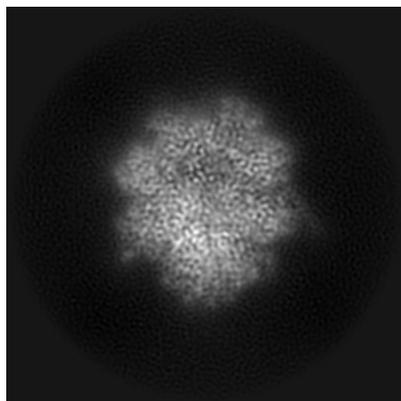
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18759. These allow visual inspection of the internal detail of the map and identification of artifacts.

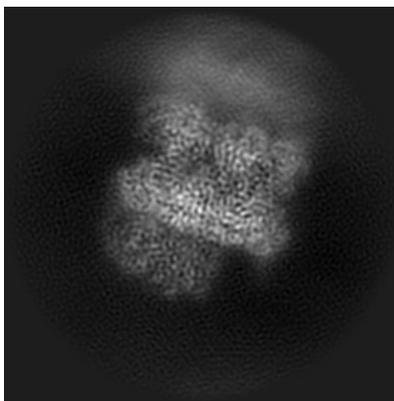
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

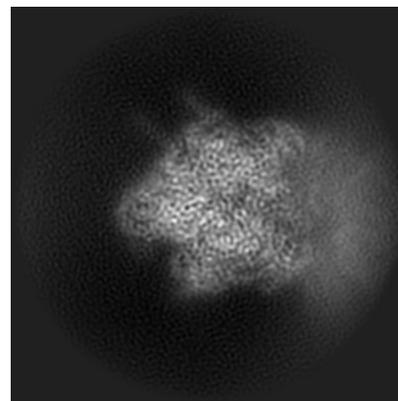
#### 6.1.1 Primary map



X

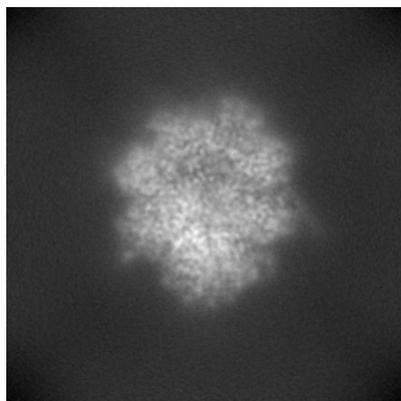


Y

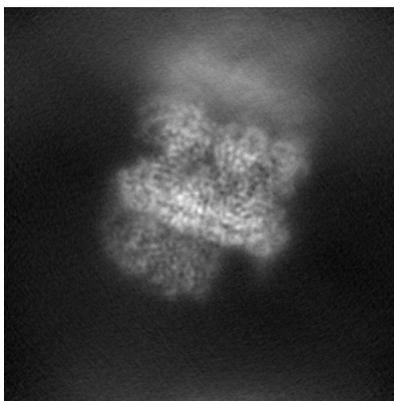


Z

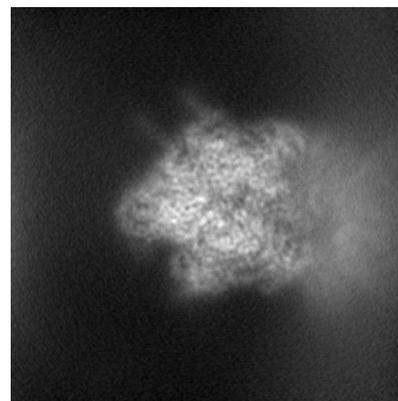
#### 6.1.2 Raw map



X



Y

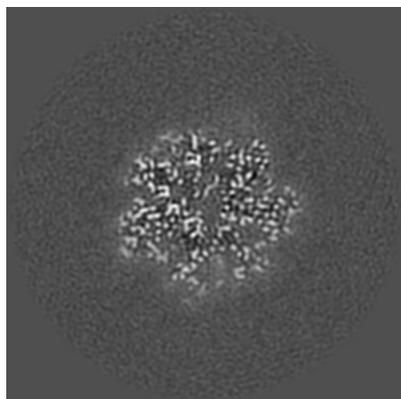


Z

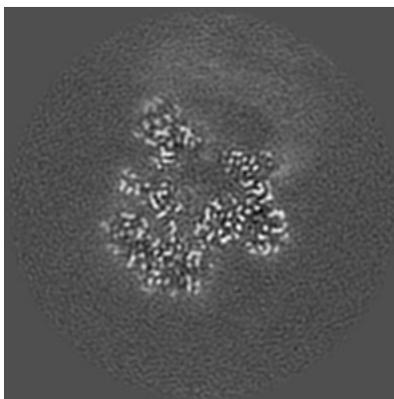
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

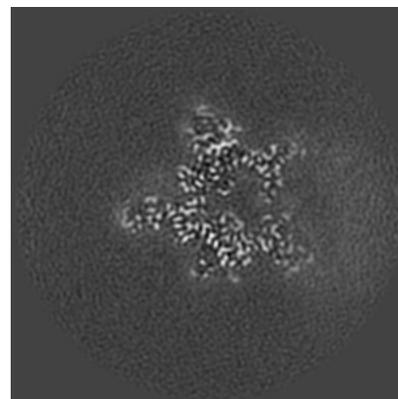
### 6.2.1 Primary map



X Index: 150

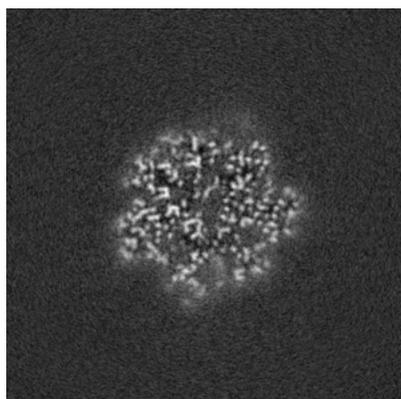


Y Index: 150

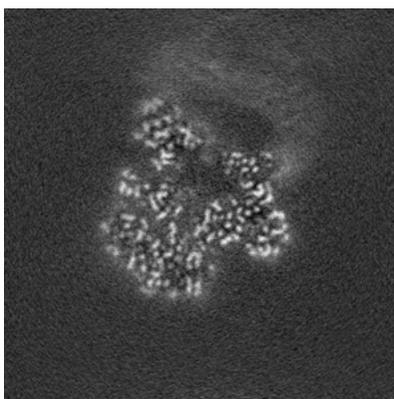


Z Index: 150

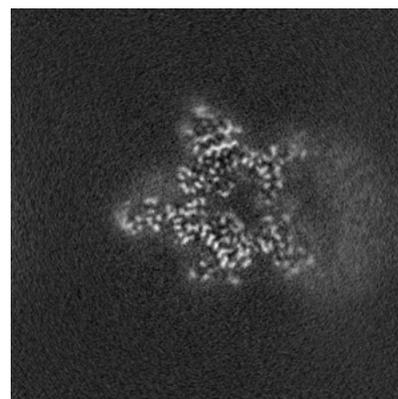
### 6.2.2 Raw map



X Index: 150



Y Index: 150

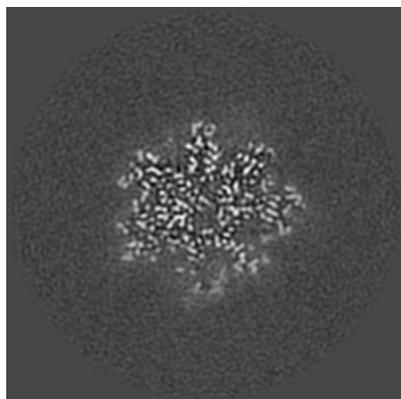


Z Index: 150

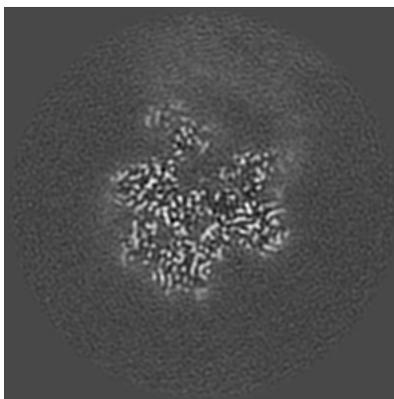
The images above show central slices of the map in three orthogonal directions.

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

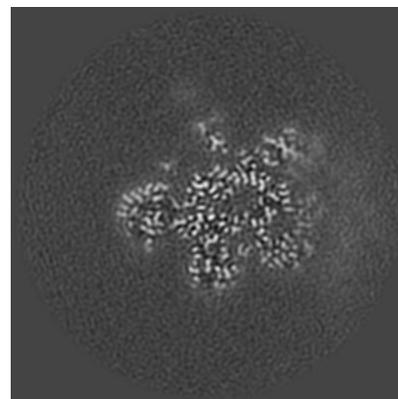
### 6.3.1 Primary map



X Index: 146

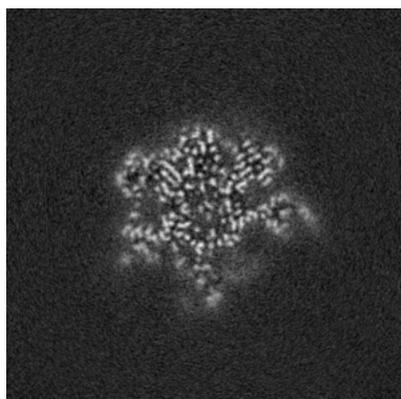


Y Index: 140

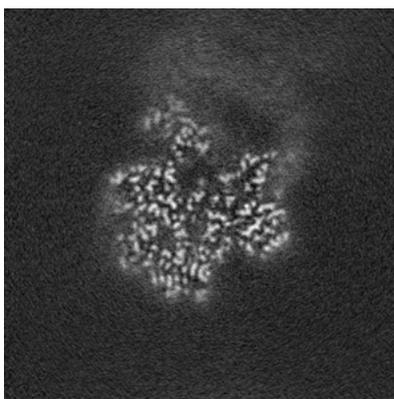


Z Index: 128

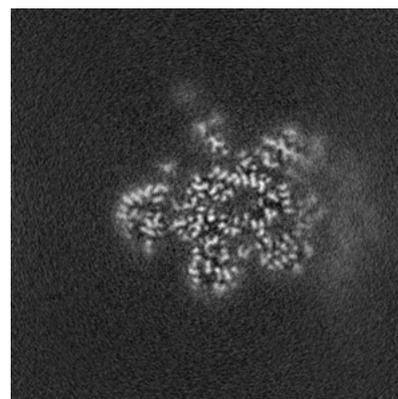
### 6.3.2 Raw map



X Index: 139



Y Index: 141

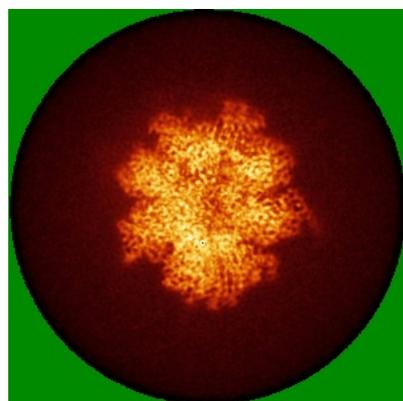


Z Index: 128

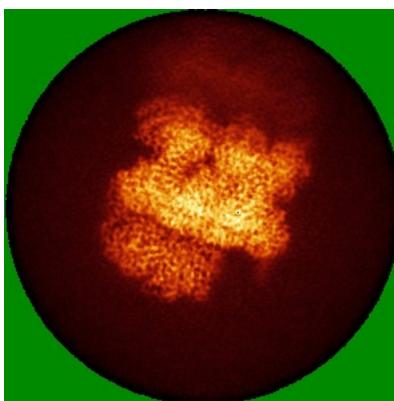
The images above show the largest variance slices of the map in three orthogonal directions.

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

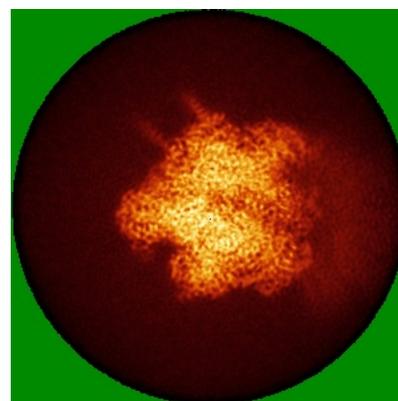
### 6.4.1 Primary map



X

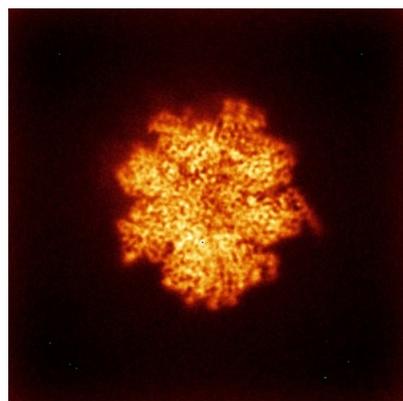


Y

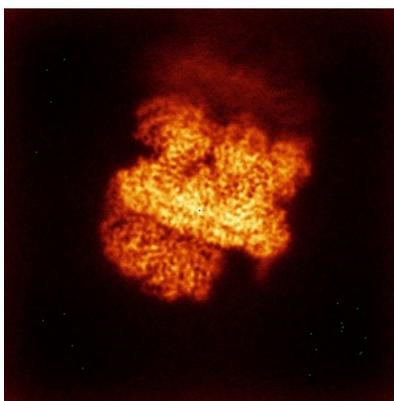


Z

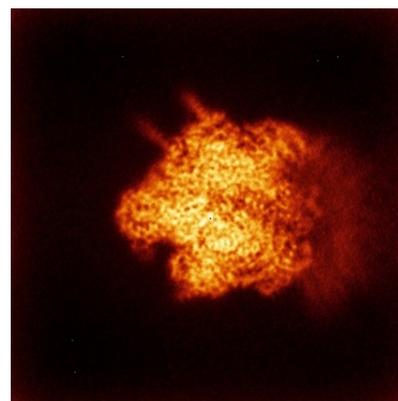
### 6.4.2 Raw map



X



Y

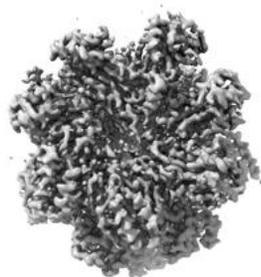


Z

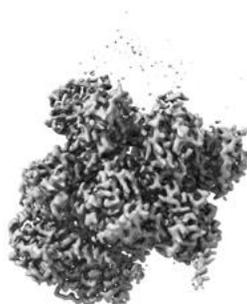
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

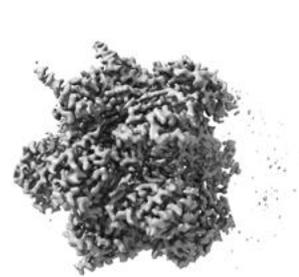
### 6.5.1 Primary map



X



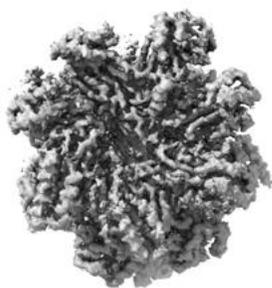
Y



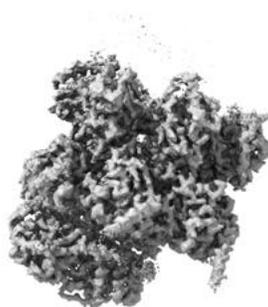
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

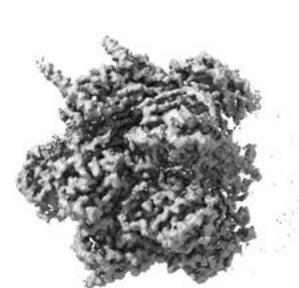
### 6.5.2 Raw map



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.

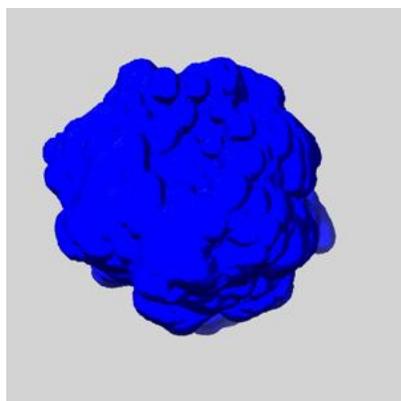
## 6.6 Mask visualisation [i](#)

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

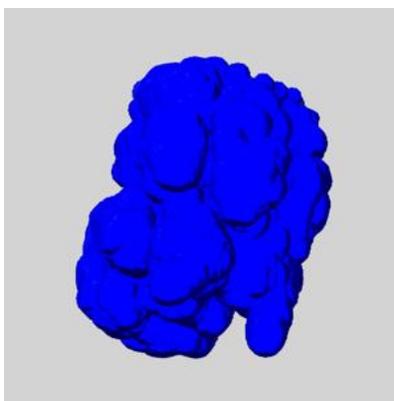
A mask typically either:

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

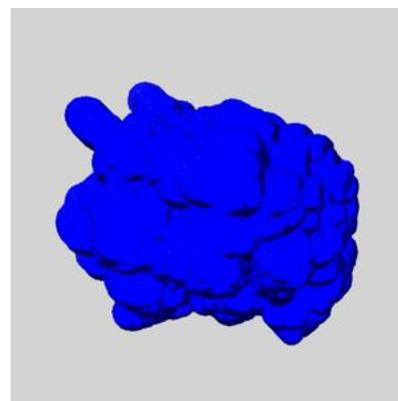
### 6.6.1 emd\_18759\_msk\_1.map [i](#)



X



Y

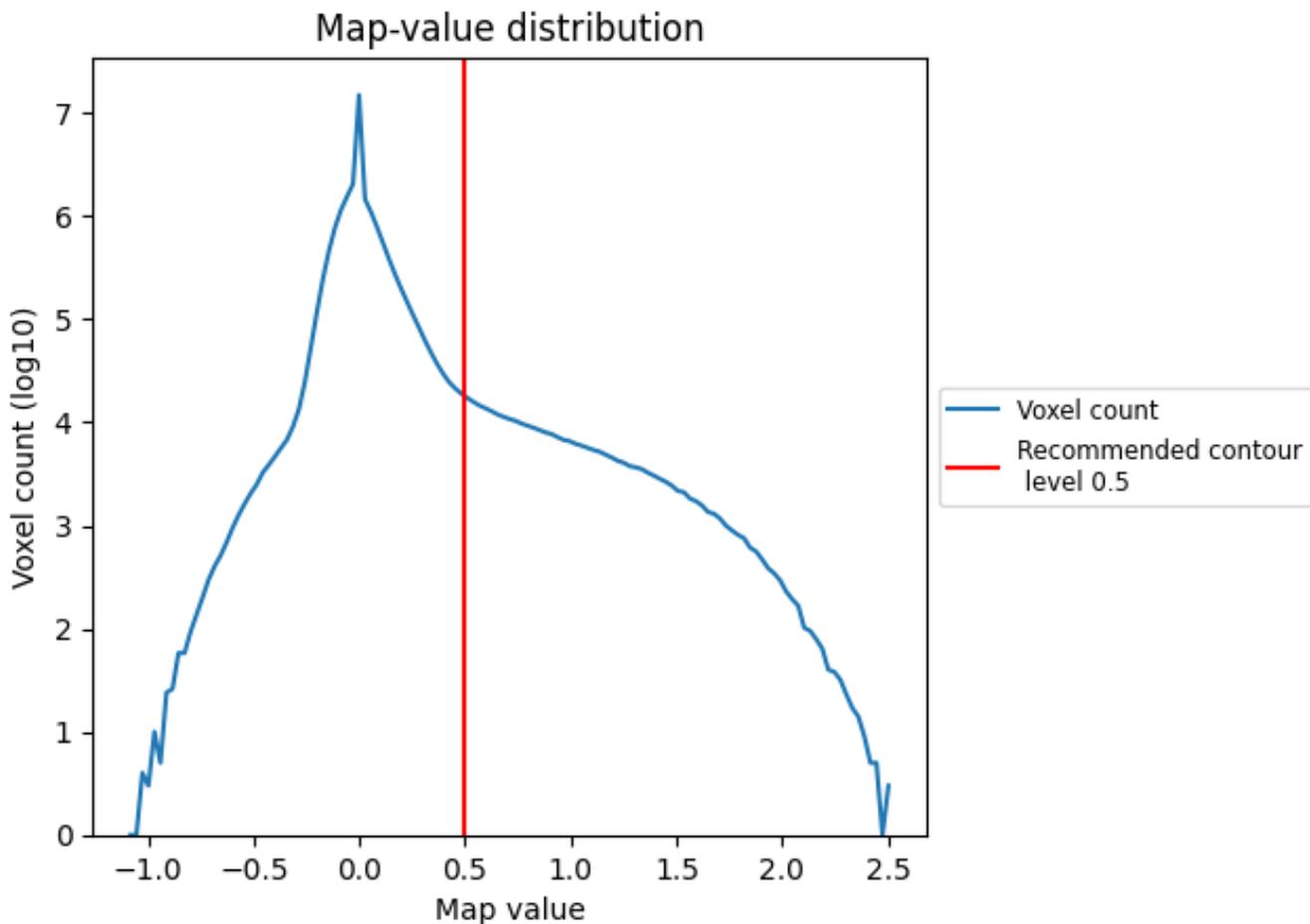


Z

## 7 Map analysis [i](#)

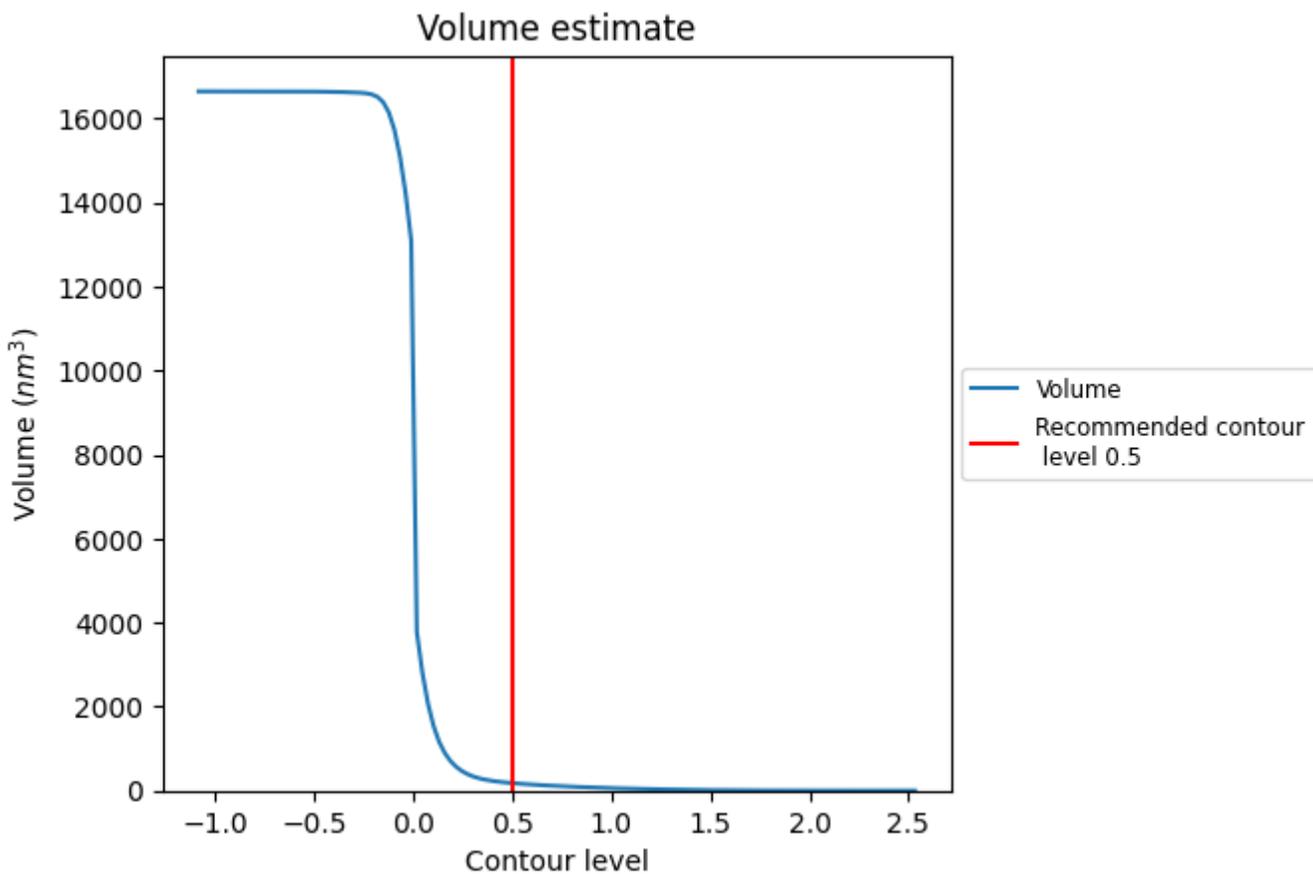
This section contains the results of statistical analysis of the map.

### 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.

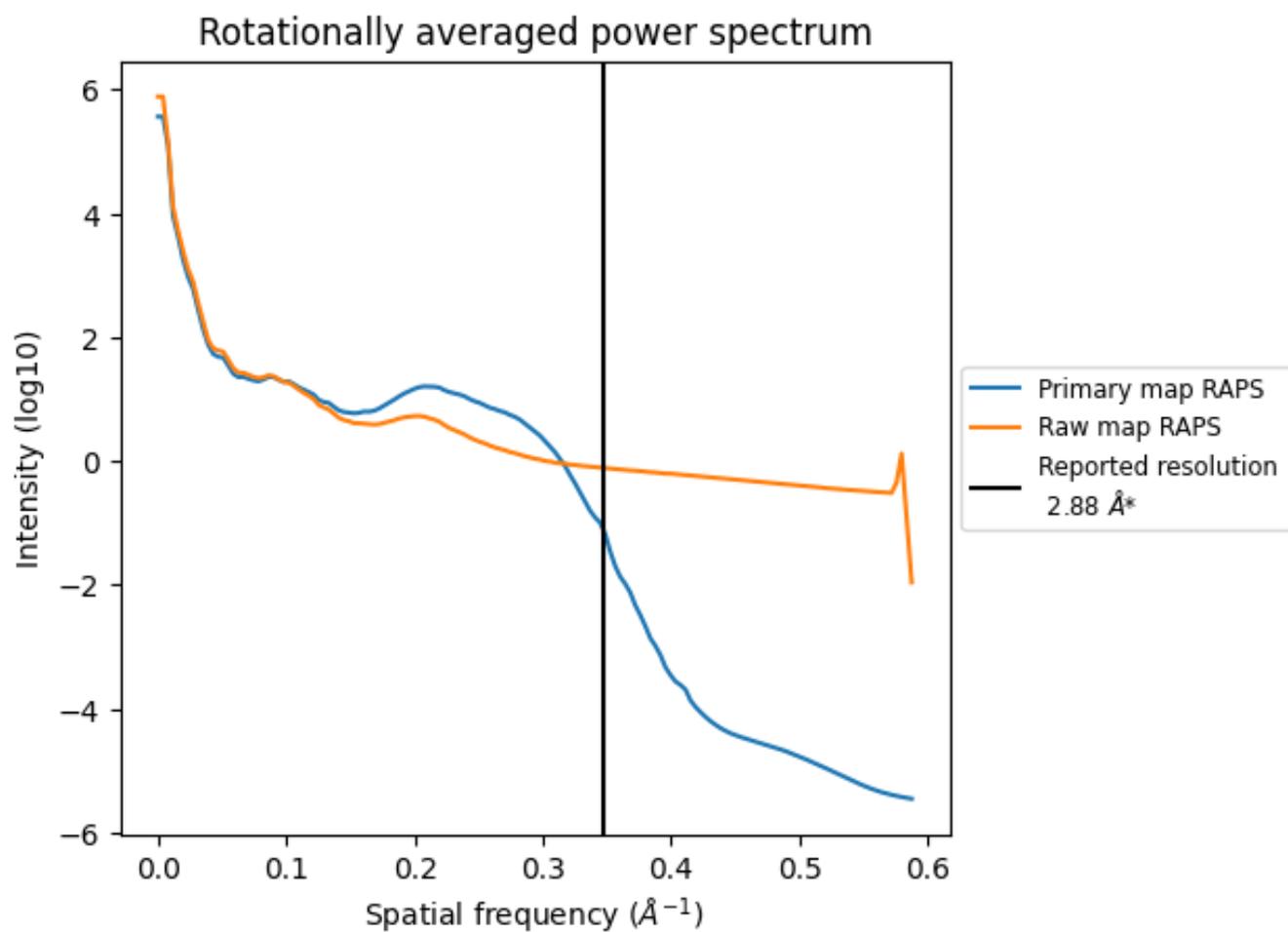
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179 nm<sup>3</sup>; this corresponds to an approximate mass of 162 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

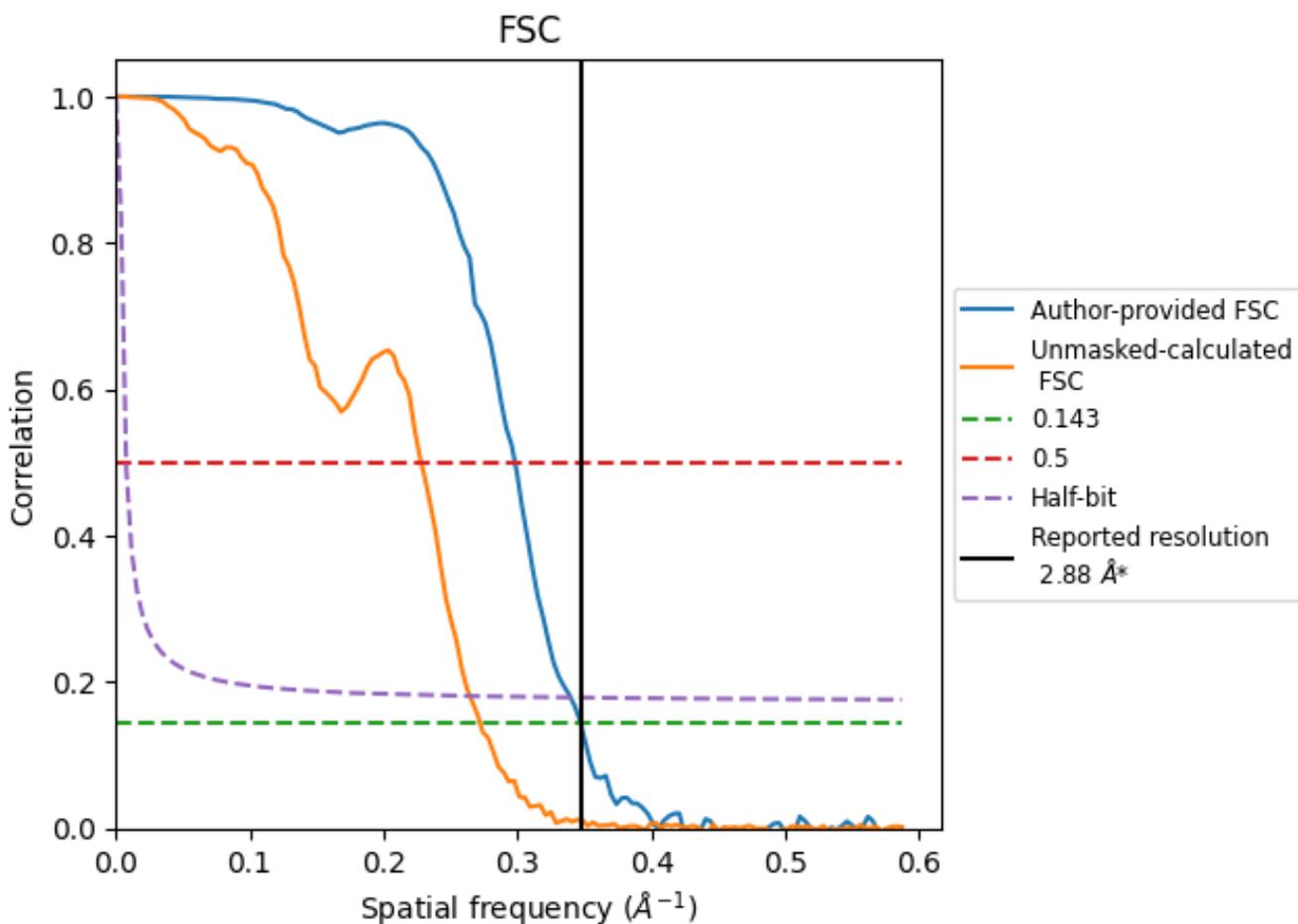


\*Reported resolution corresponds to spatial frequency of  $0.347 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

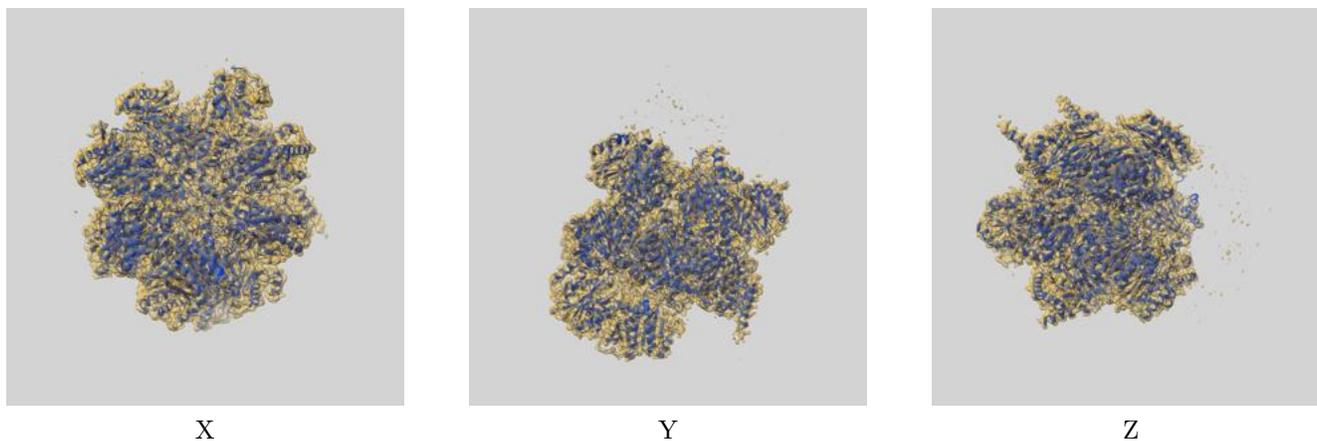
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.35	2.94
Unmasked-calculated*	3.67	4.38	3.78

\*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 3.67 differs from the reported value 2.88 by more than 10 %

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

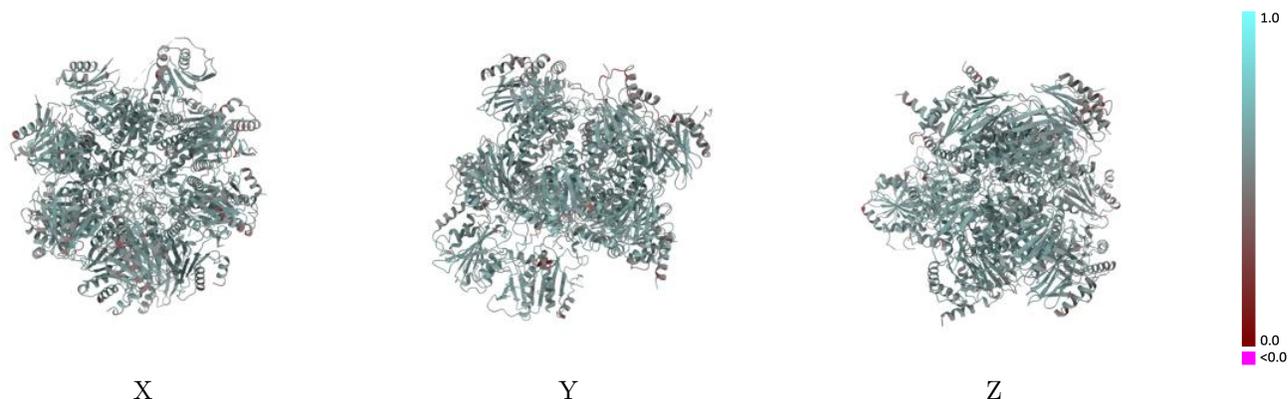
This section contains information regarding the fit between EMDB map EMD-18759 and PDB model 8QYN. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



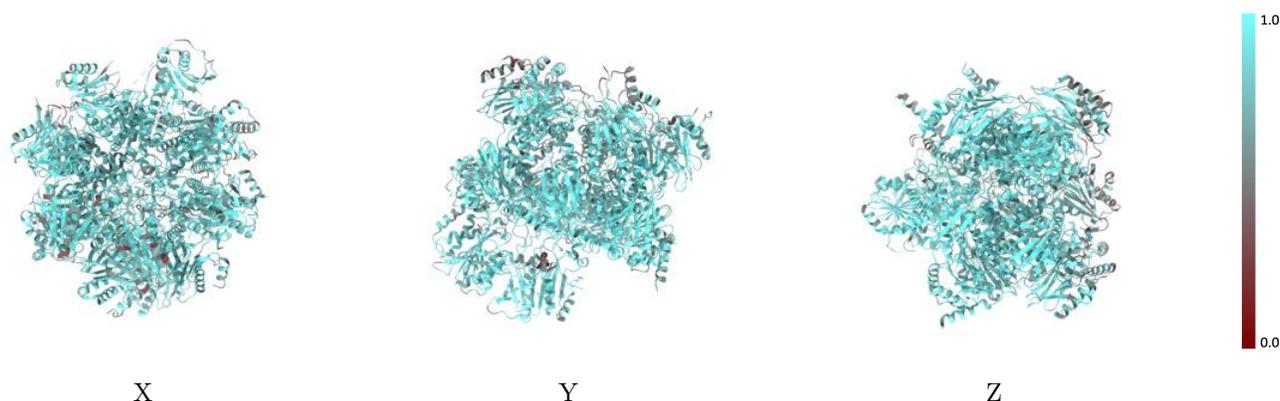
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



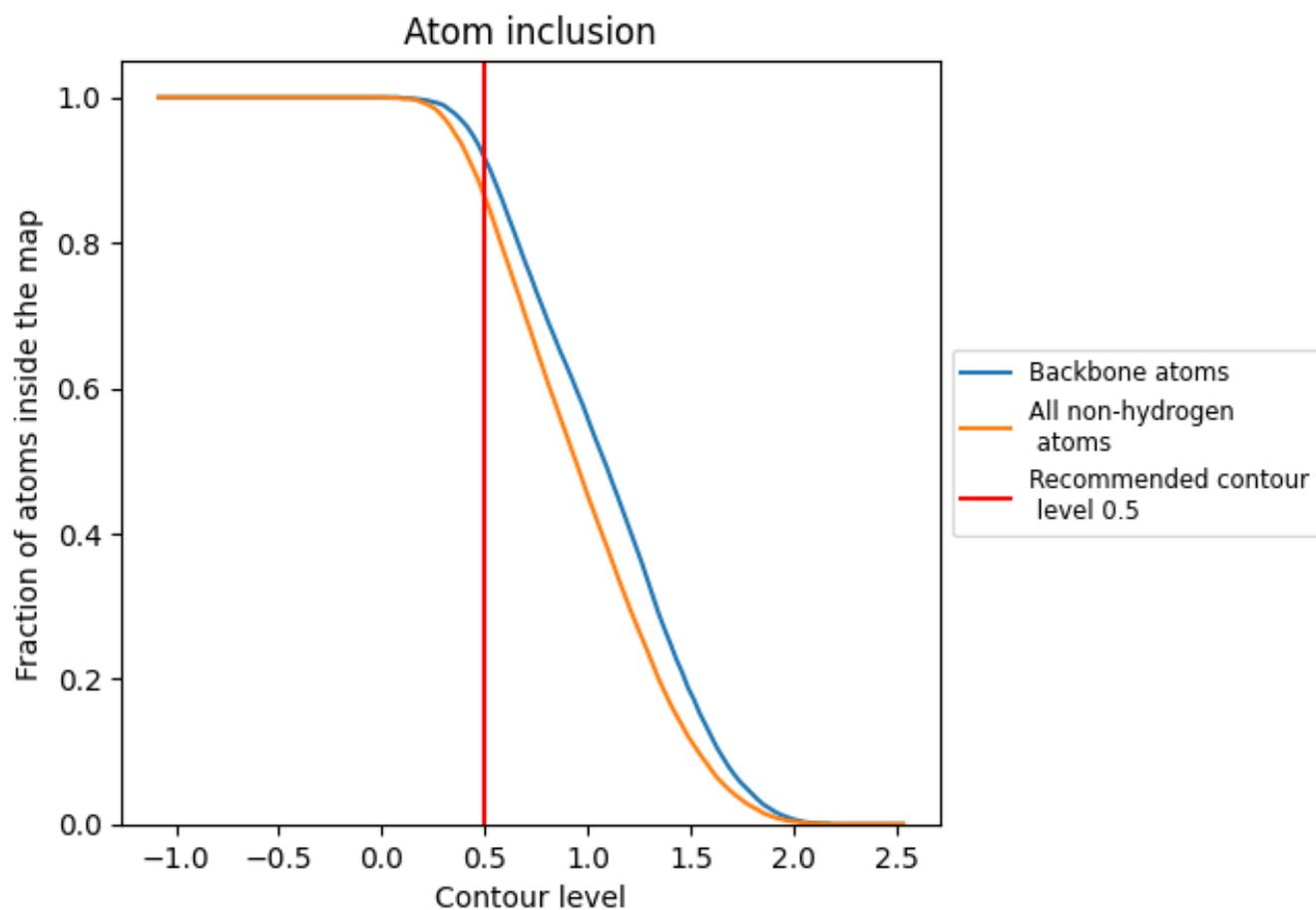
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.5710
A	 0.9350	 0.5870
B	 0.8850	 0.5780
C	 0.9020	 0.5840
D	 0.8790	 0.5720
E	 0.9250	 0.5880
F	 0.9120	 0.5840
G	 0.9170	 0.5850
H	 0.8260	 0.5800
I	 0.8220	 0.5560
J	 0.9050	 0.5790
K	 0.8620	 0.5770
L	 0.8550	 0.5580
M	 0.7660	 0.5330
N	 0.8110	 0.5580
O	 0.7680	 0.5520
P	 0.8230	 0.5630
Q	 0.8010	 0.5550

