



Full wwPDB EM Validation Report ⓘ

Sep 1, 2026 – 01:50 pm BST

PDB ID : 9TMN / pdb_00009tmn
EMDB ID : EMD-56072
Title : Human sperm 20S proteasome complex isolated from native source
Authors : Kolata, P.; Allegretti, M.
Deposited on : 2025-12-15
Resolution : 1.85 Å (reported)
Based on initial model : 6RGQ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at 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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.50

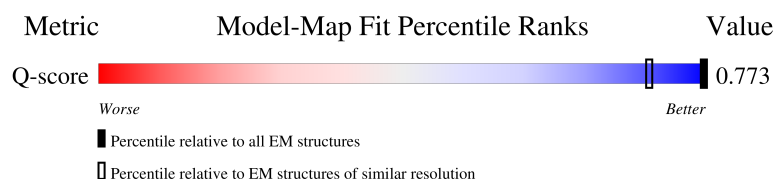
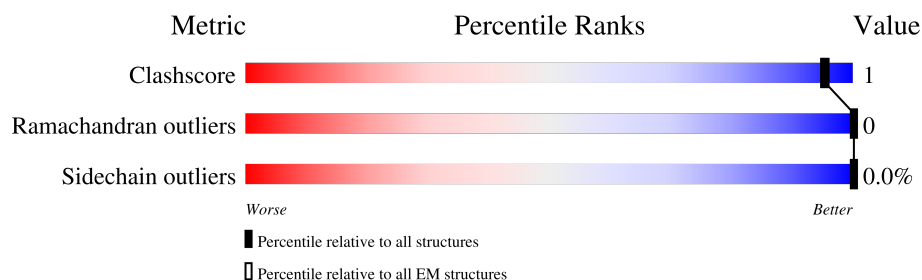
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

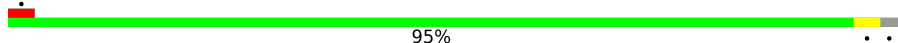
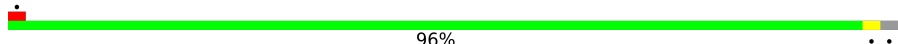
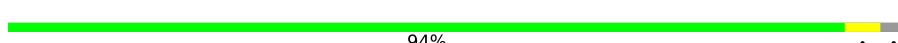
The reported resolution of this entry is 1.85 Å.

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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	944 (1.35 - 2.35)

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 ≥ 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	246	 95% ..
1	O	246	 96% ..
2	B	234	 94% ..
2	P	234	 94% ..

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Mol	Chain	Length	Quality of chain
3	C	261	 6% 92% 5%
3	Q	261	 6% 92% 5%
4	D	250	 9% 94%
4	R	250	 9% 94%
5	E	241	 94%
5	S	241	 95%
6	F	263	 86% 11%
6	T	263	 87% 11%
7	G	255	 89% 5% 6%
7	U	255	 88% 5% 6%
8	H	205	 95%
8	V	205	 95%
9	I	234	 91% 6%
9	W	234	 91% 6%
10	J	205	 98%
10	X	205	 99%
11	K	201	 97%
11	Y	201	 98%
12	M	213	 95%
12	a	213	 95%
13	N	219	 95%
13	b	219	 94%
14	L	204	 96%
14	Z	204	 95%
15	d	3	 100%

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Mol	Chain	Length	Quality of chain
15	e	3	 100%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51258 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	240	Total	C	N	O	S	0	0
			1872	1189	313	357	13		
1	O	240	Total	C	N	O	S	0	0
			1872	1189	313	357	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	228	Total	C	N	O	S	0	0
			1779	1138	300	335	6		
2	P	228	Total	C	N	O	S	0	0
			1779	1138	300	335	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1942	1228	332	372	10		
3	Q	247	Total	C	N	O	S	0	0
			1942	1228	332	372	10		

- Molecule 4 is a protein called Isoform 3 of Proteasome subunit alpha-type 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	239	Total	C	N	O	S	0	0
			1871	1177	331	358	5		
4	R	239	Total	C	N	O	S	0	0
			1871	1177	331	358	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		
5	S	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1828	1146	328	343	11		
6	T	233	Total	C	N	O	S	0	0
			1828	1146	328	343	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		
7	U	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	200	Total	C	N	O	S	0	0
			1499	939	256	292	12		
8	V	200	Total	C	N	O	S	0	0
			1499	939	256	292	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
9	W	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		
11	Y	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	212	Total	C	N	O	S	0	0
			1642	1041	280	311	10		
12	a	212	Total	C	N	O	S	0	0
			1642	1041	280	311	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	212	Total	C	N	O	S	0	0
			1655	1044	285	315	11		
13	b	212	Total	C	N	O	S	0	0
			1655	1044	285	315	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		
14	Z	200	Total	C	N	O	S	0	0
			1555	980	273	293	9		

- Molecule 15 is a protein called tripeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	d	3	Total	C	N	O	0	0
			25	16	6	3		
15	e	3	Total	C	N	O	0	0
			25	16	6	3		

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	I	1	Total 1	Mg 1	0
16	J	1	Total 1	Mg 1	0
16	W	1	Total 1	Mg 1	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	A	91	Total 91	O 91	0
17	B	71	Total 71	O 71	0
17	C	88	Total 88	O 88	0
17	D	70	Total 70	O 70	0
17	E	69	Total 69	O 69	0
17	F	85	Total 85	O 85	0
17	G	88	Total 88	O 88	0
17	H	139	Total 139	O 139	0
17	I	133	Total 133	O 133	0
17	J	129	Total 129	O 129	0
17	K	119	Total 119	O 119	0
17	M	134	Total 134	O 134	0
17	N	162	Total 162	O 162	0
17	O	88	Total 88	O 88	0
17	P	78	Total 78	O 78	0
17	Q	86	Total 86	O 86	0

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Mol	Chain	Residues	Atoms		AltConf
17	S	60	Total 60	O 60	0
17	U	77	Total 77	O 77	0
17	V	120	Total 120	O 120	0
17	W	126	Total 126	O 126	0
17	X	119	Total 119	O 119	0
17	R	63	Total 63	O 63	0
17	b	159	Total 159	O 159	0
17	L	110	Total 110	O 110	0
17	a	135	Total 135	O 135	0
17	T	85	Total 85	O 85	0
17	Y	120	Total 120	O 120	0
17	d	2	Total 2	O 2	0
17	e	2	Total 2	O 2	0
17	Z	113	Total 113	O 113	0



- Molecule 7: Proteasome subunit alpha type-3

Chain G: 89% 5% 6%



- Molecule 7: Proteasome subunit alpha type-3

Chain U: 88% 5% 6%



- Molecule 8: Proteasome subunit beta type-6

Chain H: 95% ..



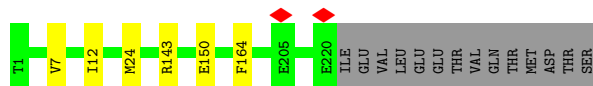
- Molecule 8: Proteasome subunit beta type-6

Chain V: 95% ..



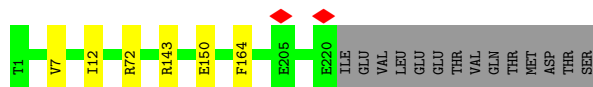
- Molecule 9: Proteasome subunit beta type-7

Chain I: 91% • 6%

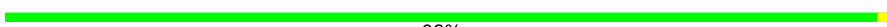


- Molecule 9: Proteasome subunit beta type-7

Chain W: 91% • 6%



- Molecule 10: Proteasome subunit beta type-3

Chain J:  98% .



- Molecule 10: Proteasome subunit beta type-3

Chain X:  99% .



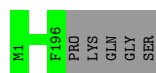
- Molecule 11: Proteasome subunit beta type-2

Chain K:  97% .

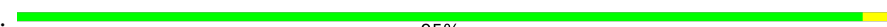


- Molecule 11: Proteasome subunit beta type-2

Chain Y:  98% .

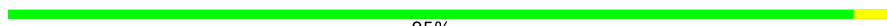


- Molecule 12: Proteasome subunit beta type-1

Chain M:  95% .

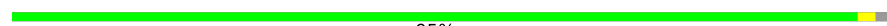


- Molecule 12: Proteasome subunit beta type-1

Chain a:  95% .



- Molecule 13: Proteasome subunit beta type-4

Chain N:  95% . .

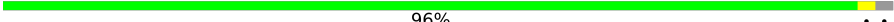


- Molecule 13: Proteasome subunit beta type-4

Chain b:  94% ..



- Molecule 14: Proteasome subunit beta type-5

Chain L:  96% ..



- Molecule 14: Proteasome subunit beta type-5

Chain Z:  95% ..

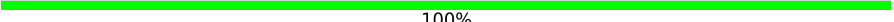


- Molecule 15: tripeptide

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: tripeptide

Chain e:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	222000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.831	Depositor
Minimum map value	-1.560	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	334.152, 334.152, 334.152	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.663, 0.663, 0.663	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/1906	0.33	0/2576
1	O	0.16	0/1906	0.33	0/2576
2	B	0.16	0/1818	0.35	0/2463
2	P	0.30	0/1818	0.49	0/2463
3	C	0.17	0/1972	0.35	0/2657
3	Q	0.16	0/1972	0.34	0/2657
4	D	0.44	0/1897	0.63	0/2558
4	R	0.44	0/1897	0.63	0/2558
5	E	0.16	0/1832	0.34	0/2475
5	S	0.15	0/1832	0.34	0/2475
6	F	0.17	0/1862	0.36	0/2517
6	T	0.17	0/1862	0.36	0/2517
7	G	0.34	0/1909	0.51	0/2570
7	U	0.40	0/1909	0.56	0/2570
8	H	0.18	0/1525	0.36	0/2064
8	V	0.18	0/1525	0.36	0/2064
9	I	0.19	0/1686	0.39	0/2282
9	W	0.18	0/1686	0.39	0/2282
10	J	0.19	0/1620	0.39	0/2184
10	X	0.18	0/1620	0.39	0/2184
11	K	0.17	0/1603	0.37	0/2168
11	Y	0.18	0/1603	0.37	0/2168
12	M	0.42	0/1672	0.66	0/2254
12	a	0.42	0/1672	0.66	0/2254
13	N	0.35	0/1687	0.55	0/2284
13	b	0.35	0/1687	0.55	0/2284
14	L	0.17	0/1586	0.36	0/2142
14	Z	0.17	0/1586	0.36	0/2142
15	d	0.25	0/24	0.51	0/31
15	e	0.26	0/24	0.51	0/31
All	All	0.26	0/49198	0.45	0/66450

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

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	1872	0	1882	5	0
1	O	1872	0	1882	3	0
2	B	1779	0	1771	5	0
2	P	1779	0	1771	5	0
3	C	1942	0	1960	4	0
3	Q	1942	0	1960	5	0
4	D	1871	0	1904	2	0
4	R	1871	0	1904	2	0
5	E	1804	0	1784	7	0
5	S	1804	0	1784	5	0
6	F	1828	0	1820	5	0
6	T	1828	0	1820	3	0
7	G	1874	0	1861	7	0
7	U	1874	0	1861	8	0
8	H	1499	0	1469	3	0
8	V	1499	0	1469	5	0
9	I	1659	0	1680	4	0
9	W	1659	0	1680	4	0
10	J	1591	0	1612	3	0
10	X	1591	0	1612	1	0
11	K	1571	0	1573	1	0
11	Y	1571	0	1573	0	0
12	M	1642	0	1640	6	0
12	a	1642	0	1640	6	0
13	N	1655	0	1634	3	0
13	b	1655	0	1634	4	0
14	L	1555	0	1520	3	0
14	Z	1555	0	1520	4	0
15	d	25	0	33	0	0
15	e	25	0	33	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	1	0	0	0	0
16	J	1	0	0	0	0
16	W	1	0	0	0	0
17	A	91	0	0	0	0
17	B	71	0	0	0	0
17	C	88	0	0	0	0
17	D	70	0	0	0	0
17	E	69	0	0	0	0
17	F	85	0	0	0	0
17	G	88	0	0	0	0
17	H	139	0	0	0	0
17	I	133	0	0	0	0
17	J	129	0	0	0	0
17	K	119	0	0	0	0
17	L	110	0	0	0	0
17	M	134	0	0	0	0
17	N	162	0	0	0	0
17	O	88	0	0	1	0
17	P	78	0	0	0	0
17	Q	86	0	0	0	0
17	R	63	0	0	0	0
17	S	60	0	0	0	0
17	T	85	0	0	0	0
17	U	77	0	0	0	0
17	V	120	0	0	0	0
17	W	126	0	0	0	0
17	X	119	0	0	0	0
17	Y	120	0	0	0	0
17	Z	113	0	0	0	0
17	a	135	0	0	0	0
17	b	159	0	0	0	0
17	d	2	0	0	0	0
17	e	2	0	0	0	0
All	All	51258	0	48286	94	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 (94) 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)
13:b:86:ARG:NH1	13:b:133:GLU:OE2	2.23	0.71
13:N:86:ARG:NH1	13:N:133:GLU:OE2	2.23	0.70
5:S:41:GLN:OE1	5:S:164:GLN:NE2	2.28	0.67
7:U:34:SER:OG	7:U:65:ARG:NH1	2.28	0.67
5:E:41:GLN:OE1	5:E:164:GLN:NE2	2.30	0.64
1:A:45:LYS:NZ	1:A:188:ASP:OD1	2.31	0.62
5:E:231:LYS:NZ	5:E:235:GLU:OE1	2.32	0.62
13:b:96:MET:HE2	13:b:110:MET:HE1	1.83	0.60
9:I:7:VAL:HG22	9:I:12:ILE:CD1	2.32	0.60
5:S:121:LEU:HD22	6:T:79:ALA:HB3	1.83	0.60
9:W:7:VAL:HG22	9:W:12:ILE:CD1	2.32	0.59
3:Q:62:SER:OG	3:Q:65:ILE:O	2.20	0.59
13:N:96:MET:HE2	13:N:110:MET:HE1	1.83	0.59
17:O:368:HOH:O	9:W:72:ARG:HD2	2.03	0.59
14:Z:9:ARG:NH2	14:Z:146:ASP:OD1	2.37	0.58
14:L:9:ARG:NH2	14:L:146:ASP:OD1	2.37	0.57
3:C:62:SER:OG	3:C:65:ILE:O	2.22	0.57
7:G:117:MET:HE2	7:G:117:MET:HA	1.87	0.56
2:B:158:LYS:NZ	3:C:54:LYS:O	2.38	0.56
5:E:121:LEU:HD22	6:F:79:ALA:HB3	1.88	0.56
7:G:34:SER:OG	7:G:65:ARG:NH1	2.38	0.56
1:O:34:GLN:NE2	7:U:17:ASP:O	2.38	0.56
12:M:38:ARG:NH2	9:W:164:PHE:O	2.39	0.55
9:I:143:ARG:NH1	9:I:150:GLU:OE2	2.39	0.54
9:I:164:PHE:O	12:a:38:ARG:NH2	2.39	0.53
12:a:145:LEU:HD21	12:a:182:ALA:HB2	1.91	0.53
12:M:145:LEU:HD21	12:M:182:ALA:HB2	1.91	0.52
8:V:14:LEU:HD23	8:V:44:CYS:SG	2.50	0.51
7:G:108:LEU:HD11	7:G:137:LEU:HB3	1.91	0.51
3:Q:11:ILE:HG22	4:R:9:ILE:HG23	1.93	0.51
7:U:108:LEU:HD11	7:U:137:LEU:HB3	1.92	0.51
3:C:11:ILE:HG22	4:D:9:ILE:HG23	1.93	0.51
3:Q:178:ASP:OD2	3:Q:195:LYS:NZ	2.26	0.50
10:J:182:MET:HE3	10:J:203:MET:HE3	1.93	0.50
3:Q:171:ALA:HB2	3:Q:200:THR:HG21	1.94	0.49
1:O:72:ILE:HG21	1:O:114:LEU:HD21	1.95	0.49
1:A:145:GLU:N	1:A:145:GLU:OE1	2.46	0.49
1:A:72:ILE:HG21	1:A:114:LEU:HD21	1.95	0.48
7:U:49:VAL:HG23	7:U:66:LEU:HD21	1.95	0.48
7:U:117:MET:HA	7:U:117:MET:HE2	1.95	0.48
6:F:41:LYS:NZ	6:F:181:GLU:OE1	2.35	0.48
8:H:14:LEU:HD23	8:H:44:CYS:SG	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:4:MET:HG3	8:V:127:ILE:HG22	1.96	0.47
10:X:182:MET:HE3	10:X:203:MET:HE3	1.98	0.46
2:P:74:VAL:HG22	2:P:75:TYR:H	1.81	0.46
7:U:42:LYS:HE3	7:U:183:GLU:HA	1.98	0.46
6:F:72:ILE:HG22	6:F:134:ILE:HG12	1.98	0.45
10:J:204:ASP:OXT	14:Z:19:ARG:NH1	2.48	0.45
1:A:130:GLU:OE1	1:A:130:GLU:N	2.43	0.45
5:S:189:MET:HE2	5:S:194:ALA:HA	1.99	0.45
1:O:145:GLU:OE1	1:O:145:GLU:N	2.46	0.45
2:B:74:VAL:HG22	2:B:75:TYR:H	1.80	0.45
8:H:129:GLY:O	8:H:132:SER:OG	2.31	0.45
2:P:64:VAL:O	2:P:219:ARG:NH1	2.48	0.45
2:B:37:ILE:HD13	2:B:189:THR:HG23	1.98	0.44
6:T:72:ILE:HG22	6:T:134:ILE:HG12	1.98	0.44
2:B:64:VAL:O	2:B:219:ARG:NH1	2.48	0.44
2:P:39:ALA:N	2:P:42:GLY:O	2.49	0.44
4:D:201:VAL:HG21	4:D:208:ILE:HG12	2.00	0.44
8:V:127:ILE:HD11	8:V:136:TYR:CD1	2.52	0.44
12:M:110:ILE:HD12	12:M:124:PHE:CE1	2.53	0.44
13:N:96:MET:HE3	13:N:127:MET:HA	1.99	0.44
4:R:201:VAL:HG21	4:R:208:ILE:HG12	2.00	0.44
2:B:39:ALA:N	2:B:42:GLY:O	2.49	0.44
7:G:49:VAL:HG23	7:G:66:LEU:HD21	1.99	0.44
12:a:83:MET:HG2	12:a:87:ALA:HB3	1.99	0.44
8:V:127:ILE:HD11	8:V:136:TYR:CE1	2.53	0.44
2:P:158:LYS:NZ	3:Q:54:LYS:O	2.51	0.43
2:P:37:ILE:HD13	2:P:189:THR:HG23	2.00	0.43
13:b:96:MET:HE3	13:b:127:MET:HA	1.99	0.43
12:a:110:ILE:HD12	12:a:124:PHE:CE1	2.53	0.43
3:C:171:ALA:HB2	3:C:200:THR:HG21	2.00	0.43
12:M:83:MET:HG2	12:M:87:ALA:HB3	2.00	0.43
7:G:202:ASP:OD1	7:G:204:VAL:HG22	2.19	0.43
5:S:167:ALA:HB3	6:T:56:LEU:HD13	2.01	0.42
7:U:39:ILE:HG21	7:U:189:ILE:HD12	2.02	0.42
9:W:143:ARG:NH1	9:W:150:GLU:OE1	2.45	0.42
14:L:20:ALA:HB2	14:L:31:VAL:HG21	2.02	0.41
12:a:127:VAL:HG23	14:Z:50:ALA:CB	2.50	0.41
8:V:14:LEU:HD21	8:V:101:ALA:HB3	2.01	0.41
5:E:167:ALA:HB3	6:F:56:LEU:HD13	2.02	0.41
10:J:64:GLN:OE1	11:K:86:ARG:NH1	2.51	0.41
5:S:9:ASP:OD2	5:S:9:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:92:LEU:CD1	13:b:112:ILE:HD11	2.51	0.41
5:E:105:GLU:OE2	12:M:75:TYR:OH	2.28	0.41
5:E:189:MET:HE2	5:E:194:ALA:HA	2.03	0.41
5:E:163:VAL:HG12	6:F:60:GLN:OE1	2.20	0.41
7:G:52:LEU:HD23	7:G:209:PHE:HB2	2.03	0.41
1:A:34:GLN:NE2	7:G:17:ASP:O	2.54	0.40
12:M:127:VAL:HG23	14:L:50:ALA:CB	2.50	0.40
14:Z:20:ALA:HB2	14:Z:31:VAL:HG21	2.02	0.40
8:H:14:LEU:HD11	8:H:179:ILE:HD12	2.04	0.40
9:I:24:MET:HE3	12:a:187:VAL:HG21	2.04	0.40
7:U:52:LEU:HD22	7:U:206:ASP:HB3	2.04	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	238/246 (97%)	237 (100%)	1 (0%)	0	100	100
1	O	238/246 (97%)	237 (100%)	1 (0%)	0	100	100
2	B	226/234 (97%)	225 (100%)	1 (0%)	0	100	100
2	P	226/234 (97%)	225 (100%)	1 (0%)	0	100	100
3	C	245/261 (94%)	240 (98%)	5 (2%)	0	100	100
3	Q	245/261 (94%)	239 (98%)	6 (2%)	0	100	100
4	D	237/250 (95%)	233 (98%)	4 (2%)	0	100	100
4	R	237/250 (95%)	233 (98%)	4 (2%)	0	100	100
5	E	234/241 (97%)	229 (98%)	5 (2%)	0	100	100
5	S	234/241 (97%)	231 (99%)	3 (1%)	0	100	100
6	F	231/263 (88%)	229 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	T	231/263 (88%)	229 (99%)	2 (1%)	0	100	100
7	G	237/255 (93%)	232 (98%)	5 (2%)	0	100	100
7	U	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
8	H	198/205 (97%)	195 (98%)	3 (2%)	0	100	100
8	V	198/205 (97%)	195 (98%)	3 (2%)	0	100	100
9	I	218/234 (93%)	215 (99%)	3 (1%)	0	100	100
9	W	218/234 (93%)	215 (99%)	3 (1%)	0	100	100
10	J	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	X	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
11	K	194/201 (96%)	191 (98%)	3 (2%)	0	100	100
11	Y	194/201 (96%)	191 (98%)	3 (2%)	0	100	100
12	M	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
12	a	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
13	N	210/219 (96%)	204 (97%)	6 (3%)	0	100	100
13	b	210/219 (96%)	204 (97%)	6 (3%)	0	100	100
14	L	198/204 (97%)	194 (98%)	4 (2%)	0	100	100
14	Z	198/204 (97%)	194 (98%)	4 (2%)	0	100	100
15	d	1/3 (33%)	1 (100%)	0	0	100	100
15	e	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6158/6468 (95%)	6063 (98%)	95 (2%)	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	205/210 (98%)	205 (100%)	0	100	100
1	O	205/210 (98%)	205 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	187/191 (98%)	187 (100%)	0	100	100
2	P	187/191 (98%)	187 (100%)	0	100	100
3	C	207/221 (94%)	207 (100%)	0	100	100
3	Q	207/221 (94%)	207 (100%)	0	100	100
4	D	200/210 (95%)	199 (100%)	1 (0%)	81	77
4	R	200/210 (95%)	199 (100%)	1 (0%)	81	77
5	E	198/203 (98%)	198 (100%)	0	100	100
5	S	198/203 (98%)	198 (100%)	0	100	100
6	F	199/224 (89%)	199 (100%)	0	100	100
6	T	199/224 (89%)	199 (100%)	0	100	100
7	G	197/212 (93%)	197 (100%)	0	100	100
7	U	197/212 (93%)	197 (100%)	0	100	100
8	H	155/159 (98%)	155 (100%)	0	100	100
8	V	155/159 (98%)	155 (100%)	0	100	100
9	I	181/195 (93%)	181 (100%)	0	100	100
9	W	181/195 (93%)	181 (100%)	0	100	100
10	J	173/174 (99%)	173 (100%)	0	100	100
10	X	173/174 (99%)	173 (100%)	0	100	100
11	K	167/171 (98%)	167 (100%)	0	100	100
11	Y	167/171 (98%)	167 (100%)	0	100	100
12	M	177/178 (99%)	177 (100%)	0	100	100
12	a	177/178 (99%)	177 (100%)	0	100	100
13	N	175/181 (97%)	175 (100%)	0	100	100
13	b	175/181 (97%)	175 (100%)	0	100	100
14	L	156/159 (98%)	156 (100%)	0	100	100
14	Z	156/159 (98%)	156 (100%)	0	100	100
15	d	3/3 (100%)	3 (100%)	0	100	100
15	e	3/3 (100%)	3 (100%)	0	100	100
All	All	5160/5382 (96%)	5158 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
4	D	150	ASP
4	R	150	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	75	ASN
2	B	62	HIS
2	B	101	GLN
3	C	166	ASN
5	E	114	GLN
6	F	8	ASN
6	F	175	HIS
7	G	110	HIS
7	G	170	GLN
8	H	123	GLN
8	H	154	GLN
8	H	187	GLN
9	I	80	ASN
9	I	172	ASN
11	K	61	GLN
11	K	82	ASN
12	M	108	ASN
12	M	157	ASN
13	N	188	GLN
1	O	12	HIS
1	O	75	ASN
1	O	100	ASN
2	P	62	HIS
3	Q	102	GLN
3	Q	155	ASN
3	Q	167	ASN
5	S	114	GLN
8	V	123	GLN
9	W	62	ASN
9	W	80	ASN
9	W	193	ASN
13	b	162	GLN
13	b	188	GLN
12	a	108	ASN
12	a	152	GLN
12	a	157	ASN

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Mol	Chain	Res	Type
11	Y	82	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

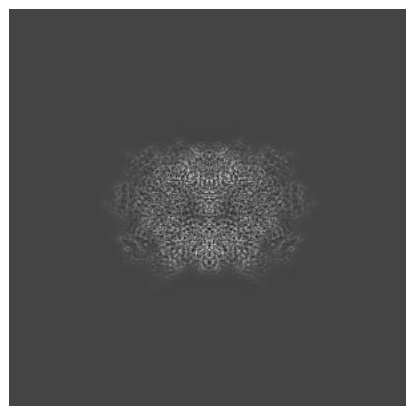
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56072. These allow visual inspection of the internal detail of the map and identification of artifacts.

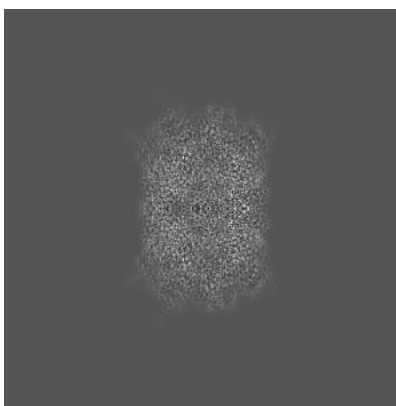
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

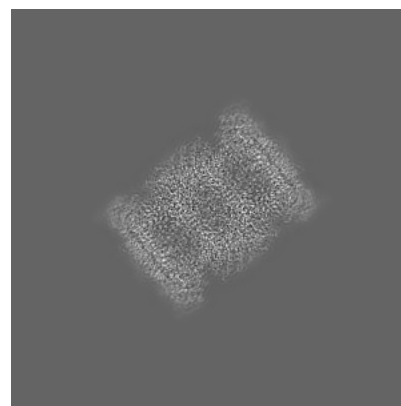
6.1.1 Primary map



X

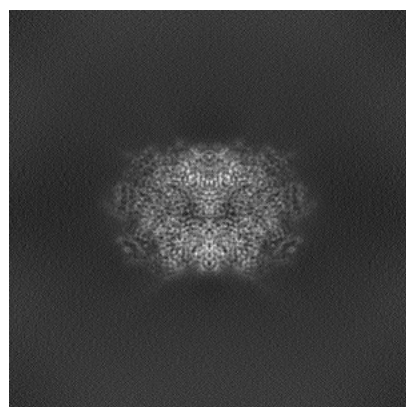


Y

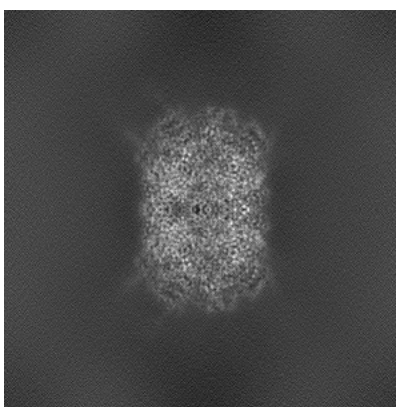


Z

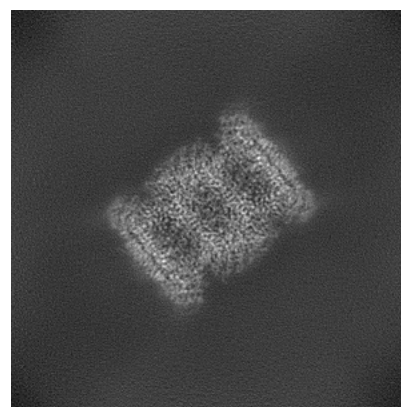
6.1.2 Raw map



X



Y

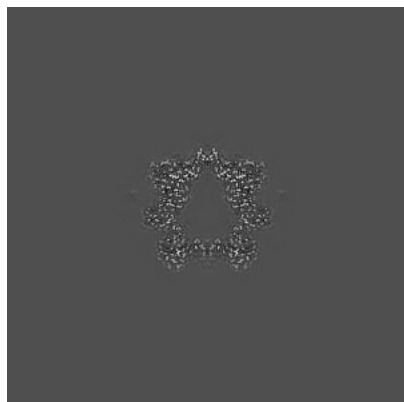


Z

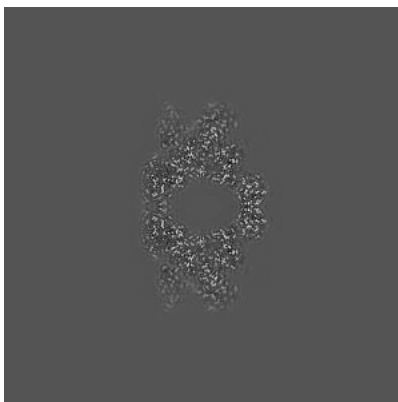
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

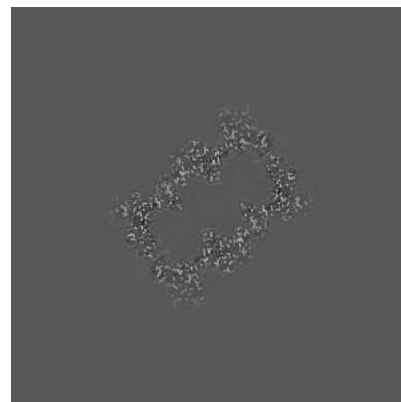
6.2.1 Primary map



X Index: 252

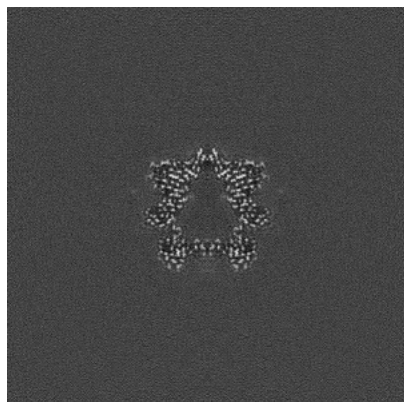


Y Index: 252

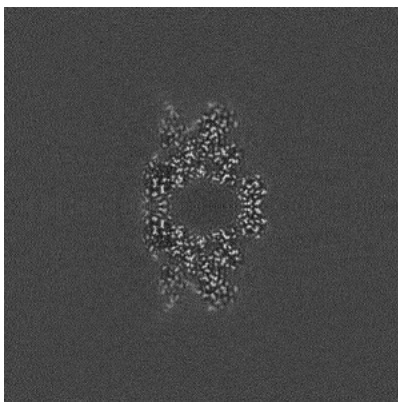


Z Index: 252

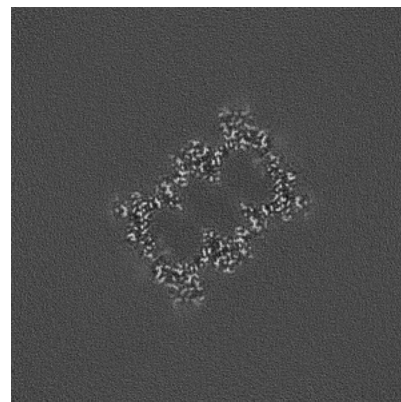
6.2.2 Raw map



X Index: 252



Y Index: 252

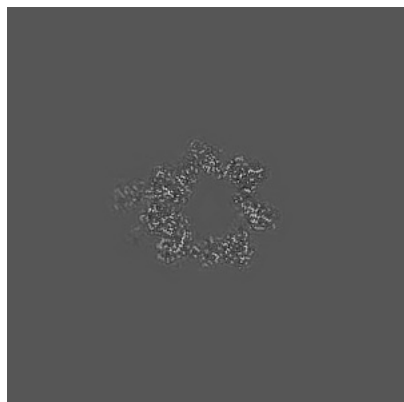


Z Index: 252

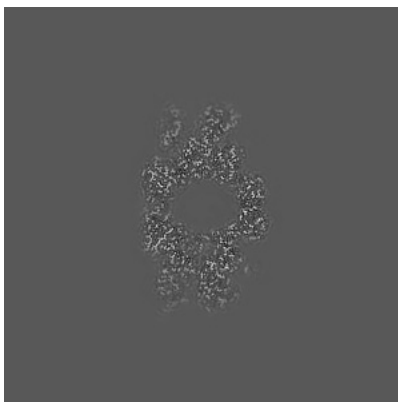
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

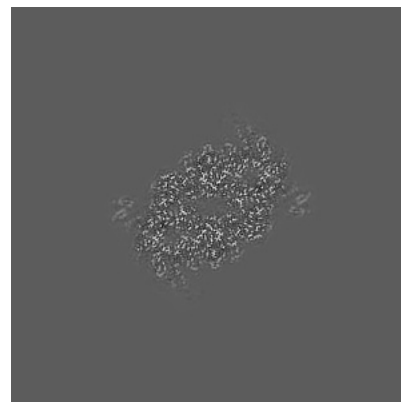
6.3.1 Primary map



X Index: 241

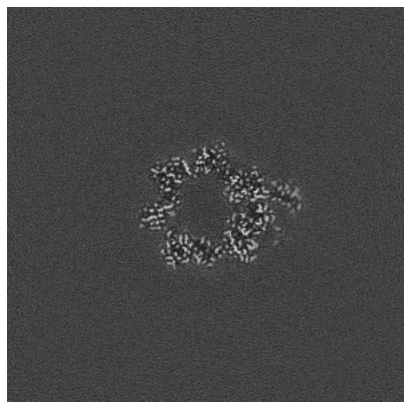


Y Index: 249

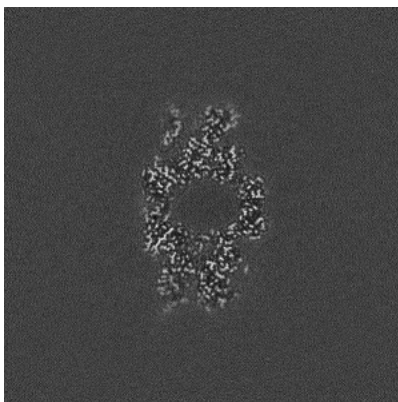


Z Index: 290

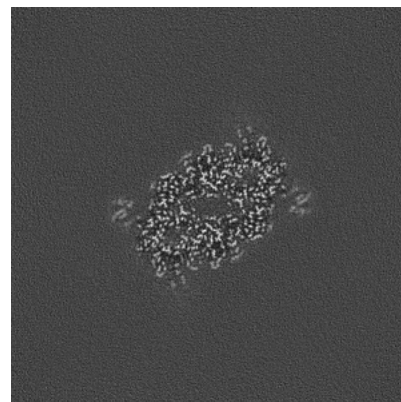
6.3.2 Raw map



X Index: 264



Y Index: 249

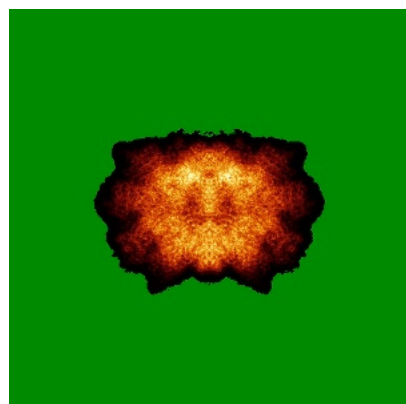


Z Index: 290

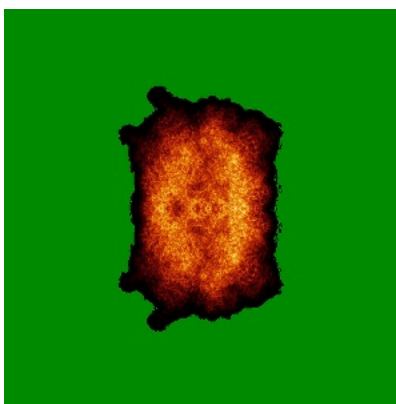
The images above show the largest variance slices of the map in three orthogonal directions.

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

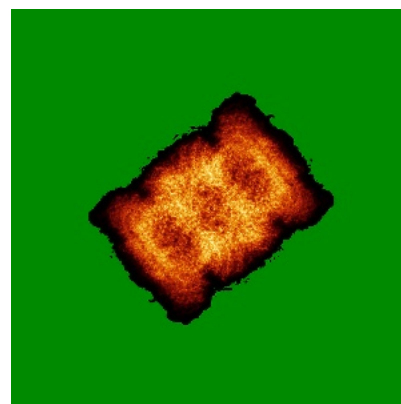
6.4.1 Primary map



X

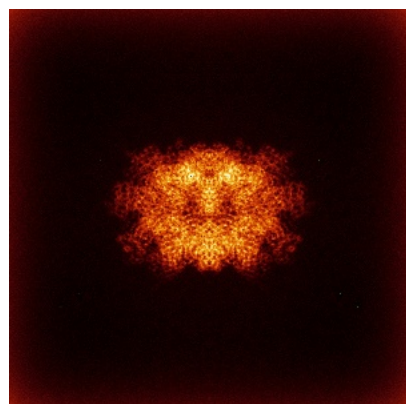


Y

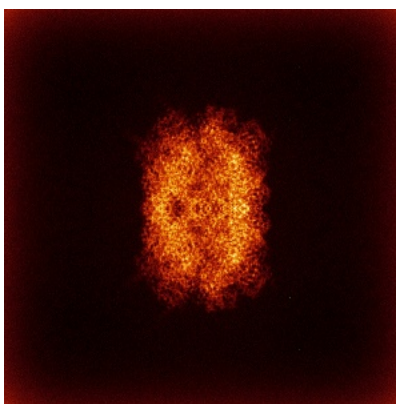


Z

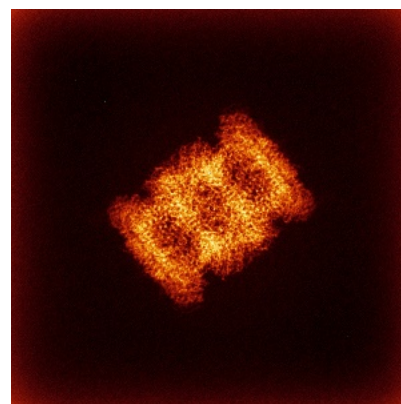
6.4.2 Raw map



X



Y

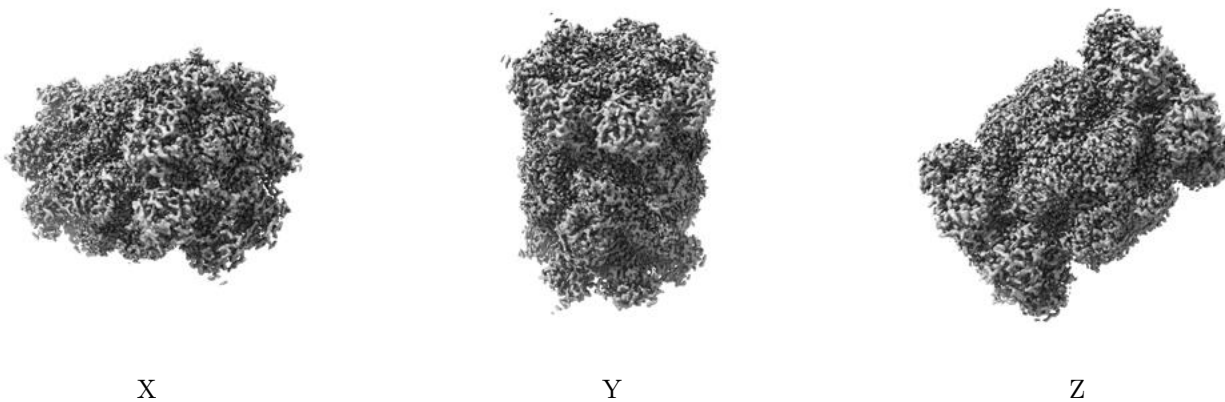


Z

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.

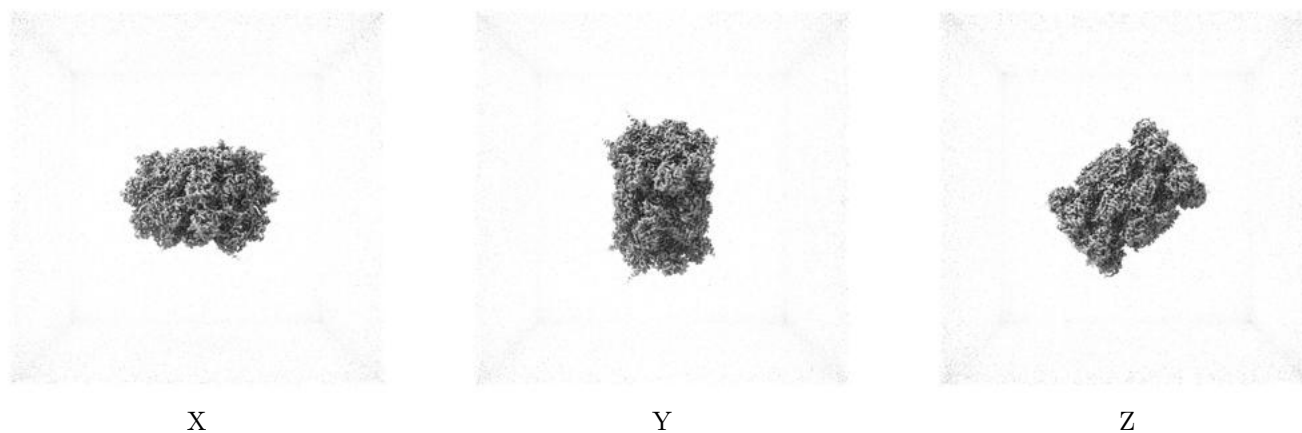
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

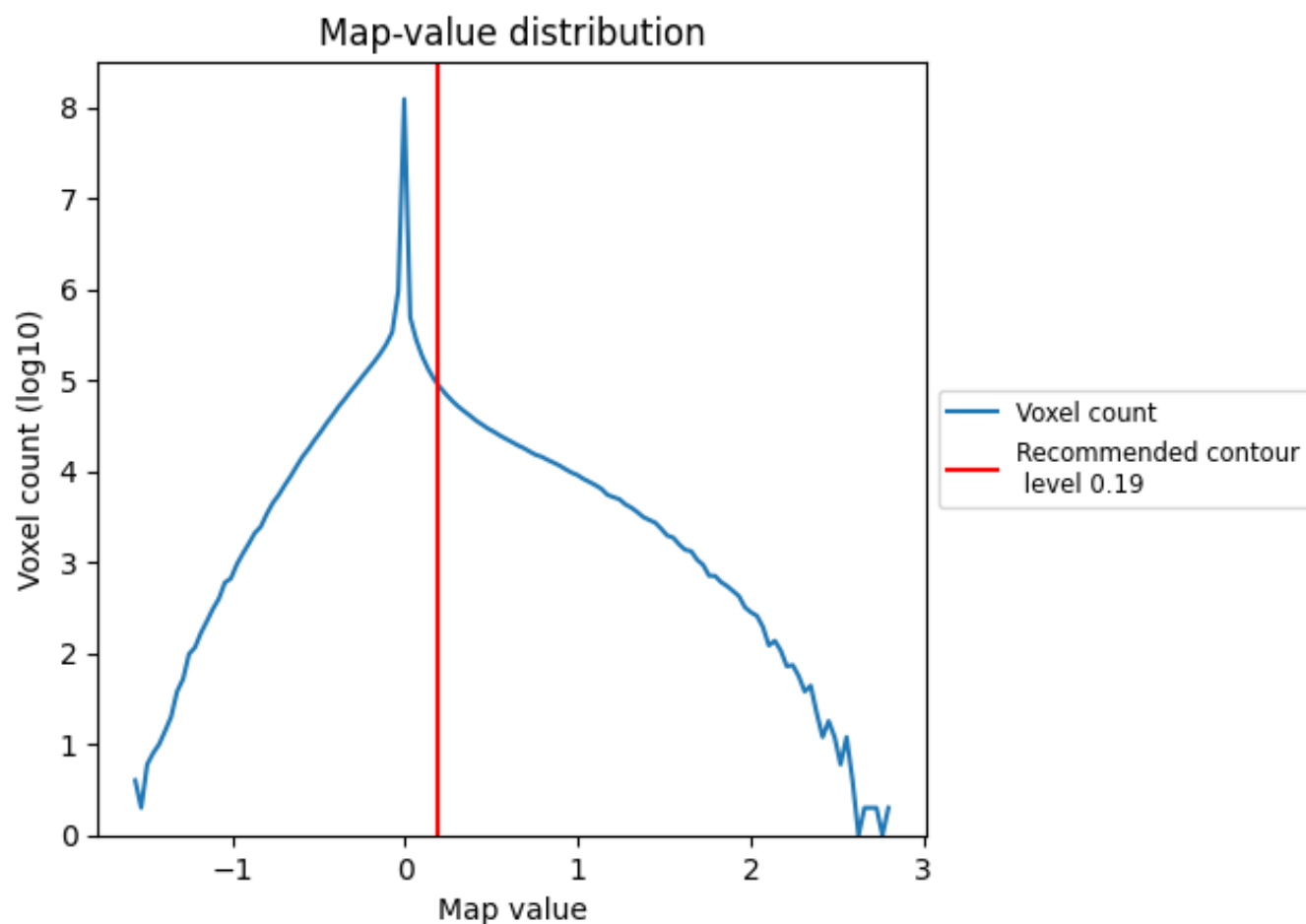
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

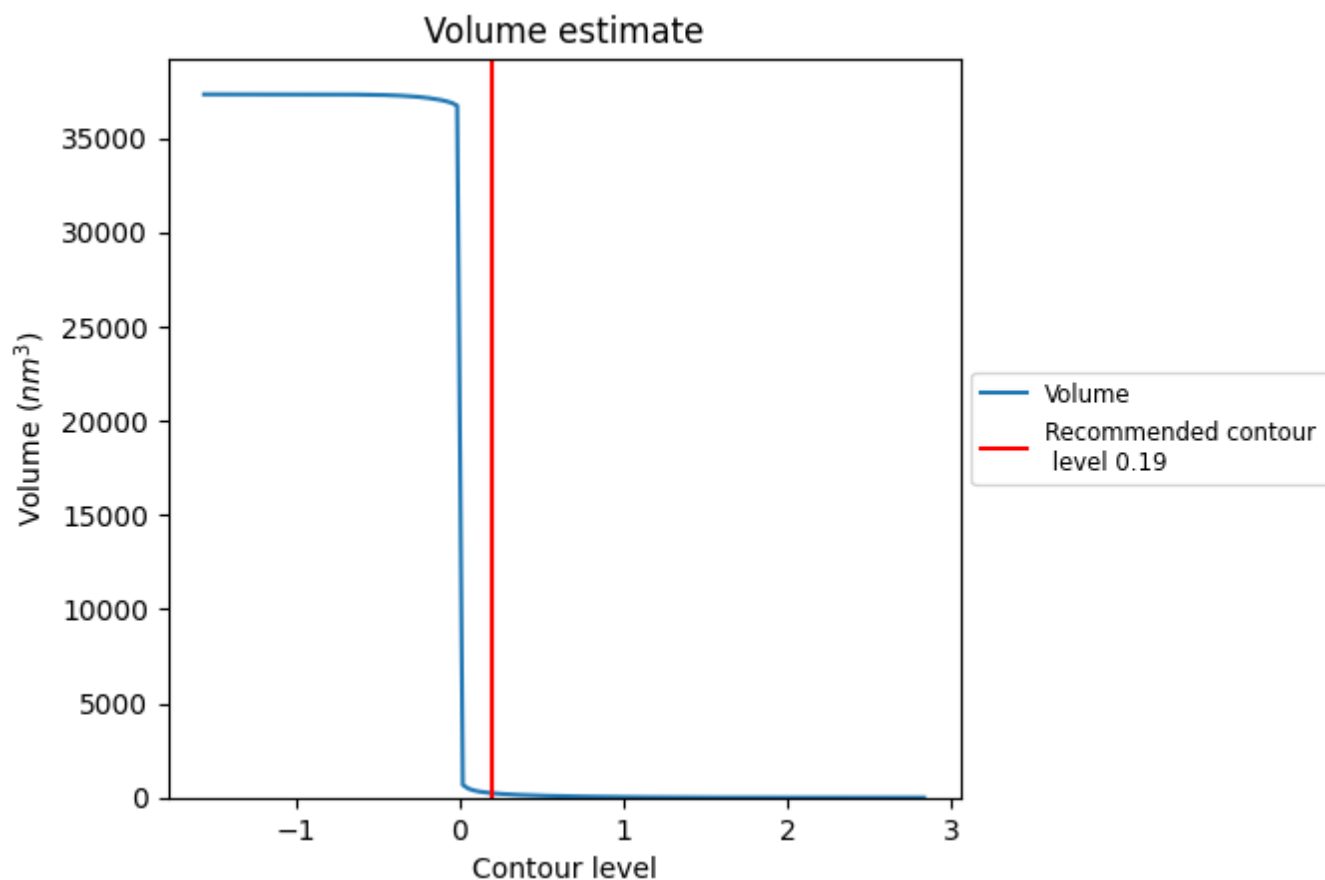
This section contains the results of statistical analysis of the map.

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.

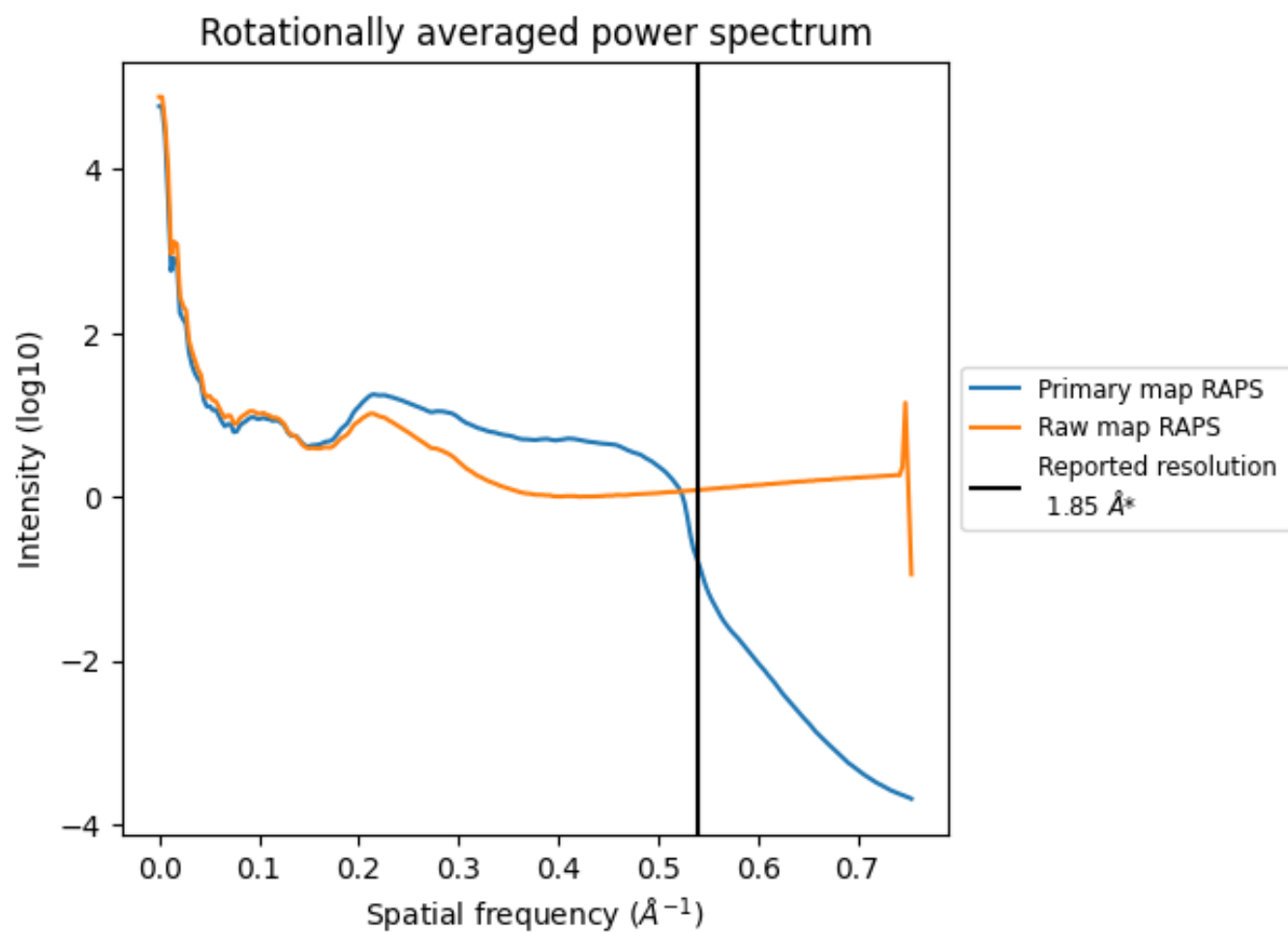
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm³; this corresponds to an approximate mass of 215 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](#)

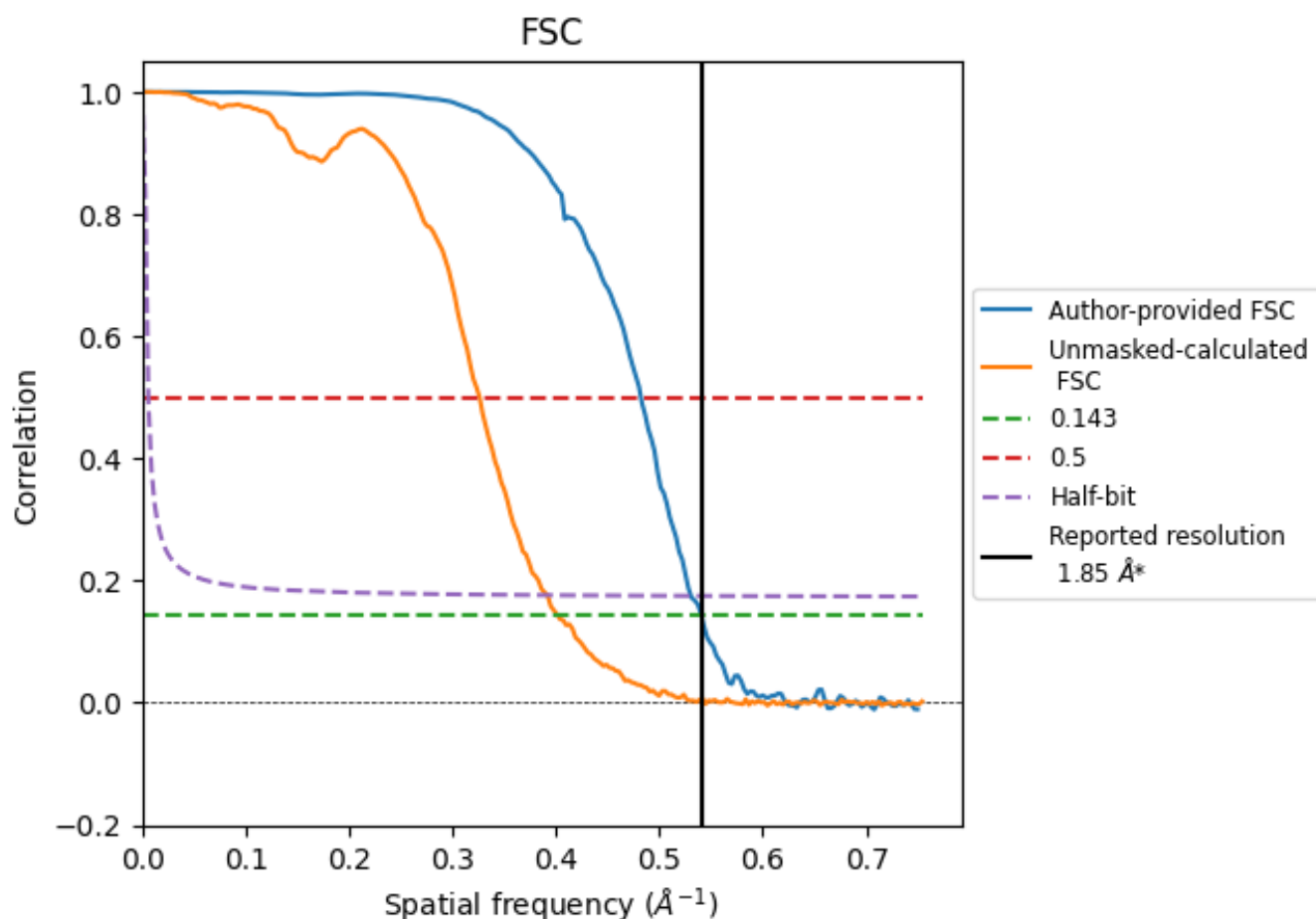


*Reported resolution corresponds to spatial frequency of 0.541 $\text{\AA}^{-1}$

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 0.541 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

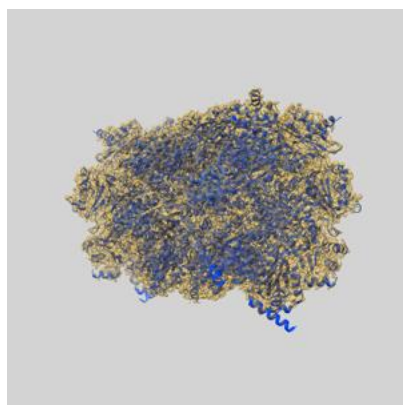
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.85	-	-
Author-provided FSC curve	1.85	2.07	1.88
Unmasked-calculated*	2.49	3.07	2.55

*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 2.49 differs from the reported value 1.85 by more than 10 %

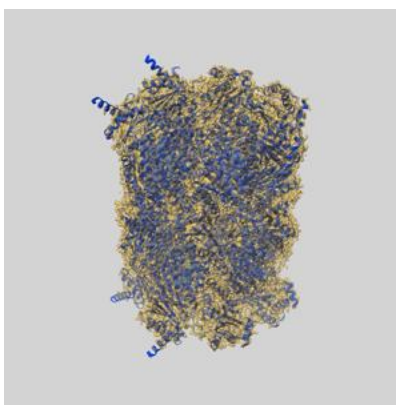
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56072 and PDB model 9TMN. Per-residue inclusion information can be found in section [3](#) on page [10](#).

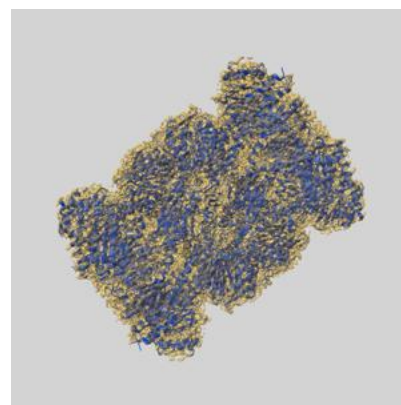
9.1 Map-model overlay [i](#)



X



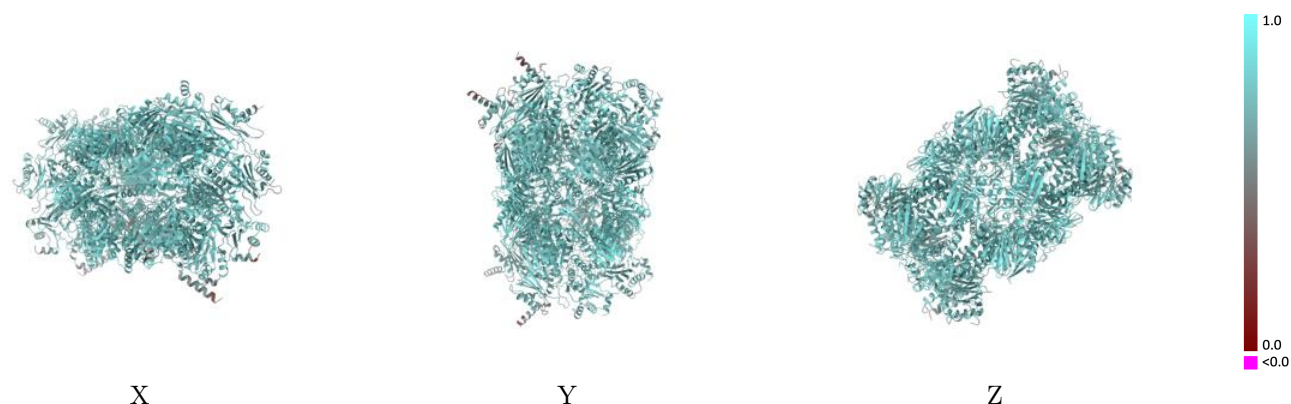
Y



Z

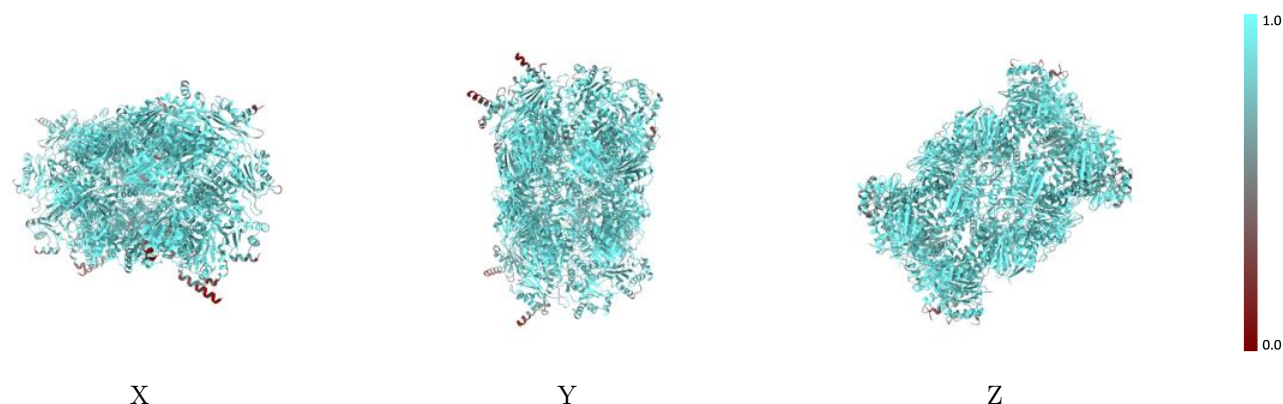
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



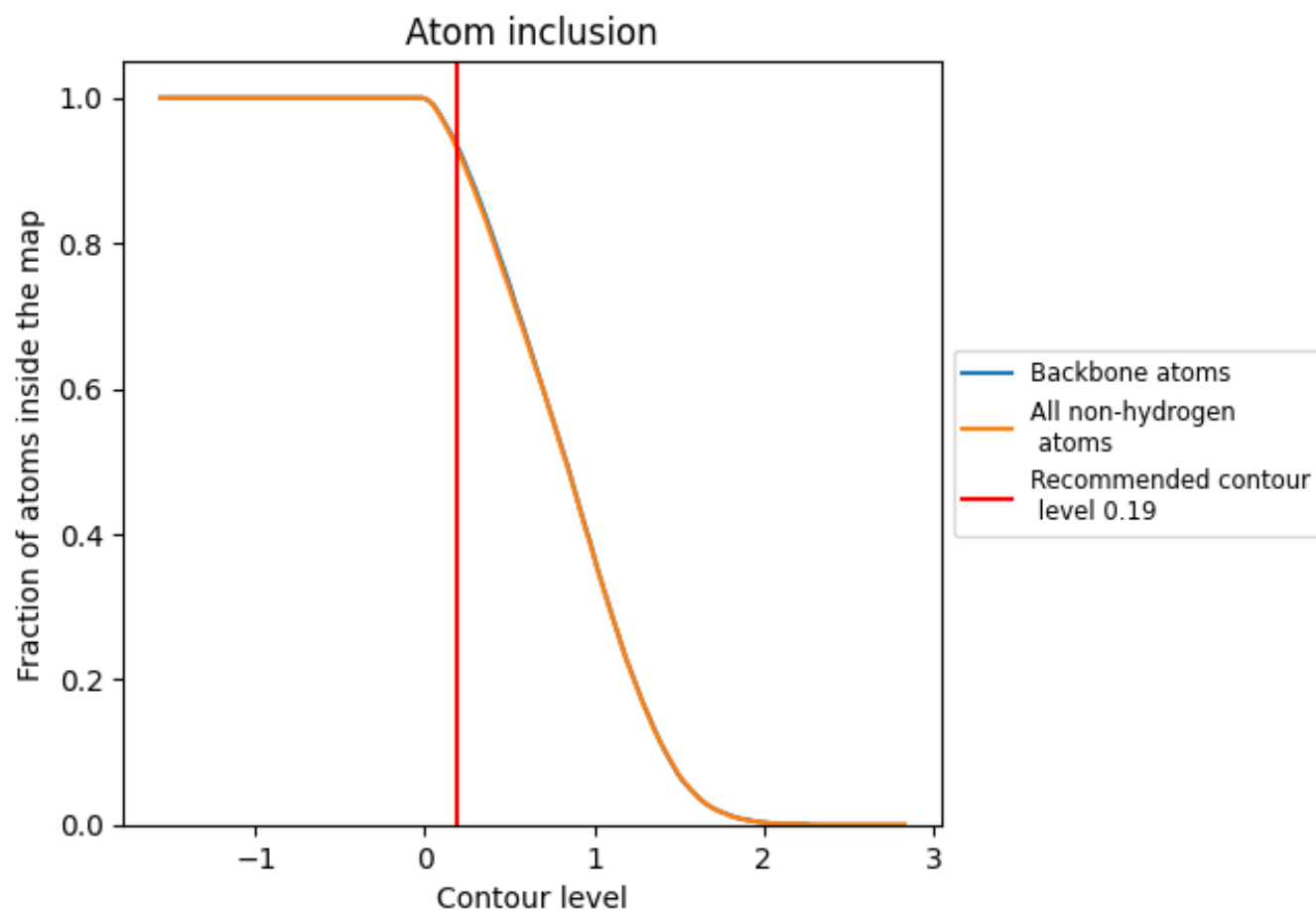
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.7730
A	 0.9150	 0.7570
B	 0.9260	 0.7640
C	 0.8740	 0.7340
D	 0.8380	 0.7160
E	 0.8910	 0.7350
F	 0.9230	 0.7490
G	 0.9030	 0.7510
H	 0.9710	 0.8140
I	 0.9690	 0.8040
J	 0.9830	 0.8080
K	 0.9750	 0.8110
L	 0.9800	 0.8090
M	 0.9680	 0.8010
N	 0.9760	 0.8070
O	 0.9160	 0.7590
P	 0.9230	 0.7620
Q	 0.8740	 0.7340
R	 0.8380	 0.7180
S	 0.8900	 0.7340
T	 0.9240	 0.7480
U	 0.9030	 0.7500
V	 0.9710	 0.8120
W	 0.9660	 0.8030
X	 0.9810	 0.8110
Y	 0.9750	 0.8110
Z	 0.9800	 0.8100
a	 0.9680	 0.8020
b	 0.9760	 0.8070
d	 0.8260	 0.7230
e	 0.8260	 0.7270

