



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 03:44 AM EST

PDB ID : 7LXV
EMDB ID : EMD-23576
Title : Structure of human 20S proteasome with bound MPI-5
Authors : Metcalfe, R.D.; Morton, C.J.; Liu, B.; Xie, S.C.; Hanssen, E.; Leis, A.P.;
Tilley, L.; Griffin, M.D.W.
Deposited on : 2021-03-05
Resolution : 3.40 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

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:

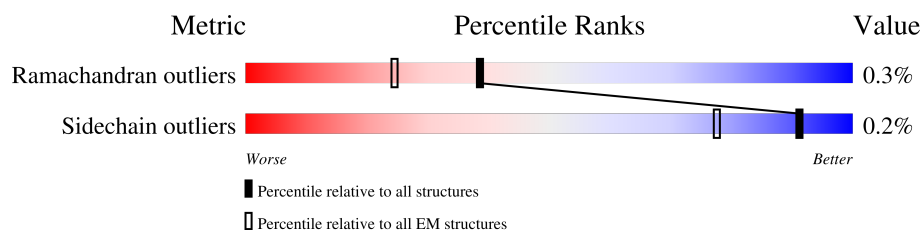
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
1	O	234	
2	B	261	
2	P	261	
3	C	248	
3	Q	248	
4	D	241	
4	R	241	
5	E	263	

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Mol	Chain	Length	Quality of chain
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	205	
14	b	205	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 48314 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
1	A	229	Total	C	N	O	S	0	0
			1787	1144	301	336	6		
1	O	229	Total	C	N	O	S	0	0
			1787	1144	301	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	239	Total	C	N	O	S	0	0
			1884	1193	322	359	10		
2	P	239	Total	C	N	O	S	0	0
			1884	1193	322	359	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	235	Total	C	N	O	S	0	0
			1852	1164	329	354	5		
3	Q	235	Total	C	N	O	S	0	0
			1852	1164	329	354	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		
4	R	236	Total	C	N	O	S	0	0
			1804	1133	297	363	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1857	1162	334	350	11		
5	S	236	Total	C	N	O	S	0	0
			1857	1162	334	350	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		
6	T	239	Total	C	N	O	S	0	0
			1874	1189	320	354	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total	C	N	O	S	0	0
			1884	1193	318	360	13		
7	U	242	Total	C	N	O	S	0	0
			1884	1193	318	360	13		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
8	V	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
9	W	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	199	Total	C	N	O	S	0	0
			1543	974	269	291	9		
11	Y	199	Total	C	N	O	S	0	0
			1543	974	269	291	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		
12	Z	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1657	1048	285	312	12		
13	a	212	Total	C	N	O	S	0	0
			1657	1048	285	312	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

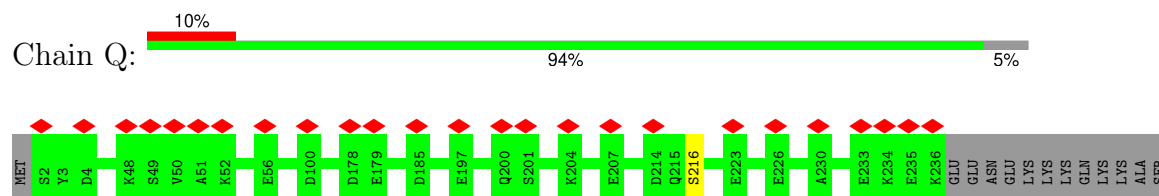
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	b	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		

- Molecule 15 is N-[(1R)-2-([1,1'-biphenyl]-4-yl)-1-boronoethyl]-1-methyl-L-prolinamide (three-letter code: YHD) (formula: C₂₀H₂₅BN₂O₃) (labeled as "Ligand of Interest" by depositor).

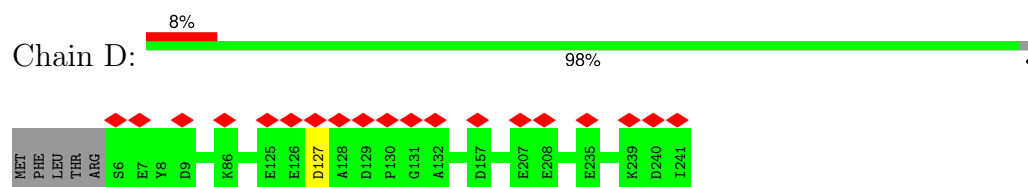


Mol	Chain	Residues	Atoms					AltConf
15	K	1	Total 26	B 1	C 20	N 2	O 3	0
15	Y	1	Total 26	B 1	C 20	N 2	O 3	0

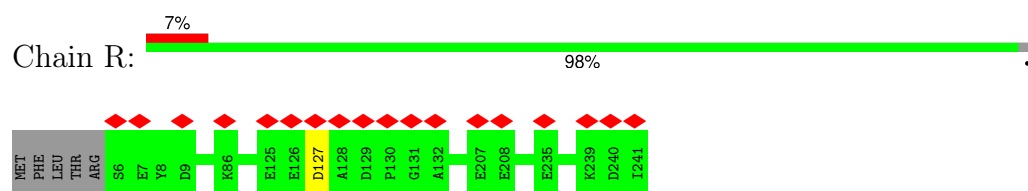
- Molecule 3: Proteasome subunit alpha type-7



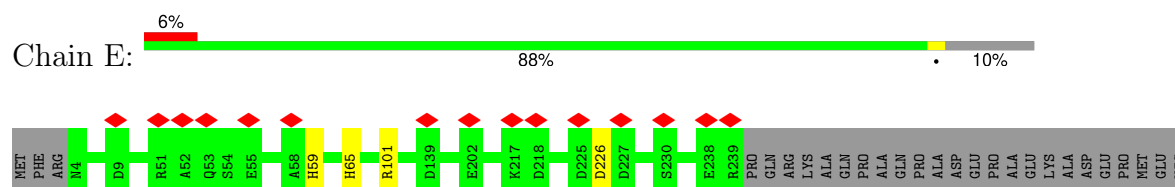
- Molecule 4: Proteasome subunit alpha type-5



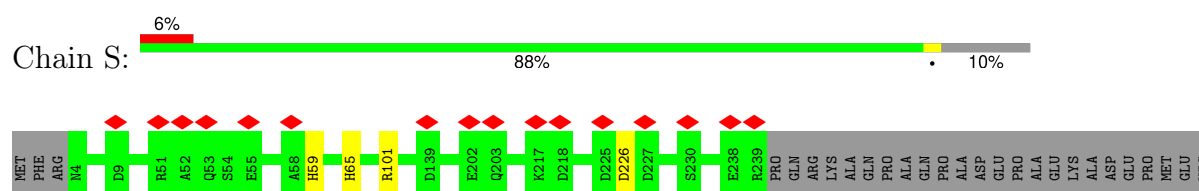
- Molecule 4: Proteasome subunit alpha type-5



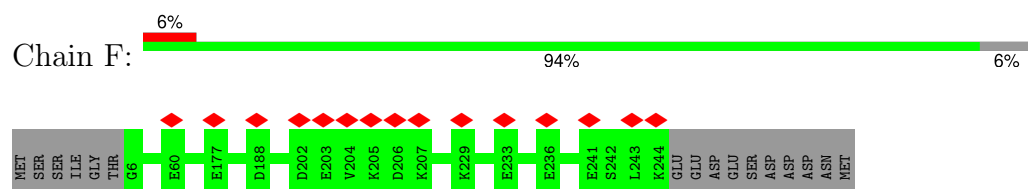
- Molecule 5: Proteasome subunit alpha type-1



- Molecule 5: Proteasome subunit alpha type-1

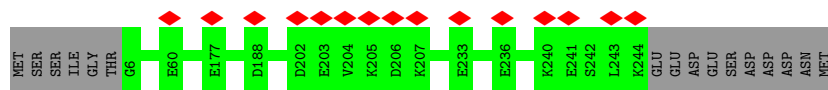


- Molecule 6: Proteasome subunit alpha type-3

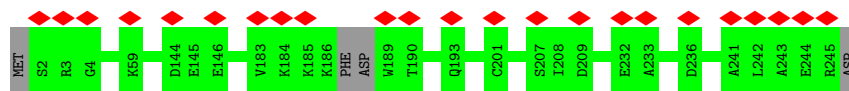


- Molecule 6: Proteasome subunit alpha type-3

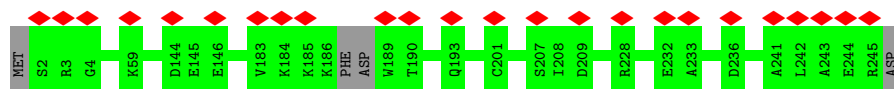




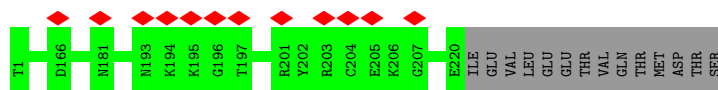
- Molecule 7: Proteasome subunit alpha type-6



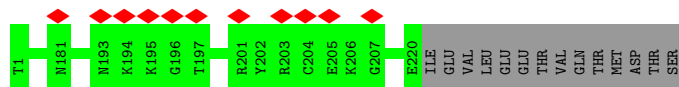
- Molecule 7: Proteasome subunit alpha type-6



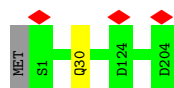
- Molecule 8: Proteasome subunit beta type-7



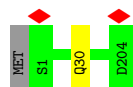
- Molecule 8: Proteasome subunit beta type-7



- Molecule 9: Proteasome subunit beta type-3

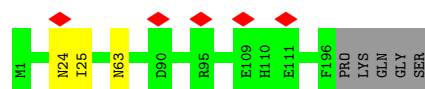


- Molecule 9: Proteasome subunit beta type-3



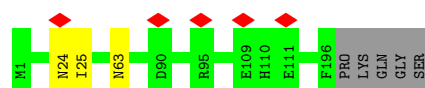
- Molecule 10: Proteasome subunit beta type-2

Chain J:  96%



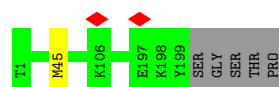
- Molecule 10: Proteasome subunit beta type-2

Chain X:  96%



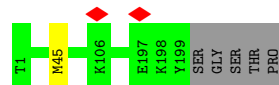
- Molecule 11: Proteasome subunit beta type-5

Chain K:  97%



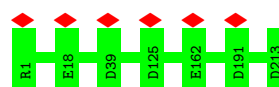
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  97%



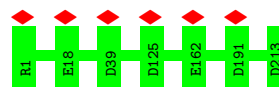
- Molecule 12: Proteasome subunit beta type-1

Chain L:  100%



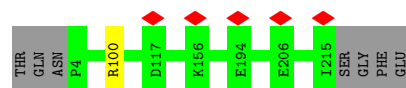
- Molecule 12: Proteasome subunit beta type-1

Chain Z:  100%



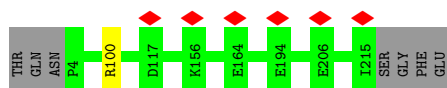
- Molecule 13: Proteasome subunit beta type-4

Chain M:  96%



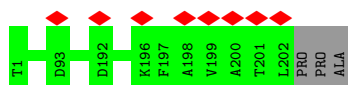
- Molecule 13: Proteasome subunit beta type-4

Chain a:  96%



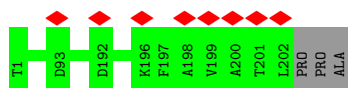
- Molecule 14: Proteasome subunit beta type-6

Chain N:  99%



- Molecule 14: Proteasome subunit beta type-6

Chain b:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.628	Depositor
Minimum map value	-20.277	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.34	0/1826	0.56	0/2474
1	O	0.34	0/1826	0.56	0/2474
2	B	0.34	0/1913	0.57	1/2577 (0.0%)
2	P	0.34	0/1913	0.57	1/2577 (0.0%)
3	C	0.33	0/1878	0.55	0/2534
3	Q	0.33	0/1878	0.55	0/2534
4	D	0.31	0/1832	0.55	0/2475
4	R	0.31	0/1832	0.55	0/2475
5	E	0.32	0/1891	0.59	0/2555
5	S	0.32	0/1891	0.59	0/2555
6	F	0.35	0/1909	0.54	0/2570
6	T	0.35	0/1909	0.54	0/2570
7	G	0.32	0/1916	0.54	0/2587
7	U	0.32	0/1916	0.54	0/2587
8	H	0.33	0/1686	0.57	0/2282
8	V	0.33	0/1686	0.57	0/2282
9	I	0.35	0/1620	0.57	0/2184
9	W	0.35	0/1620	0.57	0/2184
10	J	0.37	0/1603	0.57	0/2168
10	X	0.37	0/1603	0.56	0/2168
11	K	0.36	0/1574	0.54	1/2127 (0.0%)
11	Y	0.36	0/1574	0.54	1/2127 (0.0%)
12	L	0.34	0/1684	0.57	0/2268
12	Z	0.34	0/1684	0.58	0/2268
13	M	0.34	0/1690	0.57	0/2286
13	a	0.34	0/1690	0.57	0/2286
14	N	0.35	0/1540	0.54	0/2085
14	b	0.35	0/1540	0.54	0/2085
All	All	0.34	0/49124	0.56	4/66344 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	209	GLU	CA-CB-CG	6.98	128.75	113.40
2	B	209	GLU	CA-CB-CG	6.97	128.74	113.40
11	K	45	MET	CA-CB-CG	6.51	124.38	113.30
11	Y	45	MET	CA-CB-CG	6.50	124.35	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/234 (97%)	217 (96%)	7 (3%)	3 (1%)	10	33
1	O	227/234 (97%)	217 (96%)	7 (3%)	3 (1%)	10	33
2	B	235/261 (90%)	230 (98%)	5 (2%)	0	100	100
2	P	235/261 (90%)	230 (98%)	5 (2%)	0	100	100
3	C	233/248 (94%)	227 (97%)	5 (2%)	1 (0%)	30	60
3	Q	233/248 (94%)	227 (97%)	5 (2%)	1 (0%)	30	60
4	D	234/241 (97%)	226 (97%)	7 (3%)	1 (0%)	30	60
4	R	234/241 (97%)	226 (97%)	7 (3%)	1 (0%)	30	60
5	E	234/263 (89%)	227 (97%)	5 (2%)	2 (1%)	14	41
5	S	234/263 (89%)	227 (97%)	5 (2%)	2 (1%)	14	41
6	F	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
6	T	237/255 (93%)	234 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	238/246 (97%)	234 (98%)	4 (2%)	0	100	100
7	U	238/246 (97%)	234 (98%)	4 (2%)	0	100	100
8	H	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
8	V	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	197 (98%)	4 (2%)	1 (0%)	25	54
9	W	202/205 (98%)	197 (98%)	4 (2%)	1 (0%)	25	54
10	J	194/201 (96%)	191 (98%)	1 (0%)	2 (1%)	13	39
10	X	194/201 (96%)	191 (98%)	1 (0%)	2 (1%)	13	39
11	K	197/204 (97%)	194 (98%)	3 (2%)	0	100	100
11	Y	197/204 (97%)	194 (98%)	3 (2%)	0	100	100
12	L	211/213 (99%)	209 (99%)	2 (1%)	0	100	100
12	Z	211/213 (99%)	209 (99%)	2 (1%)	0	100	100
13	M	210/219 (96%)	205 (98%)	5 (2%)	0	100	100
13	a	210/219 (96%)	205 (98%)	5 (2%)	0	100	100
14	N	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
14	b	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
All	All	6140/6458 (95%)	6002 (98%)	118 (2%)	20 (0%)	38	66

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	226	ASP
9	I	30	GLN
5	S	226	ASP
9	W	30	GLN
3	C	216	SER
10	J	25	ILE
3	Q	216	SER
10	X	25	ILE
1	A	51	GLN
5	E	59	HIS
1	O	51	GLN
5	S	59	HIS
1	A	201	GLN
4	D	127	ASP
10	J	24	ASN

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Mol	Chain	Res	Type
1	O	201	GLN
4	R	127	ASP
10	X	24	ASN
1	A	52	LYS
1	O	52	LYS

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	188/191 (98%)	188 (100%)	0	100	100
1	O	188/191 (98%)	188 (100%)	0	100	100
2	B	201/221 (91%)	200 (100%)	1 (0%)	86	91
2	P	201/221 (91%)	200 (100%)	1 (0%)	86	91
3	C	199/211 (94%)	199 (100%)	0	100	100
3	Q	199/211 (94%)	199 (100%)	0	100	100
4	D	198/203 (98%)	198 (100%)	0	100	100
4	R	198/203 (98%)	198 (100%)	0	100	100
5	E	202/224 (90%)	200 (99%)	2 (1%)	73	83
5	S	202/224 (90%)	200 (99%)	2 (1%)	73	83
6	F	197/212 (93%)	197 (100%)	0	100	100
6	T	197/212 (93%)	197 (100%)	0	100	100
7	G	206/210 (98%)	206 (100%)	0	100	100
7	U	206/210 (98%)	206 (100%)	0	100	100
8	H	181/195 (93%)	181 (100%)	0	100	100
8	V	181/195 (93%)	181 (100%)	0	100	100
9	I	173/174 (99%)	173 (100%)	0	100	100
9	W	173/174 (99%)	173 (100%)	0	100	100
10	J	167/171 (98%)	166 (99%)	1 (1%)	84	90
10	X	167/171 (98%)	166 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	154/159 (97%)	154 (100%)	0	100	100
11	Y	154/159 (97%)	154 (100%)	0	100	100
12	L	178/178 (100%)	178 (100%)	0	100	100
12	Z	178/178 (100%)	178 (100%)	0	100	100
13	M	175/181 (97%)	174 (99%)	1 (1%)	84	90
13	a	175/181 (97%)	174 (99%)	1 (1%)	84	90
14	N	157/159 (99%)	157 (100%)	0	100	100
14	b	157/159 (99%)	157 (100%)	0	100	100
All	All	5152/5378 (96%)	5142 (100%)	10 (0%)	91	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	209	GLU
5	E	65	HIS
5	E	101	ARG
10	J	63	ASN
13	M	100	ARG
2	P	209	GLU
5	S	65	HIS
5	S	101	ARG
10	X	63	ASN
13	a	100	ARG

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	101	GLN
1	A	139	ASN
7	G	150	GLN
8	H	57	GLN
8	H	172	ASN
9	I	168	GLN
10	J	8	GLN
1	O	101	GLN
1	O	139	ASN
7	U	150	GLN
8	V	57	GLN

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Mol	Chain	Res	Type
8	V	172	ASN
9	W	168	GLN
10	X	8	GLN
12	Z	151	ASN
12	Z	152	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	YHD	K	301	11	24,28,28	1.83	6 (25%)	33,38,38	3.10	19 (57%)
15	YHD	Y	301	11	24,28,28	1.83	6 (25%)	33,38,38	3.11	19 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	YHD	K	301	11	-	8/15/30/30	0/3/3/3
15	YHD	Y	301	11	-	8/15/30/30	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	301	YHD	C14-C13	4.94	1.60	1.49
15	Y	301	YHD	C14-C13	4.94	1.60	1.49
15	Y	301	YHD	C20-C21	2.62	1.43	1.38
15	K	301	YHD	C20-C21	2.61	1.43	1.38
15	K	301	YHD	O25-C03	2.42	1.28	1.23
15	Y	301	YHD	O25-C03	2.42	1.28	1.23
15	K	301	YHD	C04-N23	2.39	1.52	1.46
15	Y	301	YHD	C04-N23	2.39	1.52	1.46
15	K	301	YHD	C12-C11	2.11	1.42	1.38
15	Y	301	YHD	C09-C10	2.11	1.56	1.51
15	K	301	YHD	C09-C10	2.08	1.56	1.51
15	Y	301	YHD	C12-C11	2.07	1.42	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	YHD	C21-C10-C11	-6.21	109.00	118.23
15	K	301	YHD	C21-C10-C11	-6.21	109.00	118.23
15	Y	301	YHD	C20-C13-C12	-5.95	107.03	117.68
15	K	301	YHD	C20-C13-C12	-5.90	107.12	117.68
15	K	301	YHD	C18-C19-C14	5.12	126.36	120.54
15	Y	301	YHD	C18-C19-C14	5.09	126.33	120.54
15	K	301	YHD	C15-C14-C19	-4.67	109.32	117.68
15	Y	301	YHD	C15-C14-C19	-4.64	109.38	117.68
15	K	301	YHD	C16-C15-C14	4.41	125.56	120.54
15	Y	301	YHD	C16-C15-C14	4.36	125.50	120.54
15	Y	301	YHD	C11-C12-C13	4.34	126.69	121.12
15	K	301	YHD	C11-C12-C13	4.29	126.63	121.12
15	Y	301	YHD	C21-C20-C13	4.20	126.52	121.12
15	K	301	YHD	C21-C20-C13	4.16	126.46	121.12
15	Y	301	YHD	C09-C02-N22	3.93	115.46	110.39
15	K	301	YHD	C09-C02-N22	3.92	115.45	110.39
15	Y	301	YHD	C20-C13-C14	3.87	127.93	121.25
15	K	301	YHD	C20-C13-C14	3.86	127.91	121.25
15	Y	301	YHD	C12-C11-C10	3.64	125.78	121.00
15	Y	301	YHD	C04-C03-N22	3.63	124.50	116.52
15	K	301	YHD	C12-C11-C10	3.62	125.76	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	YHD	C10-C09-C02	3.61	121.48	113.76
15	K	301	YHD	C04-C03-N22	3.61	124.43	116.52
15	K	301	YHD	C10-C09-C02	3.60	121.48	113.76
15	K	301	YHD	C09-C10-C21	3.36	127.15	120.90
15	Y	301	YHD	C09-C10-C21	3.33	127.11	120.90
15	K	301	YHD	C19-C14-C13	3.24	126.85	121.25
15	Y	301	YHD	C19-C14-C13	3.22	126.81	121.25
15	K	301	YHD	C20-C21-C10	3.07	125.03	121.00
15	Y	301	YHD	C20-C21-C10	3.03	124.98	121.00
15	Y	301	YHD	C18-C17-C16	-2.92	115.88	119.87
15	K	301	YHD	C18-C17-C16	-2.90	115.90	119.87
15	K	301	YHD	O25-C03-N22	-2.65	118.21	122.96
15	Y	301	YHD	O25-C03-N22	-2.65	118.22	122.96
15	Y	301	YHD	C12-C13-C14	2.19	125.04	121.25
15	K	301	YHD	C12-C13-C14	2.15	124.97	121.25
15	K	301	YHD	C07-C08-C04	2.06	108.43	104.14
15	Y	301	YHD	C07-C08-C04	2.05	108.42	104.14

There are no chirality outliers.

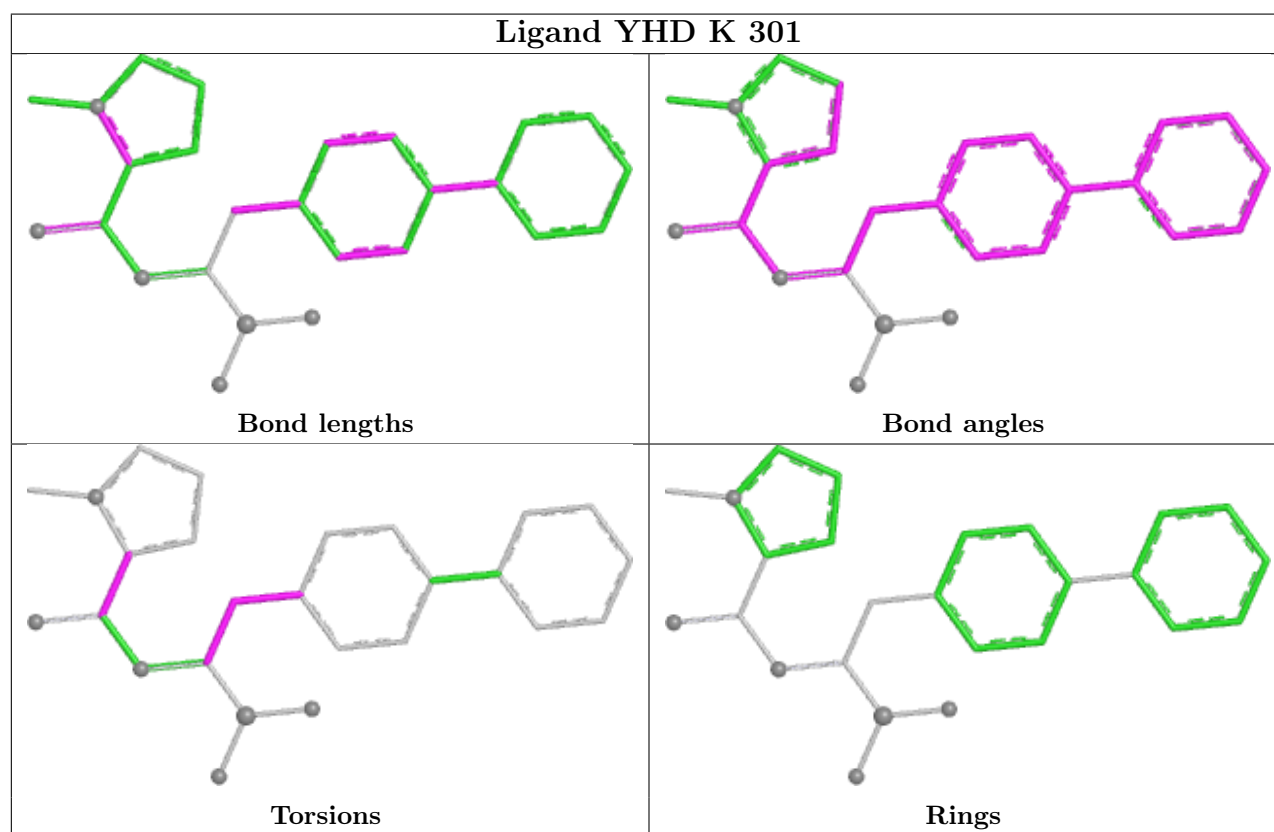
All (16) torsion outliers are listed below:

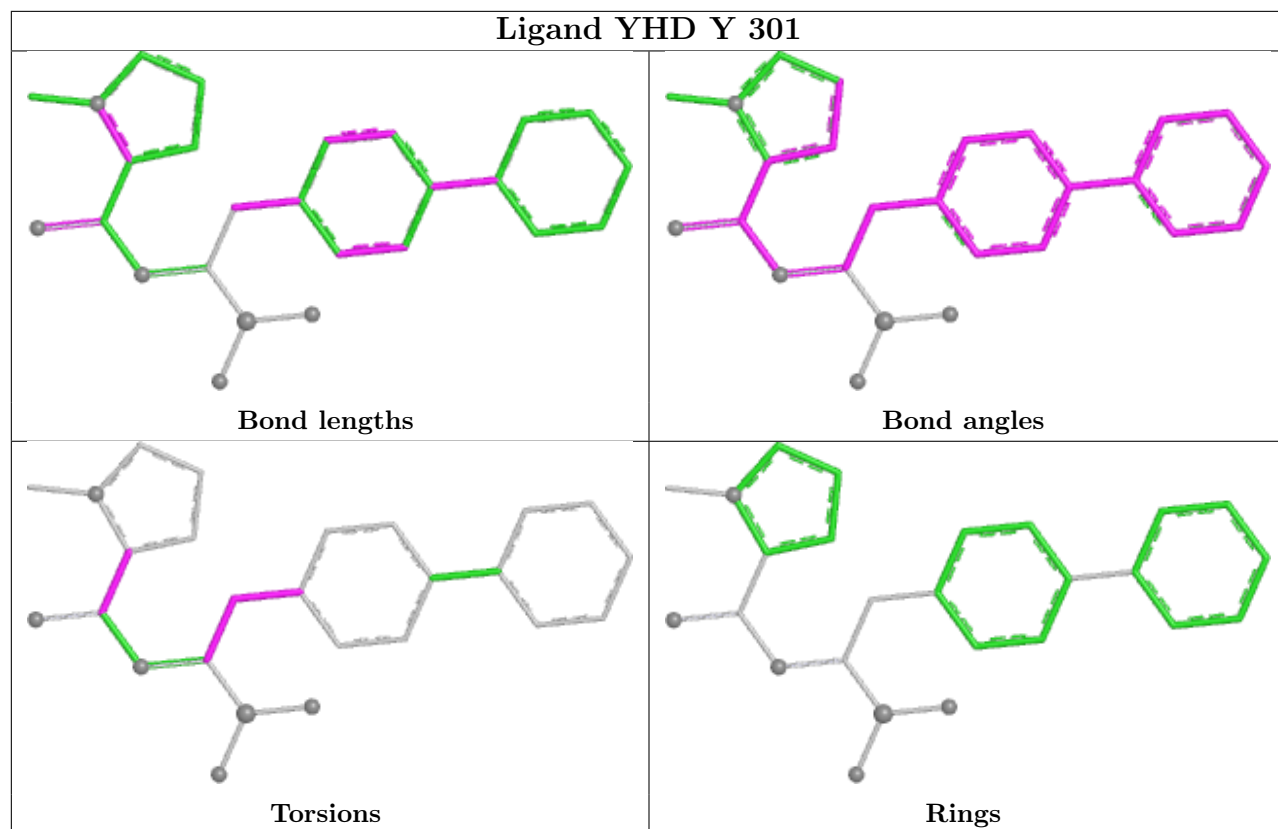
Mol	Chain	Res	Type	Atoms
15	K	301	YHD	C02-C09-C10-C11
15	K	301	YHD	C02-C09-C10-C21
15	K	301	YHD	B01-C02-C09-C10
15	Y	301	YHD	C02-C09-C10-C11
15	Y	301	YHD	C02-C09-C10-C21
15	Y	301	YHD	B01-C02-C09-C10
15	K	301	YHD	O25-C03-C04-N23
15	Y	301	YHD	O25-C03-C04-N23
15	K	301	YHD	N22-C03-C04-N23
15	Y	301	YHD	N22-C03-C04-N23
15	K	301	YHD	N22-C03-C04-C08
15	Y	301	YHD	N22-C03-C04-C08
15	K	301	YHD	O25-C03-C04-C08
15	Y	301	YHD	O25-C03-C04-C08
15	K	301	YHD	N22-C02-C09-C10
15	Y	301	YHD	N22-C02-C09-C10

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

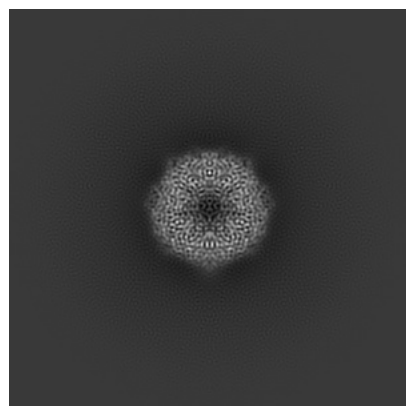
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23576. These allow visual inspection of the internal detail of the map and identification of artifacts.

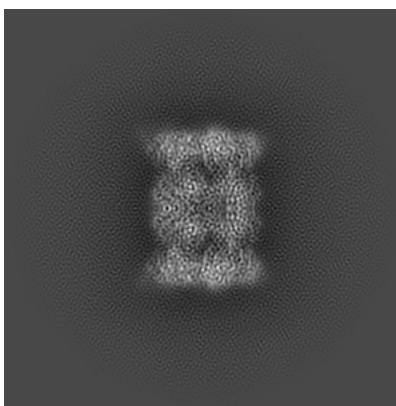
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

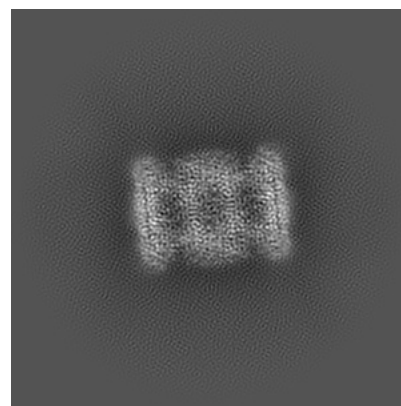
6.1.1 Primary map



X

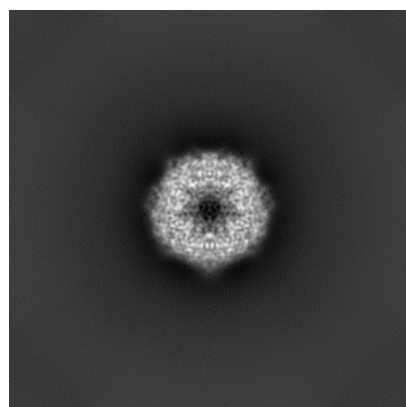


Y

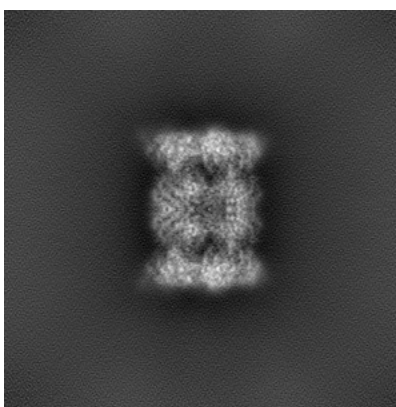


Z

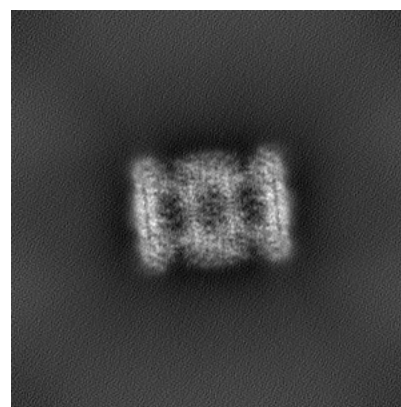
6.1.2 Raw map



X



Y

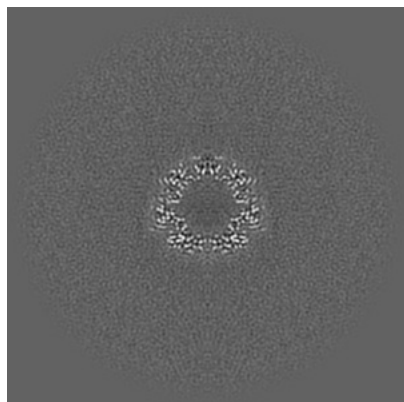


Z

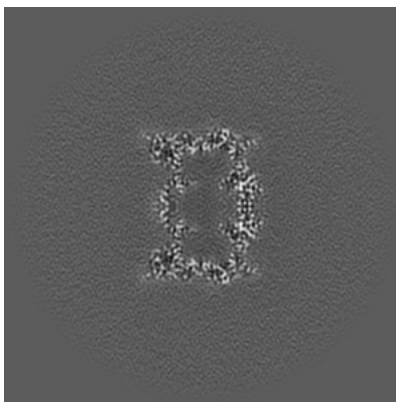
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

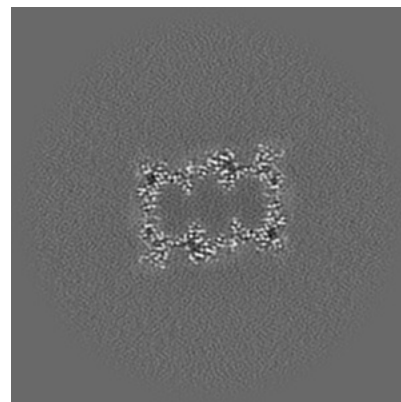
6.2.1 Primary map



X Index: 150

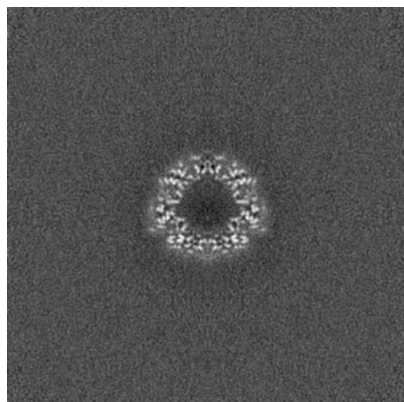


Y Index: 150

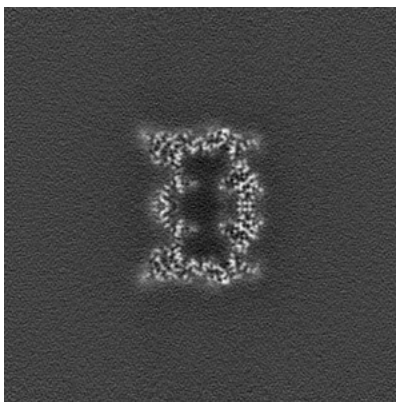


Z Index: 150

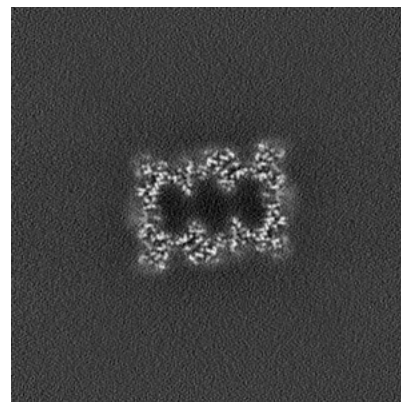
6.2.2 Raw map



X Index: 150



Y Index: 150

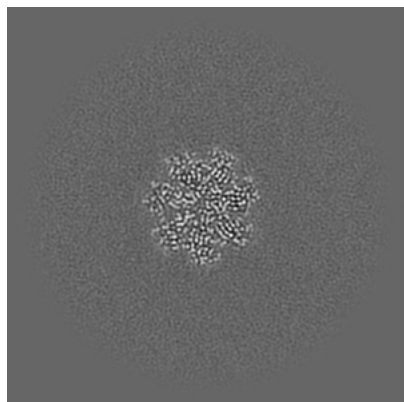


Z Index: 150

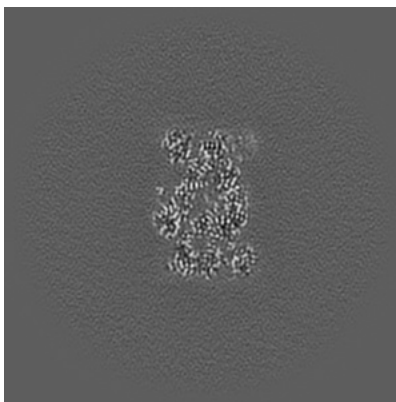
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

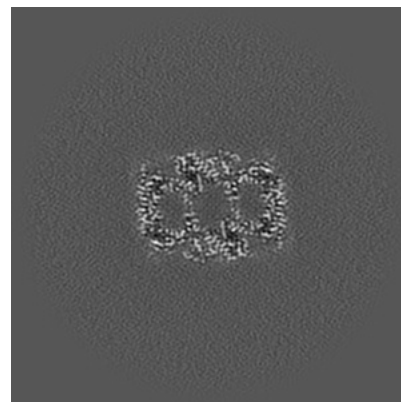
6.3.1 Primary map



X Index: 106

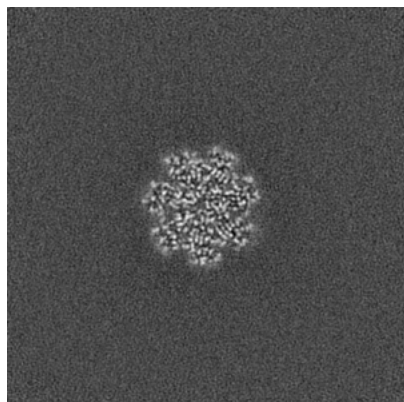


Y Index: 129

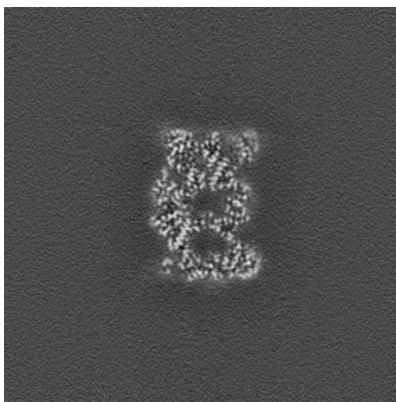


Z Index: 138

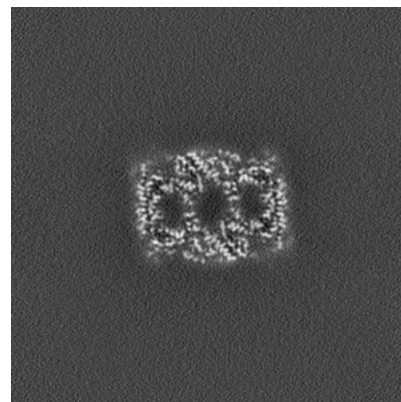
6.3.2 Raw map



X Index: 106



Y Index: 133

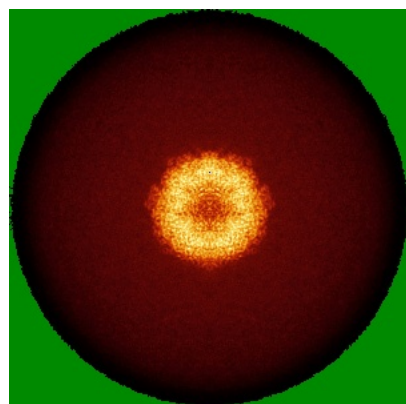


Z Index: 138

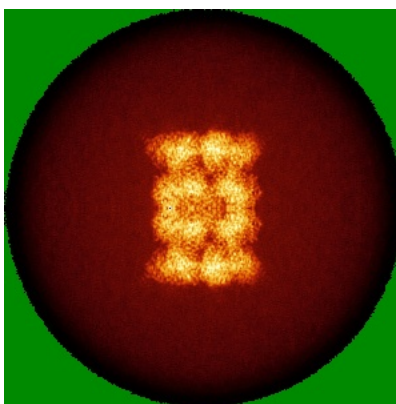
The images above show the largest variance slices of the map in three orthogonal directions.

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

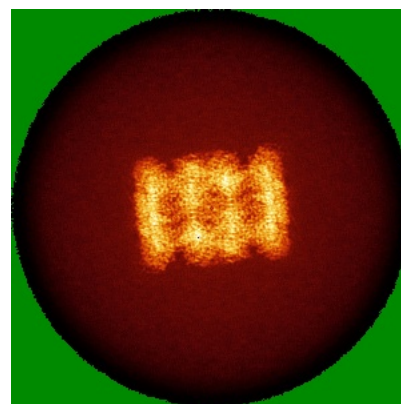
6.4.1 Primary map



X

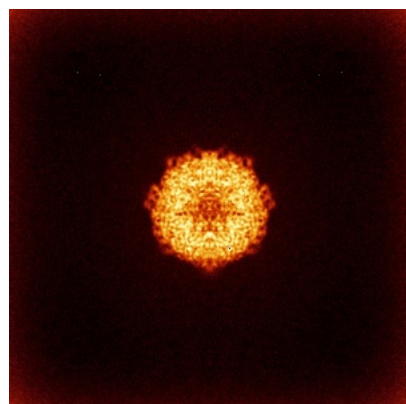


Y

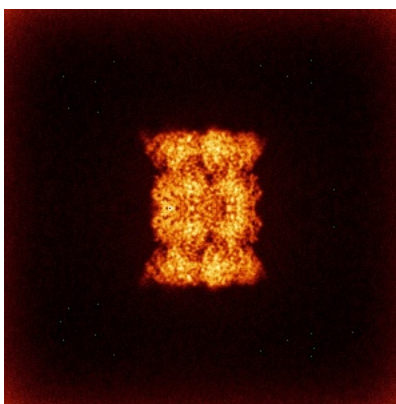


Z

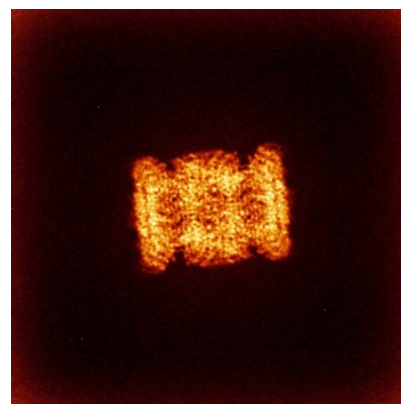
6.4.2 Raw map



X



Y

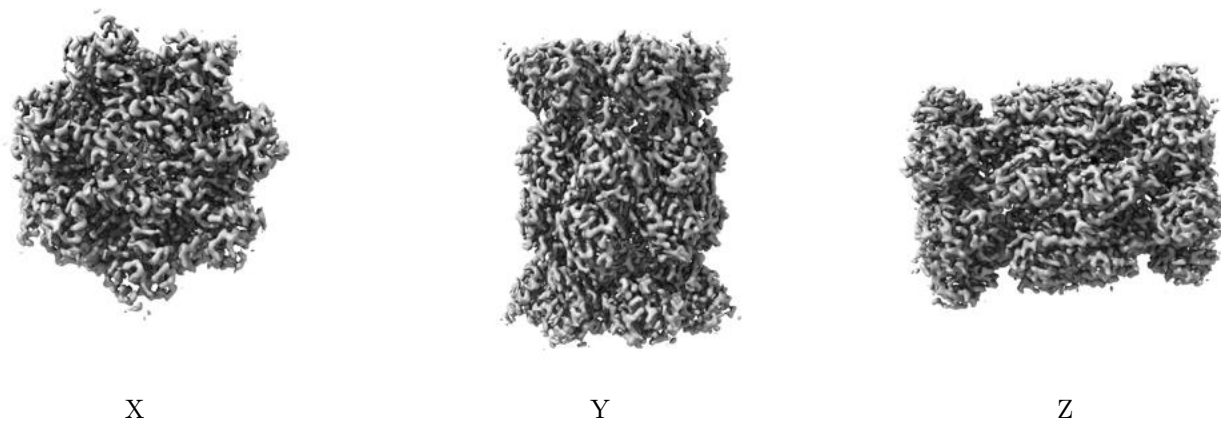


Z

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 5.0. 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.

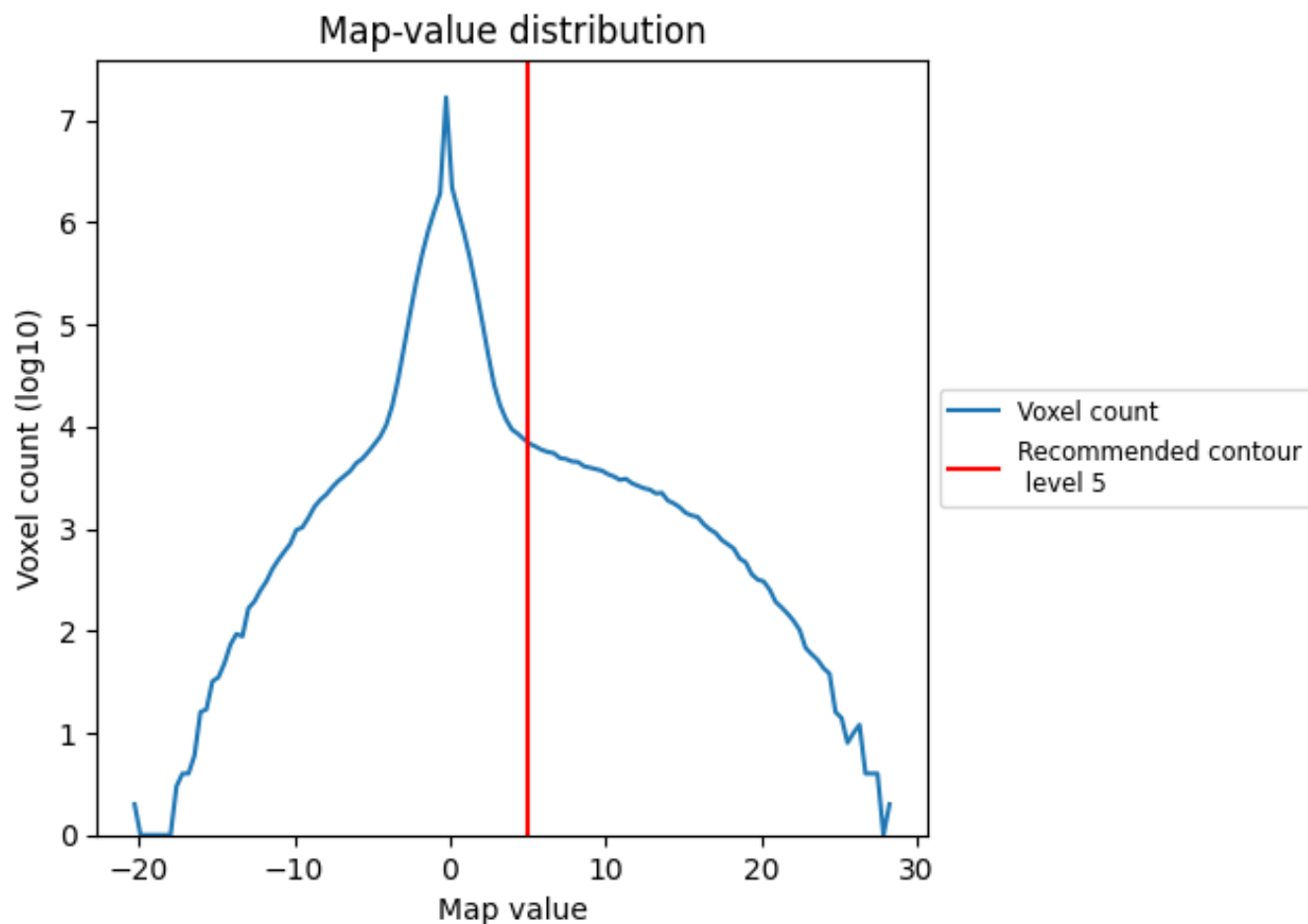
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

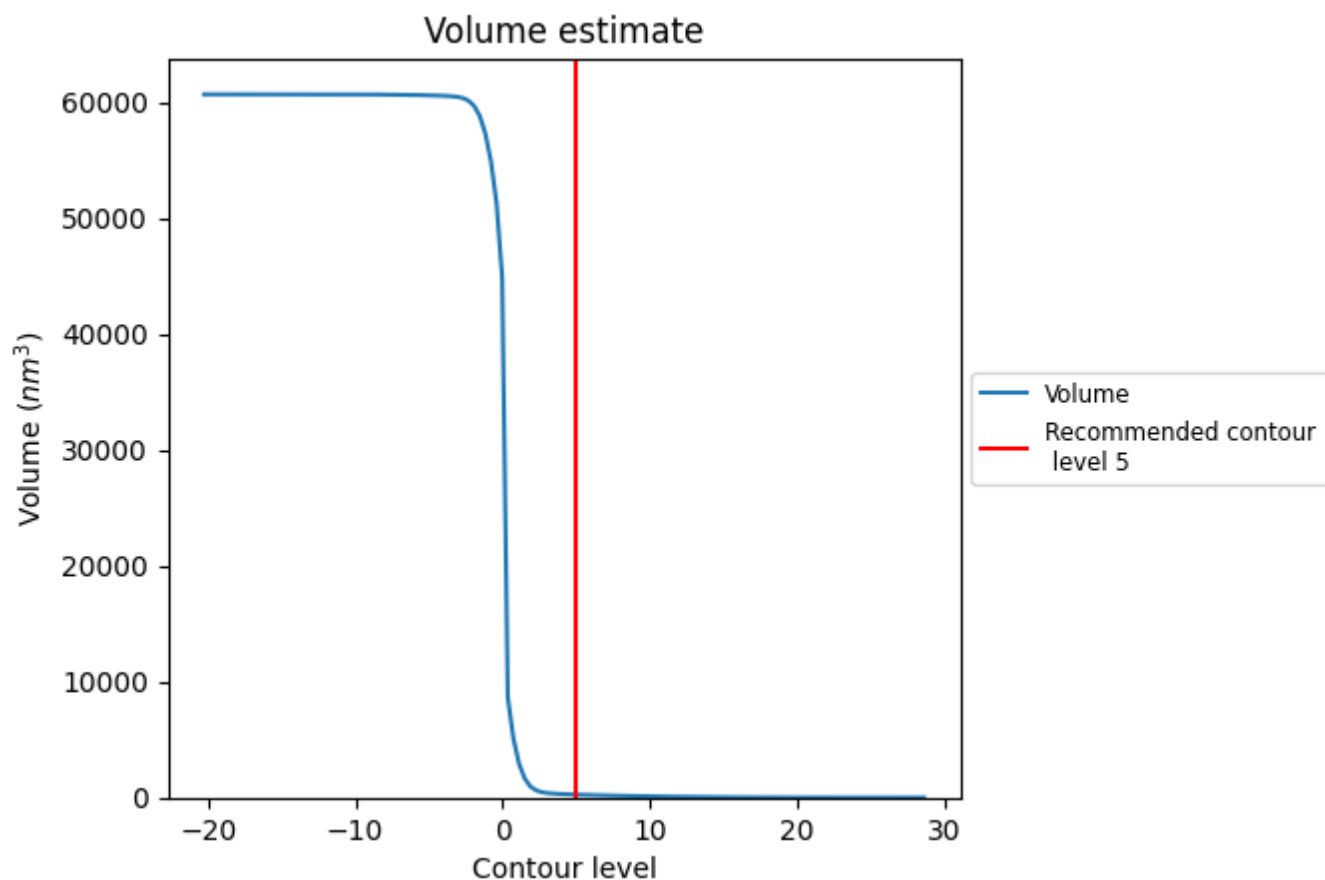
This section contains the results of statistical analysis of the map.

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.

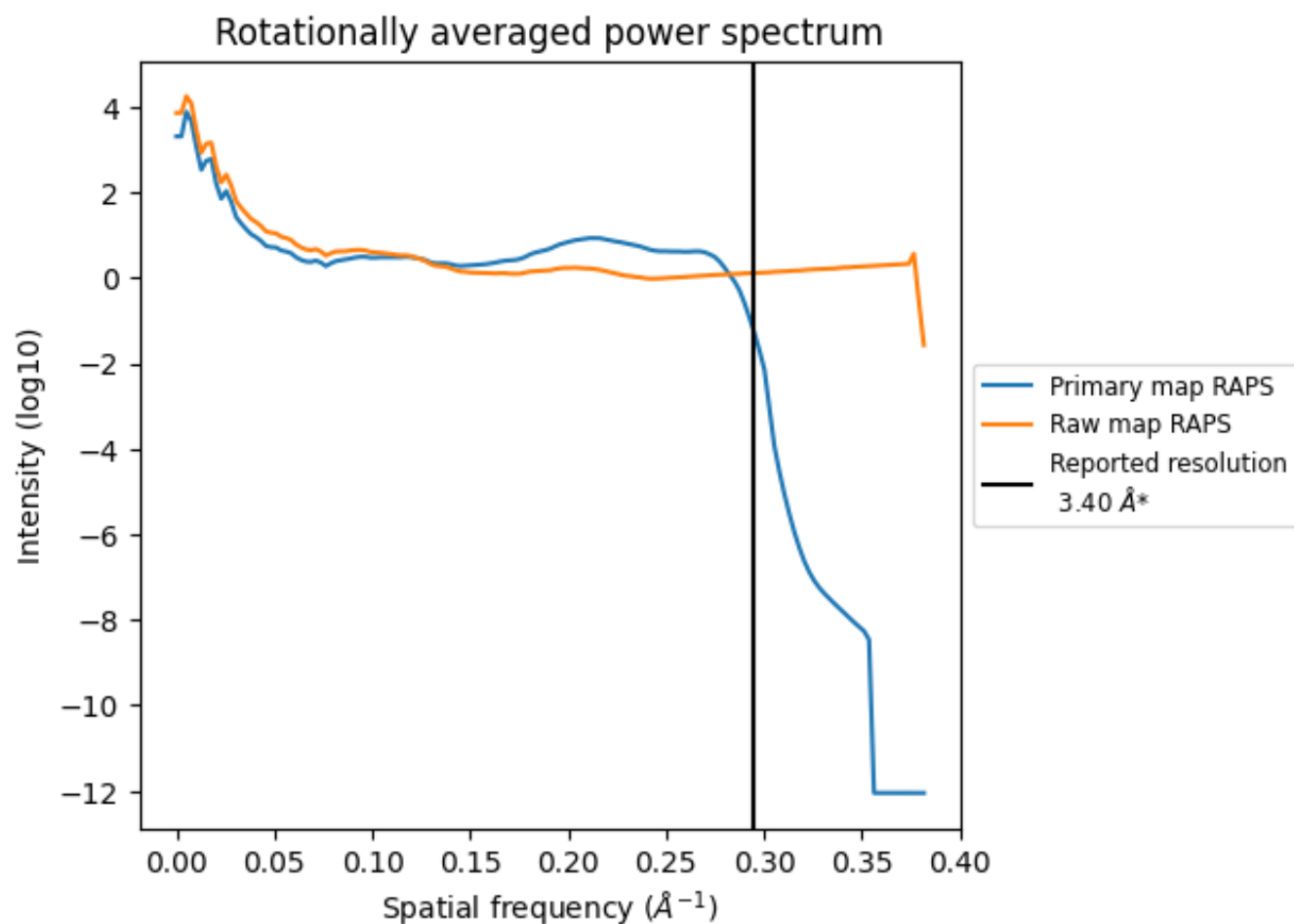
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm³; this corresponds to an approximate mass of 228 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 ⓘ

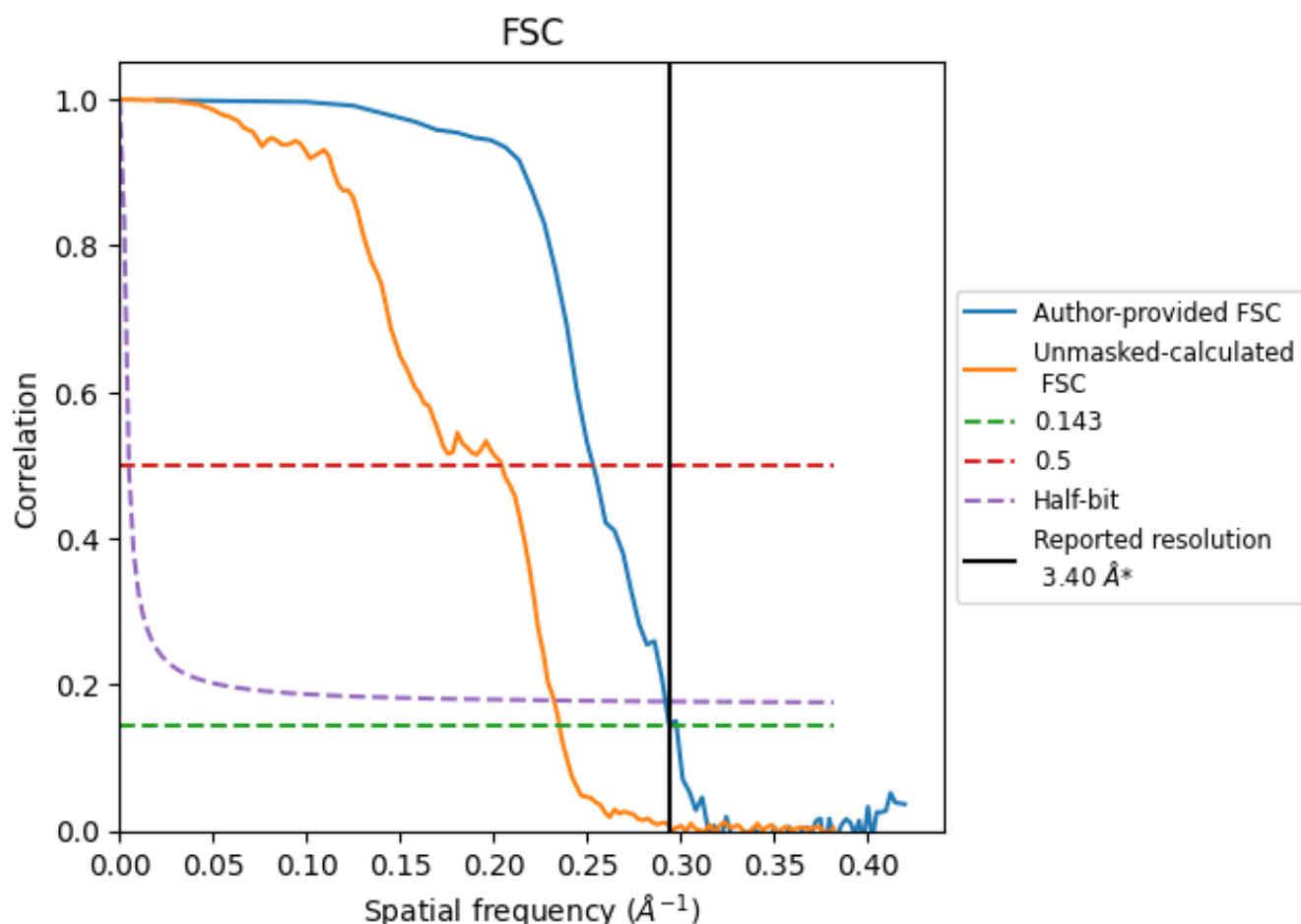


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

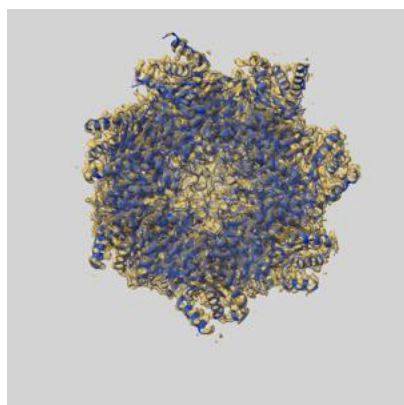
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.36	3.95	3.44
Unmasked-calculated*	4.25	4.90	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 3.4 by more than 10 %

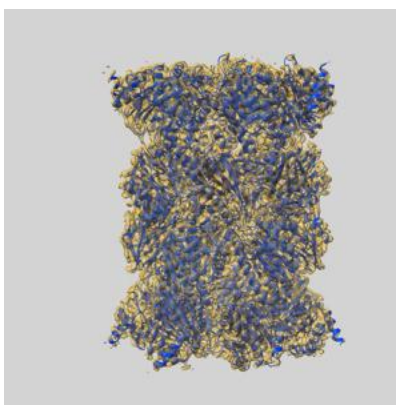
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23576 and PDB model 7LXV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

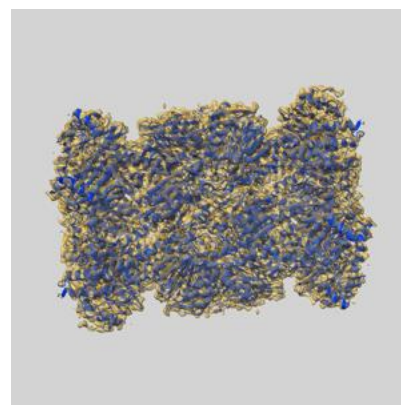
9.1 Map-model overlay [i](#)



X



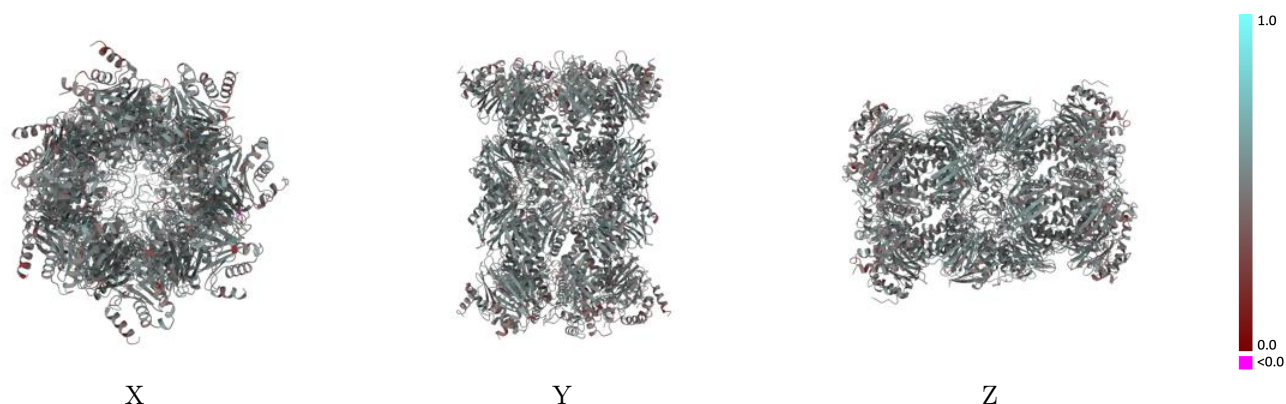
Y



Z

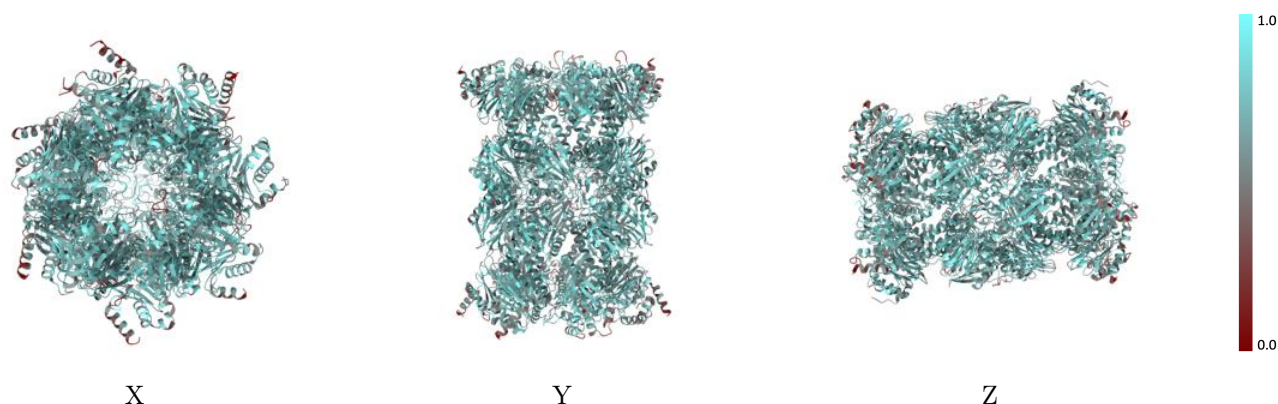
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



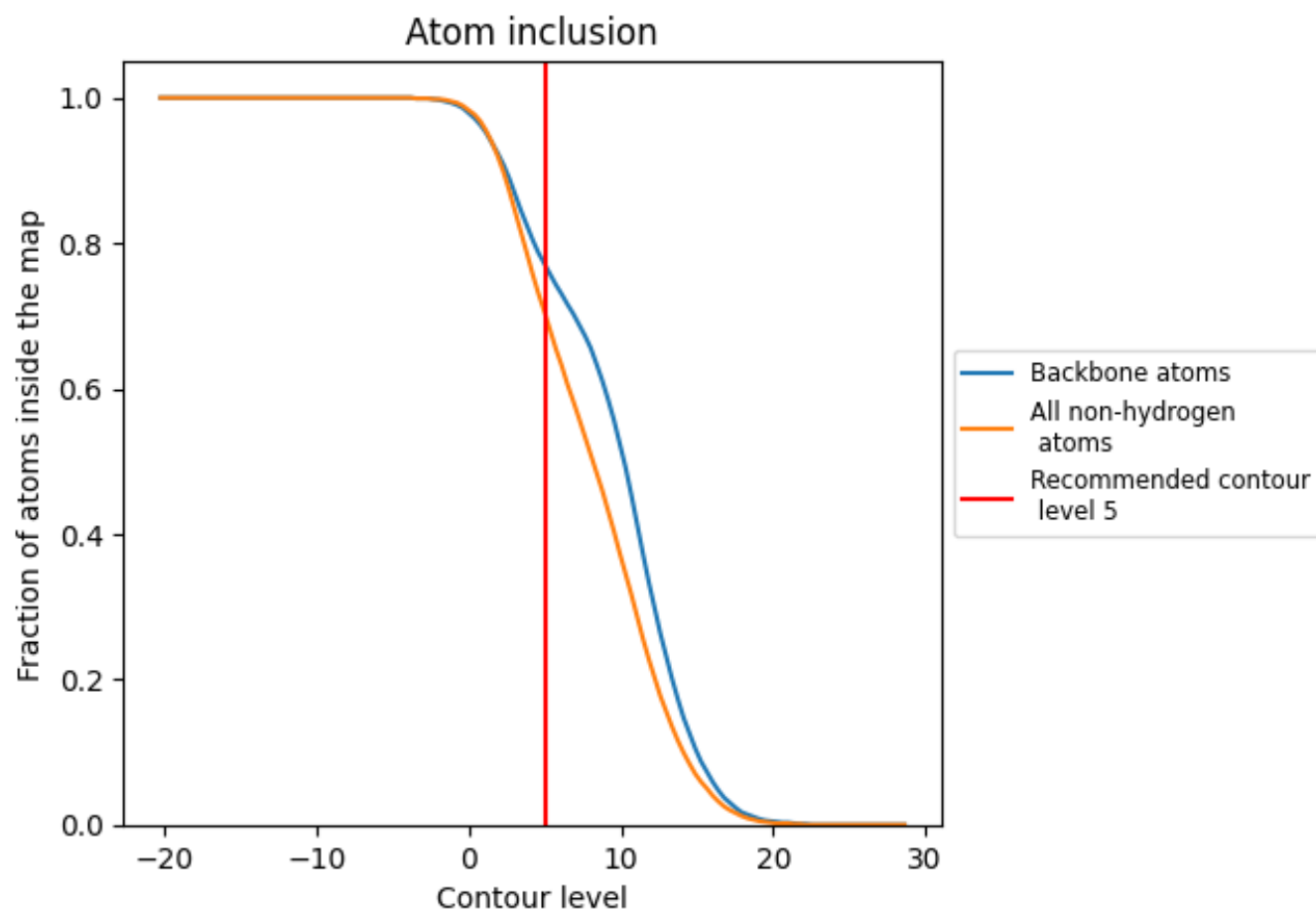
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7030	 0.4960
A	 0.6920	 0.4810
B	 0.6820	 0.4880
C	 0.6840	 0.4890
D	 0.6700	 0.4920
E	 0.6900	 0.4840
F	 0.6820	 0.4900
G	 0.6490	 0.4780
H	 0.6930	 0.5020
I	 0.7340	 0.5130
J	 0.7390	 0.5110
K	 0.7570	 0.5130
L	 0.7160	 0.4980
M	 0.7470	 0.5050
N	 0.7320	 0.5100
O	 0.6910	 0.4810
P	 0.6830	 0.4870
Q	 0.6890	 0.4870
R	 0.6690	 0.4910
S	 0.6910	 0.4850
T	 0.6810	 0.4890
U	 0.6490	 0.4770
V	 0.6940	 0.5010
W	 0.7340	 0.5140
X	 0.7390	 0.5130
Y	 0.7590	 0.5110
Z	 0.7150	 0.5000
a	 0.7470	 0.5050
b	 0.7310	 0.5100

