Full wwPDB EM Validation Report ⓘ

Apr 13, 2024 – 12:54 PM EDT

PDB ID	:	8U6Y
EMDB ID	:	EMD-41963
Title	:	Preholo-Proteasome from Beta 3 D205 deletion
Authors	:	Walsh Jr., R.M.; Rawson, S.; Velez, B.; Blickling, M.; Razi, A.; Hanna, J.
Deposited on	:	2023-09-14
Resolution	:	2.80 Å(reported)
Based on initial model	:	8T08

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:

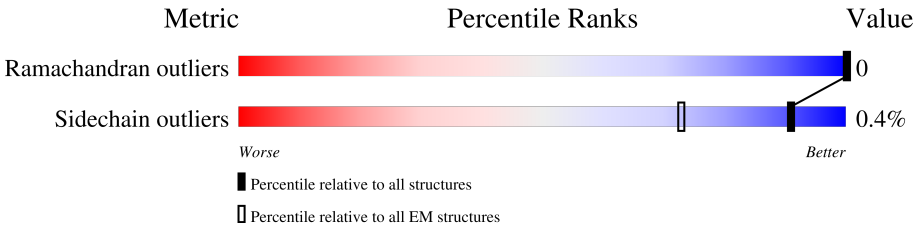
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	92% 8%
1	R	252	92% 8%
2	B	250	98%
2	S	250	98%
3	C	245	95% 5%
3	T	245	95% 5%
4	D	254	87% 13%
4	U	254	87% 13%
5	E	260	93% 7%

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Mol	Chain	Length	Quality of chain
5	V	260	93% 7%
6	F	234	99%
6	W	234	100%
7	G	288	78% 22%
7	X	288	78% 22%
8	H	148	5% 96%
8	Y	148	5% 96%
9	I	261	87% 12%
9	Z	261	87% 12%
10	J	204	86% 14%
10	a	204	86% 14%
11	K	198	82% 18%
11	b	198	82% 18%
12	L	287	6% 75% 24%
12	c	287	7% 75% 24%
13	M	241	89% 10%
13	d	241	89% 10%
14	N	215	93% 6%
14	e	215	93% 6%
15	O	276	86% 14%
15	f	276	86% 14%
16	P	267	87% 13%
16	g	267	87% 13%
17	Q	266	76% 24%
17	h	266	76% 24%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 113955 atoms, of which 56875 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	231	Total	C	H	N	O	S	0	0
			3636	1162	1813	304	349	8		
1	R	231	Total	C	H	N	O	S	0	0
			3636	1162	1813	304	349	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	247	Total	C	H	N	O	S	0	0
			3791	1204	1900	312	372	3		
2	S	247	Total	C	H	N	O	S	0	0
			3791	1204	1900	312	372	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	233	Total	C	H	N	O	S	0	0
			3661	1160	1834	303	361	3		
3	T	233	Total	C	H	N	O	S	0	0
			3661	1160	1834	303	361	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	220	Total	C	H	N	O	S	0	0
			3465	1086	1740	297	338	4		
4	U	220	Total	C	H	N	O	S	0	0
			3465	1086	1740	297	338	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	242	Total	C	H	N	O	S	0	0
			3749	1180	1868	317	376	8		
5	V	242	Total	C	H	N	O	S	0	0
			3749	1180	1868	317	376	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	234	Total	C	H	N	O	S	0	0
			3598	1134	1795	313	351	5		
6	W	234	Total	C	H	N	O	S	0	0
			3611	1134	1808	313	351	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	226	Total	C	H	N	O	S	0	0
			3496	1114	1750	304	324	4		
7	X	226	Total	C	H	N	O	S	0	0
			3496	1114	1750	304	324	4		

- Molecule 8 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	142	Total	C	H	N	O	S	0	0
			2248	698	1114	200	229	7		
8	Y	142	Total	C	H	N	O	S	0	0
			2248	698	1114	200	229	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	229	Total	C	H	N	O	S	0	0
			3464	1098	1726	301	333	6		
9	Z	229	Total	C	H	N	O	S	0	0
			3464	1098	1726	301	333	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	176	Total	C	H	N	O	S	0	0
			2737	885	1370	216	259	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	a	176	Total	C	H	N	O	S	0	0
			2737	885	1370	216	259	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	163	Total	C	H	N	O	S	0	0
			2649	835	1335	226	249	4		
11	b	163	Total	C	H	N	O	S	0	0
			2649	835	1335	226	249	4		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	217	Total	C	H	N	O	S	0	0
			3347	1080	1657	283	319	8		
12	c	217	Total	C	H	N	O	S	0	0
			3347	1080	1657	283	319	8		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	218	Total	C	H	N	O	S	0	0
			3404	1097	1676	297	330	4		
13	d	218	Total	C	H	N	O	S	0	0
			3404	1097	1676	297	330	4		

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	202	Total	C	H	N	O	S	0	0
			3066	978	1516	256	309	7		
14	e	202	Total	C	H	N	O	S	0	0
			3066	978	1516	256	309	7		

- Molecule 15 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	238	Total	C	H	N	O	S	0	0
			3739	1207	1882	288	349	13		
15	f	238	Total	C	H	N	O	S	0	0
			3739	1207	1882	288	349	13		

- Molecule 16 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	232	Total	C	H	N	O	S	0	0
			3748	1233	1858	299	351	7		
16	g	232	Total	C	H	N	O	S	0	0
			3748	1233	1858	299	351	7		

- Molecule 17 is a protein called Proteasome subunit beta type-7.

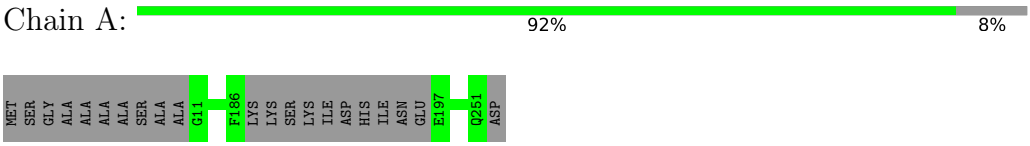
Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	202	Total	C	H	N	O	S	0	0
			3173	1000	1597	271	299	6		
17	h	202	Total	C	H	N	O	S	0	0
			3173	1000	1597	271	299	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

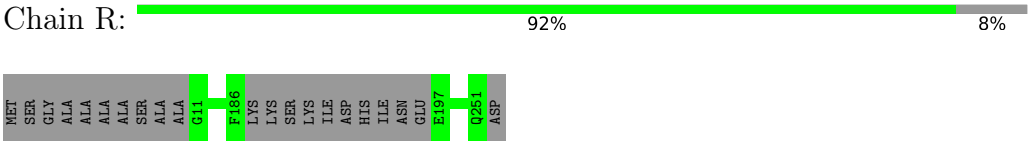
• Molecule 1: Proteasome subunit alpha type-1

Chain A:



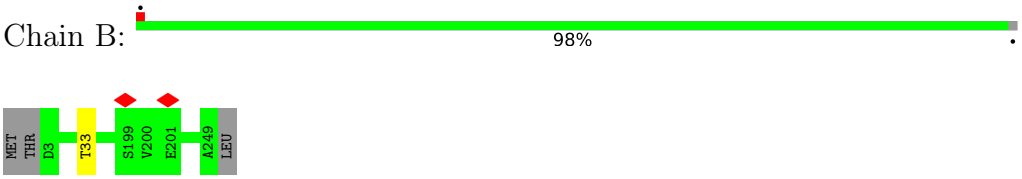
• Molecule 1: Proteasome subunit alpha type-1

Chain R:



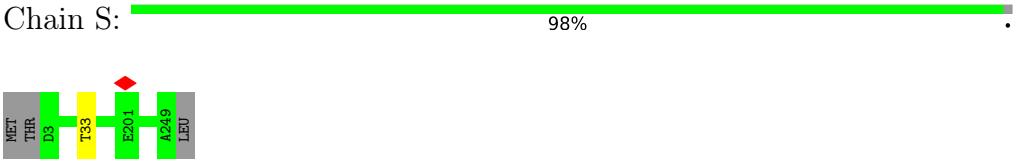
• Molecule 2: Proteasome subunit alpha type-2

Chain B:



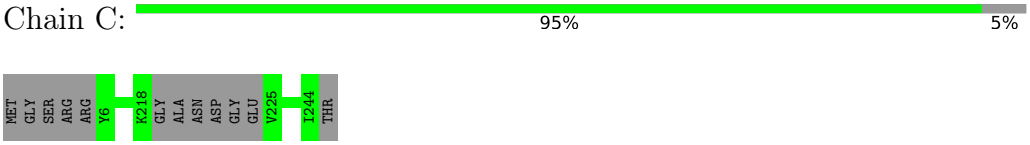
• Molecule 2: Proteasome subunit alpha type-2

Chain S:



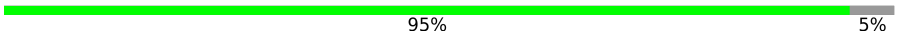
• Molecule 3: Proteasome subunit alpha type-3

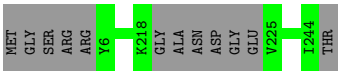
Chain C:



• Molecule 3: Proteasome subunit alpha type-3

Chain T:





• Molecule 4: Proteasome subunit alpha type-4

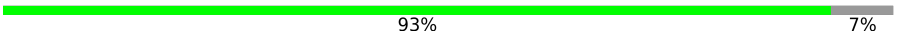
Chain D:

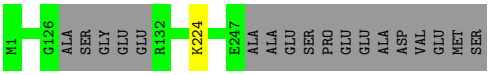
• Molecule 4: Proteasome subunit alpha type-4

Chain U:

• Molecule 5: Proteasome subunit alpha type-5

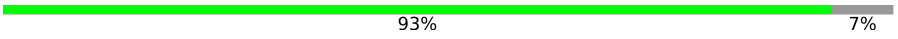
Chain E:

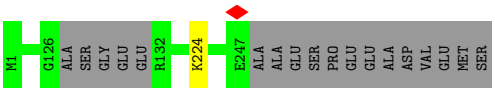




• Molecule 5: Proteasome subunit alpha type-5

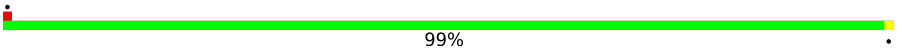
Chain V:

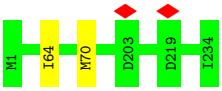




• Molecule 6: Proteasome subunit alpha type-6

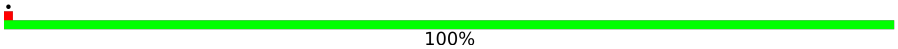
Chain F:

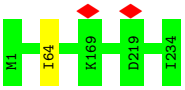




• Molecule 6: Proteasome subunit alpha type-6

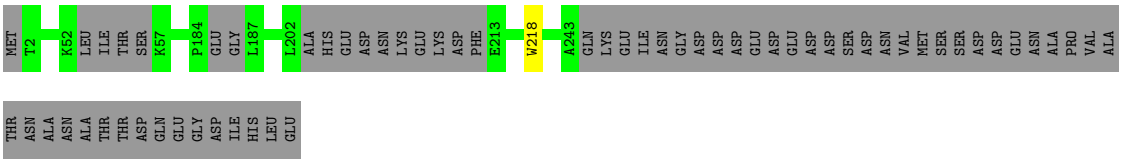
Chain W:





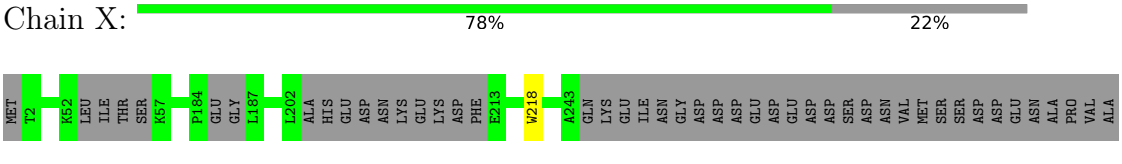
• Molecule 7: Proteasome subunit alpha type-7

Chain G:



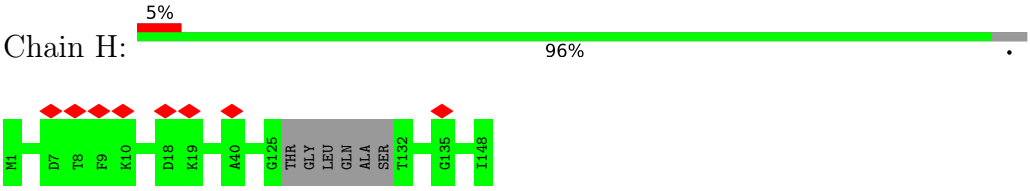
• Molecule 7: Proteasome subunit alpha type-7

Chain X:



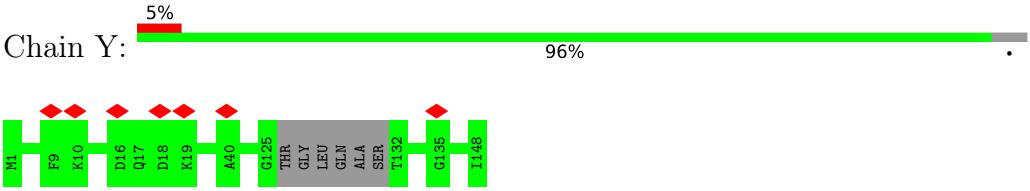
• Molecule 8: Proteasome maturation factor UMP1

Chain H:



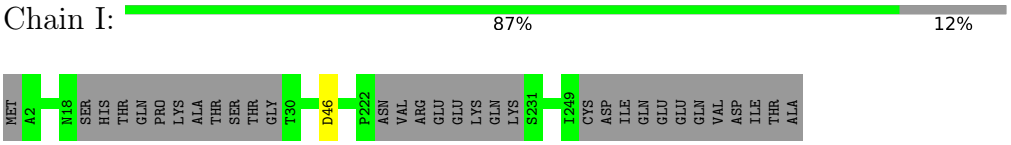
• Molecule 8: Proteasome maturation factor UMP1

Chain Y:



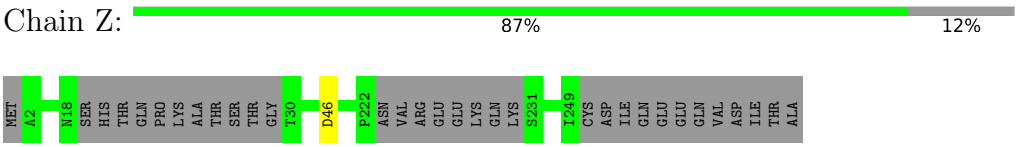
• Molecule 9: Proteasome subunit beta type-2

Chain I:



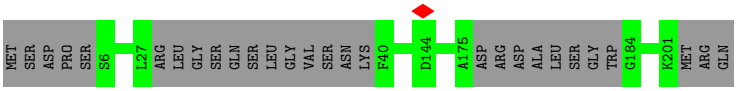
• Molecule 9: Proteasome subunit beta type-2

Chain Z:

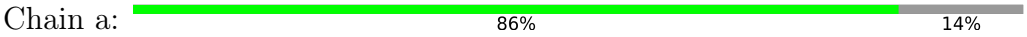


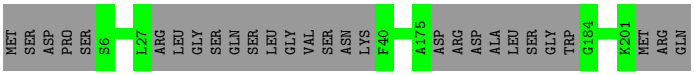
• Molecule 10: Proteasome subunit beta type-3

Chain J:

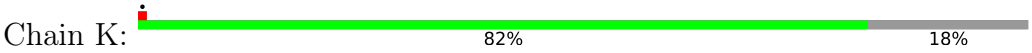


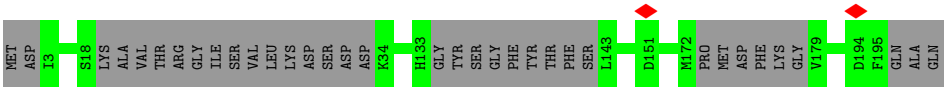
• Molecule 10: Proteasome subunit beta type-3



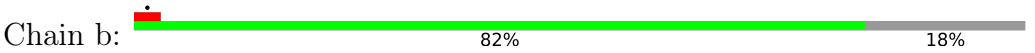


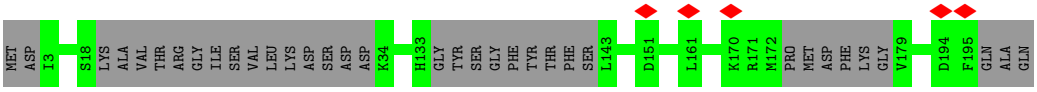
• Molecule 11: Proteasome subunit beta type-4



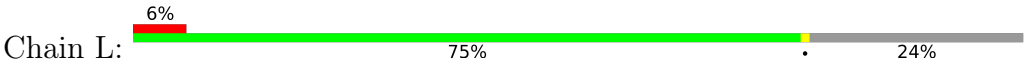


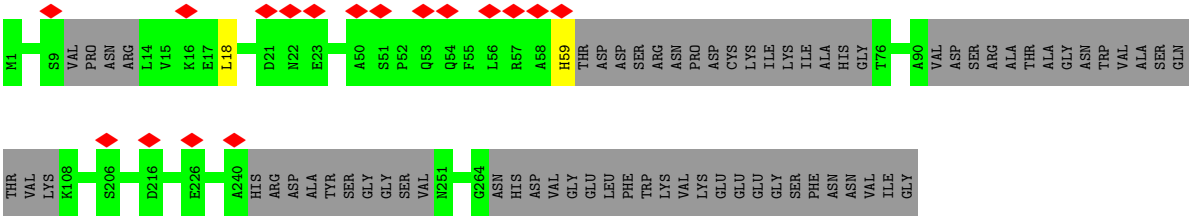
• Molecule 11: Proteasome subunit beta type-4



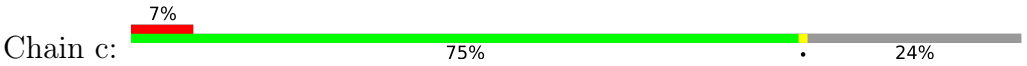


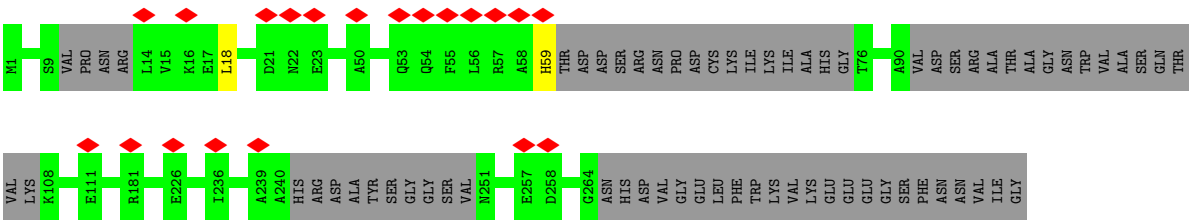
• Molecule 12: Proteasome subunit beta type-5





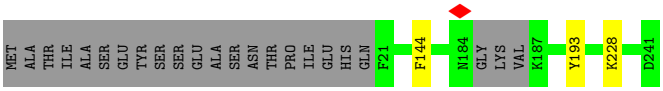
• Molecule 12: Proteasome subunit beta type-5





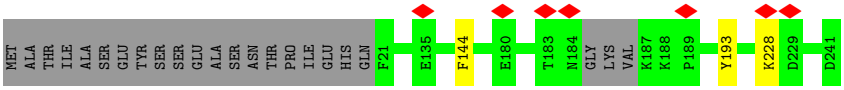
• Molecule 13: Proteasome subunit beta type-6

Chain M:



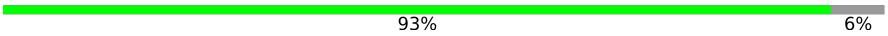
• Molecule 13: Proteasome subunit beta type-6

Chain d:



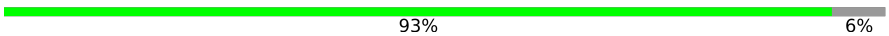
• Molecule 14: Proteasome subunit beta type-1

Chain N:



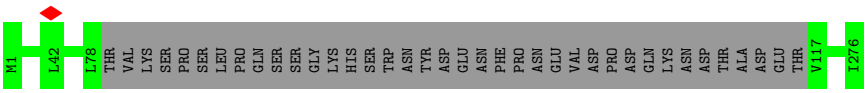
• Molecule 14: Proteasome subunit beta type-1

Chain e:



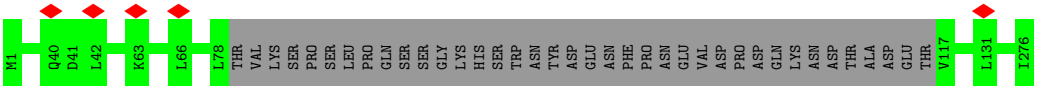
• Molecule 15: Proteasome chaperone 1

Chain O:



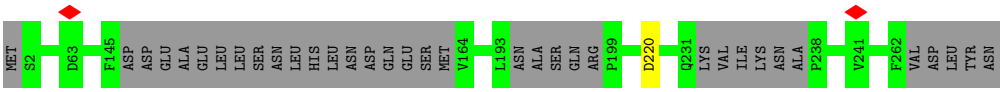
• Molecule 15: Proteasome chaperone 1

Chain f:



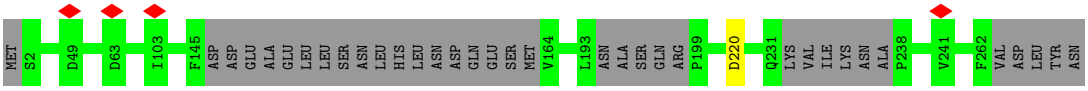
• Molecule 16: Proteasome assembly chaperone 2

Chain P:



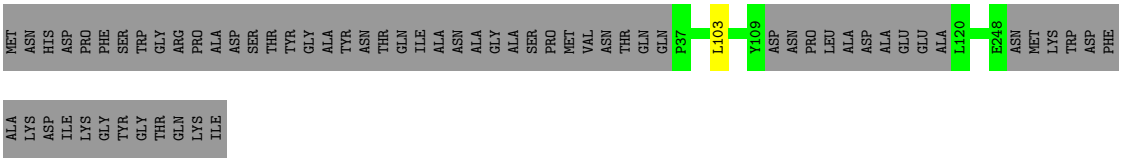
• Molecule 16: Proteasome assembly chaperone 2

Chain g:



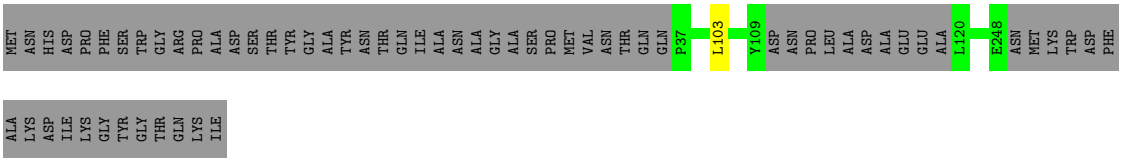
• Molecule 17: Proteasome subunit beta type-7

Chain Q:



• Molecule 17: Proteasome subunit beta type-7

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	19020	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 ($e^-/Å^2$)	57.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.327	Depositor
Minimum map value	-1.230	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.233	Depositor
Map size (Å)	375.24, 375.24, 375.24	wwPDB
Map dimensions	354, 354, 354	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/1859	0.48	0/2519
1	R	0.25	0/1859	0.48	0/2519
2	B	0.25	0/1928	0.47	0/2611
2	S	0.25	0/1928	0.47	0/2611
3	C	0.24	0/1856	0.49	0/2513
3	T	0.24	0/1856	0.49	0/2513
4	D	0.25	0/1750	0.50	0/2367
4	U	0.25	0/1750	0.51	0/2367
5	E	0.24	0/1907	0.48	0/2567
5	V	0.24	0/1907	0.48	0/2567
6	F	0.25	0/1831	0.50	0/2473
6	W	0.25	0/1831	0.52	0/2473
7	G	0.24	0/1781	0.47	0/2403
7	X	0.25	0/1781	0.47	0/2403
8	H	0.23	0/1152	0.48	0/1556
8	Y	0.23	0/1152	0.48	0/1556
9	I	0.24	0/1770	0.48	0/2400
9	Z	0.24	0/1770	0.48	0/2400
10	J	0.25	0/1392	0.46	0/1878
10	a	0.25	0/1392	0.46	0/1878
11	K	0.24	0/1333	0.49	0/1794
11	b	0.24	0/1333	0.49	0/1794
12	L	0.25	0/1724	0.46	0/2330
12	c	0.25	0/1724	0.46	0/2330
13	M	0.25	0/1765	0.48	0/2379
13	d	0.25	0/1765	0.48	0/2379
14	N	0.25	0/1579	0.48	0/2138
14	e	0.25	0/1579	0.48	0/2138
15	O	0.25	0/1901	0.44	0/2577
15	f	0.25	0/1901	0.44	0/2577
16	P	0.25	0/1938	0.46	0/2630
16	g	0.25	0/1938	0.46	0/2630
17	Q	0.25	0/1601	0.53	0/2170
17	h	0.25	0/1601	0.53	0/2170

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.25	0/58134	0.48	0/78610

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)

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	227/252 (90%)	226 (100%)	1 (0%)	0	100	100
1	R	227/252 (90%)	226 (100%)	1 (0%)	0	100	100
2	B	245/250 (98%)	244 (100%)	1 (0%)	0	100	100
2	S	245/250 (98%)	244 (100%)	1 (0%)	0	100	100
3	C	229/245 (94%)	224 (98%)	5 (2%)	0	100	100
3	T	229/245 (94%)	224 (98%)	5 (2%)	0	100	100
4	D	212/254 (84%)	209 (99%)	3 (1%)	0	100	100
4	U	212/254 (84%)	209 (99%)	3 (1%)	0	100	100
5	E	238/260 (92%)	235 (99%)	3 (1%)	0	100	100
5	V	238/260 (92%)	235 (99%)	3 (1%)	0	100	100
6	F	232/234 (99%)	226 (97%)	6 (3%)	0	100	100
6	W	232/234 (99%)	226 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	218/288 (76%)	216 (99%)	2 (1%)	0	100	100
7	X	218/288 (76%)	216 (99%)	2 (1%)	0	100	100
8	H	138/148 (93%)	132 (96%)	6 (4%)	0	100	100
8	Y	138/148 (93%)	132 (96%)	6 (4%)	0	100	100
9	I	223/261 (85%)	219 (98%)	4 (2%)	0	100	100
9	Z	223/261 (85%)	219 (98%)	4 (2%)	0	100	100
10	J	170/204 (83%)	165 (97%)	5 (3%)	0	100	100
10	a	170/204 (83%)	165 (97%)	5 (3%)	0	100	100
11	K	155/198 (78%)	153 (99%)	2 (1%)	0	100	100
11	b	155/198 (78%)	153 (99%)	2 (1%)	0	100	100
12	L	207/287 (72%)	204 (99%)	3 (1%)	0	100	100
12	c	207/287 (72%)	205 (99%)	2 (1%)	0	100	100
13	M	214/241 (89%)	211 (99%)	3 (1%)	0	100	100
13	d	214/241 (89%)	211 (99%)	3 (1%)	0	100	100
14	N	200/215 (93%)	198 (99%)	2 (1%)	0	100	100
14	e	200/215 (93%)	198 (99%)	2 (1%)	0	100	100
15	O	234/276 (85%)	230 (98%)	4 (2%)	0	100	100
15	f	234/276 (85%)	230 (98%)	4 (2%)	0	100	100
16	P	224/267 (84%)	218 (97%)	6 (3%)	0	100	100
16	g	224/267 (84%)	218 (97%)	6 (3%)	0	100	100
17	Q	198/266 (74%)	190 (96%)	8 (4%)	0	100	100
17	h	198/266 (74%)	190 (96%)	8 (4%)	0	100	100
All	All	7128/8292 (86%)	7001 (98%)	127 (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	196/210 (93%)	196 (100%)	0	100	100
1	R	196/210 (93%)	196 (100%)	0	100	100
2	B	206/209 (99%)	205 (100%)	1 (0%)	88	96
2	S	206/209 (99%)	205 (100%)	1 (0%)	88	96
3	C	196/204 (96%)	196 (100%)	0	100	100
3	T	196/204 (96%)	196 (100%)	0	100	100
4	D	195/226 (86%)	195 (100%)	0	100	100
4	U	195/226 (86%)	195 (100%)	0	100	100
5	E	202/215 (94%)	201 (100%)	1 (0%)	88	96
5	V	202/215 (94%)	201 (100%)	1 (0%)	88	96
6	F	193/193 (100%)	191 (99%)	2 (1%)	76	93
6	W	193/193 (100%)	192 (100%)	1 (0%)	88	96
7	G	185/239 (77%)	184 (100%)	1 (0%)	88	96
7	X	185/239 (77%)	184 (100%)	1 (0%)	88	96
8	H	132/136 (97%)	132 (100%)	0	100	100
8	Y	132/136 (97%)	132 (100%)	0	100	100
9	I	185/214 (86%)	184 (100%)	1 (0%)	88	96
9	Z	185/214 (86%)	184 (100%)	1 (0%)	88	96
10	J	148/172 (86%)	148 (100%)	0	100	100
10	a	148/172 (86%)	148 (100%)	0	100	100
11	K	146/175 (83%)	146 (100%)	0	100	100
11	b	146/175 (83%)	146 (100%)	0	100	100
12	L	177/235 (75%)	175 (99%)	2 (1%)	73	92
12	c	177/235 (75%)	175 (99%)	2 (1%)	73	92
13	M	182/201 (90%)	179 (98%)	3 (2%)	62	88
13	d	182/201 (90%)	179 (98%)	3 (2%)	62	88
14	N	166/178 (93%)	165 (99%)	1 (1%)	86	96
14	e	166/178 (93%)	165 (99%)	1 (1%)	86	96
15	O	215/251 (86%)	215 (100%)	0	100	100
15	f	215/251 (86%)	215 (100%)	0	100	100
16	P	212/244 (87%)	211 (100%)	1 (0%)	88	96
16	g	212/244 (87%)	211 (100%)	1 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Q	174/224 (78%)	173 (99%)	1 (1%)	86 96
17	h	174/224 (78%)	173 (99%)	1 (1%)	86 96
All	All	6220/7052 (88%)	6193 (100%)	27 (0%)	91 97

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	33	THR
5	E	224	LYS
6	F	64	ILE
6	F	70	MET
7	G	218	TRP
9	I	46	ASP
12	L	18	LEU
12	L	59	HIS
13	M	144	PHE
13	M	193	TYR
13	M	228	LYS
14	N	36	ASP
16	P	220	ASP
17	Q	103	LEU
2	S	33	THR
5	V	224	LYS
6	W	64	ILE
7	X	218	TRP
9	Z	46	ASP
12	c	18	LEU
12	c	59	HIS
13	d	144	PHE
13	d	193	TYR
13	d	228	LYS
14	e	36	ASP
16	g	220	ASP
17	h	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	31	HIS
6	F	93	ASN

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Mol	Chain	Res	Type
7	G	73	HIS
9	I	8	ASN
13	M	171	ASN
13	M	177	ASN
14	N	111	ASN
3	T	31	HIS
6	W	93	ASN
7	X	73	HIS
9	Z	8	ASN
14	e	111	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

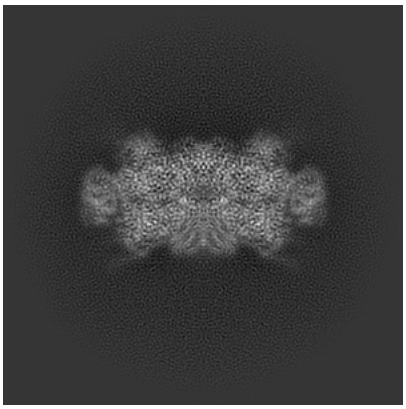
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41963. These allow visual inspection of the internal detail of the map and identification of artifacts.

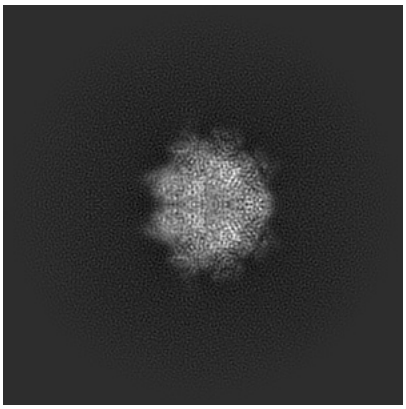
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

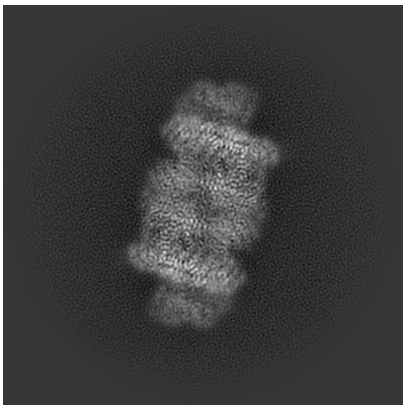
6.1.1 Primary map



X

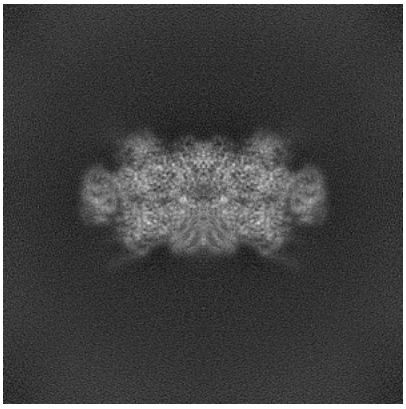


Y

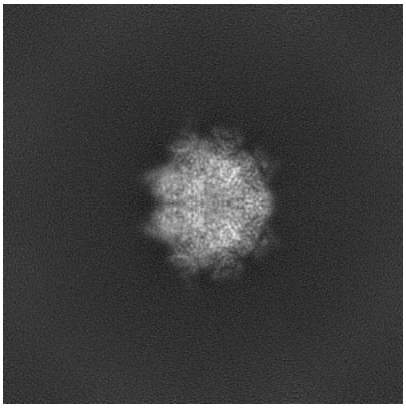


Z

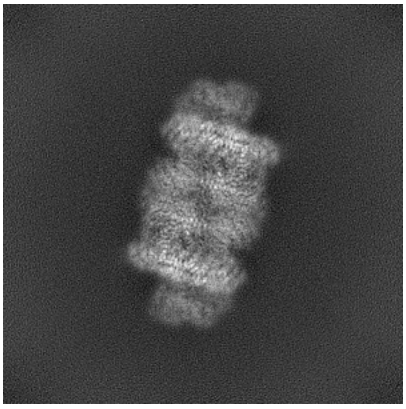
6.1.2 Raw map



X



Y

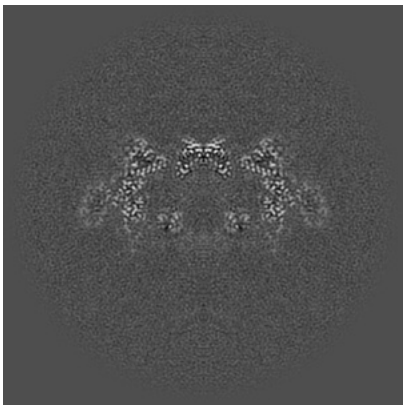


Z

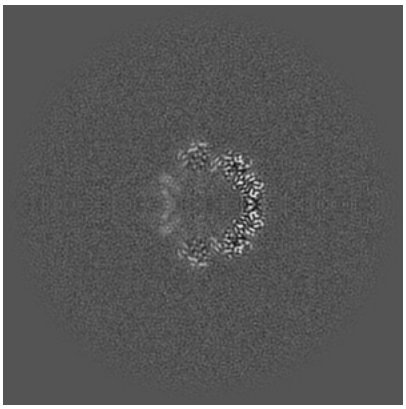
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

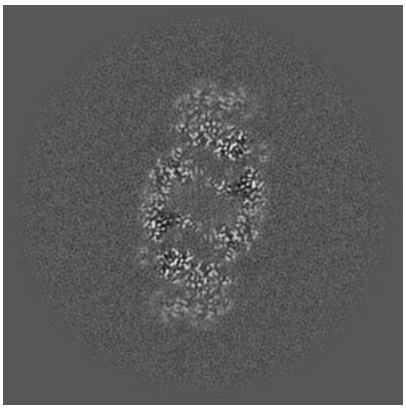
6.2.1 Primary map



X Index: 177

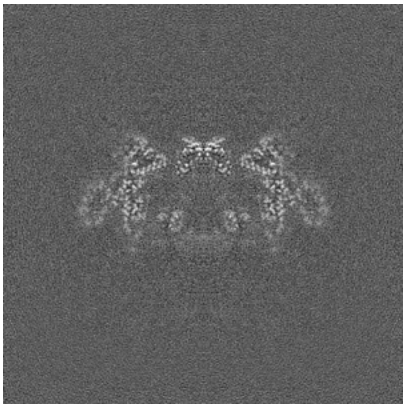


Y Index: 177

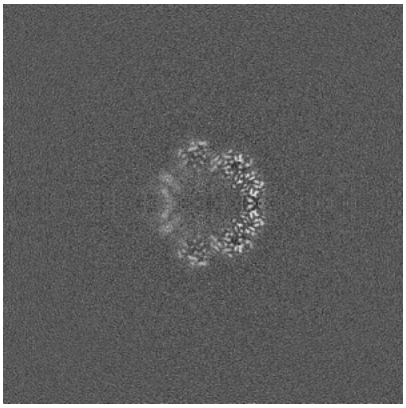


Z Index: 177

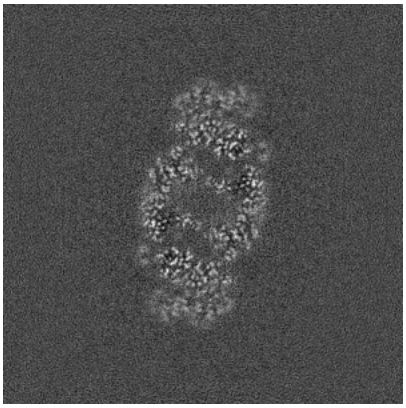
6.2.2 Raw map



X Index: 177



Y Index: 177

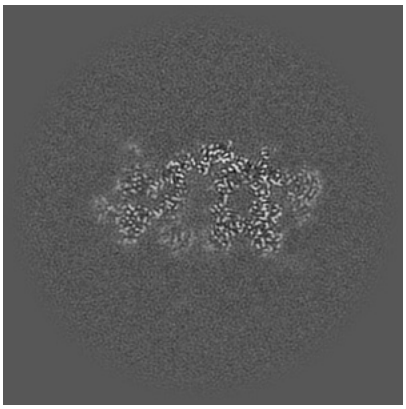


Z Index: 177

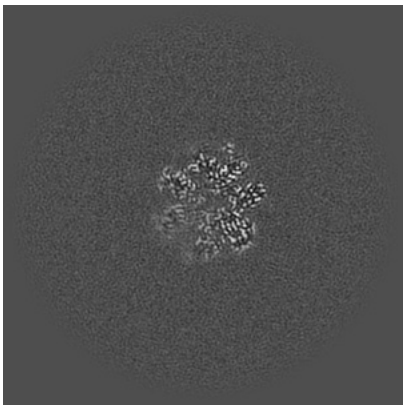
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

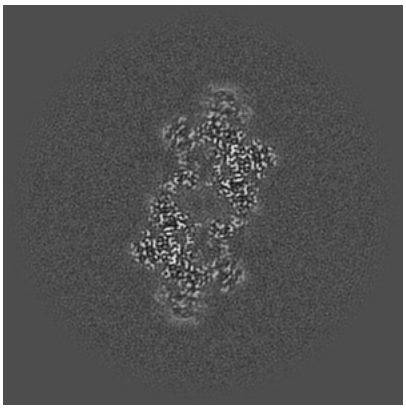
6.3.1 Primary map



X Index: 193

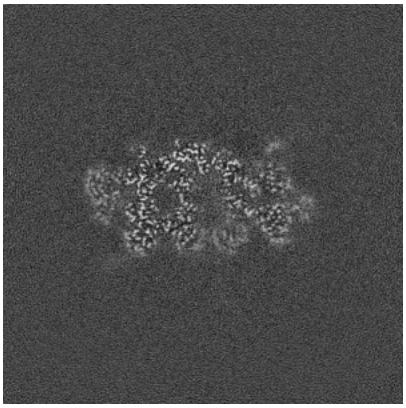


Y Index: 199

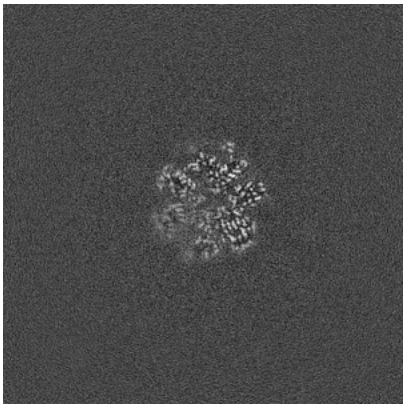


Z Index: 197

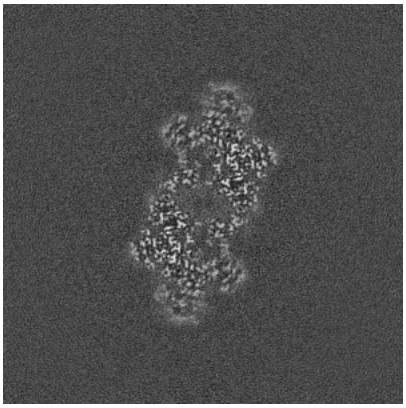
6.3.2 Raw map



X Index: 161



Y Index: 199

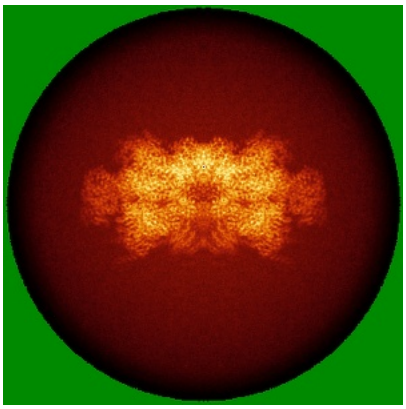


Z Index: 197

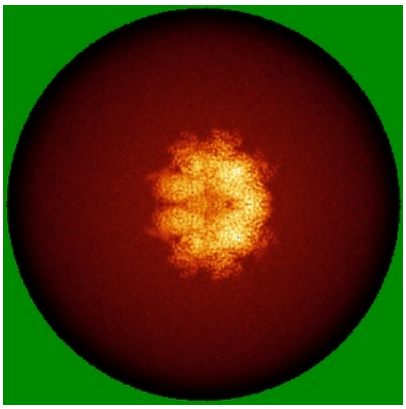
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

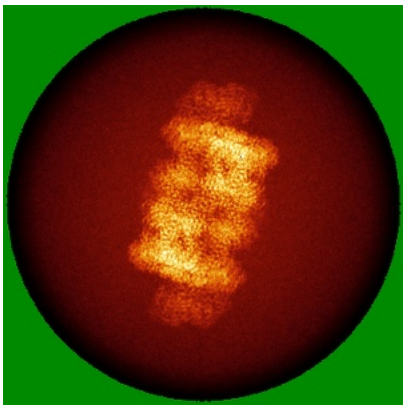
6.4.1 Primary map



X

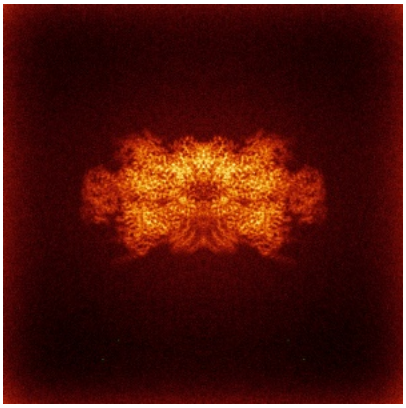


Y

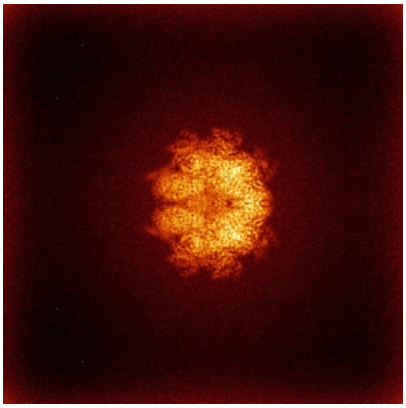


Z

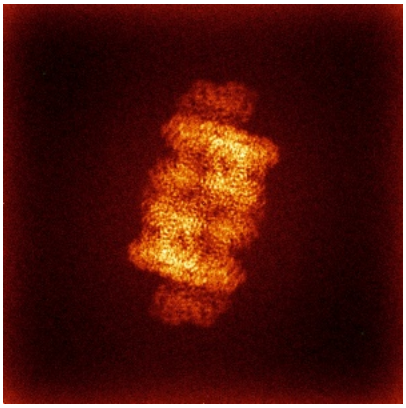
6.4.2 Raw map



X



Y

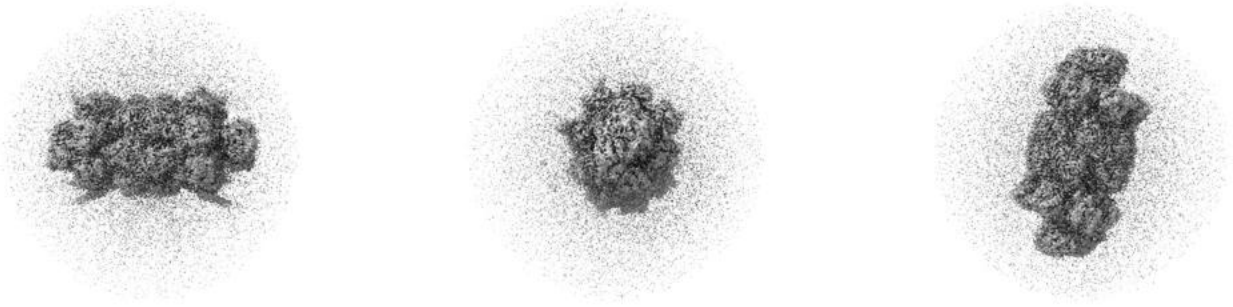


Z

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)

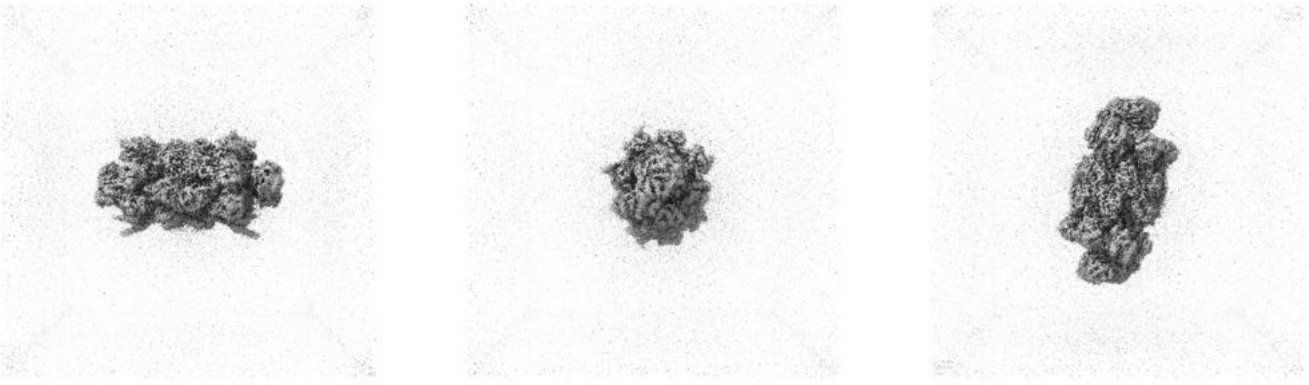
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.233. 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.

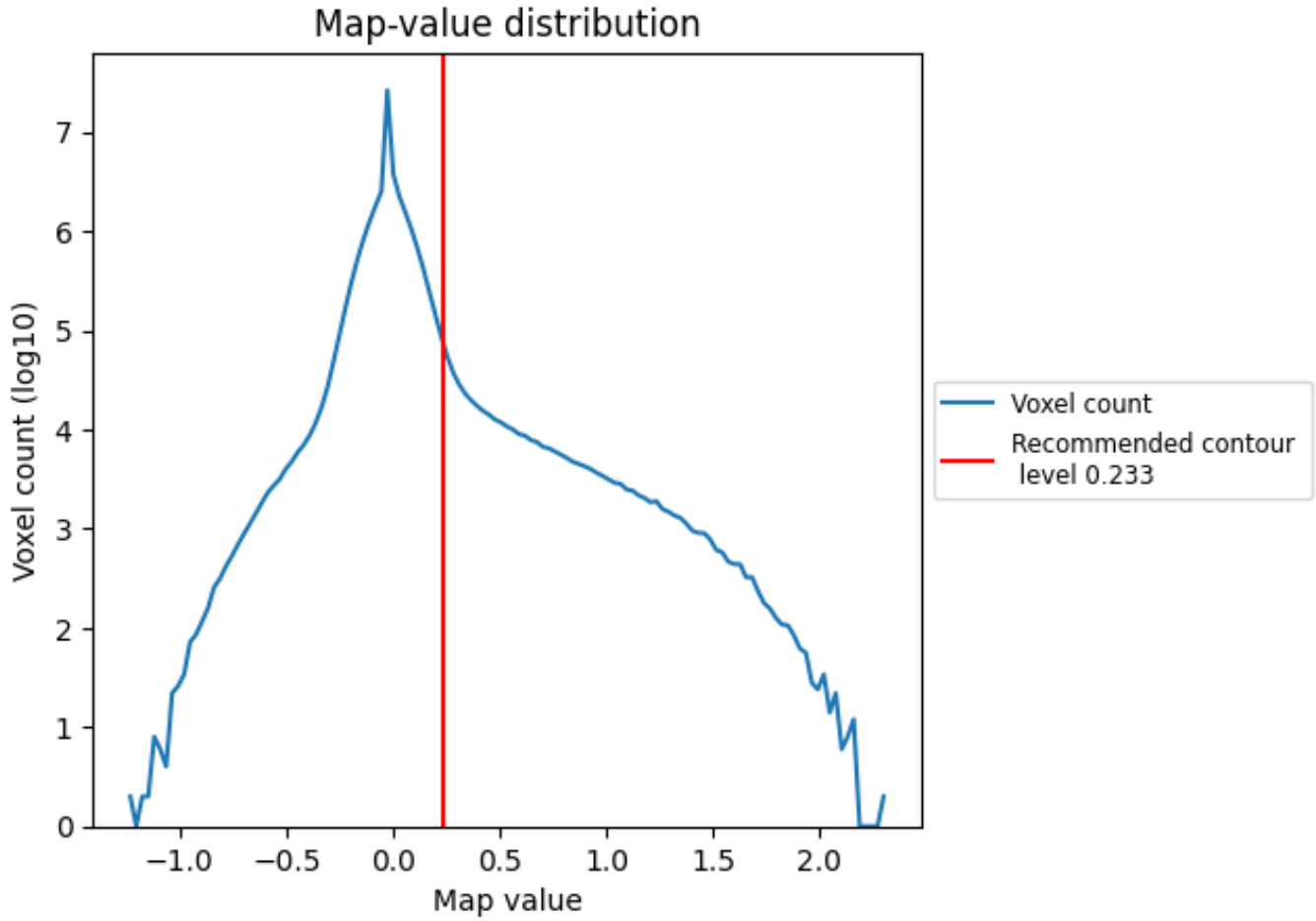
6.6 Mask visualisation (i)

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

7 Map analysis

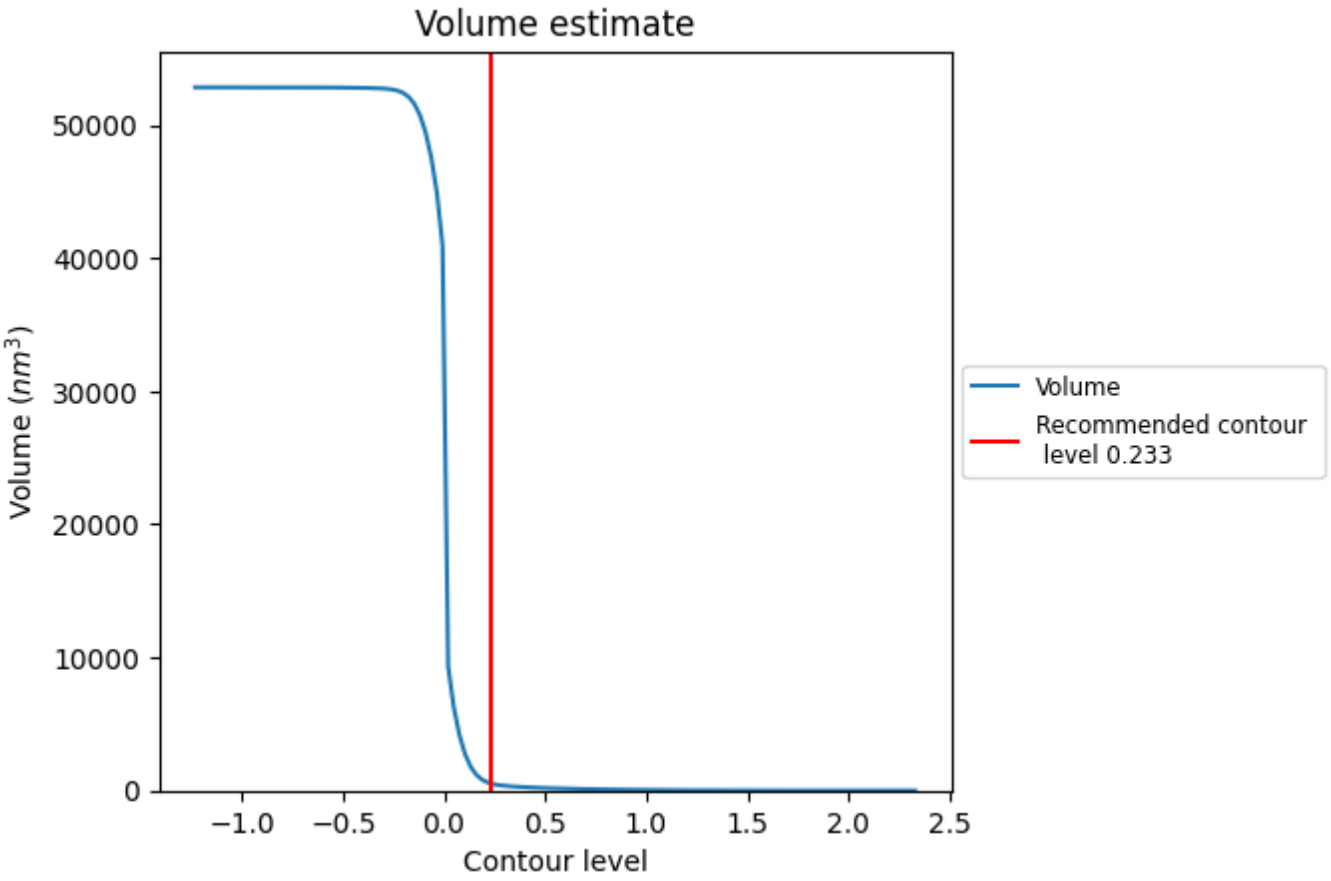
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

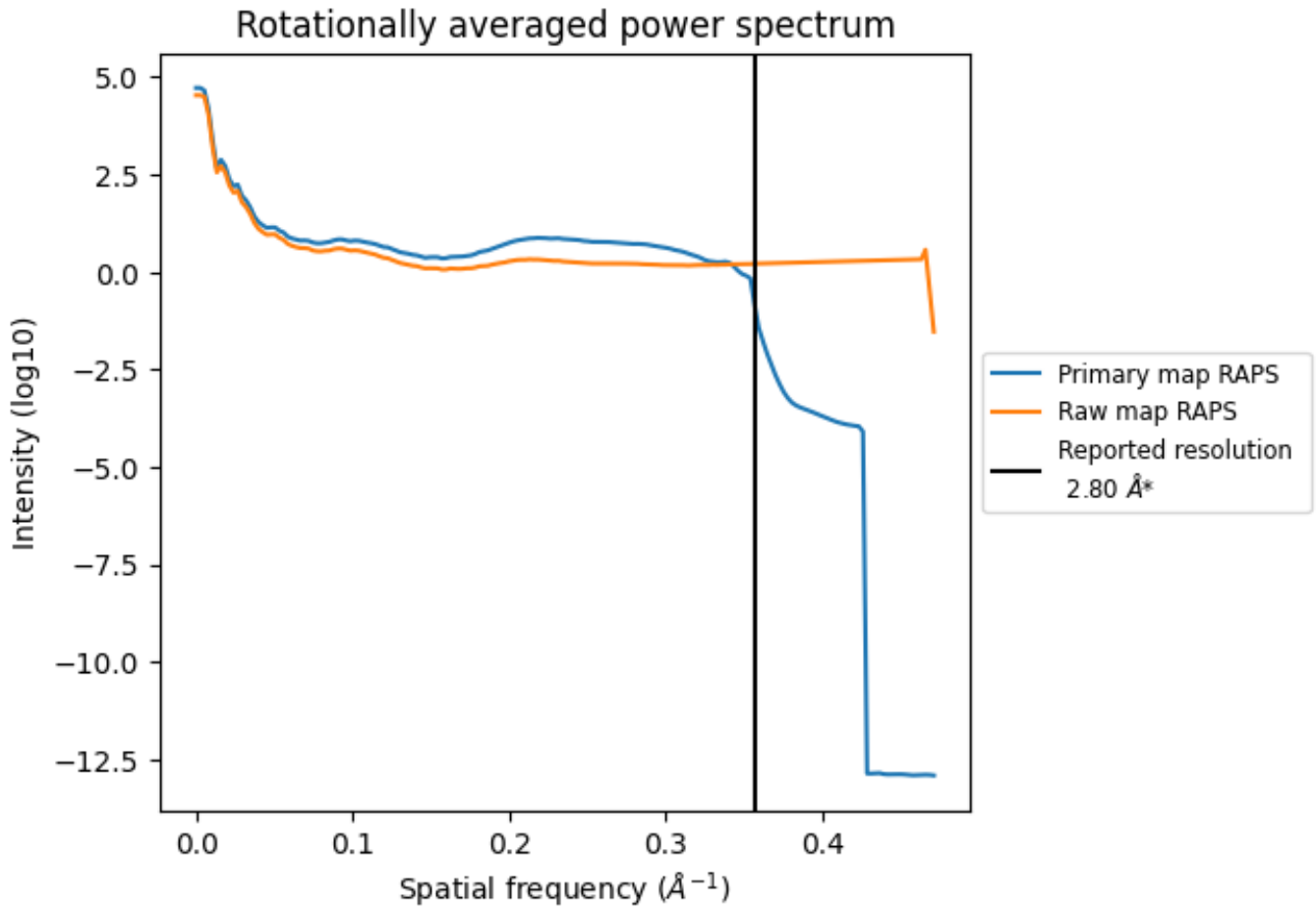
7.2 Volume estimate



The volume at the recommended contour level is 532 nm^3; this corresponds to an approximate mass of 481 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)

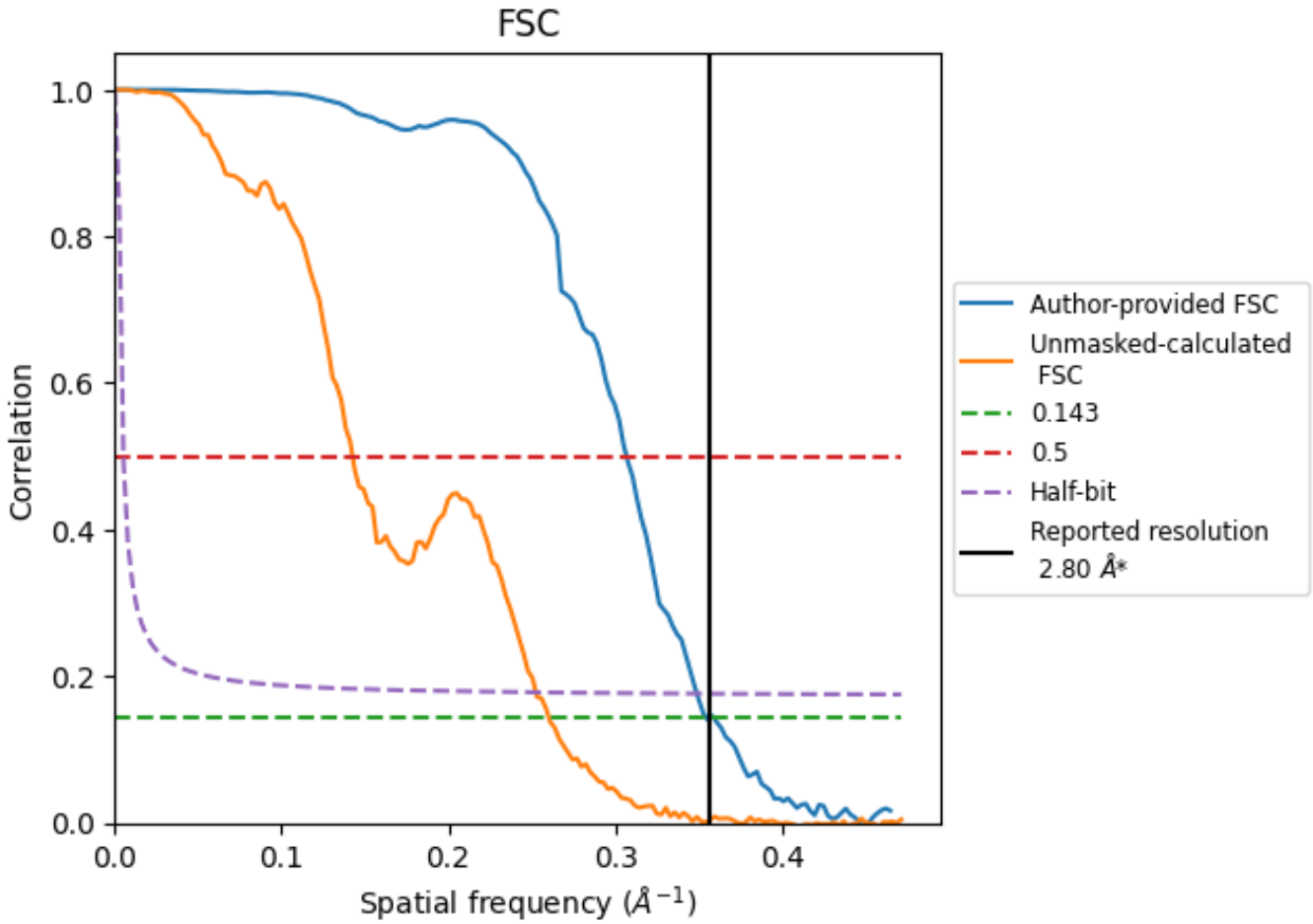


*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

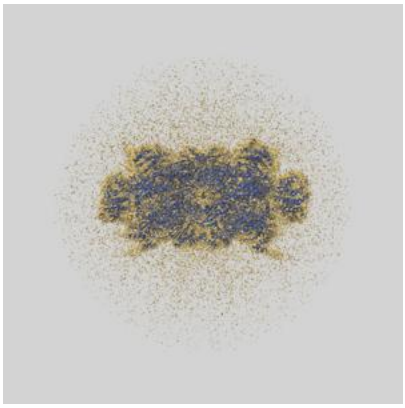
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.26	2.86
Unmasked-calculated*	3.84	7.01	3.96

*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 3.84 differs from the reported value 2.8 by more than 10 %

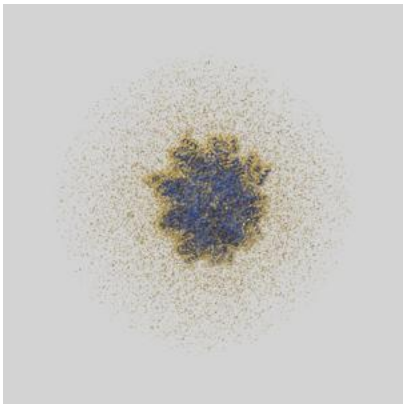
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41963 and PDB model 8U6Y. Per-residue inclusion information can be found in section 3 on page 8.

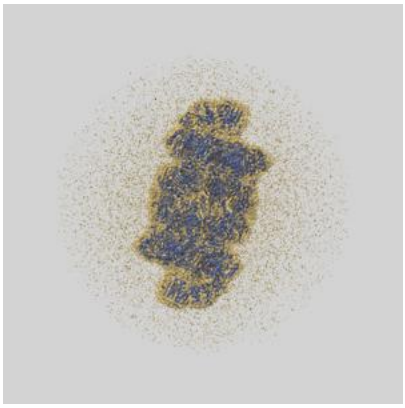
9.1 Map-model overlay



X



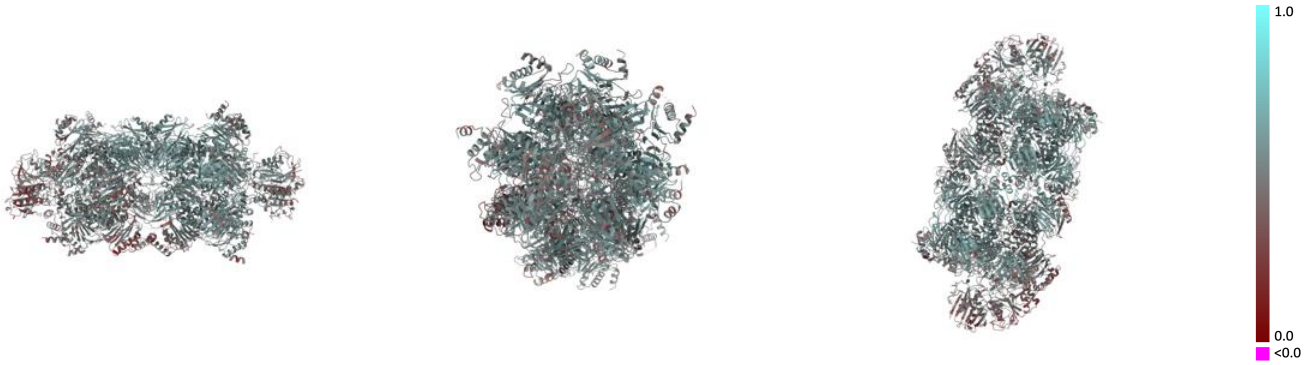
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.233 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.

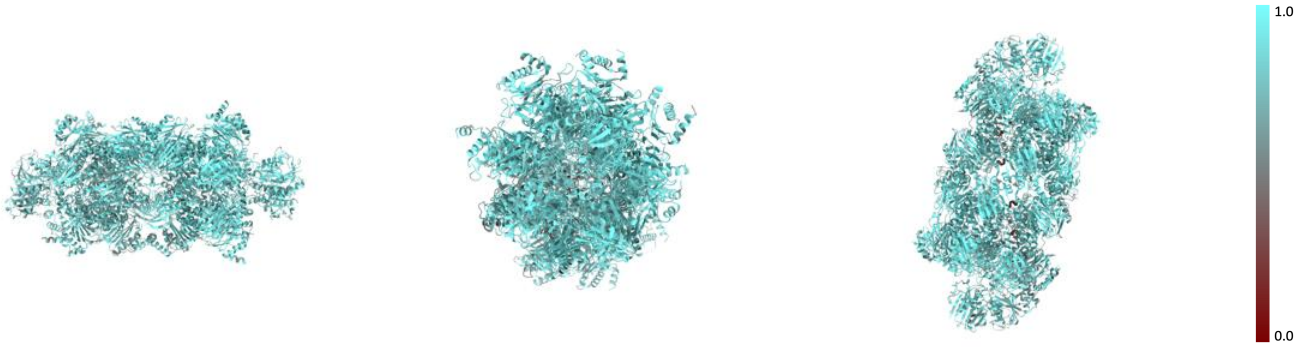
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

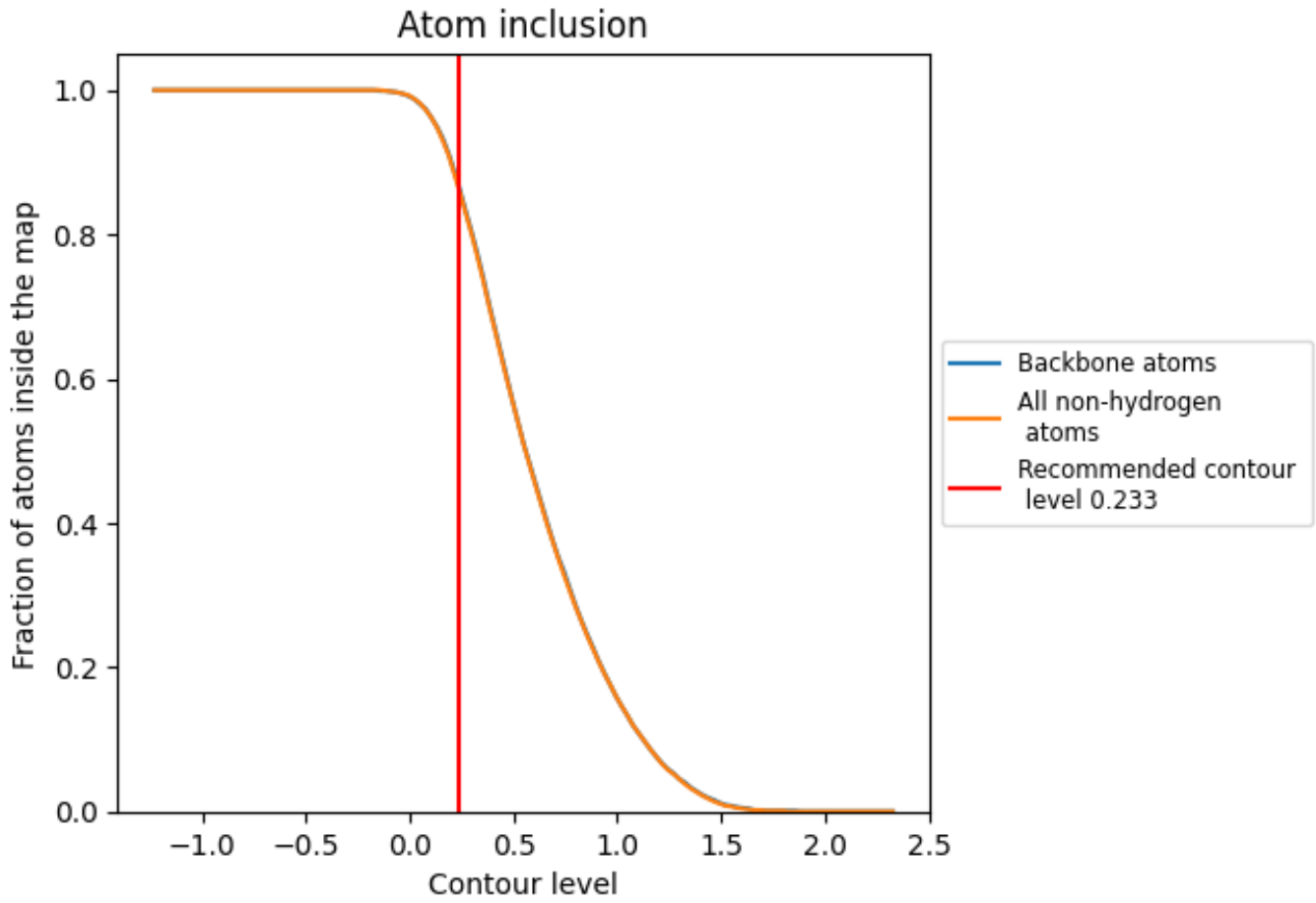
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.233).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.233) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.5130
A	0.9250	0.5560
B	0.9240	0.5660
C	0.9050	0.5490
D	0.9120	0.5420
E	0.8820	0.5390
F	0.8850	0.5220
G	0.9040	0.5430
H	0.8210	0.5300
I	0.9310	0.5710
J	0.9080	0.5460
K	0.8730	0.5030
L	0.7280	0.4380
M	0.8610	0.5250
N	0.9280	0.5730
O	0.7990	0.4600
P	0.8460	0.4640
Q	0.8870	0.5170
R	0.9120	0.5460
S	0.9040	0.5510
T	0.8920	0.5350
U	0.8860	0.5090
V	0.8310	0.4730
W	0.8440	0.4700
X	0.8840	0.5220
Y	0.8200	0.5330
Z	0.9190	0.5660
a	0.8980	0.5380
b	0.8630	0.4930
c	0.7090	0.4050
d	0.7990	0.4510
e	0.9420	0.5860
f	0.7580	0.3860
g	0.7900	0.3990
h	0.9280	0.5700