wwPDB EM Validation Summary Report (i)

Oct 6, 2024 – 03:40 PM EDT

PDB ID	:	8T08
EMDB ID	:	EMD-40938
Title	:	Preholo-Proteasome from Pre1-1 Pre4-1 Double Mutant
Authors	:	Walsh Jr., R.M.; Rawson, S.; Schnell, H.; Velez, B.; Hanna, J.
Deposited on	:	2023-05-31
Resolution	:	3.00 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

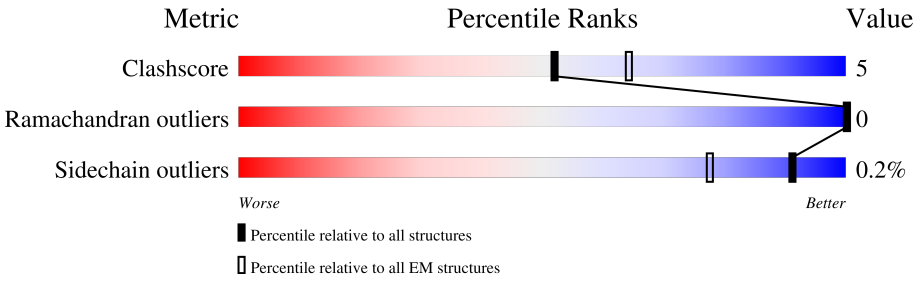
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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 <=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	81% 11% 8%
1	R	252	81% 10% 8%
2	B	250	89% 10% •
2	S	250	89% 10% •
3	C	258	74% 17% 10%
3	T	258	74% 16% 10%
4	D	254	79% 9% 12%
4	U	254	79% 9% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	260	
5	V	260	
6	F	234	
6	W	234	
7	G	288	
7	X	288	
8	H	148	
8	Y	148	
9	I	261	
9	Z	261	
10	J	205	
10	a	205	
11	K	198	
11	b	198	
12	L	287	
12	c	287	
13	M	241	
13	d	241	
14	N	215	
14	e	215	
15	O	276	
15	f	276	
16	P	267	
16	g	267	
17	Q	251	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	h	251	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 55104 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	231	Total	C	N	O	S	0	0
			1823	1162	304	349	8		
1	R	231	Total	C	N	O	S	0	0
			1823	1162	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	N	O	S	0	0
			1891	1204	312	372	3		
2	S	247	Total	C	N	O	S	0	0
			1891	1204	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	N	O	S	0	0
			1827	1160	303	361	3		
3	T	233	Total	C	N	O	S	0	0
			1827	1160	303	361	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	223	Total	C	N	O	S	0	0
			1752	1101	303	344	4		
4	U	223	Total	C	N	O	S	0	0
			1752	1101	303	344	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	242	Total	C	N	O	S	0	0
			1881	1180	317	376	8		
5	V	242	Total	C	N	O	S	0	0
			1881	1180	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	N	O	S	0	0
			1803	1134	313	351	5		
6	W	234	Total	C	N	O	S	0	0
			1803	1134	313	351	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	234	Total	C	N	O	S	0	0
			1809	1155	314	336	4		
7	X	234	Total	C	N	O	S	0	0
			1809	1155	314	336	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	122	Total	C	N	O	S	0	0
			977	603	174	194	6		
8	Y	122	Total	C	N	O	S	0	0
			977	603	174	194	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	229	Total	C	N	O	S	0	0
			1738	1098	301	333	6		
9	Z	229	Total	C	N	O	S	0	0
			1738	1098	301	333	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1359	879	215	258	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	175	Total	C	N	O	S	0	0
			1359	879	215	258	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	181	Total	C	N	O	S	0	0
			1458	931	245	278	4		
11	b	181	Total	C	N	O	S	0	0
			1458	931	245	278	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	conflict	UNP P22141
b	142	PHE	SER	conflict	UNP P22141

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	101	Total	C	N	O	S	0	0
			821	528	139	148	6		
12	c	101	Total	C	N	O	S	0	0
			821	528	139	148	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	202	Total	C	N	O	S	0	0
			1590	1006	274	306	4		
13	d	202	Total	C	N	O	S	0	0
			1590	1006	274	306	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1550	978	256	309	7		
14	e	202	Total	C	N	O	S	0	0
			1550	978	256	309	7		

- Molecule 15 is a protein called Proteasome chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	237	Total	C	N	O	S	0	0
			1845	1199	286	347	13		
15	f	237	Total	C	N	O	S	0	0
			1845	1199	286	347	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	227	Total	C	N	O	S	0	0
			1852	1214	294	337	7		
16	g	227	Total	C	N	O	S	0	0
			1852	1214	294	337	7		

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

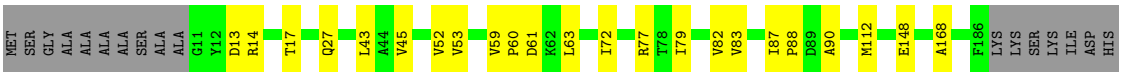
Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	202	Total	C	N	O	S	0	0
			1576	1000	271	299	6		
17	h	202	Total	C	N	O	S	0	0
			1576	1000	271	299	6		

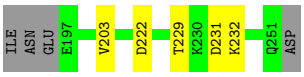
3 Residue-property plots (i)

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

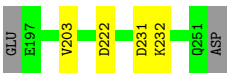
Chain A:





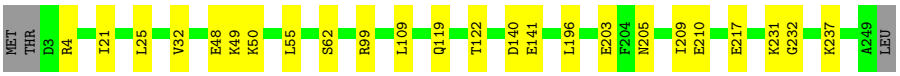
• Molecule 1: Proteasome subunit alpha type-1

Chain R:



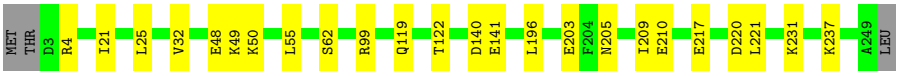
• Molecule 2: Proteasome subunit alpha type-2

Chain B:



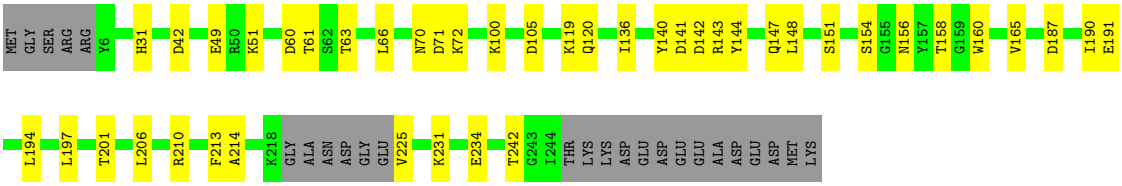
• Molecule 2: Proteasome subunit alpha type-2

Chain S:



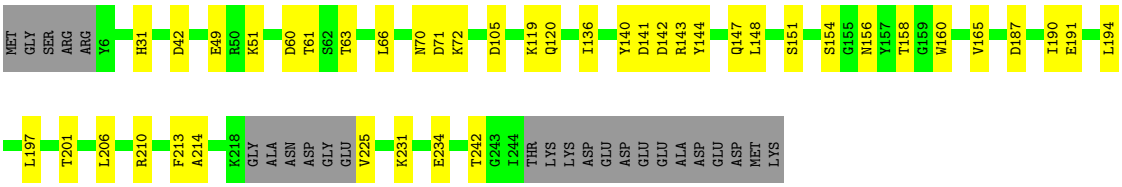
• Molecule 3: Proteasome subunit alpha type-3

Chain C:



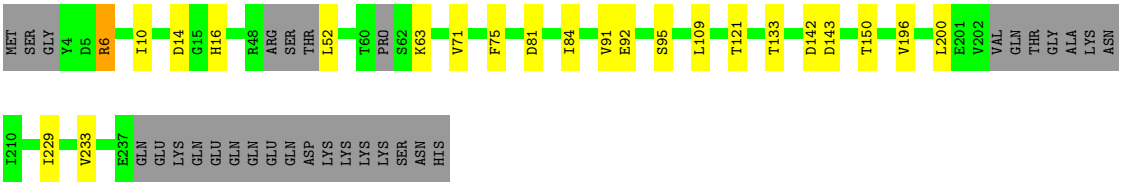
• Molecule 3: Proteasome subunit alpha type-3

Chain T:



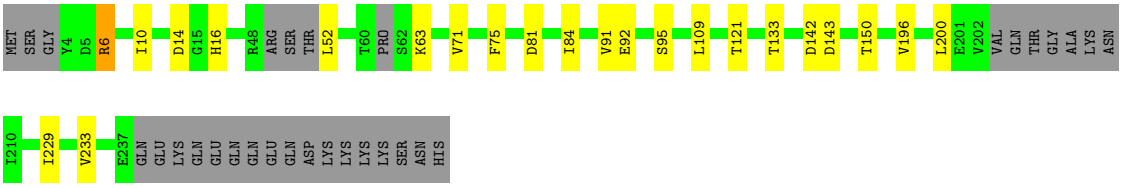
• Molecule 4: Proteasome subunit alpha type-4

Chain D:



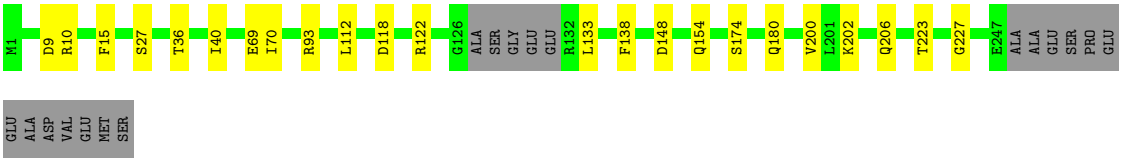
• Molecule 4: Proteasome subunit alpha type-4

Chain U:



• Molecule 5: Proteasome subunit alpha type-5

Chain E:

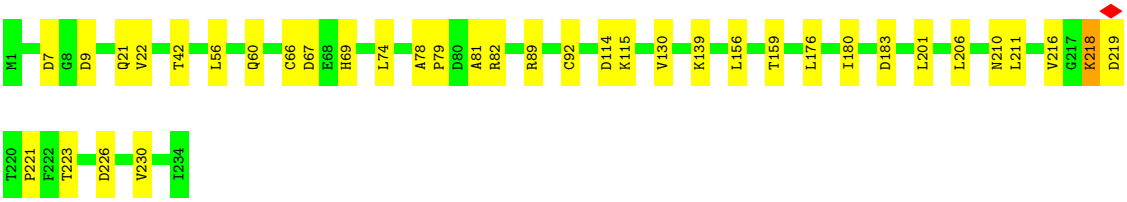


• Molecule 5: Proteasome subunit alpha type-5

Chain V:

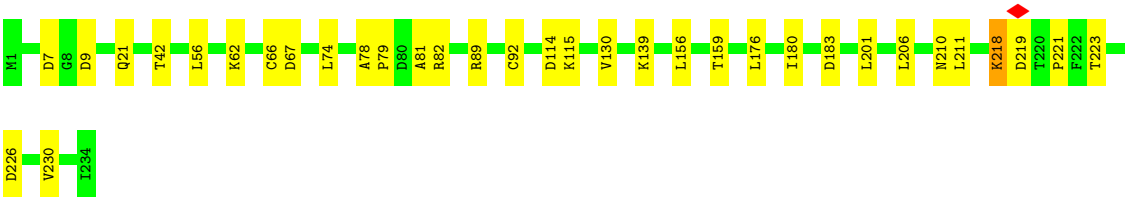
• Molecule 6: Proteasome subunit alpha type-6

Chain F:



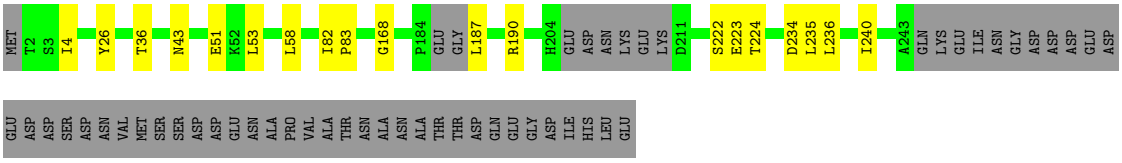
• Molecule 6: Proteasome subunit alpha type-6

Chain W:



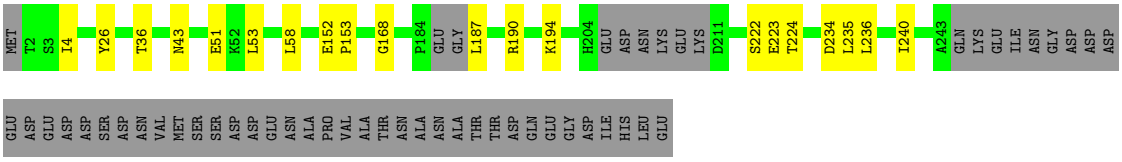
• Molecule 7: Proteasome subunit alpha type-7

Chain G:



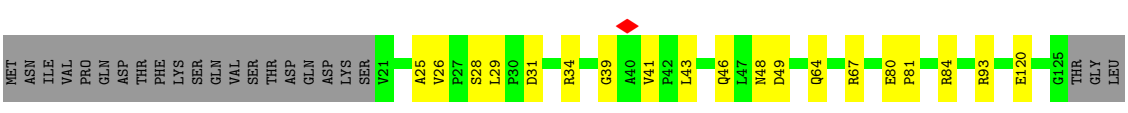
• Molecule 7: Proteasome subunit alpha type-7

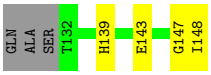
Chain X:



• Molecule 8: Proteasome maturation factor UMP1

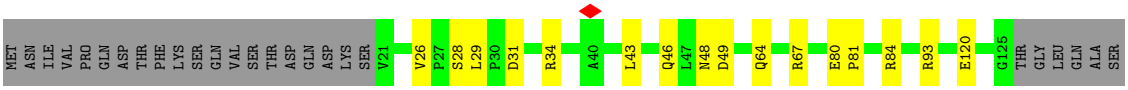
Chain H:





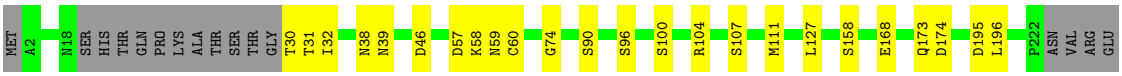
• Molecule 8: Proteasome maturation factor UMP1

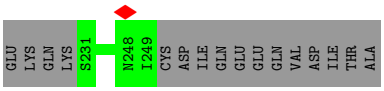
Chain Y:



• Molecule 9: Proteasome subunit beta type-2

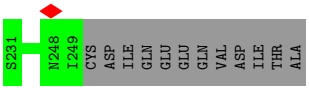
Chain I:





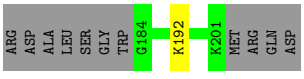
• Molecule 9: Proteasome subunit beta type-2

Chain Z:



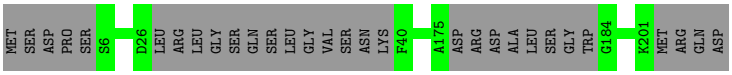
• Molecule 10: Proteasome subunit beta type-3

Chain J:



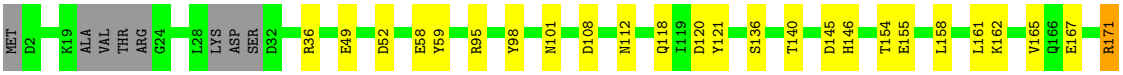
• Molecule 10: Proteasome subunit beta type-3

Chain a:



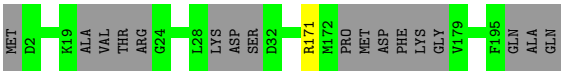
• Molecule 11: Proteasome subunit beta type-4

Chain K:



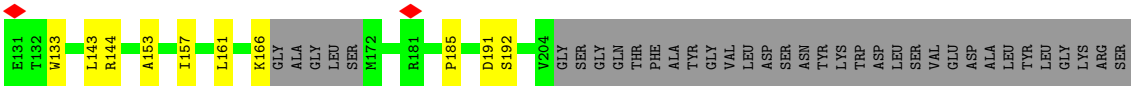
• Molecule 11: Proteasome subunit beta type-4

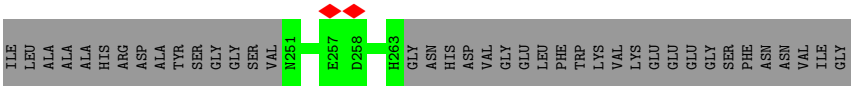
Chain b:



• Molecule 12: Proteasome subunit beta type-5

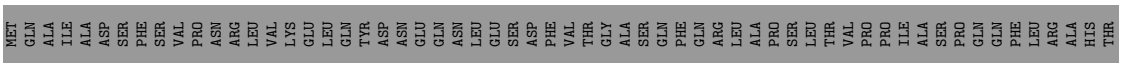
Chain L:

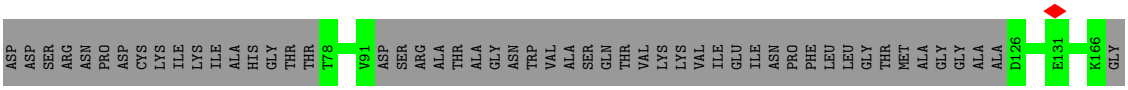


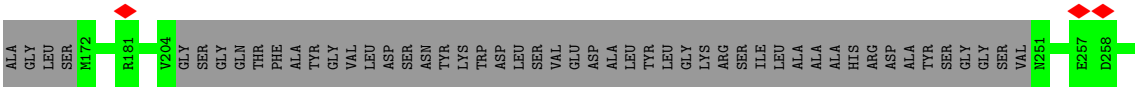


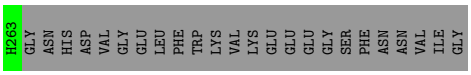
• Molecule 12: Proteasome subunit beta type-5

Chain c:



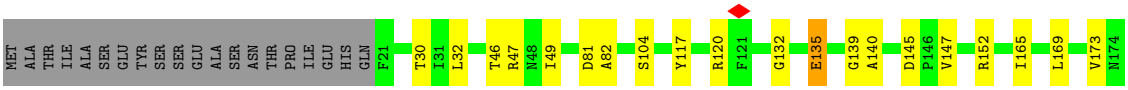






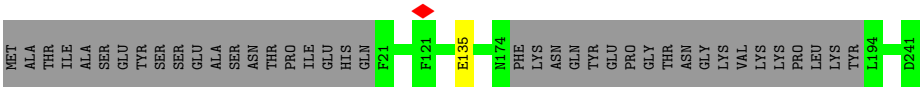
• Molecule 13: Proteasome subunit beta type-6

Chain M:



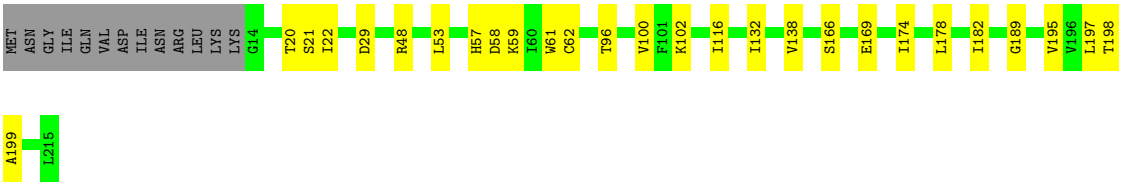
• Molecule 13: Proteasome subunit beta type-6

Chain d:



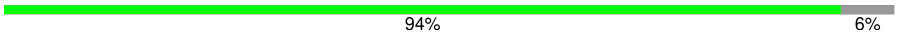
• Molecule 14: Proteasome subunit beta type-1

Chain N:



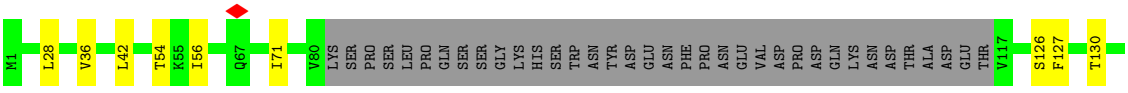
• Molecule 14: Proteasome subunit beta type-1

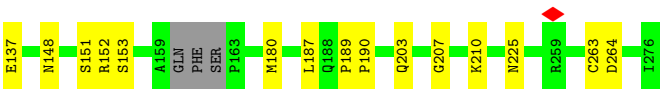
Chain e:



• Molecule 15: Proteasome chaperone 1

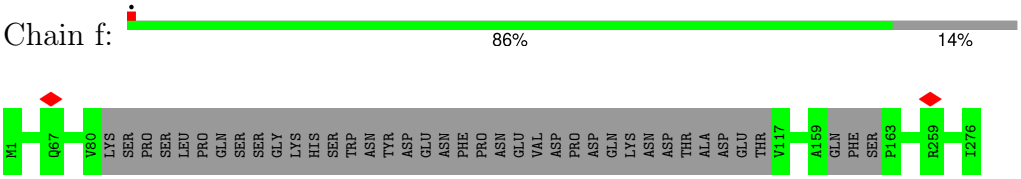
Chain O:





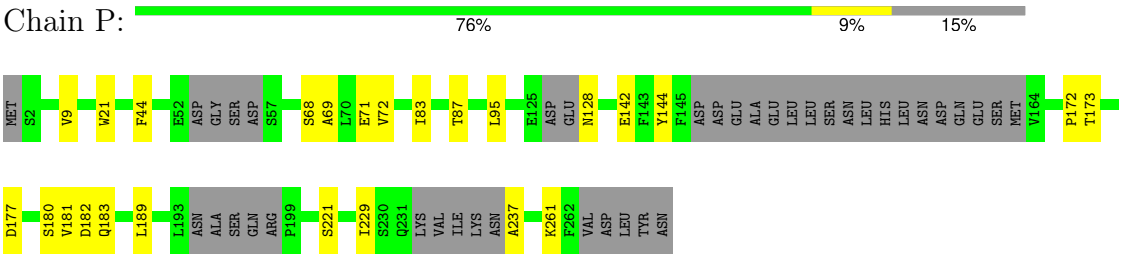
• Molecule 15: Proteasome chaperone 1

Chain f:



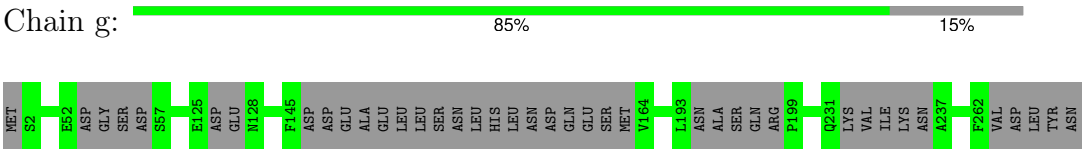
• Molecule 16: Proteasome assembly chaperone 2

Chain P:



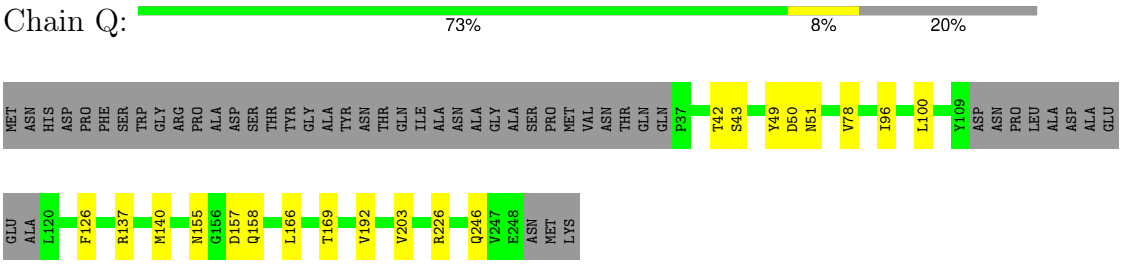
• Molecule 16: Proteasome assembly chaperone 2

Chain g:



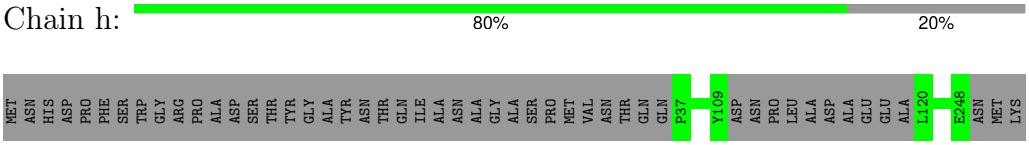
• Molecule 17: Proteasome subunit beta type-7

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	68930	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 ($e^-/Å^2$)	54.3	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	3.594	Depositor
Minimum map value	-1.707	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.305	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/1859	0.48	0/2519
1	R	0.26	0/1859	0.48	0/2519
2	B	0.27	0/1928	0.47	0/2611
2	S	0.27	0/1928	0.47	0/2611
3	C	0.26	0/1856	0.47	0/2513
3	T	0.26	0/1856	0.47	0/2513
4	D	0.25	0/1777	0.48	0/2403
4	U	0.25	0/1777	0.48	0/2403
5	E	0.25	0/1907	0.47	0/2567
5	V	0.25	0/1907	0.47	0/2567
6	F	0.25	0/1831	0.48	0/2473
6	W	0.26	0/1831	0.48	0/2473
7	G	0.26	0/1847	0.46	0/2495
7	X	0.26	0/1847	0.46	0/2495
8	H	0.24	0/993	0.48	0/1341
8	Y	0.24	0/993	0.48	0/1341
9	I	0.26	0/1770	0.48	0/2400
9	Z	0.26	0/1770	0.48	0/2400
10	J	0.26	0/1384	0.45	0/1867
10	a	0.26	0/1384	0.44	0/1867
11	K	0.25	0/1482	0.47	0/1995
11	b	0.25	0/1482	0.48	0/1995
12	L	0.24	0/838	0.49	0/1128
12	c	0.24	0/838	0.49	0/1128
13	M	0.26	0/1622	0.50	0/2187
13	d	0.26	0/1622	0.50	0/2187
14	N	0.26	0/1579	0.47	0/2138
14	e	0.26	0/1579	0.47	0/2138
15	O	0.26	0/1887	0.46	0/2557
15	f	0.26	0/1887	0.46	0/2557
16	P	0.24	0/1898	0.43	0/2574
16	g	0.24	0/1898	0.43	0/2574
17	Q	0.25	0/1601	0.51	0/2170
17	h	0.25	0/1601	0.51	0/2170

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.26	0/56118	0.47	0/75876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1823	0	1811	20	0
1	R	1823	0	1811	18	0
2	B	1891	0	1899	16	0
2	S	1891	0	1899	16	0
3	C	1827	0	1832	29	0
3	T	1827	0	1832	28	0
4	D	1752	0	1762	17	0
4	U	1752	0	1762	16	0
5	E	1881	0	1866	16	0
5	V	1881	0	1866	11	0
6	F	1803	0	1807	27	0
6	W	1803	0	1807	25	0
7	G	1809	0	1806	14	0
7	X	1809	0	1806	15	0
8	H	977	0	959	21	0
8	Y	977	0	959	16	0
9	I	1738	0	1722	18	0
9	Z	1738	0	1722	17	0
10	J	1359	0	1356	13	0
10	a	1359	0	1356	0	0
11	K	1458	0	1457	21	0
11	b	1458	0	1457	0	0
12	L	821	0	799	12	0
12	c	821	0	799	0	0
13	M	1590	0	1534	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	d	1590	0	1534	0	0
14	N	1550	0	1515	24	0
14	e	1550	0	1515	0	0
15	O	1845	0	1875	18	0
15	f	1845	0	1875	0	0
16	P	1852	0	1832	16	0
16	g	1852	0	1832	0	0
17	Q	1576	0	1596	12	0
17	h	1576	0	1596	0	0
All	All	55104	0	54856	432	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 5.

The worst 5 of 432 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:20:THR:CG2	14:N:22:ILE:HG23	1.62	1.28
14:N:20:THR:HG22	14:N:22:ILE:HG23	1.26	1.12
14:N:20:THR:CG2	14:N:22:ILE:CG2	2.38	1.00
14:N:20:THR:HG21	14:N:22:ILE:CG2	1.98	0.94
14:N:20:THR:HG21	14:N:22:ILE:HG23	1.50	0.92

There are no symmetry-related clashes.

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%)	225 (99%)	2 (1%)	0	100	100
1	R	227/252 (90%)	225 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	245/250 (98%)	242 (99%)	3 (1%)	0	100	100
2	S	245/250 (98%)	242 (99%)	3 (1%)	0	100	100
3	C	229/258 (89%)	225 (98%)	4 (2%)	0	100	100
3	T	229/258 (89%)	225 (98%)	4 (2%)	0	100	100
4	D	215/254 (85%)	214 (100%)	1 (0%)	0	100	100
4	U	215/254 (85%)	214 (100%)	1 (0%)	0	100	100
5	E	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
5	V	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
6	F	232/234 (99%)	228 (98%)	4 (2%)	0	100	100
6	W	232/234 (99%)	228 (98%)	4 (2%)	0	100	100
7	G	228/288 (79%)	225 (99%)	3 (1%)	0	100	100
7	X	228/288 (79%)	225 (99%)	3 (1%)	0	100	100
8	H	118/148 (80%)	114 (97%)	4 (3%)	0	100	100
8	Y	118/148 (80%)	114 (97%)	4 (3%)	0	100	100
9	I	223/261 (85%)	218 (98%)	5 (2%)	0	100	100
9	Z	223/261 (85%)	218 (98%)	5 (2%)	0	100	100
10	J	169/205 (82%)	165 (98%)	4 (2%)	0	100	100
10	a	169/205 (82%)	165 (98%)	4 (2%)	0	100	100
11	K	173/198 (87%)	169 (98%)	4 (2%)	0	100	100
11	b	173/198 (87%)	169 (98%)	4 (2%)	0	100	100
12	L	93/287 (32%)	93 (100%)	0	0	100	100
12	c	93/287 (32%)	93 (100%)	0	0	100	100
13	M	198/241 (82%)	195 (98%)	3 (2%)	0	100	100
13	d	198/241 (82%)	195 (98%)	3 (2%)	0	100	100
14	N	200/215 (93%)	195 (98%)	5 (2%)	0	100	100
14	e	200/215 (93%)	195 (98%)	5 (2%)	0	100	100
15	O	231/276 (84%)	229 (99%)	2 (1%)	0	100	100
15	f	231/276 (84%)	229 (99%)	2 (1%)	0	100	100
16	P	215/267 (80%)	211 (98%)	4 (2%)	0	100	100
16	g	215/267 (80%)	211 (98%)	4 (2%)	0	100	100
17	Q	198/251 (79%)	190 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	h	198/251 (79%)	190 (96%)	8 (4%)	0	100	100
All	All	6864/8290 (83%)	6742 (98%)	122 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/210 (93%)	196 (100%)	0	100	100
1	R	196/210 (93%)	196 (100%)	0	100	100
2	B	206/209 (99%)	206 (100%)	0	100	100
2	S	206/209 (99%)	206 (100%)	0	100	100
3	C	196/216 (91%)	196 (100%)	0	100	100
3	T	196/216 (91%)	196 (100%)	0	100	100
4	D	198/226 (88%)	197 (100%)	1 (0%)	86	94
4	U	198/226 (88%)	197 (100%)	1 (0%)	86	94
5	E	202/215 (94%)	202 (100%)	0	100	100
5	V	202/215 (94%)	202 (100%)	0	100	100
6	F	193/193 (100%)	191 (99%)	2 (1%)	73	88
6	W	193/193 (100%)	191 (99%)	2 (1%)	73	88
7	G	192/239 (80%)	192 (100%)	0	100	100
7	X	192/239 (80%)	192 (100%)	0	100	100
8	H	112/136 (82%)	112 (100%)	0	100	100
8	Y	112/136 (82%)	112 (100%)	0	100	100
9	I	185/214 (86%)	185 (100%)	0	100	100
9	Z	185/214 (86%)	185 (100%)	0	100	100
10	J	147/173 (85%)	147 (100%)	0	100	100
10	a	147/173 (85%)	147 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	161/175 (92%)	160 (99%)	1 (1%)	84 93
11	b	161/175 (92%)	160 (99%)	1 (1%)	84 93
12	L	87/235 (37%)	87 (100%)	0	100 100
12	c	87/235 (37%)	87 (100%)	0	100 100
13	M	167/201 (83%)	166 (99%)	1 (1%)	84 93
13	d	167/201 (83%)	166 (99%)	1 (1%)	84 93
14	N	166/178 (93%)	166 (100%)	0	100 100
14	e	166/178 (93%)	166 (100%)	0	100 100
15	O	214/251 (85%)	214 (100%)	0	100 100
15	f	214/251 (85%)	214 (100%)	0	100 100
16	P	207/244 (85%)	207 (100%)	0	100 100
16	g	207/244 (85%)	207 (100%)	0	100 100
17	Q	174/212 (82%)	174 (100%)	0	100 100
17	h	174/212 (82%)	174 (100%)	0	100 100
All	All	6006/7054 (85%)	5996 (100%)	10 (0%)	91 97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	W	218	LYS
11	b	171	ARG
13	d	135	GLU
11	K	171	ARG
13	M	135	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
17	h	227	ASN
11	b	118	GLN
5	V	147	HIS
17	Q	227	ASN
11	b	101	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 oligosaccharides 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.

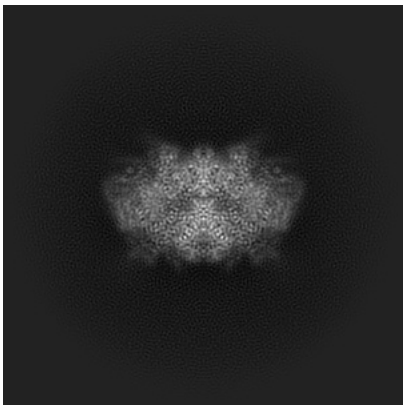
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40938. These allow visual inspection of the internal detail of the map and identification of artifacts.

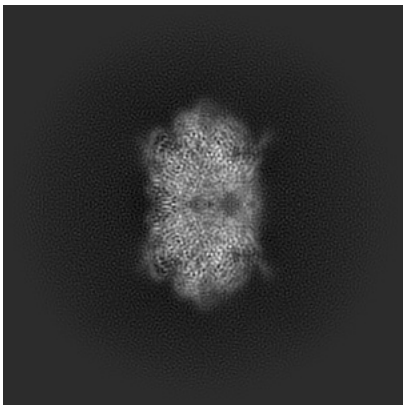
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

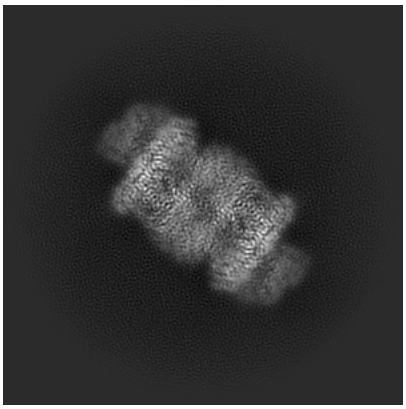
6.1.1 Primary map



X

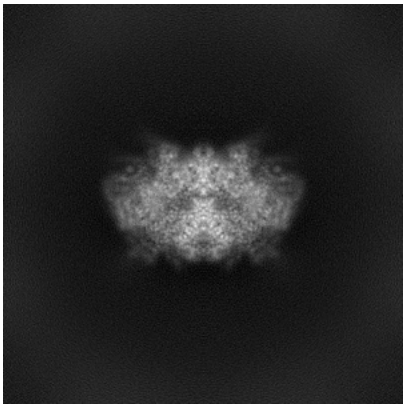


Y

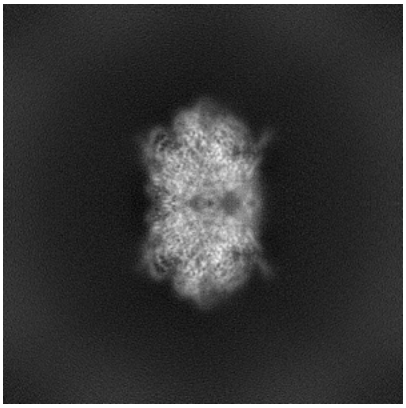


Z

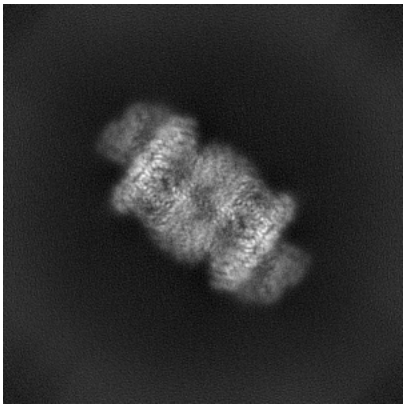
6.1.2 Raw map



X



Y

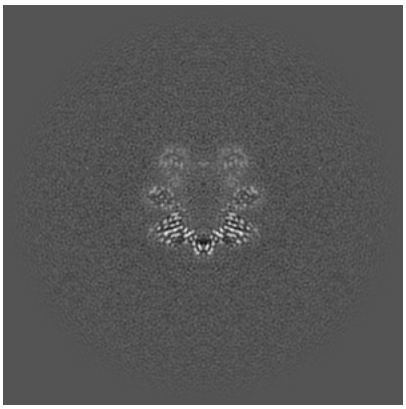


Z

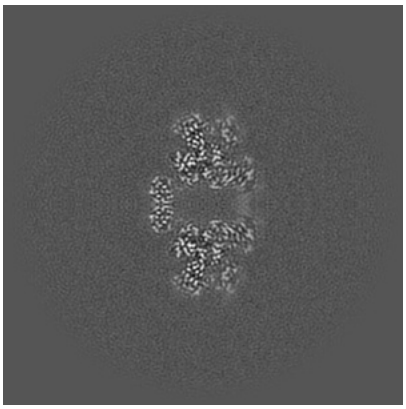
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

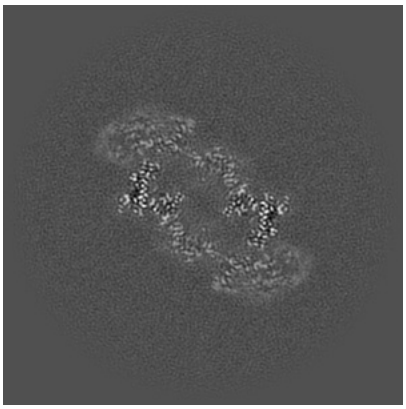
6.2.1 Primary map



X Index: 180

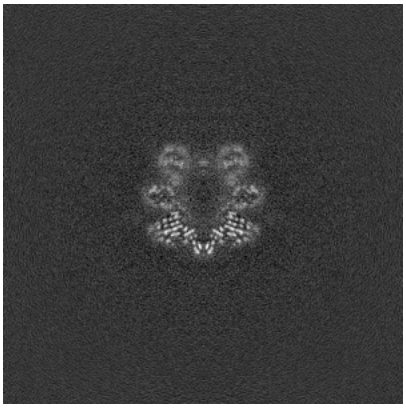


Y Index: 180

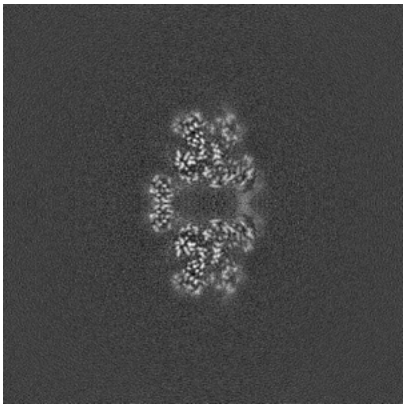


Z Index: 180

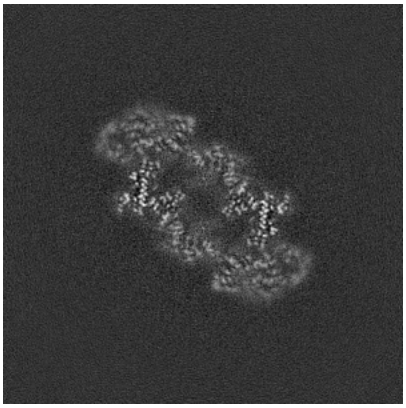
6.2.2 Raw map



X Index: 180



Y Index: 180

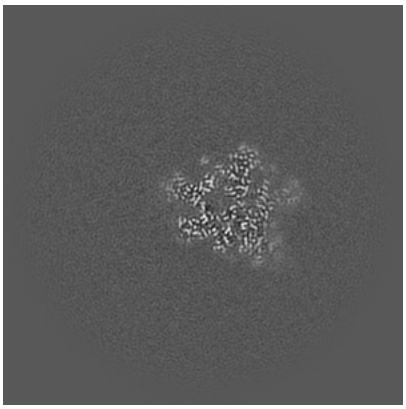


Z Index: 180

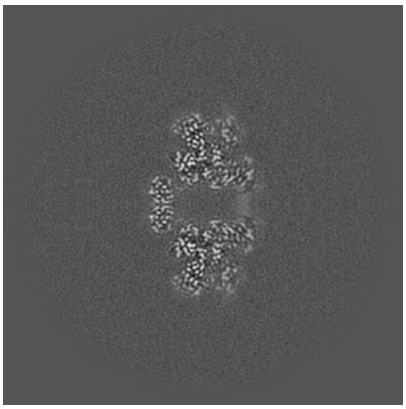
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

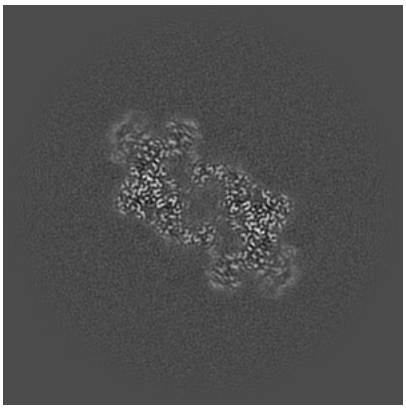
6.3.1 Primary map



X Index: 139

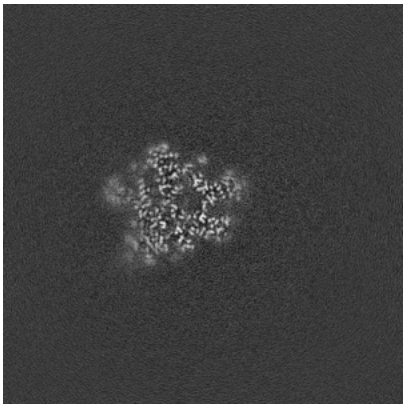


Y Index: 180

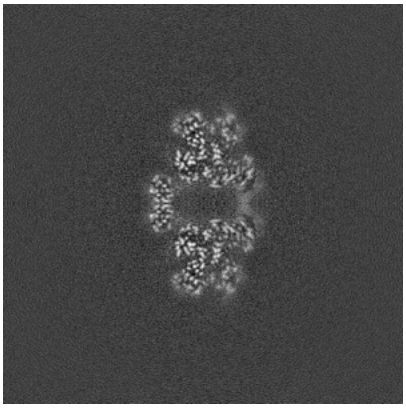


Z Index: 168

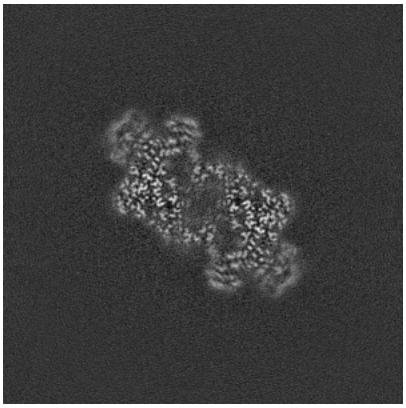
6.3.2 Raw map



X Index: 221



Y Index: 180

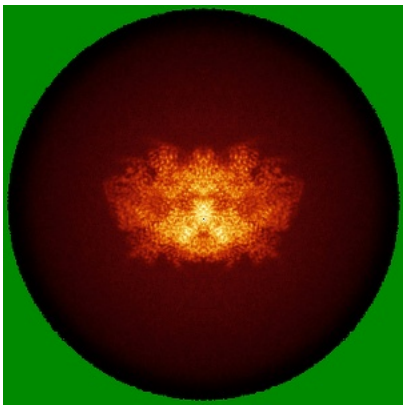


Z Index: 168

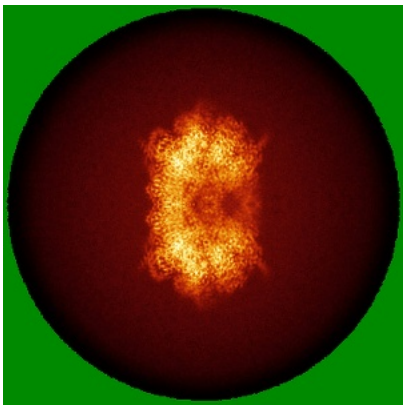
The images above show the largest variance slices of the map in three orthogonal directions.

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

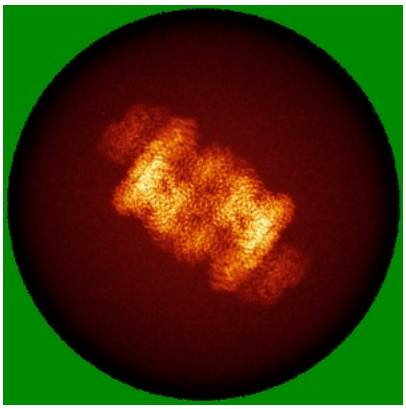
6.4.1 Primary map



X

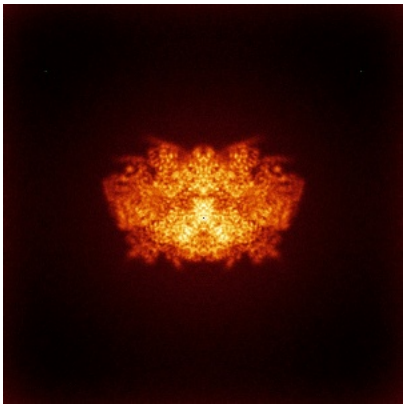


Y

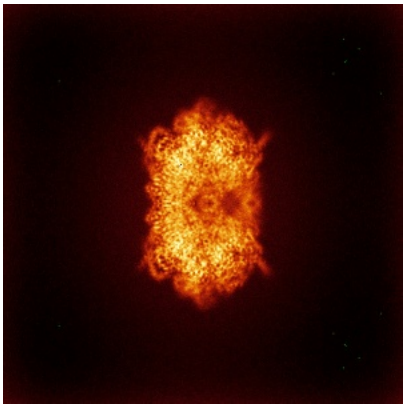


Z

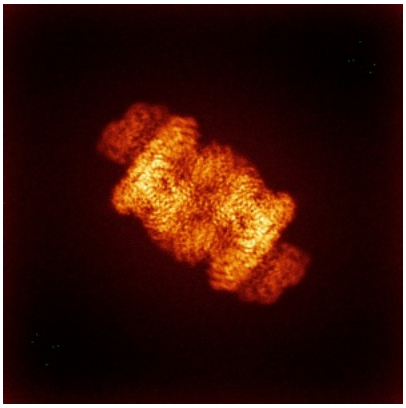
6.4.2 Raw map



X



Y

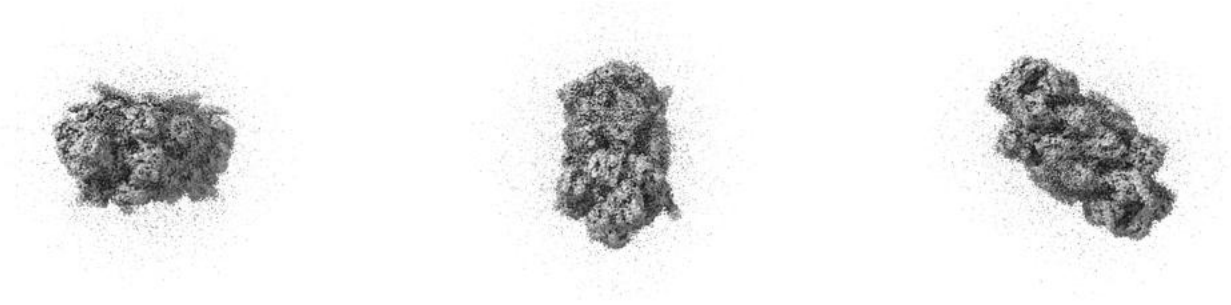


Z

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)

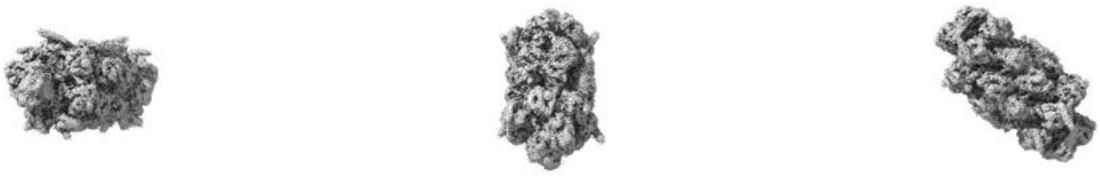
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.305. 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.

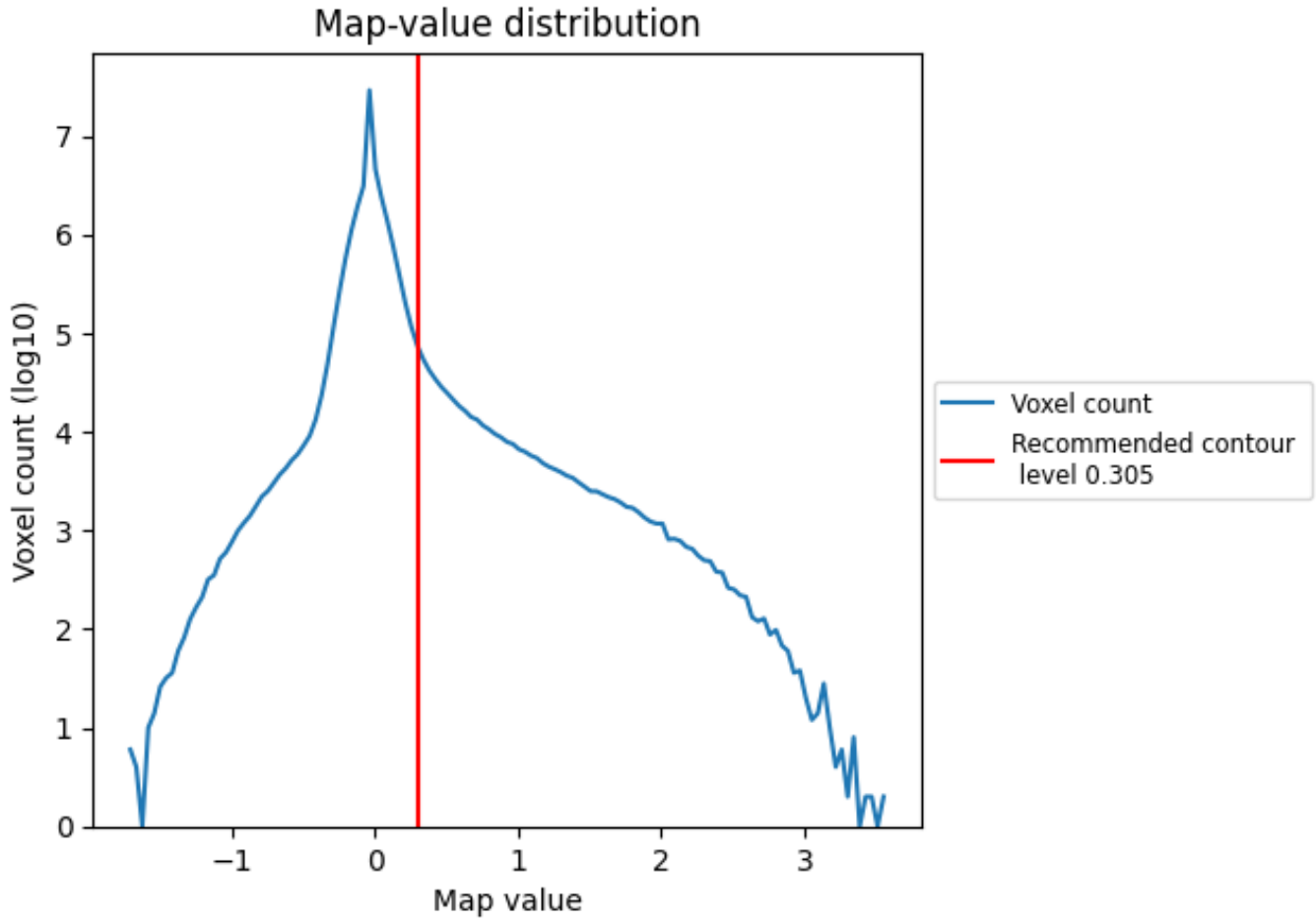
6.6 Mask visualisation (i)

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

7 Map analysis

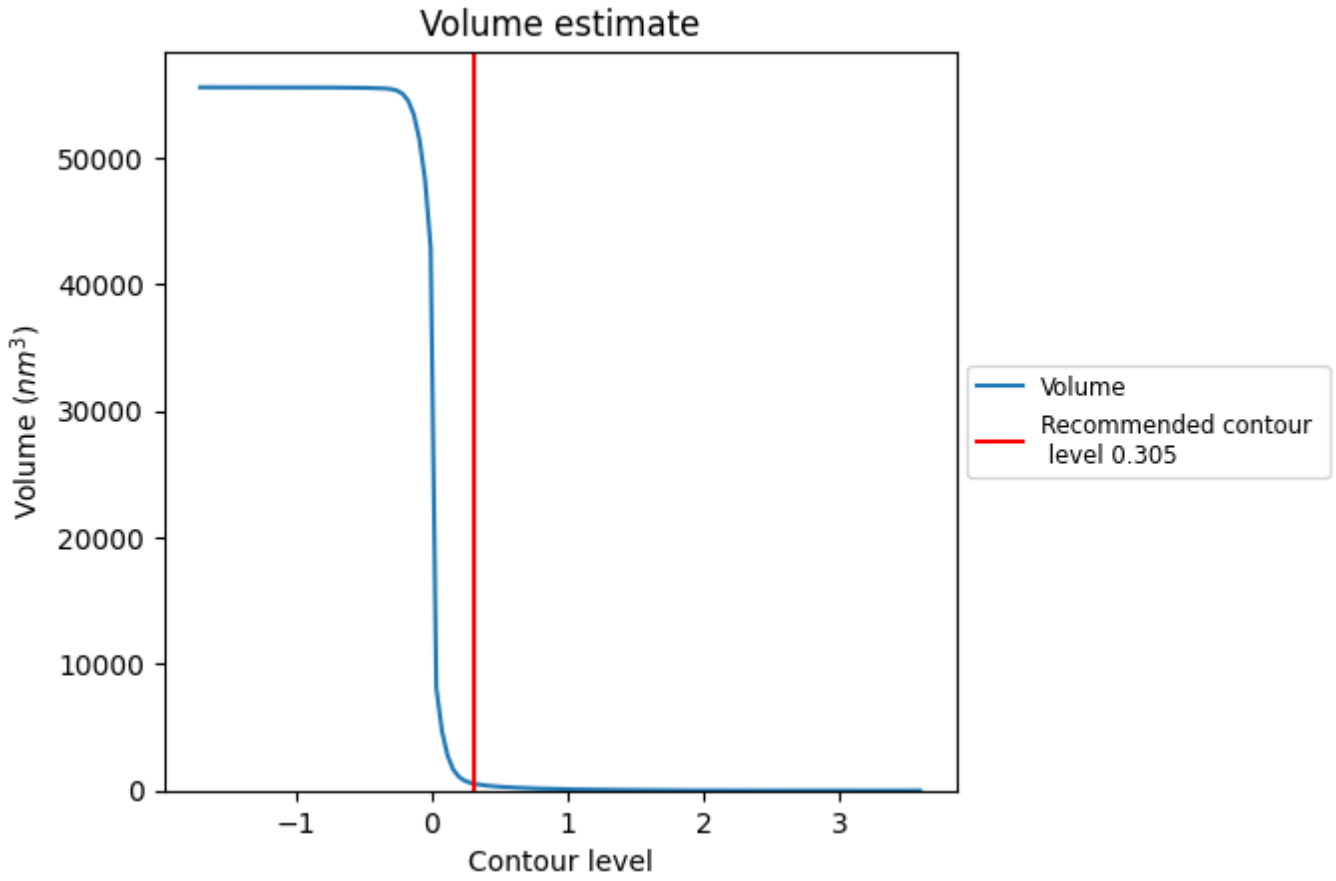
This section contains the results of statistical analysis of the map.

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.

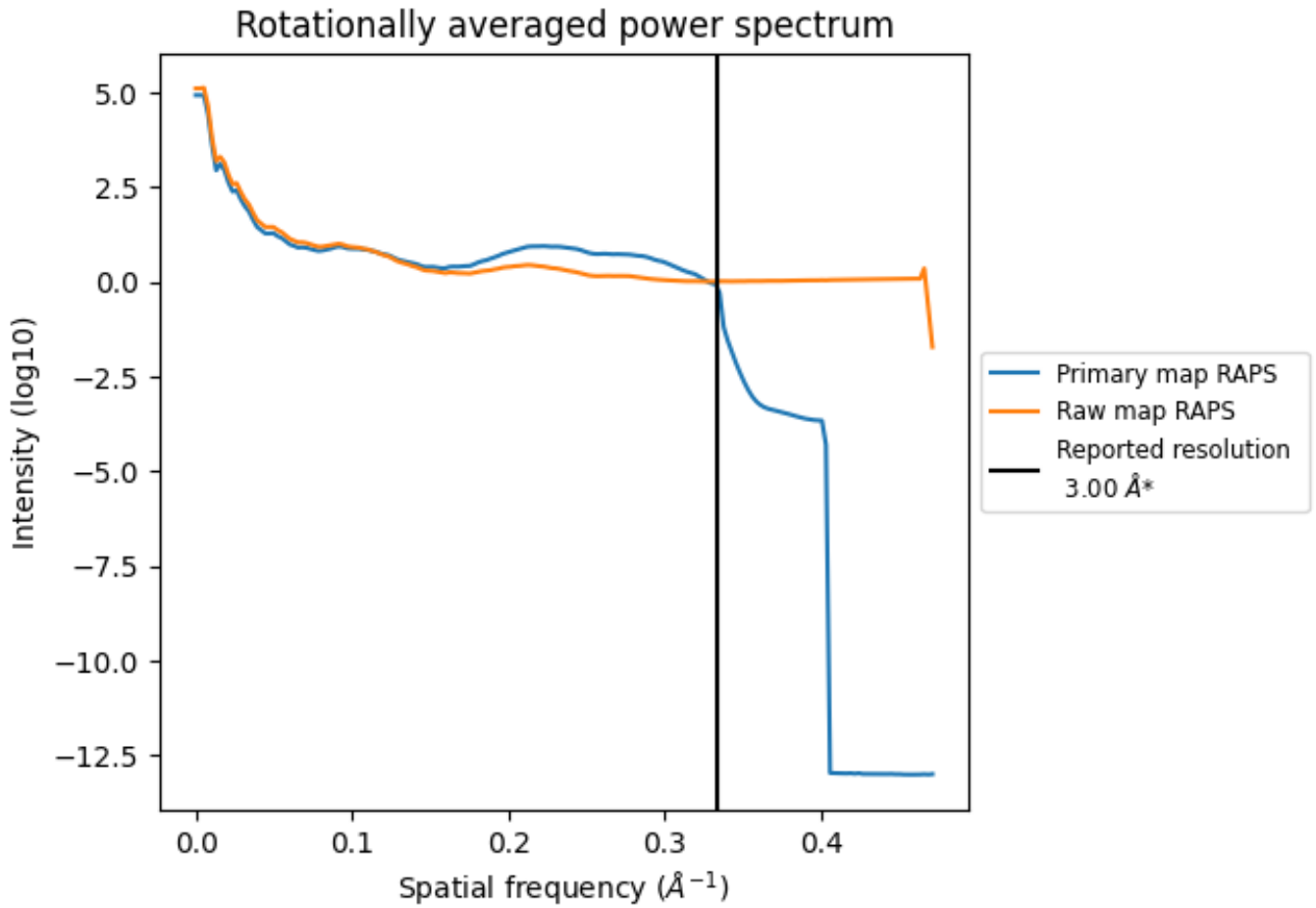
7.2 Volume estimate (i)



The volume at the recommended contour level is 561 nm^3; this corresponds to an approximate mass of 507 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)

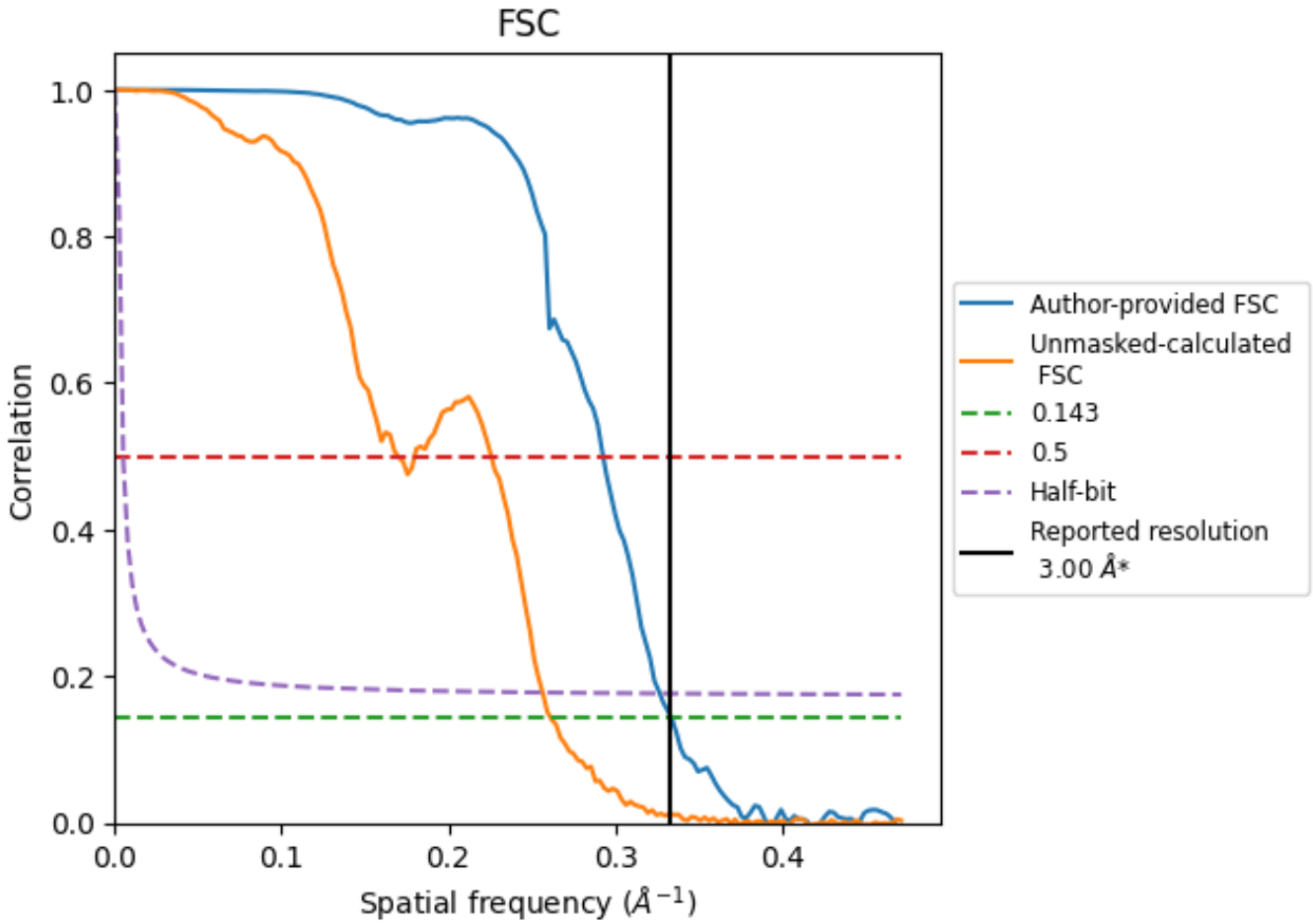


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

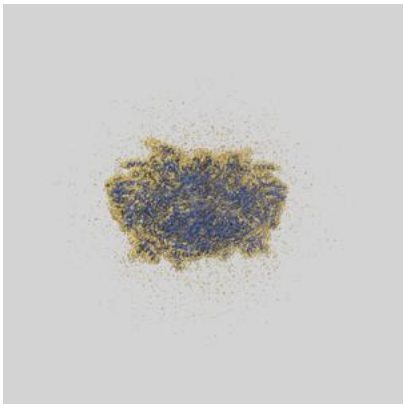
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.42	3.06
Unmasked-calculated*	3.83	5.89	3.90

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

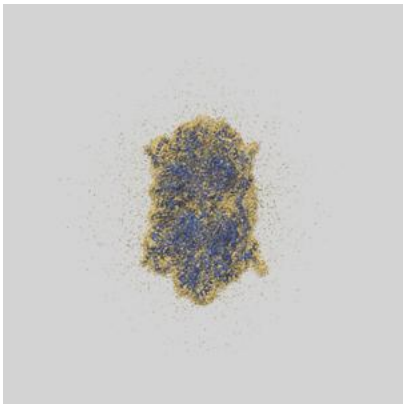
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40938 and PDB model 8T08. Per-residue inclusion information can be found in section 3 on page 9.

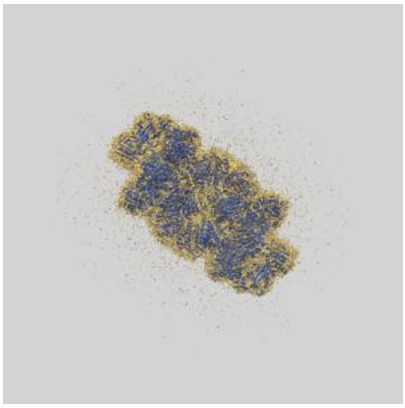
9.1 Map-model overlay



X



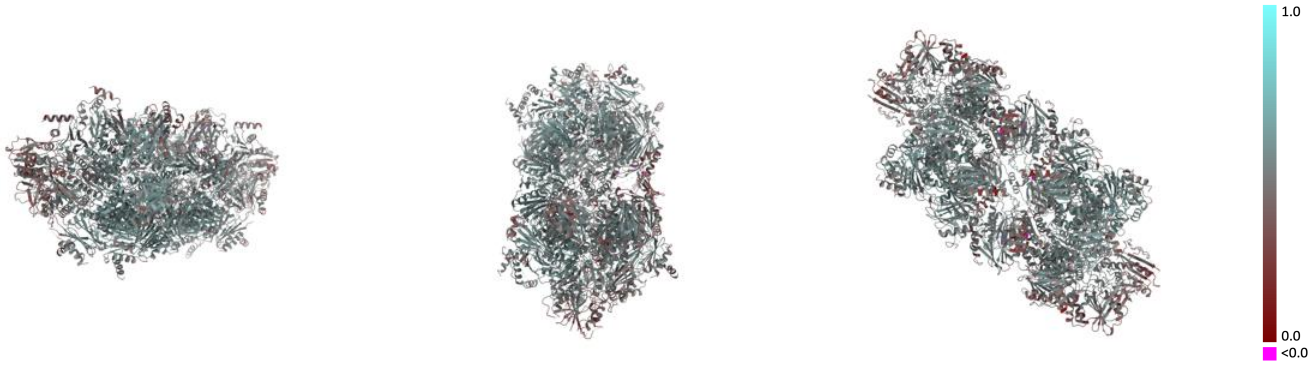
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.305 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.

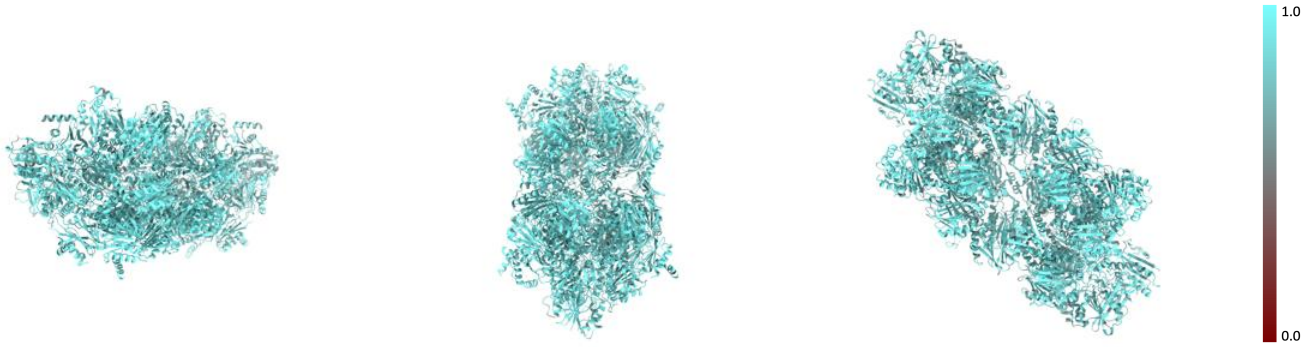
9.2 Q-score mapped to coordinate model



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.

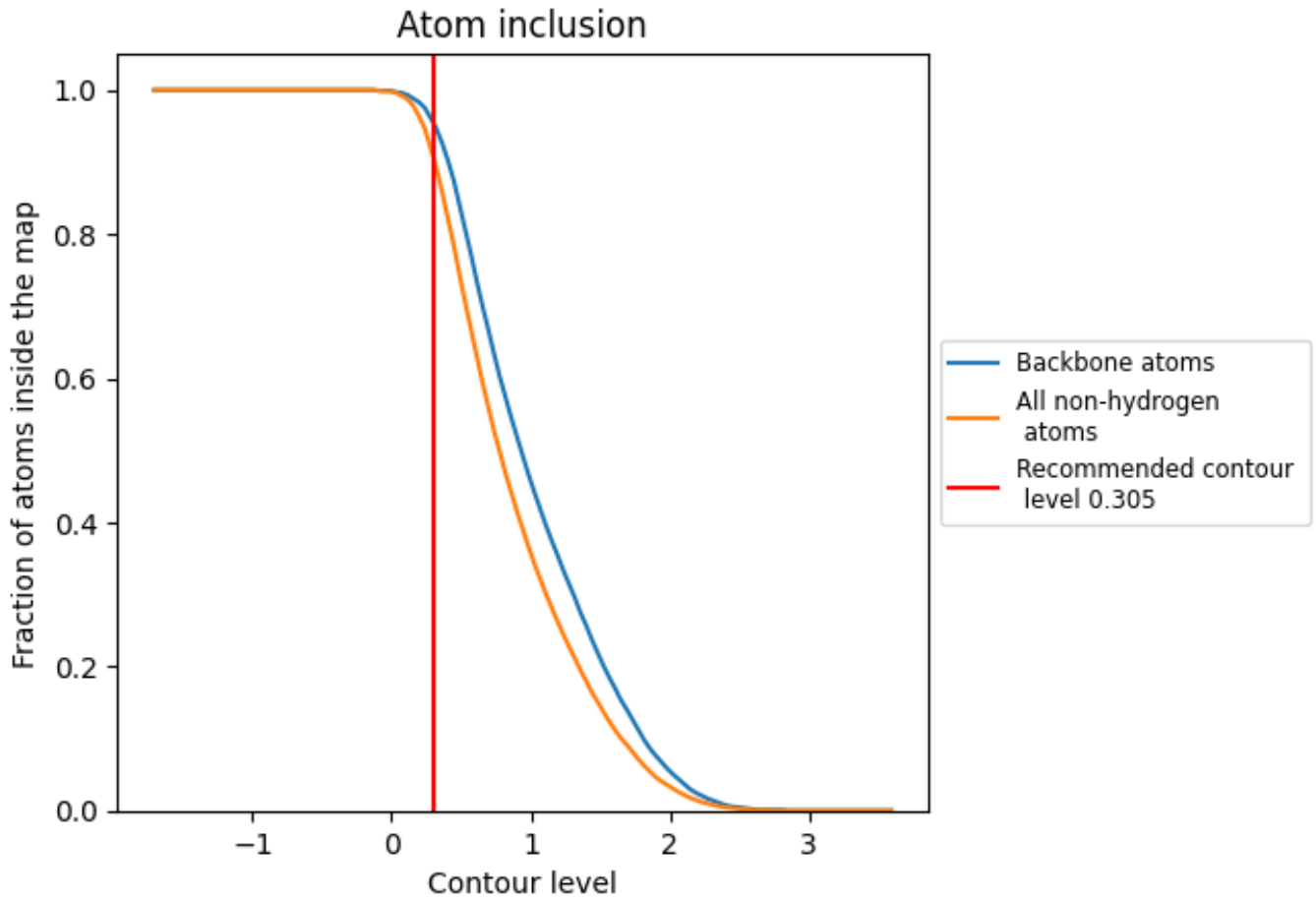
9.3 Atom inclusion mapped to coordinate model



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 (0.305).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9040	0.5040
A	0.9340	0.5420
B	0.9300	0.5460
C	0.9330	0.5360
D	0.9190	0.5190
E	0.8860	0.4900
F	0.9000	0.4800
G	0.9300	0.5230
H	0.8640	0.5230
I	0.9250	0.5430
J	0.9180	0.5280
K	0.9000	0.4750
L	0.8440	0.4060
M	0.8960	0.4970
N	0.9320	0.5470
O	0.8180	0.4220
P	0.8650	0.4260
Q	0.9410	0.5400
R	0.9330	0.5440
S	0.9310	0.5440
T	0.9330	0.5350
U	0.9190	0.5180
V	0.8840	0.4930
W	0.8980	0.4790
X	0.9310	0.5220
Y	0.8630	0.5220
Z	0.9250	0.5430
a	0.9180	0.5280
b	0.9010	0.4780
c	0.8440	0.4050
d	0.8910	0.4950
e	0.9320	0.5470
f	0.8160	0.4260
g	0.8640	0.4240
h	0.9400	0.5400