



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2024 – 05:27 pm BST

PDB ID : 8RVQ
EMDB ID : EMD-19529
Title : 20S proteasome from pre1-1
Authors : Mark, E.; Ramos, P.C.; Kayser, F.; Hoekendorff, J.; Dohmen, R.J.; Wendler, P.
Deposited on : 2024-02-01
Resolution : 2.02 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 ⓘ 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:

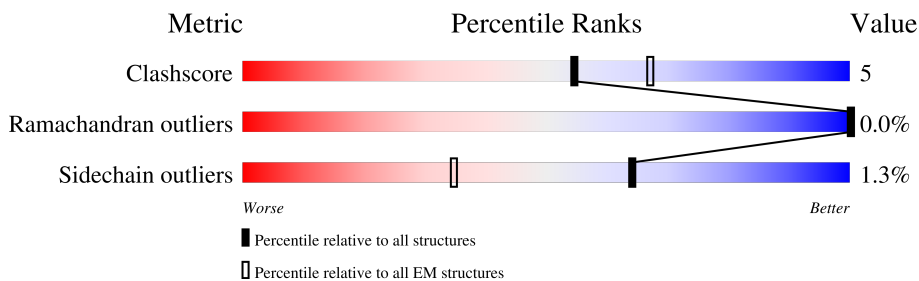
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.02 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.





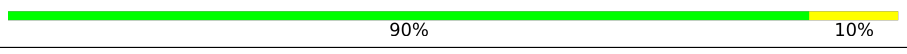
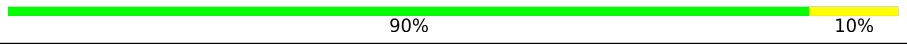


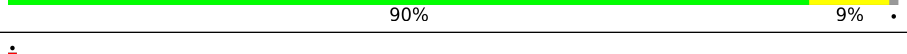
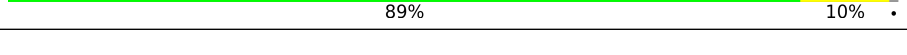
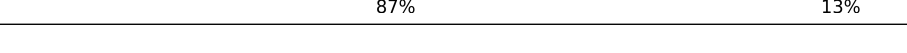
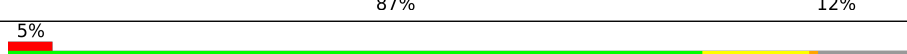
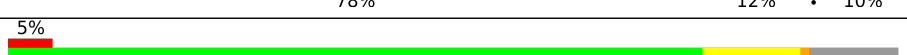

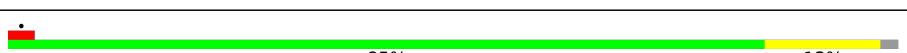
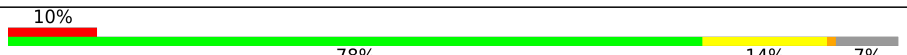
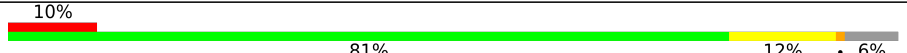





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	1	222	
1	M	222	
2	2	233	
2	N	233	
3	D	254	
3	R	254	
4	F	234	
4	T	234	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	G	288	 74% 9% 17%
5	U	288	 73% 9% 17%
6	H	196	 90% 10%
6	V	196	 90% 10%
7	I	232	 83% 12% 5%
7	W	232	 81% 13% 5%
8	J	205	 90% 9%
8	X	205	 89% 10%
9	L	212	 87% 13%
9	Z	212	 87% 12%
10	A	252	 5% 78% 12% 10%
10	O	252	 5% 78% 11% 10%
11	B	250	 5% 82% 16%
11	P	250	 5% 85% 13%
12	C	258	 10% 78% 14% 7%
12	Q	258	 10% 81% 12% 6%
13	E	260	 5% 81% 11% 8%
13	S	260	 5% 82% 9% 9%
14	K	212	 5% 73% 15% 12%
14	Y	212	 5% 75% 12% 12%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 51191 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 beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	222	Total	C	N	O	S	0	0
			1756	1115	303	334	4		
1	M	222	Total	C	N	O	S	0	0
			1756	1115	303	334	4		

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		
2	N	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
3	R	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	231	Total	C	N	O	S	0	0
			1772	1114	307	347	4		
4	T	231	Total	C	N	O	S	0	0
			1772	1114	307	347	4		

- Molecule 5 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	240	Total	C	N	O	S	0	0
			1867	1188	325	350	4		
5	U	240	Total	C	N	O	S	0	0
			1867	1188	325	350	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	196	Total	C	N	O	S	0	0
			1511	955	250	299	7		
6	V	196	Total	C	N	O	S	0	0
			1511	955	250	299	7		

- Molecule 7 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	220	Total	C	N	O	S	0	0
			1670	1054	291	319	6		
7	W	220	Total	C	N	O	S	0	0
			1670	1054	291	319	6		

- Molecule 8 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	203	Total	C	N	O	S	0	0
			1574	1007	257	302	8		
8	X	203	Total	C	N	O	S	0	0
			1574	1007	257	302	8		

- Molecule 9 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	212	Total	C	N	O	S	0	0
			1643	1045	280	311	7		
9	Z	212	Total	C	N	O	S	0	0
			1643	1045	280	311	7		

- Molecule 10 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	228	Total	C	N	O	S	0	0
			1814	1155	305	346	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	O	228	1814	1155	305	346	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	245	1875	1194	309	369	3	0	0
11	P	245	1875	1194	309	369	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	C	240	1882	1189	318	372	3	0	0
12	Q	243	1900	1200	321	376	3	0	0

- Molecule 13 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	238	1829	1145	310	367	7	0	0
13	S	237	1821	1140	309	365	7	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	187	1495	952	252	287	4	0	0
14	Y	187	1496	952	252	288	4	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	engineered mutation	UNP P22141
K	199	ASP	-	expression tag	UNP P22141
K	200	TYR	-	expression tag	UNP P22141
K	201	LYS	-	expression tag	UNP P22141

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	202	ASP	-	expression tag	UNP P22141
K	203	ASP	-	expression tag	UNP P22141
K	204	ASP	-	expression tag	UNP P22141
K	205	ASP	-	expression tag	UNP P22141
K	206	LYS	-	expression tag	UNP P22141
K	207	HIS	-	expression tag	UNP P22141
K	208	HIS	-	expression tag	UNP P22141
K	209	HIS	-	expression tag	UNP P22141
K	210	HIS	-	expression tag	UNP P22141
K	211	HIS	-	expression tag	UNP P22141
K	212	HIS	-	expression tag	UNP P22141
Y	142	PHE	SER	engineered mutation	UNP P22141
Y	199	ASP	-	expression tag	UNP P22141
Y	200	TYR	-	expression tag	UNP P22141
Y	201	LYS	-	expression tag	UNP P22141
Y	202	ASP	-	expression tag	UNP P22141
Y	203	ASP	-	expression tag	UNP P22141
Y	204	ASP	-	expression tag	UNP P22141
Y	205	ASP	-	expression tag	UNP P22141
Y	206	LYS	-	expression tag	UNP P22141
Y	207	HIS	-	expression tag	UNP P22141
Y	208	HIS	-	expression tag	UNP P22141
Y	209	HIS	-	expression tag	UNP P22141
Y	210	HIS	-	expression tag	UNP P22141
Y	211	HIS	-	expression tag	UNP P22141
Y	212	HIS	-	expression tag	UNP P22141

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	AltConf
15	1	95	Total O 95 95	0
15	2	97	Total O 97 97	0
15	D	95	Total O 95 95	0
15	F	92	Total O 92 92	0
15	G	74	Total O 74 74	0
15	H	72	Total O 72 72	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
15	I	101	Total 101	O 101	0
15	J	72	Total 72	O 72	0
15	L	80	Total 80	O 80	0
15	M	99	Total 99	O 99	0
15	N	99	Total 99	O 99	0
15	R	100	Total 100	O 100	0
15	T	86	Total 86	O 86	0
15	U	76	Total 76	O 76	0
15	V	68	Total 68	O 68	0
15	W	100	Total 100	O 100	0
15	X	76	Total 76	O 76	0
15	Z	81	Total 81	O 81	0
15	A	91	Total 91	O 91	0
15	B	83	Total 83	O 83	0
15	C	73	Total 73	O 73	0
15	E	103	Total 103	O 103	0
15	K	73	Total 73	O 73	0
15	O	91	Total 91	O 91	0
15	P	85	Total 85	O 85	0
15	Q	78	Total 78	O 78	0
15	S	102	Total 102	O 102	0

Continued on next page...

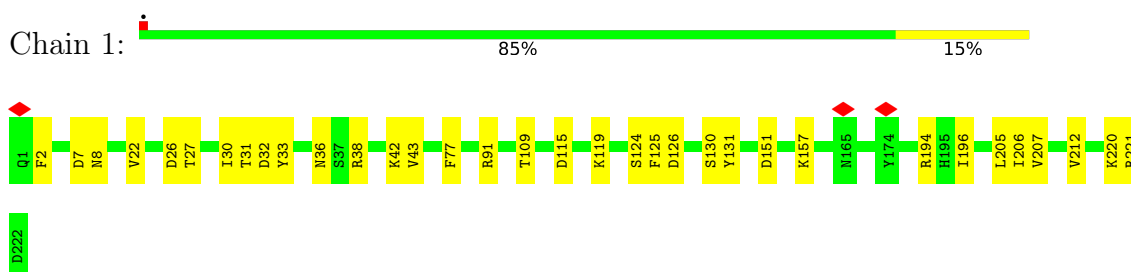
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
15	Y	70	Total	O	0
			70	70	

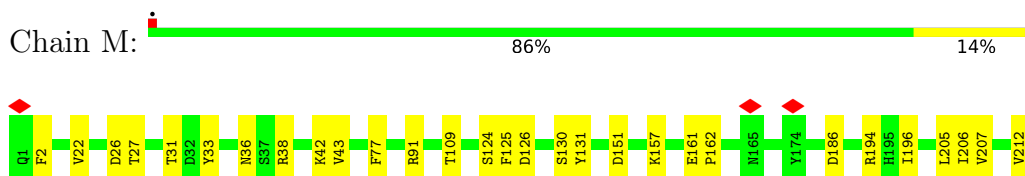
3 Residue-property plots [i](#)

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.

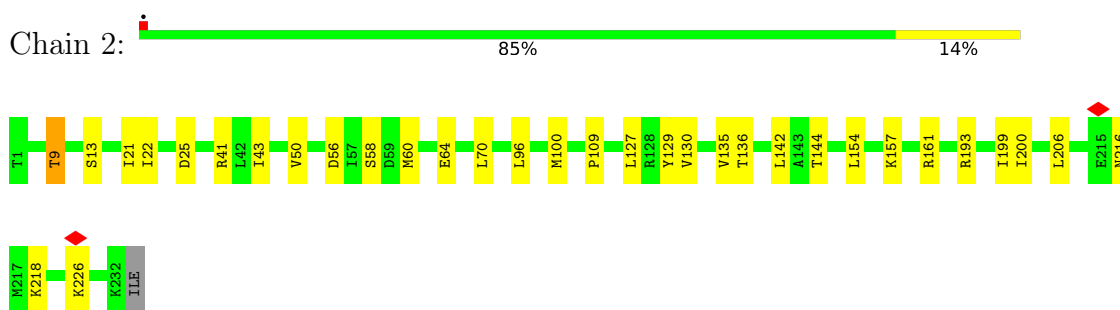
- Molecule 1: Proteasome subunit beta type-6



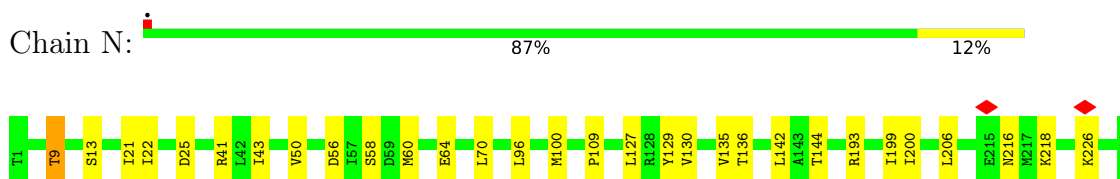
- Molecule 1: Proteasome subunit beta type-6



- Molecule 2: Proteasome subunit beta type-7



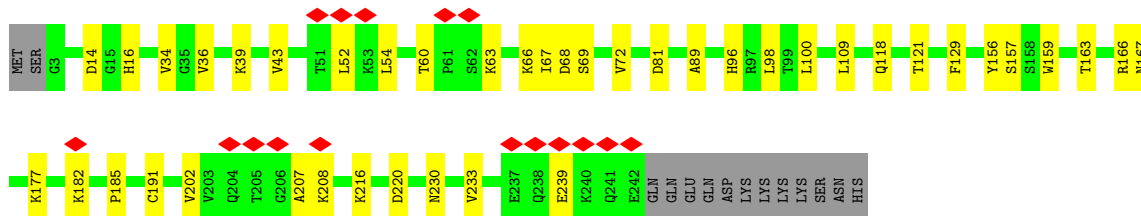
- Molecule 2: Proteasome subunit beta type-7



IILE

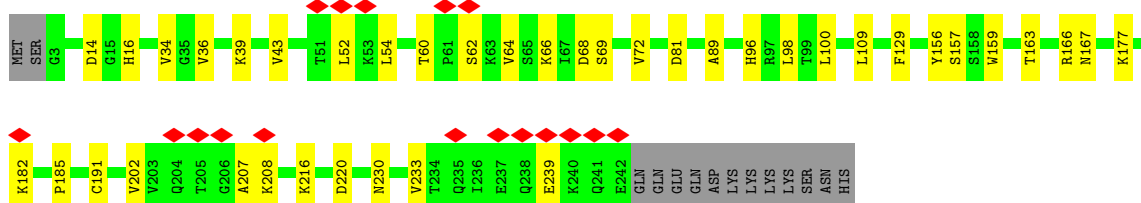
- Molecule 3: Proteasome subunit alpha type-4

Chain D: 6% 78% 17% 6%



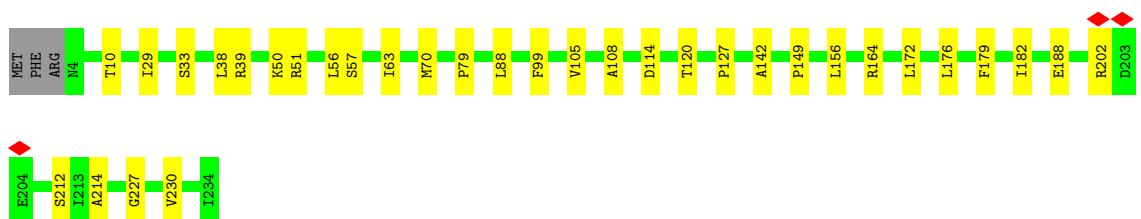
- Molecule 3: Proteasome subunit alpha type-4

Chain R: 7% 79% 16% 6%



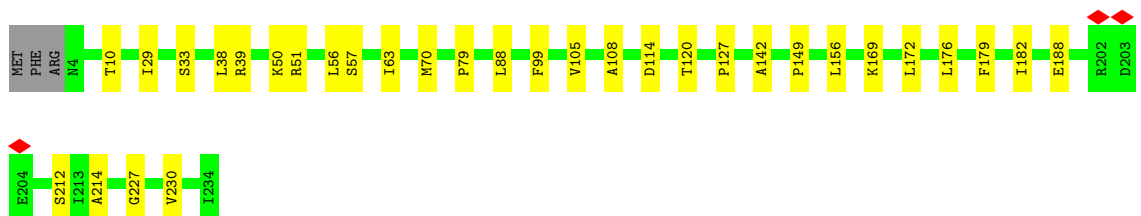
- Molecule 4: Proteasome subunit alpha type-6

Chain F: 85% 14%



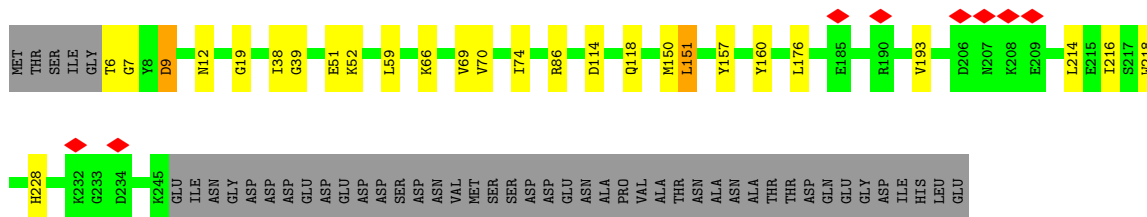
- Molecule 4: Proteasome subunit alpha type-6

Chain T: 85% 14%

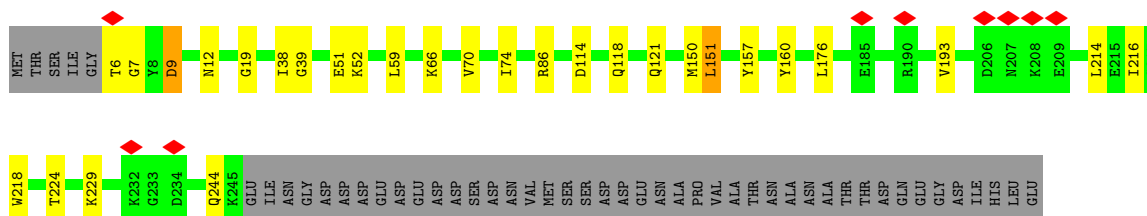


- Molecule 5: Probable proteasome subunit alpha type-7

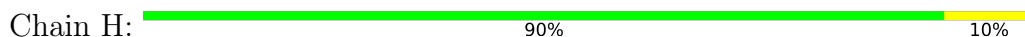
Chain G: 74% 9% 17%



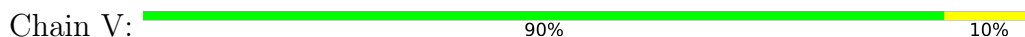
• Molecule 5: Probable proteasome subunit alpha type-7



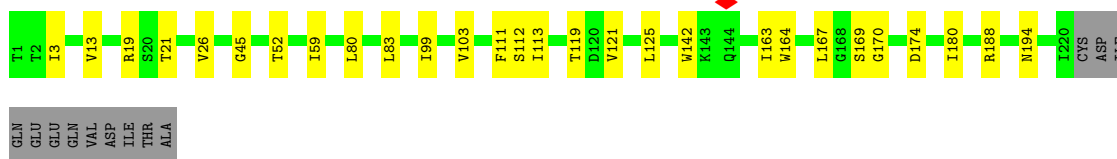
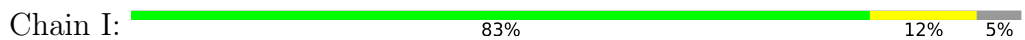
• Molecule 6: Proteasome subunit beta type-1



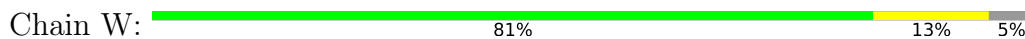
• Molecule 6: Proteasome subunit beta type-1

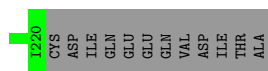


• Molecule 7: Proteasome subunit beta type-2

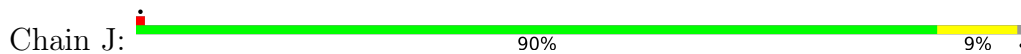


• Molecule 7: Proteasome subunit beta type-2

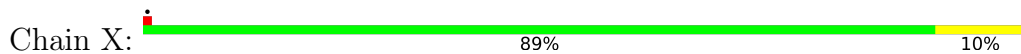




• Molecule 8: Proteasome subunit beta type-3



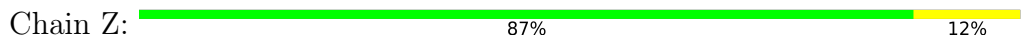
• Molecule 8: Proteasome subunit beta type-3



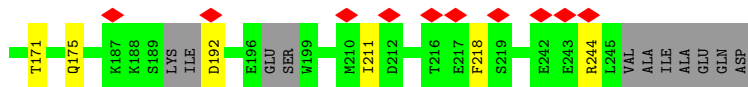
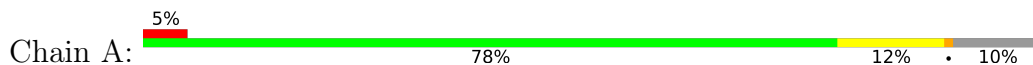
• Molecule 9: Proteasome subunit beta type-5



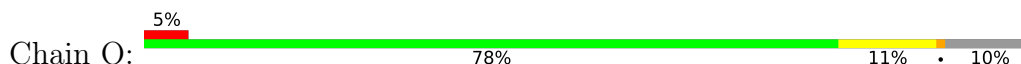
• Molecule 9: Proteasome subunit beta type-5

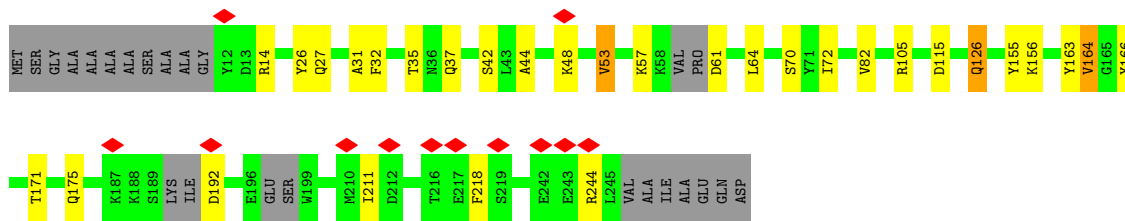


• Molecule 10: Proteasome subunit alpha type-1

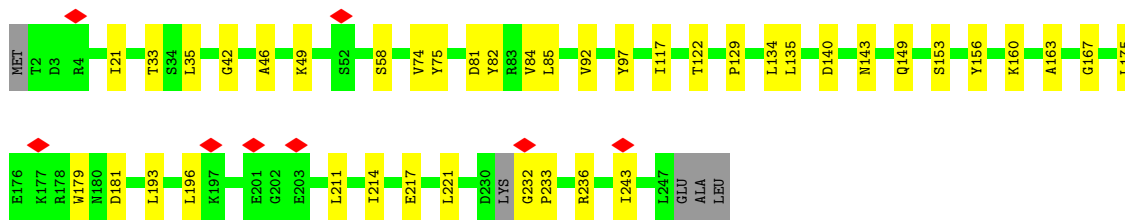
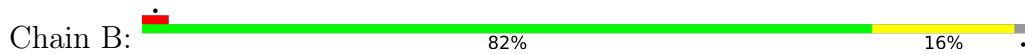


• Molecule 10: Proteasome subunit alpha type-1

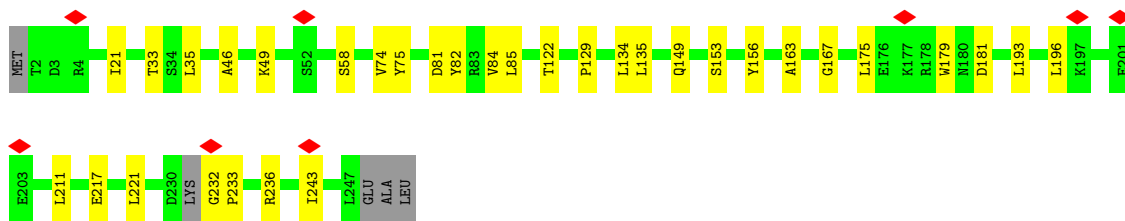
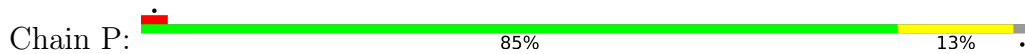




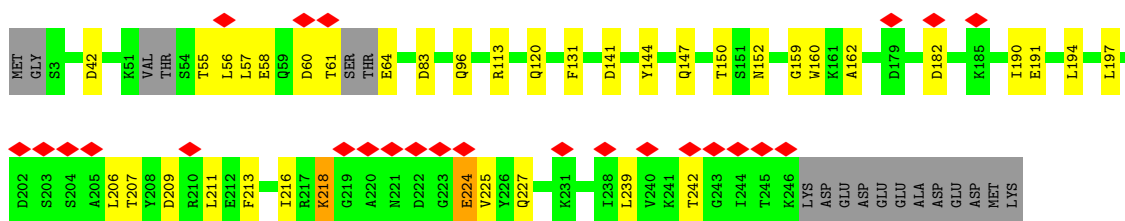
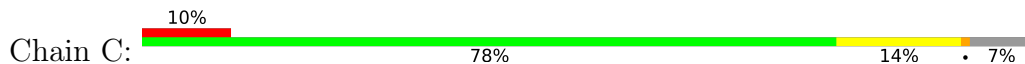
• Molecule 11: Proteasome subunit alpha type-2



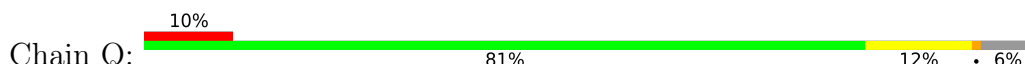
• Molecule 11: Proteasome subunit alpha type-2

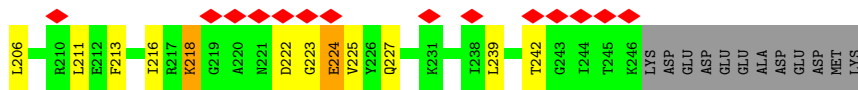


• Molecule 12: Proteasome subunit alpha type-3

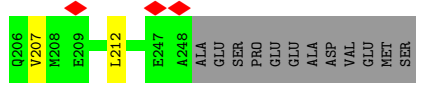
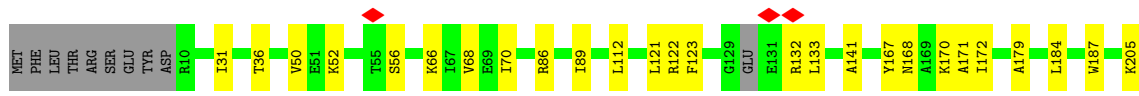
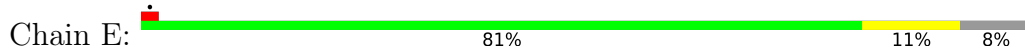


• Molecule 12: Proteasome subunit alpha type-3

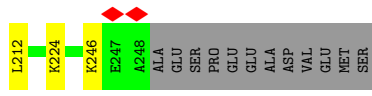
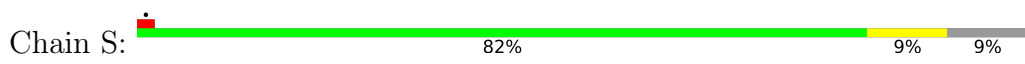




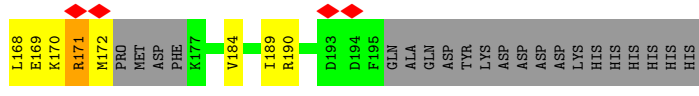
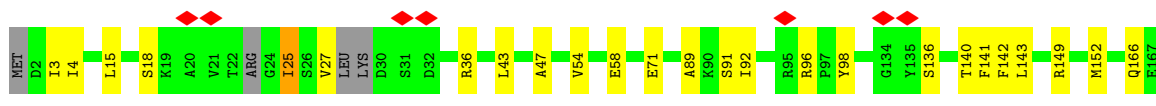
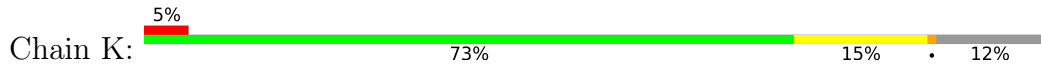
• Molecule 13: Proteasome subunit alpha type-5



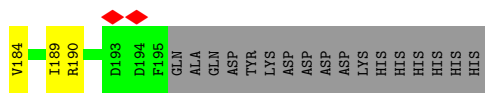
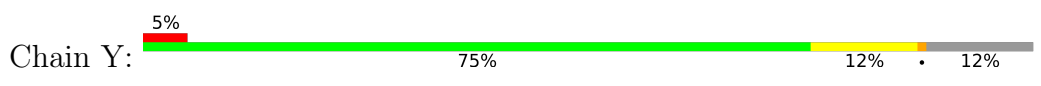
• Molecule 13: Proteasome subunit alpha type-5



• Molecule 14: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	341154	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.948	Depositor
Minimum map value	-1.197	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.276	Depositor
Map size (\AA)	500.4, 500.4, 500.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.834, 0.834, 0.834	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	1	0.25	0/1794	0.47	0/2420
1	M	0.25	0/1794	0.47	0/2420
2	2	0.25	0/1846	0.50	0/2503
2	N	0.25	0/1846	0.50	0/2503
3	D	0.25	0/1910	0.49	0/2586
3	R	0.25	0/1910	0.49	0/2586
4	F	0.24	0/1799	0.49	0/2433
4	T	0.24	0/1799	0.49	0/2433
5	G	0.25	0/1907	0.47	0/2575
5	U	0.25	0/1907	0.47	0/2575
6	H	0.25	0/1540	0.48	0/2087
6	V	0.25	0/1540	0.47	0/2087
7	I	0.24	0/1701	0.48	0/2307
7	W	0.24	0/1701	0.48	0/2307
8	J	0.25	0/1604	0.47	0/2166
8	X	0.25	0/1604	0.48	0/2166
9	L	0.25	0/1680	0.47	0/2274
9	Z	0.25	0/1680	0.47	0/2274
10	A	0.25	0/1848	0.48	0/2497
10	O	0.25	0/1848	0.48	0/2497
11	B	0.25	0/1911	0.48	0/2588
11	P	0.25	0/1911	0.48	0/2588
12	C	0.25	0/1910	0.48	0/2580
12	Q	0.24	0/1929	0.48	0/2608
13	E	0.24	0/1853	0.47	0/2494
13	S	0.24	0/1845	0.47	0/2484
14	K	0.24	0/1519	0.47	0/2044
14	Y	0.24	0/1520	0.47	0/2046
All	All	0.25	0/49656	0.48	0/67128

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	1	1756	0	1711	23	0
1	M	1756	0	1711	21	0
2	2	1815	0	1821	23	0
2	N	1815	0	1821	21	0
3	D	1881	0	1892	26	0
3	R	1881	0	1892	25	0
4	F	1772	0	1775	22	0
4	T	1772	0	1775	23	0
5	G	1867	0	1860	16	0
5	U	1867	0	1860	17	0
6	H	1511	0	1481	11	0
6	V	1511	0	1481	10	0
7	I	1670	0	1679	18	0
7	W	1670	0	1679	20	0
8	J	1574	0	1566	13	0
8	X	1574	0	1566	13	0
9	L	1643	0	1595	17	0
9	Z	1643	0	1595	16	0
10	A	1814	0	1800	19	0
10	O	1814	0	1800	19	0
11	B	1875	0	1881	24	0
11	P	1875	0	1881	19	0
12	C	1882	0	1881	26	0
12	Q	1900	0	1901	24	0
13	E	1829	0	1814	19	0
13	S	1821	0	1808	17	0
14	K	1495	0	1492	23	0
14	Y	1496	0	1492	18	0
15	1	95	0	0	2	0
15	2	97	0	0	2	0
15	A	91	0	0	3	0
15	B	83	0	0	1	0
15	C	73	0	0	2	0
15	D	95	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	103	0	0	1	0
15	F	92	0	0	0	0
15	G	74	0	0	0	0
15	H	72	0	0	0	0
15	I	101	0	0	1	0
15	J	72	0	0	2	0
15	K	73	0	0	3	0
15	L	80	0	0	2	0
15	M	99	0	0	2	0
15	N	99	0	0	1	0
15	O	91	0	0	3	0
15	P	85	0	0	1	0
15	Q	78	0	0	2	0
15	R	100	0	0	1	0
15	S	102	0	0	1	0
15	T	86	0	0	0	0
15	U	76	0	0	1	0
15	V	68	0	0	0	0
15	W	100	0	0	1	0
15	X	76	0	0	2	0
15	Y	70	0	0	2	0
15	Z	81	0	0	1	0
All	All	51191	0	48510	480	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 480 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:160:LYS:HB2	12:C:57:LEU:HD12	1.68	0.75
1:M:196:ILE:HD11	7:W:21:THR:HG21	1.73	0.70
1:1:196:ILE:HD11	7:I:21:THR:HG21	1.73	0.70
1:M:151:ASP:HB3	1:M:157:LYS:HD2	1.75	0.69
1:1:151:ASP:HB3	1:1:157:LYS:HD2	1.75	0.68

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	1	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
1	M	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
2	2	230/233 (99%)	218 (95%)	12 (5%)	0	100	100
2	N	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
3	D	238/254 (94%)	229 (96%)	9 (4%)	0	100	100
3	R	238/254 (94%)	230 (97%)	8 (3%)	0	100	100
4	F	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
4	T	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
5	G	238/288 (83%)	235 (99%)	3 (1%)	0	100	100
5	U	238/288 (83%)	235 (99%)	3 (1%)	0	100	100
6	H	194/196 (99%)	192 (99%)	2 (1%)	0	100	100
6	V	194/196 (99%)	192 (99%)	2 (1%)	0	100	100
7	I	218/232 (94%)	217 (100%)	1 (0%)	0	100	100
7	W	218/232 (94%)	217 (100%)	1 (0%)	0	100	100
8	J	201/205 (98%)	192 (96%)	9 (4%)	0	100	100
8	X	201/205 (98%)	191 (95%)	10 (5%)	0	100	100
9	L	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
9	Z	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
10	A	220/252 (87%)	214 (97%)	6 (3%)	0	100	100
10	O	220/252 (87%)	214 (97%)	6 (3%)	0	100	100
11	B	241/250 (96%)	234 (97%)	7 (3%)	0	100	100
11	P	241/250 (96%)	234 (97%)	7 (3%)	0	100	100
12	C	234/258 (91%)	226 (97%)	8 (3%)	0	100	100
12	Q	239/258 (93%)	231 (97%)	8 (3%)	0	100	100
13	E	234/260 (90%)	229 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	S	233/260 (90%)	230 (99%)	3 (1%)	0	100	100
14	K	179/212 (84%)	175 (98%)	3 (2%)	1 (1%)	22	16
14	Y	179/212 (84%)	175 (98%)	3 (2%)	1 (1%)	22	16
All	All	6176/6616 (93%)	6011 (97%)	163 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	K	25	ILE
14	Y	25	ILE

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	1	185/185 (100%)	182 (98%)	3 (2%)	58	62
1	M	185/185 (100%)	183 (99%)	2 (1%)	70	75
2	2	198/199 (100%)	196 (99%)	2 (1%)	73	77
2	N	198/199 (100%)	196 (99%)	2 (1%)	73	77
3	D	212/226 (94%)	207 (98%)	5 (2%)	44	46
3	R	212/226 (94%)	207 (98%)	5 (2%)	44	46
4	F	190/193 (98%)	190 (100%)	0	100	100
4	T	190/193 (98%)	190 (100%)	0	100	100
5	G	198/239 (83%)	193 (98%)	5 (2%)	42	44
5	U	198/239 (83%)	192 (97%)	6 (3%)	36	36
6	H	162/162 (100%)	162 (100%)	0	100	100
6	V	162/162 (100%)	162 (100%)	0	100	100
7	I	179/190 (94%)	177 (99%)	2 (1%)	70	75
7	W	179/190 (94%)	177 (99%)	2 (1%)	70	75
8	J	171/173 (99%)	169 (99%)	2 (1%)	67	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	X	171/173 (99%)	168 (98%)	3 (2%)	54	57
9	L	169/169 (100%)	166 (98%)	3 (2%)	54	57
9	Z	169/169 (100%)	166 (98%)	3 (2%)	54	57
10	A	196/210 (93%)	190 (97%)	6 (3%)	35	34
10	O	196/210 (93%)	191 (97%)	5 (3%)	41	42
11	B	205/209 (98%)	205 (100%)	0	100	100
11	P	205/209 (98%)	205 (100%)	0	100	100
12	C	200/216 (93%)	195 (98%)	5 (2%)	42	44
12	Q	202/216 (94%)	198 (98%)	4 (2%)	50	53
13	E	195/215 (91%)	195 (100%)	0	100	100
13	S	194/215 (90%)	193 (100%)	1 (0%)	86	90
14	K	165/189 (87%)	163 (99%)	2 (1%)	67	72
14	Y	165/189 (87%)	163 (99%)	2 (1%)	67	72
All	All	5251/5550 (95%)	5181 (99%)	70 (1%)	64	70

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	K	171	ARG
10	O	53	VAL
12	Q	218	LYS
2	N	9	THR
1	M	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
12	C	147	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

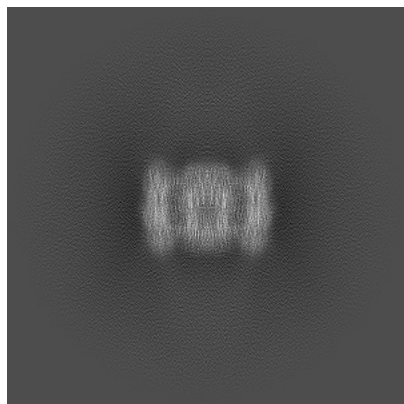
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19529. These allow visual inspection of the internal detail of the map and identification of artifacts.

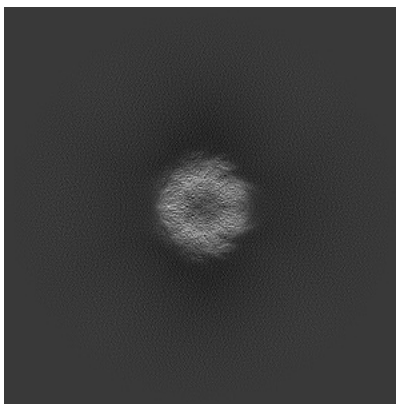
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

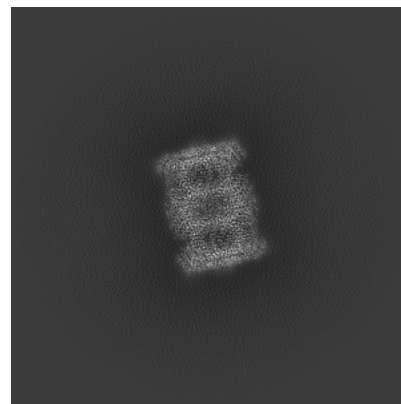
6.1.1 Primary map



X

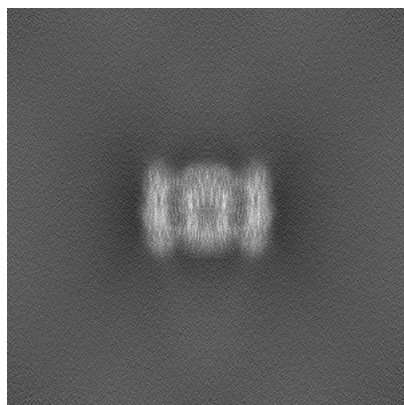


Y

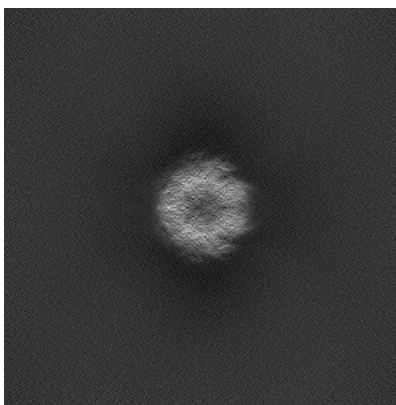


Z

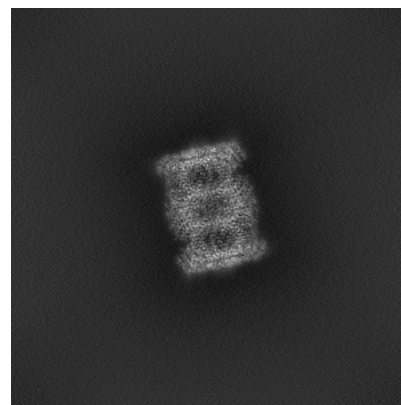
6.1.2 Raw map



X



Y

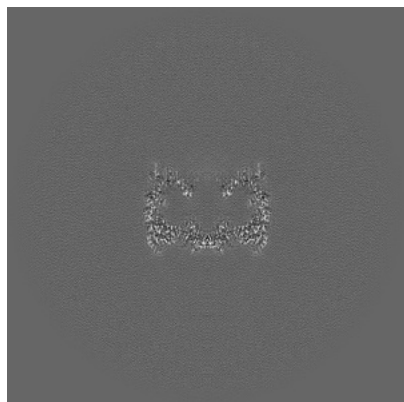


Z

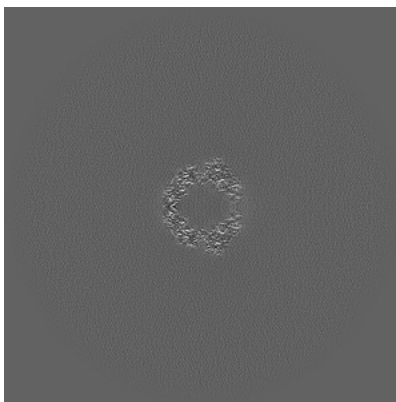
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

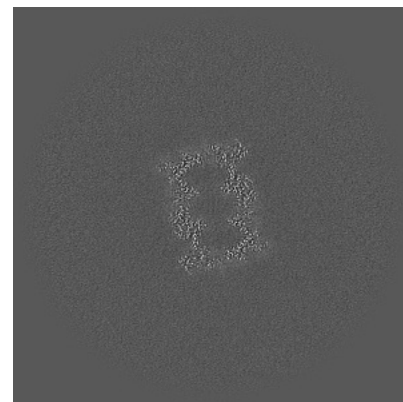
6.2.1 Primary map



X Index: 300

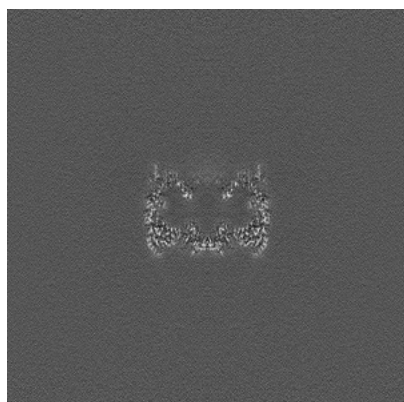


Y Index: 300

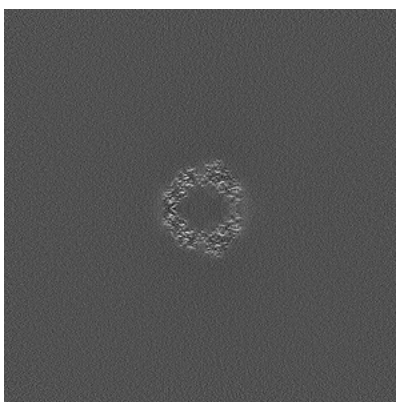


Z Index: 300

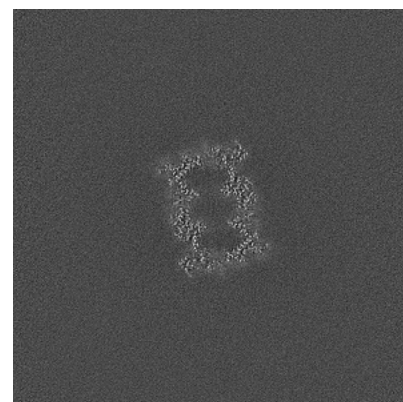
6.2.2 Raw map



X Index: 300



Y Index: 300

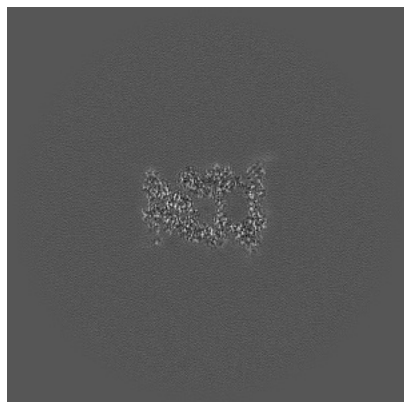


Z Index: 300

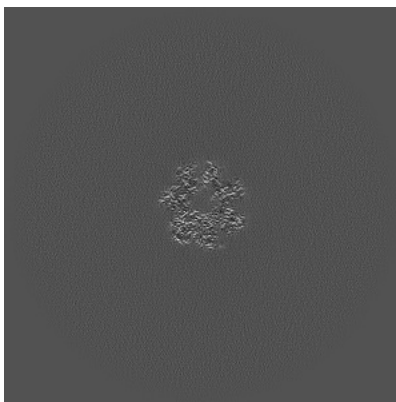
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

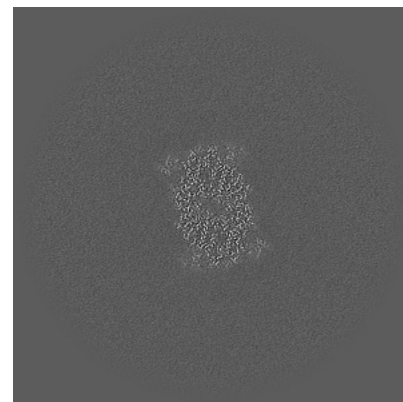
6.3.1 Primary map



X Index: 273

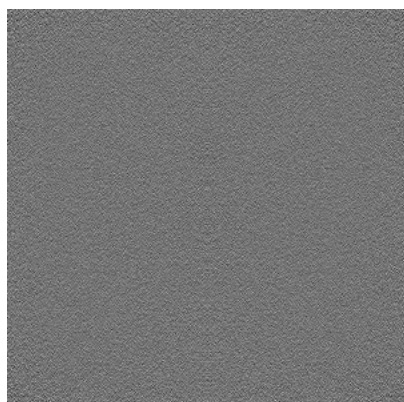


Y Index: 273

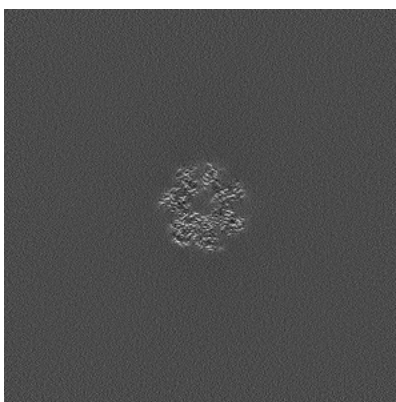


Z Index: 268

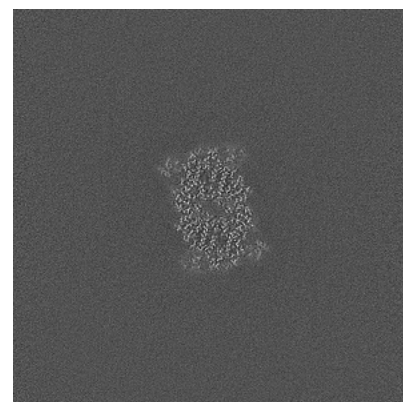
6.3.2 Raw map



X Index: 0



Y Index: 273

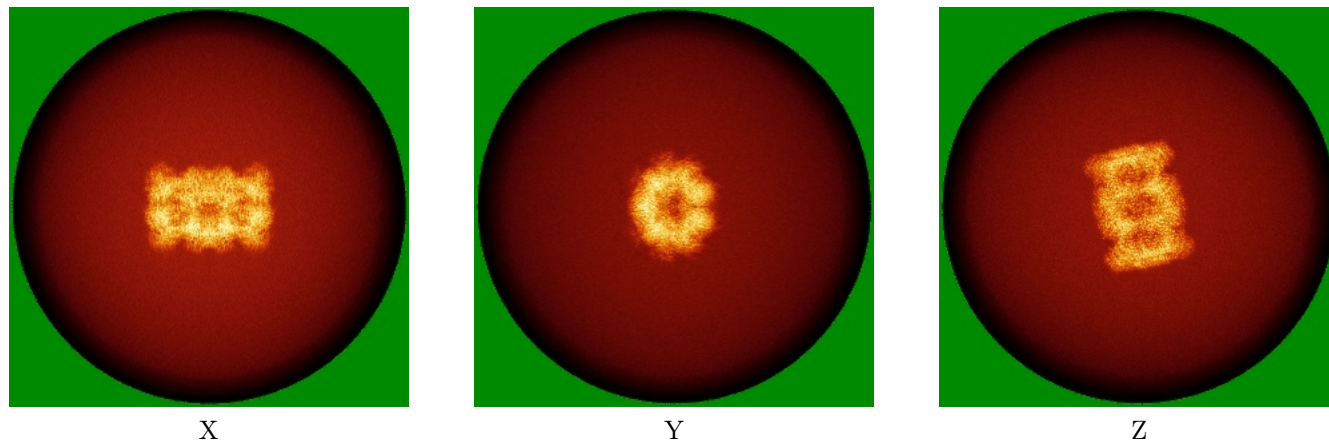


Z Index: 268

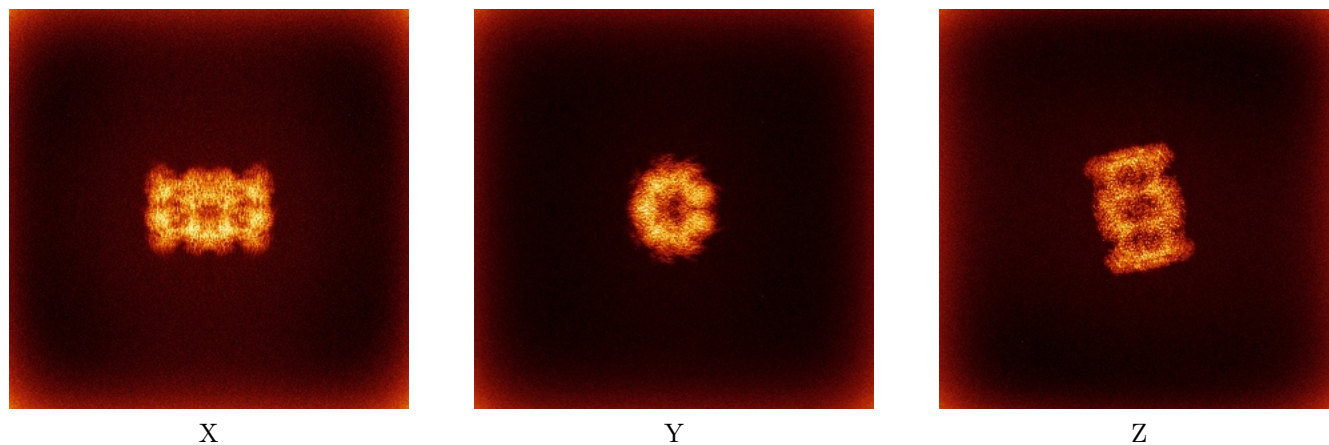
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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



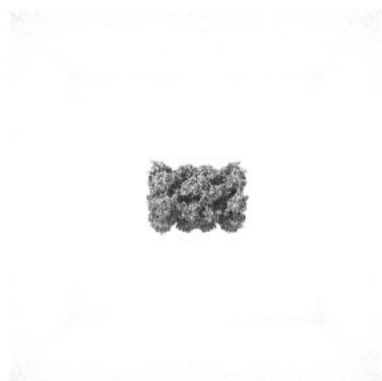
Y



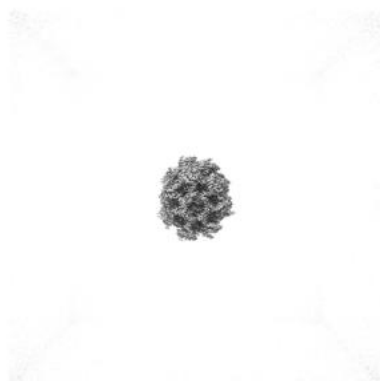
Z

The images above show the 3D surface view of the map at the recommended contour level 0.276. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

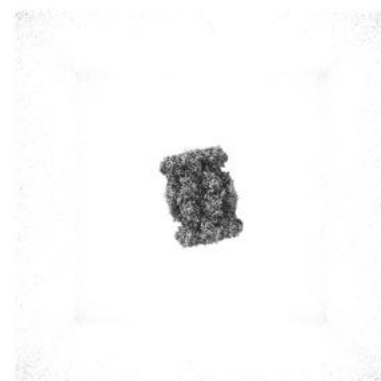
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

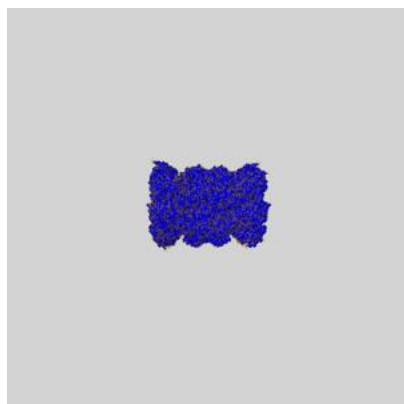
6.6 Mask visualisation [i](#)

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

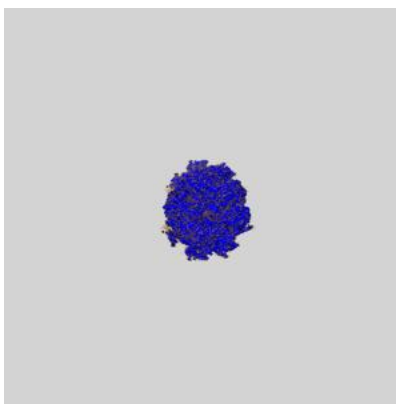
A mask typically either:

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

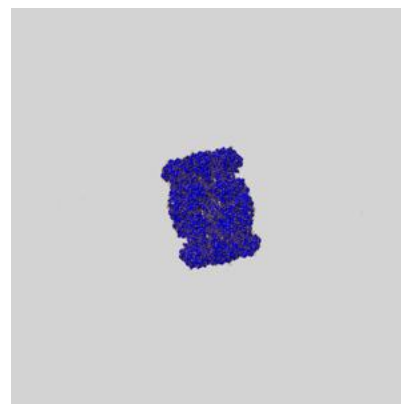
6.6.1 emd_19529_msk_1.map [i](#)



X



Y

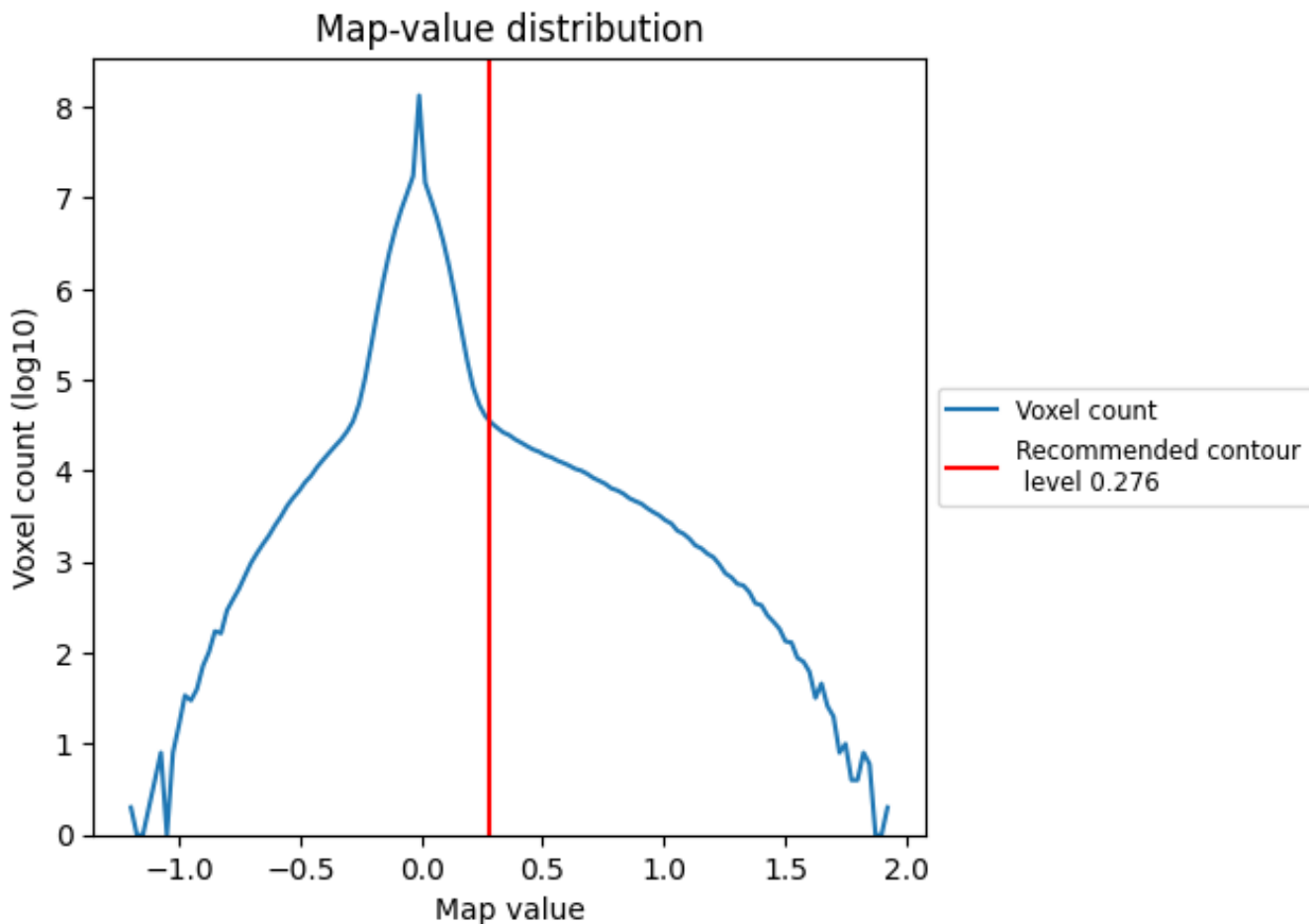


Z

7 Map analysis [i](#)

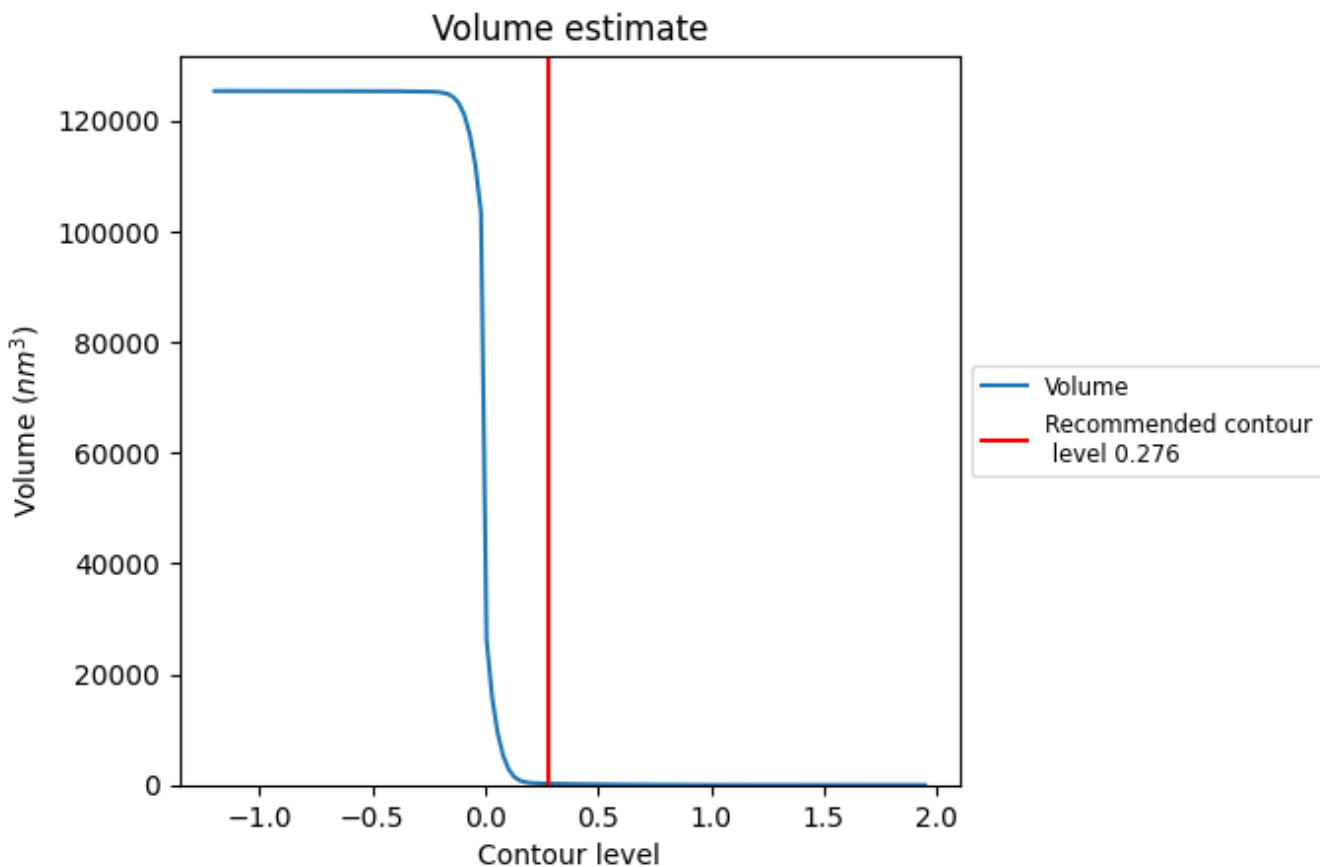
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

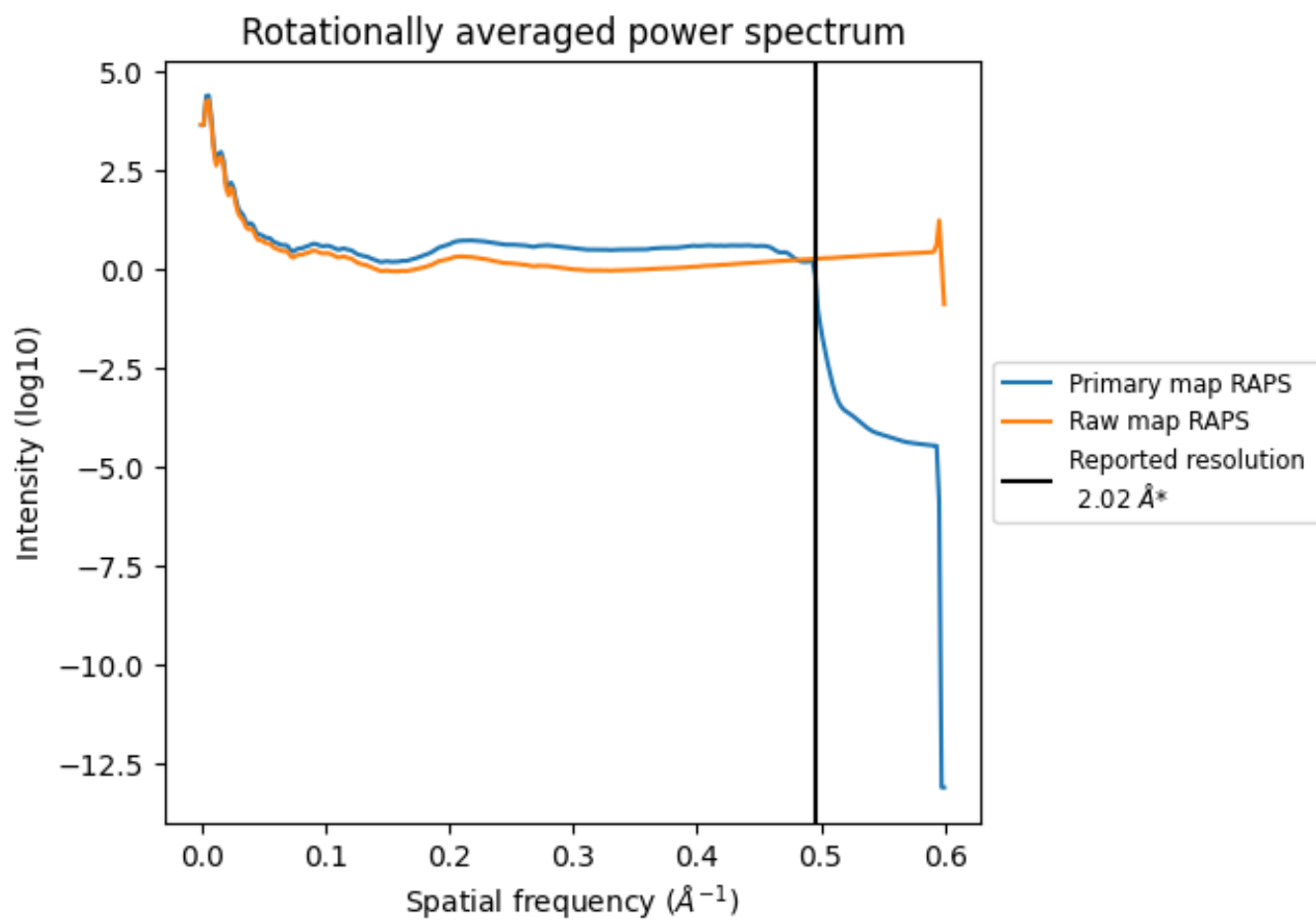
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm³; this corresponds to an approximate mass of 217 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](#)

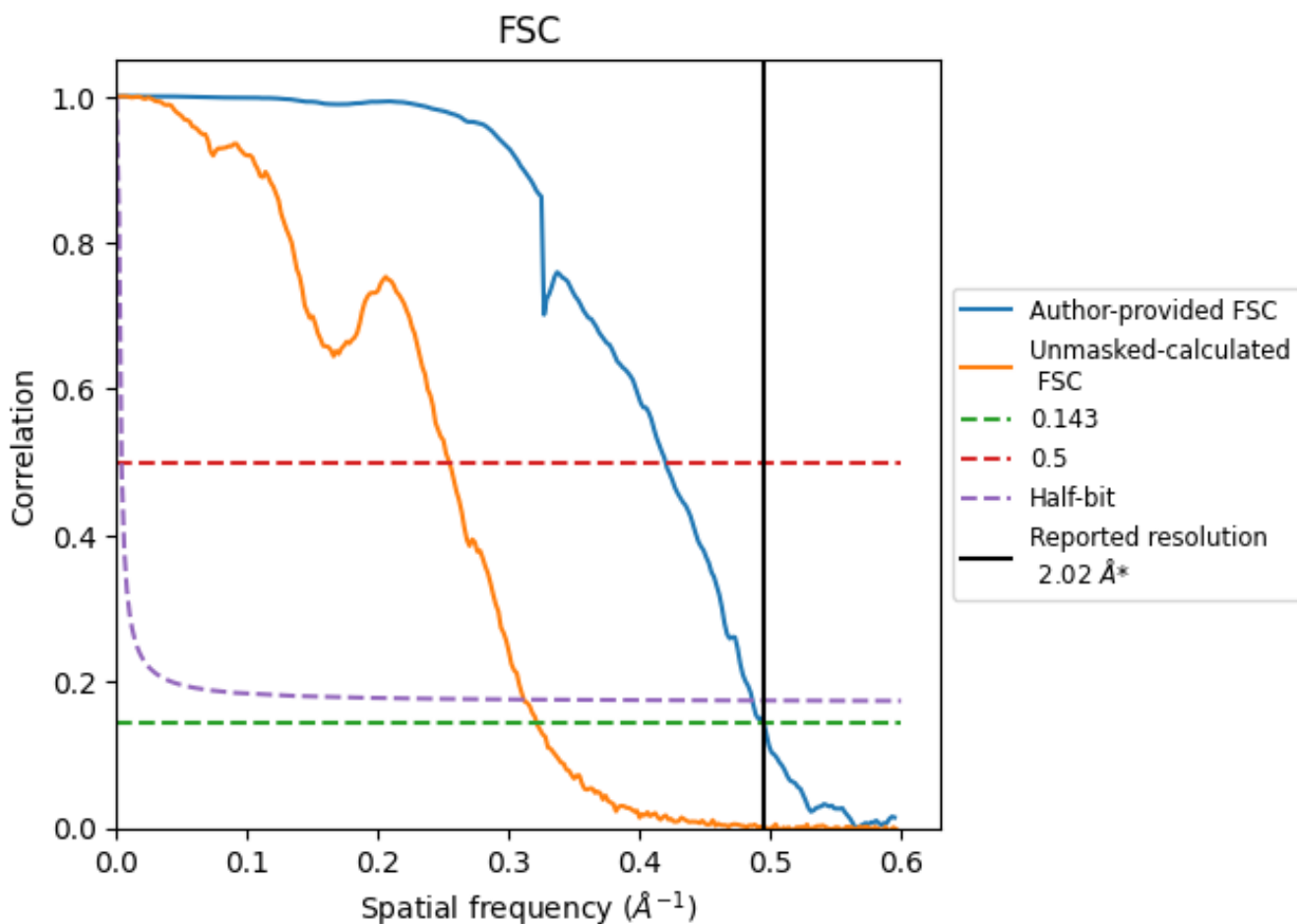


*Reported resolution corresponds to spatial frequency of 0.495 Å⁻¹

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 0.495 \AA^{-1}

8.2 Resolution estimates [i](#)

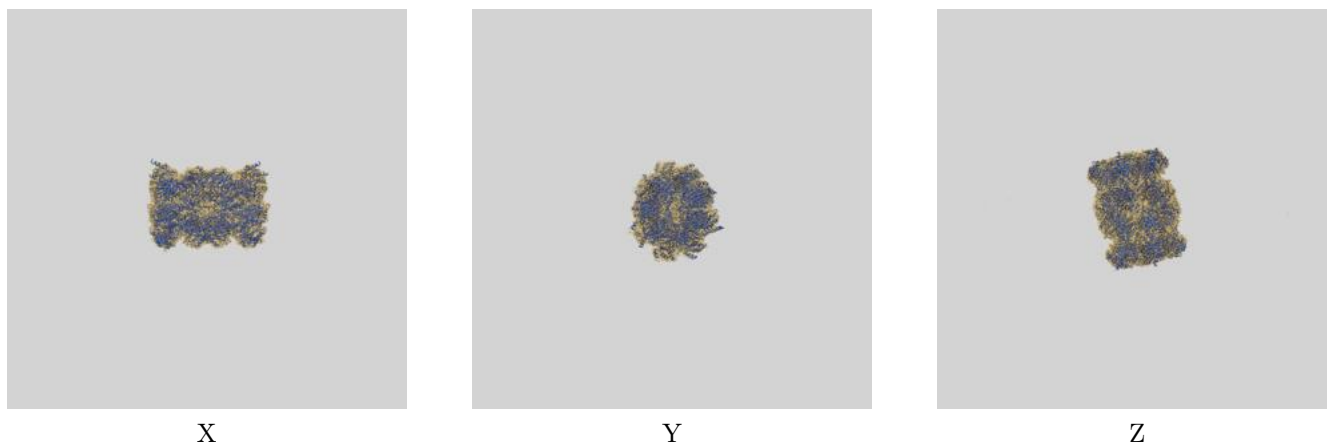
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.02	-	-
Author-provided FSC curve	2.02	2.38	2.06
Unmasked-calculated*	3.11	3.93	3.21

*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 3.11 differs from the reported value 2.02 by more than 10 %

9 Map-model fit [i](#)

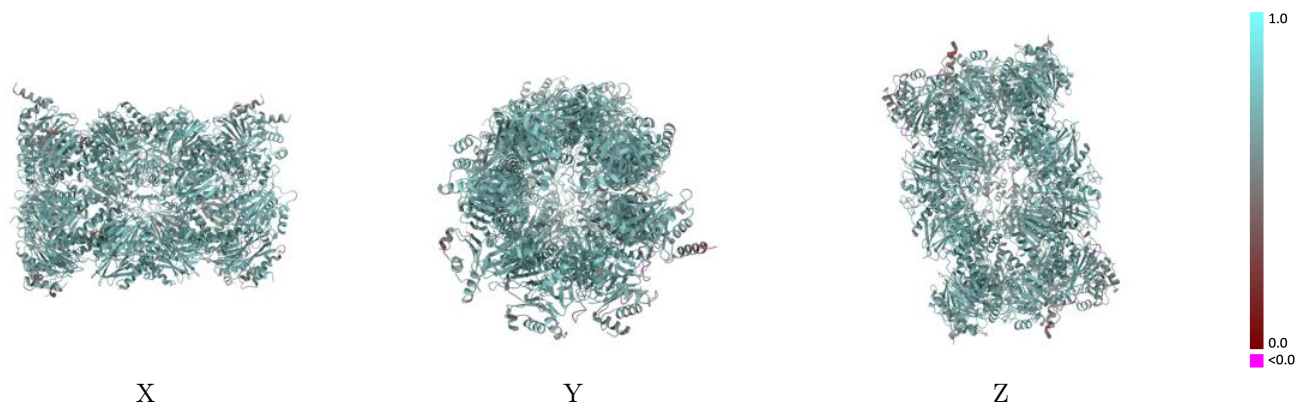
This section contains information regarding the fit between EMDB map EMD-19529 and PDB model 8RVQ. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



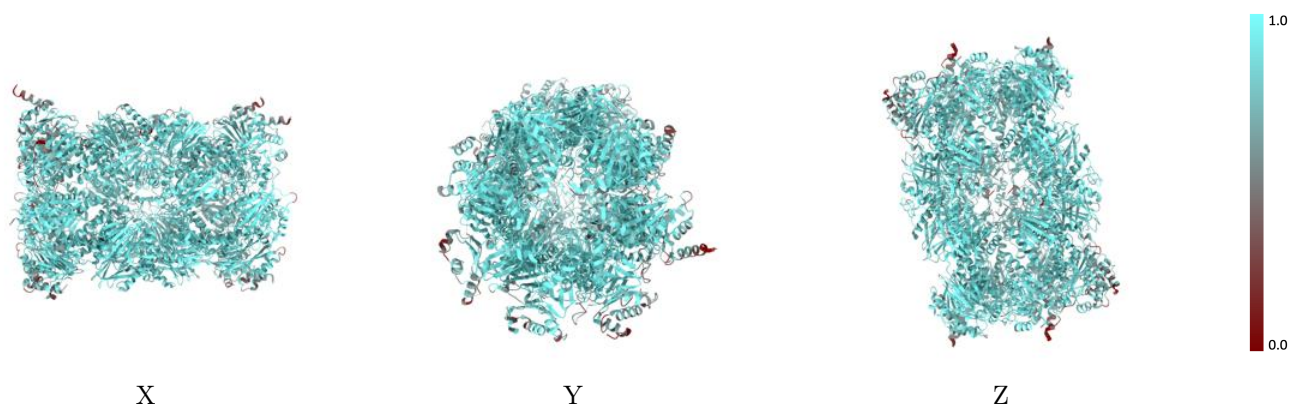
The images above show the 3D surface view of the map at the recommended contour level 0.276 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



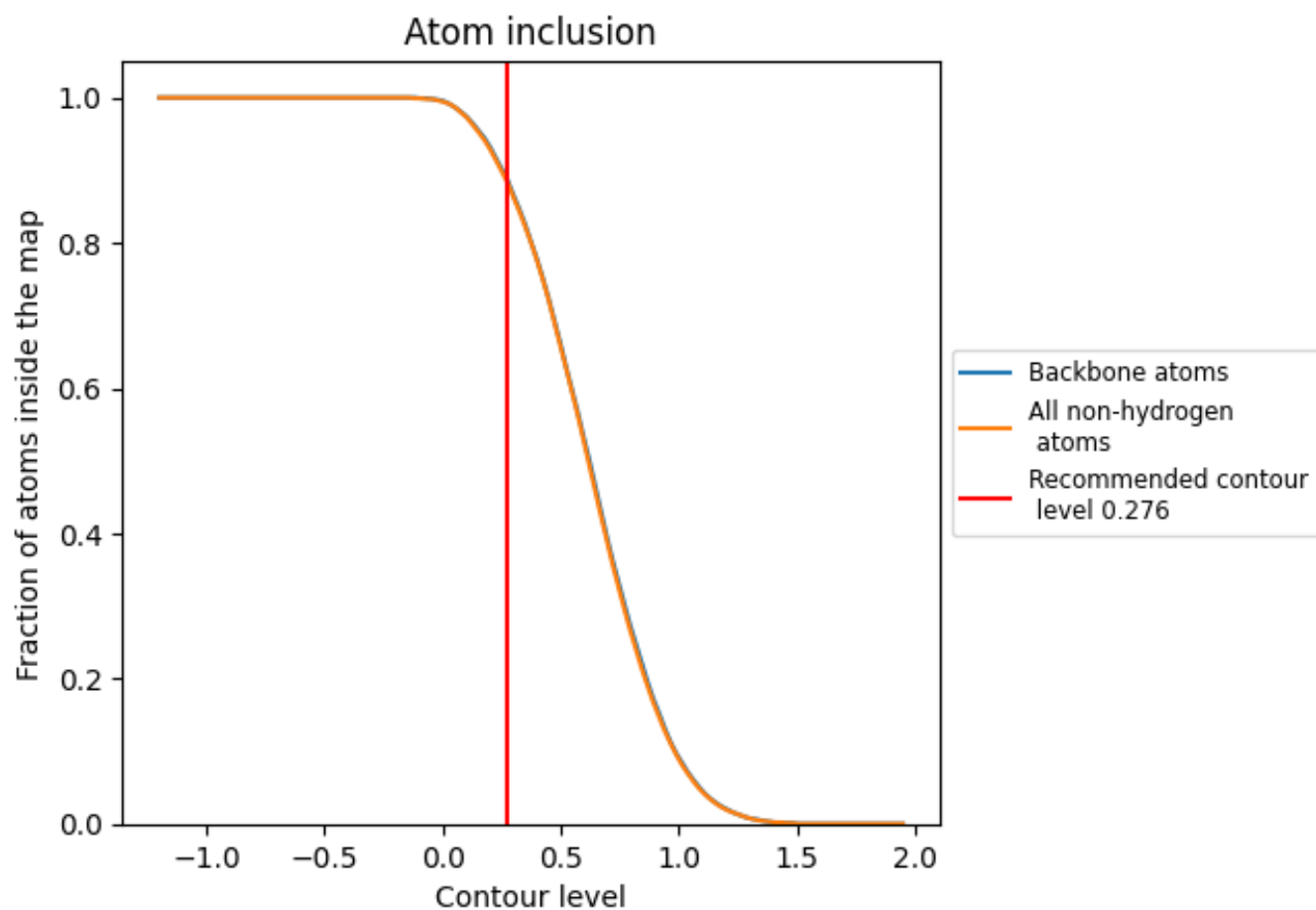
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.276).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.276) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.6590
1	 0.9210	 0.6720
2	 0.9320	 0.6820
A	 0.8340	 0.6460
B	 0.8630	 0.6430
C	 0.7960	 0.6180
D	 0.8120	 0.6160
E	 0.8890	 0.6580
F	 0.9220	 0.6730
G	 0.8720	 0.6570
H	 0.9410	 0.6910
I	 0.9370	 0.6820
J	 0.9300	 0.6760
K	 0.8440	 0.6420
L	 0.9250	 0.6780
M	 0.9200	 0.6730
N	 0.9330	 0.6820
O	 0.8320	 0.6410
P	 0.8630	 0.6410
Q	 0.7900	 0.6180
R	 0.8090	 0.6200
S	 0.8910	 0.6620
T	 0.9220	 0.6750
U	 0.8720	 0.6570
V	 0.9410	 0.6900
W	 0.9370	 0.6810
X	 0.9290	 0.6750
Y	 0.8440	 0.6410
Z	 0.9250	 0.6790

