



wwPDB EM Validation Summary Report ⓘ

Aug 17, 2024 – 12:43 pm BST

PDB ID : 8QYO
EMDB ID : EMD-18760
Title : Human proteasome 20S core particle
Authors : Schulman, B.A.; Hanna, J.W.; Harper, J.W.; Adolf, F.; Du, J.; Rawson, S.D.;
Walsh Jr, R.M.; Goodall, E.A.
Deposited on : 2023-10-26
Resolution : 2.84 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

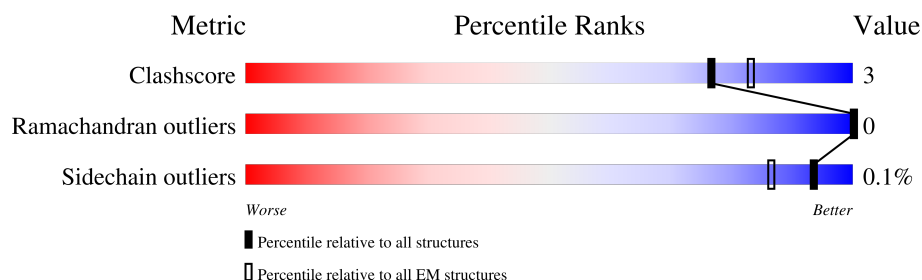
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	<div> <div>22%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	O	234	<div> <div>23%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
2	B	261	<div> <div>23%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
2	P	261	<div> <div>23%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
3	C	248	<div> <div>31%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
3	Q	248	<div> <div>29%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
4	D	241	<div> <div>19%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
4	R	241	<div> <div>18%</div> <div>85%</div> <div>10%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	263	
11	Y	263	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	239	
14	b	239	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 47940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1783	1141	300	336	6		
1	O	229	Total	C	N	O	S	0	0
			1783	1141	300	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	245	Total	C	N	O	S	0	0
			1922	1212	332	368	10		
2	P	245	Total	C	N	O	S	0	0
			1922	1212	332	368	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	237	Total	C	N	O	S	0	0
			1867	1171	331	360	5		
3	Q	237	Total	C	N	O	S	0	0
			1867	1171	331	360	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	227	Total	C	N	O	S	0	0
			1736	1093	288	344	11		
4	R	227	Total	C	N	O	S	0	0
			1736	1093	288	344	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	234	Total	C	N	O	S	0	0
			1837	1151	329	346	11		
5	S	234	Total	C	N	O	S	0	0
			1837	1151	329	346	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	239	Total	C	N	O	S	0	0
			1870	1187	320	352	11		
6	T	239	Total	C	N	O	S	0	0
			1870	1187	320	352	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	237	Total	C	N	O	S	0	0
			1839	1163	310	353	13		
7	U	237	Total	C	N	O	S	0	0
			1839	1163	310	353	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	219	Total	C	N	O	S	0	0
			1650	1039	282	317	12		
8	V	219	Total	C	N	O	S	0	0
			1650	1039	282	317	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1561	1001	264	287	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	0	0
			1561	1001	264	287	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1553	979	271	294	9		
11	Y	201	Total	C	N	O	S	0	0
			1553	979	271	294	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	208	Total	C	N	O	S	0	0
			1613	1022	276	305	10		
12	Z	208	Total	C	N	O	S	0	0
			1613	1022	276	305	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	215	Total	C	N	O	S	0	0
			1680	1059	290	319	12		
13	a	215	Total	C	N	O	S	0	0
			1680	1059	290	319	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	234	THR	ILE	variant	UNP P28070
a	234	THR	ILE	variant	UNP P28070

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	196	Total	C	N	O	S	0	0
			1468	916	252	288	12		
14	b	196	Total	C	N	O	S	0	0
			1468	916	252	288	12		

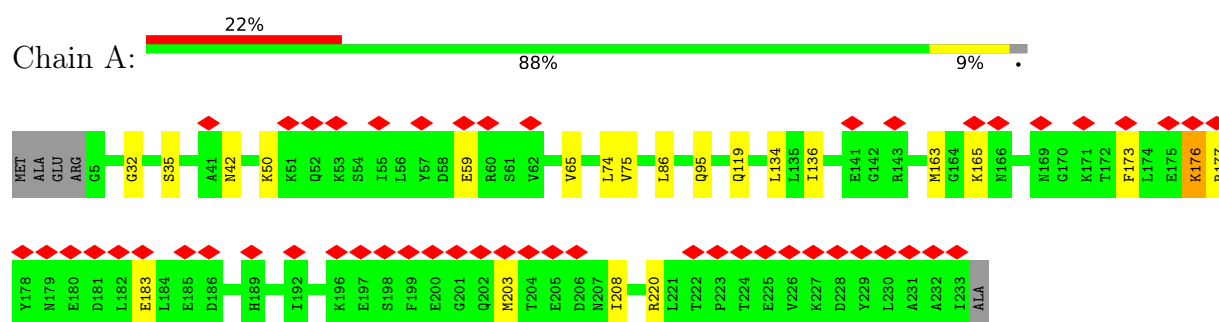
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	145	GLY	VAL	variant	UNP P28072
b	145	GLY	VAL	variant	UNP P28072

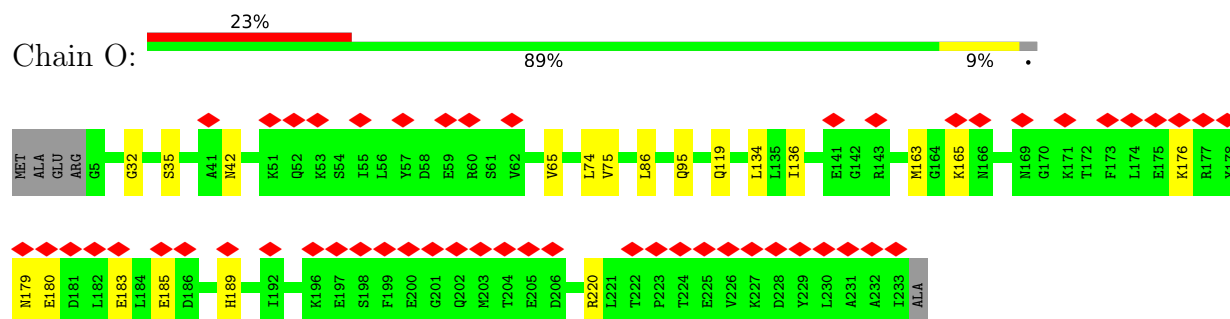
3 Residue-property plots [i](#)

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.

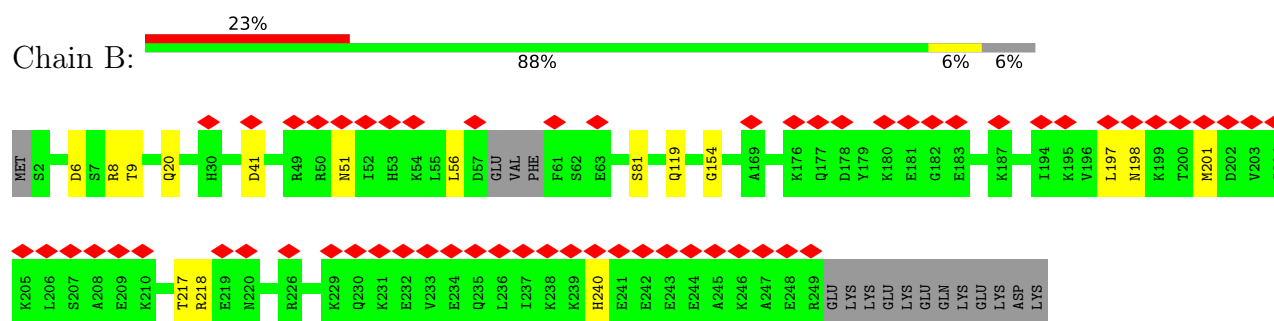
- Molecule 1: Proteasome subunit alpha type-2



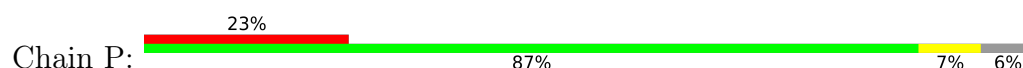
- Molecule 1: Proteasome subunit alpha type-2

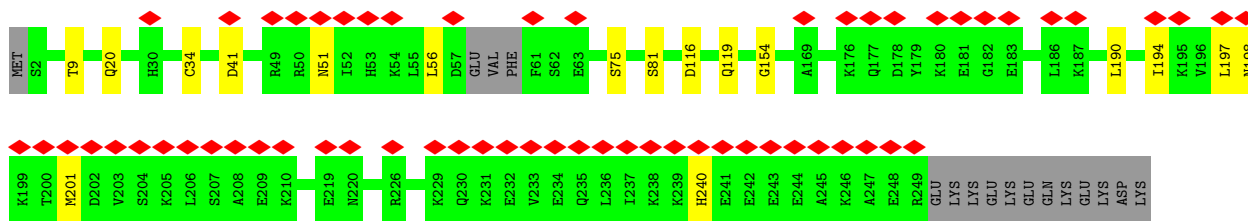


- Molecule 2: Proteasome subunit alpha type-4

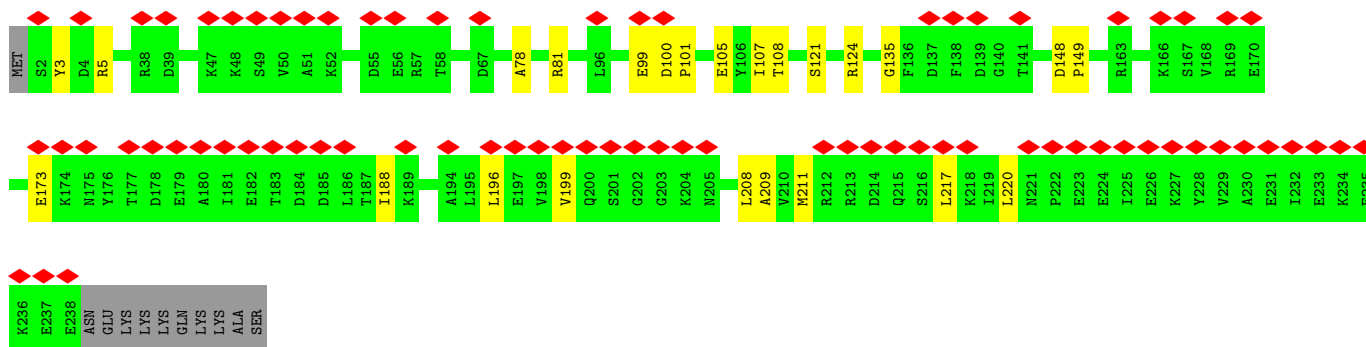
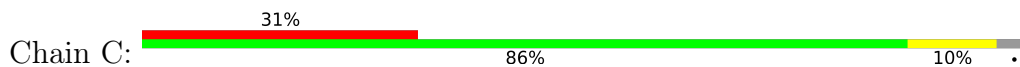


- Molecule 2: Proteasome subunit alpha type-4

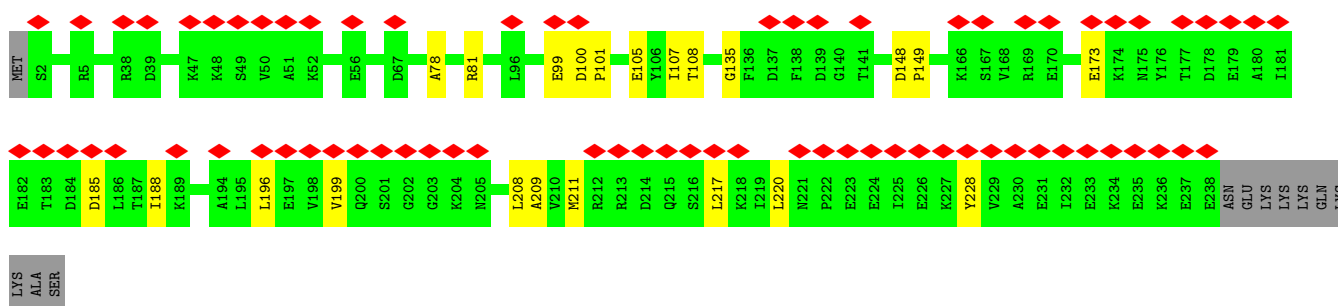
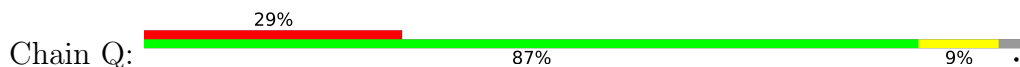




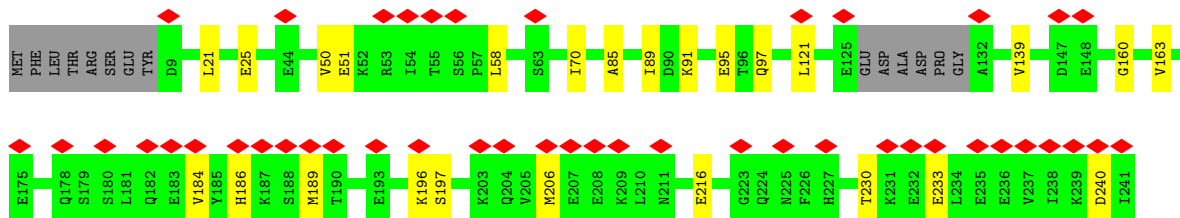
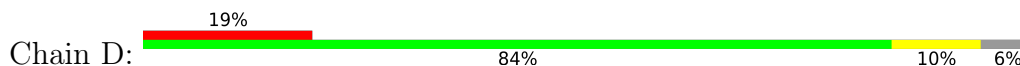
• Molecule 3: Proteasome subunit alpha type-7



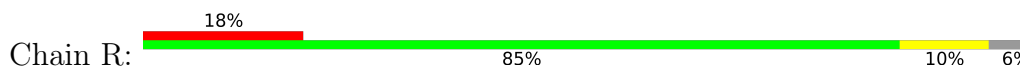
• Molecule 3: Proteasome subunit alpha type-7

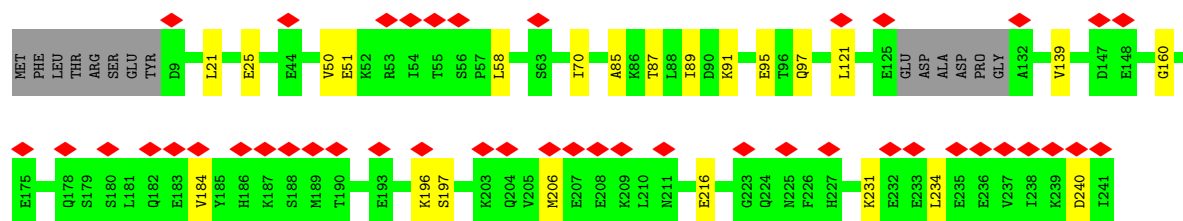


• Molecule 4: Proteasome subunit alpha type-5

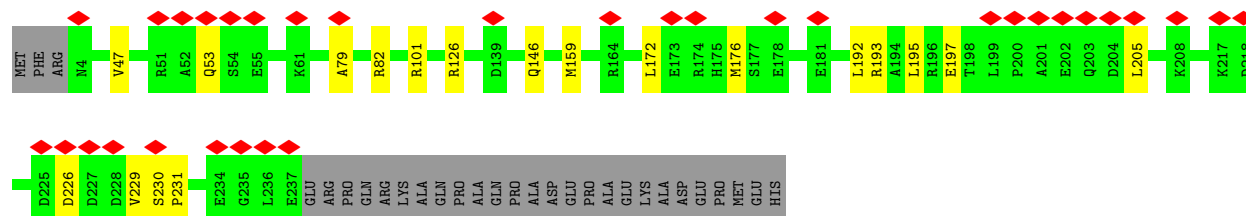
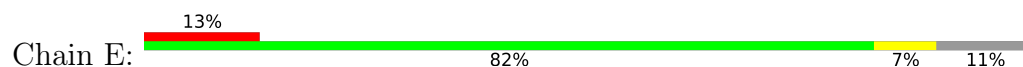


• Molecule 4: Proteasome subunit alpha type-5

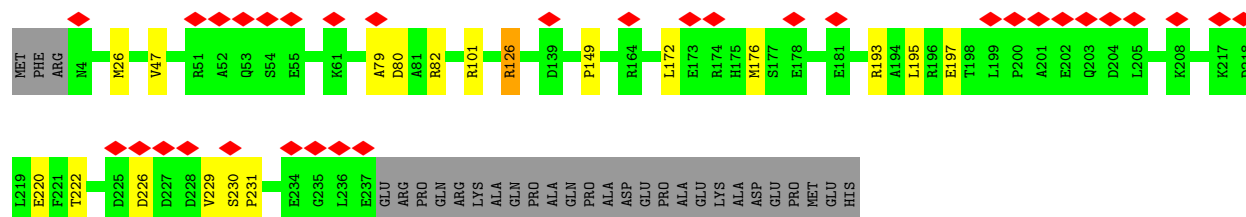
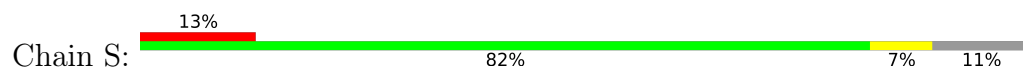




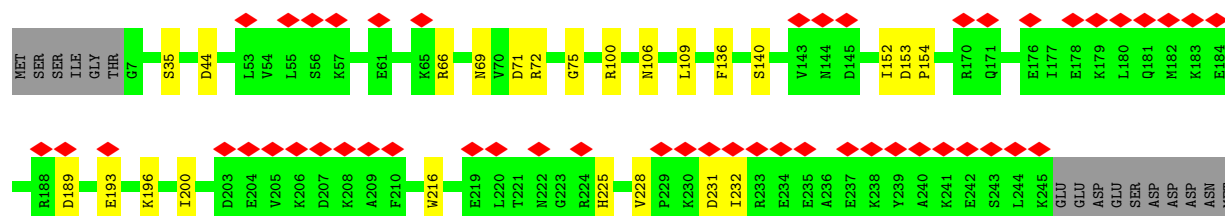
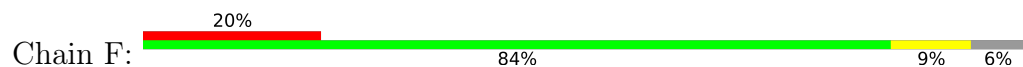
• Molecule 5: Proteasome subunit alpha type-1



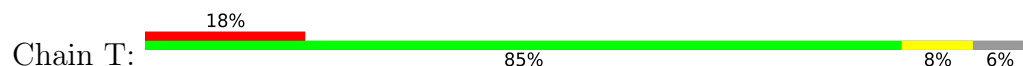
• Molecule 5: Proteasome subunit alpha type-1

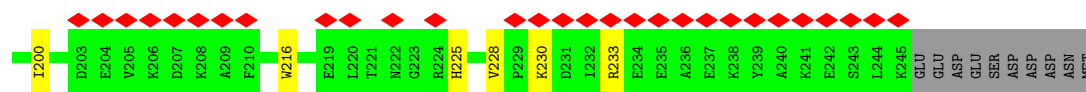


• Molecule 6: Proteasome subunit alpha type-3

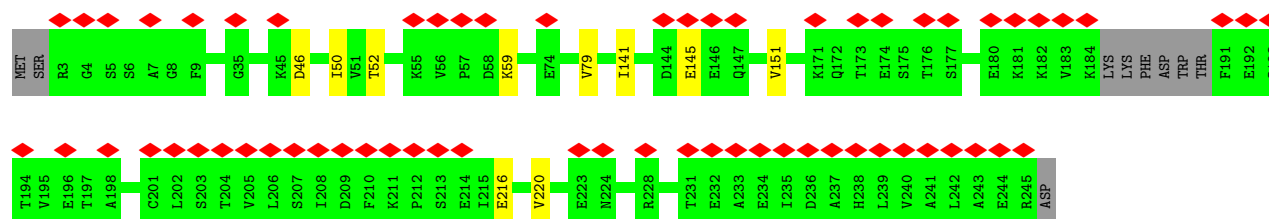


• Molecule 6: Proteasome subunit alpha type-3

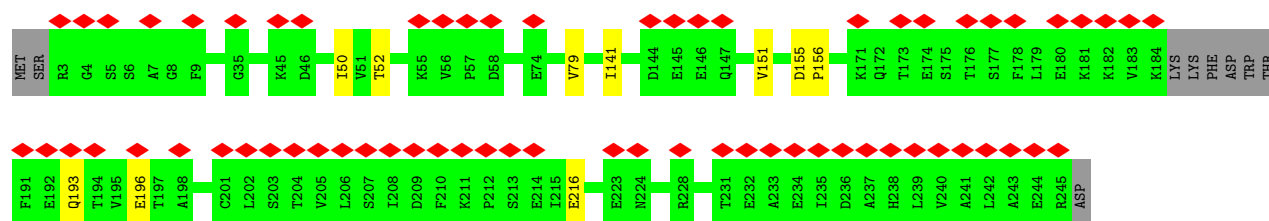




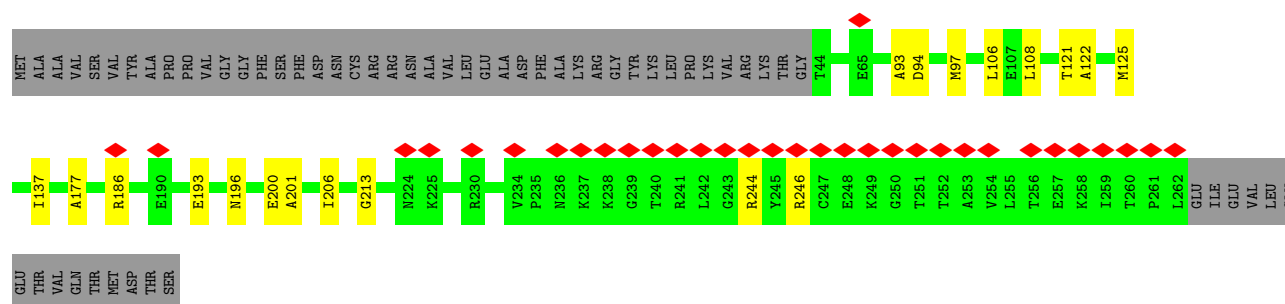
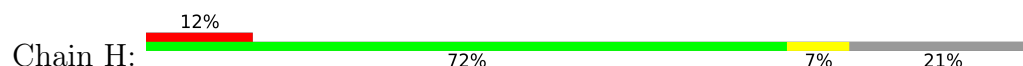
• Molecule 7: Proteasome subunit alpha type-6



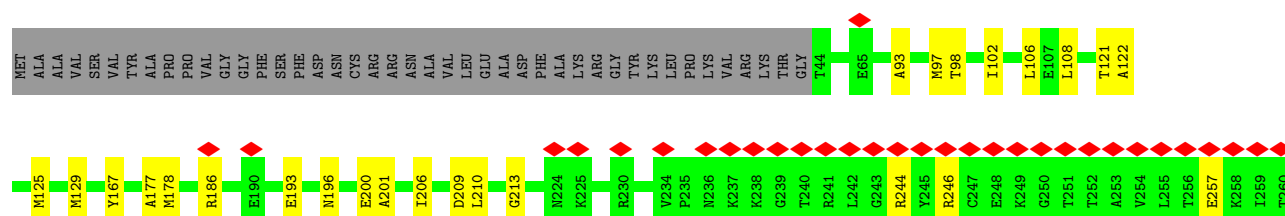
• Molecule 7: Proteasome subunit alpha type-6

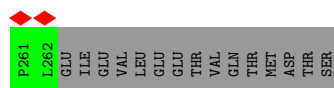


• Molecule 8: Proteasome subunit beta type-7

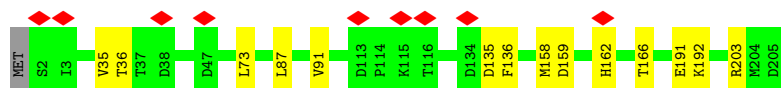


• Molecule 8: Proteasome subunit beta type-7

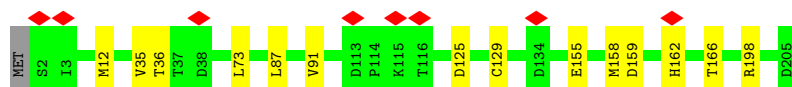




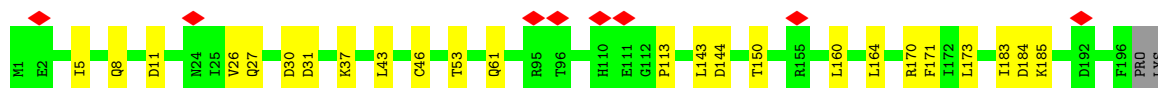
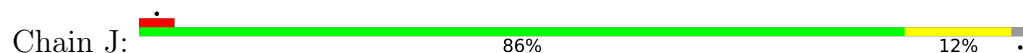
- Molecule 9: Proteasome subunit beta type-3



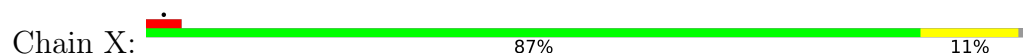
- Molecule 9: Proteasome subunit beta type-3



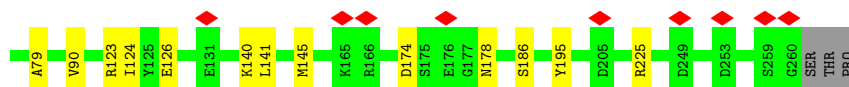
- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-5




- Molecule 11: Proteasome subunit beta type-5

Chain Y:  72% 5% 24%

MET ALA LEU SER ALA VAL LEU ARG PRO LEU PRO VAL ASN GLN ARG PHE PHE GLY LEU GLY ARG ASP LEU LEU ASP LEU LEU GLY PRO GLY SER LEU SER ASP GLY LEU SER LEU ALA PRO GLY TRP VAL PRO GLU PRO GLU ILE ILE MET LEU HIS GLY T60

A79 V90 R123 I124 Y125 E126 E131 K140 L141 M145 K165 R166 D174 S175 E176 G177 N178 D205 R225 D249 N250 D253 S259 G260 SER THR PRO


- Molecule 12: Proteasome subunit beta type-1

Chain L:  7% 82% 14%

MET LEU SER THR ALA MET TYR SER ALA PRO GLY ARG ASP LEU MET GLY MET GLU PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU R29 A44 G45 E46 D47 F48 R56 F61 D67 K73 L74 T75 D76 E143 E144 G145 K146 V149 F183 M186 Q187 ASN VAL

GLU HIS VAL P193 R198 D219 K228 E229 G230 I231 D241


- Molecule 12: Proteasome subunit beta type-1

Chain Z:  7% 83% 14%

MET LEU SER THR ALA MET TYR SER ALA PRO GLY ARG ASP LEU MET GLY MET GLU PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU R29 A44 G45 E46 D47 F48 R56 F61 D67 K73 D76 E143 E144 G145 K146 V149 K164 F183 M186 Q187 ASN

VAL GLU HIS VAL P193 R198 D219 K228 E229 G230 I231 D241


- Molecule 13: Proteasome subunit beta type-4

Chain M:  5% 75% 7% 19%

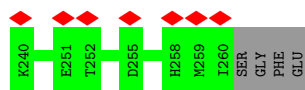
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D162 L167 G168 Y169 V170 M172 L182 A183 T184 K201 Q202 R211 E215 R231 F232 T238 E239 K240 E251 T252 D255 H258 N259 I260 SER GLY PHE GLU

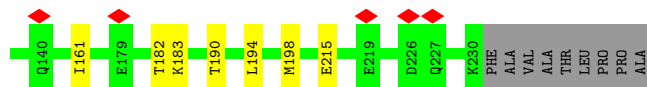
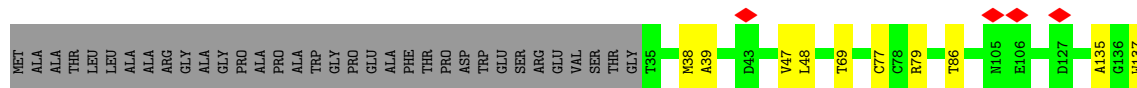
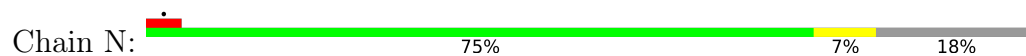
- Molecule 13: Proteasome subunit beta type-4

Chain a:  6% 81% 19%

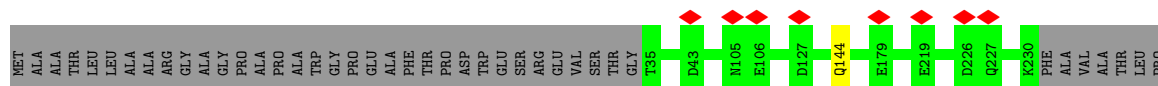
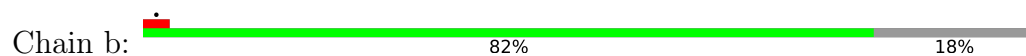
MET GLU ALA PHE LEU GLY SER ARG GLY LEU TRP ALA GLY GLY PRO PRO ALA ALA GLY GLN PHE TYR ARG ILE SER THR PRO ASP PHE MET ASP PRO ALA SER ALA LEU TYR ARG GLY PRO ILE THR ARG T46 Q47 H48 G123 D124 D162 G163 E164 E200 K201 Q202



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	569831	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.35	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.052	Depositor
Minimum map value	-2.057	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.112	Depositor
Recommended contour level	0.636	Depositor
Map size (\AA)	330.68, 330.68, 330.68	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.181, 1.181, 1.181	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/1822	0.50	0/2470
1	O	0.33	0/1822	0.51	0/2470
2	B	0.31	0/1950	0.51	0/2626
2	P	0.31	0/1950	0.51	0/2626
3	C	0.30	0/1893	0.53	0/2554
3	Q	0.30	0/1893	0.53	0/2554
4	D	0.29	0/1761	0.50	0/2376
4	R	0.30	0/1761	0.50	0/2376
5	E	0.29	0/1871	0.53	0/2529
5	S	0.30	0/1871	0.54	0/2529
6	F	0.32	0/1905	0.53	0/2565
6	T	0.32	0/1905	0.53	0/2565
7	G	0.33	0/1869	0.51	0/2524
7	U	0.32	0/1869	0.51	0/2524
8	H	0.32	0/1677	0.53	0/2270
8	V	0.32	0/1677	0.54	0/2270
9	I	0.33	0/1620	0.55	0/2184
9	W	0.33	0/1620	0.54	0/2184
10	J	0.35	0/1593	0.54	0/2156
10	X	0.36	0/1593	0.54	0/2156
11	K	0.36	0/1584	0.55	0/2140
11	Y	0.35	0/1584	0.55	0/2140
12	L	0.33	0/1641	0.56	0/2206
12	Z	0.33	0/1641	0.55	0/2206
13	M	0.36	0/1713	0.58	0/2319
13	a	0.36	0/1713	0.57	0/2319
14	N	0.34	0/1493	0.55	0/2019
14	b	0.35	0/1493	0.56	0/2019
All	All	0.33	0/48784	0.53	0/65876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1783	0	1771	14	0
1	O	1783	0	1771	12	0
2	B	1922	0	1937	13	0
2	P	1922	0	1937	11	0
3	C	1867	0	1884	18	0
3	Q	1867	0	1884	15	0
4	D	1736	0	1734	16	0
4	R	1736	0	1734	15	0
5	E	1837	0	1826	10	0
5	S	1837	0	1826	10	0
6	F	1870	0	1857	14	0
6	T	1870	0	1857	13	0
7	G	1839	0	1849	8	0
7	U	1839	0	1849	5	0
8	H	1650	0	1672	11	0
8	V	1650	0	1672	14	0
9	I	1591	0	1609	8	0
9	W	1591	0	1609	9	0
10	J	1561	0	1558	17	0
10	X	1561	0	1558	14	0
11	K	1553	0	1509	10	0
11	Y	1553	0	1509	8	0
12	L	1613	0	1616	5	0
12	Z	1613	0	1616	5	0
13	M	1680	0	1654	11	0
13	a	1680	0	1654	0	0
14	N	1468	0	1432	10	0
14	b	1468	0	1432	0	0
All	All	47940	0	47816	264	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 3.

The worst 5 of 264 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)
2:P:9:THR:HG23	2:P:20:GLN:HG3	1.69	0.75
13:M:83:ASN:OD1	13:M:231:ARG:NH2	2.22	0.72
14:N:69:THR:OG1	14:N:77:CYS:SG	2.55	0.65
4:D:121:LEU:HD12	5:E:79:ALA:HB3	1.79	0.65
10:J:27:GLN:NE2	10:J:30:ASP:OD1	2.30	0.64

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	227/234 (97%)	223 (98%)	4 (2%)	0	100	100
1	O	227/234 (97%)	225 (99%)	2 (1%)	0	100	100
2	B	241/261 (92%)	236 (98%)	5 (2%)	0	100	100
2	P	241/261 (92%)	237 (98%)	4 (2%)	0	100	100
3	C	235/248 (95%)	232 (99%)	3 (1%)	0	100	100
3	Q	235/248 (95%)	232 (99%)	3 (1%)	0	100	100
4	D	223/241 (92%)	218 (98%)	5 (2%)	0	100	100
4	R	223/241 (92%)	217 (97%)	6 (3%)	0	100	100
5	E	232/263 (88%)	226 (97%)	6 (3%)	0	100	100
5	S	232/263 (88%)	226 (97%)	6 (3%)	0	100	100
6	F	237/255 (93%)	233 (98%)	4 (2%)	0	100	100
6	T	237/255 (93%)	233 (98%)	4 (2%)	0	100	100
7	G	233/246 (95%)	228 (98%)	5 (2%)	0	100	100
7	U	233/246 (95%)	229 (98%)	4 (2%)	0	100	100
8	H	217/277 (78%)	213 (98%)	4 (2%)	0	100	100
8	V	217/277 (78%)	212 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
10	J	194/201 (96%)	188 (97%)	6 (3%)	0	100	100
10	X	194/201 (96%)	189 (97%)	5 (3%)	0	100	100
11	K	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
11	Y	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
12	L	204/241 (85%)	195 (96%)	9 (4%)	0	100	100
12	Z	204/241 (85%)	197 (97%)	7 (3%)	0	100	100
13	M	213/264 (81%)	204 (96%)	9 (4%)	0	100	100
13	a	213/264 (81%)	205 (96%)	8 (4%)	0	100	100
14	N	194/239 (81%)	187 (96%)	7 (4%)	0	100	100
14	b	194/239 (81%)	187 (96%)	7 (4%)	0	100	100
All	All	6102/6876 (89%)	5943 (97%)	159 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/191 (98%)	186 (100%)	1 (0%)	88	94
1	O	187/191 (98%)	186 (100%)	1 (0%)	88	94
2	B	204/221 (92%)	204 (100%)	0	100	100
2	P	204/221 (92%)	204 (100%)	0	100	100
3	C	200/211 (95%)	200 (100%)	0	100	100
3	Q	200/211 (95%)	200 (100%)	0	100	100
4	D	191/203 (94%)	191 (100%)	0	100	100
4	R	191/203 (94%)	191 (100%)	0	100	100
5	E	200/224 (89%)	198 (99%)	2 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	200/224 (89%)	198 (99%)	2 (1%)	76	88
6	F	196/212 (92%)	196 (100%)	0	100	100
6	T	196/212 (92%)	196 (100%)	0	100	100
7	G	201/210 (96%)	201 (100%)	0	100	100
7	U	201/210 (96%)	201 (100%)	0	100	100
8	H	180/228 (79%)	180 (100%)	0	100	100
8	V	180/228 (79%)	180 (100%)	0	100	100
9	I	173/174 (99%)	173 (100%)	0	100	100
9	W	173/174 (99%)	173 (100%)	0	100	100
10	J	165/171 (96%)	165 (100%)	0	100	100
10	X	165/171 (96%)	165 (100%)	0	100	100
11	K	155/202 (77%)	155 (100%)	0	100	100
11	Y	155/202 (77%)	155 (100%)	0	100	100
12	L	173/199 (87%)	173 (100%)	0	100	100
12	Z	173/199 (87%)	173 (100%)	0	100	100
13	M	178/215 (83%)	178 (100%)	0	100	100
13	a	178/215 (83%)	178 (100%)	0	100	100
14	N	152/180 (84%)	152 (100%)	0	100	100
14	b	152/180 (84%)	151 (99%)	1 (1%)	84	91
All	All	5110/5682 (90%)	5103 (100%)	7 (0%)	93	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	176	LYS
5	S	101	ARG
14	b	144	GLN
5	S	126	ARG
5	E	126	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
10	X	8	GLN

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Mol	Chain	Res	Type
10	X	24	ASN
10	X	27	GLN
10	J	27	GLN
2	B	240	HIS

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 monosaccharides 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.

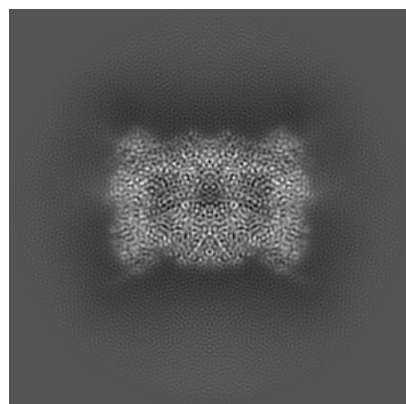
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18760. These allow visual inspection of the internal detail of the map and identification of artifacts.

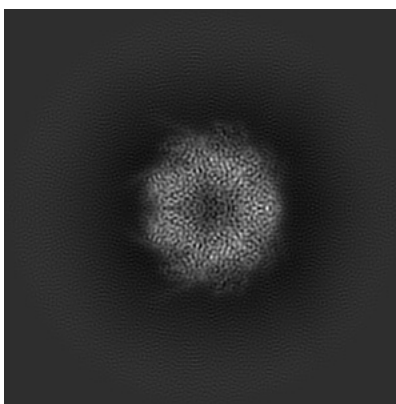
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

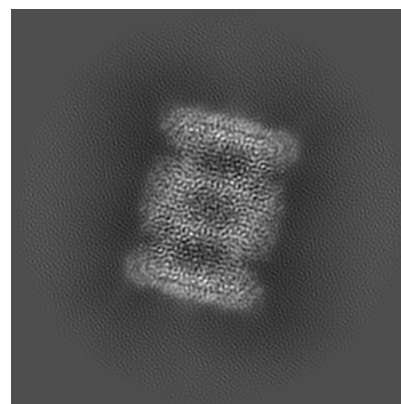
6.1.1 Primary map



X

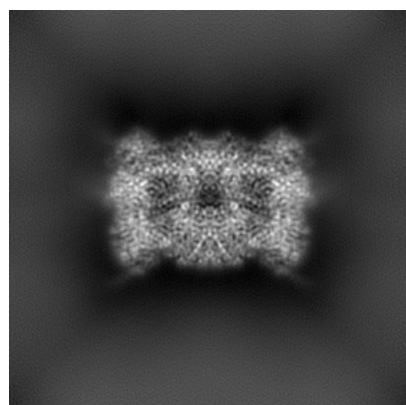


Y

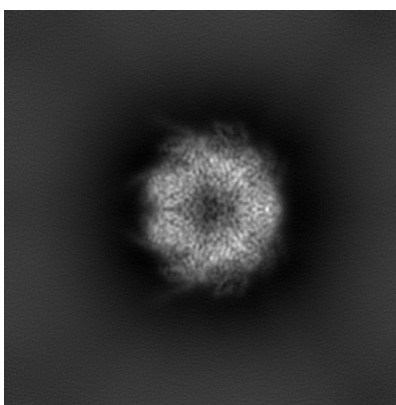


Z

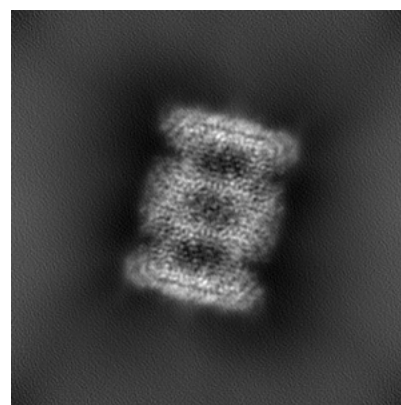
6.1.2 Raw map



X



Y

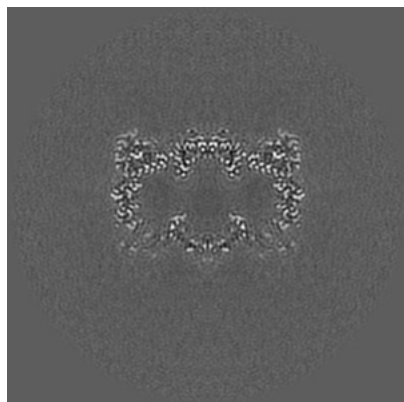


Z

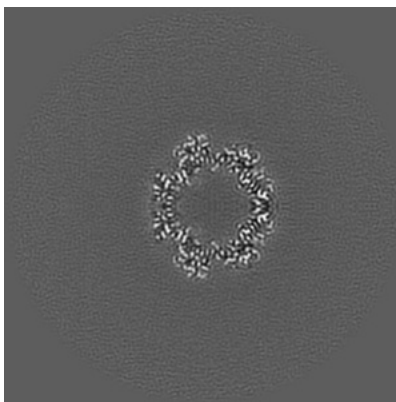
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

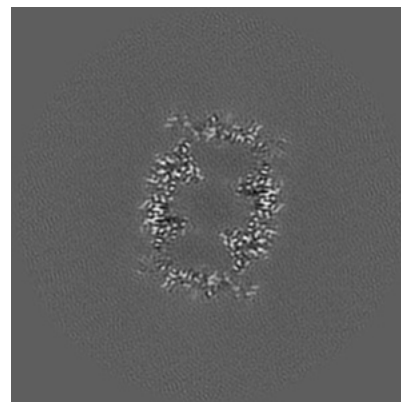
6.2.1 Primary map



X Index: 140

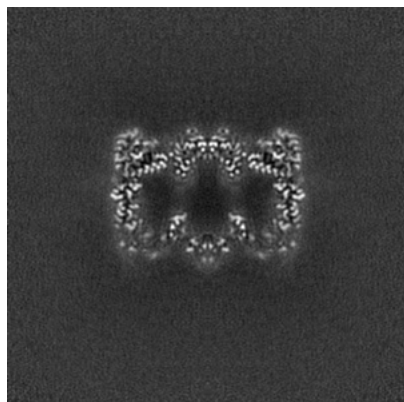


Y Index: 140

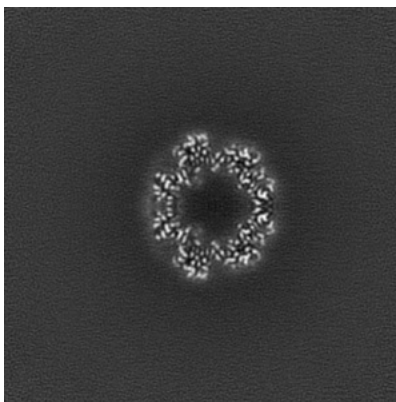


Z Index: 140

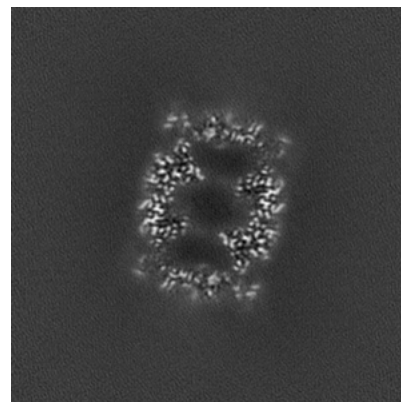
6.2.2 Raw map



X Index: 140



Y Index: 140

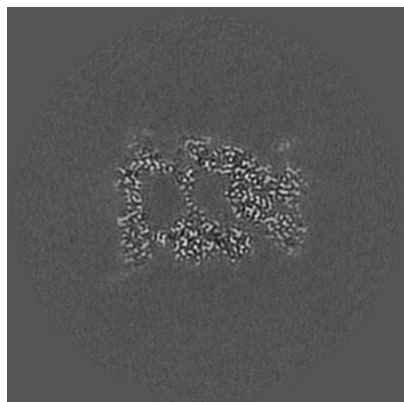


Z Index: 140

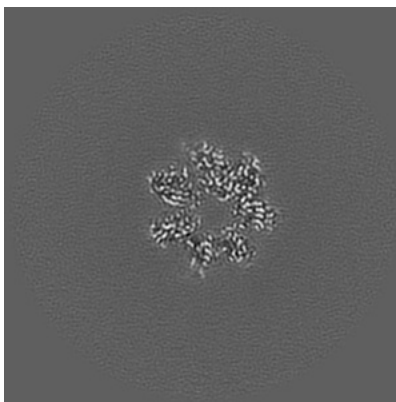
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

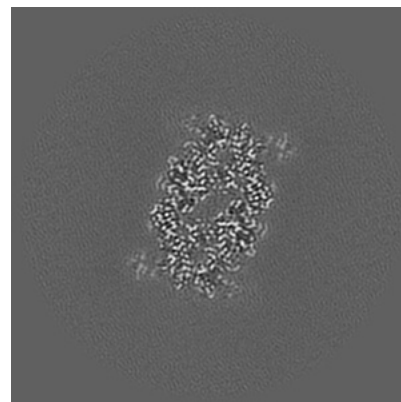
6.3.1 Primary map



X Index: 122

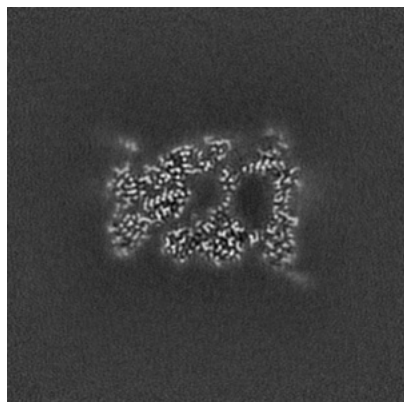


Y Index: 122

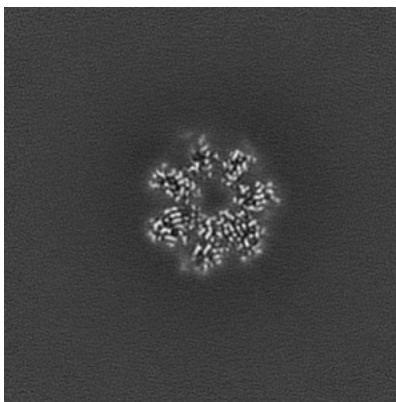


Z Index: 168

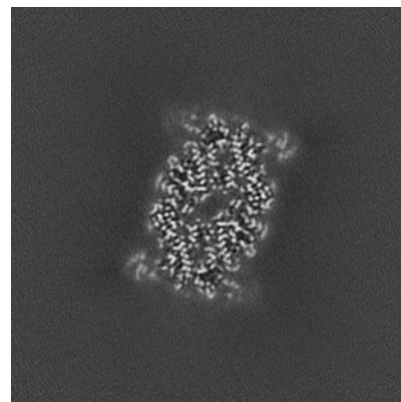
6.3.2 Raw map



X Index: 158



Y Index: 159

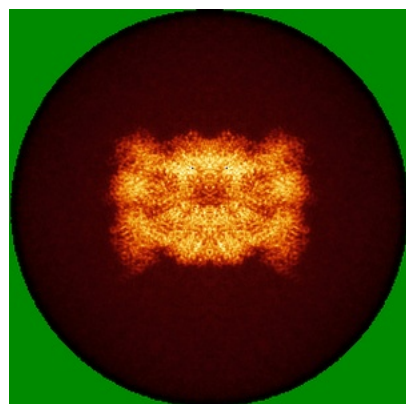


Z Index: 168

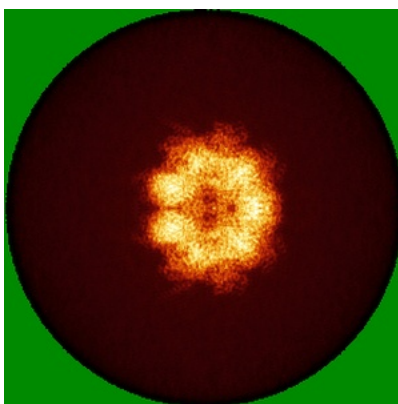
The images above show the largest variance slices of the map in three orthogonal directions.

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

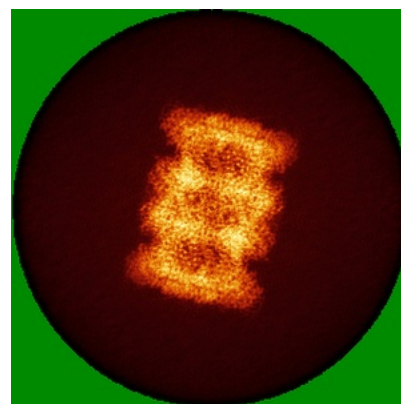
6.4.1 Primary map



X

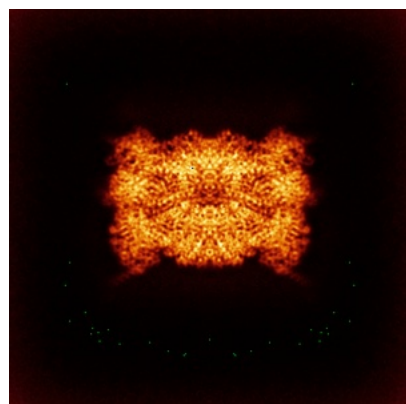


Y

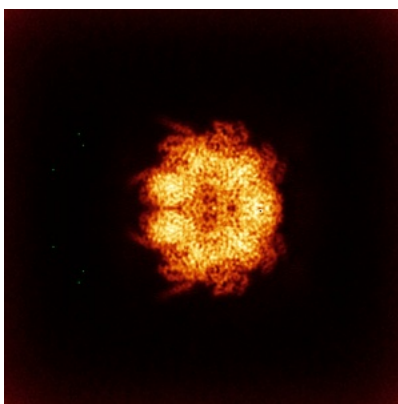


Z

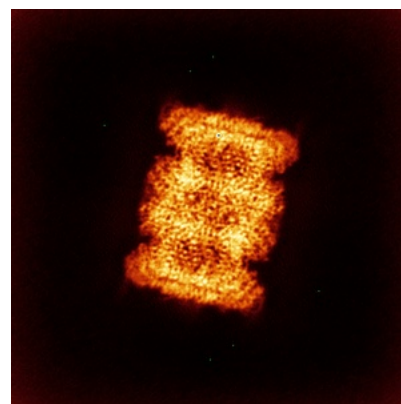
6.4.2 Raw map



X



Y

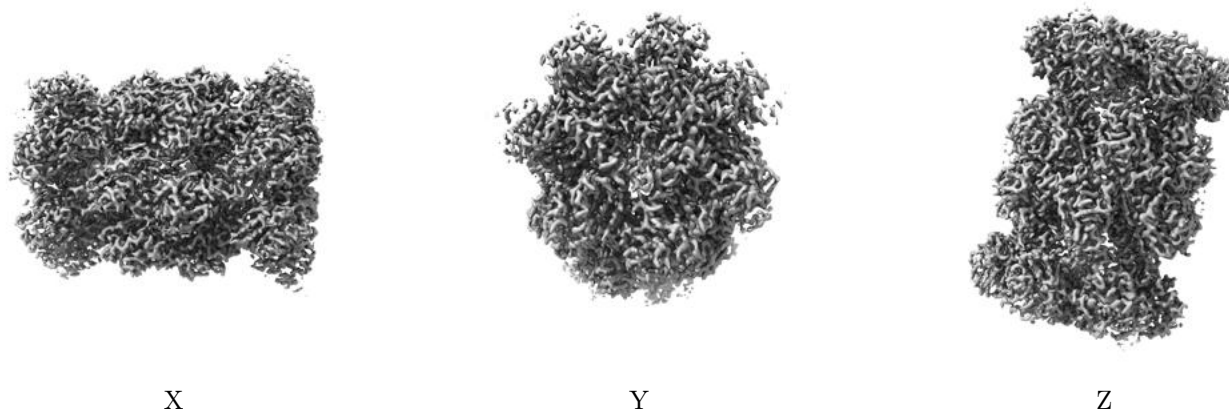


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.636. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

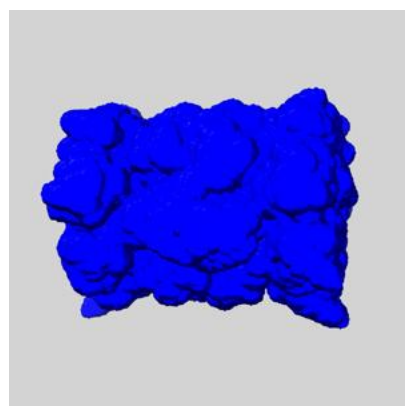
6.6 Mask visualisation [i](#)

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

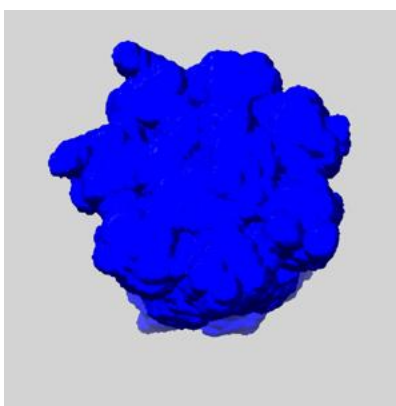
A mask typically either:

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

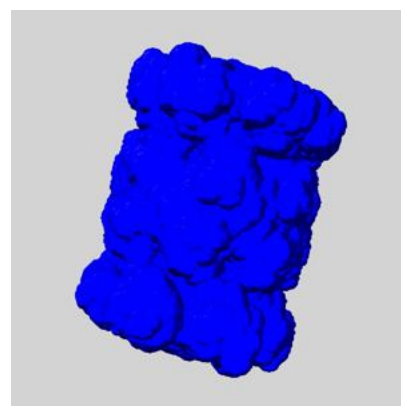
6.6.1 emd_18760_msk_1.map [i](#)



X



Y

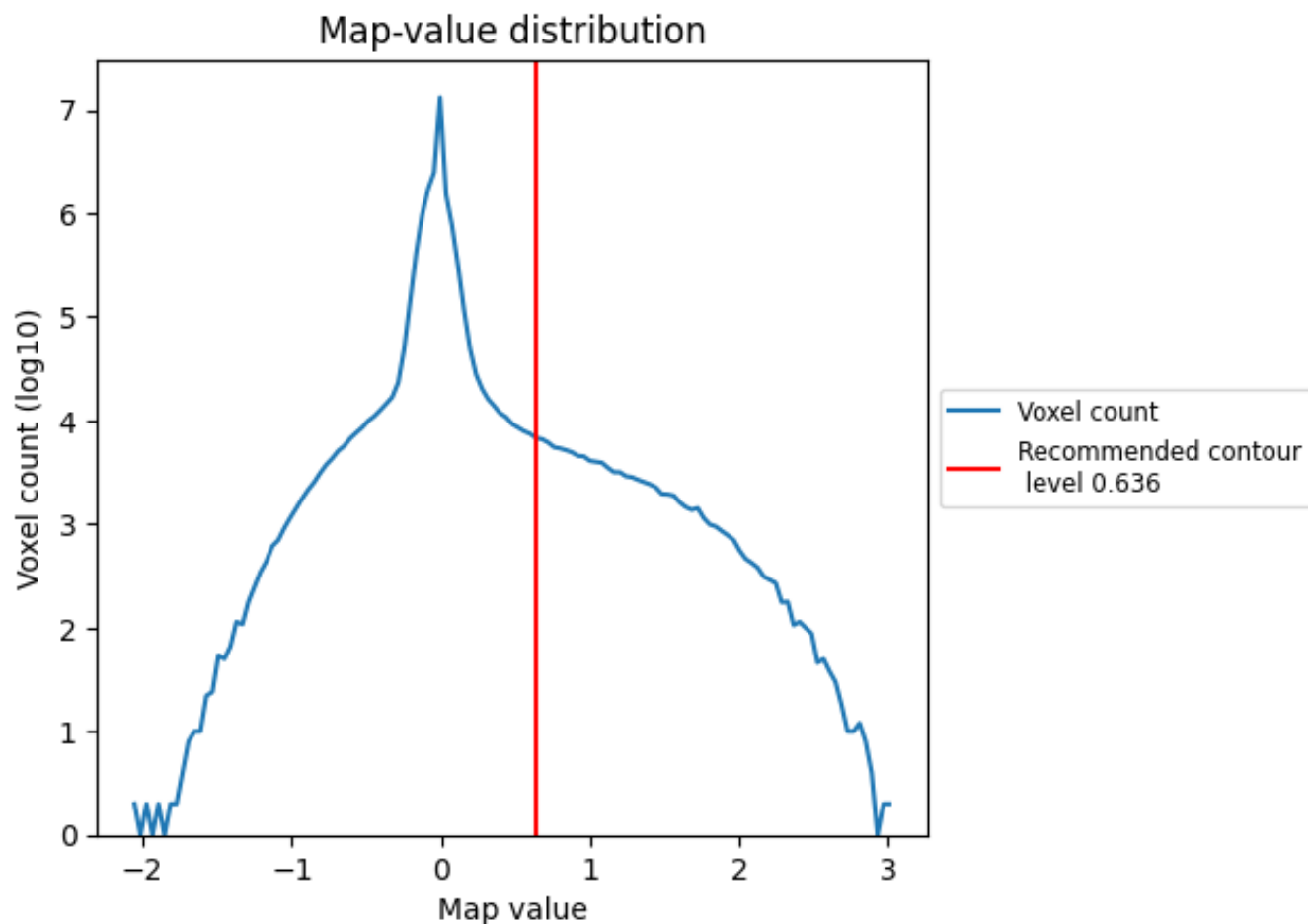


Z

7 Map analysis [i](#)

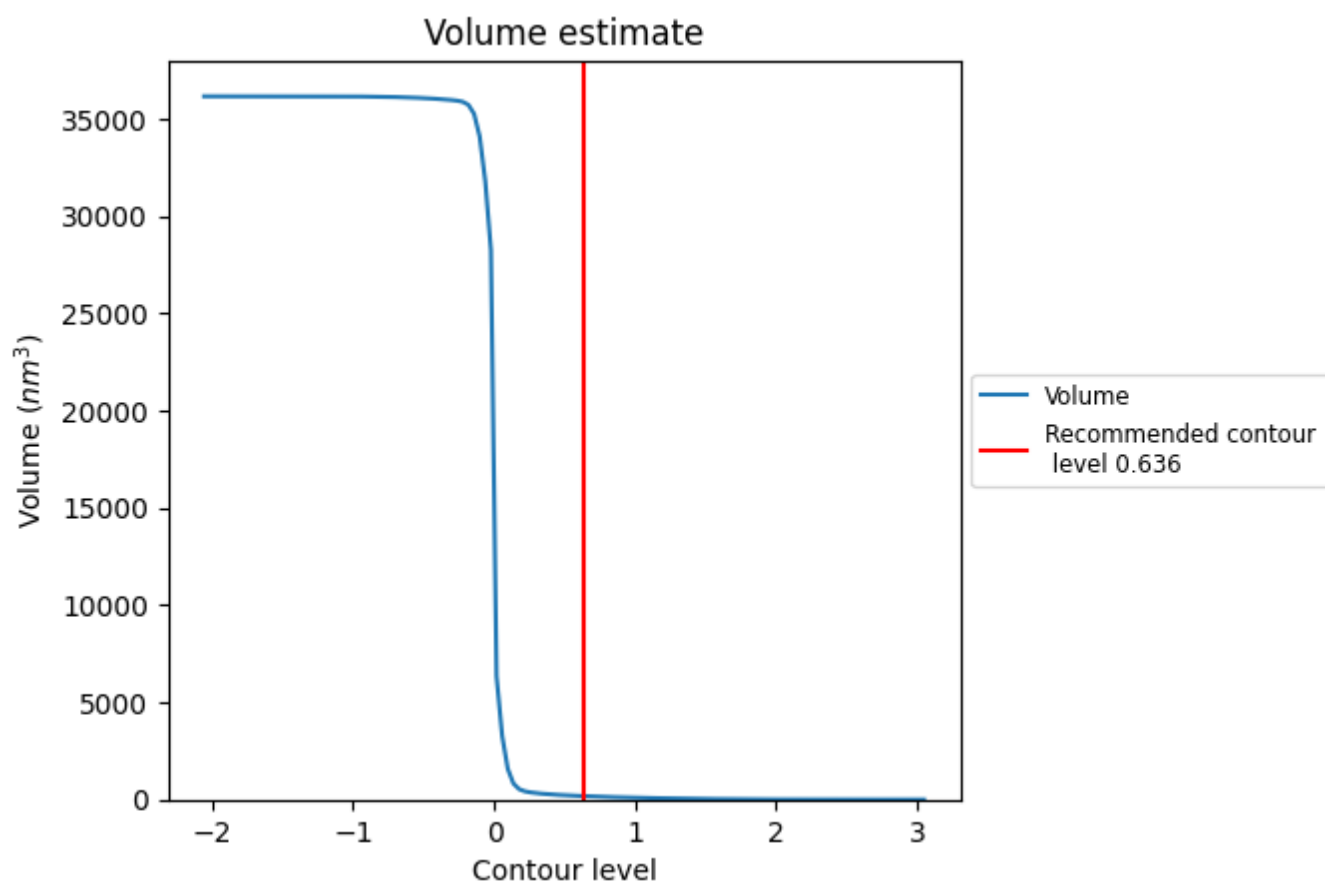
This section contains the results of statistical analysis of the map.

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.

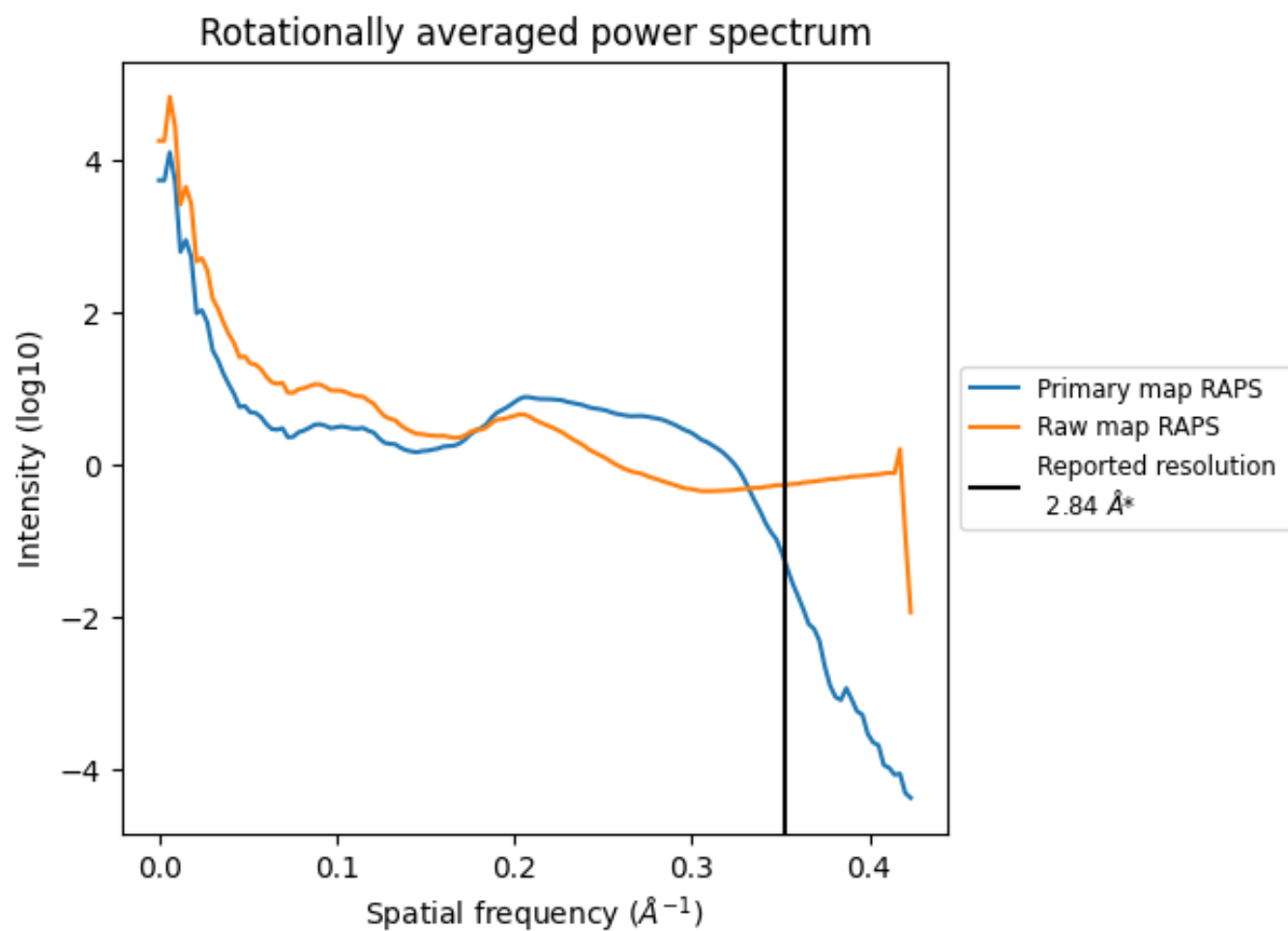
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm³; this corresponds to an approximate mass of 161 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

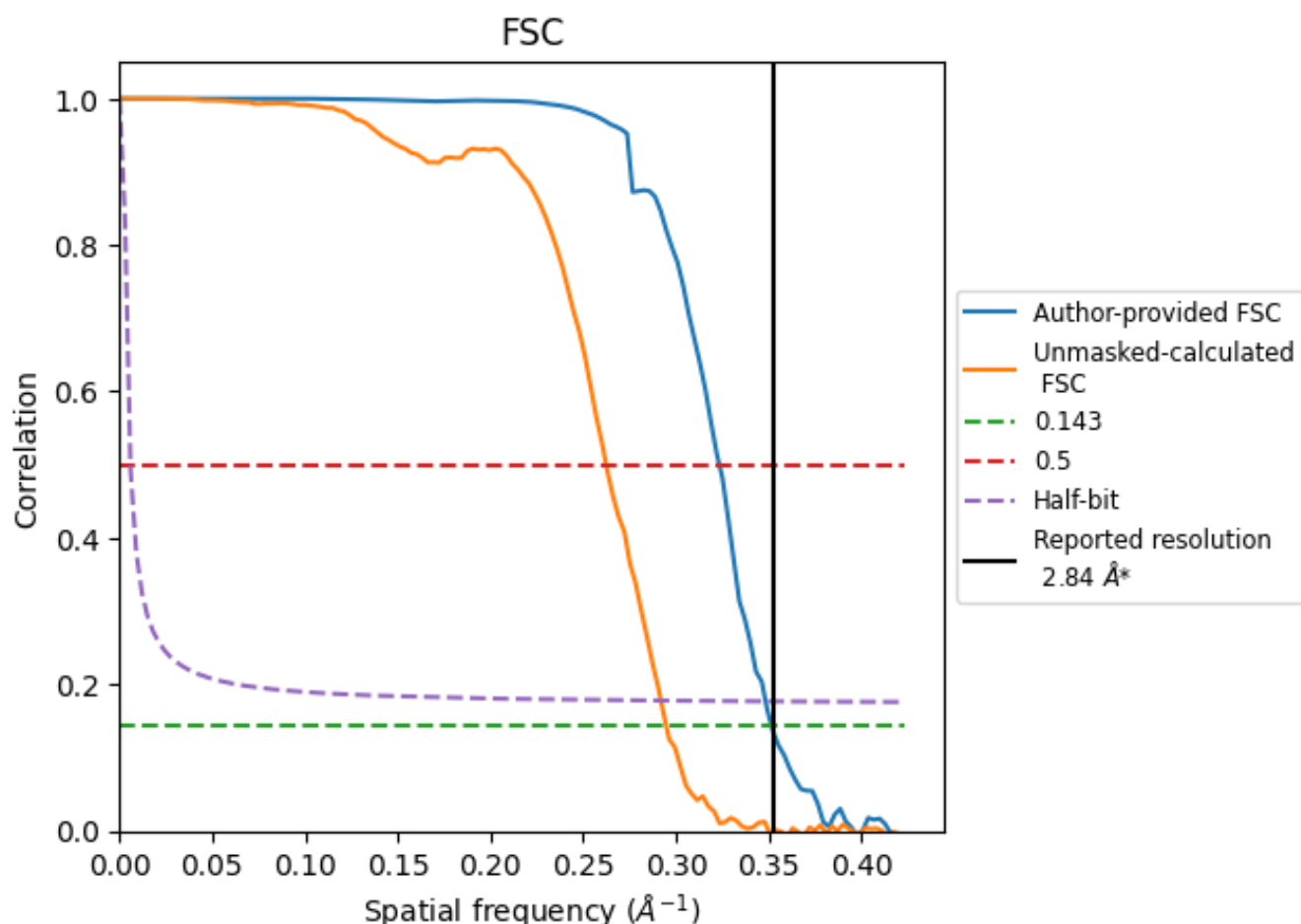


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

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 0.352 Å⁻¹

8.2 Resolution estimates [i](#)

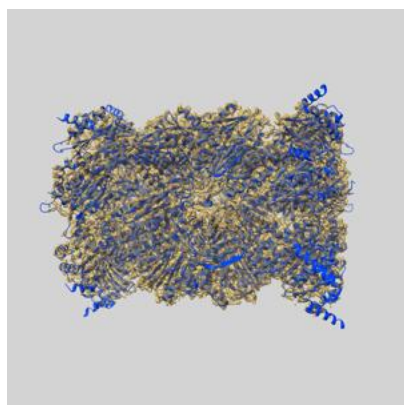
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.09	2.87
Unmasked-calculated*	3.39	3.81	3.43

*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 3.39 differs from the reported value 2.84 by more than 10 %

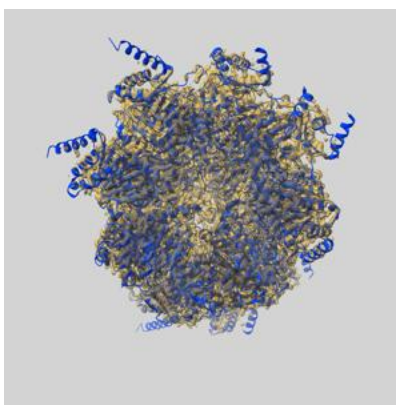
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18760 and PDB model 8QYO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

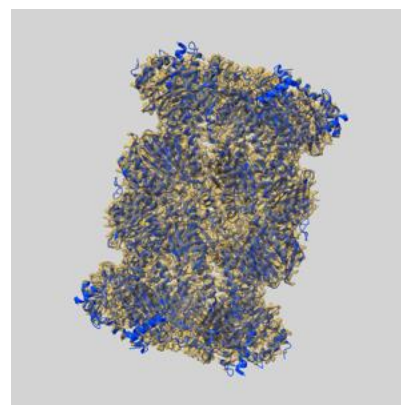
9.1 Map-model overlay [i](#)



X



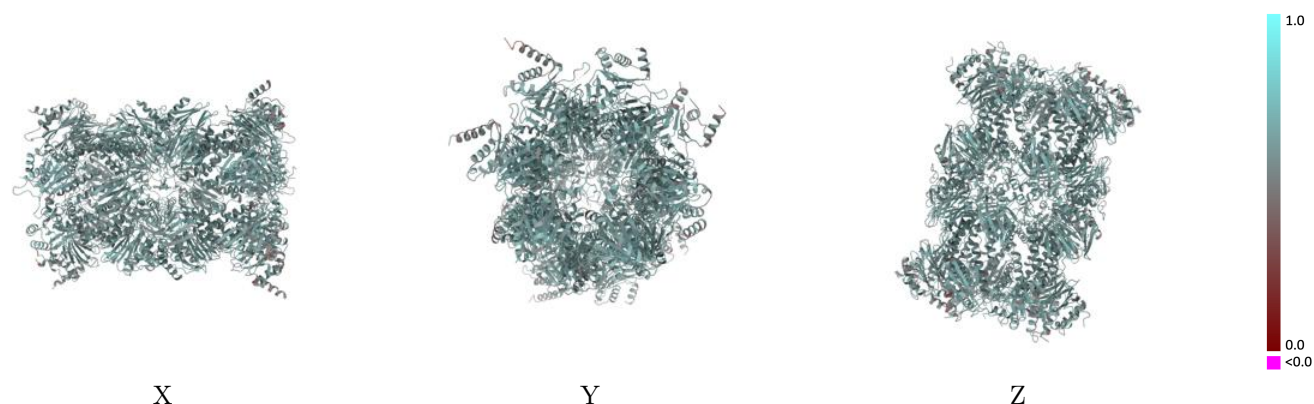
Y



Z

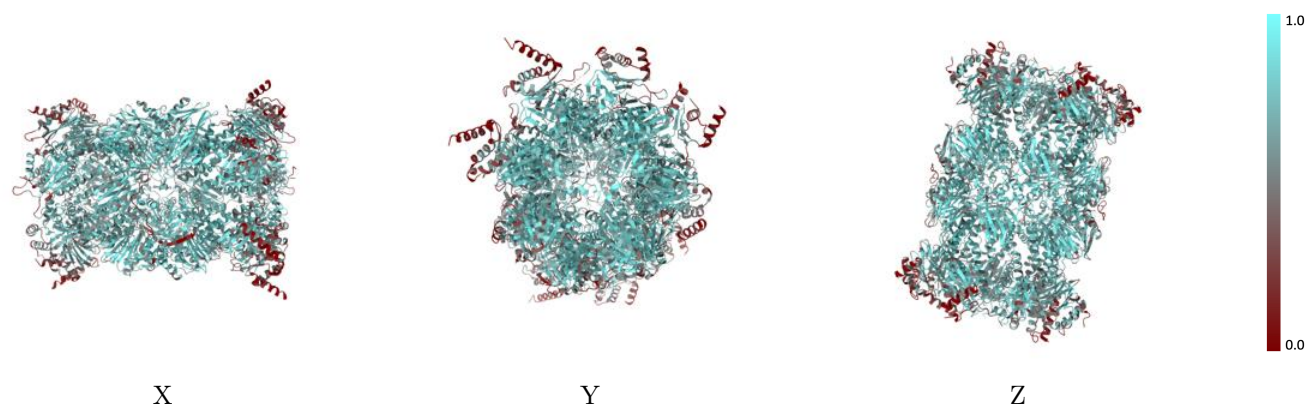
The images above show the 3D surface view of the map at the recommended contour level 0.636 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



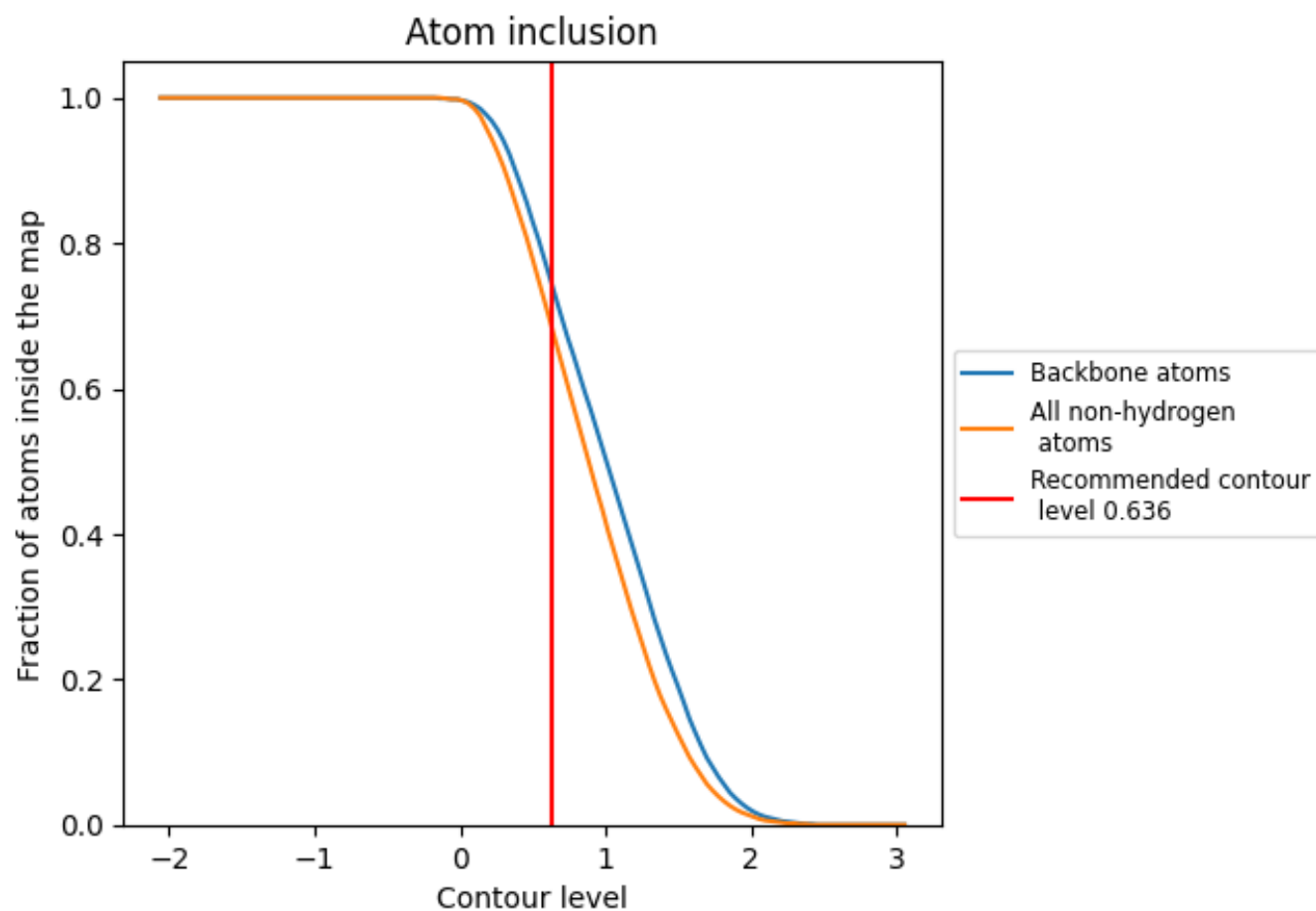
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.636).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.636) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.5960
A	 0.6300	 0.5950
B	 0.5850	 0.5820
C	 0.5600	 0.5810
D	 0.6140	 0.5890
E	 0.6700	 0.5990
F	 0.6300	 0.5870
G	 0.5900	 0.5770
H	 0.7000	 0.6030
I	 0.7690	 0.6090
J	 0.7840	 0.6100
K	 0.7800	 0.6090
L	 0.7280	 0.5960
M	 0.7700	 0.6070
N	 0.7850	 0.6100
O	 0.6310	 0.5940
P	 0.5840	 0.5830
Q	 0.5610	 0.5790
R	 0.6150	 0.5900
S	 0.6710	 0.5970
T	 0.6300	 0.5860
U	 0.5880	 0.5760
V	 0.7000	 0.6050
W	 0.7640	 0.6080
X	 0.7820	 0.6080
Y	 0.7800	 0.6120
Z	 0.7290	 0.5980
a	 0.7670	 0.6030
b	 0.7880	 0.6080

