wwPDB EM Validation Summary Report (i)

May 12, 2024 – 12:26 pm BST

PDB ID	:	6R70
EMDB ID	:	EMD-4738
Title	:	Endogeneous native human 20S proteasome
Authors	:	Schmidli, C.; Albiez, S.; Rima, L.; Righetto, R.; Mohammed, I.; Oliva, P.; Kovacik, L.; Stahlberg, H.; Braun, T.
Deposited on	:	2019-03-28
Resolution	:	3.50 Å(reported)
Based on initial model	:	5LE5

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:

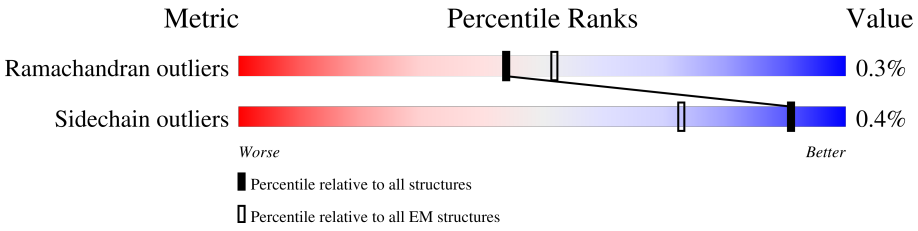
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	M	216	100%
1	a	216	100%
2	A	230	100%
2	O	230	100%
3	B	248	15% 98%
3	P	248	14% 94%
4	C	237	38% 96%
4	Q	237	35% 96%
5	D	233	21% 100%

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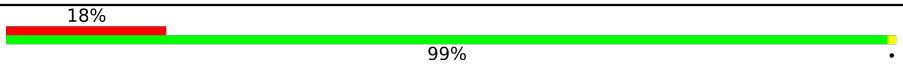
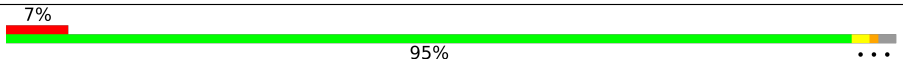
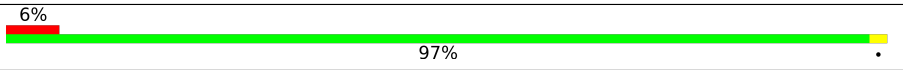
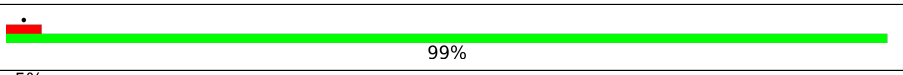
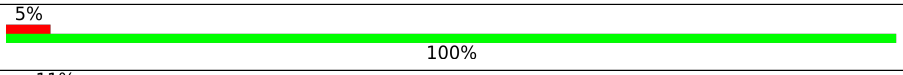
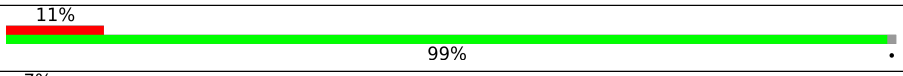
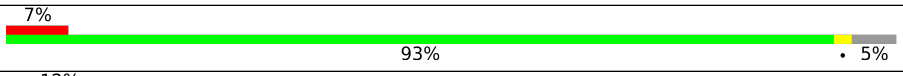
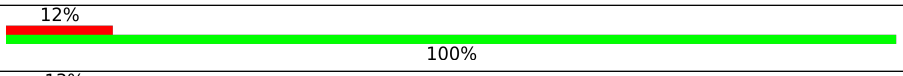
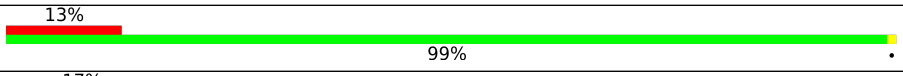
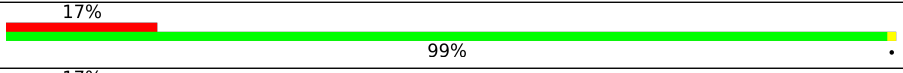
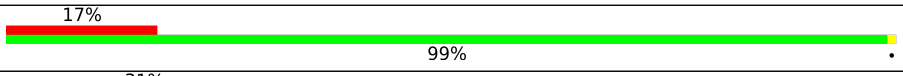
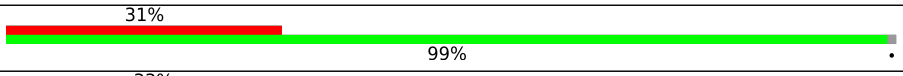
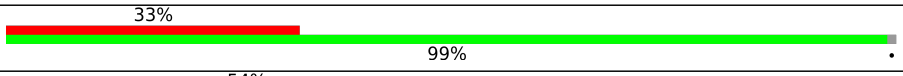
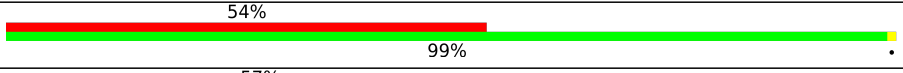
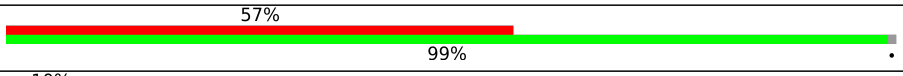
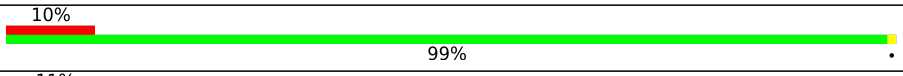
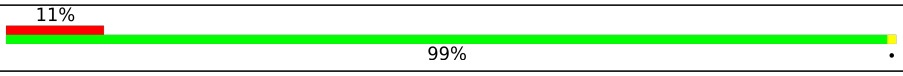
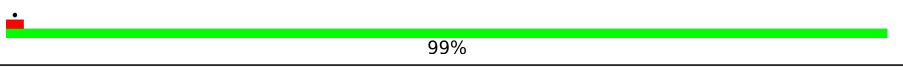
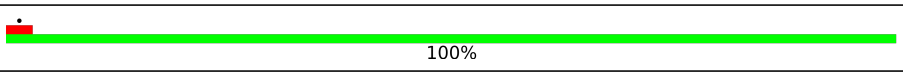
Mol	Chain	Length	Quality of chain
5	R	233	
6	E	238	
6	S	238	
7	F	240	
7	T	240	
8	G	244	
8	U	244	
9	H	220	
9	V	220	
10	I	204	
10	W	204	
11	J	196	
11	X	196	
12	K	201	
12	Y	201	
13	L	213	
13	Z	213	
14	N	203	
14	b	203	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 48581 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-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		
1	a	216	Total	C	N	O	S	1	0
			1692	1067	291	322	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	230	Total	C	N	O	S	2	0
			1811	1158	308	339	6		
2	O	230	Total	C	N	O	S	0	0
			1798	1150	305	337	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	248	Total	C	N	O	S	1	0
			1958	1238	336	373	11		
3	P	247	Total	C	N	O	S	2	0
			1950	1234	332	373	11		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	236	Total	C	N	O	S	0	0
			1864	1171	330	359	4		
4	Q	231	Total	C	N	O	S	0	0
			1832	1153	323	352	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	233	Total	C	N	O	S	2	0
			1791	1124	296	360	11		
5	R	233	Total	C	N	O	S	1	0
			1783	1119	295	358	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	233	Total	C	N	O	S	0	0
			1831	1148	328	345	10		
6	S	237	Total	C	N	O	S	3	0
			1888	1184	341	353	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	239	Total	C	N	O	S	4	0
			1894	1202	323	357	12		
7	T	240	Total	C	N	O	S	1	0
			1884	1195	321	356	12		

- Molecule 8 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	241	Total	C	N	O	S	2	0
			1892	1203	317	362	10		
8	U	232	Total	C	N	O	S	0	0
			1798	1138	304	346	10		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	220	Total	C	N	O	S	2	0
			1672	1053	286	320	13		
9	V	220	Total	C	N	O	S	2	0
			1669	1051	283	322	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	204	Total	C	N	O	S	6	0
			1633	1039	274	301	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	204	Total	C	N	O	S	2	0
			1608	1024	270	295	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	195	Total	C	N	O	S	2	0
			1580	1013	269	289	9		
11	X	195	Total	C	N	O	S	2	0
			1575	1010	268	288	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
12	Y	199	Total	C	N	O	S	3	0
			1570	991	278	291	10		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	213	Total	C	N	O	S	2	0
			1660	1051	284	314	11		
13	Z	213	Total	C	N	O	S	1	0
			1657	1049	284	313	11		

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

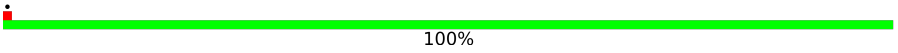
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	1	0
			1519	953	258	295	13		
14	b	203	Total	C	N	O	S	1	0
			1526	958	259	296	13		

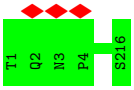
3 Residue-property plots (i)

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-4

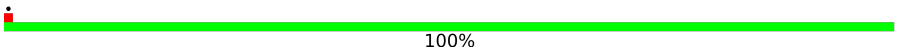
Chain M:

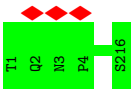




• Molecule 1: Proteasome subunit beta type-4

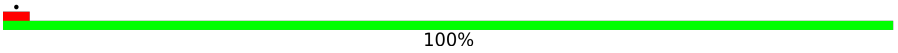
Chain a:





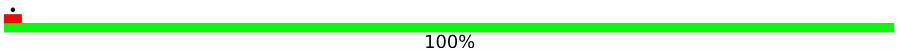
• Molecule 2: Proteasome subunit alpha type-2

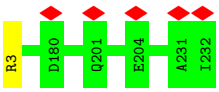
Chain A:



• Molecule 2: Proteasome subunit alpha type-2

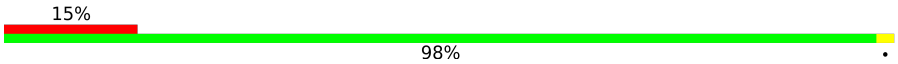
Chain O:

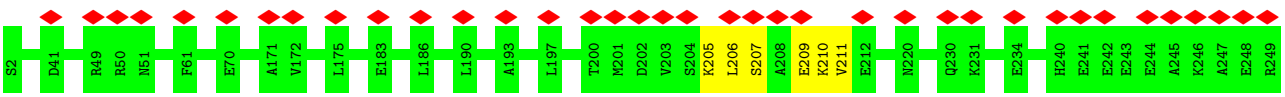




• Molecule 3: Proteasome subunit alpha type-4

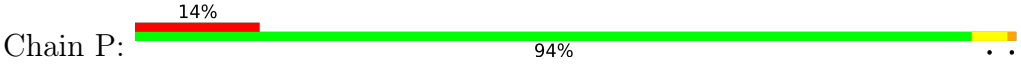
Chain B:

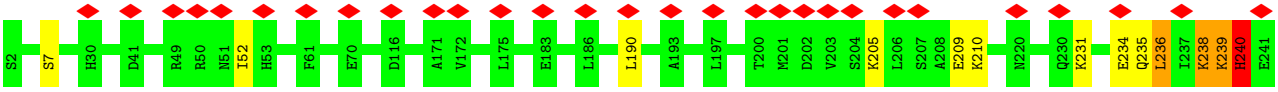


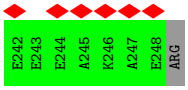


• Molecule 3: Proteasome subunit alpha type-4

Chain P:

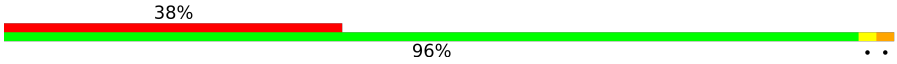


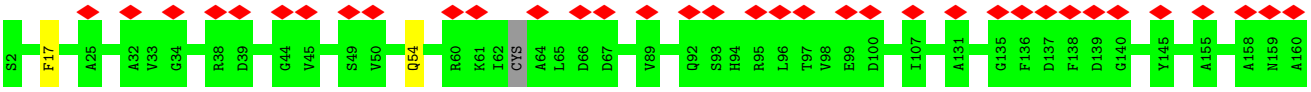


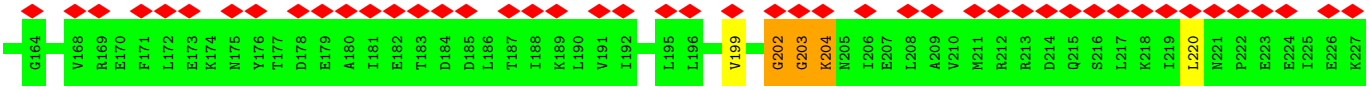


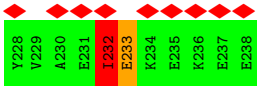
• Molecule 4: Proteasome subunit alpha type-7

Chain C:



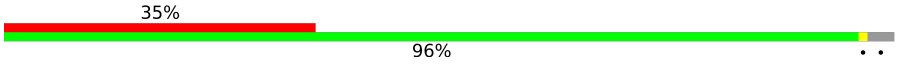


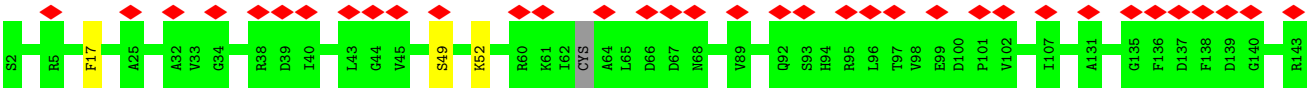


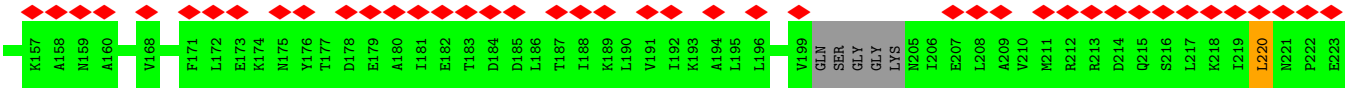


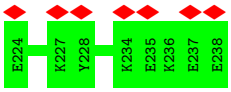
• Molecule 4: Proteasome subunit alpha type-7

Chain Q:



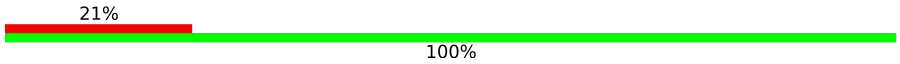


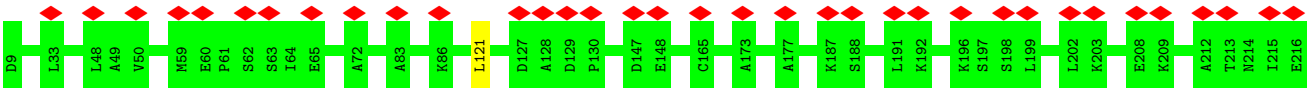


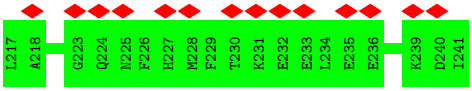


• Molecule 5: Proteasome subunit alpha type-5

Chain D:

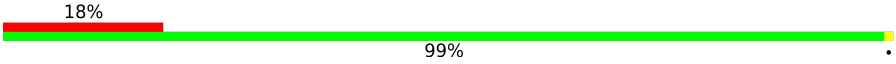


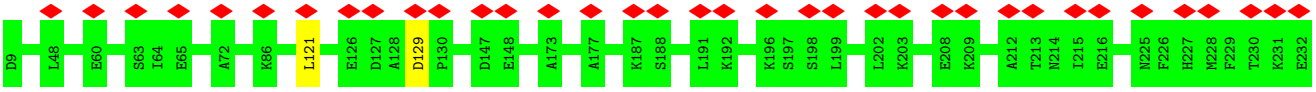


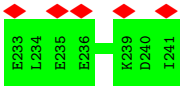


• Molecule 5: Proteasome subunit alpha type-5

Chain R:

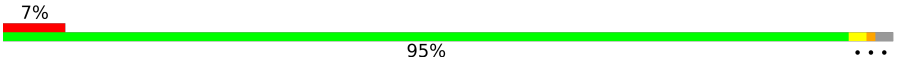


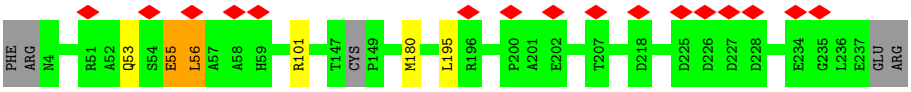




• Molecule 6: Proteasome subunit alpha type-1

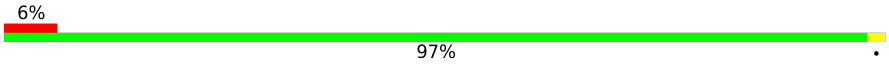
Chain E:

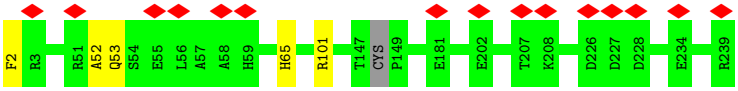




• Molecule 6: Proteasome subunit alpha type-1

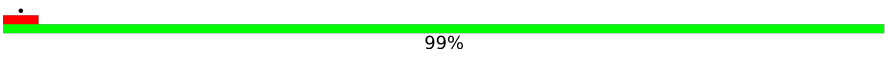
Chain S:

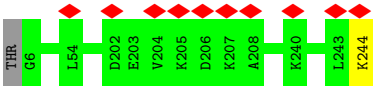




• Molecule 7: Proteasome subunit alpha type-3

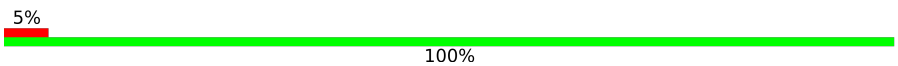
Chain F:

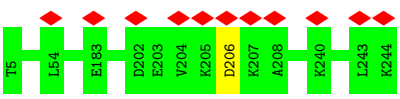




• Molecule 7: Proteasome subunit alpha type-3

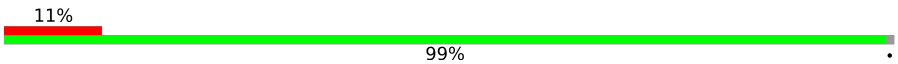
Chain T:

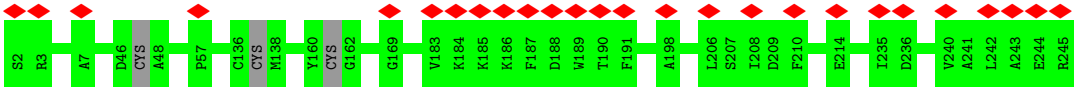




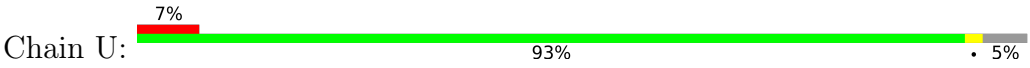
• Molecule 8: Proteasome subunit alpha type-6

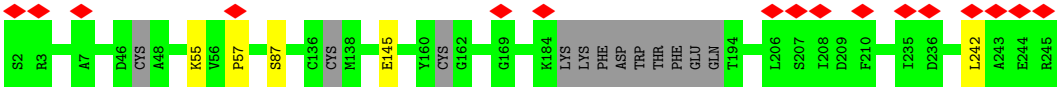
Chain G:



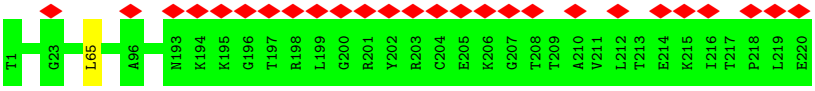


• Molecule 8: Proteasome subunit alpha type-6

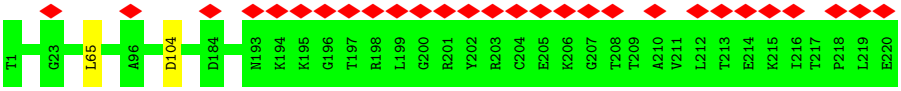




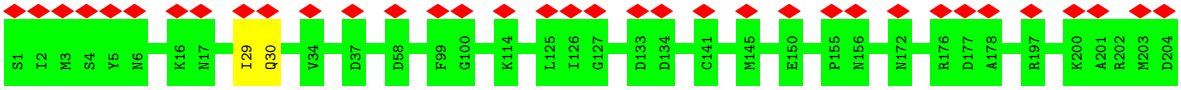
• Molecule 9: Proteasome subunit beta type-7



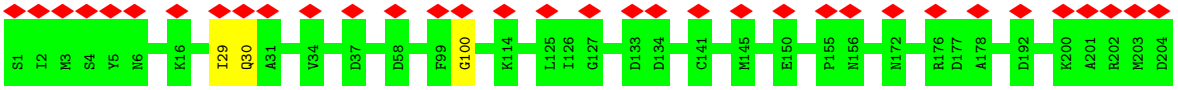
• Molecule 9: Proteasome subunit beta type-7



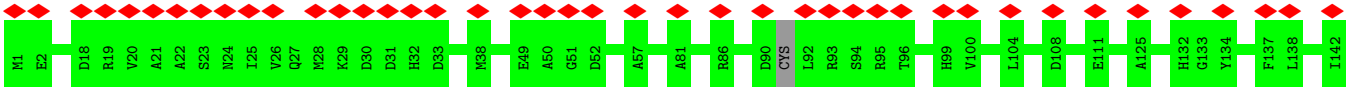
• Molecule 10: Proteasome subunit beta type-3

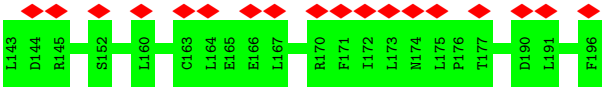


• Molecule 10: Proteasome subunit beta type-3



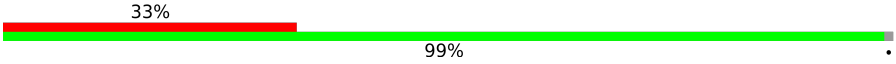
• Molecule 11: Proteasome subunit beta type-2

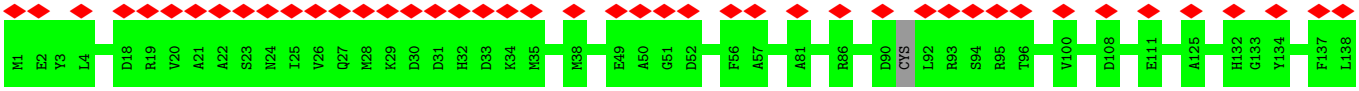


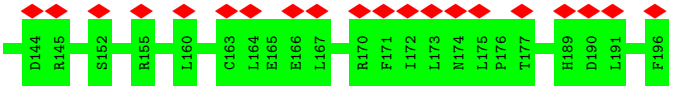


• Molecule 11: Proteasome subunit beta type-2

Chain X:

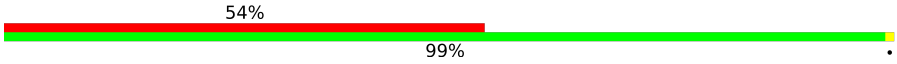


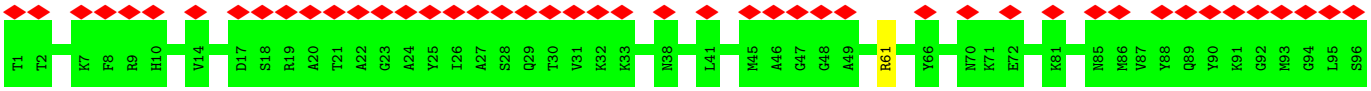


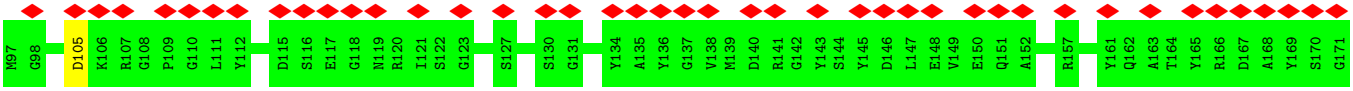


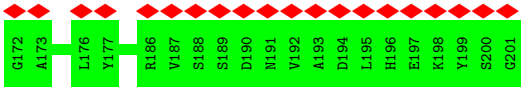
• Molecule 12: Proteasome subunit beta type-5

Chain K:



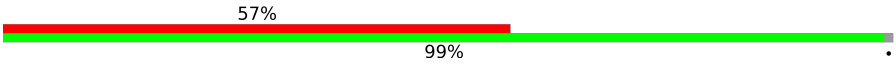


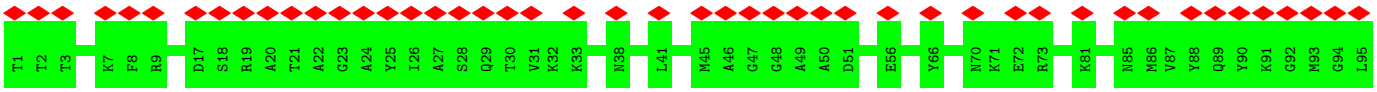


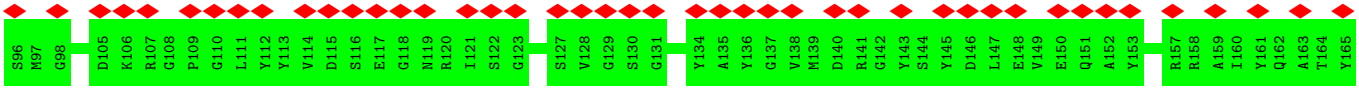


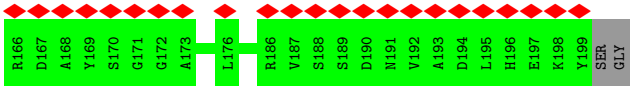
• Molecule 12: Proteasome subunit beta type-5

Chain Y:



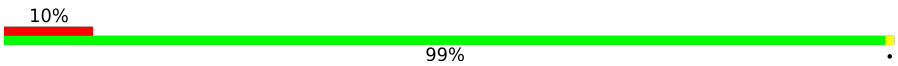


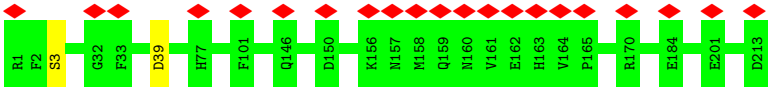




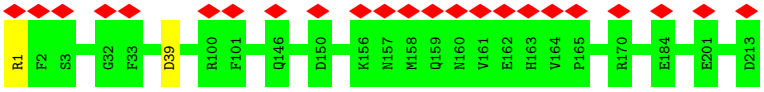
• Molecule 13: Proteasome subunit beta type-1

Chain L:

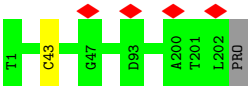




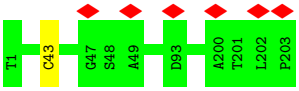
• Molecule 13: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-6



• Molecule 14: Proteasome subunit beta type-6



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	16015	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 ($e^-/Å^2$)	72	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	389.76, 389.76, 389.76	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.015, 1.015, 1.015	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	M	0.48	0/1720	0.57	0/2328
1	a	0.49	0/1728	0.62	0/2339
2	A	0.47	0/1856	0.57	0/2514
2	O	0.47	0/1837	0.58	0/2488
3	B	0.40	0/1991	0.69	1/2681 (0.0%)
3	P	0.61	6/1986 (0.3%)	0.89	12/2675 (0.4%)
4	C	0.38	0/1889	0.71	4/2547 (0.2%)
4	Q	0.36	0/1856	0.62	1/2503 (0.0%)
5	D	0.40	0/1818	0.64	0/2456
5	R	0.38	0/1810	0.61	0/2444
6	E	0.42	0/1864	0.64	0/2517
6	S	0.43	0/1932	0.66	0/2607
7	F	0.48	0/1941	0.59	0/2612
7	T	0.49	0/1922	0.64	1/2588 (0.0%)
8	G	0.46	0/1929	0.55	0/2602
8	U	0.46	0/1824	0.58	2/2459 (0.1%)
9	H	0.40	0/1705	0.61	1/2307 (0.0%)
9	V	0.41	0/1702	0.64	1/2303 (0.0%)
10	I	0.32	0/1668	0.54	0/2247
10	W	0.32	0/1640	0.59	0/2209
11	J	0.32	0/1615	0.59	0/2182
11	X	0.32	0/1613	0.58	0/2180
12	K	0.30	0/1590	0.55	0/2147
12	Y	0.30	0/1610	0.59	0/2172
13	L	0.35	0/1696	0.63	1/2285 (0.0%)
13	Z	0.36	0/1690	0.62	1/2276 (0.0%)
14	N	0.50	0/1548	0.58	0/2095
14	b	0.50	0/1556	0.59	0/2107
All	All	0.42	6/49536 (0.0%)	0.62	25/66870 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	4
3	P	0	7
4	C	0	4
4	Q	0	2
5	R	0	1
6	E	0	3
6	S	0	2
8	U	0	1
10	I	0	1
10	W	0	2
13	Z	0	1
All	All	0	28

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	239	LYS	CB-CG	7.36	1.72	1.52
3	P	239	LYS	CG-CD	6.86	1.75	1.52
3	P	239	LYS	CD-CE	6.86	1.68	1.51
3	P	235	GLN	CB-CG	-6.43	1.35	1.52
3	P	239	LYS	CE-NZ	6.18	1.64	1.49

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	239	LYS	C-N-CA	12.72	153.50	121.70
3	P	236	LEU	CA-CB-CG	10.56	139.60	115.30
3	P	239	LYS	CD-CE-NZ	8.60	131.47	111.70
4	C	232	ILE	CG1-CB-CG2	-8.39	92.95	111.40
7	T	206	ASP	CB-CG-OD1	8.24	125.72	118.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	205	LYS	Peptide
3	B	207	SER	Peptide
3	B	209	GLU	Peptide
3	B	211	VAL	Peptide
4	C	199	VAL	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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	M	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
1	a	215/216 (100%)	207 (96%)	8 (4%)	0	100	100
2	A	230/230 (100%)	221 (96%)	9 (4%)	0	100	100
2	O	228/230 (99%)	219 (96%)	9 (4%)	0	100	100
3	B	247/248 (100%)	237 (96%)	9 (4%)	1 (0%)	34	72
3	P	247/248 (100%)	234 (95%)	10 (4%)	3 (1%)	13	50
4	C	232/237 (98%)	215 (93%)	12 (5%)	5 (2%)	6	37
4	Q	225/237 (95%)	212 (94%)	12 (5%)	1 (0%)	34	72
5	D	233/233 (100%)	221 (95%)	11 (5%)	1 (0%)	34	72
5	R	232/233 (100%)	221 (95%)	10 (4%)	1 (0%)	34	72
6	E	229/238 (96%)	215 (94%)	12 (5%)	2 (1%)	17	56
6	S	236/238 (99%)	227 (96%)	8 (3%)	1 (0%)	34	72
7	F	241/240 (100%)	237 (98%)	4 (2%)	0	100	100
7	T	239/240 (100%)	231 (97%)	8 (3%)	0	100	100
8	G	235/244 (96%)	230 (98%)	5 (2%)	0	100	100
8	U	222/244 (91%)	215 (97%)	6 (3%)	1 (0%)	29	68
9	H	220/220 (100%)	217 (99%)	3 (1%)	0	100	100
9	V	220/220 (100%)	215 (98%)	5 (2%)	0	100	100
10	I	208/204 (102%)	202 (97%)	5 (2%)	1 (0%)	29	68
10	W	204/204 (100%)	195 (96%)	8 (4%)	1 (0%)	29	68
11	J	193/196 (98%)	179 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	X	193/196 (98%)	186 (96%)	7 (4%)	0	100	100
12	K	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
12	Y	200/201 (100%)	194 (97%)	6 (3%)	0	100	100
13	L	213/213 (100%)	204 (96%)	9 (4%)	0	100	100
13	Z	212/213 (100%)	203 (96%)	9 (4%)	0	100	100
14	N	201/203 (99%)	194 (96%)	7 (4%)	0	100	100
14	b	202/203 (100%)	193 (96%)	9 (4%)	0	100	100
All	All	6170/6246 (99%)	5923 (96%)	229 (4%)	18 (0%)	44	75

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	203	GLY
4	C	204	LYS
4	C	233	GLU
6	E	56	LEU
3	P	239	LYS

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	M	179/179 (100%)	179 (100%)	0	100	100
1	a	180/179 (101%)	180 (100%)	0	100	100
2	A	191/189 (101%)	190 (100%)	1 (0%)	88	94
2	O	189/189 (100%)	188 (100%)	1 (0%)	88	94
3	B	209/208 (100%)	209 (100%)	0	100	100
3	P	209/208 (100%)	207 (99%)	2 (1%)	76	88
4	C	200/201 (100%)	198 (99%)	2 (1%)	76	88
4	Q	197/201 (98%)	196 (100%)	1 (0%)	88	94
5	D	196/195 (100%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	195/195 (100%)	195 (100%)	0	100	100
6	E	199/204 (98%)	196 (98%)	3 (2%)	65	84
6	S	206/204 (101%)	203 (98%)	3 (2%)	65	84
7	F	201/198 (102%)	200 (100%)	1 (0%)	88	94
7	T	199/198 (100%)	199 (100%)	0	100	100
8	G	207/208 (100%)	207 (100%)	0	100	100
8	U	196/208 (94%)	195 (100%)	1 (0%)	88	94
9	H	183/181 (101%)	183 (100%)	0	100	100
9	V	183/181 (101%)	181 (99%)	2 (1%)	73	88
10	I	178/173 (103%)	178 (100%)	0	100	100
10	W	175/173 (101%)	175 (100%)	0	100	100
11	J	168/167 (101%)	168 (100%)	0	100	100
11	X	168/167 (101%)	168 (100%)	0	100	100
12	K	156/156 (100%)	154 (99%)	2 (1%)	69	86
12	Y	158/156 (101%)	158 (100%)	0	100	100
13	L	180/178 (101%)	178 (99%)	2 (1%)	73	88
13	Z	179/178 (101%)	179 (100%)	0	100	100
14	N	158/158 (100%)	157 (99%)	1 (1%)	86	94
14	b	159/158 (101%)	158 (99%)	1 (1%)	86	94
All	All	5198/5190 (100%)	5175 (100%)	23 (0%)	91	96

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	7[B]	SER
6	S	65[B]	HIS
6	S	65[A]	HIS
6	S	101	ARG
7	F	244	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	18	GLN

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Mol	Chain	Res	Type
10	W	156	ASN
4	Q	175	ASN
5	R	182	GLN
11	X	27	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 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.

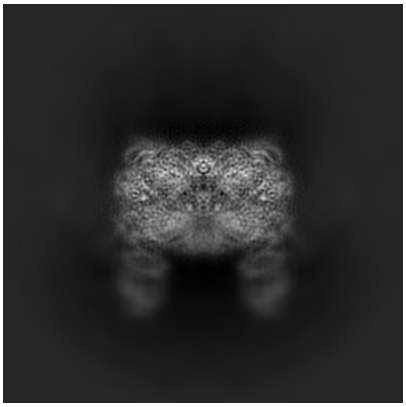
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4738. These allow visual inspection of the internal detail of the map and identification of artifacts.

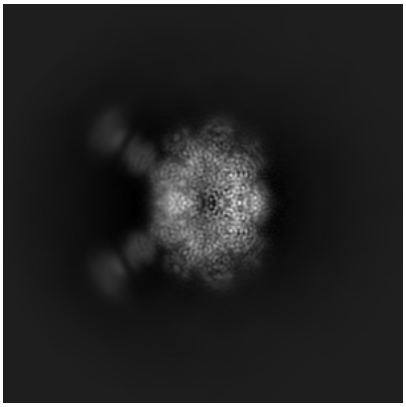
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

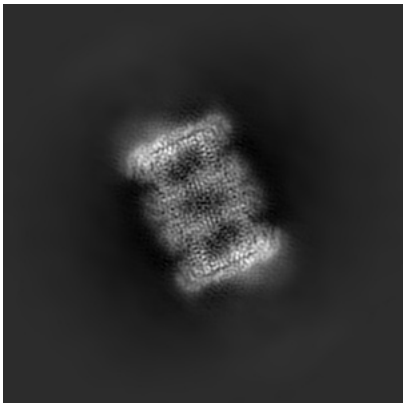
6.1.1 Primary map



X



Y



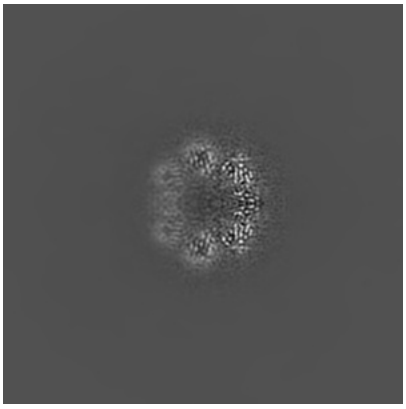
Z

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

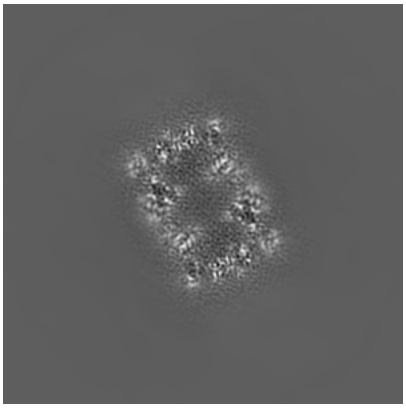
6.2 Central slices

6.2.1 Primary map

X Index: 192



Y Index: 192



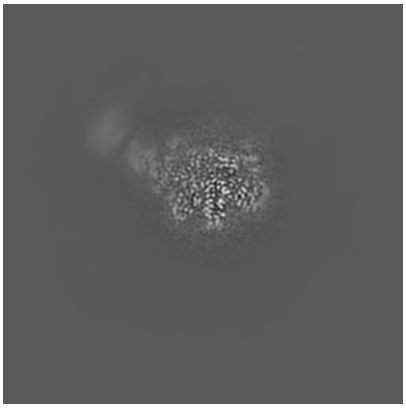
Z Index: 192

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

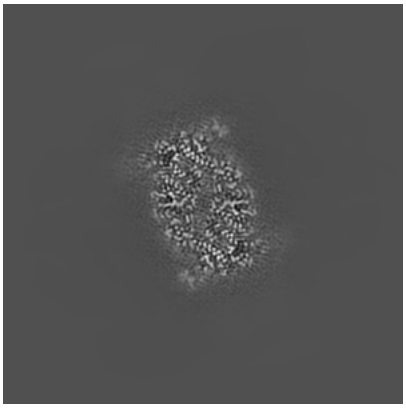
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 192



Y Index: 135

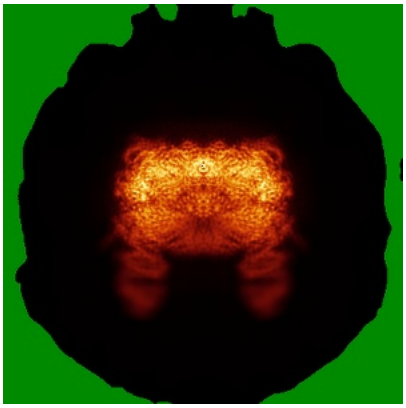


Z Index: 223

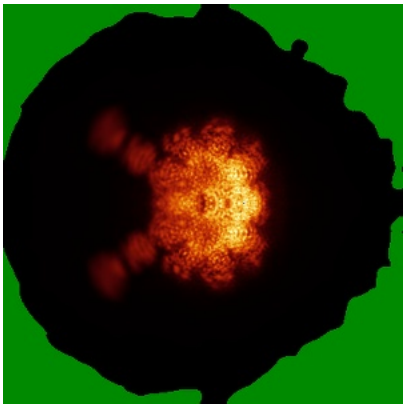
The images above show the largest variance slices of the map in three orthogonal directions.

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

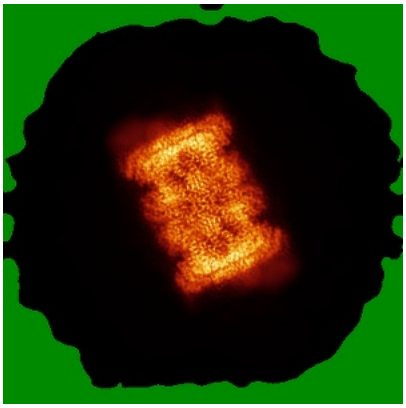
6.4.1 Primary map



X



Y

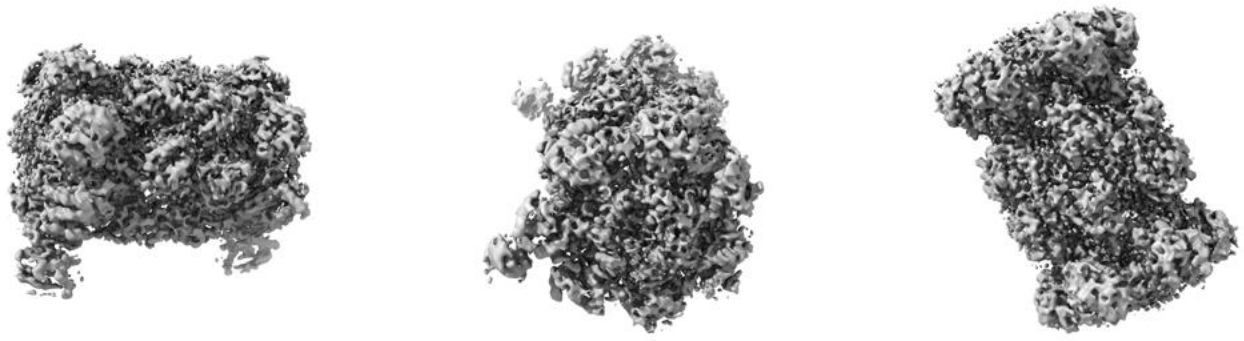


Z

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

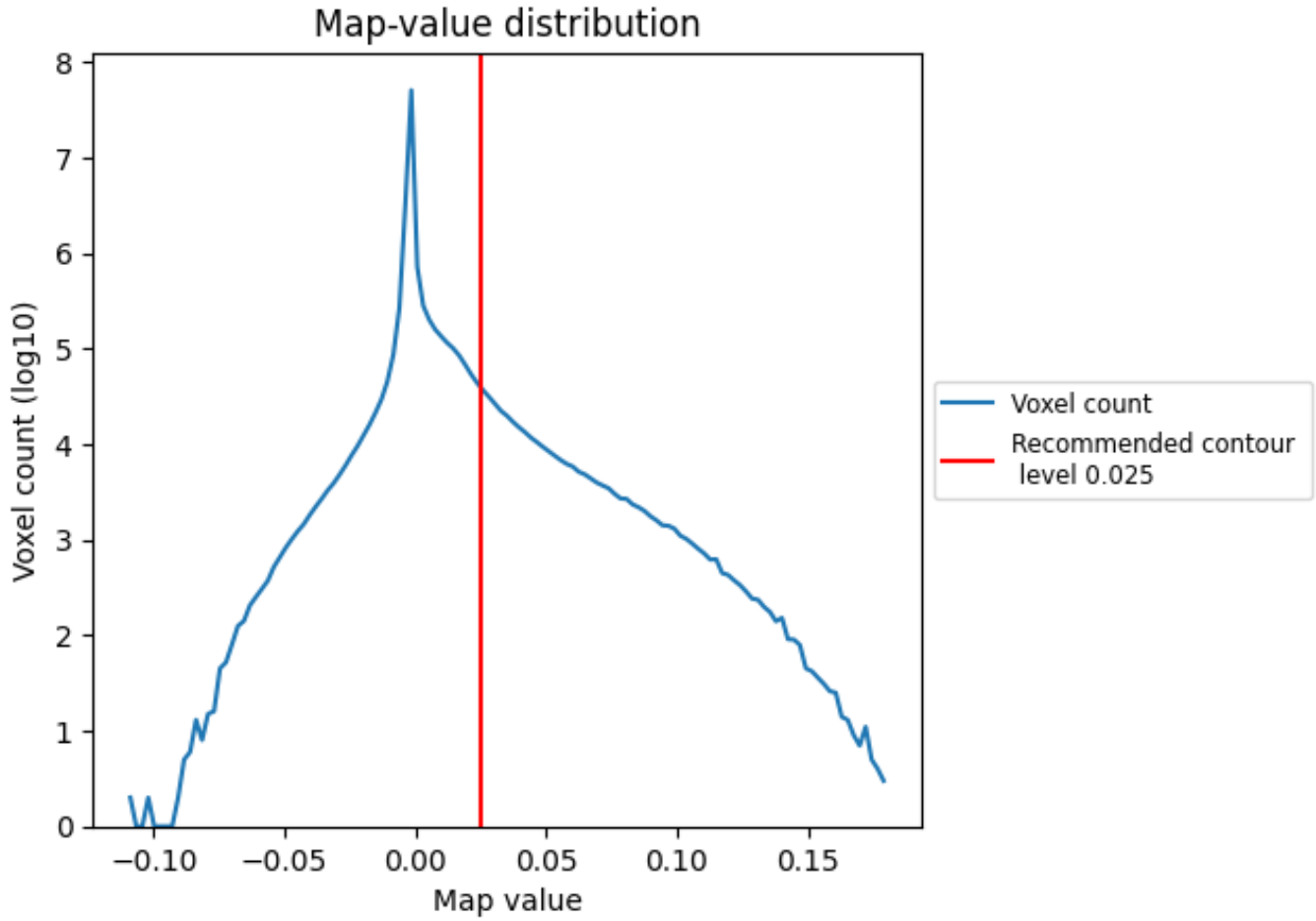
6.6 Mask visualisation (i)

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

7 Map analysis

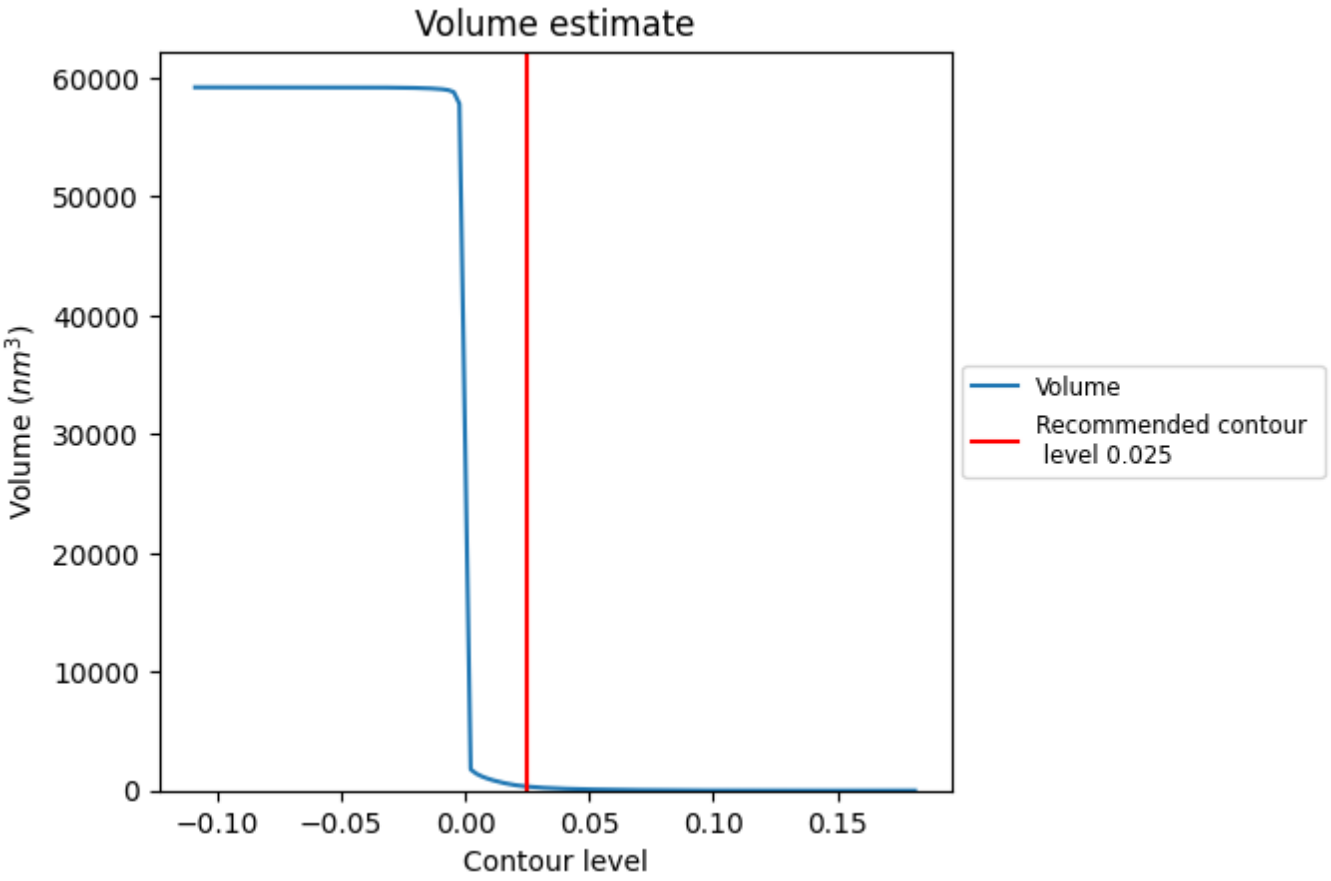
This section contains the results of statistical analysis of the map.

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.

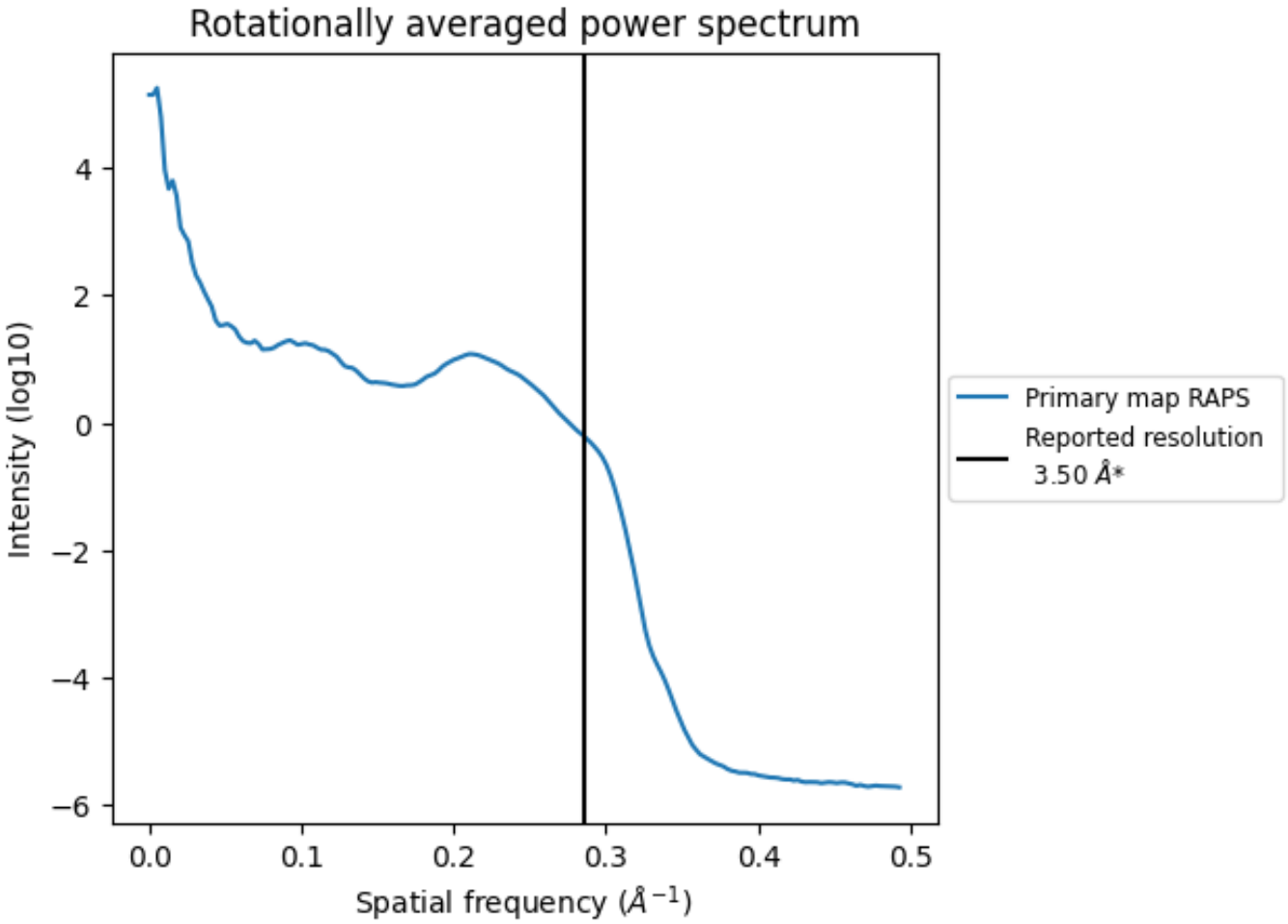
7.2 Volume estimate (i)



The volume at the recommended contour level is 337 nm^3; this corresponds to an approximate mass of 304 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)

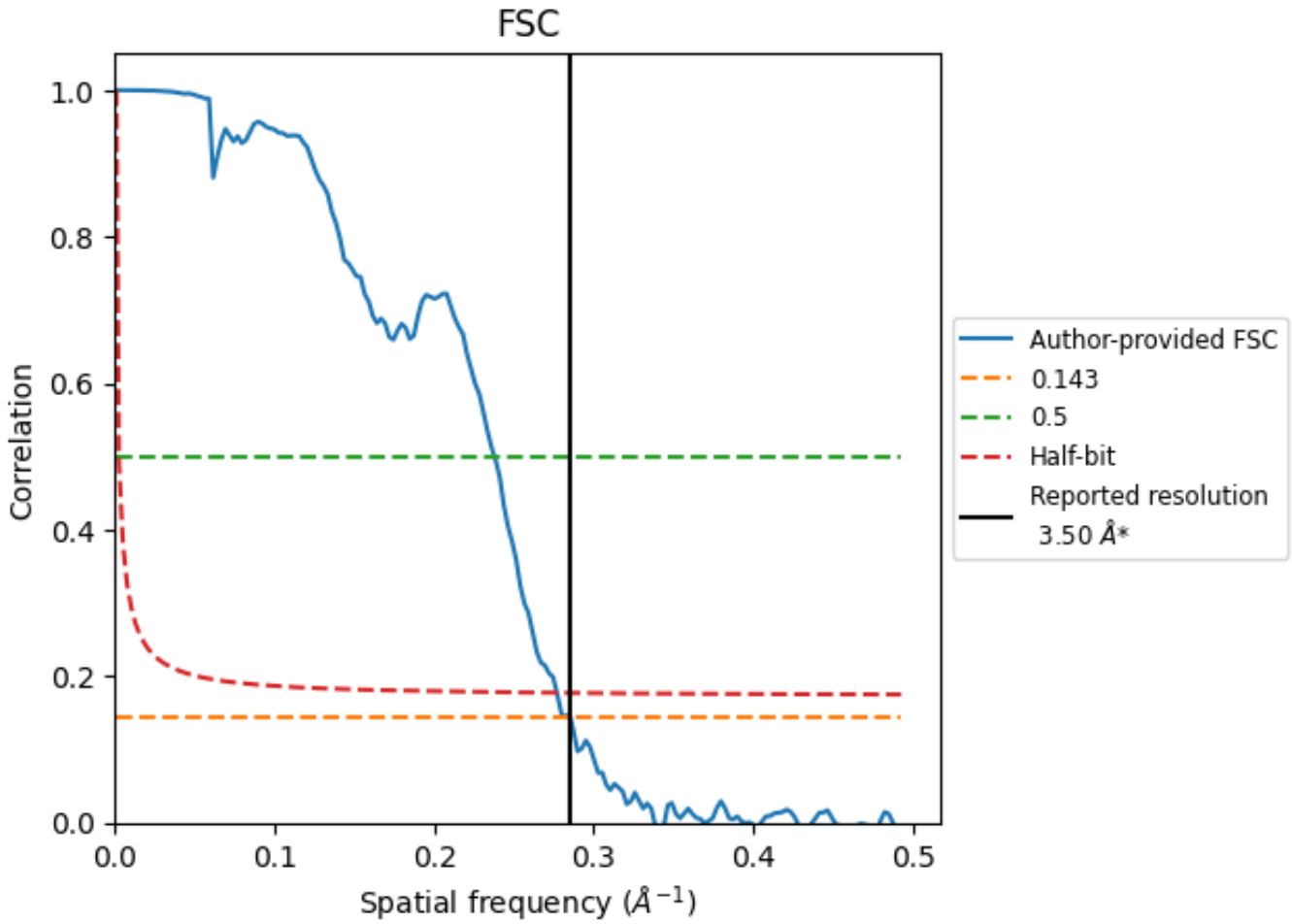


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

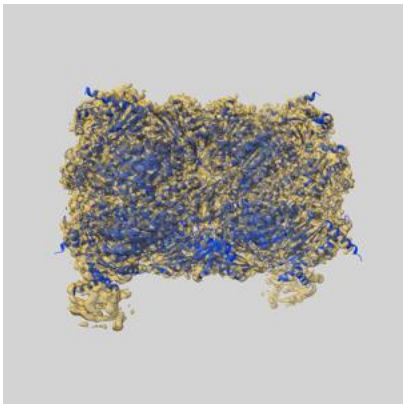
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	4.21	3.61
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

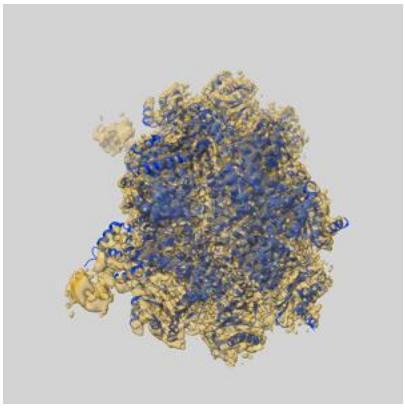
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4738 and PDB model 6R70. Per-residue inclusion information can be found in section 3 on page 7.

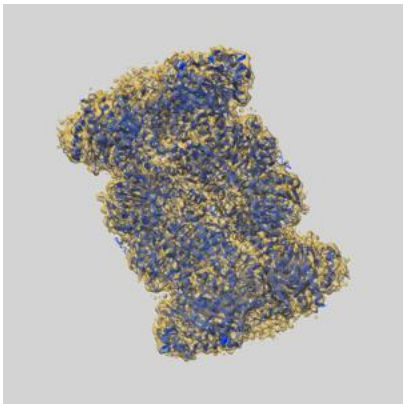
9.1 Map-model overlay



X



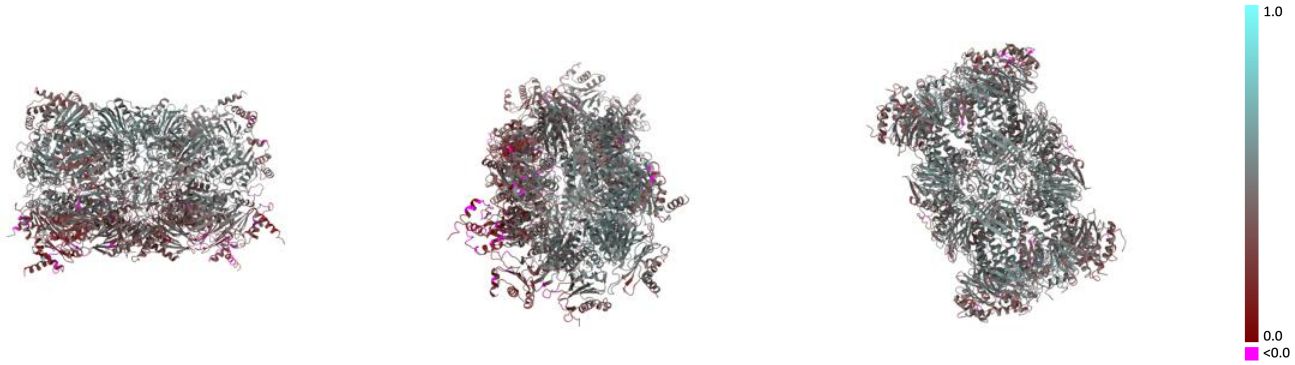
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

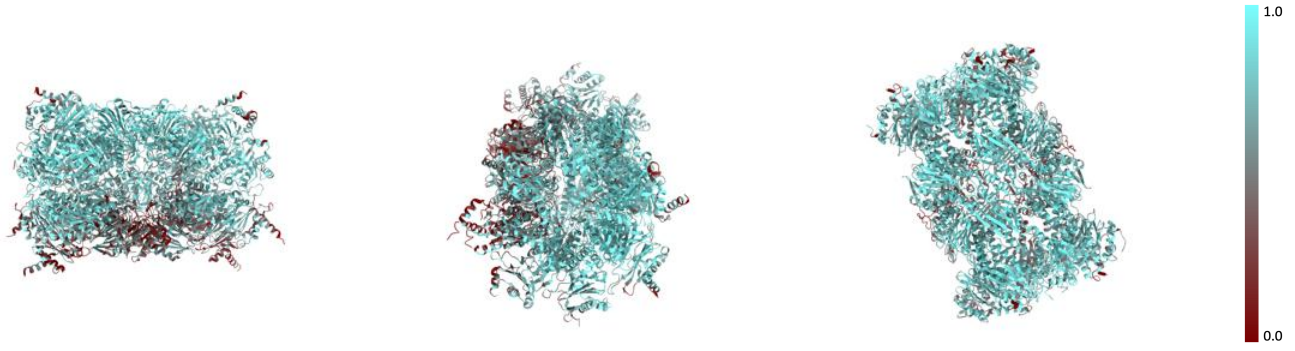
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

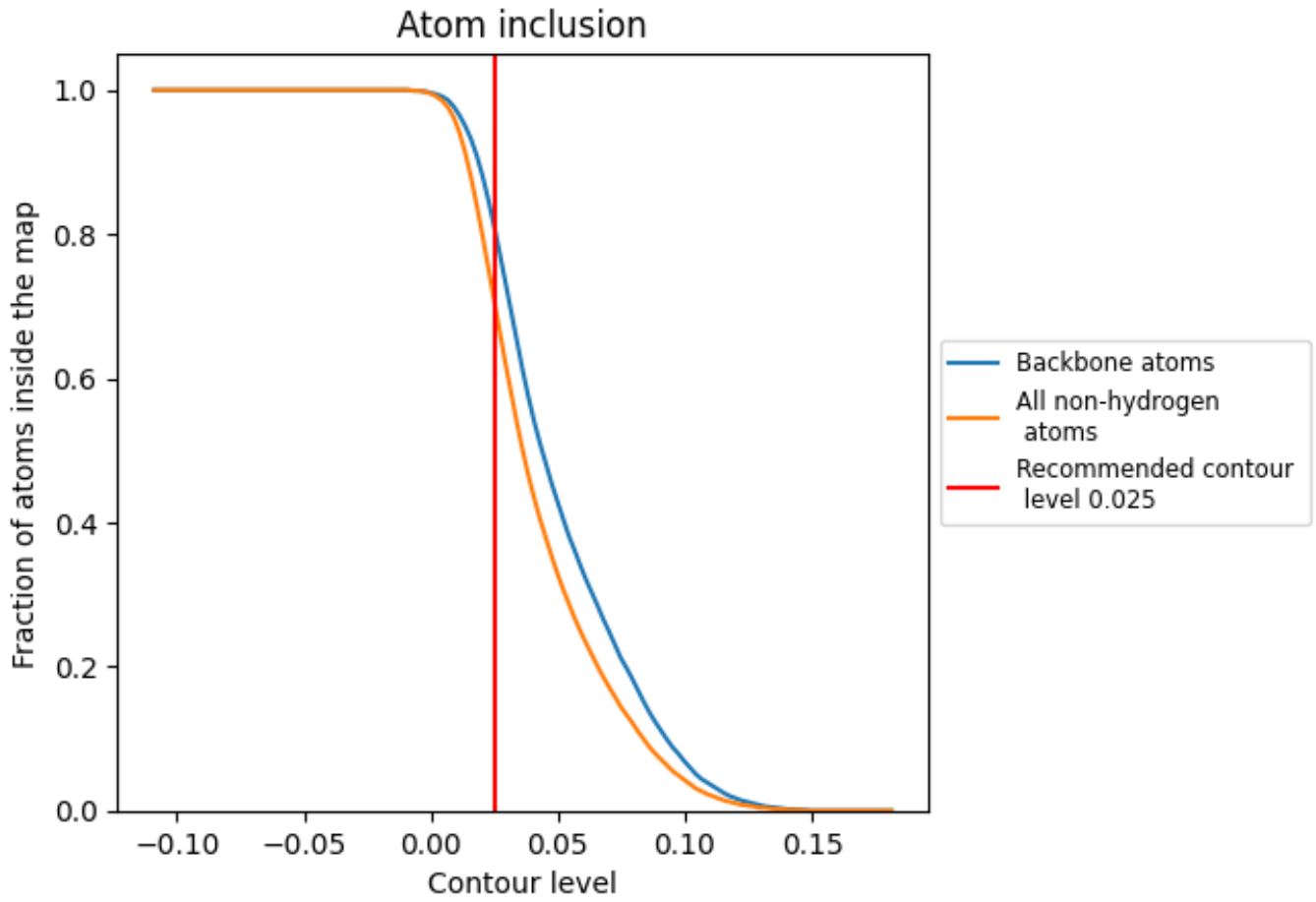
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 71% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7060	0.4190
A	0.8140	0.4670
B	0.7100	0.3890
C	0.5190	0.2580
D	0.6520	0.3420
E	0.7930	0.4180
F	0.8120	0.4710
G	0.7730	0.4540
H	0.7260	0.4450
I	0.6570	0.4190
J	0.5220	0.3580
K	0.3960	0.3450
L	0.7080	0.4380
M	0.8790	0.5220
N	0.8720	0.5080
O	0.8210	0.4740
P	0.7100	0.3960
Q	0.5410	0.2760
R	0.6700	0.3560
S	0.7810	0.4220
T	0.8160	0.4700
U	0.8200	0.4770
V	0.7330	0.4550
W	0.6600	0.4210
X	0.4930	0.3600
Y	0.3660	0.3400
Z	0.7060	0.4400
a	0.8710	0.5120
b	0.8680	0.5050