wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 01:01 pm GMT

PDB ID	:	8QZ9
EMDB ID	:	EMD-18773
Title	:	Human 20S proteasome assembly intermediate structure 4
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	:	2.95 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:

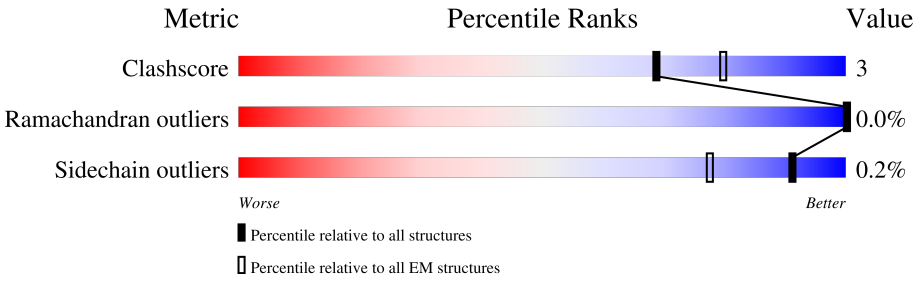
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.95 Å.

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



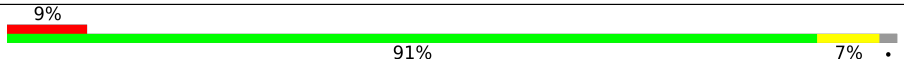
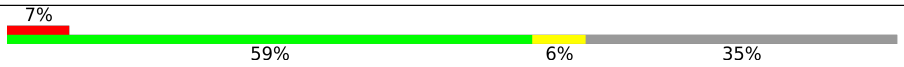
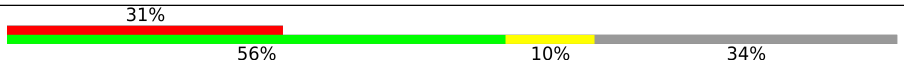
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	234	92% 6% •
2	B	261	88% 5% 7%
3	C	248	86% 8% 5%
4	D	242	86% 11% •
5	E	264	84% 6% 9%
6	F	255	83% 11% 6%
7	G	247	85% 12% •
8	H	141	72% 8% • 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	288	
10	J	265	
11	K	332	
12	L	205	
13	M	202	
14	N	263	
15	O	241	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 24217 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
			Total	C	N	O	S		
1	A	229	1731	1114	295	316	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	242	1786	1132	312	332	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	235	1780	1121	318	336	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	236	1758	1109	293	344	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ACE	-	acetylation	UNP P28066

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	240	1852	1162	336	343	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ACE	-	acetylation	UNP P25786

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	240	Total	C	N	O	S	0	0
			1834	1163	312	348	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total	C	N	O	S	0	0
			1819	1157	310	340	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ACE	-	acetylation	UNP P60900

- Molecule 8 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	113	Total	C	N	O	S	0	0
			901	573	152	171	5		

- Molecule 9 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	269	Total	C	N	O	S	0	0
			2056	1320	337	384	15		

- Molecule 10 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	249	Total	C	N	O	S	0	0
			1888	1218	307	349	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ACE	-	acetylation	UNP Q969U7

- Molecule 11 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	231	Total	C	N	O	S	0	0
			1646	1047	281	308	10		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	237P	GLU	-	expression tag	UNP Q99436
K	237Q	ASP	-	expression tag	UNP Q99436
K	237R	LEU	-	expression tag	UNP Q99436
K	237S	TYR	-	expression tag	UNP Q99436
K	237T	PHE	-	expression tag	UNP Q99436
K	237U	GLN	-	expression tag	UNP Q99436
K	237V	SER	-	expression tag	UNP Q99436
K	237W	VAL	-	expression tag	UNP Q99436
K	237X	ASP	-	expression tag	UNP Q99436
K	237Y	SER	-	expression tag	UNP Q99436
K	237Z	ALA	-	expression tag	UNP Q99436
K	238A	TRP	-	expression tag	UNP Q99436
K	238B	SER	-	expression tag	UNP Q99436
K	238C	HIS	-	expression tag	UNP Q99436
K	238D	PRO	-	expression tag	UNP Q99436
K	238E	GLN	-	expression tag	UNP Q99436
K	238F	PHE	-	expression tag	UNP Q99436
K	238G	GLU	-	expression tag	UNP Q99436
K	238H	LYS	-	expression tag	UNP Q99436
K	238I	GLY	-	expression tag	UNP Q99436
K	238J	GLY	-	expression tag	UNP Q99436
K	238K	GLY	-	expression tag	UNP Q99436
K	238L	SER	-	expression tag	UNP Q99436
K	238M	GLY	-	expression tag	UNP Q99436
K	238N	GLY	-	expression tag	UNP Q99436
K	238O	GLY	-	expression tag	UNP Q99436
K	238P	SER	-	expression tag	UNP Q99436
K	238Q	GLY	-	expression tag	UNP Q99436
K	238R	GLY	-	expression tag	UNP Q99436
K	238S	SER	-	expression tag	UNP Q99436
K	238T	ALA	-	expression tag	UNP Q99436
K	238U	TRP	-	expression tag	UNP Q99436
K	238V	SER	-	expression tag	UNP Q99436
K	238W	HIS	-	expression tag	UNP Q99436
K	238X	PRO	-	expression tag	UNP Q99436
K	238Y	GLN	-	expression tag	UNP Q99436

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	238Z	PHE	-	expression tag	UNP Q99436
K	239A	GLU	-	expression tag	UNP Q99436
K	239B	LYS	-	expression tag	UNP Q99436
K	247	UNK	-	expression tag	UNP Q99436
K	248	UNK	-	expression tag	UNP Q99436
K	249	UNK	-	expression tag	UNP Q99436
K	250	UNK	-	expression tag	UNP Q99436
K	251	UNK	-	expression tag	UNP Q99436
K	252	UNK	-	expression tag	UNP Q99436
K	253	UNK	-	expression tag	UNP Q99436
K	254	UNK	-	expression tag	UNP Q99436
K	255	UNK	-	expression tag	UNP Q99436
K	256	UNK	-	expression tag	UNP Q99436
K	257	UNK	-	expression tag	UNP Q99436
K	258	UNK	-	expression tag	UNP Q99436
K	259	UNK	-	expression tag	UNP Q99436
K	260	UNK	-	expression tag	UNP Q99436
K	261	UNK	-	expression tag	UNP Q99436
K	262	UNK	-	expression tag	UNP Q99436

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	179	Total	C	N	O	S	0	0
			1343	865	224	238	16		

- Molecule 13 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	197	Total	C	N	O	S	0	0
			1462	940	249	265	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	ACE	-	acetylation	UNP P49721

- Molecule 14 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	172	Total	C	N	O	S	0	0
			1250	800	215	228	7		

- Molecule 15 is a protein called Proteasome subunit beta type-1.

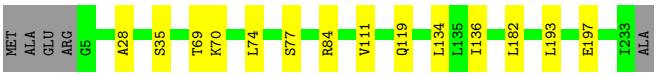
Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	160	Total	C	N	O	S	0	0
			1111	704	188	211	8		

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.

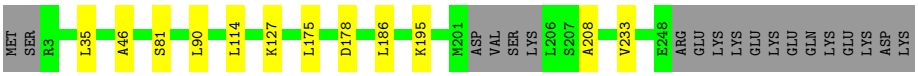
- Molecule 1: Proteasome subunit alpha type-2

Chain A:



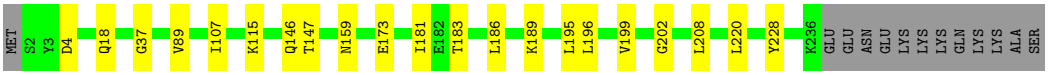
- Molecule 2: Proteasome subunit alpha type-4

Chain B:



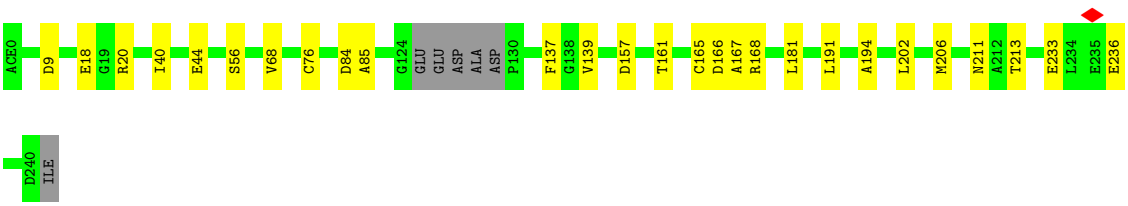
- Molecule 3: Proteasome subunit alpha type-7

Chain C:



- Molecule 4: Proteasome subunit alpha type-5

Chain D:

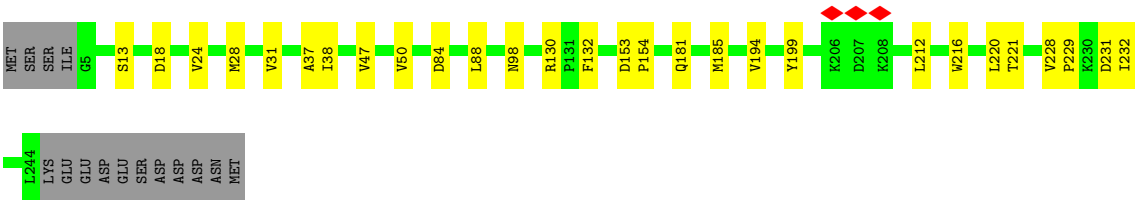


- Molecule 5: Proteasome subunit alpha type-1

Chain E:

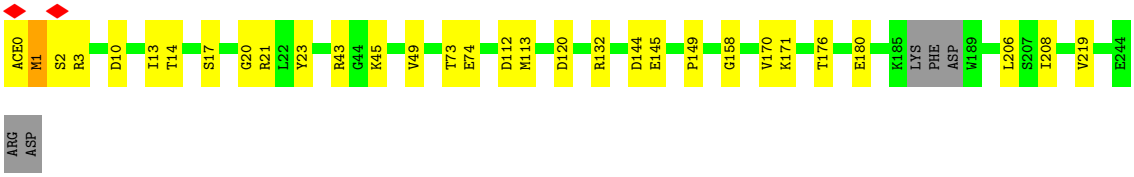
• Molecule 6: Proteasome subunit alpha type-3

Chain F:



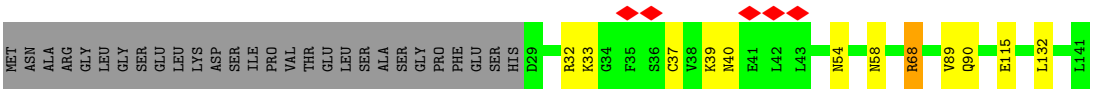
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



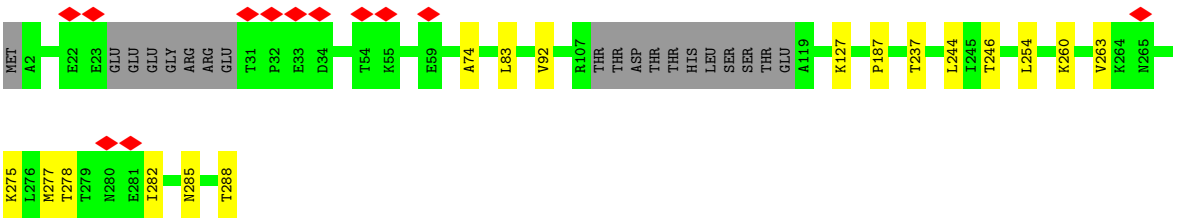
• Molecule 8: Proteasome maturation protein

Chain H:



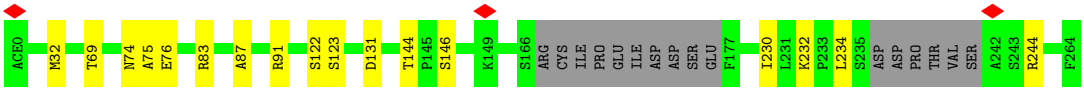
• Molecule 9: Proteasome assembly chaperone 1

Chain I:

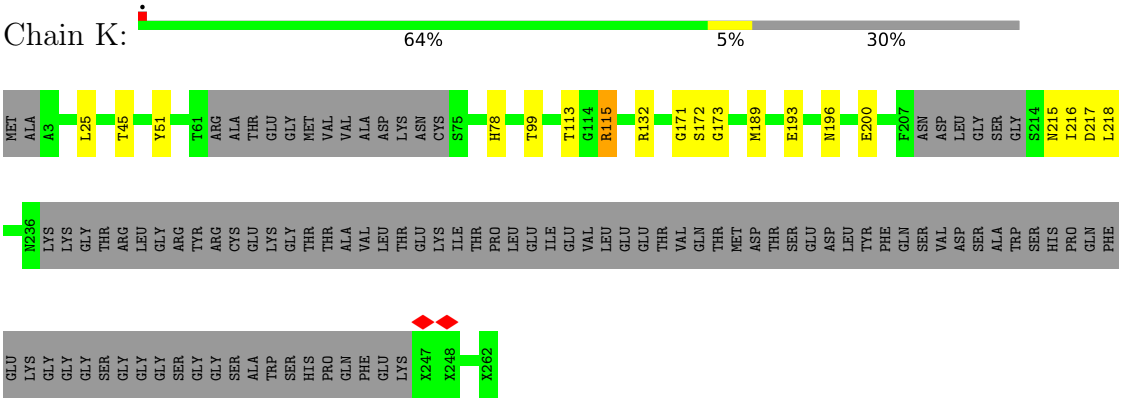


• Molecule 10: Proteasome assembly chaperone 2

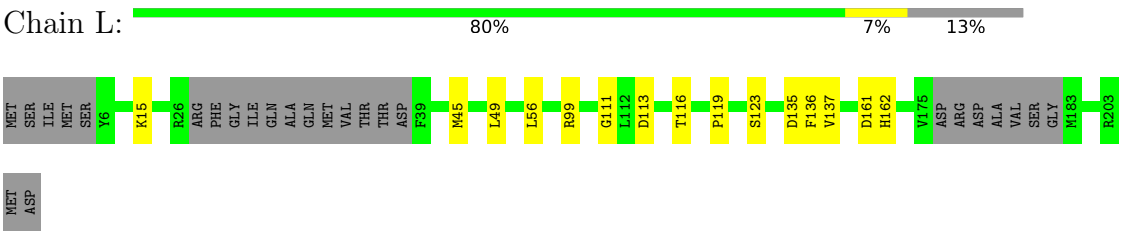
Chain J:



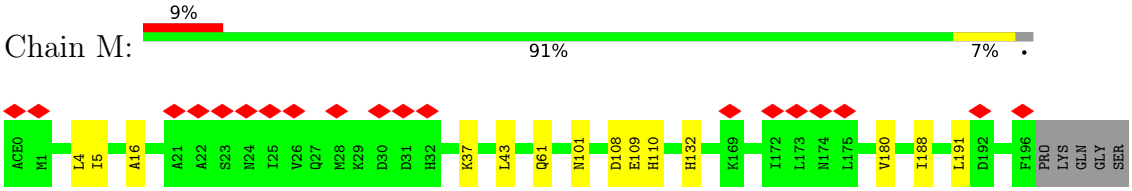
• Molecule 11: Proteasome subunit beta type-7



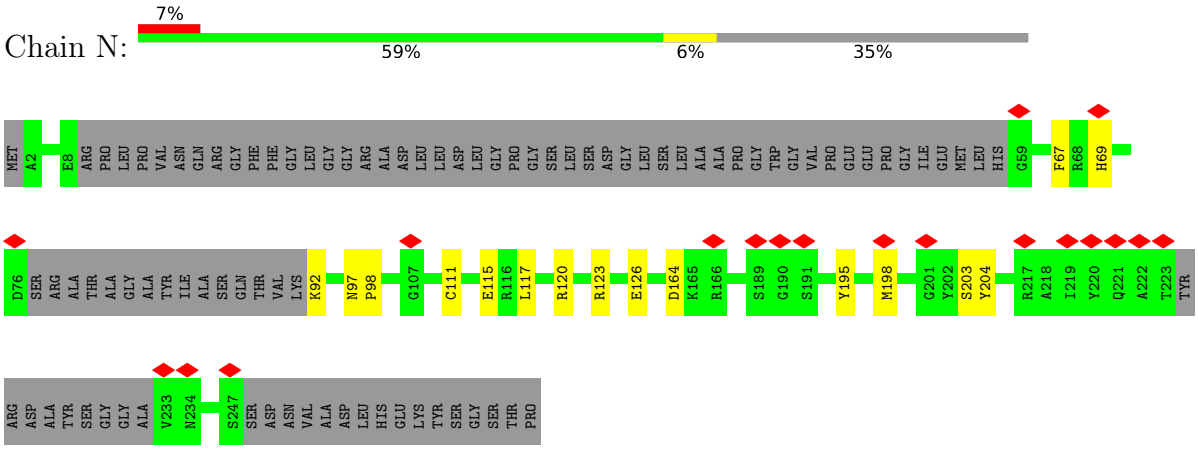
• Molecule 12: Proteasome subunit beta type-3



• Molecule 13: Proteasome subunit beta type-2

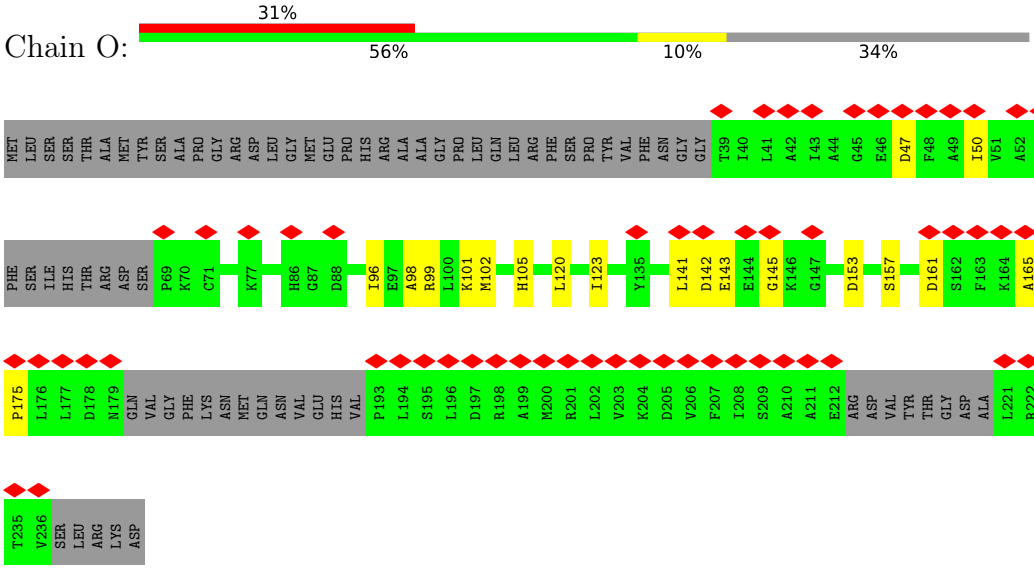


• Molecule 14: Proteasome subunit beta type-5



• Molecule 15: Proteasome subunit beta type-1

Chain O:


31%
56%
10%
34%
MET LEU SER SER THR ALA MET TYR SER ALA PRO GLY ARG ASP LEU GLY MET GLU PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU ARG PHE SER PRO TYR VAL PHE ASN GLY GLY T39 I40 L41 A42 I43 A44 G45 E46 D47 F48 A49 I50 V51 A52 S53 D54 THR ARG LEU SER GLU GLY
PHE SER ILE HIS THR ARG ASP SER P69 K70 C71 K77 H86 G87 D88 I96 E97 A98 R99 L100 K101 M102 H105 L120 I123 Y135 L141 D142 E143 E144 G145 K146 G147 D153 S157 D161 S162 F163 K164 A165 G166 GLY SER ALA S170 A171 M172 L173 Q174
P175 L176 L177 D178 N179 GLN VAL GLY PHE LYS ASN MET GLN ASN VAL GLU HIS VAL P193 L194 S195 L196 D197 R198 A199 M200 R201 L202 V203 K204 D205 V206 F207 I208 S209 A210 A211 E212 ARG ASP VAL TYR THR GLY ASP ALA L221 R222 I223 C224 I225 V226 T227 K228 E229 G230 I231 R232 E233 E234
T235 V236 SER LEU ARG LYS ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41421	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 ($e^-/Å^2$)	66.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.624	Depositor
Minimum map value	-1.099	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	255.36, 255.36, 255.36	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8512, 0.8512, 0.8512	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE

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	0.26	0/1770	0.46	0/2407
2	B	0.26	0/1813	0.48	0/2461
3	C	0.25	0/1806	0.50	0/2451
4	D	0.25	0/1784	0.47	0/2417
5	E	0.25	0/1885	0.51	0/2553
6	F	0.26	0/1869	0.48	0/2527
7	G	0.26	0/1849	0.48	0/2507
8	H	0.25	0/916	0.46	0/1232
9	I	0.25	0/2100	0.45	0/2863
10	J	0.25	0/1926	0.48	0/2617
11	K	0.26	0/1596	0.47	0/2171
12	L	0.26	0/1367	0.48	0/1850
13	M	0.26	0/1490	0.48	0/2029
14	N	0.24	0/1271	0.47	0/1723
15	O	0.23	0/1123	0.48	0/1522
All	All	0.25	0/24565	0.48	0/33330

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	1731	0	1702	11	0
2	B	1786	0	1729	8	0
3	C	1780	0	1747	14	0
4	D	1758	0	1713	18	0
5	E	1852	0	1816	13	0
6	F	1834	0	1776	19	0
7	G	1819	0	1798	20	0
8	H	901	0	909	10	0
9	I	2056	0	1982	11	0
10	J	1888	0	1884	11	0
11	K	1646	0	1548	11	0
12	L	1343	0	1321	8	0
13	M	1462	0	1389	8	0
14	N	1250	0	1188	10	0
15	O	1111	0	1047	13	0
All	All	24217	0	23549	166	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 166 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)
4:D:85:ALA:HB2	4:D:139:VAL:HG21	1.76	0.67
1:A:69:THR:HG22	1:A:70:LYS:H	1.59	0.67
1:A:74:LEU:HD21	1:A:134:LEU:HD22	1.77	0.67
3:C:89:VAL:HG11	8:H:32:ARG:HE	1.61	0.66
5:E:120:THR:O	6:F:130:ARG:NH2	2.28	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%)	220 (97%)	7 (3%)	0	100	100
2	B	238/261 (91%)	233 (98%)	5 (2%)	0	100	100
3	C	233/248 (94%)	223 (96%)	10 (4%)	0	100	100
4	D	232/242 (96%)	219 (94%)	13 (6%)	0	100	100
5	E	238/264 (90%)	226 (95%)	12 (5%)	0	100	100
6	F	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
7	G	238/247 (96%)	232 (98%)	5 (2%)	1 (0%)	30	54
8	H	111/141 (79%)	106 (96%)	5 (4%)	0	100	100
9	I	263/288 (91%)	247 (94%)	16 (6%)	0	100	100
10	J	243/265 (92%)	231 (95%)	12 (5%)	0	100	100
11	K	209/332 (63%)	202 (97%)	7 (3%)	0	100	100
12	L	173/205 (84%)	167 (96%)	6 (4%)	0	100	100
13	M	195/202 (96%)	185 (95%)	10 (5%)	0	100	100
14	N	164/263 (62%)	157 (96%)	7 (4%)	0	100	100
15	O	150/241 (62%)	139 (93%)	11 (7%)	0	100	100
All	All	3152/3688 (86%)	3021 (96%)	130 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	1	MET

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/191 (91%)	174 (100%)	0	100	100
2	B	173/221 (78%)	173 (100%)	0	100	100
3	C	180/211 (85%)	180 (100%)	0	100	100
4	D	186/203 (92%)	186 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	195/224 (87%)	195 (100%)	0	100 100
6	F	187/212 (88%)	187 (100%)	0	100 100
7	G	189/210 (90%)	189 (100%)	0	100 100
8	H	104/128 (81%)	102 (98%)	2 (2%)	52 73
9	I	220/262 (84%)	220 (100%)	0	100 100
10	J	208/237 (88%)	208 (100%)	0	100 100
11	K	160/257 (62%)	159 (99%)	1 (1%)	84 91
12	L	135/174 (78%)	134 (99%)	1 (1%)	81 90
13	M	139/171 (81%)	139 (100%)	0	100 100
14	N	115/202 (57%)	115 (100%)	0	100 100
15	O	104/199 (52%)	104 (100%)	0	100 100
All	All	2469/3102 (80%)	2465 (100%)	4 (0%)	91 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	33	LYS
8	H	68	ARG
11	K	115	ARG
12	L	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
8	H	58	ASN
13	M	101	ASN

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.

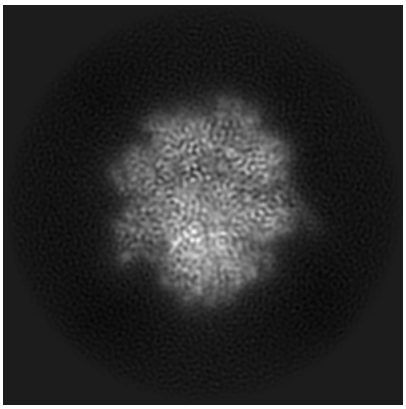
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18773. These allow visual inspection of the internal detail of the map and identification of artifacts.

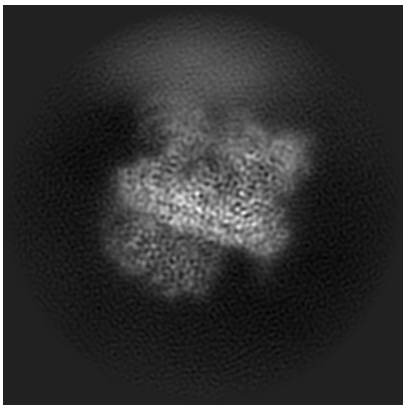
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

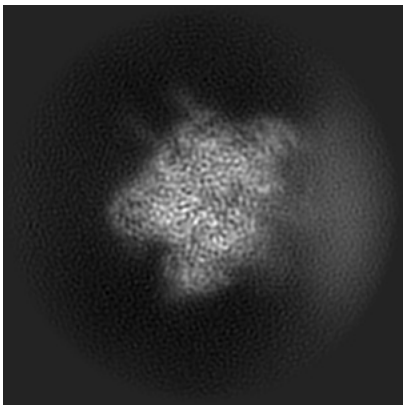
6.1.1 Primary map



X

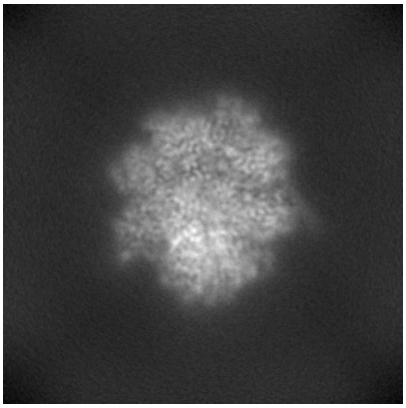


Y

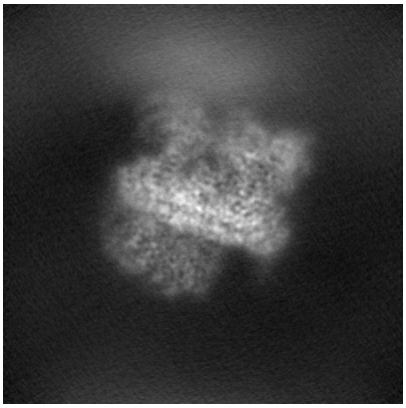


Z

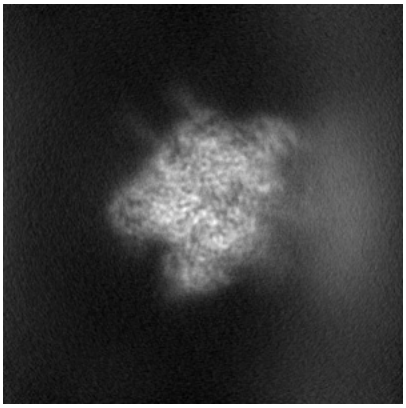
6.1.2 Raw map



X



Y

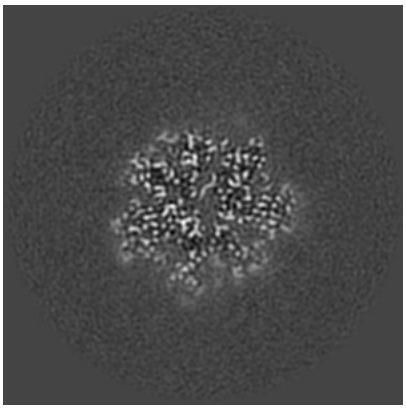


Z

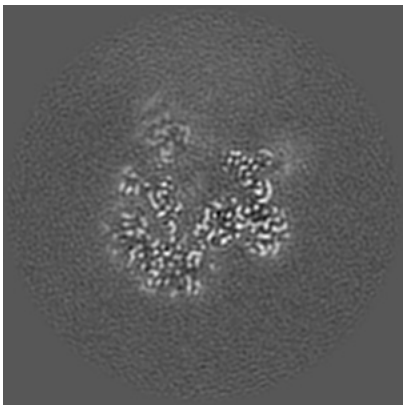
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

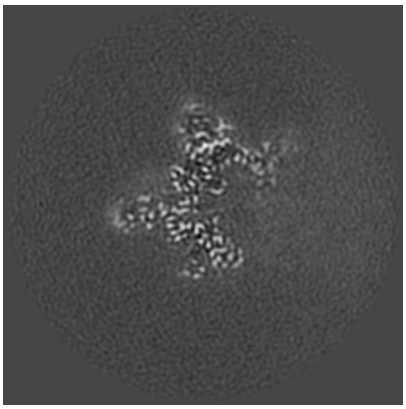
6.2.1 Primary map



X Index: 150

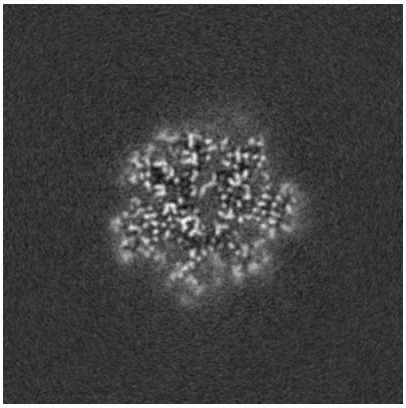


Y Index: 150

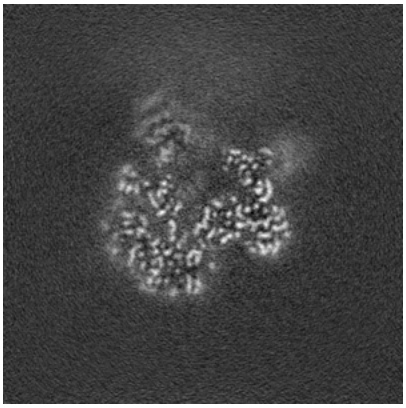


Z Index: 150

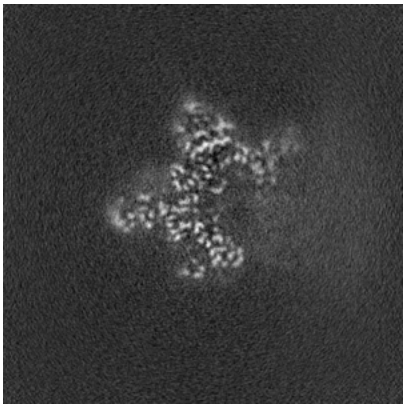
6.2.2 Raw map



X Index: 150



Y Index: 150

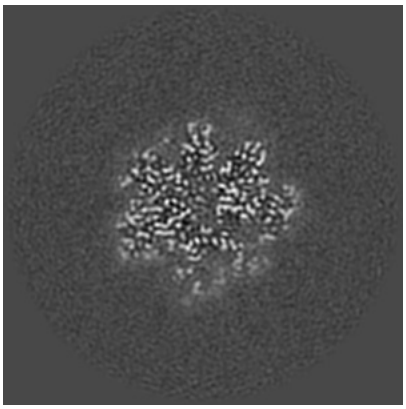


Z Index: 150

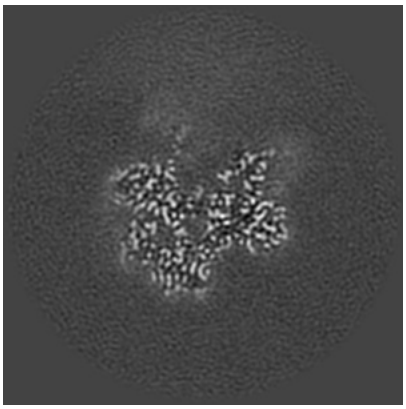
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

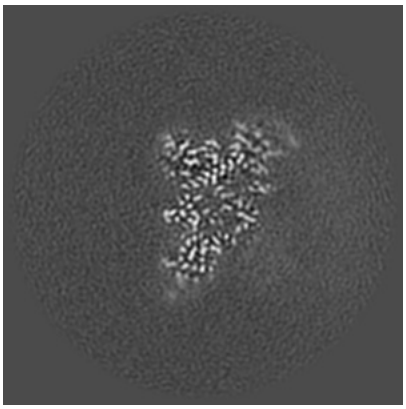
6.3.1 Primary map



X Index: 147

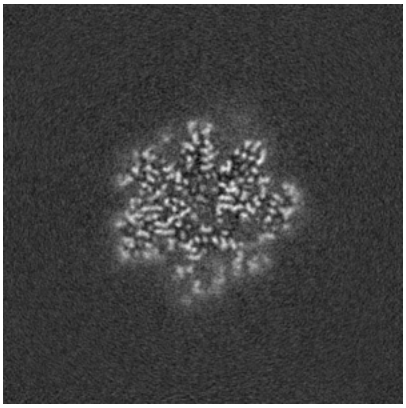


Y Index: 141

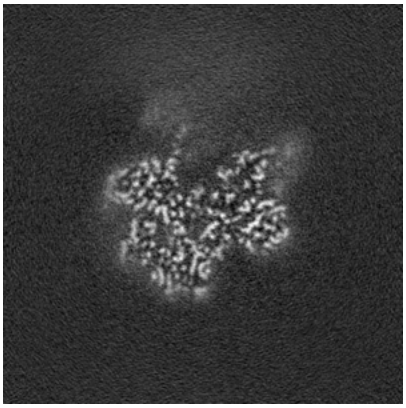


Z Index: 179

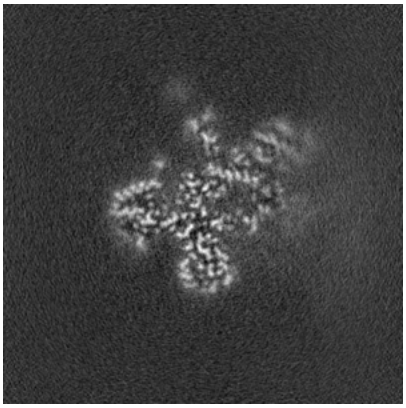
6.3.2 Raw map



X Index: 147



Y Index: 140

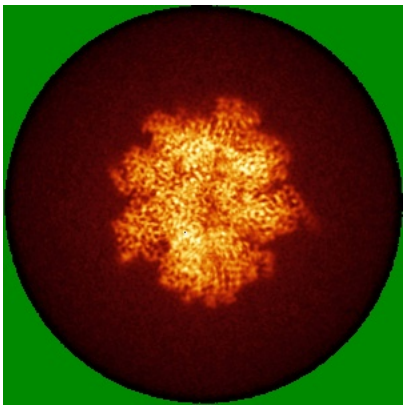


Z Index: 129

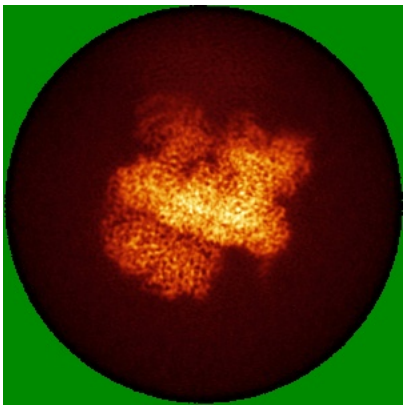
The images above show the largest variance slices of the map in three orthogonal directions.

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

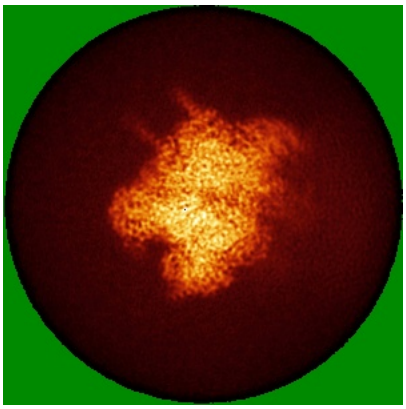
6.4.1 Primary map



X

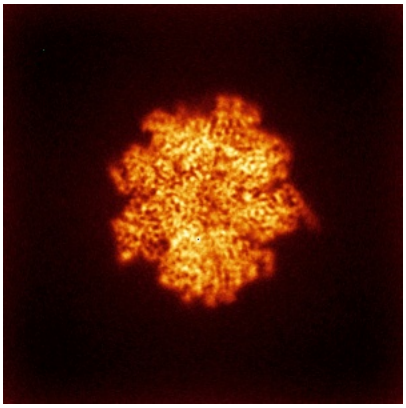


Y

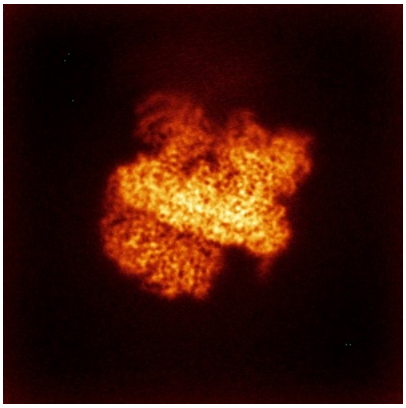


Z

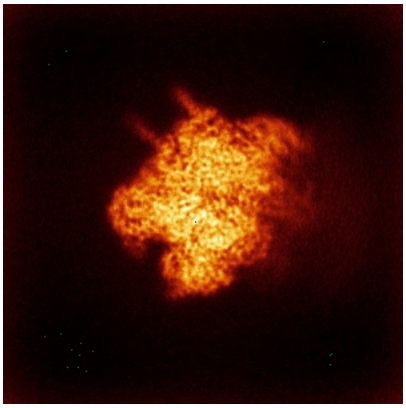
6.4.2 Raw map



X



Y

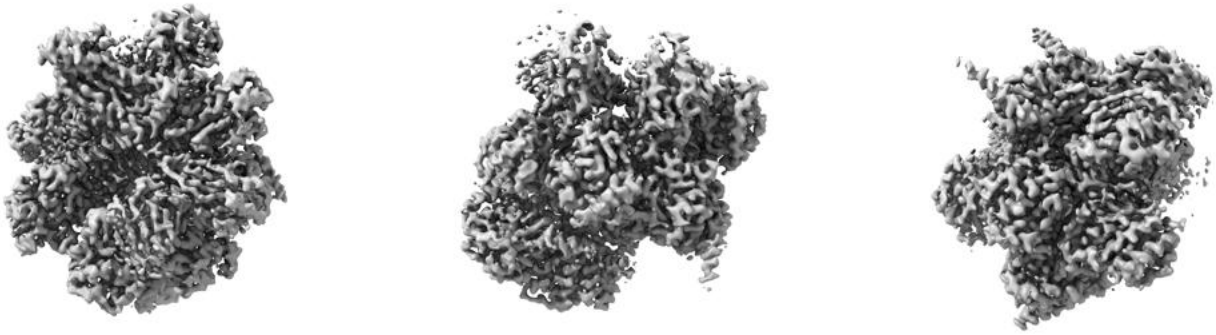


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

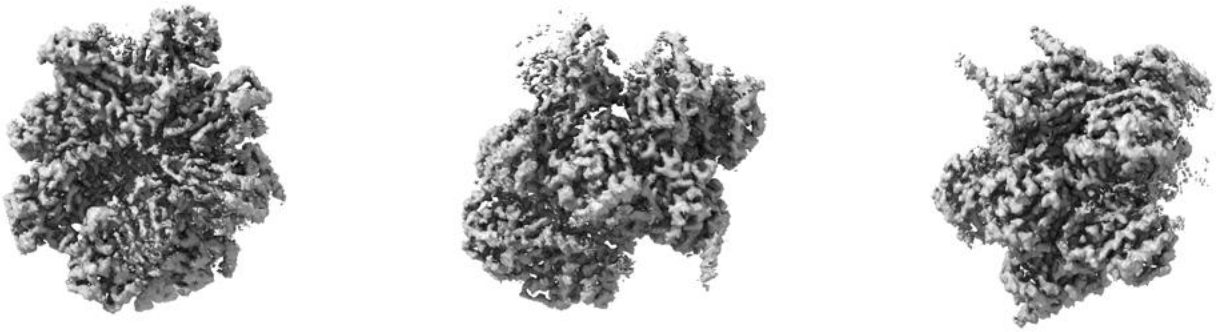
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

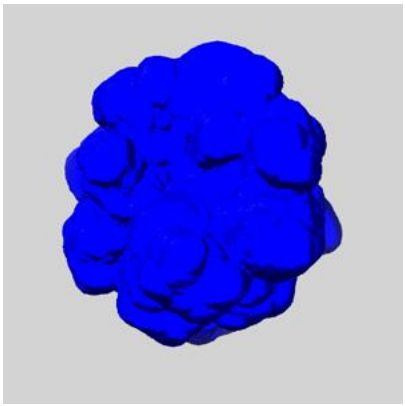
6.6 Mask visualisation (i)

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

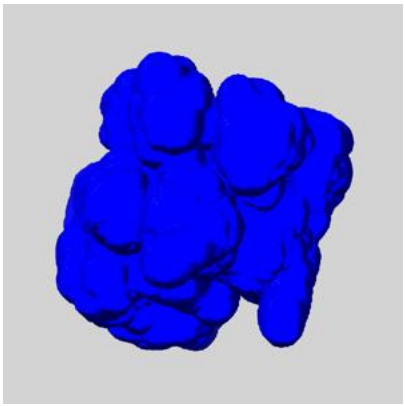
A mask typically either:

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

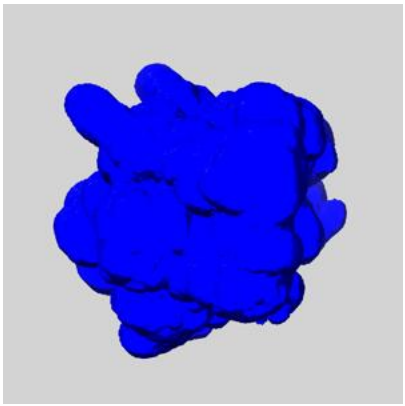
6.6.1 emd_18773_msk_1.map (i)



X



Y

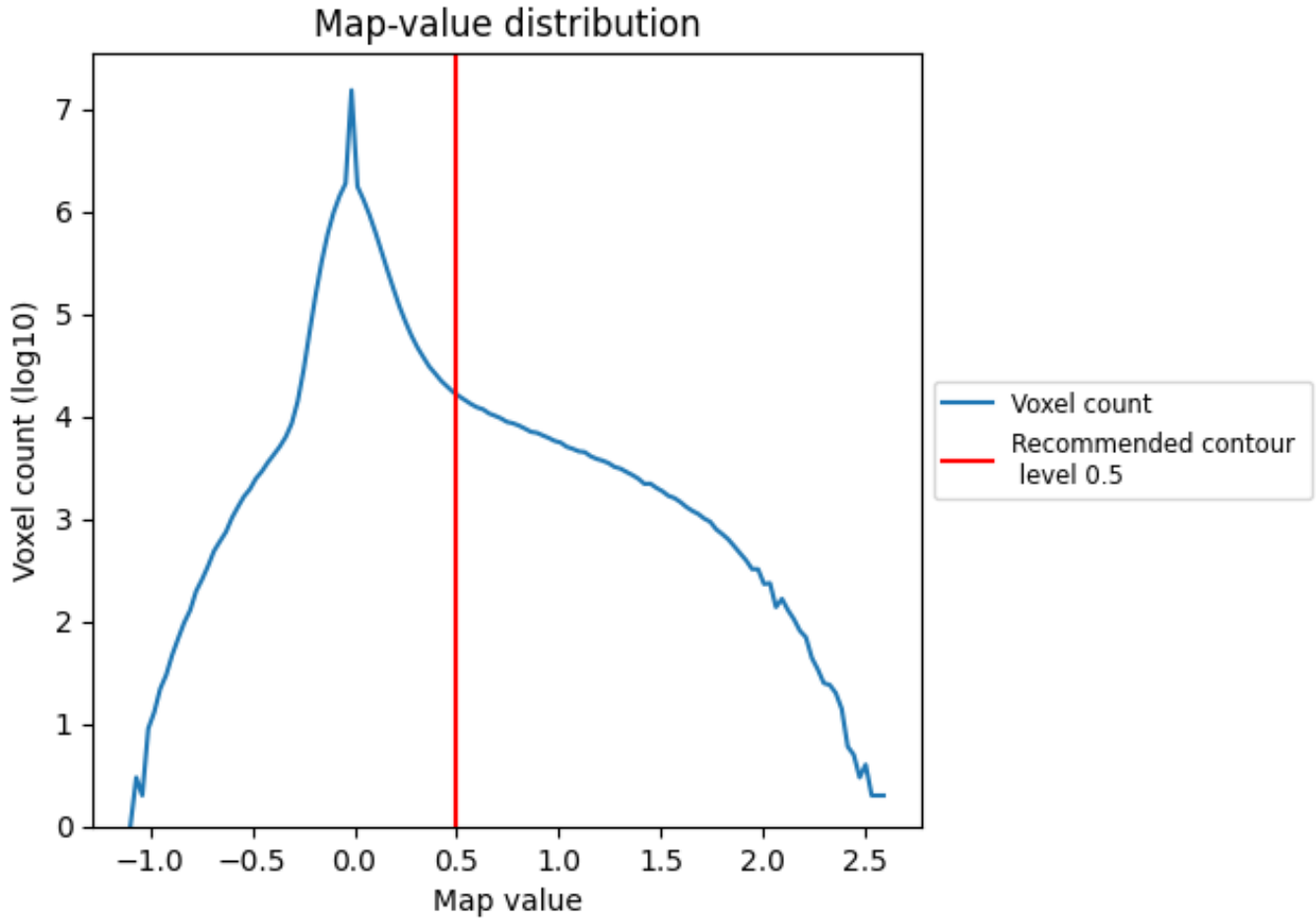


Z

7 Map analysis

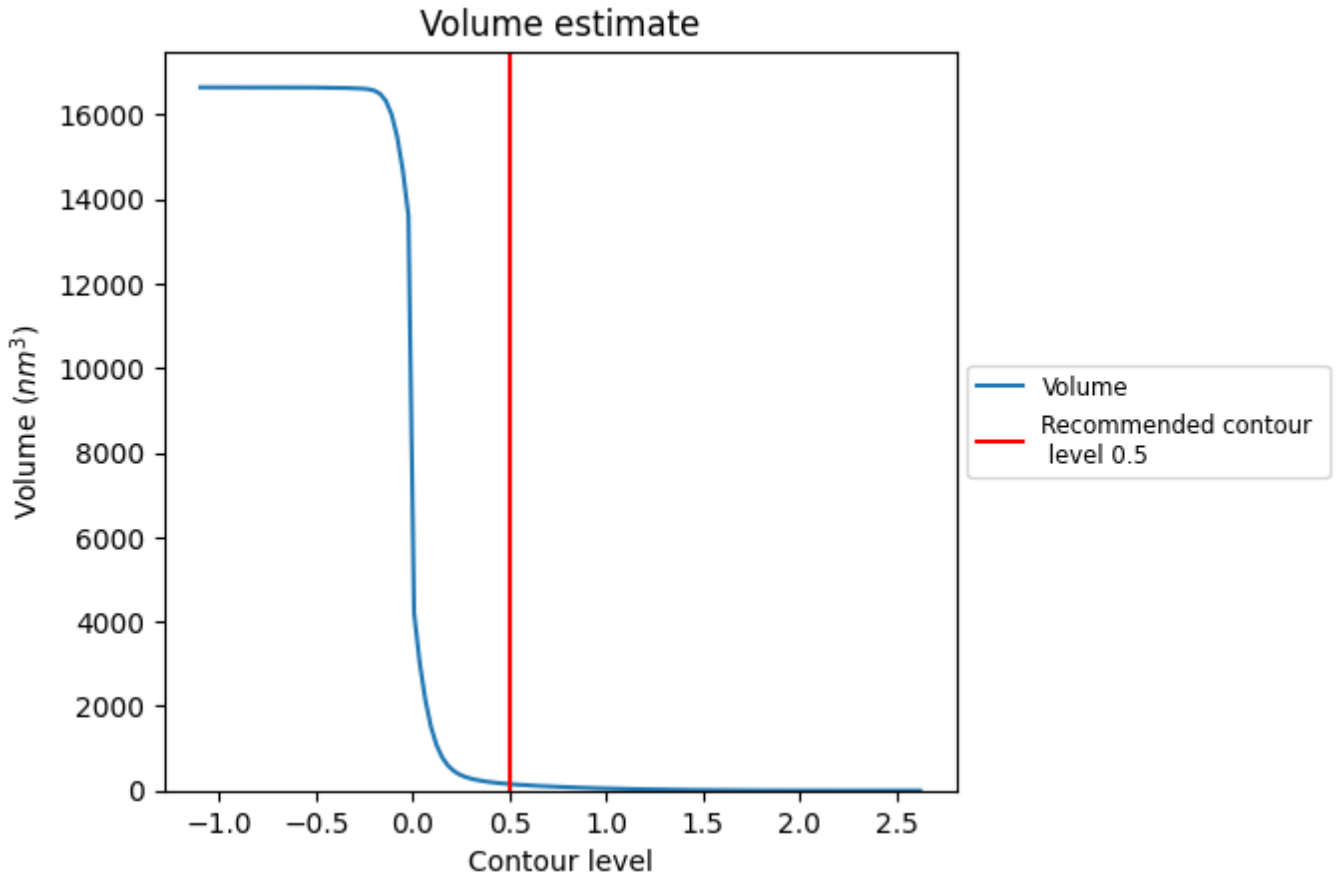
This section contains the results of statistical analysis of the map.

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.

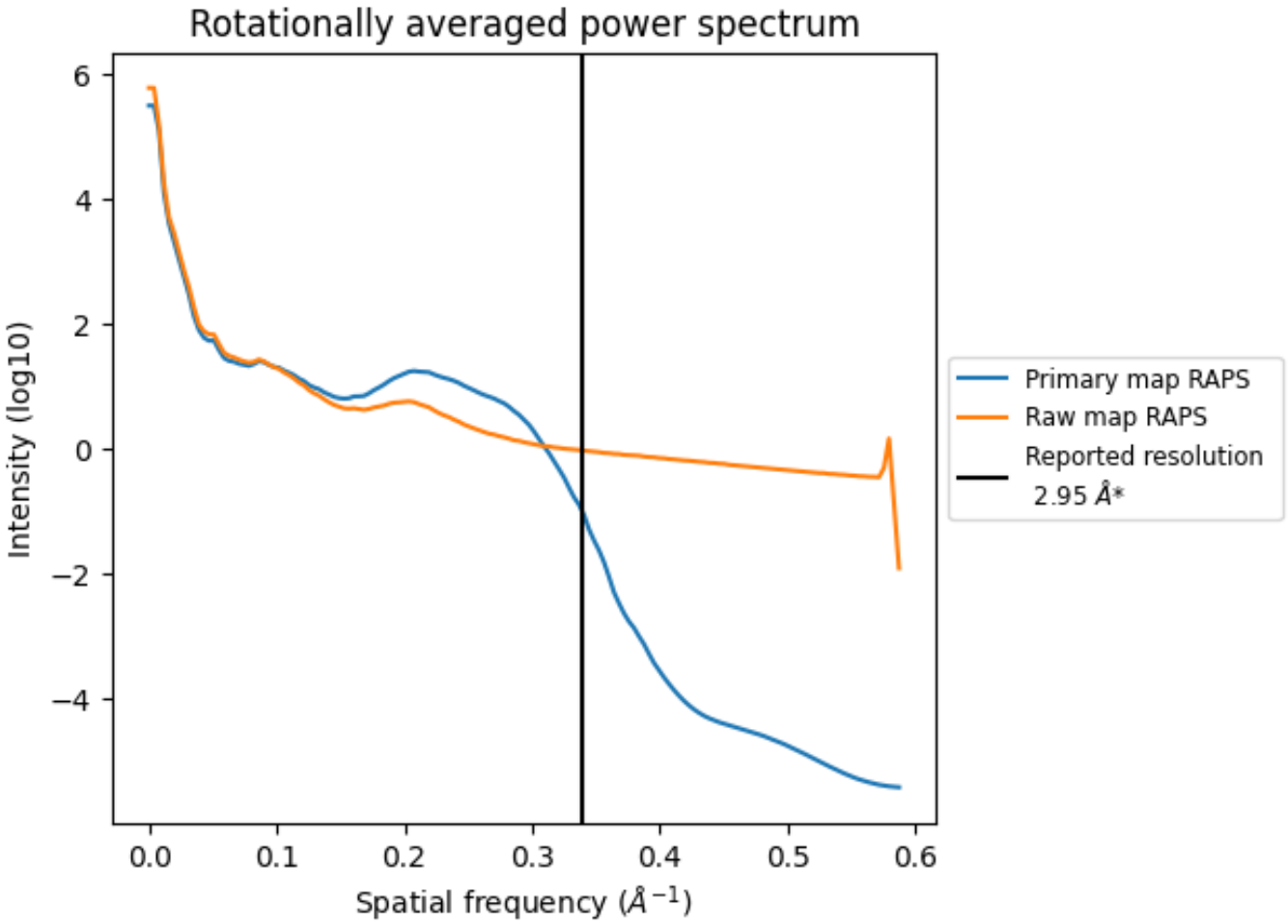
7.2 Volume estimate (i)



The volume at the recommended contour level is 154 nm^3; this corresponds to an approximate mass of 139 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)

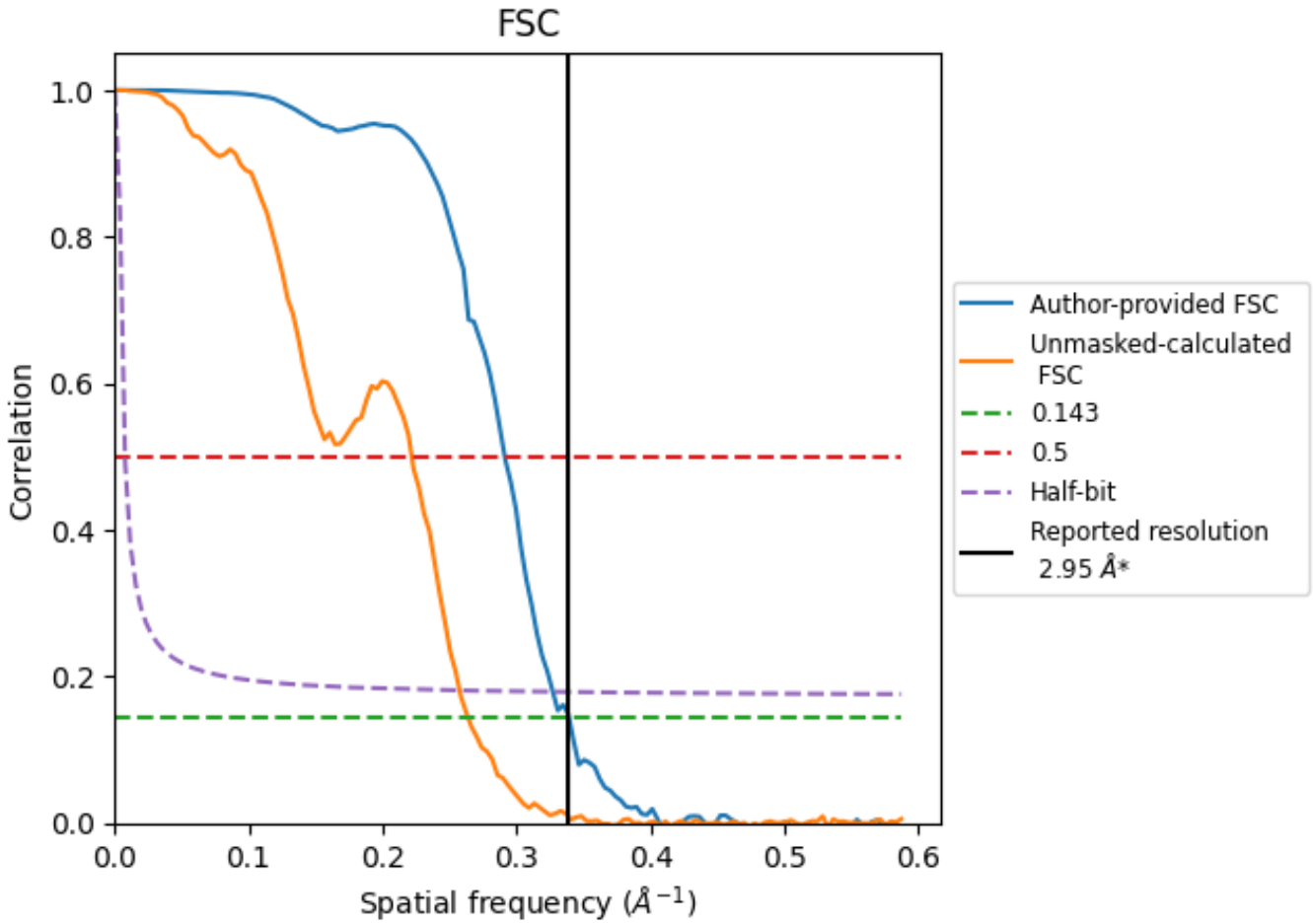


*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

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 0.339 Å^{-1}

8.2 Resolution estimates (i)

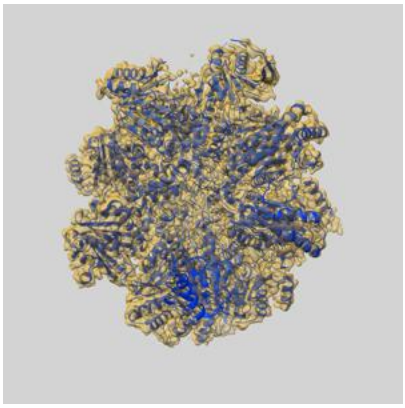
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.43	3.06
Unmasked-calculated*	3.79	4.51	3.88

*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 3.79 differs from the reported value 2.95 by more than 10 %

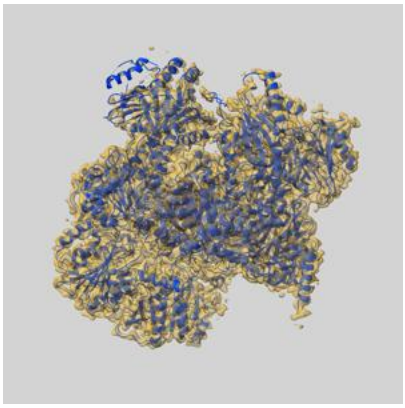
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18773 and PDB model 8QZ9. Per-residue inclusion information can be found in section 3 on page 9.

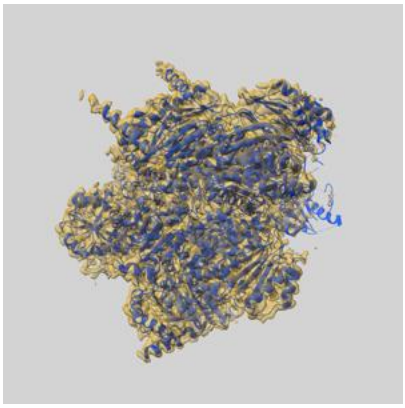
9.1 Map-model overlay



X



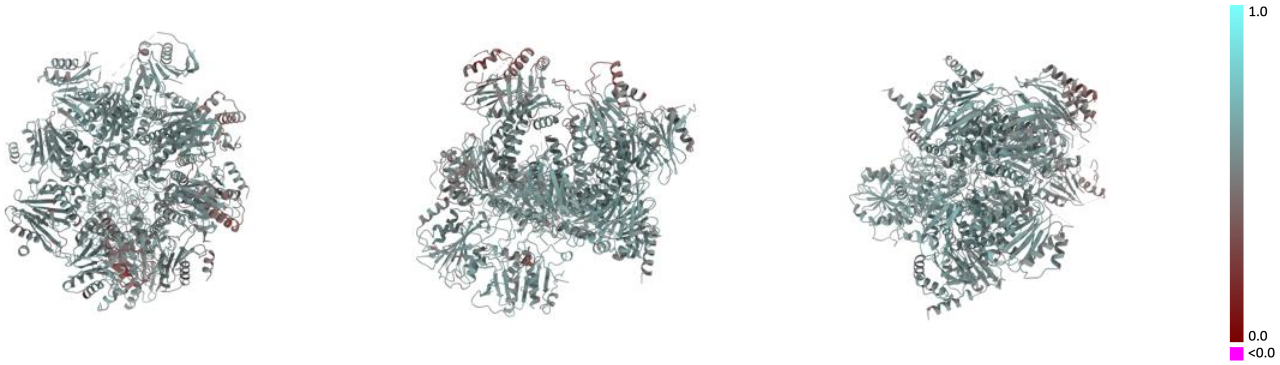
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

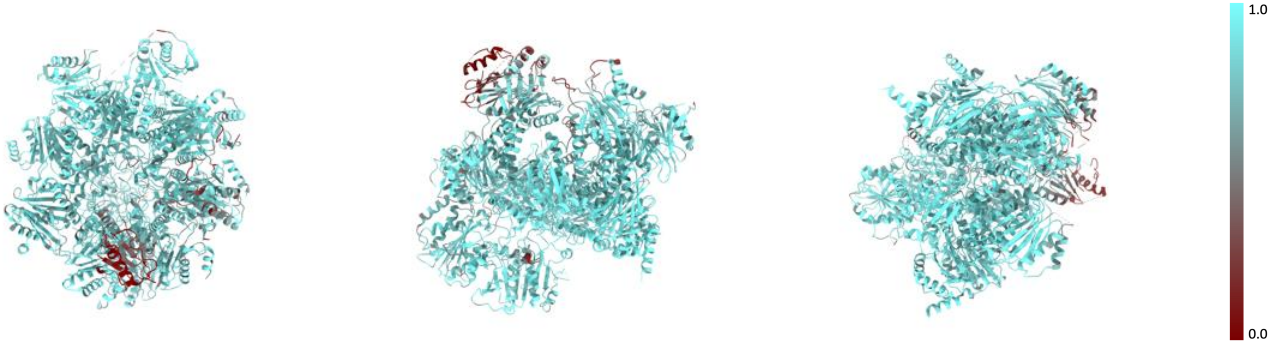
9.2 Q-score mapped to coordinate model (i)



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.

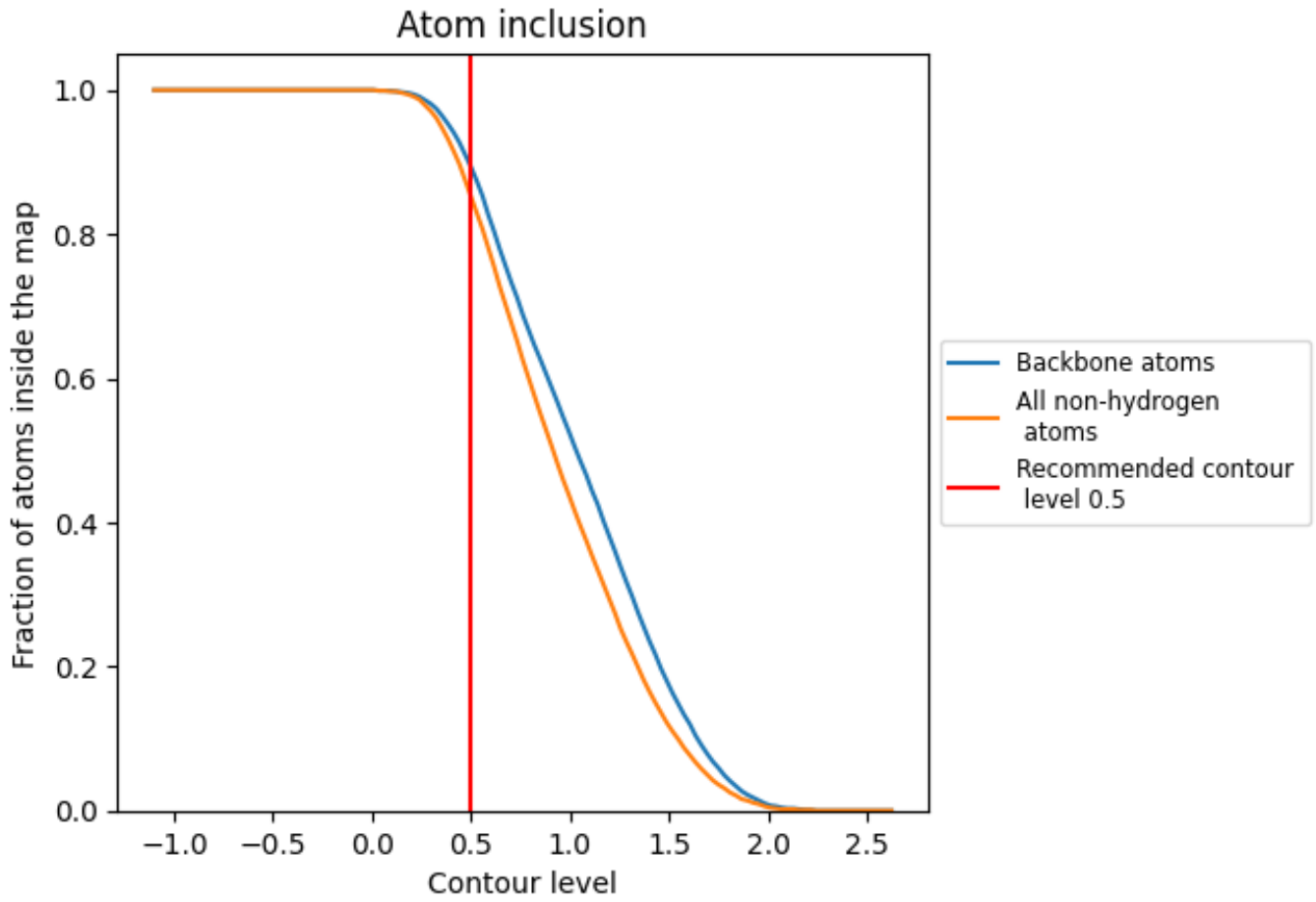
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.5550
A	0.9410	0.5860
B	0.9300	0.5810
C	0.9190	0.5720
D	0.8640	0.5400
E	0.9060	0.5670
F	0.8870	0.5610
G	0.9230	0.5770
H	0.8250	0.5630
I	0.8170	0.5450
J	0.8940	0.5680
K	0.8740	0.5650
L	0.8800	0.5550
M	0.7700	0.5150
N	0.7070	0.5150
O	0.4460	0.4720