Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:45 am GMT

PDB ID	:	6RGQ
EMDB ID	:	EMD-4877
Title	:	Human 20S Proteasome
Authors	:	Toste Rego, A.; da Fonseca, P.C.A.
Deposited on	:	2019-04-17
Resolution	:	2.60 Å(reported)
Based on initial model	:	5LE5

This is a Full wwPDB EM Validation 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:

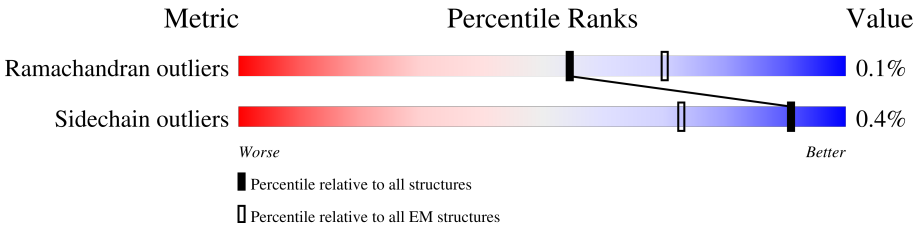
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.60 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	A	246	96%
1	O	246	96%
2	B	234	97%
2	P	234	97%
3	C	261	94% 5%
3	Q	261	94% 5%
4	D	248	5% 93% 6%
4	R	248	5% 93% 6%
5	E	241	96%

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Mol	Chain	Length	Quality of chain
5	S	241	96%
6	F	263	87% 11%
6	T	263	87% 11%
7	G	255	93% 6%
7	U	255	93% 6%
8	H	205	99%
8	V	205	99%
9	I	234	94% 6%
9	W	234	94% 6%
10	J	205	99%
10	X	205	99%
11	K	201	95%
11	Y	201	95%
12	L	204	97%
12	Z	204	97%
13	M	213	99%
13	a	213	99%
14	N	219	96%
14	b	219	96%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 45340 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		
1	O	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		
2	P	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		
3	Q	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		
4	R	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		
5	S	233	Total	C	N	O	S	0	0
			1659	1056	287	305	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		
6	T	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		
7	U	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		
8	V	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		
9	W	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		
11	Y	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		
12	Z	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		
13	a	212	Total	C	N	O	S	0	0
			1583	1016	279	278	10		

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

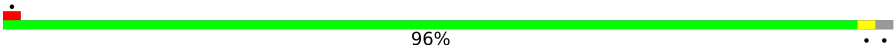
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		
14	b	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		

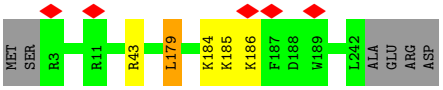
3 Residue-property plots (i)

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-6

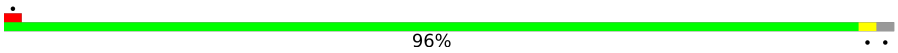
Chain A:

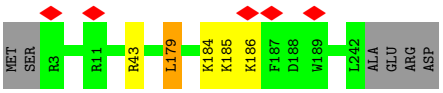




• Molecule 1: Proteasome subunit alpha type-6

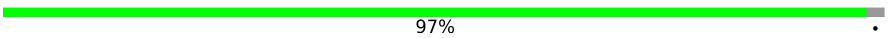
Chain O:





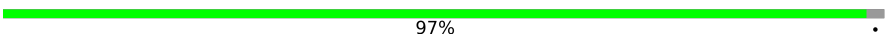
• Molecule 2: Proteasome subunit alpha type-2

Chain B:



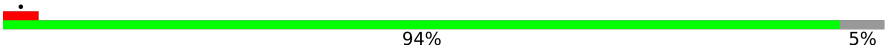
• Molecule 2: Proteasome subunit alpha type-2

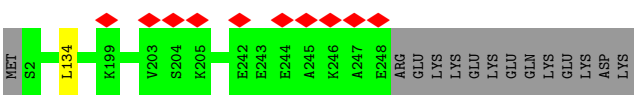
Chain P:



• Molecule 3: Proteasome subunit alpha type-4

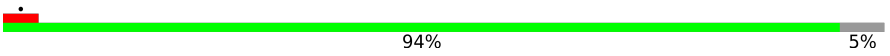
Chain C:

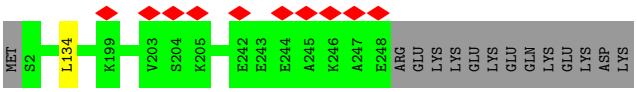




• Molecule 3: Proteasome subunit alpha type-4

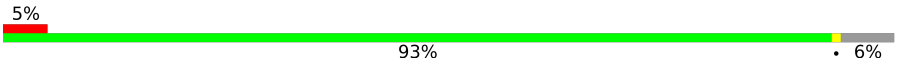
Chain Q:

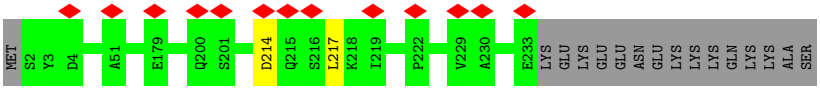




• Molecule 4: Proteasome subunit alpha type-7

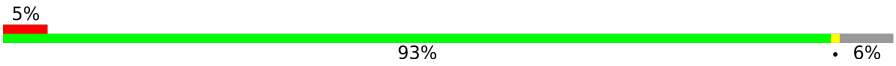
Chain D:

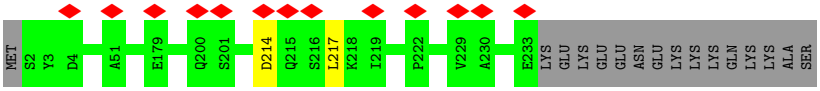




• Molecule 4: Proteasome subunit alpha type-7

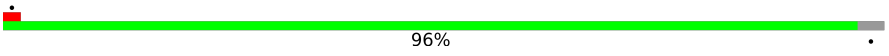
Chain R:

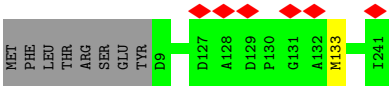




• Molecule 5: Proteasome subunit alpha type-5

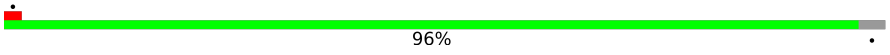
Chain E:

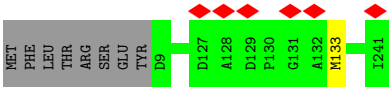




• Molecule 5: Proteasome subunit alpha type-5

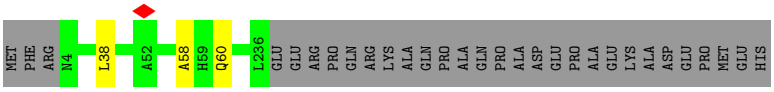
Chain S:





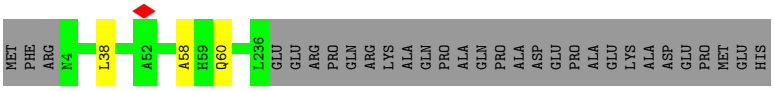
• Molecule 6: Proteasome subunit alpha type-1

Chain F:



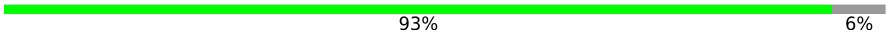
• Molecule 6: Proteasome subunit alpha type-1

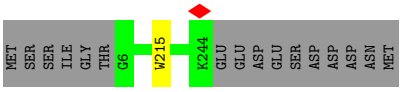
Chain T:



• Molecule 7: Proteasome subunit alpha type-3

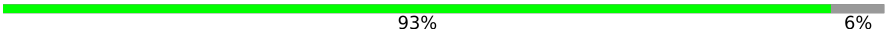
Chain G:

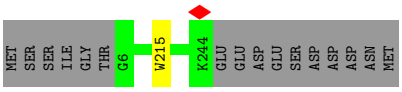




• Molecule 7: Proteasome subunit alpha type-3

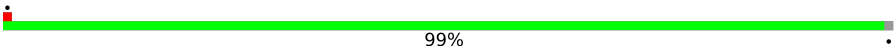
Chain U:

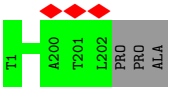




• Molecule 8: Proteasome subunit beta type-6

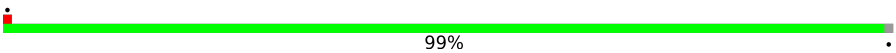
Chain H:

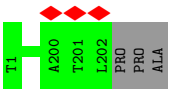




• Molecule 8: Proteasome subunit beta type-6

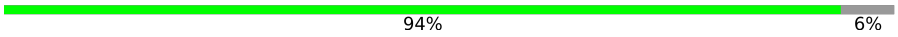
Chain V:

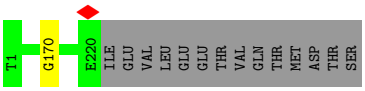




• Molecule 9: Proteasome subunit beta type-7

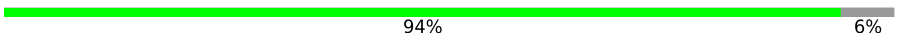
Chain I:

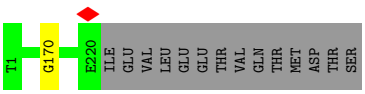




• Molecule 9: Proteasome subunit beta type-7

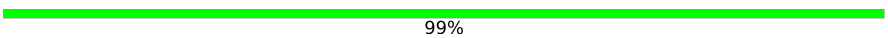
Chain W:

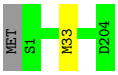




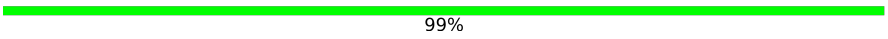
• Molecule 10: Proteasome subunit beta type-3

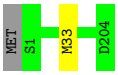
Chain J:



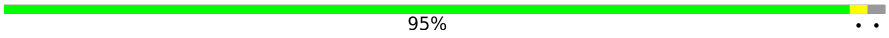


• Molecule 10: Proteasome subunit beta type-3

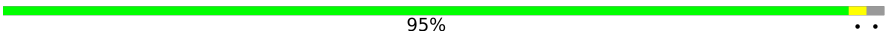
Chain X: 



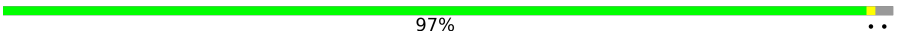
• Molecule 11: Proteasome subunit beta type-2

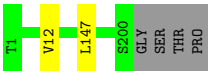
Chain K: 

• Molecule 11: Proteasome subunit beta type-2

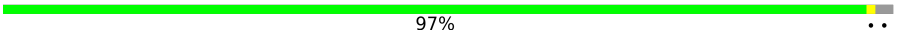
Chain Y: 

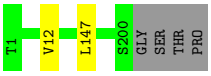
• Molecule 12: Proteasome subunit beta type-5

Chain L: 

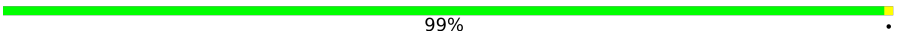


• Molecule 12: Proteasome subunit beta type-5

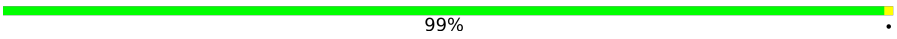
Chain Z: 

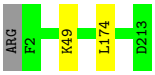


• Molecule 13: Proteasome subunit beta type-1

Chain M: 

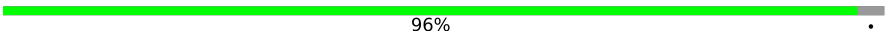
• Molecule 13: Proteasome subunit beta type-1

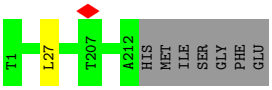
Chain a: 



• Molecule 14: Proteasome subunit beta type-4

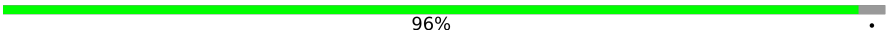
Chain N:

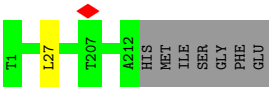




• Molecule 14: Proteasome subunit beta type-4

Chain b:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	50885	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 ($e^-/Å^2$)	45.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	95000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	18.005	Depositor
Minimum map value	-9.676	Depositor
Average map value	-0.019	Depositor
Map value standard deviation	0.769	Depositor
Recommended contour level	2.6	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	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	0.46	0/1763	0.62	2/2393 (0.1%)
1	O	0.46	0/1763	0.62	2/2393 (0.1%)
2	B	0.47	0/1701	0.60	1/2318 (0.0%)
2	P	0.47	0/1701	0.60	1/2318 (0.0%)
3	C	0.42	0/1815	0.60	1/2466 (0.0%)
3	Q	0.42	0/1815	0.60	1/2466 (0.0%)
4	D	0.39	0/1657	0.57	1/2261 (0.0%)
4	R	0.39	0/1657	0.57	1/2261 (0.0%)
5	E	0.40	0/1685	0.57	0/2290
5	S	0.40	0/1685	0.57	0/2290
6	F	0.42	0/1738	0.58	0/2364
6	T	0.42	0/1738	0.58	0/2364
7	G	0.45	0/1795	0.56	0/2434
7	U	0.45	0/1795	0.56	0/2434
8	H	0.46	0/1491	0.58	0/2021
8	V	0.46	0/1491	0.58	0/2021
9	I	0.45	0/1603	0.66	1/2180 (0.0%)
9	W	0.45	0/1603	0.66	1/2180 (0.0%)
10	J	0.44	0/1563	0.63	0/2113
10	X	0.44	0/1563	0.63	0/2113
11	K	0.48	0/1538	0.65	3/2088 (0.1%)
11	Y	0.48	0/1538	0.65	3/2088 (0.1%)
12	L	0.54	0/1531	0.67	1/2076 (0.0%)
12	Z	0.54	0/1531	0.67	1/2076 (0.0%)
13	M	0.46	0/1613	0.66	1/2178 (0.0%)
13	a	0.46	0/1613	0.65	1/2178 (0.0%)
14	N	0.47	0/1598	0.64	1/2170 (0.0%)
14	b	0.47	0/1598	0.64	1/2170 (0.0%)
All	All	0.45	0/46182	0.61	24/62704 (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
1	A	0	2
1	O	0	2
4	D	0	1
4	R	0	1
6	F	0	2
6	T	0	2
11	K	0	1
11	Y	0	1
All	All	0	12

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	LEU	CA-CB-CG	6.82	130.97	115.30
1	O	179	LEU	CA-CB-CG	6.80	130.95	115.30
2	B	133	LEU	CB-CG-CD1	-6.70	99.61	111.00
2	P	133	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	A	179	LEU	CB-CG-CD2	-6.32	100.25	111.00
1	O	179	LEU	CB-CG-CD2	-6.32	100.25	111.00
13	a	174	LEU	CA-CB-CG	5.97	129.02	115.30
13	M	174	LEU	CA-CB-CG	5.96	129.01	115.30
11	K	103	LEU	CA-CB-CG	5.78	128.60	115.30
12	L	147	LEU	CA-CB-CG	5.78	128.58	115.30
12	Z	147	LEU	CA-CB-CG	5.77	128.56	115.30
11	Y	103	LEU	CA-CB-CG	5.75	128.53	115.30
11	Y	92	LEU	CA-CB-CG	5.67	128.33	115.30
11	K	92	LEU	CA-CB-CG	5.64	128.28	115.30
4	D	217	LEU	CA-CB-CG	5.33	127.55	115.30
4	R	217	LEU	CA-CB-CG	5.33	127.55	115.30
11	K	183	ILE	CG1-CB-CG2	-5.11	100.16	111.40
11	Y	183	ILE	CG1-CB-CG2	-5.11	100.17	111.40
3	Q	134	LEU	CA-CB-CG	5.10	127.02	115.30
3	C	134	LEU	CA-CB-CG	5.09	127.00	115.30
14	N	27	LEU	CA-CB-CG	5.07	126.96	115.30
9	I	170	GLY	C-N-CA	5.06	134.35	121.70
9	W	170	GLY	C-N-CA	5.05	134.32	121.70
14	b	27	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	LYS	Peptide
1	A	186	LYS	Peptide
4	D	214	ASP	Peptide
6	F	58	ALA	Peptide
6	F	60	GLN	Peptide
11	K	24	ASN	Peptide
1	O	185	LYS	Peptide
1	O	186	LYS	Peptide
4	R	214	ASP	Peptide
6	T	58	ALA	Peptide
6	T	60	GLN	Peptide
11	Y	24	ASN	Peptide

5.2 Too-close contacts (i)

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

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	238/246 (97%)	224 (94%)	13 (6%)	1 (0%)	34 57
1	O	238/246 (97%)	224 (94%)	13 (6%)	1 (0%)	34 57
2	B	227/234 (97%)	220 (97%)	7 (3%)	0	100 100
2	P	227/234 (97%)	220 (97%)	7 (3%)	0	100 100
3	C	245/261 (94%)	232 (95%)	13 (5%)	0	100 100
3	Q	245/261 (94%)	232 (95%)	13 (5%)	0	100 100
4	D	230/248 (93%)	219 (95%)	11 (5%)	0	100 100
4	R	230/248 (93%)	219 (95%)	11 (5%)	0	100 100
5	E	231/241 (96%)	220 (95%)	11 (5%)	0	100 100
5	S	231/241 (96%)	220 (95%)	11 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	231/263 (88%)	222 (96%)	9 (4%)	0	100	100
6	T	231/263 (88%)	222 (96%)	9 (4%)	0	100	100
7	G	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
7	U	237/255 (93%)	229 (97%)	8 (3%)	0	100	100
8	H	200/205 (98%)	194 (97%)	6 (3%)	0	100	100
8	V	200/205 (98%)	194 (97%)	6 (3%)	0	100	100
9	I	218/234 (93%)	206 (94%)	12 (6%)	0	100	100
9	W	218/234 (93%)	206 (94%)	12 (6%)	0	100	100
10	J	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
10	X	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
11	K	194/201 (96%)	179 (92%)	14 (7%)	1 (0%)	29	52
11	Y	194/201 (96%)	179 (92%)	14 (7%)	1 (0%)	29	52
12	L	198/204 (97%)	189 (96%)	9 (4%)	0	100	100
12	Z	198/204 (97%)	189 (96%)	9 (4%)	0	100	100
13	M	210/213 (99%)	198 (94%)	12 (6%)	0	100	100
13	a	210/213 (99%)	198 (94%)	12 (6%)	0	100	100
14	N	210/219 (96%)	196 (93%)	14 (7%)	0	100	100
14	b	210/219 (96%)	196 (93%)	14 (7%)	0	100	100
All	All	6142/6458 (95%)	5836 (95%)	302 (5%)	4 (0%)	54	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	25	ILE
11	Y	25	ILE
1	A	184	LYS
1	O	184	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	A	163/210 (78%)	161 (99%)	2 (1%)	71 87
1	O	163/210 (78%)	161 (99%)	2 (1%)	71 87
2	B	150/191 (78%)	150 (100%)	0	100 100
2	P	150/191 (78%)	150 (100%)	0	100 100
3	C	160/221 (72%)	160 (100%)	0	100 100
3	Q	160/221 (72%)	160 (100%)	0	100 100
4	D	136/211 (64%)	136 (100%)	0	100 100
4	R	136/211 (64%)	136 (100%)	0	100 100
5	E	158/203 (78%)	157 (99%)	1 (1%)	86 95
5	S	158/203 (78%)	157 (99%)	1 (1%)	86 95
6	F	160/224 (71%)	159 (99%)	1 (1%)	86 95
6	T	160/224 (71%)	159 (99%)	1 (1%)	86 95
7	G	162/212 (76%)	161 (99%)	1 (1%)	86 95
7	U	162/212 (76%)	161 (99%)	1 (1%)	86 95
8	H	140/159 (88%)	140 (100%)	0	100 100
8	V	140/159 (88%)	140 (100%)	0	100 100
9	I	157/195 (80%)	157 (100%)	0	100 100
9	W	157/195 (80%)	157 (100%)	0	100 100
10	J	155/174 (89%)	154 (99%)	1 (1%)	86 95
10	X	155/174 (89%)	154 (99%)	1 (1%)	86 95
11	K	148/171 (86%)	148 (100%)	0	100 100
11	Y	148/171 (86%)	148 (100%)	0	100 100
12	L	138/159 (87%)	137 (99%)	1 (1%)	84 94
12	Z	138/159 (87%)	137 (99%)	1 (1%)	84 94
13	M	158/178 (89%)	157 (99%)	1 (1%)	86 95
13	a	158/178 (89%)	157 (99%)	1 (1%)	86 95
14	N	149/181 (82%)	149 (100%)	0	100 100
14	b	149/181 (82%)	149 (100%)	0	100 100
All	All	4268/5378 (79%)	4252 (100%)	16 (0%)	91 97

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	179	LEU
5	E	133	MET
6	F	38	LEU
7	G	215	TRP
10	J	33	MET
12	L	12	VAL
13	M	49	LYS
1	O	43	ARG
1	O	179	LEU
5	S	133	MET
6	T	38	LEU
7	U	215	TRP
10	X	33	MET
12	Z	12	VAL
13	a	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	92	GLN
1	A	193	GLN
2	B	87	HIS
2	B	108	GLN
3	C	109	GLN
3	C	240	HIS
4	D	54	GLN
9	I	80	ASN
10	J	71	ASN
10	J	92	ASN
11	K	27	GLN
11	K	71	ASN
11	K	82	ASN
11	K	101	ASN
11	K	189	HIS
1	O	24	GLN
1	O	92	GLN
1	O	193	GLN
2	P	87	HIS
2	P	108	GLN
3	Q	109	GLN
3	Q	240	HIS

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Mol	Chain	Res	Type
4	R	54	GLN
9	W	80	ASN
10	X	71	ASN
10	X	92	ASN
11	Y	71	ASN
11	Y	82	ASN
11	Y	101	ASN
11	Y	189	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.

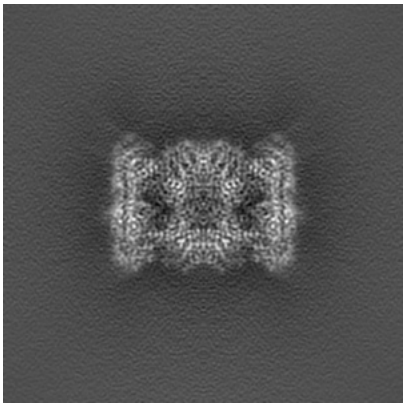
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4877. These allow visual inspection of the internal detail of the map and identification of artifacts.

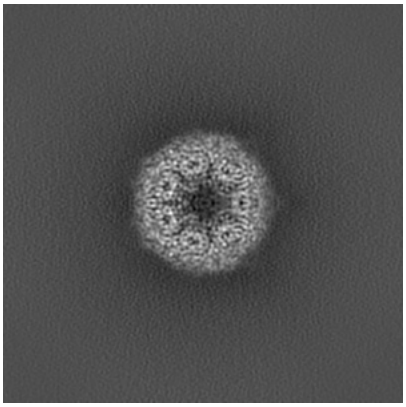
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

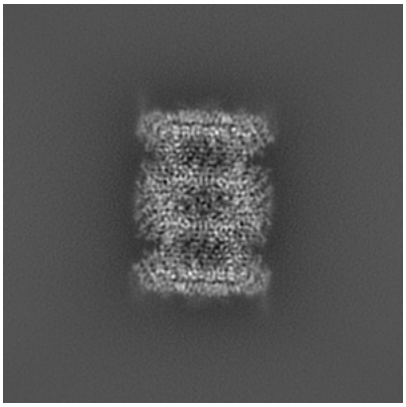
6.1.1 Primary map



X



Y

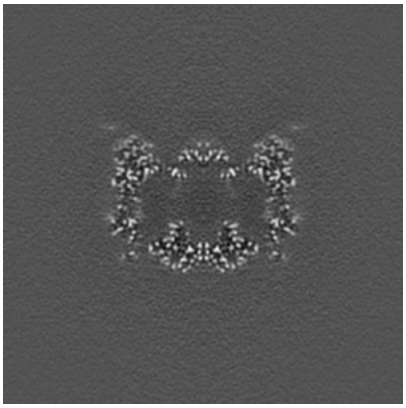


Z

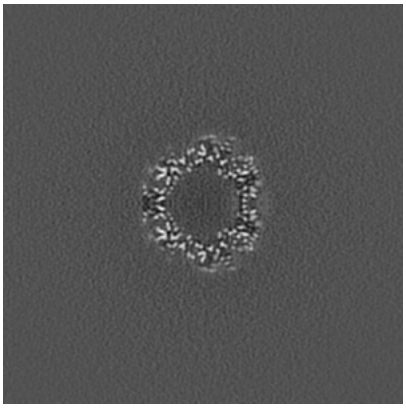
The images above show the map projected in three orthogonal directions.

6.2 Central slices

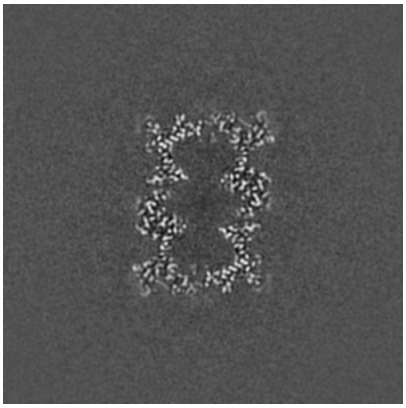
6.2.1 Primary map



X Index: 200



Y Index: 200

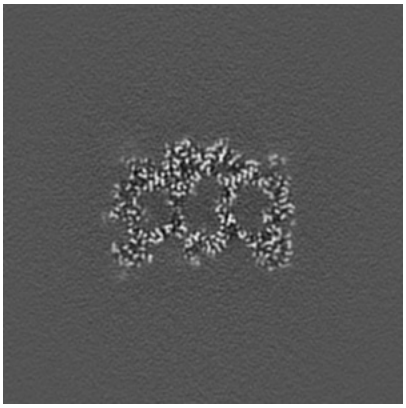


Z Index: 200

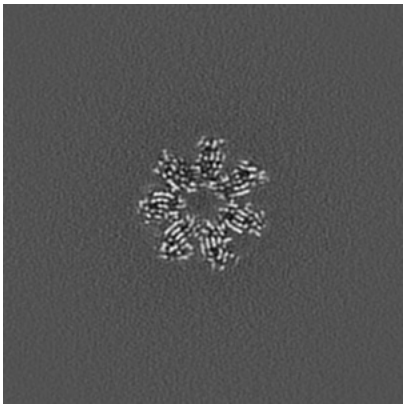
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

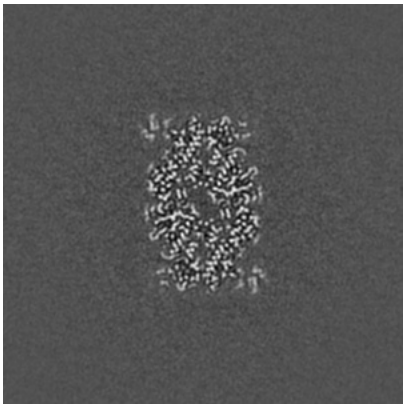
6.3.1 Primary map



X Index: 224



Y Index: 224

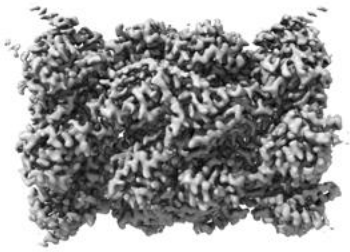


Z Index: 167

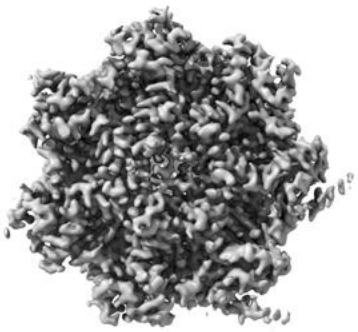
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

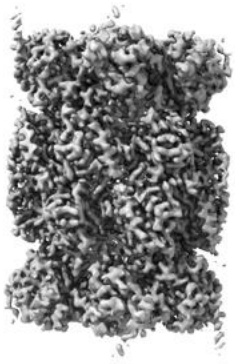
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

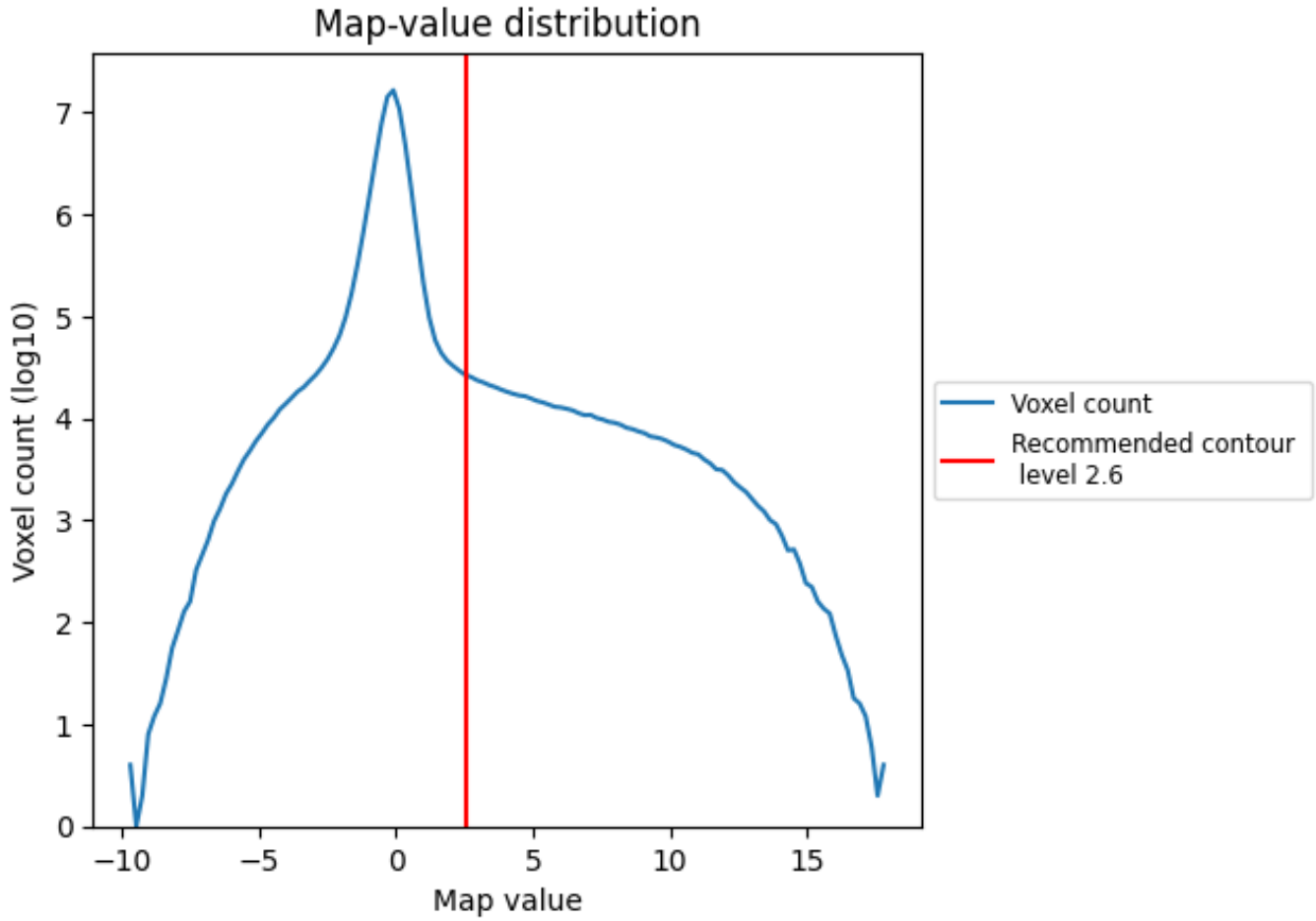
6.5 Mask visualisation (i)

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

7 Map analysis

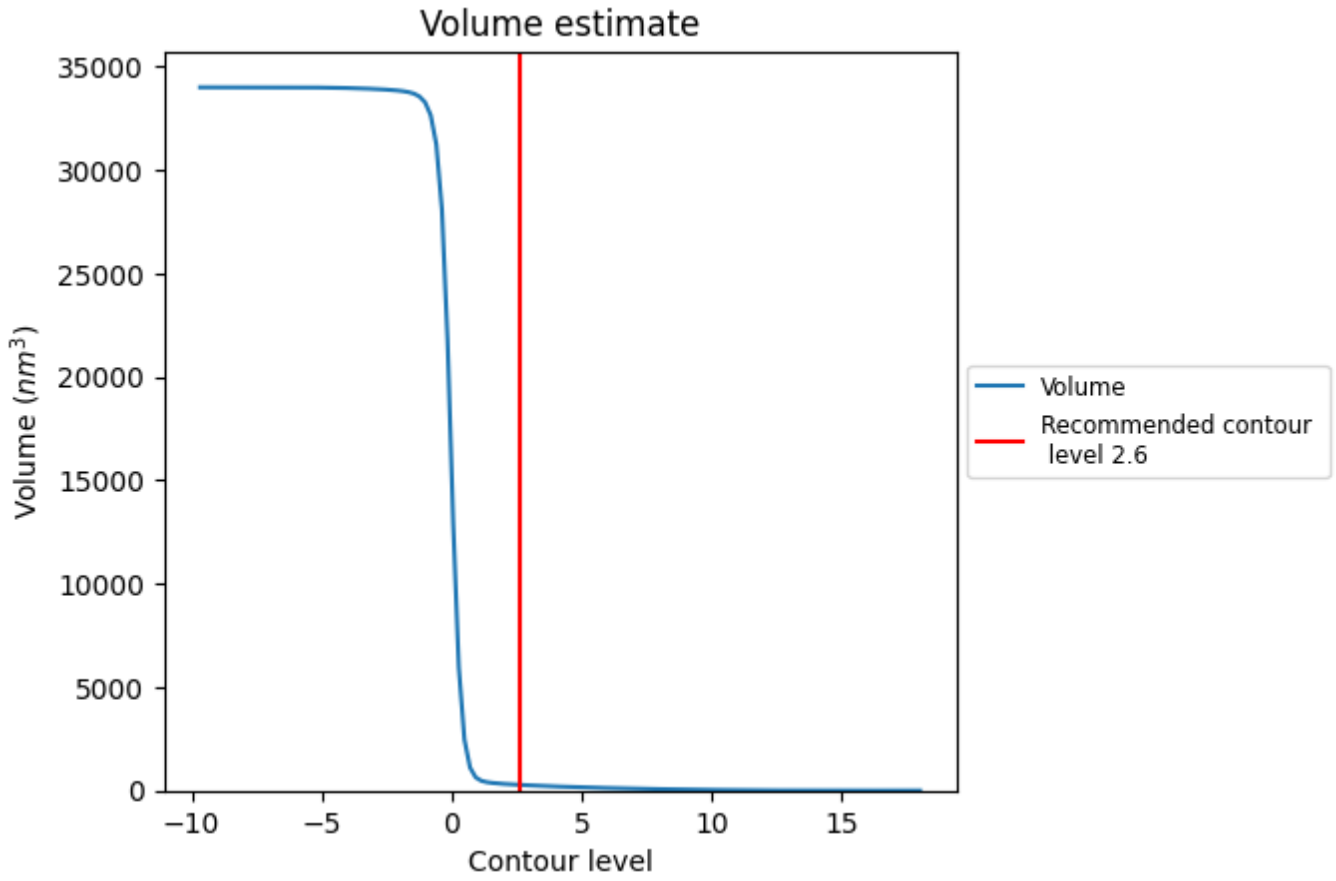
This section contains the results of statistical analysis of the map.

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.

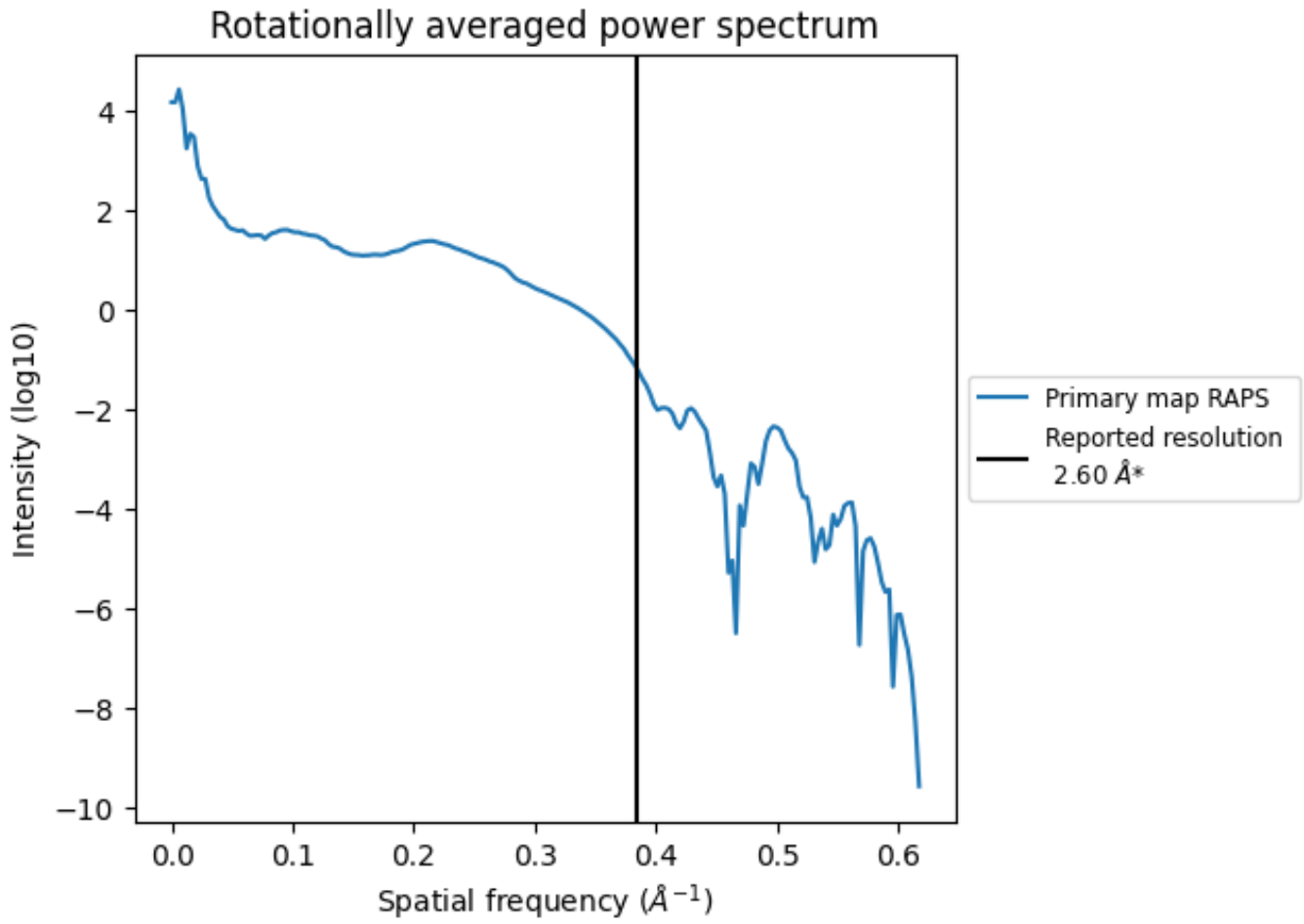
7.2 Volume estimate



The volume at the recommended contour level is 276 nm^3; this corresponds to an approximate mass of 250 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)

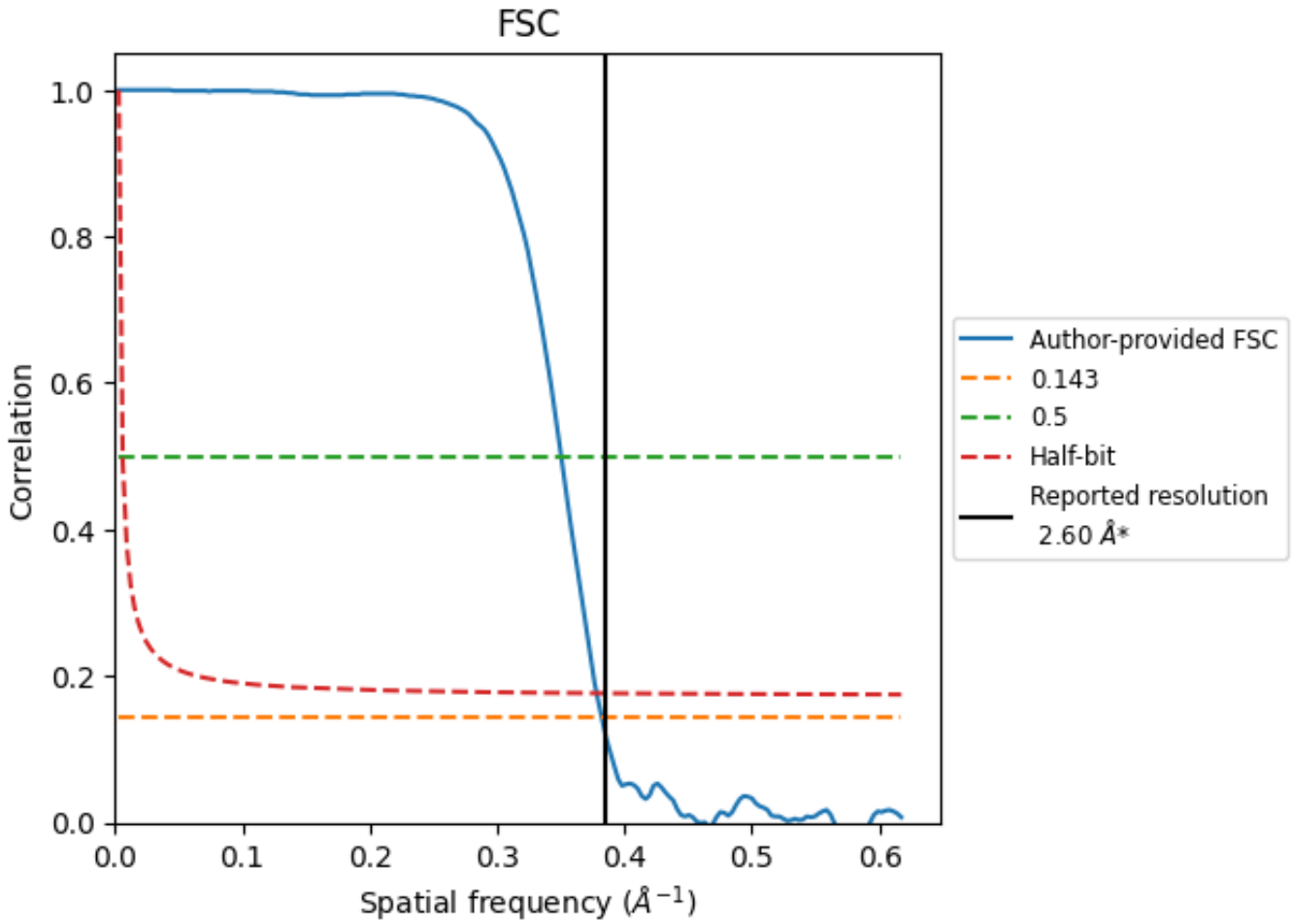


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

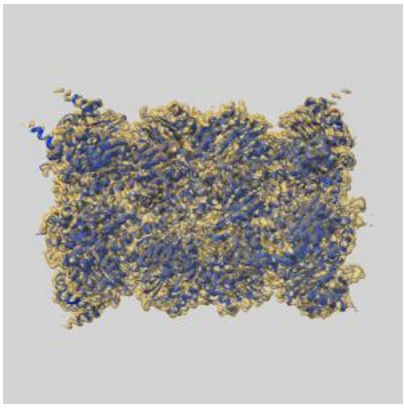
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	2.85	2.64
Unmasked-calculated*	-	-	-

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

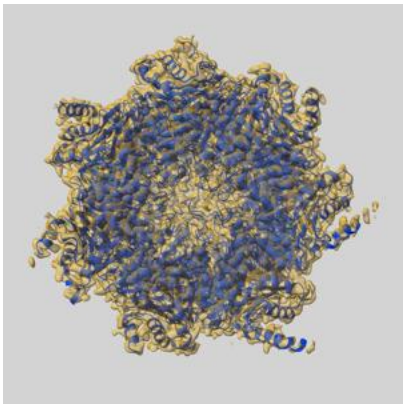
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4877 and PDB model 6RGQ. Per-residue inclusion information can be found in section 3 on page 7.

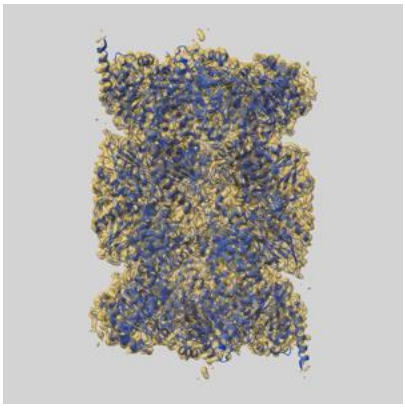
9.1 Map-model overlay



X



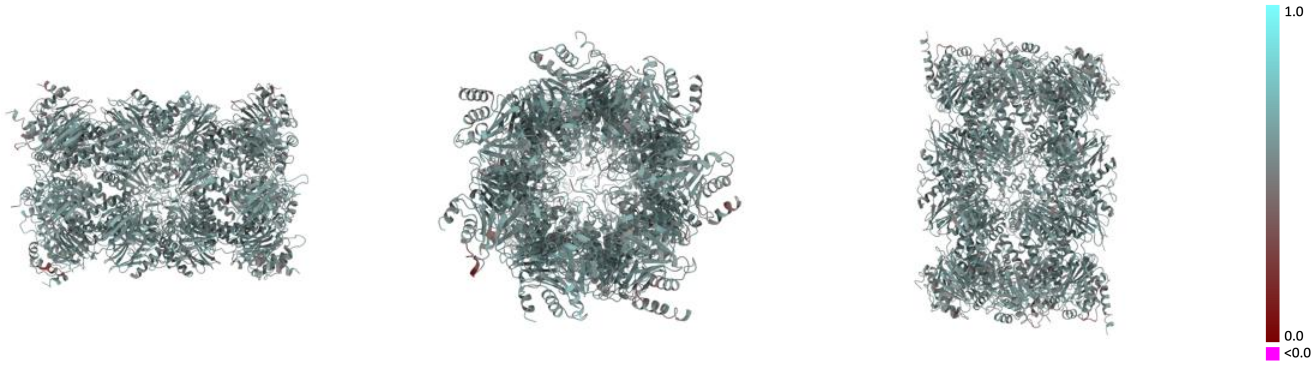
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.6 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.

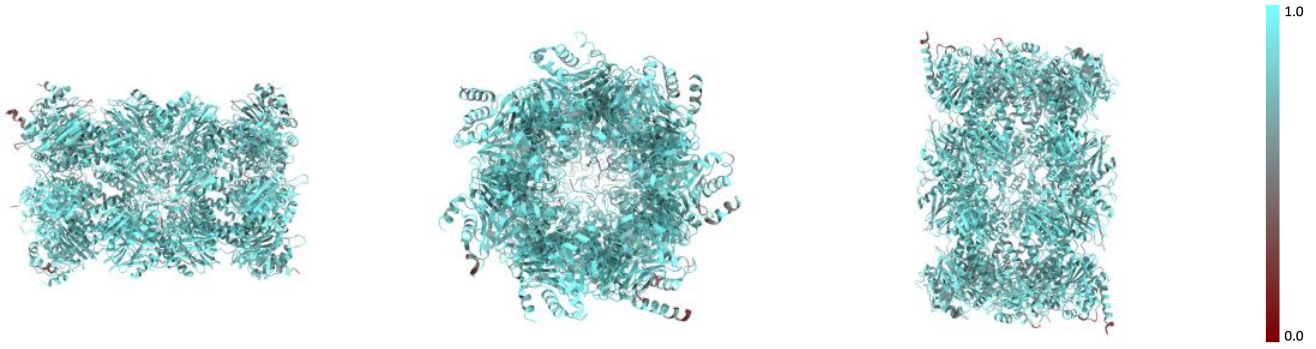
9.2 Q-score mapped to coordinate model (i)



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.

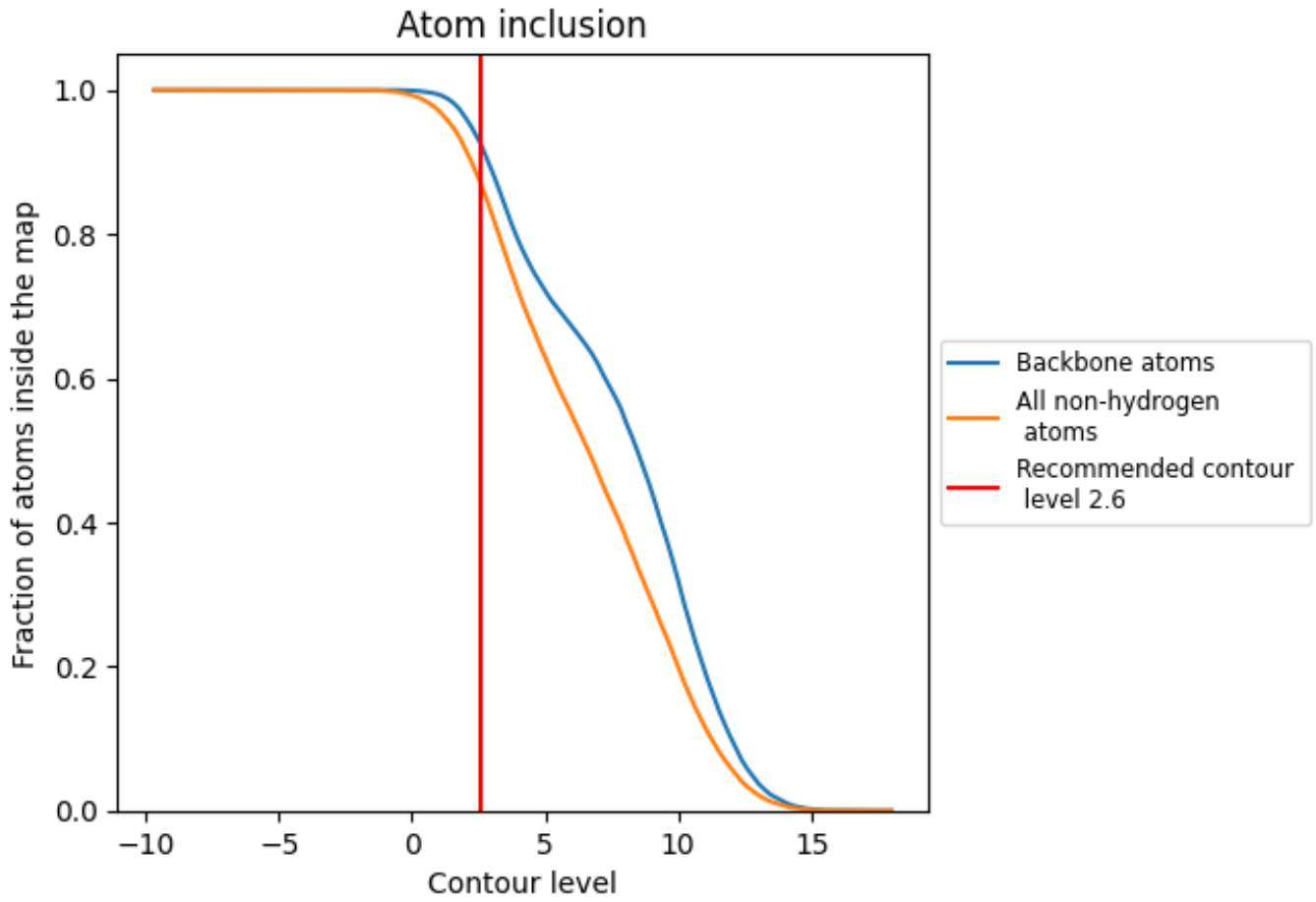
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.6).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (2.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8693	0.5630
A	0.8487	0.5530
B	0.8950	0.5720
C	0.8246	0.5520
D	0.8093	0.5460
E	0.8077	0.5540
F	0.8655	0.5590
G	0.8652	0.5600
H	0.8995	0.5670
I	0.8846	0.5680
J	0.8957	0.5740
K	0.8988	0.5730
L	0.9028	0.5690
M	0.8844	0.5710
N	0.9094	0.5760
O	0.8481	0.5530
P	0.8943	0.5730
Q	0.8240	0.5500
R	0.8099	0.5470
S	0.8083	0.5550
T	0.8655	0.5580
U	0.8646	0.5590
V	0.8995	0.5670
W	0.8852	0.5690
X	0.8957	0.5750
Y	0.8982	0.5710
Z	0.9021	0.5690
a	0.8844	0.5690
b	0.9094	0.5750