Full wwPDB EM Validation Report

Dec 30, 2024 – 07:17 am GMT

PDB ID	:	9F9P
EMDB ID	:	EMD-50258
Title	:	CryoEM structure of recombinant Trypanosoma cruzi apo proteasome 20S subunit
Authors	:	Rowland, P.
Deposited on	:	2024-05-08
Resolution	:	2.25 Å(reported)

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:

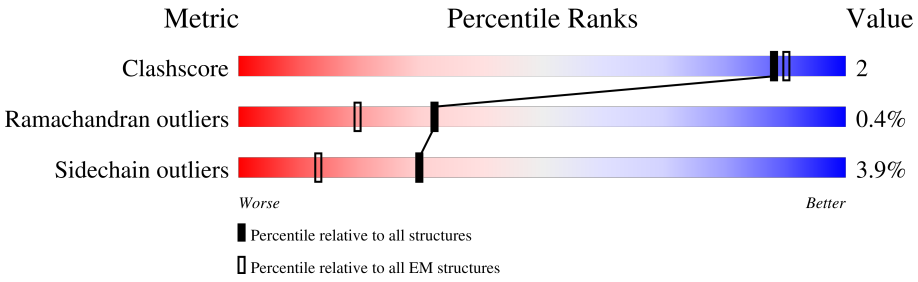
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.25 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	268	86% 5% 9%
1	O	268	86% 5% 9%
2	B	231	94% 5% •
2	P	231	94% 5% •
3	C	286	83% 11% 5%
3	Q	286	83% 11% • 5%
4	D	247	85% 9% • 5%
4	R	247	84% 9% • 5%

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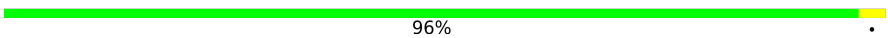
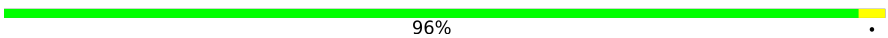
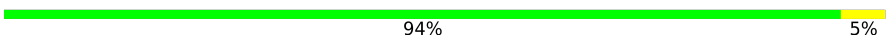
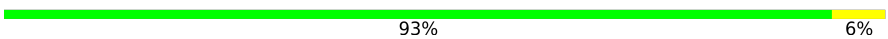
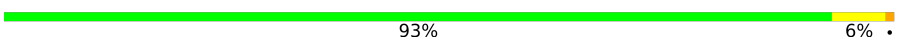
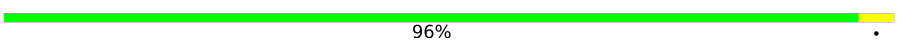
Mol	Chain	Length	Quality of chain
5	E	245	
5	S	245	
6	F	265	
6	T	265	
7	G	237	
7	U	237	
8	H	284	
8	V	284	
9	I	292	
9	W	292	
10	J	205	
10	X	205	
11	K	206	
11	Y	206	
12	L	311	
12	Z	311	
13	M	246	
13	a	246	
14	N	218	
14	b	218	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 49596 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1884	1190	328	353	13		
1	O	244	Total	C	N	O	S	0	0
			1884	1190	328	353	13		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ALA	-	expression tag	UNP A0A2V2W7U6
A	252	GLU	-	expression tag	UNP A0A2V2W7U6
A	253	ASN	-	expression tag	UNP A0A2V2W7U6
A	254	LEU	-	expression tag	UNP A0A2V2W7U6
A	255	TYR	-	expression tag	UNP A0A2V2W7U6
A	256	PHE	-	expression tag	UNP A0A2V2W7U6
A	257	GLN	-	expression tag	UNP A0A2V2W7U6
A	258	SER	-	expression tag	UNP A0A2V2W7U6
A	259	HIS	-	expression tag	UNP A0A2V2W7U6
A	260	HIS	-	expression tag	UNP A0A2V2W7U6
A	261	HIS	-	expression tag	UNP A0A2V2W7U6
A	262	HIS	-	expression tag	UNP A0A2V2W7U6
A	263	HIS	-	expression tag	UNP A0A2V2W7U6
A	264	HIS	-	expression tag	UNP A0A2V2W7U6
A	265	HIS	-	expression tag	UNP A0A2V2W7U6
A	266	HIS	-	expression tag	UNP A0A2V2W7U6
A	267	HIS	-	expression tag	UNP A0A2V2W7U6
A	268	HIS	-	expression tag	UNP A0A2V2W7U6
O	251	ALA	-	expression tag	UNP A0A2V2W7U6
O	252	GLU	-	expression tag	UNP A0A2V2W7U6
O	253	ASN	-	expression tag	UNP A0A2V2W7U6
O	254	LEU	-	expression tag	UNP A0A2V2W7U6
O	255	TYR	-	expression tag	UNP A0A2V2W7U6
O	256	PHE	-	expression tag	UNP A0A2V2W7U6
O	257	GLN	-	expression tag	UNP A0A2V2W7U6
O	258	SER	-	expression tag	UNP A0A2V2W7U6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	259	HIS	-	expression tag	UNP A0A2V2W7U6
O	260	HIS	-	expression tag	UNP A0A2V2W7U6
O	261	HIS	-	expression tag	UNP A0A2V2W7U6
O	262	HIS	-	expression tag	UNP A0A2V2W7U6
O	263	HIS	-	expression tag	UNP A0A2V2W7U6
O	264	HIS	-	expression tag	UNP A0A2V2W7U6
O	265	HIS	-	expression tag	UNP A0A2V2W7U6
O	266	HIS	-	expression tag	UNP A0A2V2W7U6
O	267	HIS	-	expression tag	UNP A0A2V2W7U6
O	268	HIS	-	expression tag	UNP A0A2V2W7U6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	228	Total	C	N	O	S	0	0
			1737	1095	292	342	8		
2	P	228	Total	C	N	O	S	0	0
			1737	1095	292	342	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2126	1338	367	413	8		
3	Q	271	Total	C	N	O	S	0	0
			2126	1338	367	413	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	234	Total	C	N	O	S	0	0
			1864	1173	329	355	7		
4	R	234	Total	C	N	O	S	0	0
			1864	1173	329	355	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	223	ARG	HIS	conflict	UNP A0A2V2WZ04
R	223	ARG	HIS	conflict	UNP A0A2V2WZ04

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	227	Total	C	N	O	S	0	0
			1757	1102	302	344	9		
5	S	227	Total	C	N	O	S	0	0
			1757	1102	302	344	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	221	Total	C	N	O	S	0	0
			1722	1095	298	320	9		
6	T	221	Total	C	N	O	S	0	0
			1722	1095	298	320	9		

- Molecule 7 is a protein called Putative proteasome alpha 7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	227	Total	C	N	O	S	0	0
			1724	1078	297	336	13		
7	U	227	Total	C	N	O	S	0	0
			1724	1078	297	336	13		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	228	Total	C	N	O	S	0	0
			1723	1081	290	339	13		
8	V	228	Total	C	N	O	S	0	0
			1723	1081	290	339	13		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1663	1043	294	315	11		
9	W	219	Total	C	N	O	S	0	0
			1663	1043	294	315	11		

- Molecule 10 is a protein called Putative proteasome beta 3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1555	976	265	299	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total 1555	C 976	N 265	O 299	S 15	0	0

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total 1586	C 995	N 275	O 299	S 17	0	0
11	Y	206	Total 1586	C 995	N 275	O 299	S 17	0	0

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total 1578	C 995	N 274	O 300	S 9	0	0
12	Z	201	Total 1578	C 995	N 274	O 300	S 9	0	0

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	208	Total 1647	C 1042	N 279	O 314	S 12	0	0
13	a	208	Total 1647	C 1042	N 279	O 314	S 12	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	245	ASN	LYS	conflict	UNP A0A2V2VW62
a	245	ASN	LYS	conflict	UNP A0A2V2VW62

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total 1695	C 1075	N 290	O 313	S 17	0	0
14	b	218	Total 1695	C 1075	N 290	O 313	S 17	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	AltConf
15	A	39	Total O 39 39	0
15	B	33	Total O 33 33	0
15	C	33	Total O 33 33	0
15	D	21	Total O 21 21	0
15	E	22	Total O 22 22	0
15	F	26	Total O 26 26	0
15	G	33	Total O 33 33	0
15	H	52	Total O 52 52	0
15	I	44	Total O 44 44	0
15	J	50	Total O 50 50	0
15	K	37	Total O 37 37	0
15	L	29	Total O 29 29	0
15	M	48	Total O 48 48	0
15	N	69	Total O 69 69	0
15	O	39	Total O 39 39	0
15	P	33	Total O 33 33	0
15	Q	33	Total O 33 33	0
15	R	21	Total O 21 21	0
15	S	22	Total O 22 22	0
15	T	26	Total O 26 26	0
15	U	33	Total O 33 33	0
15	V	52	Total O 52 52	0

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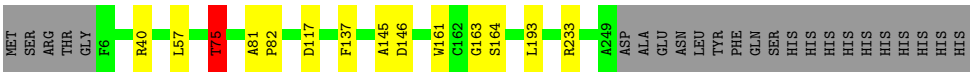
Mol	Chain	Residues	Atoms	AltConf
15	W	45	Total O 45 45	0
15	X	50	Total O 50 50	0
15	Y	37	Total O 37 37	0
15	Z	29	Total O 29 29	0
15	a	48	Total O 48 48	0
15	b	70	Total O 70 70	0

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.

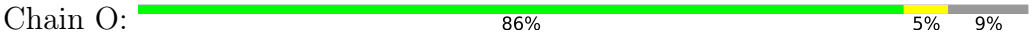
• Molecule 1: Proteasome subunit alpha type

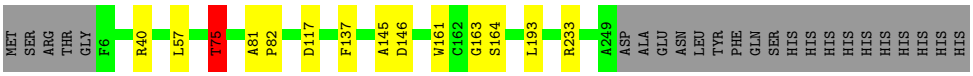
Chain A:



• Molecule 1: Proteasome subunit alpha type

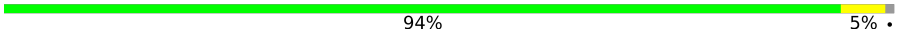
Chain O:

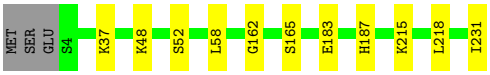




• Molecule 2: Proteasome subunit alpha type

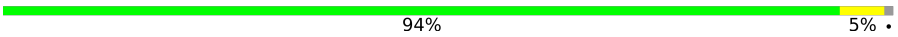
Chain B:

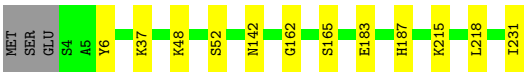




• Molecule 2: Proteasome subunit alpha type

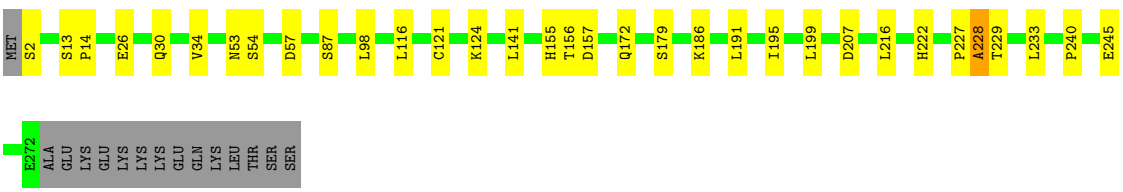
Chain P:





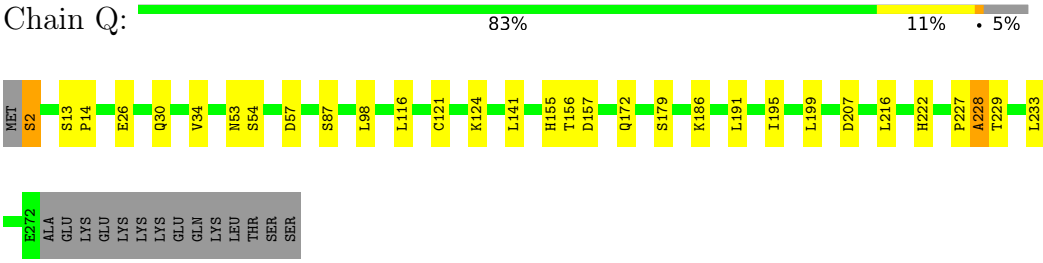
• Molecule 3: Proteasome subunit alpha type

Chain C:



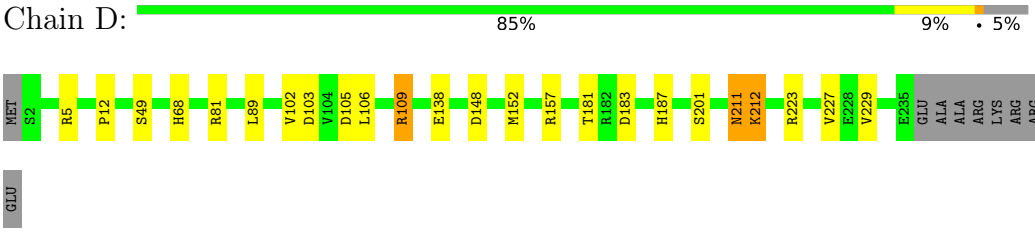
• Molecule 3: Proteasome subunit alpha type

Chain Q:



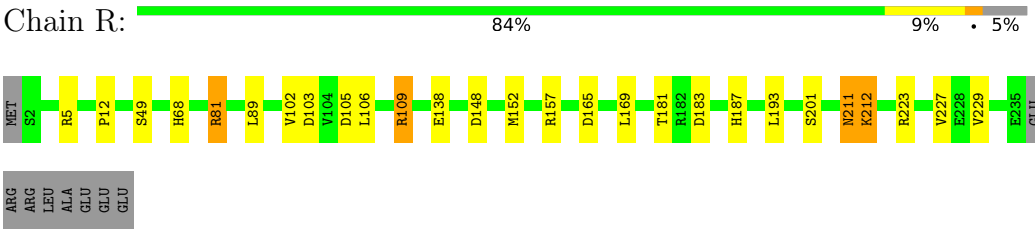
• Molecule 4: Proteasome subunit alpha type

Chain D:



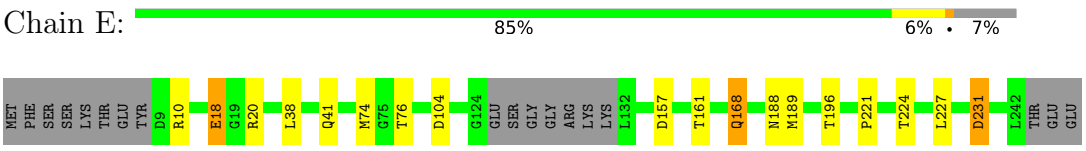
• Molecule 4: Proteasome subunit alpha type

Chain R:



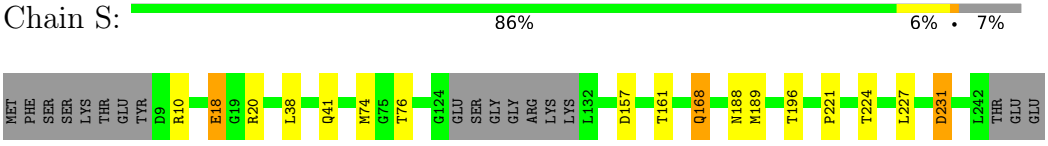
• Molecule 5: Proteasome subunit alpha type

Chain E:



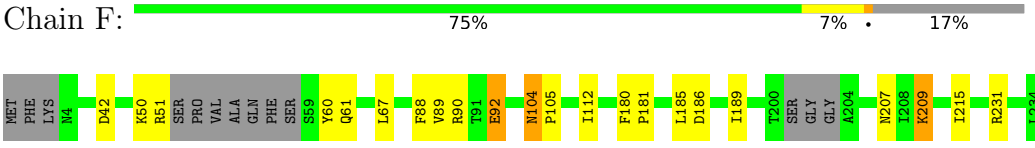
• Molecule 5: Proteasome subunit alpha type

Chain S:



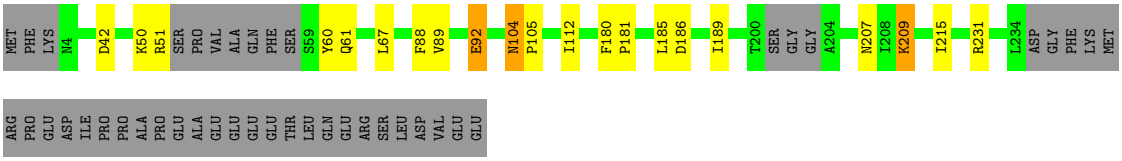
• Molecule 6: Proteasome subunit alpha type

Chain F:



• Molecule 6: Proteasome subunit alpha type

Chain T:



• Molecule 7: Putative proteasome alpha 7 subunit

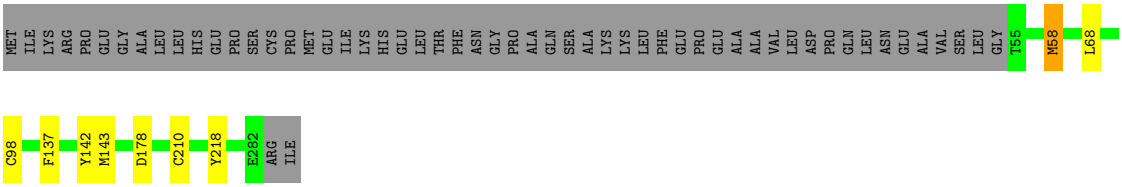
Chain G:

• Molecule 7: Putative proteasome alpha 7 subunit

Chain U:

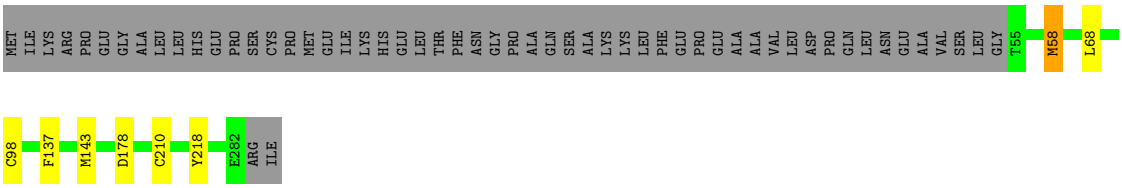
• Molecule 8: Proteasome subunit beta

Chain H:



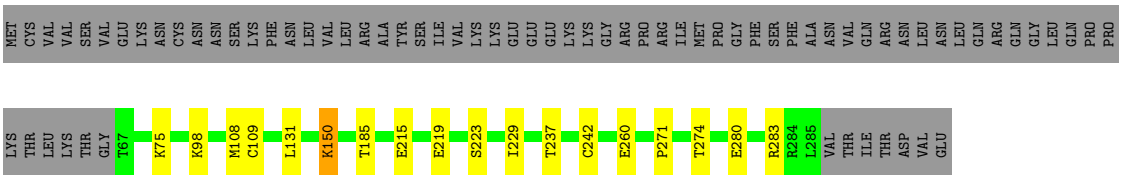
• Molecule 8: Proteasome subunit beta

Chain V:



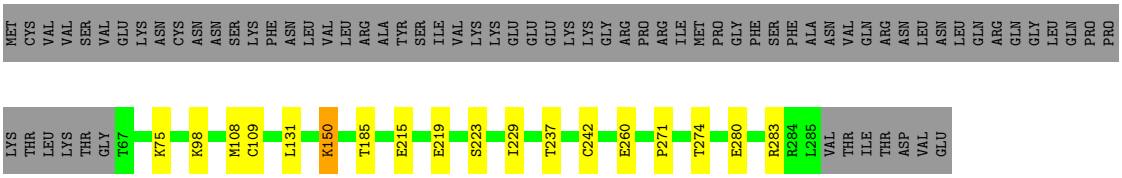
• Molecule 9: Proteasome subunit beta

Chain I:



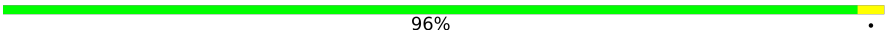
• Molecule 9: Proteasome subunit beta

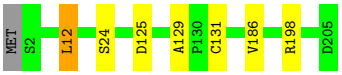
Chain W:



• Molecule 10: Putative proteasome beta 3 subunit

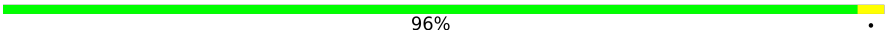
Chain J:





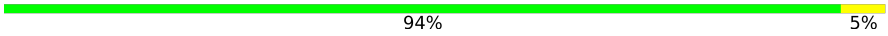
• Molecule 10: Putative proteasome beta 3 subunit

Chain X:



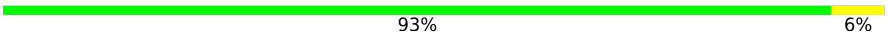
• Molecule 11: Proteasome subunit beta

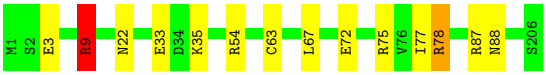
Chain K:



• Molecule 11: Proteasome subunit beta

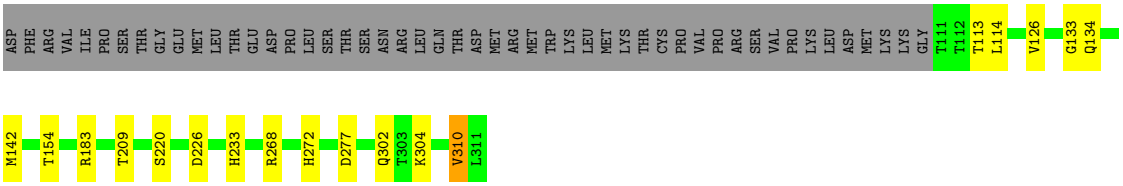
Chain Y:





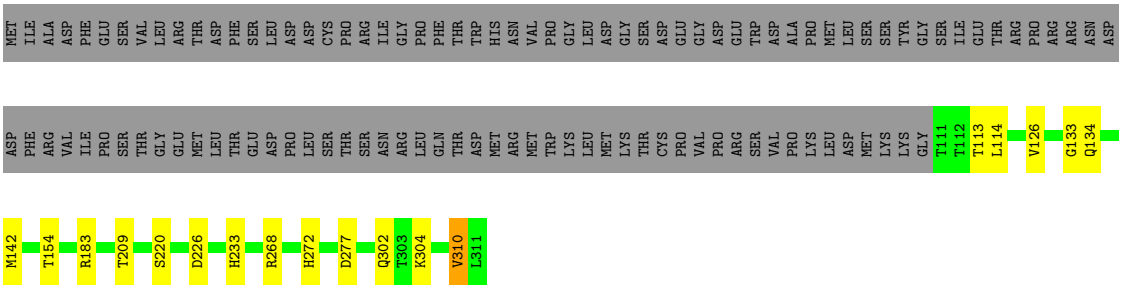
• Molecule 12: Proteasome subunit beta

Chain L:



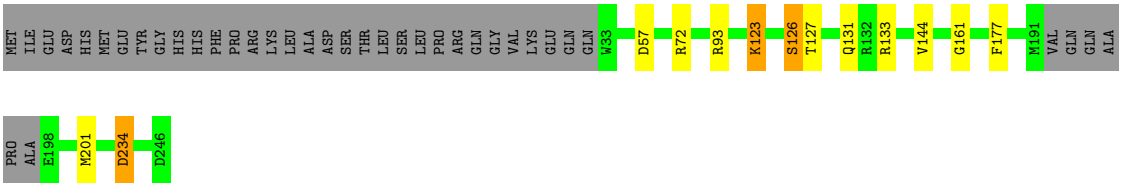
• Molecule 12: Proteasome subunit beta

Chain Z:



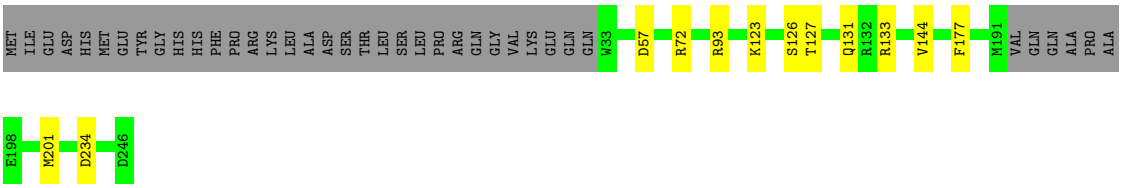
• Molecule 13: Proteasome subunit beta

Chain M:



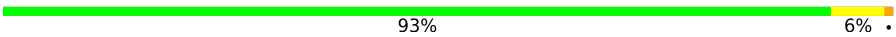
• Molecule 13: Proteasome subunit beta

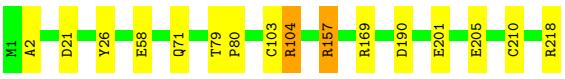
Chain a:



• Molecule 14: Proteasome subunit beta

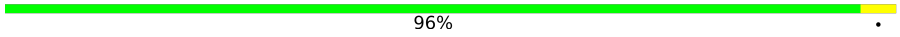
Chain N:





• Molecule 14: Proteasome subunit beta

Chain b:




M1
Y26
Q71
C103
R104
R157
D190
E205
C210
R218

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92013	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 ($e^-/Å^2$)	1.05	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

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	0.51	0/1922	0.85	2/2605 (0.1%)
1	O	0.51	0/1922	0.85	2/2605 (0.1%)
2	B	0.52	0/1770	0.82	1/2398 (0.0%)
2	P	0.52	0/1770	0.82	1/2398 (0.0%)
3	C	0.47	0/2168	0.74	0/2939
3	Q	0.47	0/2168	0.74	0/2939
4	D	0.44	0/1894	0.79	1/2549 (0.0%)
4	R	0.44	0/1894	0.79	1/2549 (0.0%)
5	E	0.43	0/1783	0.74	1/2417 (0.0%)
5	S	0.43	0/1783	0.74	1/2417 (0.0%)
6	F	0.49	0/1757	0.84	1/2375 (0.0%)
6	T	0.49	0/1757	0.84	0/2375
7	G	0.54	0/1755	0.82	0/2379
7	U	0.55	0/1755	0.82	0/2379
8	H	0.57	0/1757	0.87	1/2380 (0.0%)
8	V	0.57	0/1757	0.87	1/2380 (0.0%)
9	I	0.56	0/1690	0.93	0/2286
9	W	0.56	0/1690	0.93	0/2286
10	J	0.60	0/1580	0.87	0/2131
10	X	0.60	0/1580	0.87	0/2131
11	K	0.54	0/1612	0.88	3/2177 (0.1%)
11	Y	0.54	0/1612	0.88	3/2177 (0.1%)
12	L	0.56	0/1611	0.83	0/2178
12	Z	0.56	0/1611	0.83	0/2178
13	M	0.53	0/1682	0.90	2/2270 (0.1%)
13	a	0.54	0/1682	0.90	2/2270 (0.1%)
14	N	0.61	0/1733	0.91	2/2344 (0.1%)
14	b	0.61	0/1733	0.91	2/2344 (0.1%)
All	All	0.53	0/49428	0.84	27/66856 (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
4	D	0	2
4	R	0	2
5	E	0	1
5	S	0	1
7	G	0	2
7	U	0	2
11	K	0	2
11	Y	0	2
12	L	0	1
12	Z	0	1
13	M	0	1
13	a	0	1
14	N	0	2
14	b	0	2
All	All	0	22

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	104	ARG	NE-CZ-NH2	-7.04	116.78	120.30
14	b	103	CYS	CB-CA-C	-6.94	96.53	110.40
14	N	103	CYS	CB-CA-C	-6.93	96.55	110.40
14	N	104	ARG	NE-CZ-NH2	-6.89	116.85	120.30
2	P	48	LYS	CB-CA-C	-6.69	97.02	110.40
2	B	48	LYS	CB-CA-C	-6.67	97.05	110.40
11	K	9	ARG	CG-CD-NE	-6.56	98.03	111.80
11	Y	9	ARG	CG-CD-NE	-6.52	98.11	111.80
8	H	58	MET	CG-SD-CE	-6.41	89.95	100.20
8	V	58	MET	CG-SD-CE	-6.41	89.95	100.20
13	a	177	PHE	CB-CA-C	-6.06	98.29	110.40
13	M	177	PHE	CB-CA-C	-6.04	98.31	110.40
11	Y	87	ARG	NE-CZ-NH1	-5.90	117.35	120.30
4	D	12	PRO	N-CA-C	5.74	127.02	112.10
11	K	87	ARG	NE-CZ-NH1	-5.72	117.44	120.30
4	R	12	PRO	N-CA-C	5.72	126.97	112.10
5	E	74	MET	CB-CA-C	-5.65	99.11	110.40
5	S	74	MET	CB-CA-C	-5.62	99.16	110.40
13	M	93	ARG	NE-CZ-NH2	5.61	123.10	120.30
13	a	93	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	O	75	THR	CB-CA-C	-5.50	96.74	111.60
1	O	117	ASP	CB-CA-C	-5.50	99.40	110.40
1	A	75	THR	CB-CA-C	-5.50	96.76	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	ASP	CB-CA-C	-5.41	99.59	110.40
11	Y	78	ARG	CB-CA-C	-5.18	100.04	110.40
11	K	78	ARG	CB-CA-C	-5.16	100.08	110.40
6	F	90	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	109	ARG	Sidechain
4	D	157	ARG	Sidechain
5	E	10	ARG	Sidechain
7	G	113	ARG	Sidechain
7	G	42	ASP	Peptide
11	K	78	ARG	Sidechain
11	K	9	ARG	Sidechain
12	L	183	ARG	Sidechain
13	M	72	ARG	Sidechain
14	N	104	ARG	Sidechain
14	N	157	ARG	Sidechain
4	R	109	ARG	Sidechain
4	R	157	ARG	Sidechain
5	S	10	ARG	Sidechain
7	U	113	ARG	Sidechain
7	U	42	ASP	Peptide
11	Y	78	ARG	Sidechain
11	Y	9	ARG	Sidechain
12	Z	183	ARG	Sidechain
13	a	72	ARG	Sidechain
14	b	104	ARG	Sidechain
14	b	157	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1884	0	1874	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1884	0	1874	4	0
2	B	1737	0	1716	4	0
2	P	1737	0	1716	5	0
3	C	2126	0	2090	13	0
3	Q	2126	0	2090	15	0
4	D	1864	0	1861	9	0
4	R	1864	0	1861	12	0
5	E	1757	0	1755	8	0
5	S	1757	0	1755	7	0
6	F	1722	0	1703	8	0
6	T	1722	0	1703	8	0
7	G	1724	0	1691	8	0
7	U	1724	0	1691	8	0
8	H	1723	0	1694	4	0
8	V	1723	0	1694	3	0
9	I	1663	0	1698	7	0
9	W	1663	0	1698	7	0
10	J	1555	0	1549	5	0
10	X	1555	0	1549	5	0
11	K	1586	0	1573	5	0
11	Y	1586	0	1573	5	0
12	L	1578	0	1526	9	0
12	Z	1578	0	1526	9	0
13	M	1647	0	1594	3	0
13	a	1647	0	1594	0	0
14	N	1695	0	1654	6	0
14	b	1695	0	1654	0	0
15	A	39	0	0	0	0
15	B	33	0	0	0	0
15	C	33	0	0	0	0
15	D	21	0	0	0	0
15	E	22	0	0	2	0
15	F	26	0	0	1	0
15	G	33	0	0	0	0
15	H	52	0	0	0	0
15	I	44	0	0	1	0
15	J	50	0	0	0	0
15	K	37	0	0	2	0
15	L	29	0	0	1	0
15	M	48	0	0	0	0
15	N	69	0	0	2	0
15	O	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	33	0	0	0	0
15	Q	33	0	0	0	0
15	R	21	0	0	0	0
15	S	22	0	0	2	0
15	T	26	0	0	1	0
15	U	33	0	0	0	0
15	V	52	0	0	0	0
15	W	45	0	0	1	0
15	X	50	0	0	0	0
15	Y	37	0	0	2	0
15	Z	29	0	0	1	0
15	a	48	0	0	0	0
15	b	70	0	0	0	0
All	All	49596	0	47956	168	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 2.

All (168) 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)
14:N:157:ARG:HD3	15:N:348:HOH:O	1.60	0.98
11:Y:22:ASN:ND2	11:Y:33:GLU:OE1	2.21	0.72
6:F:189:ILE:HD11	6:F:215:ILE:HD11	1.75	0.67
6:F:209:LYS:HG2	15:F:319:HOH:O	1.95	0.67
6:T:189:ILE:HD11	6:T:215:ILE:HD11	1.75	0.67
6:T:209:LYS:HG2	15:T:319:HOH:O	1.95	0.66
11:K:22:ASN:ND2	11:K:33:GLU:OE1	2.21	0.66
11:Y:88:ASN:HB2	15:Y:317:HOH:O	1.96	0.66
11:K:88:ASN:HB2	15:K:317:HOH:O	1.96	0.65
10:X:12:LEU:C	10:X:12:LEU:HD23	2.18	0.64
10:J:125:ASP:OD2	10:J:129:ALA:HB3	1.98	0.64
10:J:12:LEU:C	10:J:12:LEU:HD23	2.18	0.64
10:X:125:ASP:OD2	10:X:129:ALA:HB3	1.97	0.63
4:R:148:ASP:OD1	4:R:152:MET:HB3	1.99	0.62
4:D:148:ASP:OD1	4:D:152:MET:HB3	1.99	0.61
5:S:20:ARG:NH1	15:S:302:HOH:O	2.35	0.60
6:F:92:GLU:HG2	6:F:112:ILE:HD13	1.83	0.60
3:C:121:CYS:SG	3:C:156:THR:HG23	2.42	0.60
3:Q:121:CYS:SG	3:Q:156:THR:HG23	2.42	0.59
14:N:169:ARG:HD3	14:N:201:GLU:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:LEU:HD23	11:K:67:LEU:HD21	1.85	0.59
6:T:92:GLU:HG2	6:T:112:ILE:HD13	1.83	0.58
5:E:20:ARG:NH1	15:E:302:HOH:O	2.35	0.58
4:R:89:LEU:HD23	11:Y:67:LEU:HD21	1.85	0.58
11:K:3:GLU:HG2	11:K:35:LYS:NZ	2.19	0.57
7:G:150:ASP:HB2	7:G:151:PRO:CD	2.35	0.57
12:L:310:VAL:O	12:L:310:VAL:CG1	2.51	0.57
12:Z:310:VAL:CG1	12:Z:310:VAL:O	2.51	0.57
11:Y:3:GLU:HG2	11:Y:35:LYS:NZ	2.19	0.57
3:Q:199:LEU:HD23	3:Q:216:LEU:HD23	1.87	0.57
7:U:150:ASP:HB2	7:U:151:PRO:CD	2.35	0.57
4:D:223:ARG:O	4:D:227:VAL:HG23	2.05	0.56
12:L:268:ARG:HE	12:L:272:HIS:HE1	1.53	0.56
4:R:223:ARG:O	4:R:227:VAL:HG23	2.05	0.56
4:D:68:HIS:HE1	4:D:102:VAL:O	1.88	0.56
12:L:277:ASP:O	15:L:401:HOH:O	2.18	0.56
4:R:68:HIS:HE1	4:R:102:VAL:O	1.88	0.56
12:L:310:VAL:O	12:L:310:VAL:HG13	2.06	0.56
12:Z:268:ARG:HE	12:Z:272:HIS:HE1	1.53	0.56
12:Z:277:ASP:O	15:Z:401:HOH:O	2.18	0.55
12:Z:310:VAL:O	12:Z:310:VAL:HG13	2.06	0.55
7:G:117:PHE:O	7:G:120:VAL:HG12	2.07	0.55
3:C:199:LEU:HD23	3:C:216:LEU:HD23	1.87	0.55
7:U:117:PHE:O	7:U:120:VAL:HG12	2.07	0.55
4:D:211:ASN:O	4:D:212:LYS:HB2	2.07	0.55
3:Q:124:LYS:NZ	3:Q:156:THR:HG22	2.22	0.55
5:E:221:PRO:HG2	5:E:224:THR:HG22	1.89	0.54
4:R:211:ASN:O	4:R:212:LYS:HB2	2.07	0.54
8:H:58:MET:HE2	8:H:210:CYS:SG	2.48	0.54
3:C:124:LYS:NZ	3:C:156:THR:HG22	2.22	0.54
5:S:221:PRO:HG2	5:S:224:THR:HG22	1.89	0.53
8:V:58:MET:HE2	8:V:210:CYS:SG	2.48	0.53
3:Q:157:ASP:OD1	3:Q:157:ASP:C	2.47	0.53
14:N:21:ASP:OD1	14:N:21:ASP:C	2.48	0.53
13:M:234:ASP:OD1	13:M:234:ASP:N	2.42	0.52
3:C:157:ASP:C	3:C:157:ASP:OD1	2.48	0.52
5:S:18:GLU:HG3	15:S:302:HOH:O	2.10	0.51
9:W:229:ILE:O	15:W:301:HOH:O	2.19	0.51
1:O:75:THR:HG23	1:O:137:PHE:CD1	2.46	0.51
5:E:18:GLU:HG3	15:E:302:HOH:O	2.09	0.50
9:I:150:LYS:HE2	9:I:185:THR:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:114:LEU:C	12:L:114:LEU:HD12	2.32	0.50
5:S:231:ASP:N	5:S:231:ASP:OD1	2.44	0.50
1:A:75:THR:HG23	1:A:137:PHE:CD1	2.46	0.50
9:W:150:LYS:HE2	9:W:185:THR:CG2	2.42	0.50
12:Z:114:LEU:C	12:Z:114:LEU:HD12	2.32	0.50
2:B:187:HIS:CE1	2:B:231:ILE:HG22	2.47	0.50
5:E:231:ASP:N	5:E:231:ASP:OD1	2.44	0.49
2:P:187:HIS:CE1	2:P:231:ILE:HG22	2.48	0.49
7:U:150:ASP:HB2	7:U:151:PRO:HD2	1.95	0.49
1:A:161:TRP:CH2	1:A:163:GLY:HA3	2.48	0.49
3:Q:199:LEU:CD2	3:Q:216:LEU:HD23	2.43	0.49
3:C:199:LEU:CD2	3:C:216:LEU:HD23	2.43	0.48
7:G:150:ASP:HB2	7:G:151:PRO:HD2	1.94	0.48
9:I:280:GLU:OE1	10:J:198:ARG:NE	2.40	0.48
1:O:161:TRP:CH2	1:O:163:GLY:HA3	2.48	0.48
9:I:229:ILE:O	15:I:301:HOH:O	2.20	0.48
3:C:34:VAL:HG12	3:C:141:LEU:HD12	1.97	0.47
3:C:233:LEU:HD23	10:J:186:VAL:HG11	1.96	0.47
9:I:271:PRO:O	9:I:274:THR:OG1	2.25	0.47
3:Q:233:LEU:HD23	10:X:186:VAL:HG11	1.96	0.47
12:L:233:HIS:HE1	15:Y:329:HOH:O	1.98	0.47
9:W:280:GLU:OE1	10:X:198:ARG:NE	2.40	0.47
3:Q:228:ALA:HB2	9:W:283:ARG:HD3	1.96	0.47
5:E:168:GLN:HE21	5:E:168:GLN:HA	1.80	0.47
3:Q:34:VAL:HG12	3:Q:141:LEU:HD12	1.96	0.47
3:C:228:ALA:HB2	9:I:283:ARG:HD3	1.97	0.46
2:P:162:GLY:O	2:P:165:SER:HB3	2.14	0.46
12:Z:154:THR:O	12:Z:209:THR:HG23	2.16	0.46
2:B:162:GLY:O	2:B:165:SER:HB3	2.15	0.46
7:G:74:VAL:HG13	7:G:134:VAL:HG13	1.98	0.46
6:F:88:PHE:CE2	6:F:112:ILE:HD12	2.51	0.46
9:W:271:PRO:O	9:W:274:THR:OG1	2.25	0.46
12:L:154:THR:O	12:L:209:THR:HG23	2.16	0.45
5:S:157:ASP:C	5:S:157:ASP:OD1	2.55	0.45
7:U:55:ARG:HH11	7:U:55:ARG:HG3	1.81	0.45
5:E:157:ASP:OD1	5:E:157:ASP:C	2.55	0.45
6:F:180:PHE:N	6:F:181:PRO:CD	2.79	0.45
3:Q:124:LYS:HZ2	3:Q:156:THR:HG22	1.81	0.45
5:S:168:GLN:HE21	5:S:168:GLN:HA	1.81	0.45
2:B:37:LYS:HE2	3:C:57:ASP:OD2	2.17	0.45
6:T:88:PHE:CE2	6:T:112:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:55:ARG:HG3	7:G:55:ARG:HH11	1.81	0.45
6:T:180:PHE:N	6:T:181:PRO:CD	2.79	0.45
7:U:74:VAL:HG13	7:U:134:VAL:HG13	1.98	0.45
2:P:37:LYS:HE2	3:Q:57:ASP:OD2	2.17	0.45
3:Q:191:LEU:O	3:Q:195:ILE:HG13	2.18	0.44
10:X:12:LEU:HD23	10:X:12:LEU:O	2.17	0.44
5:E:38:LEU:C	5:E:38:LEU:HD12	2.38	0.44
10:J:12:LEU:HD23	10:J:12:LEU:O	2.17	0.44
15:K:327:HOH:O	12:Z:233:HIS:HE1	1.99	0.44
12:Z:113:THR:HG22	12:Z:126:VAL:HG12	2.00	0.44
6:T:104:ASN:HD22	6:T:105:PRO:HD2	1.82	0.44
6:F:185:LEU:O	6:F:189:ILE:HG13	2.18	0.44
4:R:68:HIS:CE1	4:R:102:VAL:O	2.70	0.44
6:F:104:ASN:HD22	6:F:105:PRO:HD2	1.82	0.43
12:L:113:THR:HG22	12:L:126:VAL:HG12	2.00	0.43
5:S:38:LEU:C	5:S:38:LEU:HD12	2.38	0.43
13:M:126:SER:OG	13:M:161:GLY:O	2.36	0.43
14:N:79:THR:HB	14:N:80:PRO:HD2	2.00	0.43
4:D:68:HIS:CE1	4:D:102:VAL:O	2.70	0.43
3:C:191:LEU:O	3:C:195:ILE:HG13	2.18	0.43
3:Q:13:SER:HB3	3:Q:14:PRO:CD	2.48	0.43
4:D:211:ASN:O	4:D:212:LYS:CB	2.67	0.43
2:P:6:TYR:OH	3:Q:2:SER:O	2.28	0.43
6:T:185:LEU:O	6:T:189:ILE:HG13	2.18	0.43
3:C:53:ASN:OD1	3:C:54:SER:N	2.52	0.43
7:G:218:SER:O	7:G:219:ASN:HB2	2.19	0.43
8:V:58:MET:HE2	8:V:210:CYS:CB	2.49	0.43
3:C:13:SER:HB3	3:C:14:PRO:CD	2.48	0.43
4:R:187:HIS:CE1	4:R:229:VAL:HG22	2.54	0.42
2:P:37:LYS:NZ	2:P:142:ASN:O	2.50	0.42
9:W:108:MET:HG3	9:W:242:CYS:SG	2.59	0.42
8:H:58:MET:HE2	8:H:210:CYS:CB	2.49	0.42
8:H:68:LEU:HD23	8:H:98:CYS:SG	2.59	0.42
3:Q:53:ASN:OD1	3:Q:54:SER:N	2.52	0.42
4:D:187:HIS:CE1	4:D:229:VAL:HG22	2.54	0.42
9:I:108:MET:HG3	9:I:242:CYS:SG	2.59	0.42
4:R:193:LEU:HD23	4:R:193:LEU:HA	1.89	0.42
6:F:67:LEU:HD13	6:F:89:VAL:HG11	2.02	0.42
6:T:67:LEU:HD13	6:T:89:VAL:HG11	2.02	0.42
5:E:104:ASP:HB2	13:M:123:LYS:HG2	2.01	0.42
4:R:211:ASN:O	4:R:212:LYS:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:3:GLU:HG2	11:K:35:LYS:HZ3	1.84	0.42
7:U:218:SER:O	7:U:219:ASN:HB2	2.19	0.42
12:Z:268:ARG:HE	12:Z:272:HIS:CE1	2.37	0.42
3:Q:116:LEU:C	3:Q:116:LEU:HD13	2.40	0.41
8:V:68:LEU:HD23	8:V:98:CYS:SG	2.59	0.41
4:D:106:LEU:HD13	4:D:109:ARG:HH12	1.84	0.41
7:G:86:VAL:HG11	7:G:134:VAL:HG21	2.02	0.41
4:R:81:ARG:HH21	4:R:81:ARG:HD3	1.69	0.41
4:R:106:LEU:HD13	4:R:109:ARG:HH12	1.84	0.41
9:I:150:LYS:HE2	9:I:185:THR:HG23	2.02	0.41
7:U:86:VAL:HG11	7:U:134:VAL:HG21	2.02	0.41
7:U:158:TYR:CE1	7:U:161:ILE:HD13	2.56	0.41
4:R:165:ASP:O	4:R:169:LEU:HB2	2.21	0.41
8:H:142:TYR:CE2	14:N:58:GLU:HG3	2.56	0.41
9:W:150:LYS:HE2	9:W:185:THR:HG23	2.03	0.41
11:Y:54:ARG:HH21	11:Y:54:ARG:HD2	1.73	0.41
12:L:268:ARG:HE	12:L:272:HIS:CE1	2.37	0.40
14:N:2:ALA:N	15:N:306:HOH:O	2.54	0.40
3:C:116:LEU:HD13	3:C:116:LEU:C	2.40	0.40
7:G:158:TYR:CE1	7:G:161:ILE:HD13	2.56	0.40
1:A:81:ALA:N	1:A:82:PRO:HD2	2.36	0.40
1:O:81:ALA:N	1:O:82:PRO:HD2	2.37	0.40
1:O:75:THR:HG23	1:O:137:PHE:CE1	2.56	0.40
1:A:75:THR:HG23	1:A:137:PHE:CE1	2.56	0.40
2:B:58:LEU:HD23	2:B:58:LEU:HA	1.92	0.40

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	242/268 (90%)	237 (98%)	4 (2%)	1 (0%)	30 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	O	242/268 (90%)	237 (98%)	4 (2%)	1 (0%)	30 32
2	B	226/231 (98%)	222 (98%)	4 (2%)	0	100 100
2	P	226/231 (98%)	222 (98%)	4 (2%)	0	100 100
3	C	269/286 (94%)	257 (96%)	8 (3%)	4 (2%)	8 5
3	Q	269/286 (94%)	257 (96%)	8 (3%)	4 (2%)	8 5
4	D	232/247 (94%)	220 (95%)	8 (3%)	4 (2%)	7 4
4	R	232/247 (94%)	220 (95%)	8 (3%)	4 (2%)	7 4
5	E	223/245 (91%)	214 (96%)	9 (4%)	0	100 100
5	S	223/245 (91%)	214 (96%)	9 (4%)	0	100 100
6	F	215/265 (81%)	209 (97%)	6 (3%)	0	100 100
6	T	215/265 (81%)	209 (97%)	6 (3%)	0	100 100
7	G	225/237 (95%)	219 (97%)	6 (3%)	0	100 100
7	U	225/237 (95%)	218 (97%)	7 (3%)	0	100 100
8	H	226/284 (80%)	222 (98%)	4 (2%)	0	100 100
8	V	226/284 (80%)	222 (98%)	4 (2%)	0	100 100
9	I	217/292 (74%)	208 (96%)	8 (4%)	1 (0%)	25 25
9	W	217/292 (74%)	208 (96%)	8 (4%)	1 (0%)	25 25
10	J	202/205 (98%)	197 (98%)	5 (2%)	0	100 100
10	X	202/205 (98%)	197 (98%)	5 (2%)	0	100 100
11	K	204/206 (99%)	200 (98%)	3 (2%)	1 (0%)	25 25
11	Y	204/206 (99%)	200 (98%)	3 (2%)	1 (0%)	25 25
12	L	199/311 (64%)	191 (96%)	7 (4%)	1 (0%)	25 25
12	Z	199/311 (64%)	191 (96%)	7 (4%)	1 (0%)	25 25
13	M	204/246 (83%)	199 (98%)	4 (2%)	1 (0%)	25 25
13	a	204/246 (83%)	199 (98%)	4 (2%)	1 (0%)	25 25
14	N	216/218 (99%)	211 (98%)	5 (2%)	0	100 100
14	b	216/218 (99%)	211 (98%)	5 (2%)	0	100 100
All	All	6200/7082 (88%)	6011 (97%)	163 (3%)	26 (0%)	32 32

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	212	LYS

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Mol	Chain	Res	Type
4	R	212	LYS
3	C	172	GLN
3	Q	172	GLN
3	C	227	PRO
4	D	201	SER
11	K	72	GLU
3	Q	227	PRO
4	R	201	SER
11	Y	72	GLU
4	D	49	SER
4	D	211	ASN
4	R	49	SER
4	R	211	ASN
1	A	145	ALA
3	C	207	ASP
9	I	237	THR
13	M	133	ARG
1	O	145	ALA
3	Q	207	ASP
3	Q	228	ALA
9	W	237	THR
13	a	133	ARG
3	C	228	ALA
12	L	133	GLY
12	Z	133	GLY

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	199/221 (90%)	192 (96%)	7 (4%)	31	38
1	O	199/221 (90%)	192 (96%)	7 (4%)	31	38
2	B	187/190 (98%)	183 (98%)	4 (2%)	48	57
2	P	187/190 (98%)	183 (98%)	4 (2%)	48	57
3	C	225/239 (94%)	213 (95%)	12 (5%)	19	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	225/239 (94%)	213 (95%)	12 (5%)	19	19
4	D	201/211 (95%)	194 (96%)	7 (4%)	31	38
4	R	201/211 (95%)	194 (96%)	7 (4%)	31	38
5	E	191/207 (92%)	181 (95%)	10 (5%)	19	20
5	S	191/207 (92%)	181 (95%)	10 (5%)	19	20
6	F	179/217 (82%)	168 (94%)	11 (6%)	15	14
6	T	179/217 (82%)	168 (94%)	11 (6%)	15	14
7	G	188/196 (96%)	178 (95%)	10 (5%)	19	19
7	U	188/196 (96%)	178 (95%)	10 (5%)	19	19
8	H	187/234 (80%)	183 (98%)	4 (2%)	48	57
8	V	187/234 (80%)	183 (98%)	4 (2%)	48	57
9	I	179/246 (73%)	170 (95%)	9 (5%)	20	22
9	W	179/246 (73%)	170 (95%)	9 (5%)	20	22
10	J	166/167 (99%)	163 (98%)	3 (2%)	54	64
10	X	166/167 (99%)	163 (98%)	3 (2%)	54	64
11	K	168/168 (100%)	164 (98%)	4 (2%)	44	53
11	Y	168/168 (100%)	164 (98%)	4 (2%)	44	53
12	L	164/265 (62%)	157 (96%)	7 (4%)	25	28
12	Z	164/265 (62%)	157 (96%)	7 (4%)	25	28
13	M	175/208 (84%)	167 (95%)	8 (5%)	23	25
13	a	175/208 (84%)	167 (95%)	8 (5%)	23	25
14	N	177/177 (100%)	171 (97%)	6 (3%)	32	40
14	b	177/177 (100%)	171 (97%)	6 (3%)	32	40
All	All	5172/5892 (88%)	4968 (96%)	204 (4%)	30	33

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	57	LEU
1	A	75	THR
1	A	146	ASP
1	A	164	SER
1	A	193	LEU

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Mol	Chain	Res	Type
1	A	233	ARG
2	B	52	SER
2	B	183	GLU
2	B	215	LYS
2	B	218	LEU
3	C	2	SER
3	C	26	GLU
3	C	30	GLN
3	C	87	SER
3	C	98	LEU
3	C	155	HIS
3	C	179	SER
3	C	186	LYS
3	C	222	HIS
3	C	229	THR
3	C	240	PRO
3	C	245	GLU
4	D	5	ARG
4	D	81	ARG
4	D	103	ASP
4	D	105	ASP
4	D	138	GLU
4	D	181	THR
4	D	183	ASP
5	E	18	GLU
5	E	41	GLN
5	E	76	THR
5	E	161	THR
5	E	168	GLN
5	E	188	ASN
5	E	189	MET
5	E	196	THR
5	E	227	LEU
5	E	231	ASP
6	F	42	ASP
6	F	50	LYS
6	F	51	ARG
6	F	60	TYR
6	F	61	GLN
6	F	92	GLU
6	F	104	ASN
6	F	186	ASP

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Mol	Chain	Res	Type
6	F	207	ASN
6	F	209	LYS
6	F	231	ARG
7	G	27	LYS
7	G	40	CYS
7	G	41	THR
7	G	55	ARG
7	G	84	ARG
7	G	103	THR
7	G	139	TYR
7	G	171	LYS
7	G	204	ASP
7	G	213	TRP
8	H	137	PHE
8	H	143	MET
8	H	178	ASP
8	H	218	TYR
9	I	75	LYS
9	I	98	LYS
9	I	109	CYS
9	I	131	LEU
9	I	150	LYS
9	I	215	GLU
9	I	219	GLU
9	I	223	SER
9	I	260	GLU
10	J	12	LEU
10	J	24	SER
10	J	131	CYS
11	K	9	ARG
11	K	63	CYS
11	K	75	ARG
11	K	77	ILE
12	L	134	GLN
12	L	142	MET
12	L	220	SER
12	L	226	ASP
12	L	302	GLN
12	L	304	LYS
12	L	310	VAL
13	M	57	ASP
13	M	123	LYS

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Mol	Chain	Res	Type
13	M	126	SER
13	M	127	THR
13	M	131	GLN
13	M	144	VAL
13	M	201	MET
13	M	234	ASP
14	N	26	TYR
14	N	71	GLN
14	N	190	ASP
14	N	205	GLU
14	N	210	CYS
14	N	218	ARG
1	O	40	ARG
1	O	57	LEU
1	O	75	THR
1	O	146	ASP
1	O	164	SER
1	O	193	LEU
1	O	233	ARG
2	P	52	SER
2	P	183	GLU
2	P	215	LYS
2	P	218	LEU
3	Q	2	SER
3	Q	26	GLU
3	Q	30	GLN
3	Q	87	SER
3	Q	98	LEU
3	Q	155	HIS
3	Q	179	SER
3	Q	186	LYS
3	Q	222	HIS
3	Q	229	THR
3	Q	240	PRO
3	Q	245	GLU
4	R	5	ARG
4	R	81	ARG
4	R	103	ASP
4	R	105	ASP
4	R	138	GLU
4	R	181	THR
4	R	183	ASP

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Mol	Chain	Res	Type
5	S	18	GLU
5	S	41	GLN
5	S	76	THR
5	S	161	THR
5	S	168	GLN
5	S	188	ASN
5	S	189	MET
5	S	196	THR
5	S	227	LEU
5	S	231	ASP
6	T	42	ASP
6	T	50	LYS
6	T	51	ARG
6	T	60	TYR
6	T	61	GLN
6	T	92	GLU
6	T	104	ASN
6	T	186	ASP
6	T	207	ASN
6	T	209	LYS
6	T	231	ARG
7	U	27	LYS
7	U	40	CYS
7	U	41	THR
7	U	55	ARG
7	U	84	ARG
7	U	103	THR
7	U	139	TYR
7	U	171	LYS
7	U	204	ASP
7	U	213	TRP
8	V	137	PHE
8	V	143	MET
8	V	178	ASP
8	V	218	TYR
9	W	75	LYS
9	W	98	LYS
9	W	109	CYS
9	W	131	LEU
9	W	150	LYS
9	W	215	GLU
9	W	219	GLU

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Mol	Chain	Res	Type
9	W	223	SER
9	W	260	GLU
10	X	12	LEU
10	X	24	SER
10	X	131	CYS
11	Y	9	ARG
11	Y	63	CYS
11	Y	75	ARG
11	Y	77	ILE
12	Z	134	GLN
12	Z	142	MET
12	Z	220	SER
12	Z	226	ASP
12	Z	302	GLN
12	Z	304	LYS
12	Z	310	VAL
13	a	57	ASP
13	a	123	LYS
13	a	126	SER
13	a	127	THR
13	a	131	GLN
13	a	144	VAL
13	a	201	MET
13	a	234	ASP
14	b	26	TYR
14	b	71	GLN
14	b	190	ASP
14	b	205	GLU
14	b	210	CYS
14	b	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
3	C	94	ASN
3	C	149	HIS
3	C	230	GLN
4	D	68	HIS
5	E	41	GLN
5	E	65	ASN
5	E	155	GLN

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Mol	Chain	Res	Type
5	E	168	GLN
5	E	188	ASN
6	F	104	ASN
7	G	178	ASN
7	G	223	GLN
8	H	112	GLN
8	H	211	GLN
9	I	259	ASN
11	K	11	ASN
11	K	73	HIS
11	K	186	ASN
12	L	233	HIS
12	L	272	HIS
1	O	89	GLN
3	Q	94	ASN
3	Q	230	GLN
4	R	68	HIS
5	S	41	GLN
5	S	65	ASN
5	S	155	GLN
5	S	168	GLN
5	S	188	ASN
6	T	104	ASN
7	U	178	ASN
7	U	223	GLN
8	V	112	GLN
8	V	211	GLN
9	W	259	ASN
11	Y	11	ASN
11	Y	186	ASN
12	Z	233	HIS
12	Z	272	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 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.

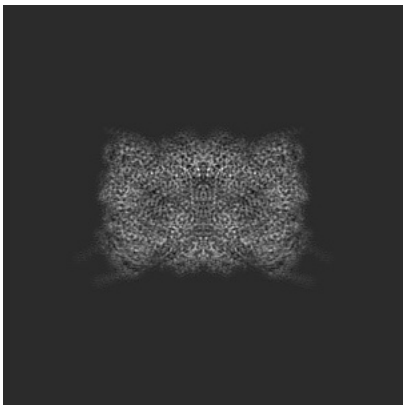
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50258. These allow visual inspection of the internal detail of the map and identification of artifacts.

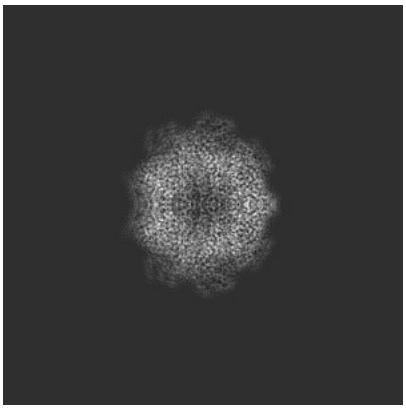
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

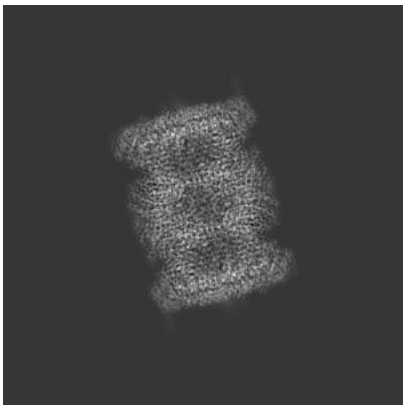
6.1.1 Primary map



X

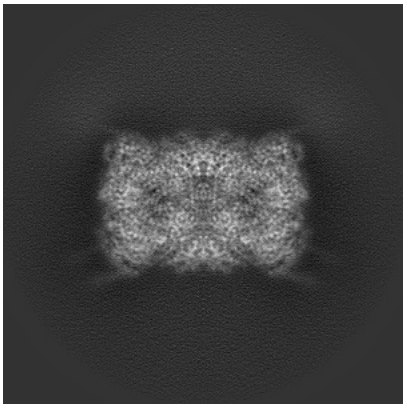


Y

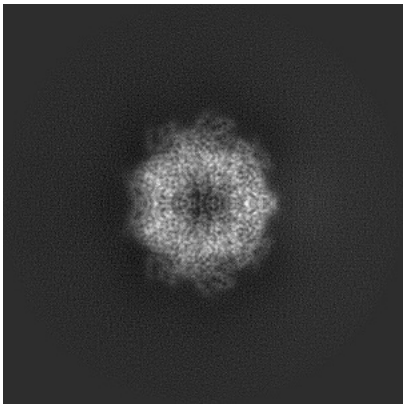


Z

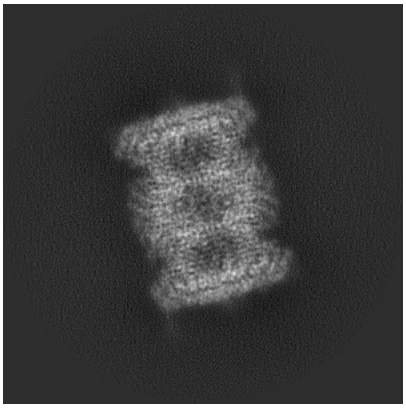
6.1.2 Raw map



X



Y

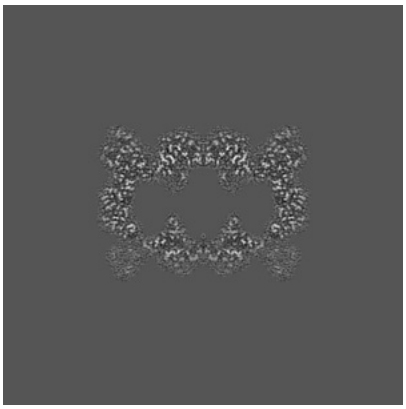


Z

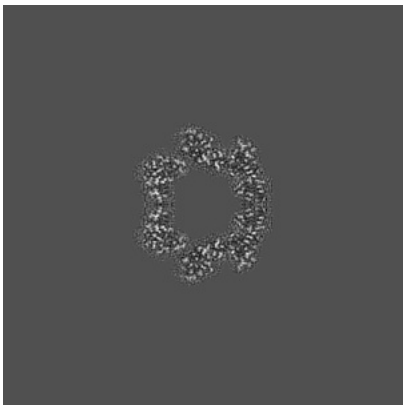
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

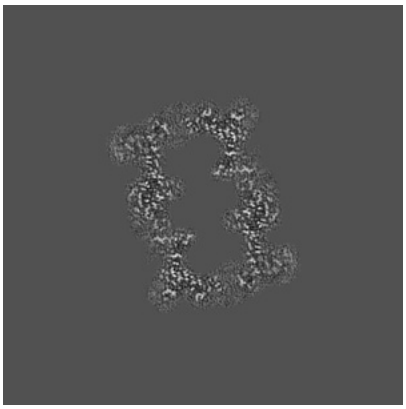
6.2.1 Primary map



X Index: 240

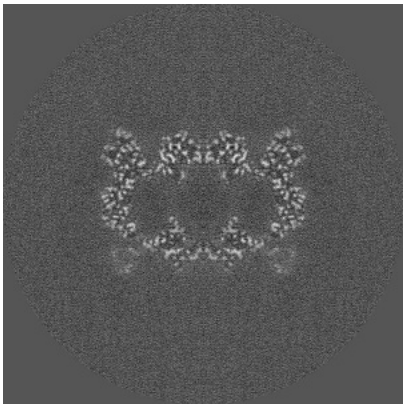


Y Index: 240

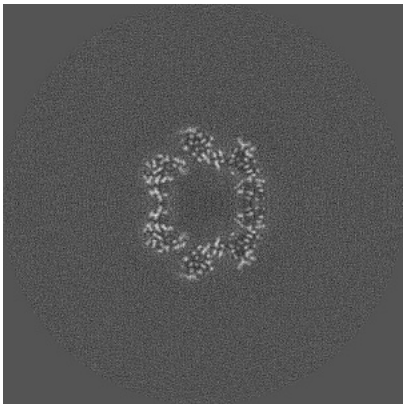


Z Index: 240

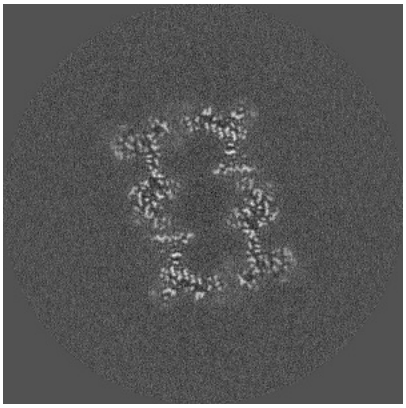
6.2.2 Raw map



X Index: 240



Y Index: 240



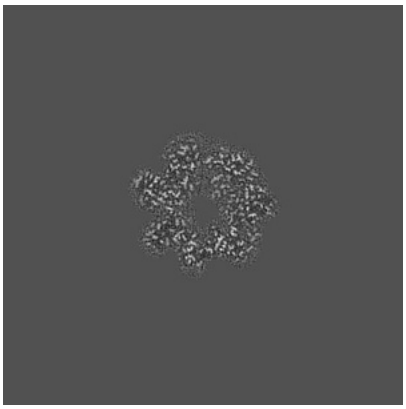
Z Index: 240

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

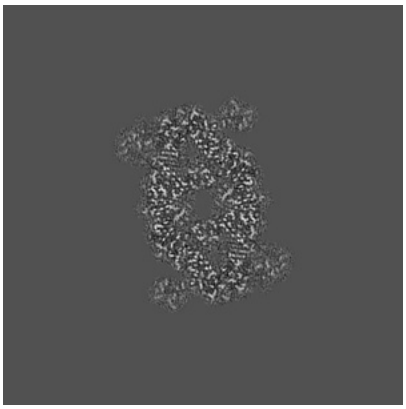
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 212

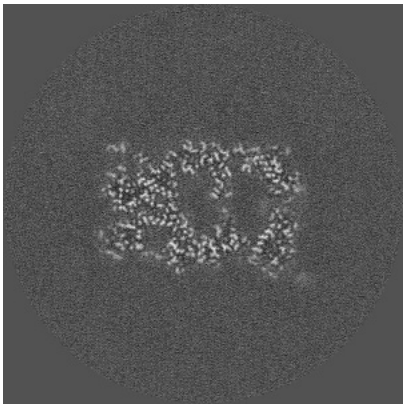


Y Index: 271

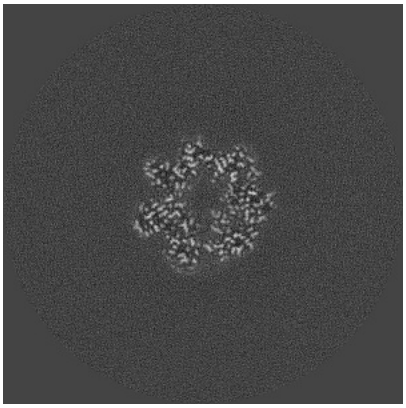


Z Index: 277

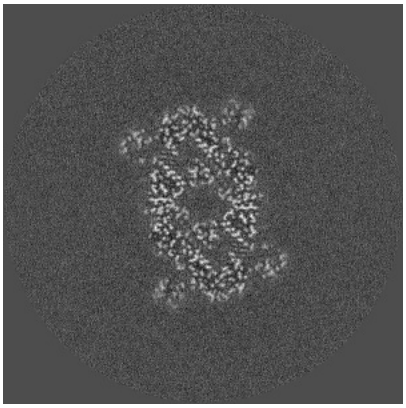
6.3.2 Raw map



X Index: 212



Y Index: 209

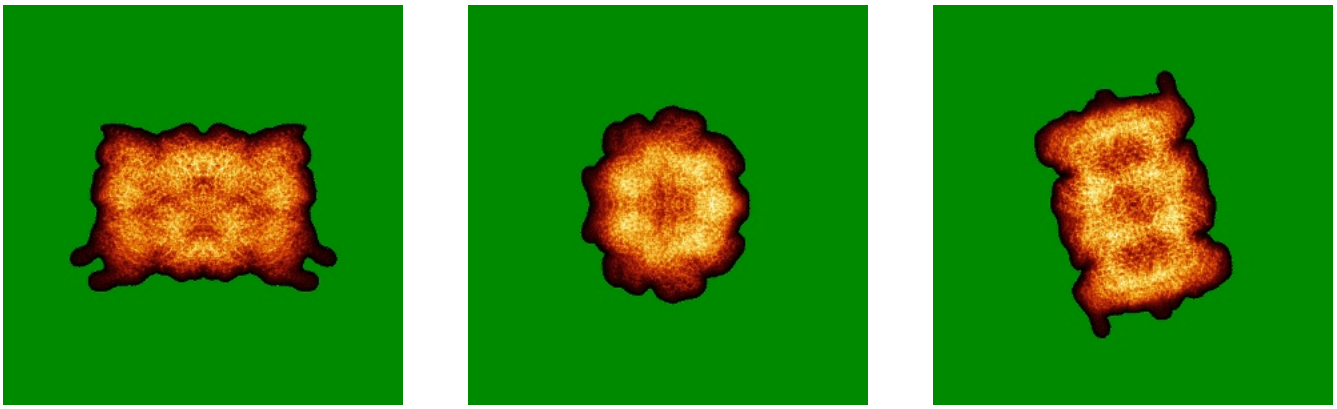


Z Index: 276

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

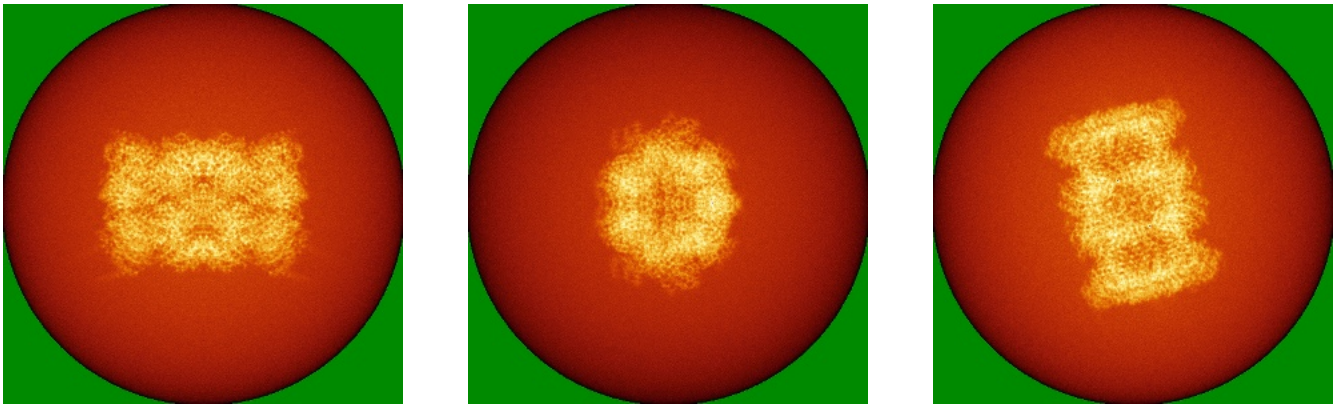
6.4 Orthogonal standard-deviation projections (False-color) (i)

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.

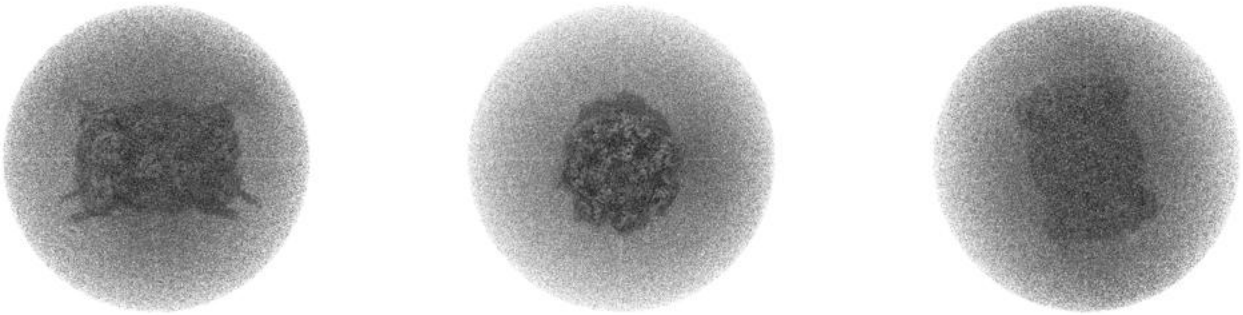
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.001. 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.

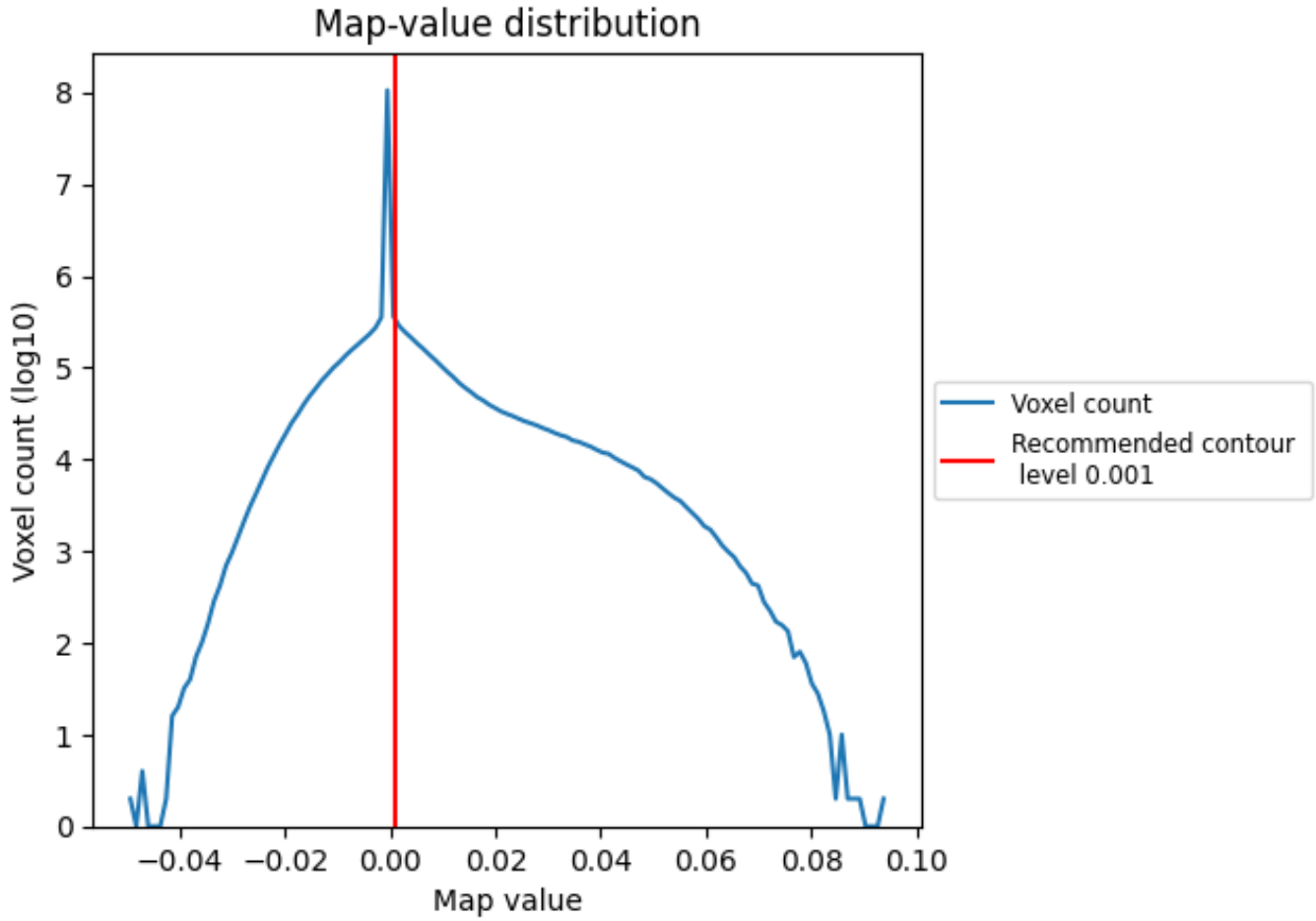
6.6 Mask visualisation (i)

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

7 Map analysis

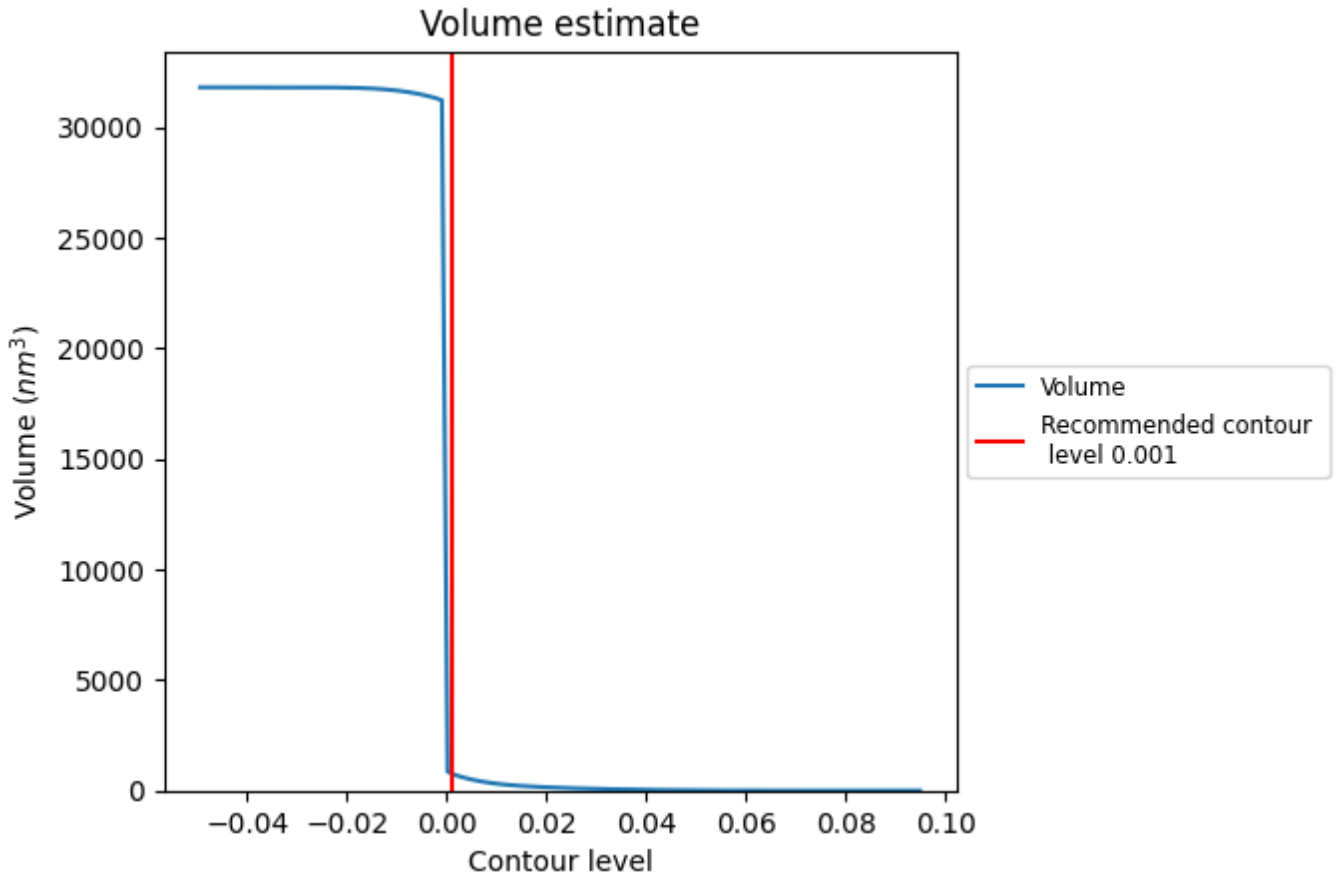
This section contains the results of statistical analysis of the map.

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.

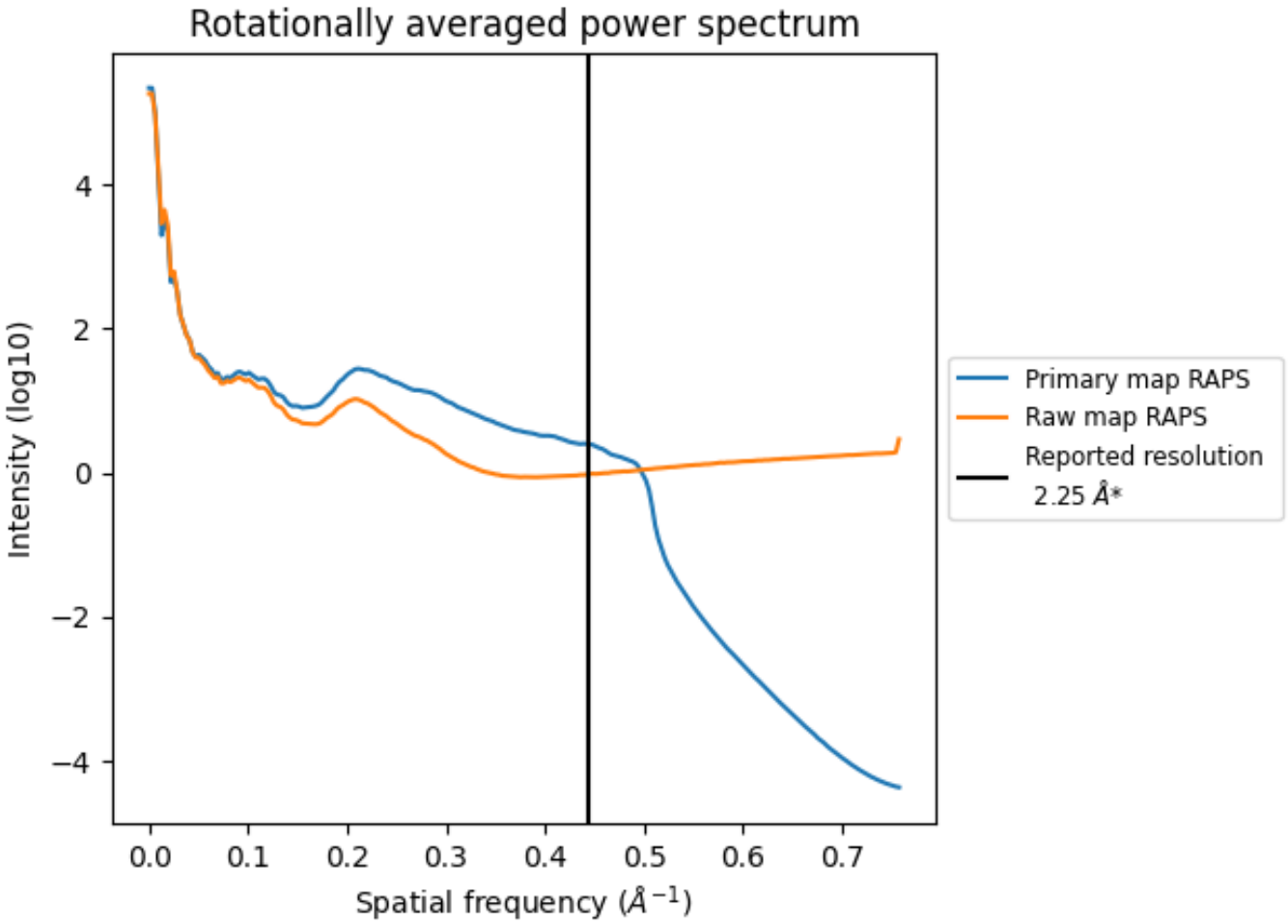
7.2 Volume estimate



The volume at the recommended contour level is 771 nm^3; this corresponds to an approximate mass of 696 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)

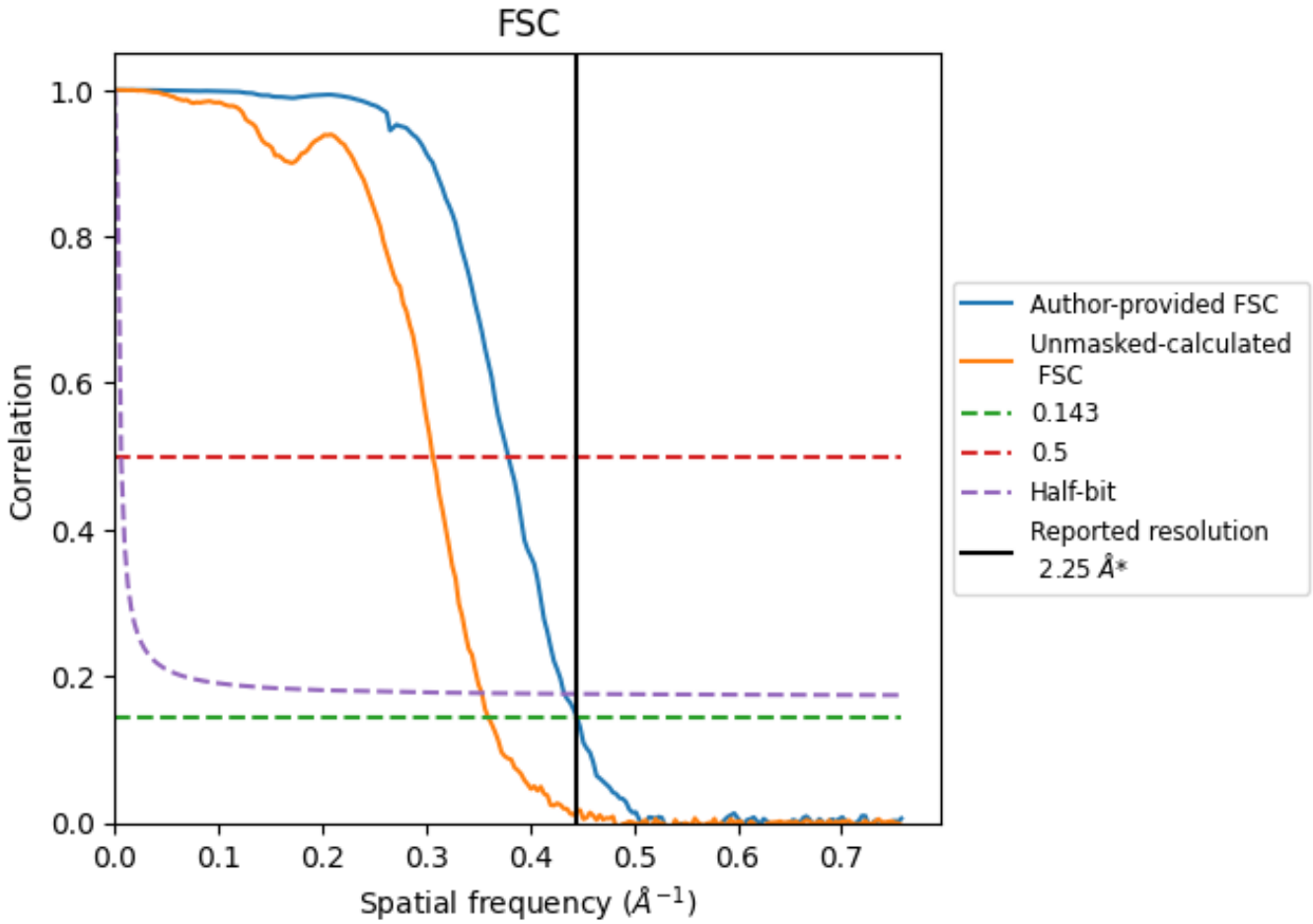


*Reported resolution corresponds to spatial frequency of 0.444 Å^{-1}

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 0.444 $Å^{-1}$

8.2 Resolution estimates (i)

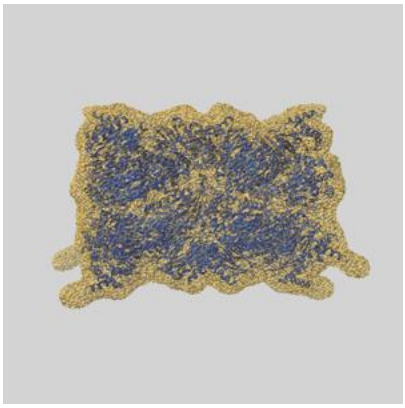
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.64	2.31
Unmasked-calculated*	2.78	3.27	2.83

*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 2.78 differs from the reported value 2.25 by more than 10 %

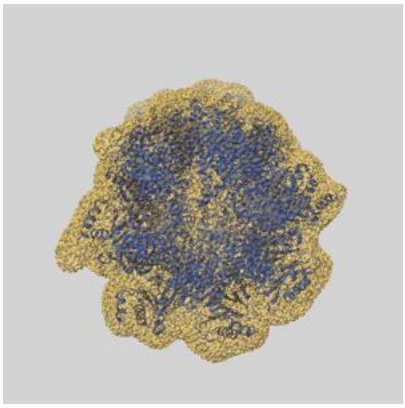
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50258 and PDB model 9F9P. Per-residue inclusion information can be found in section 3 on page 10.

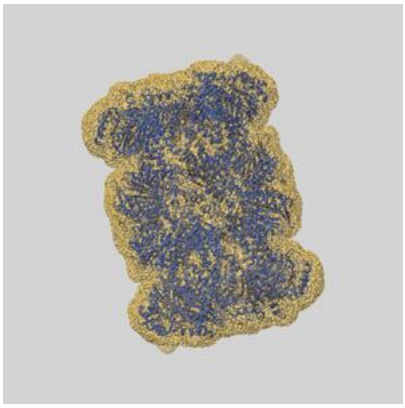
9.1 Map-model overlay



X



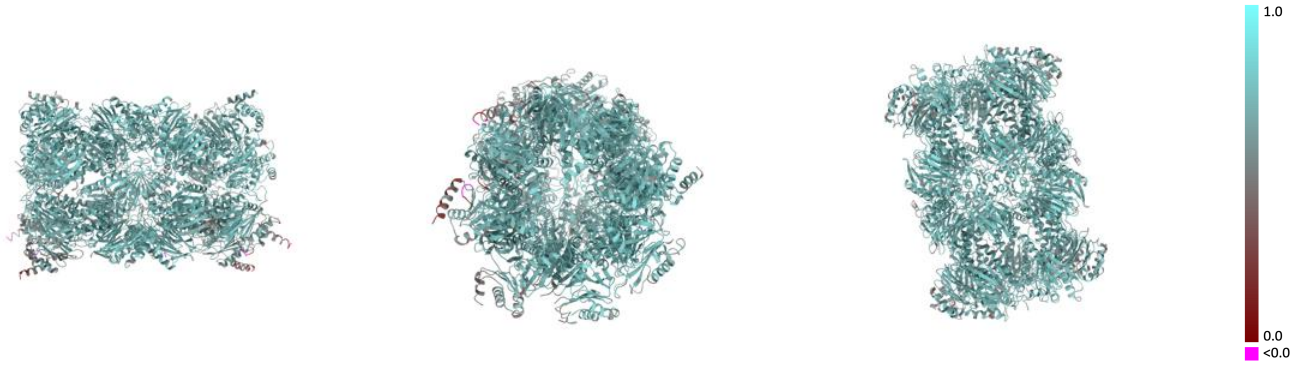
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.001 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.

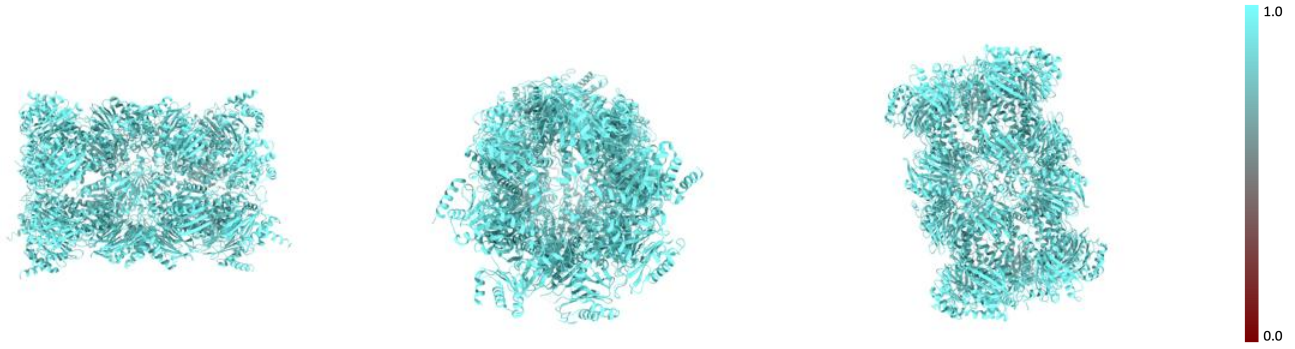
9.2 Q-score mapped to coordinate model (i)



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.

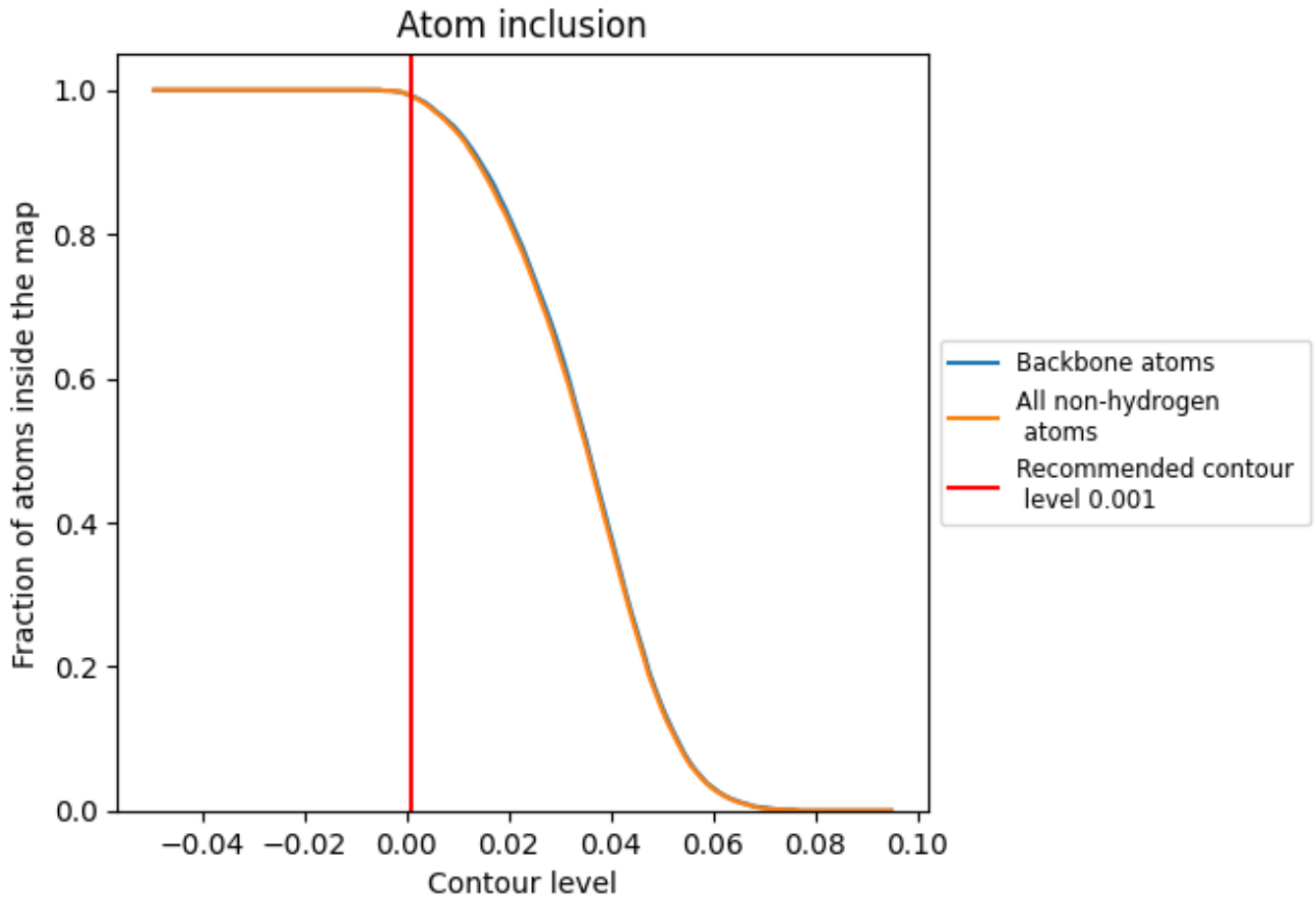
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.001).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9910	0.6990
A	0.9940	0.7080
B	0.9920	0.7050
C	0.9810	0.6550
D	0.9770	0.6310
E	0.9970	0.6420
F	0.9880	0.6900
G	0.9920	0.7040
H	0.9930	0.7380
I	0.9930	0.7090
J	0.9990	0.7360
K	0.9960	0.7150
L	0.9950	0.7230
M	0.9950	0.7230
N	0.9920	0.7390
O	0.9940	0.7080
P	0.9920	0.7040
Q	0.9810	0.6560
R	0.9770	0.6280
S	0.9970	0.6430
T	0.9880	0.6900
U	0.9920	0.7020
V	0.9930	0.7370
W	0.9940	0.7110
X	0.9990	0.7350
Y	0.9960	0.7150
Z	0.9950	0.7240
a	0.9950	0.7220
b	0.9920	0.7370