



wwPDB EM Validation Summary 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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
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

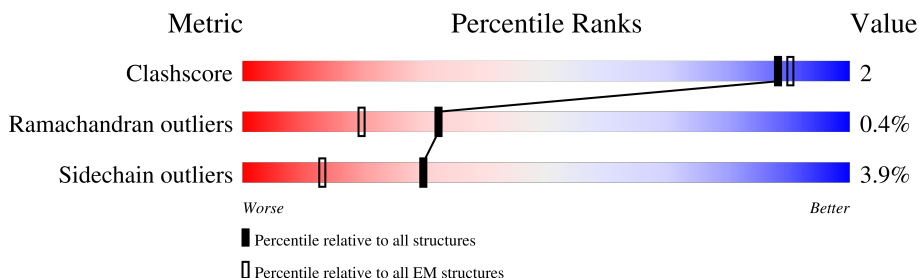
1 Overall quality at a glance

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.













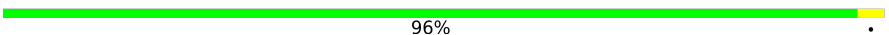
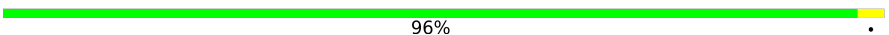
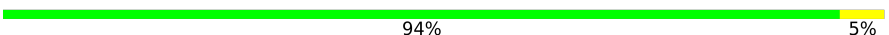






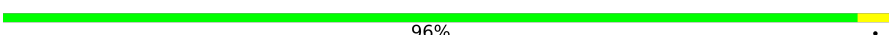
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	 85%6% • 7%
5	S	245	 86%6% • 7%
6	F	265	 75%7% • 17%
6	T	265	 75%7% • 17%
7	G	237	 86%9% •
7	U	237	 86%9% •
8	H	284	 77% • 20%
8	V	284	 77% • 20%
9	I	292	 69%6% 25%
9	W	292	 69%6% 25%
10	J	205	 96% •
10	X	205	 96% •
11	K	206	 94%5%
11	Y	206	 93%6%
12	L	311	 59%5% 35%
12	Z	311	 59%5% 35%
13	M	246	 79% • • 15%
13	a	246	 80%5% 15%
14	N	218	 93%6% •
14	b	218	 96% •

2 Entry composition

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	C	N	O	S	0	0
			1555	976	265	299	15		

- Molecule 11 is a protein called Proteasome subunit beta.

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

- Molecule 12 is a protein called Proteasome subunit beta.

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

- Molecule 13 is a protein called Proteasome subunit beta.

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

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	C	N	O	S	0	0
			1695	1075	290	313	17		
14	b	218	Total	C	N	O	S	0	0
			1695	1075	290	313	17		

- Molecule 15 is water.


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

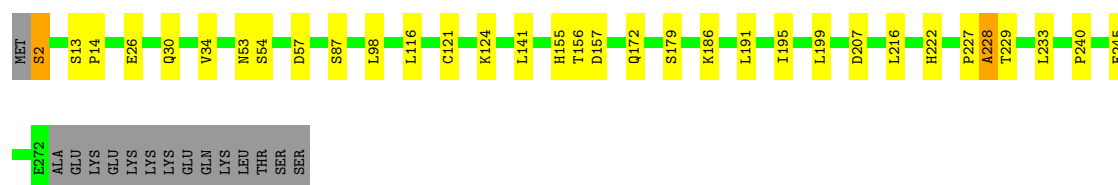
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Mol	Chain	Residues	Atoms		AltConf
15	W	45	Total 45	O 45	0
15	X	50	Total 50	O 50	0
15	Y	37	Total 37	O 37	0
15	Z	29	Total 29	O 29	0
15	a	48	Total 48	O 48	0
15	b	70	Total 70	O 70	0

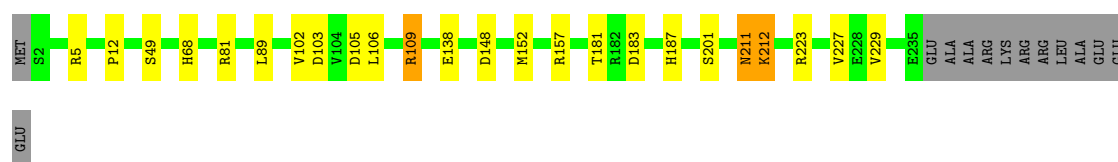
- Molecule 3: Proteasome subunit alpha type

Chain Q:  83% 11% • 5%




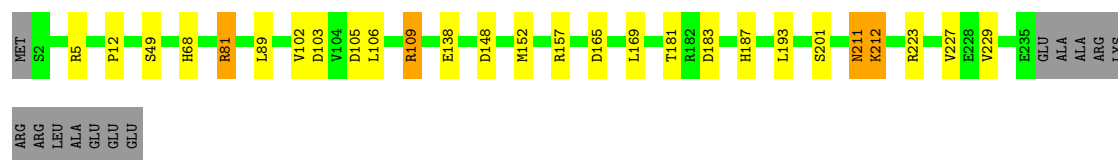
- Molecule 4: Proteasome subunit alpha type

Chain D:  85% 9% • 5%




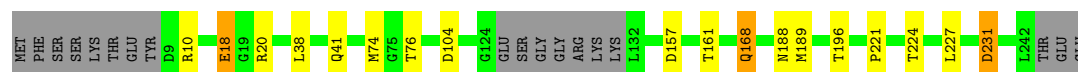
- Molecule 4: Proteasome subunit alpha type

Chain R:  84% 9% • 5%




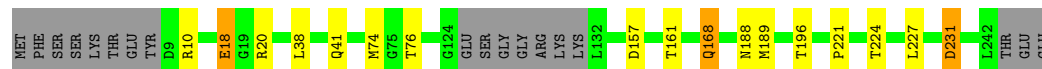
- Molecule 5: Proteasome subunit alpha type

Chain E:  85% 6% • 7%



- Molecule 5: Proteasome subunit alpha type

Chain S:  86% 6% • 7%




- Molecule 6: Proteasome subunit alpha type

Chain F:  75% 7% • 17%



MET ARG
PRO SER
GLU LYS
ASP
ILE
PRO
PRO
PRO
ALA
GLU
GLU
GLU
GLU
THR
LEU
GLN
GLU
ARG
SER
SER
LEU
ASP
VAL
GLU
GLU


• Molecule 6: Proteasome subunit alpha type

Chain T:  75% 7% 17%

MET PHE
SER
GLY
H4
D42
K50
R51
SER
PRO
GLU
VAL
ALA
GLN
PHE
SER
SS9
Y60
Q61
L67
F88
V89
E92
M104
P105
I112
F180
P181
L185
D186
I189
T200
SER
GLY
GLY
A204
N207
I208
K209
I215
R231
L234
ASP
GLY
PHE
LYS
MET


ARG
PRO
GLU
ASP
ILE
PRO
PRO
ALA
GLU
GLU
GLU
THR
SER
LEU
GLN
GLU
ARG
SER
SER
ASP
VAL
GLU
GLU

• Molecule 7: Putative proteasome alpha 7 subunit

Chain G:  86% 9% 5%


MET SER
GLY
T4
K27
C40
T41
D42
R55
V74
R84
A85
V86
T103
R113
F117
V120
V134
Y139
D150
P151
Y158
I161
K171
D204
W213
S218
N219
I230
PRO
LYS
PRO
PRO
ALA
SER
GLN

• Molecule 7: Putative proteasome alpha 7 subunit

Chain U:  86% 9% 5%

MET SER
GLY
T4
K27
C40
T41
D42
R55
V74
R84
A85
V86
T103
R113
F117
V120
V134
Y139
D150
P151
Y158
I161
K171
D204
W213
S218
N219
I230
PRO
LYS
PRO
PRO
ALA
SER
GLN


• Molecule 8: Proteasome subunit beta

Chain H:  77% 20% 3%

MET ILE
LYS ARG
PRO
GLU
GLY
ALA
LEU
LEU
HIS
HIS
PRO
SER
CYS
PRO
MET
MET
ILE
LYS
HIS
GLU
LEU
LEU
THR
PHE
ASN
GLY
PRO
ALA
GLN
GLN
SER
SER
ALA
LYS
LYS
LEU
LEU
PHE
GLU
PRO
GLU
ALA
ALA
VAL
VAL
LEU
ASP
PRO
GLN
LEU
LEU
ASN
ASN
GLU
ALA
VAL
SER
SER
GLY
T55
M58
L68

C98
F137
M143
D178
C210
Y218
E282
ARG
ILE

• Molecule 8: Proteasome subunit beta

Chain V:  77% 20% 3%

MET ILE
LYS ARG
PRO
GLU
GLY
ALA
LEU
LEU
HIS
HIS
PRO
SER
CYS
PRO
MET
MET
ILE
LYS
HIS
GLU
LEU
LEU
THR
PHE
ASN
GLY
PRO
ALA
GLN
GLN
SER
SER
ALA
LYS
LYS
LEU
LEU
PHE
GLU
PRO
GLU
ALA
ALA
VAL
VAL
LEU
ASP
PRO
GLN
LEU
LEU
ASN
ASN
GLU
ALA
VAL
SER
SER
GLY
T55
M58
L68

C98
F137
M143
D178
C210
Y218
E282
ARG
ILE

• Molecule 9: Proteasome subunit beta

Chain I:  69% 6% 25%

MET CYS VAL VAL SER VAL GLU LYS ASN CYS ASN SER LYS PHE ASN LEU VAL LEU ARG ALA TYR SER ILE VAL LYS LYS GLU GLU LYS LYS GLY ARG ARG ARG MET PRO GLY PHE SER PHE ALA ASN VAL VAL GLN THR ARG ASN ASP LEU LEU LEU GLN ARG GLN GLY LEU GLN PRO PRO

LYS THR LEU LYS THR GLY T67 K75 K98 M108 C109 L131 K150 T185 E215 E219 S223 I229 T237 C242 E260 P271 T274 E280 R283 R284 L285 VAL THR ILE THR THR ASP VAL GLU

• Molecule 9: Proteasome subunit beta

Chain W:  69% 6% 25%

MET CYS VAL VAL SER VAL GLU LYS ASN CYS ASN SER LYS PHE ASN LEU VAL LEU ARG ALA TYR SER ILE VAL LYS LYS GLU GLU LYS LYS GLY ARG ARG ARG MET PRO GLY PHE SER PHE ALA ASN VAL VAL GLN THR ARG ASN ASP LEU LEU LEU GLN ARG GLN GLY LEU GLN PRO PRO

LYS THR LEU LYS THR GLY T67 K75 K98 M108 C109 L131 K150 T185 E215 E219 S223 I229 T237 C242 E260 P271 T274 E280 R283 R284 L285 VAL THR ILE THR THR ASP VAL GLU

• Molecule 10: Putative proteasome beta 3 subunit

Chain J:  96%

MET S2 L12 S24 D125 A129 P130 C131 V186 R198 D205

• Molecule 10: Putative proteasome beta 3 subunit

Chain X:  96%

MET S2 L12 S24 D125 A129 P130 C131 V186 R198 D205

• Molecule 11: Proteasome subunit beta

Chain K:  94% 5%

H1 S2 E3 R9 N22 E33 D34 K35 C63 L67 E72 R75 V78 I77 R78 R87 N88 S206

• Molecule 11: Proteasome subunit beta

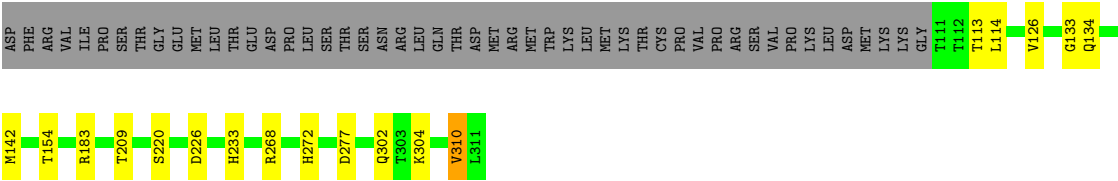
Chain Y:  93% 6%

H1 S2 E3 R9 N22 E33 D34 K35 R54 C63 L67 E72 R75 V78 I77 R78 R87 N88 S206

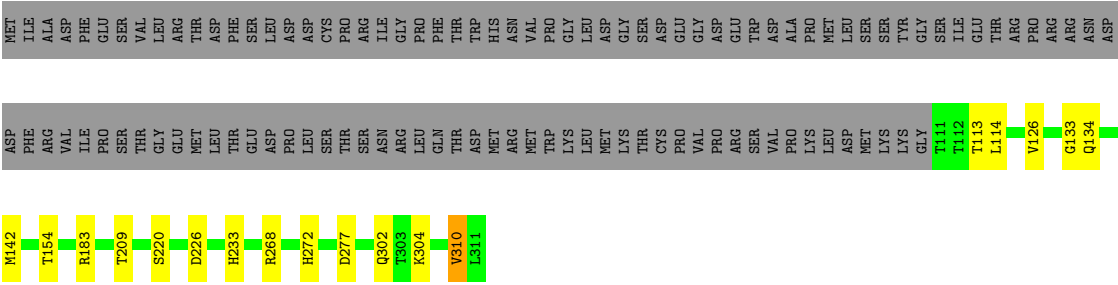
• Molecule 12: Proteasome subunit beta

Chain L:  59% 5% 35%

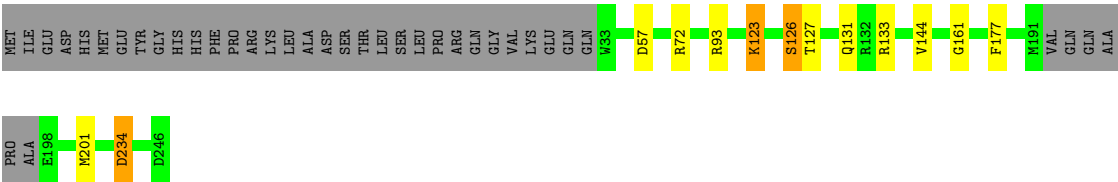
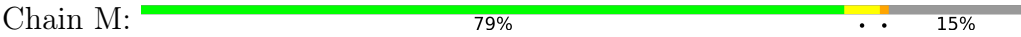
MET ILE ALA ASP PHE GLU SER VAL LEU LEU ARG D34 THR ASP PHE SER LEU ASP ASP CYS PRO ARG ILE GLY PRO PRO GLY LEU ASP GLY GLY ASP TRP ASP ASP ALA PRO MET LEU LEU SER SER TYR GLY SER ILE GLU THR ARG ARG ARG ASP



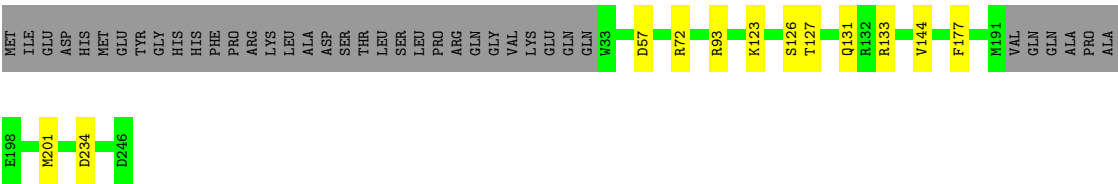
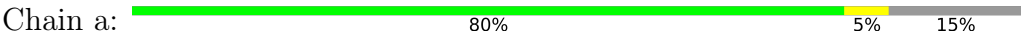
• Molecule 12: Proteasome subunit beta



• Molecule 13: Proteasome subunit beta



• Molecule 13: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 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

5.2 Too-close contacts

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

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

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/268 (90%)	237 (98%)	4 (2%)	1 (0%)	30	32
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

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	212	LYS
4	R	212	LYS
3	C	172	GLN
3	Q	172	GLN
3	C	227	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	30	GLN
6	T	50	LYS
14	b	71	GLN
3	Q	179	SER
4	R	181	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	168	GLN
9	W	259	ASN
5	S	188	ASN
7	U	223	GLN
11	Y	186	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

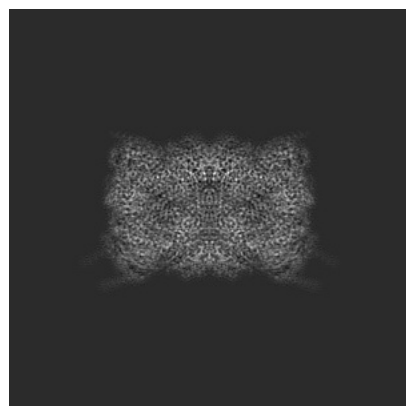
6 Map visualisation [i](#)

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.

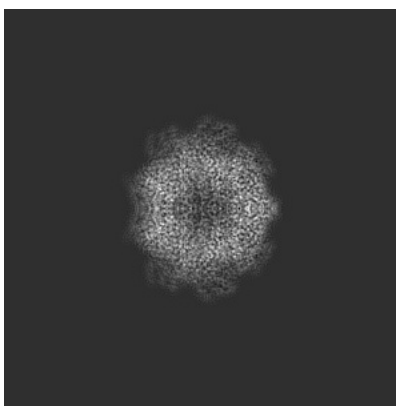
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

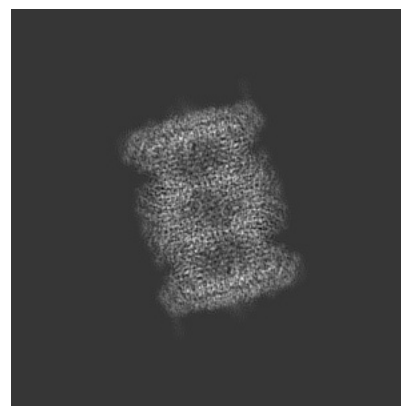
6.1.1 Primary map



X

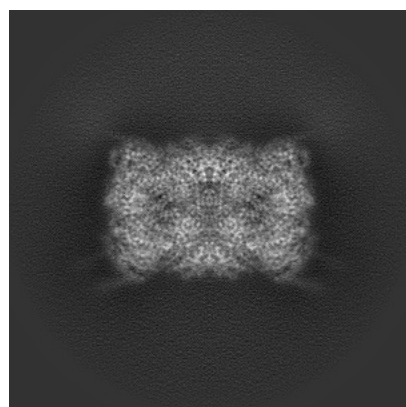


Y

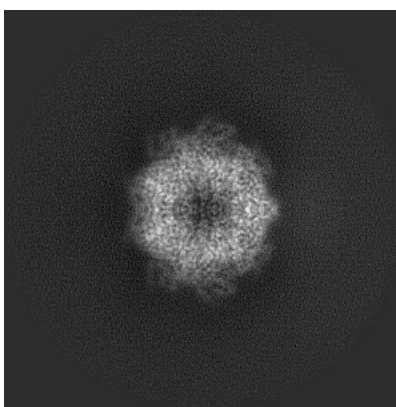


Z

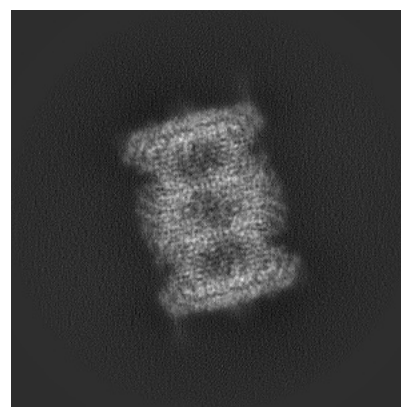
6.1.2 Raw map



X



Y

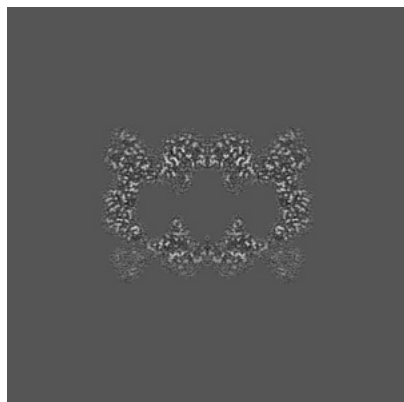


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

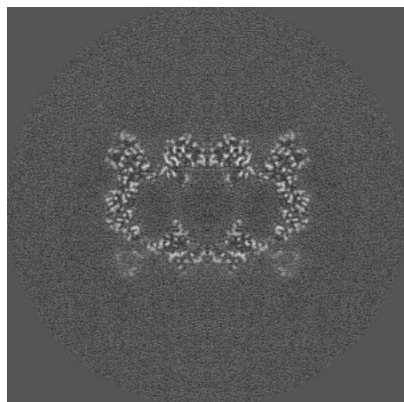


Y Index: 240

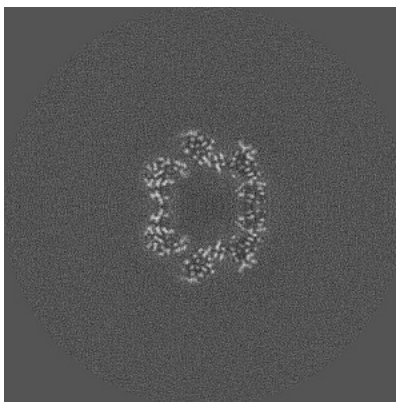


Z Index: 240

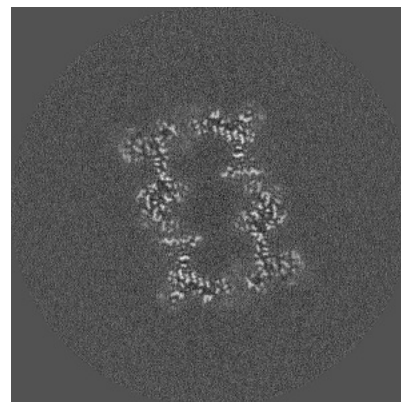
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

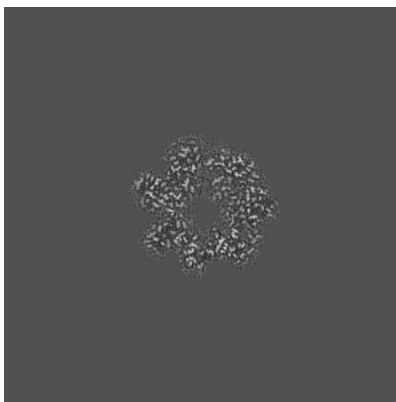
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

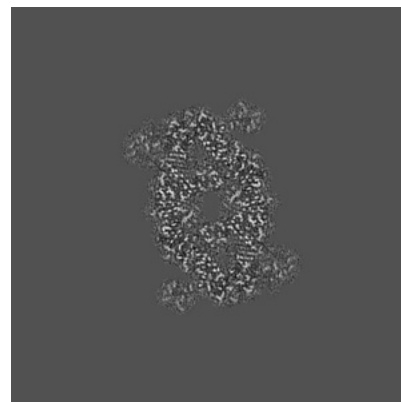
6.3.1 Primary map



X Index: 212

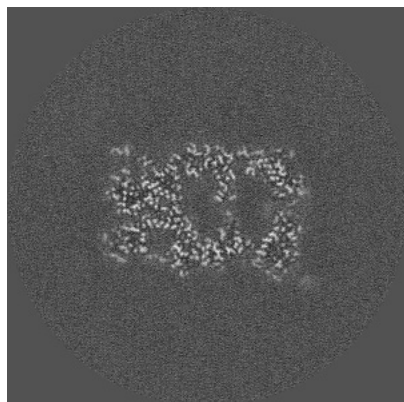


Y Index: 271

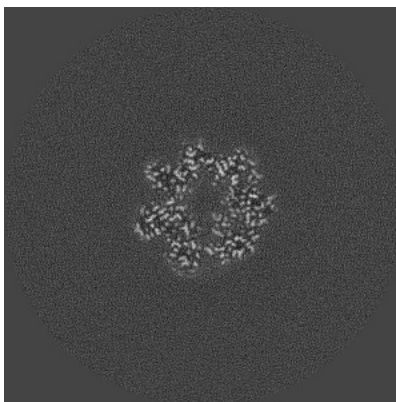


Z Index: 277

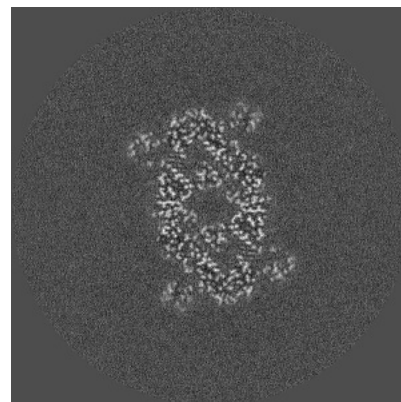
6.3.2 Raw map



X Index: 212



Y Index: 209

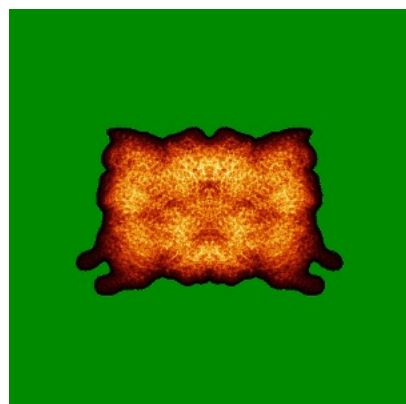


Z Index: 276

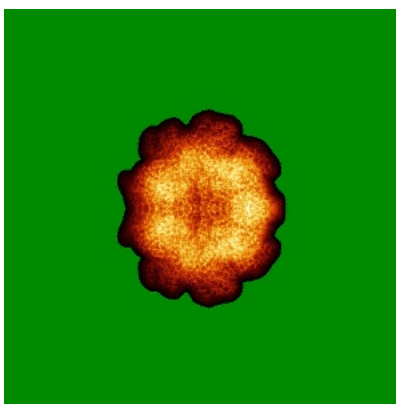
The images above show the largest variance slices of the map in three orthogonal directions.

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

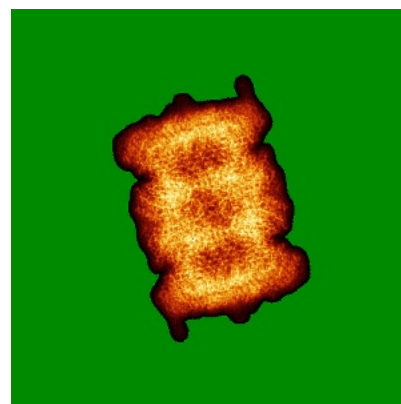
6.4.1 Primary map



X

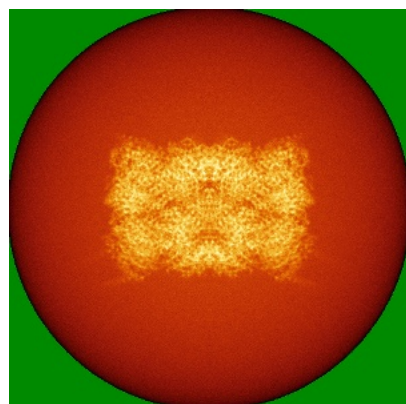


Y

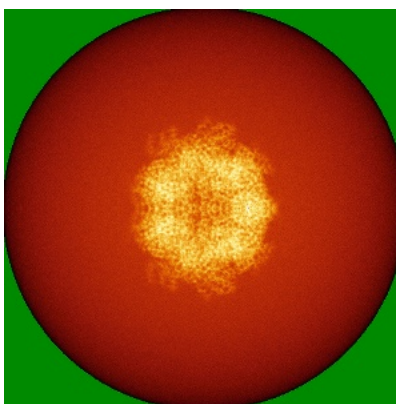


Z

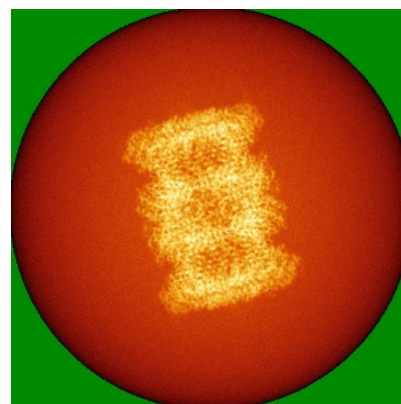
6.4.2 Raw map



X



Y

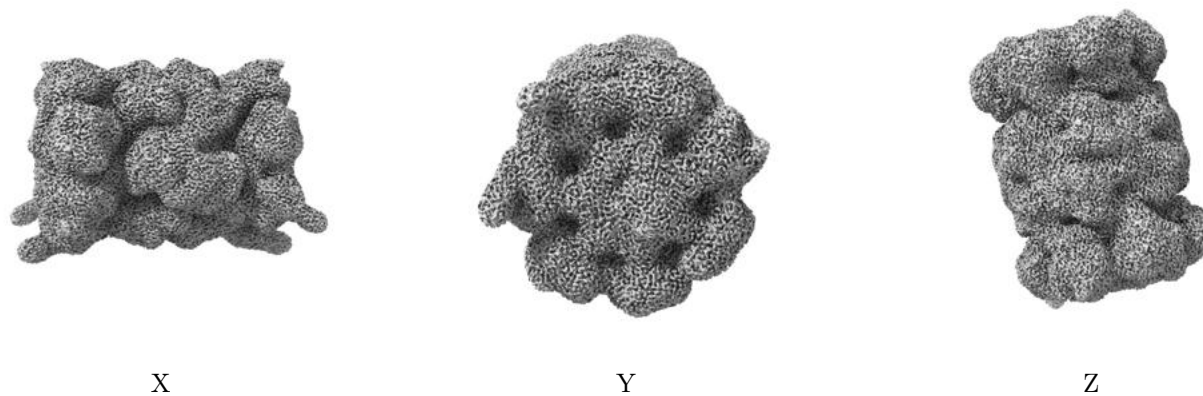


Z

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.

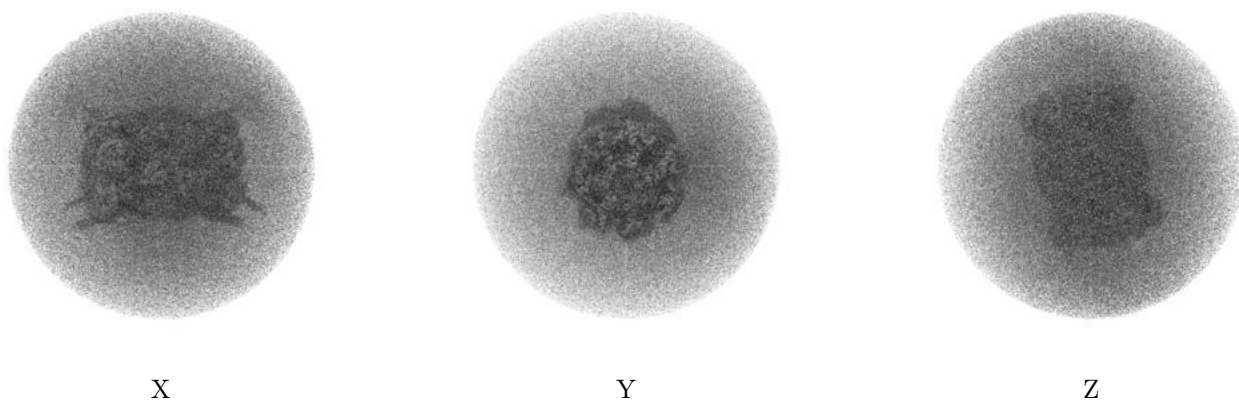
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

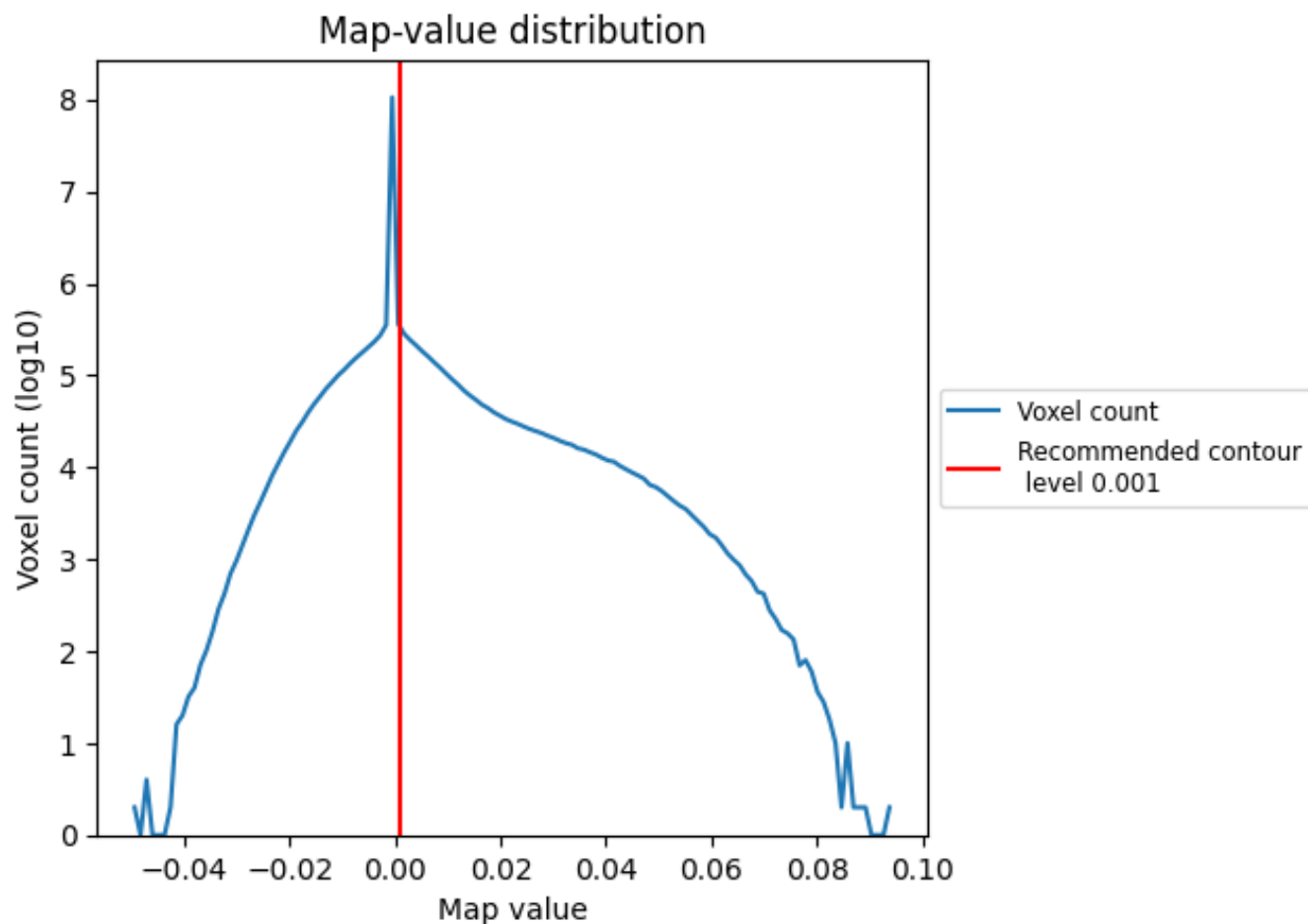
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

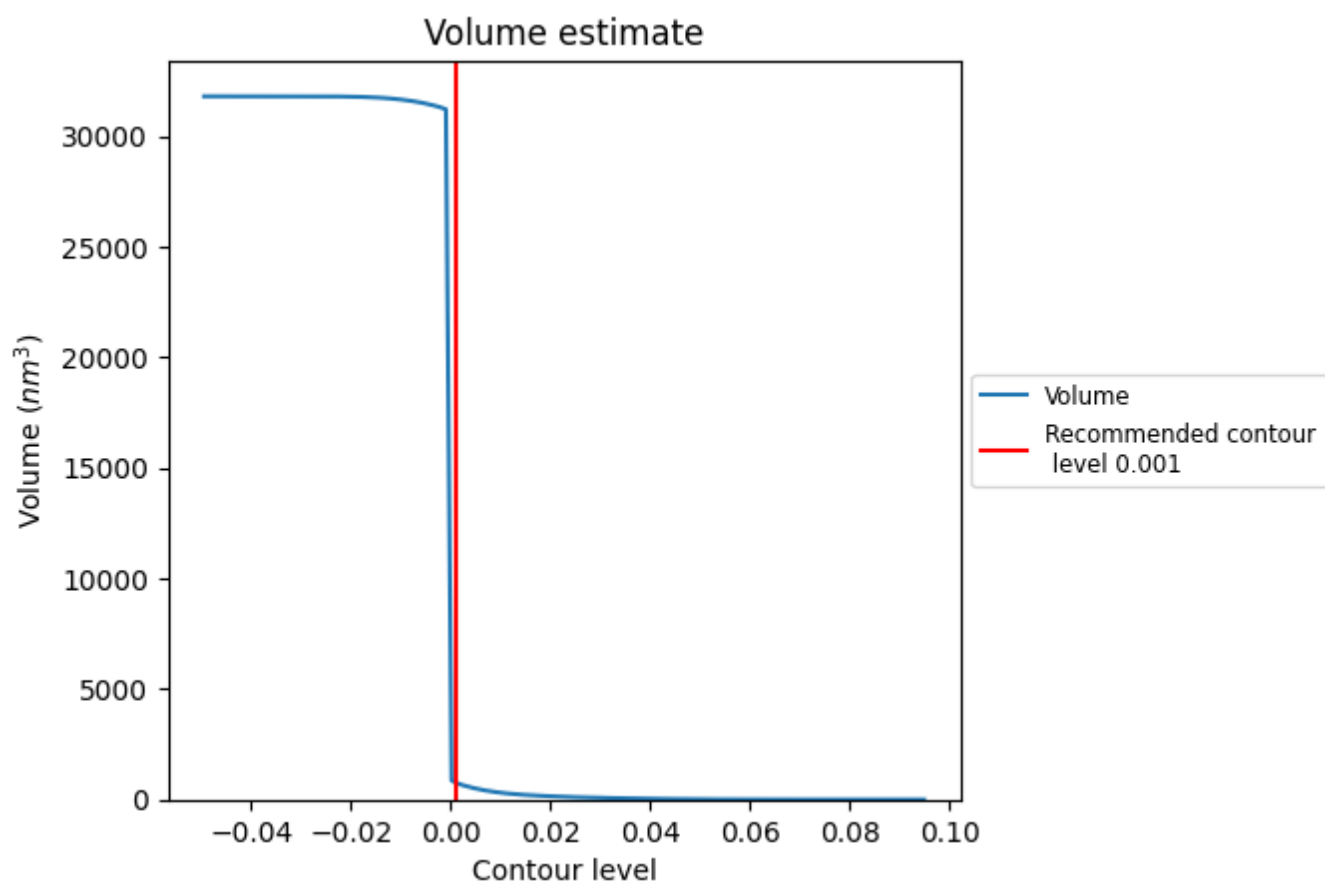
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

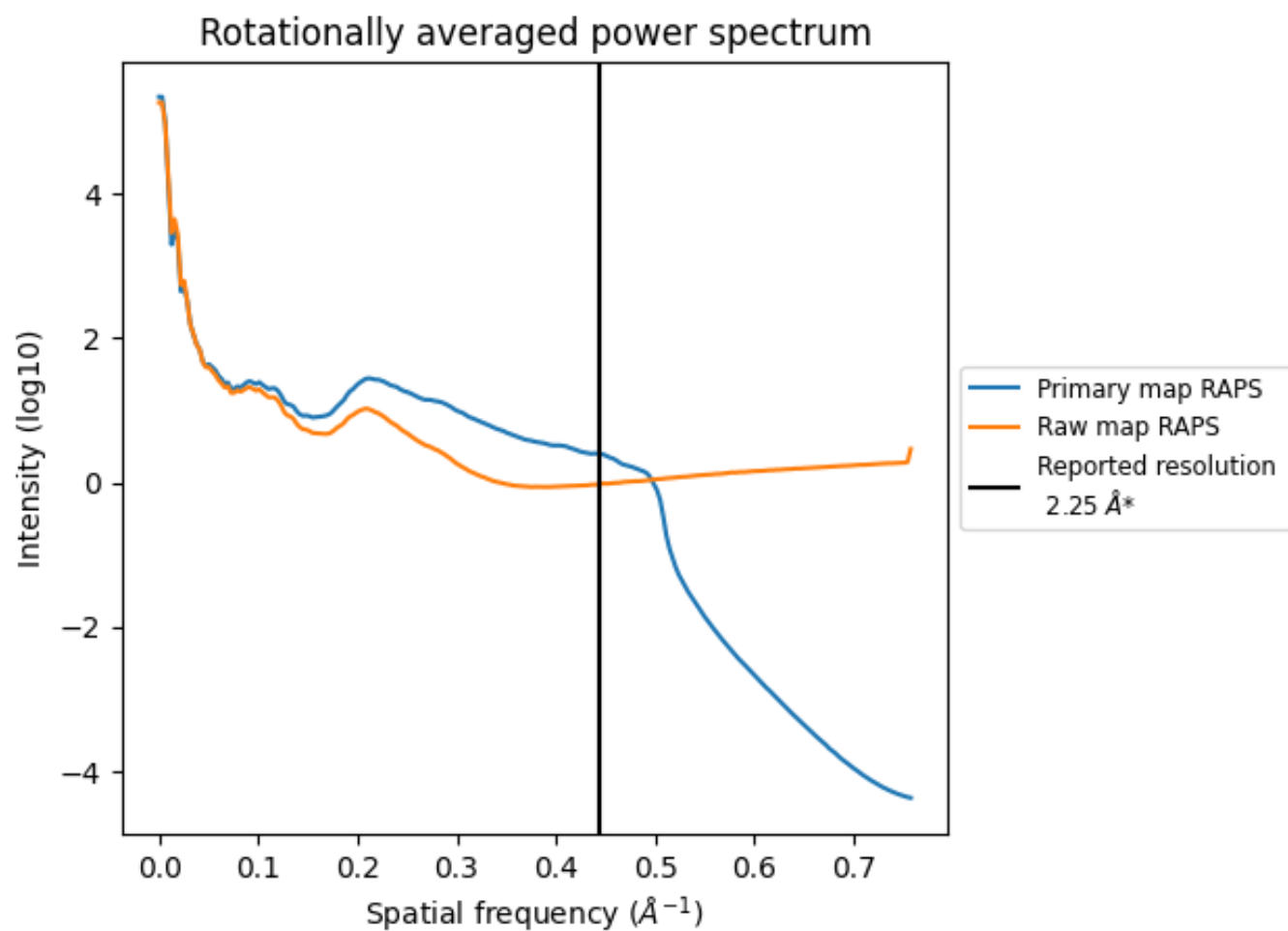
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

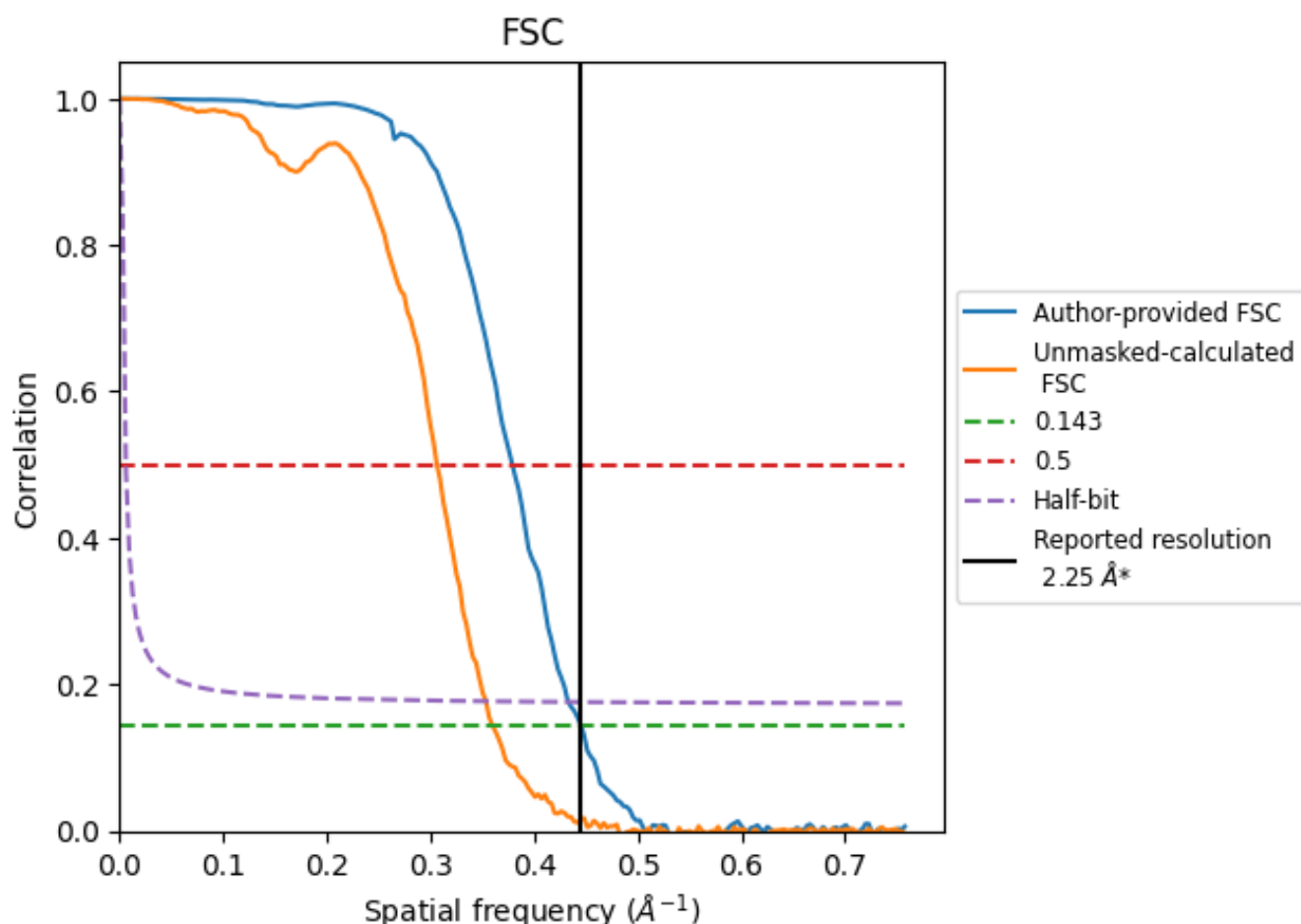


*Reported resolution corresponds to spatial frequency of 0.444 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

8.2 Resolution estimates [i](#)

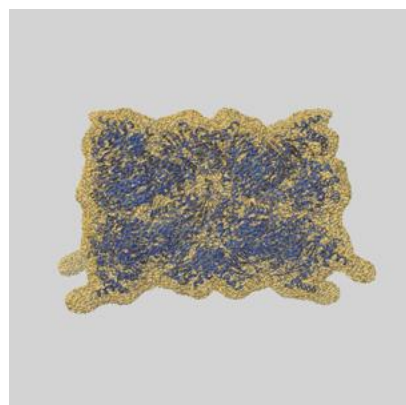
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.64	2.31
Unmasked-calculated*	2.78	3.27	2.83

*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 %

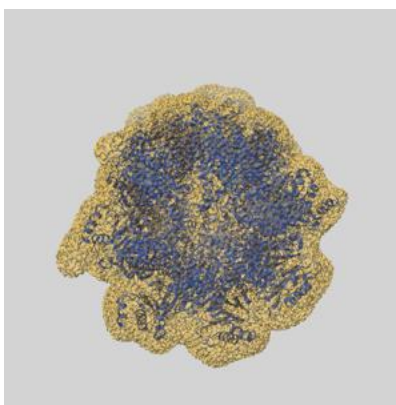
9 Map-model fit [i](#)

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](#).

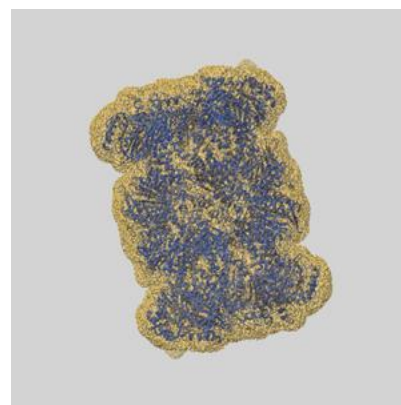
9.1 Map-model overlay [i](#)



X



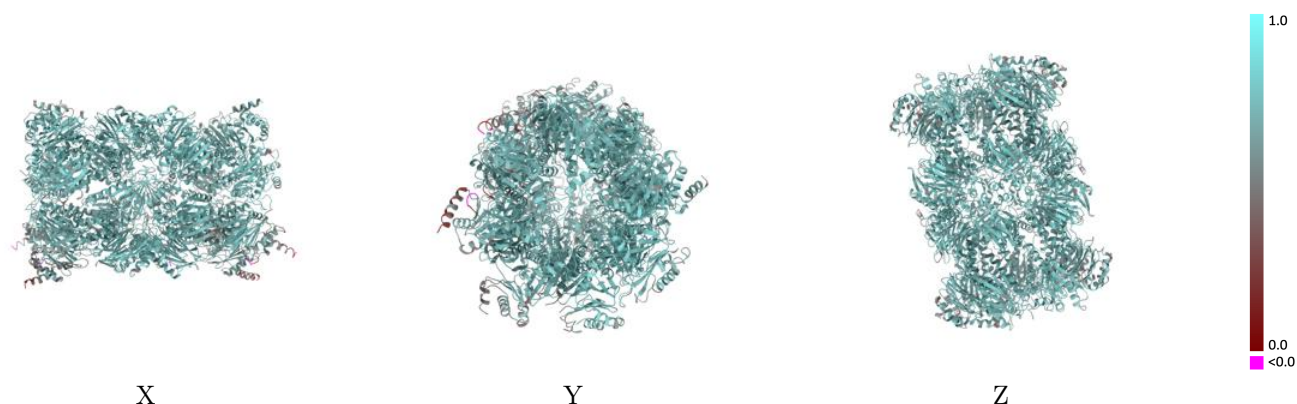
Y



Z

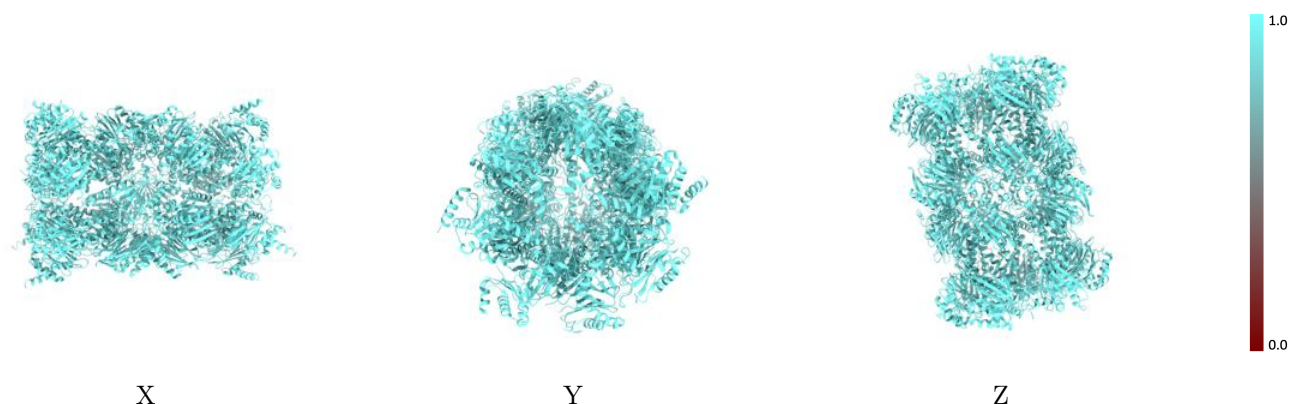
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



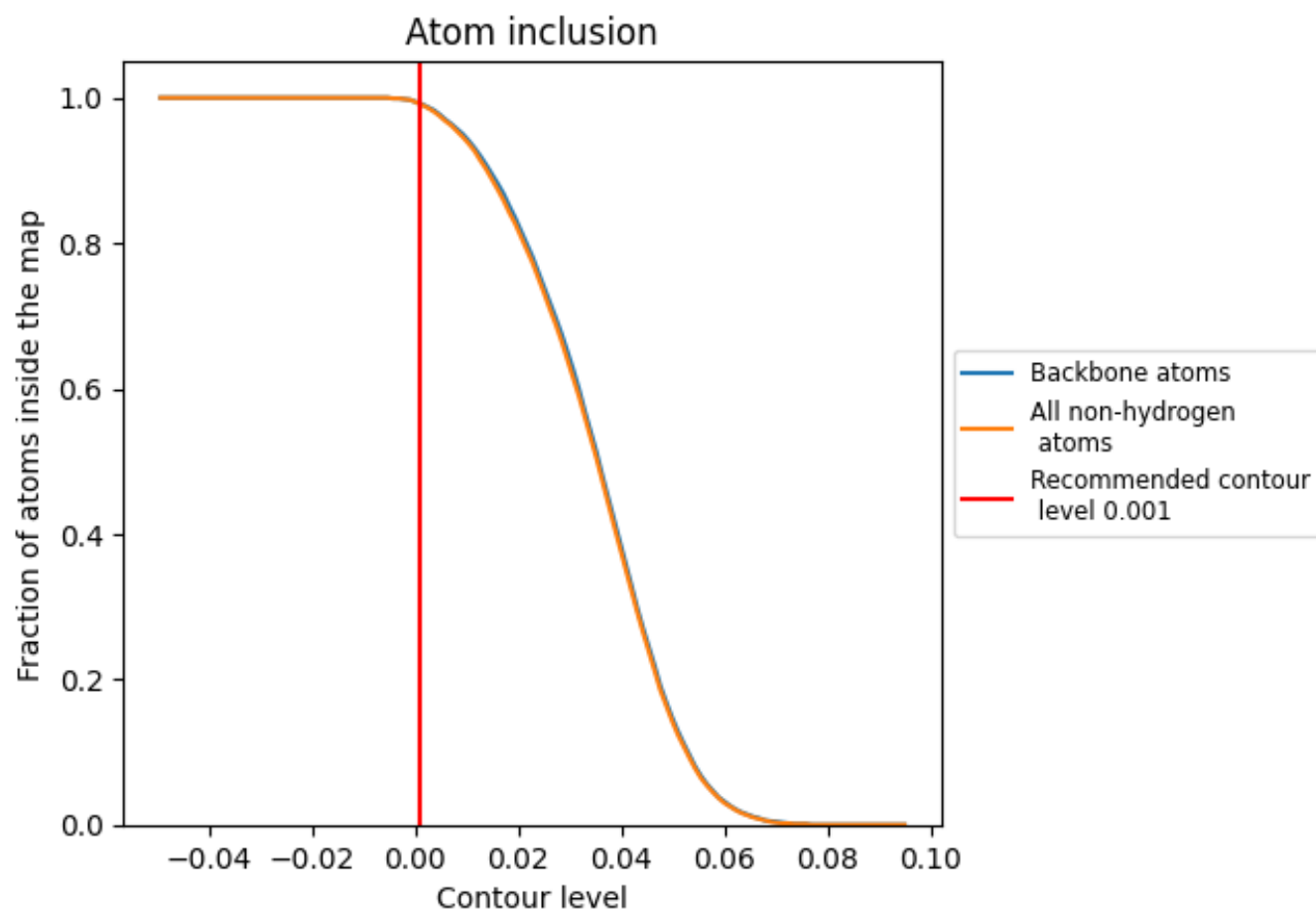
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.001).



























































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

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

