



wwPDB EM Validation Summary Report ⓘ

Apr 13, 2024 – 12:50 PM EDT

PDB ID : 8U7U
EMDB ID : EMD-41993
Title : Proteasome 20S Core Particle from Beta 3 D205 deletion
Authors : Walsh Jr., R.M.; Rawson, S.; Velez, B.; Blickling, M.; Razi, A.; Hanna, J.
Deposited on : 2023-09-15
Resolution : 2.16 Å (reported)
Based on initial model : 8T08

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:

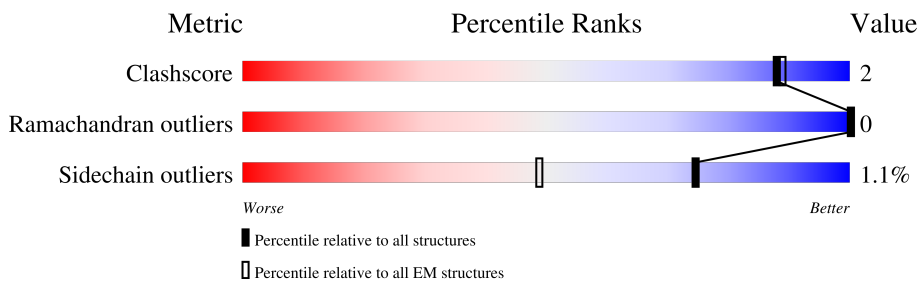
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

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 2.16 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	E	260	
1	S	260	
2	B	250	
2	P	250	
3	H	215	
3	V	215	
4	F	234	
4	T	234	

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Mol	Chain	Length	Quality of chain
5	1	241	85% 6% 9%
5	M	241	87% 9%
6	K	198	92% 6%
6	Y	198	91% 7%
7	G	288	82% 15%
7	U	288	81% 15%
8	2	266	82% 13%
8	N	266	82% 5% 13%
9	I	261	80% 16%
9	W	261	80% 16%
10	L	287	67% 5% 27%
10	Z	287	68% 5% 27%
11	C	258	87% 5% 7%
11	Q	258	88% 5% 7%
12	A	252	92% 5%
12	O	252	91% 5%
13	J	204	87% 7% 6%
13	X	204	88% 6% 6%
14	D	254	82% 6% 11%
14	R	254	83% 6% 11%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 97056 atoms, of which 48422 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-5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	E	237	Total	C	H	N	O	S	0	0
			3637	1147	1808	306	369	7		
1	S	237	Total	C	H	N	O	S	0	0
			3637	1147	1808	306	369	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	248	Total	C	H	N	O	S	0	0
			3811	1210	1911	313	374	3		
2	P	248	Total	C	H	N	O	S	0	0
			3811	1210	1911	313	374	3		

- Molecule 3 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	H	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		
3	V	196	Total	C	H	N	O	S	0	0
			2991	955	1479	250	300	7		

- Molecule 4 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	F	231	Total	C	H	N	O	S	0	0
			3550	1114	1777	307	348	4		
4	T	231	Total	C	H	N	O	S	0	0
			3550	1114	1777	307	348	4		

- Molecule 5 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	M	220	3436	1106	1697	300	329	4	0	0
5	1	220	3436	1106	1697	300	329	4	0	0

- Molecule 6 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	K	193	3098	979	1556	262	295	6	0	0
6	Y	193	3098	979	1556	262	295	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	244	3784	1205	1888	330	357	4	0	0
7	U	244	3784	1205	1888	330	357	4	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	N	231	3620	1144	1812	310	347	7	0	0
8	2	231	3620	1144	1812	310	347	7	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	220	3347	1054	1677	291	319	6	0	0
9	W	220	3347	1054	1677	291	319	6	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	L	210	3210	1037	1579	278	309	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	Z	210	3210	1037	1579	278	309	7	0	0

- Molecule 11 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	C	239	3756	1186	1881	315	371	3	0	0
11	Q	239	3756	1186	1881	315	371	3	0	0

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	A	239	3781	1203	1890	318	362	8	0	0
12	O	239	3781	1203	1890	318	362	8	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	J	192	2979	953	1490	245	284	7	0	0
13	X	192	2979	953	1490	245	284	7	0	0

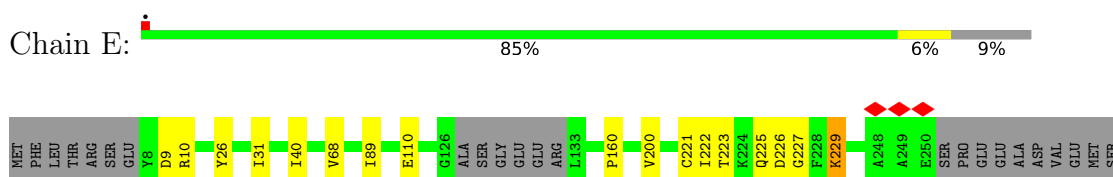
- Molecule 14 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	D	225	3528	1106	1766	303	349	4	0	0
14	R	225	3528	1106	1766	303	349	4	0	0

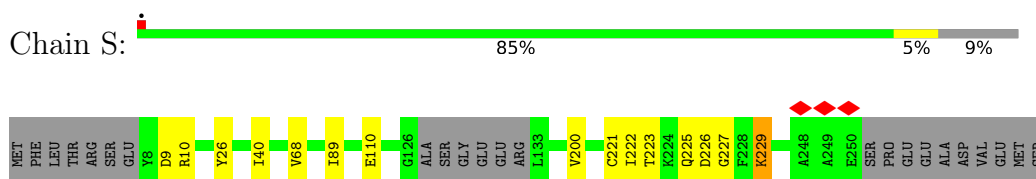
3 Residue-property plots [i](#)

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.

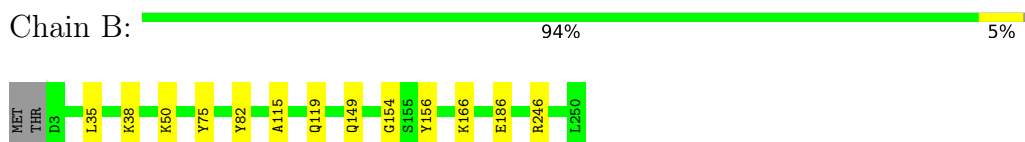
- Molecule 1: Proteasome subunit alpha type-5



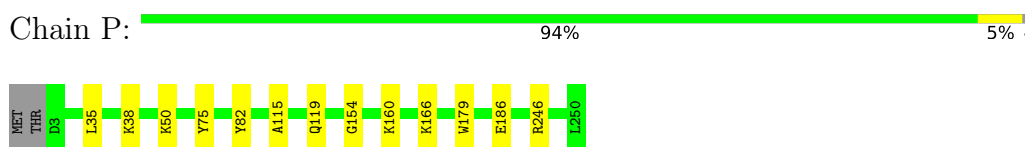
- Molecule 1: Proteasome subunit alpha type-5



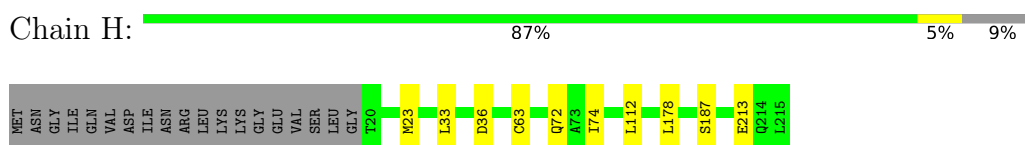
- Molecule 2: Proteasome subunit alpha type-2




- Molecule 2: Proteasome subunit alpha type-2



- Molecule 3: Proteasome subunit beta type-1



- Molecule 3: Proteasome subunit beta type-1

Chain V:  87% 5% 9%



- Molecule 4: Proteasome subunit alpha type-6

Chain F:  91% 7%




- Molecule 4: Proteasome subunit alpha type-6

Chain T:  92% 6%




- Molecule 5: Proteasome subunit beta type-6

Chain M:  87% 9%



- Molecule 5: Proteasome subunit beta type-6

Chain 1:  85% 6% 9%



- Molecule 6: Proteasome subunit beta type-4

Chain K:  92% 6%

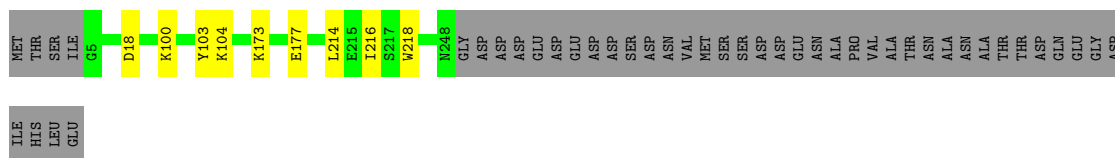
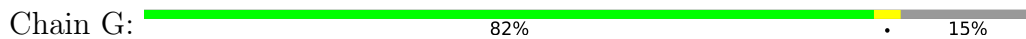


- Molecule 6: Proteasome subunit beta type-4

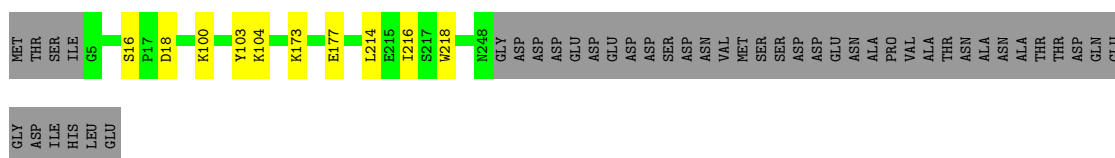
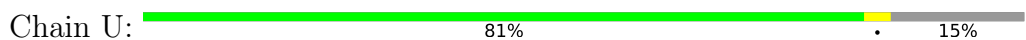
Chain Y:  91% 7%



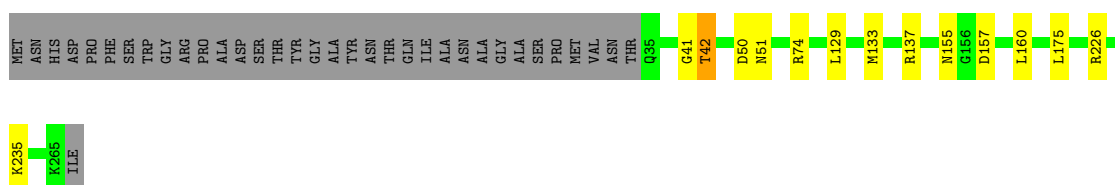
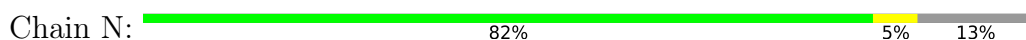
- Molecule 7: Proteasome subunit alpha type-7



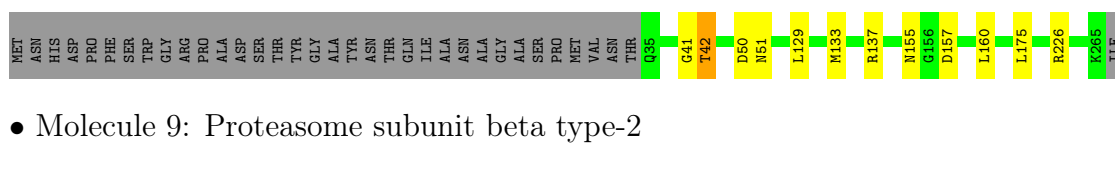
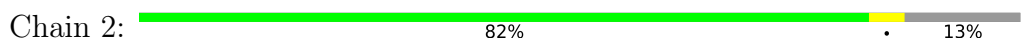
• Molecule 7: Proteasome subunit alpha type-7



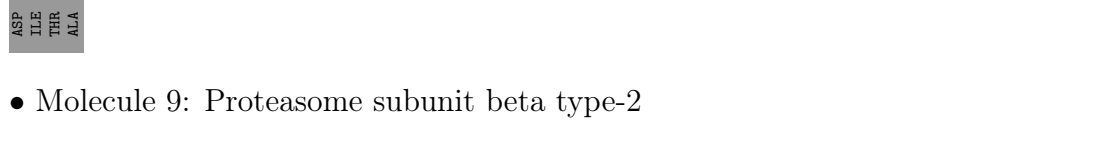
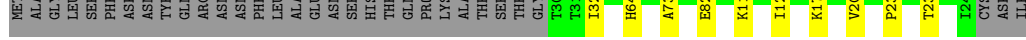
• Molecule 8: Proteasome subunit beta type-7



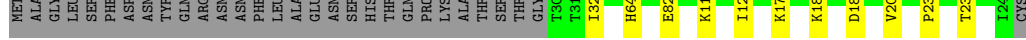
• Molecule 8: Proteasome subunit beta type-7



• Molecule 9: Proteasome subunit beta type-2



• Molecule 9: Proteasome subunit beta type-2



GLN
VAL
ASP
ILE
THR
ALA

• Molecule 10: Proteasome subunit beta type-5



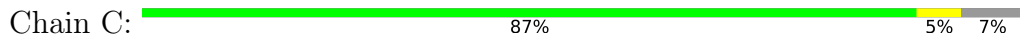
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SER ILE ARG ASP THR ALA
ASP ALA ASP ASP THR ALA
SER ASP ASP THR ALA
PHE PHE SER LYS
SER SER ILE VAL
VAL VAL PRO PRO
PRO PRO LYS LYS
ASN ASN ARG ARG
LEU LEU VAL VAL
GLY T76
LYS Q84
LEU Q84
GLU Q84
LEU Q84
GLN Q84
TYR D92
ASP D92
ASN A95
GLU A95
ASN A95
GLN V106
ASN V106
LEU M120
GLU M120
SER G123
SER G123
ASP A124
ASP A124
PHE S150
VAL S150
THR V151
GLY V151
ALA A152
SER S171
GLN S171
PHE Y179
GLN Y179
ARG T180
LEU R181
ALA D191
PRO S192
PRO S192
SER L223
LEU L223
THR E270
VAL E270
PRO N284
PRO N284
ILE V285
ALA V285
SER ILE
PRO SER
GLN PRO
GLN GLN
PHE PHE
LEU LEU
ARG ARG
HIS HIS
THR THR

• Molecule 10: Proteasome subunit beta type-5



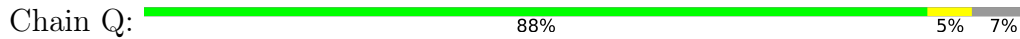
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SER ILE ARG ASP THR ALA
ASP ALA ASP ASP THR ALA
SER ASP ASP THR ALA
PHE PHE SER LYS
SER SER ILE VAL
VAL VAL PRO PRO
PRO PRO LYS LYS
ASN ASN ARG ARG
LEU LEU VAL VAL
GLY T76
LYS Q84
LEU Q84
GLU Q84
LEU Q84
GLN Q84
TYR D92
ASP D92
ASN A95
GLU A95
ASN A95
GLN V106
ASN V106
LEU M120
GLU M120
SER G123
SER G123
ASP A124
ASP A124
PHE S150
VAL S150
THR V171
GLY V171
ALA S171
SER Y179
GLN Y179
PHE R181
GLN R181
ARG D191
LEU S192
PRO S192
SER L223
LEU L223
THR E270
VAL E270
PRO N284
PRO N284
ILE V285
ALA V285
SER ILE
PRO SER
GLN PRO
GLN GLN
PHE PHE
LEU LEU
ARG ARG
HIS HIS
THR THR

• Molecule 11: Proteasome subunit alpha type-3



MET G2
SER G2
GLY E58
ALA E58
ALA E64
ALA E64
SER D83
SER D83
SER E109
SER E109
SER Q120
SER Q120
SER L148
SER L148
SER M152
SER M152
SER P153
SER P153
SER I163
SER I163
SER G166
SER G166
SER T169
SER T169
SER D183
SER D183
SER D209
SER D209
SER K218
SER K218
SER ALA
SER ASN
SER ASP
SER GLY
SER E224
SER E224
SER T242
SER T242
SER T245
SER T245
LYS LYS
ASP LYS
GLU LYS
ASP ASP
GLU ASP
GLU ASP
GLU ASP
ALA ASP
ALA ASP
ASP ASP
MET MET
LYS LYS

• Molecule 11: Proteasome subunit alpha type-3



MET G2
SER G2
GLY E58
ALA E58
ALA E64
ALA E64
SER D83
SER D83
SER E109
SER E109
SER Q120
SER Q120
SER L148
SER L148
SER M152
SER M152
SER P153
SER P153
SER I163
SER I163
SER G166
SER G166
SER T169
SER T169
SER D183
SER D183
SER K218
SER K218
SER ALA
SER ASN
SER ASP
SER GLY
SER E224
SER E224
SER T242
SER T242
SER T245
SER T245
LYS LYS
ASP LYS
GLU LYS
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ALA ASP
ASP ASP
MET MET
LYS LYS

• Molecule 12: Proteasome subunit alpha type-1



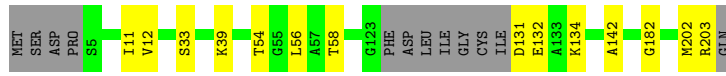
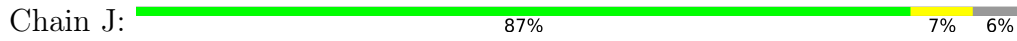
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SER GLY
GLY ALA
ALA ALA
ALA ALA
SER ALA
SER ALA
SER ALA
SER ALA
SER ALA
SER ALA
TYR TYR
D13 D13
R14 R14
V83 V83
A90 A90
S125 S125
T129 T129
M181 M181
K188 K188
S189 S189
K190 K190
I191 I191
H209 H209
S219 S219
Q251 Q251
ASP ASP

• Molecule 12: Proteasome subunit alpha type-1

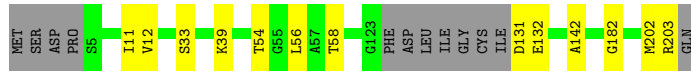
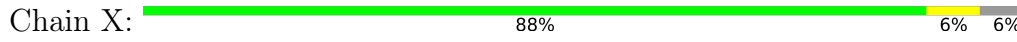


MET SER
SER GLY
GLY ALA
ALA ALA
ALA ALA
SER ALA
SER ALA
SER ALA
SER ALA
SER ALA
SER ALA
TYR TYR
D13 D13
R14 R14
V83 V83
A90 A90
S125 S125
T129 T129
M181 M181
K188 K188
S189 S189
K190 K190
I191 I191
D192 D192
H193 H193
H209 H209
S219 S219
Q251 Q251
ASP ASP

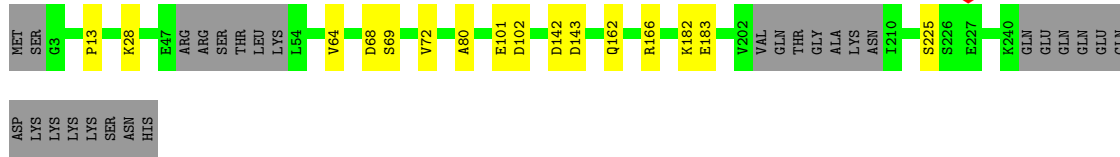
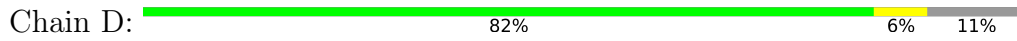
• Molecule 13: Proteasome subunit beta type-3



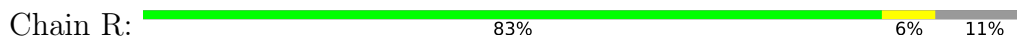
• Molecule 13: Proteasome subunit beta type-3



• Molecule 14: Proteasome subunit alpha type-4



• Molecule 14: Proteasome subunit alpha type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	240235	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 ($e^-/\text{\AA}^2$)	57.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47169	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.360	Depositor
Minimum map value	-2.318	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.34	Depositor
Map size (Å)	375.24, 375.24, 375.24	wwPDB
Map dimensions	354, 354, 354	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.36	0/1854	0.54	0/2498
1	S	0.37	0/1854	0.54	0/2498
2	B	0.46	0/1937	0.56	0/2622
2	P	0.46	0/1937	0.56	0/2622
3	H	0.50	0/1541	0.55	0/2087
3	V	0.50	0/1541	0.55	0/2087
4	F	0.41	0/1800	0.57	0/2433
4	T	0.41	0/1800	0.57	0/2433
5	1	0.43	0/1777	0.56	0/2397
5	M	0.43	0/1777	0.57	0/2397
6	K	0.40	0/1569	0.57	0/2115
6	Y	0.40	0/1569	0.57	0/2115
7	G	0.48	0/1936	0.56	0/2614
7	U	0.48	0/1936	0.56	0/2614
8	2	0.48	0/1839	0.61	0/2493
8	N	0.48	0/1839	0.61	0/2493
9	I	0.44	0/1701	0.57	0/2307
9	W	0.44	0/1701	0.57	0/2307
10	L	0.39	0/1668	0.58	0/2258
10	Z	0.39	0/1668	0.58	0/2258
11	C	0.43	0/1904	0.57	0/2576
11	Q	0.43	0/1904	0.57	0/2576
12	A	0.48	0/1928	0.55	0/2611
12	O	0.48	0/1928	0.55	0/2611
13	J	0.46	0/1516	0.55	0/2044
13	X	0.46	0/1516	0.56	0/2044
14	D	0.44	0/1789	0.57	0/2422
14	R	0.44	0/1789	0.57	0/2422
All	All	0.44	0/49518	0.57	0/66954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1829	1808	1806	10	0
1	S	1829	1808	1806	9	0
2	B	1900	1911	1910	7	0
2	P	1900	1911	1910	7	0
3	H	1512	1479	1478	5	0
3	V	1512	1479	1478	5	0
4	F	1773	1777	1775	9	0
4	T	1773	1777	1775	8	0
5	1	1739	1697	1696	9	0
5	M	1739	1697	1696	7	0
6	K	1542	1556	1556	6	0
6	Y	1542	1556	1556	7	0
7	G	1896	1888	1886	5	0
7	U	1896	1888	1886	6	0
8	2	1808	1812	1811	6	0
8	N	1808	1812	1811	8	0
9	I	1670	1677	1676	6	0
9	W	1670	1677	1676	6	0
10	L	1631	1579	1578	8	0
10	Z	1631	1579	1578	7	0
11	C	1875	1881	1879	8	0
11	Q	1875	1881	1879	7	0
12	A	1891	1890	1889	4	0
12	O	1891	1890	1889	4	0
13	J	1489	1490	1488	8	0
13	X	1489	1490	1488	7	0
14	D	1762	1766	1763	9	0
14	R	1762	1766	1763	8	0
All	All	48634	48422	48382	179	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 179 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)
10:L:284:ASN:O	13:X:39:LYS:NZ	2.17	0.77
13:J:39:LYS:NZ	10:Z:284:ASN:O	2.19	0.75
10:Z:84:GLN:NE2	10:Z:223:LEU:O	2.21	0.73
13:J:203:ARG:NH1	10:Z:270:GLU:OE1	2.24	0.71
13:X:11:ILE:HG21	13:X:142:ALA:HB3	1.72	0.70

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	E	233/260 (90%)	231 (99%)	2 (1%)	0	100	100
1	S	233/260 (90%)	231 (99%)	2 (1%)	0	100	100
2	B	246/250 (98%)	240 (98%)	6 (2%)	0	100	100
2	P	246/250 (98%)	240 (98%)	6 (2%)	0	100	100
3	H	194/215 (90%)	193 (100%)	1 (0%)	0	100	100
3	V	194/215 (90%)	193 (100%)	1 (0%)	0	100	100
4	F	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
4	T	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	1	218/241 (90%)	215 (99%)	3 (1%)	0	100	100
5	M	218/241 (90%)	215 (99%)	3 (1%)	0	100	100
6	K	191/198 (96%)	188 (98%)	3 (2%)	0	100	100
6	Y	191/198 (96%)	188 (98%)	3 (2%)	0	100	100
7	G	242/288 (84%)	240 (99%)	2 (1%)	0	100	100
7	U	242/288 (84%)	240 (99%)	2 (1%)	0	100	100
8	2	229/266 (86%)	223 (97%)	6 (3%)	0	100	100
8	N	229/266 (86%)	223 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	218/261 (84%)	215 (99%)	3 (1%)	0	100	100
9	W	218/261 (84%)	215 (99%)	3 (1%)	0	100	100
10	L	208/287 (72%)	204 (98%)	4 (2%)	0	100	100
10	Z	208/287 (72%)	204 (98%)	4 (2%)	0	100	100
11	C	235/258 (91%)	232 (99%)	3 (1%)	0	100	100
11	Q	235/258 (91%)	232 (99%)	3 (1%)	0	100	100
12	A	237/252 (94%)	235 (99%)	2 (1%)	0	100	100
12	O	237/252 (94%)	235 (99%)	2 (1%)	0	100	100
13	J	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
13	X	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
14	D	219/254 (86%)	216 (99%)	3 (1%)	0	100	100
14	R	219/254 (86%)	216 (99%)	3 (1%)	0	100	100
All	All	6174/6936 (89%)	6076 (98%)	98 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	E	195/215 (91%)	192 (98%)	3 (2%)	65	69
1	S	195/215 (91%)	192 (98%)	3 (2%)	65	69
2	B	207/209 (99%)	205 (99%)	2 (1%)	76	81
2	P	207/209 (99%)	205 (99%)	2 (1%)	76	81
3	H	162/178 (91%)	160 (99%)	2 (1%)	71	76
3	V	162/178 (91%)	160 (99%)	2 (1%)	71	76
4	F	190/193 (98%)	188 (99%)	2 (1%)	73	78
4	T	190/193 (98%)	188 (99%)	2 (1%)	73	78
5	1	183/201 (91%)	181 (99%)	2 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	M	183/201 (91%)	181 (99%)	2 (1%)	73	78
6	K	171/175 (98%)	170 (99%)	1 (1%)	86	90
6	Y	171/175 (98%)	170 (99%)	1 (1%)	86	90
7	G	201/239 (84%)	200 (100%)	1 (0%)	88	92
7	U	201/239 (84%)	200 (100%)	1 (0%)	88	92
8	2	197/224 (88%)	195 (99%)	2 (1%)	76	81
8	N	197/224 (88%)	195 (99%)	2 (1%)	76	81
9	I	179/214 (84%)	179 (100%)	0	100	100
9	W	179/214 (84%)	179 (100%)	0	100	100
10	L	168/235 (72%)	162 (96%)	6 (4%)	35	33
10	Z	168/235 (72%)	162 (96%)	6 (4%)	35	33
11	C	201/216 (93%)	198 (98%)	3 (2%)	65	69
11	Q	201/216 (93%)	198 (98%)	3 (2%)	65	69
12	A	205/210 (98%)	203 (99%)	2 (1%)	76	81
12	O	205/210 (98%)	203 (99%)	2 (1%)	76	81
13	J	161/172 (94%)	160 (99%)	1 (1%)	86	90
13	X	161/172 (94%)	160 (99%)	1 (1%)	86	90
14	D	199/226 (88%)	196 (98%)	3 (2%)	65	69
14	R	199/226 (88%)	196 (98%)	3 (2%)	65	69
All	All	5238/5814 (90%)	5178 (99%)	60 (1%)	74	78

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	D	182	LYS
12	O	219	SER
3	V	36	ASP
12	O	14	ARG
14	R	225	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	190	HIS

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Mol	Chain	Res	Type
6	Y	10	GLN
9	W	95	HIS
8	2	135	GLN
9	I	95	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

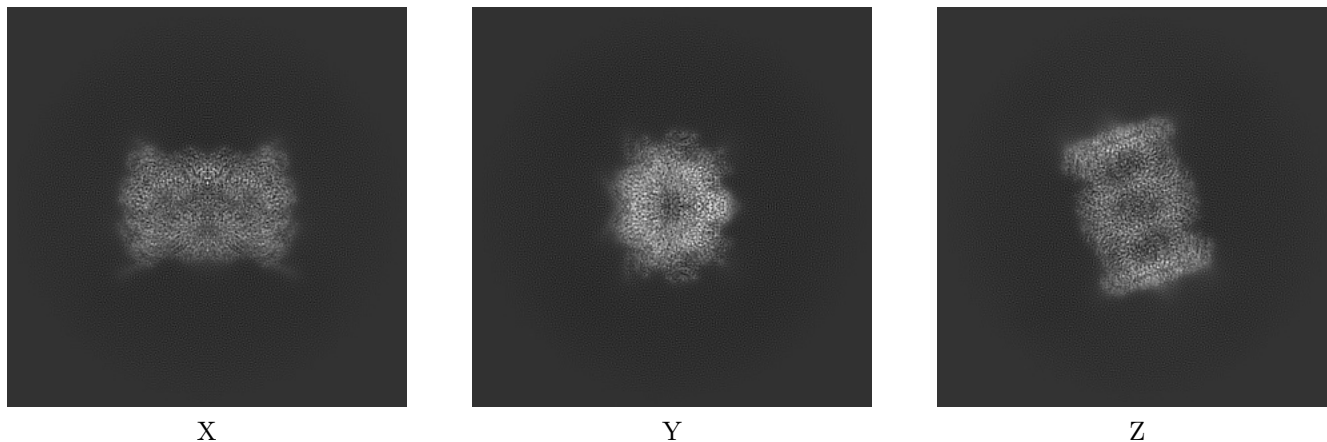
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41993. These allow visual inspection of the internal detail of the map and identification of artifacts.

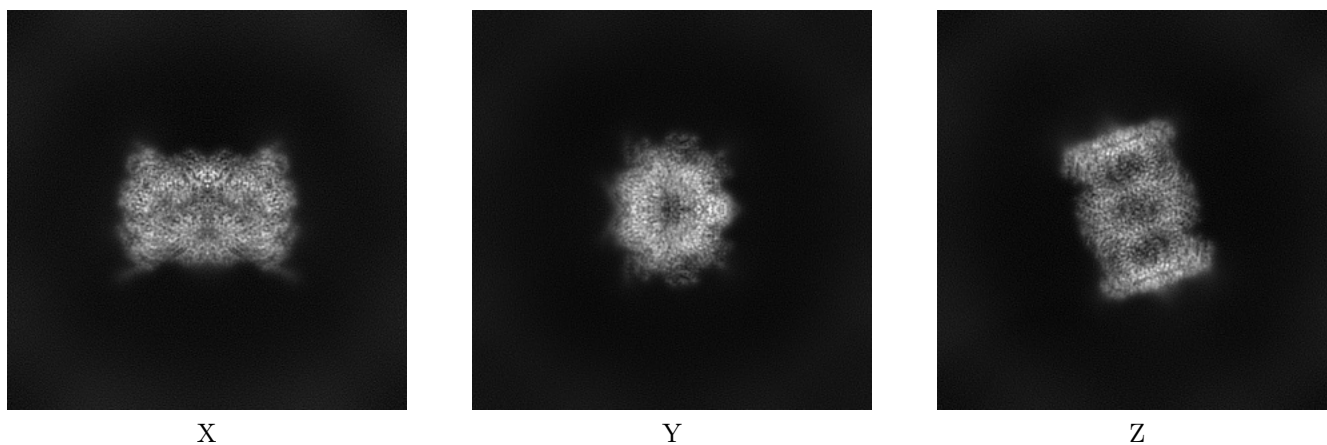
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



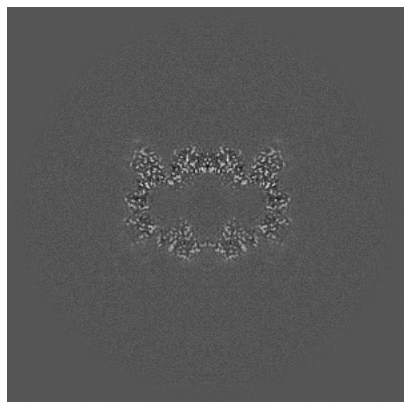
6.1.2 Raw map



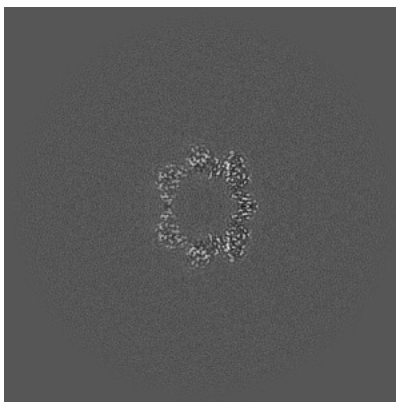
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

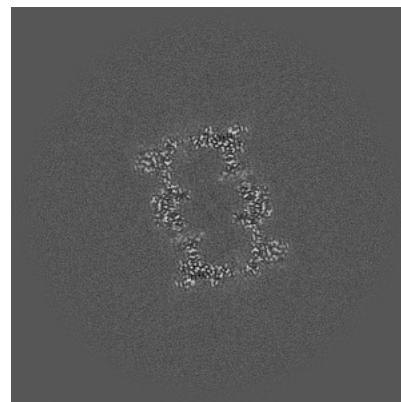
6.2.1 Primary map



X Index: 177

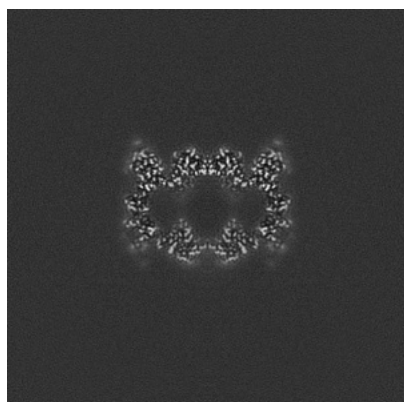


Y Index: 177

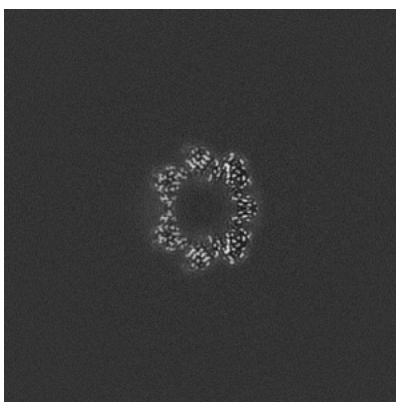


Z Index: 177

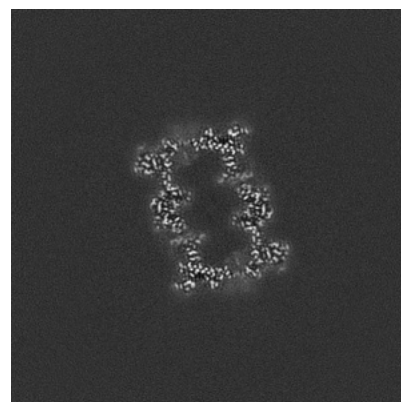
6.2.2 Raw map



X Index: 177



Y Index: 177

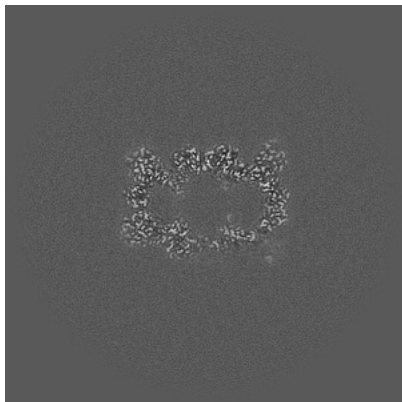


Z Index: 177

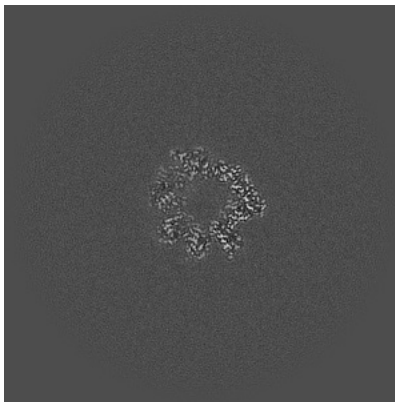
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

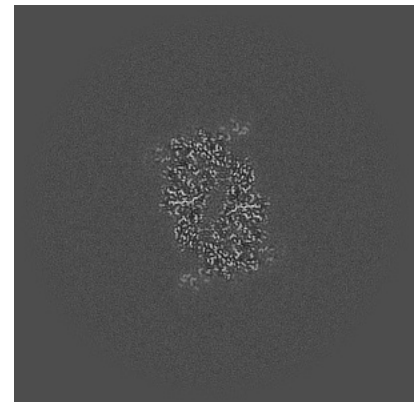
6.3.1 Primary map



X Index: 173

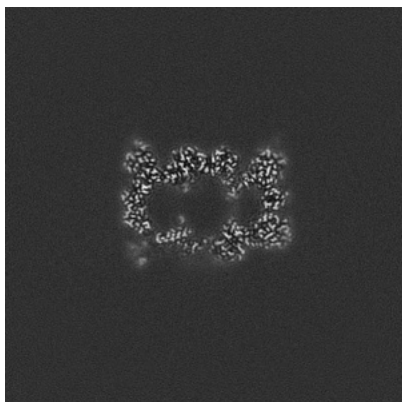


Y Index: 192

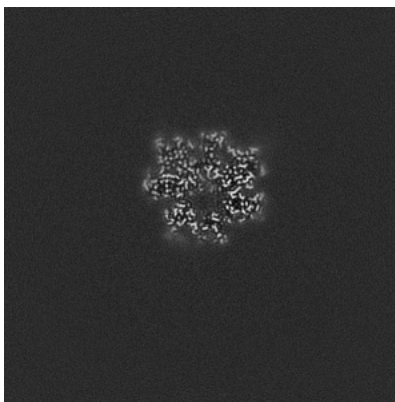


Z Index: 202

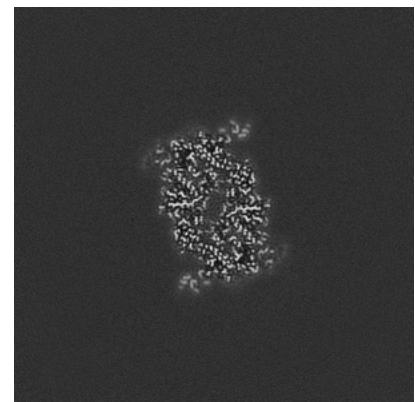
6.3.2 Raw map



X Index: 181



Y Index: 128

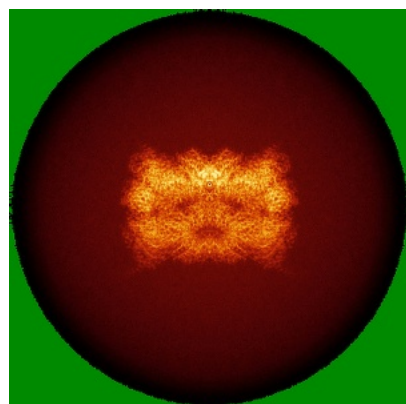


Z Index: 202

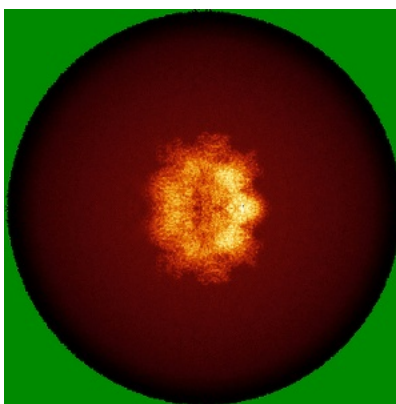
The images above show the largest variance slices of the map in three orthogonal directions.

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

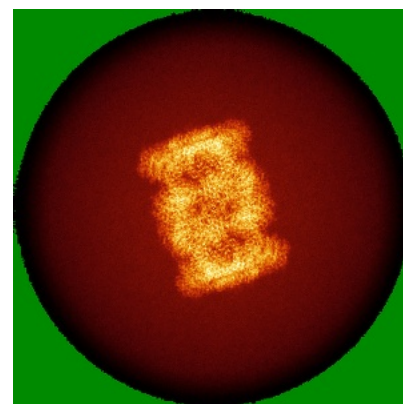
6.4.1 Primary map



X

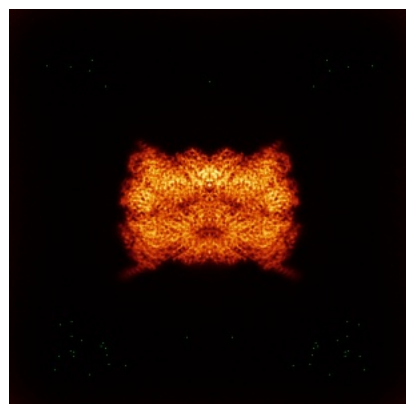


Y

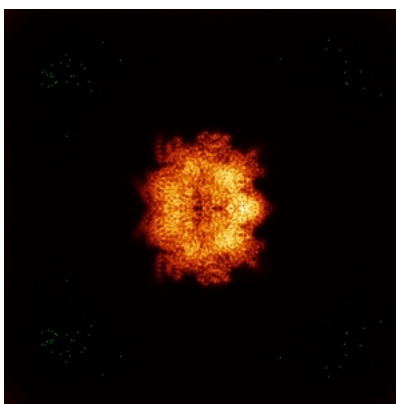


Z

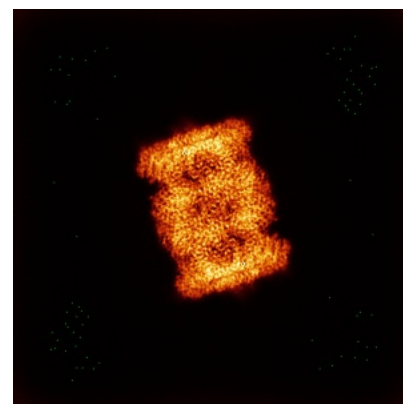
6.4.2 Raw map



X



Y

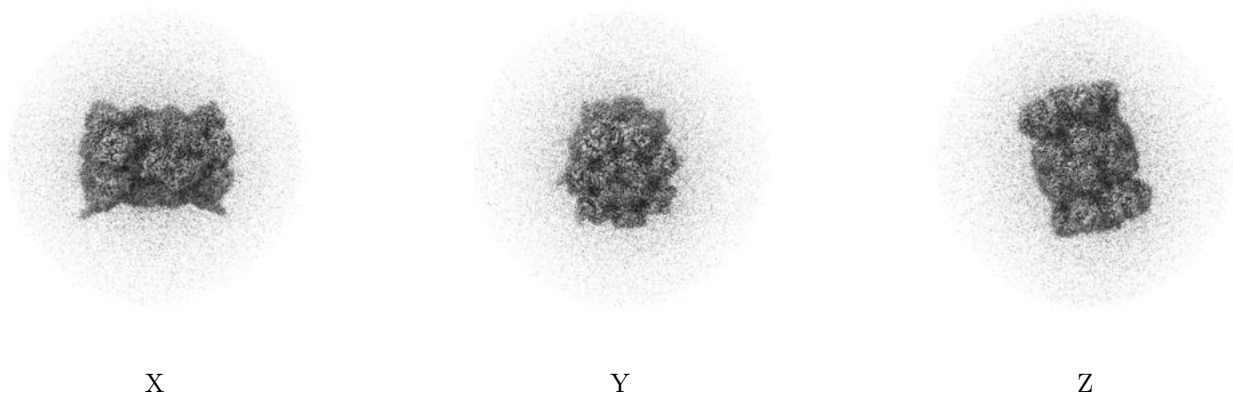


Z

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.

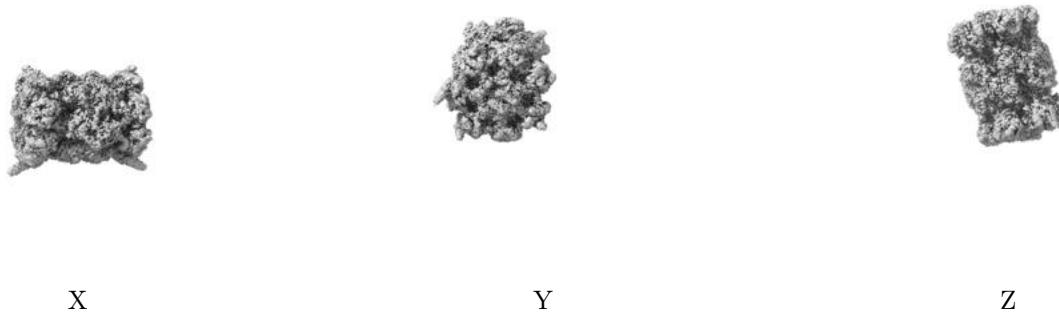
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.34. 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.

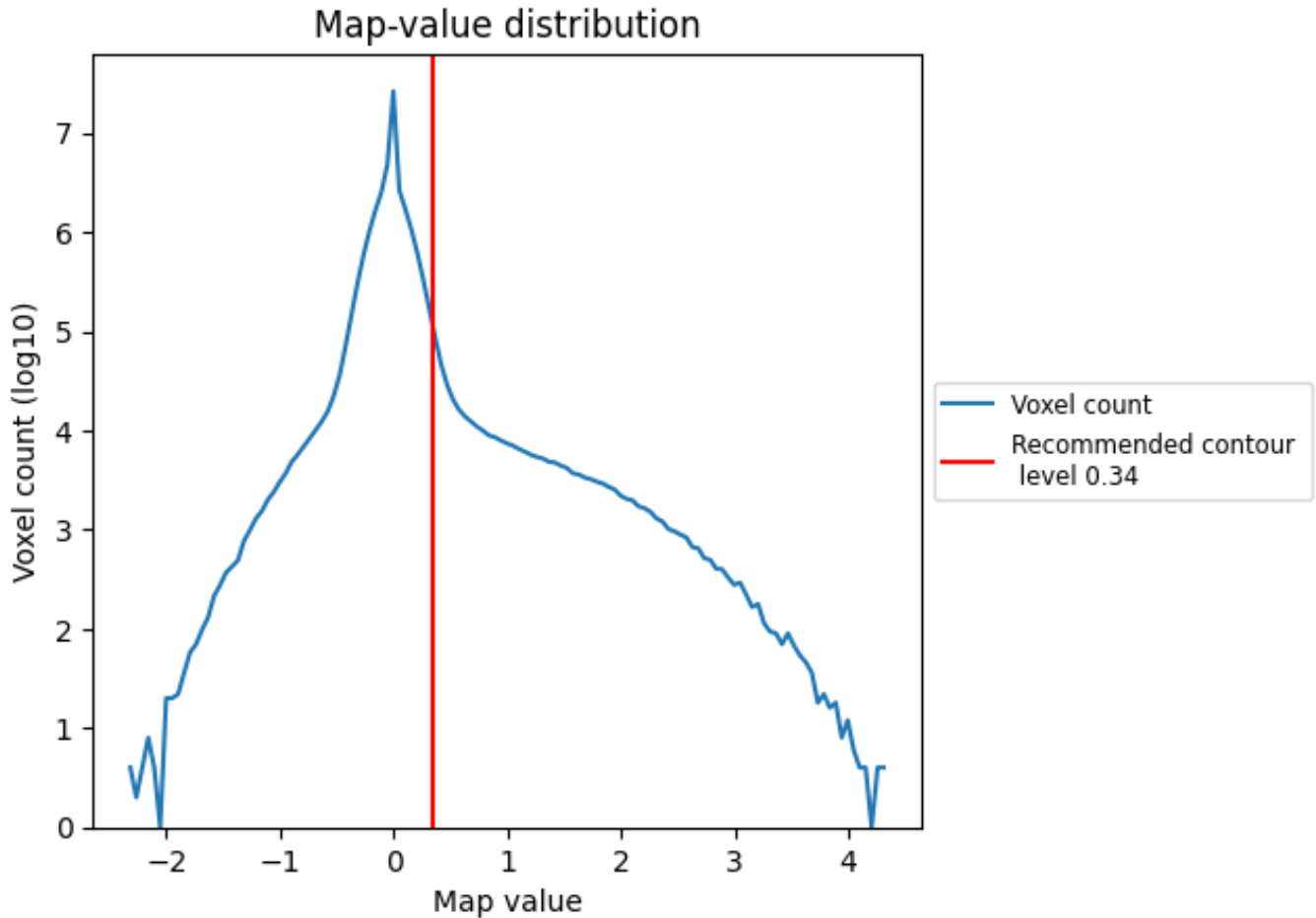
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

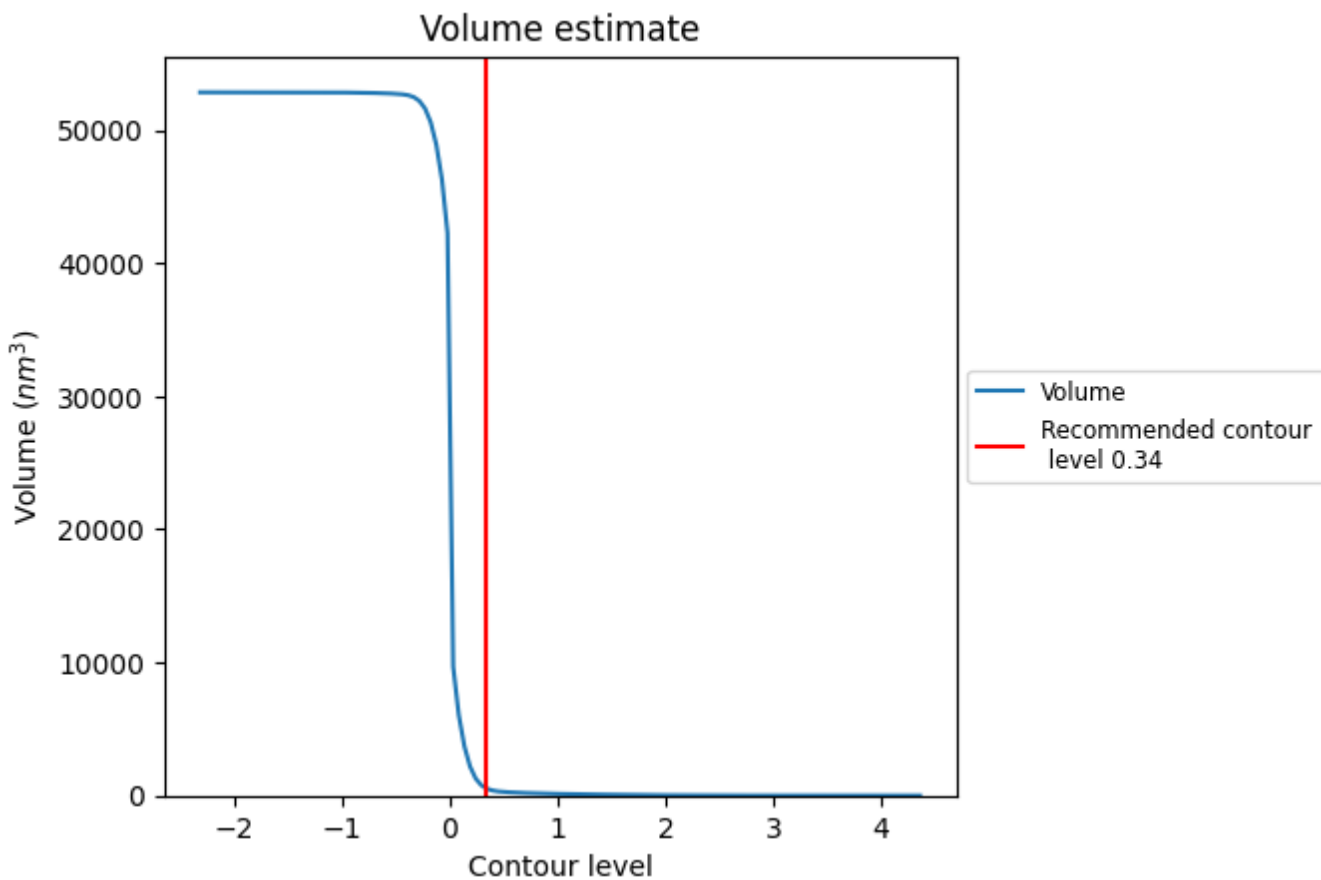
This section contains the results of statistical analysis of the map.

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.

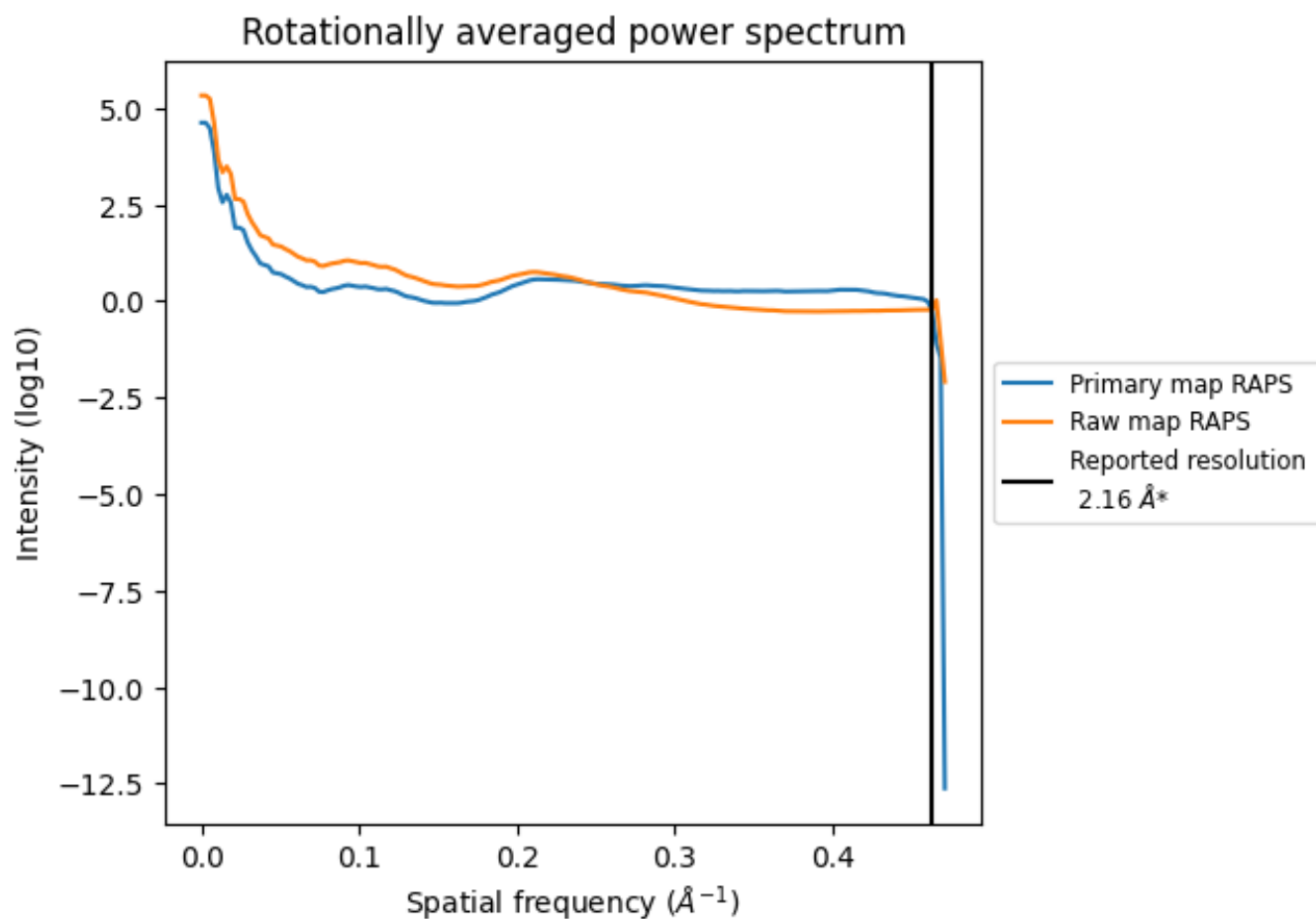
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 531 nm³; this corresponds to an approximate mass of 479 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

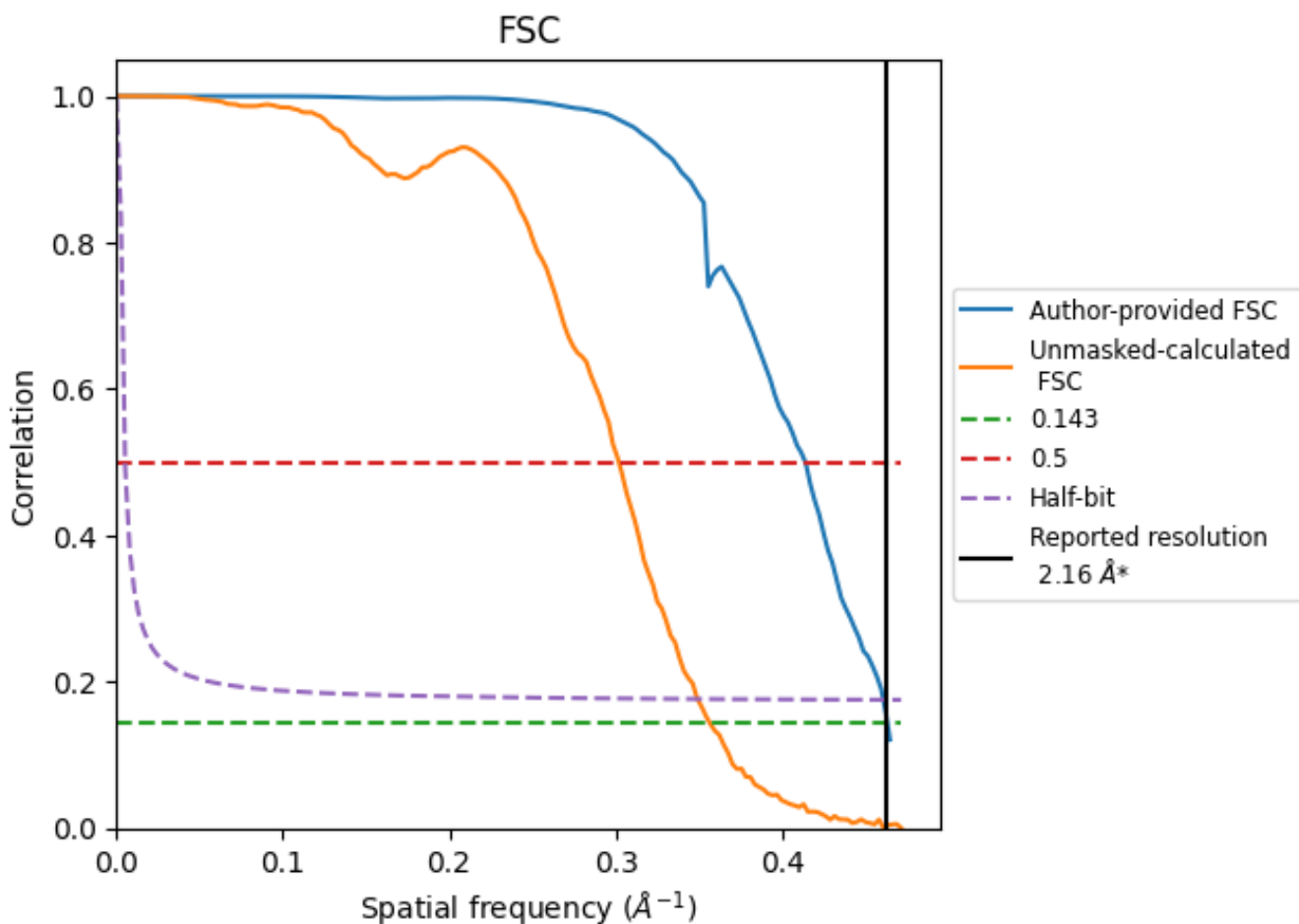


*Reported resolution corresponds to spatial frequency of 0.463 Å⁻¹

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 0.463 Å⁻¹

8.2 Resolution estimates [i](#)

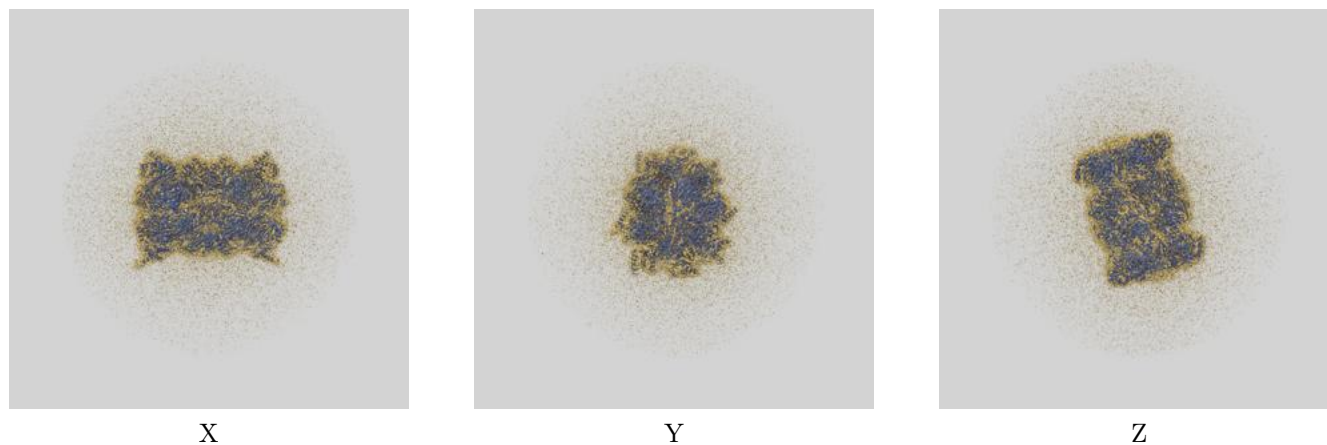
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.16	-	-
Author-provided FSC curve	2.16	2.41	2.17
Unmasked-calculated*	2.80	3.31	2.86

*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 2.80 differs from the reported value 2.16 by more than 10 %

9 Map-model fit [i](#)

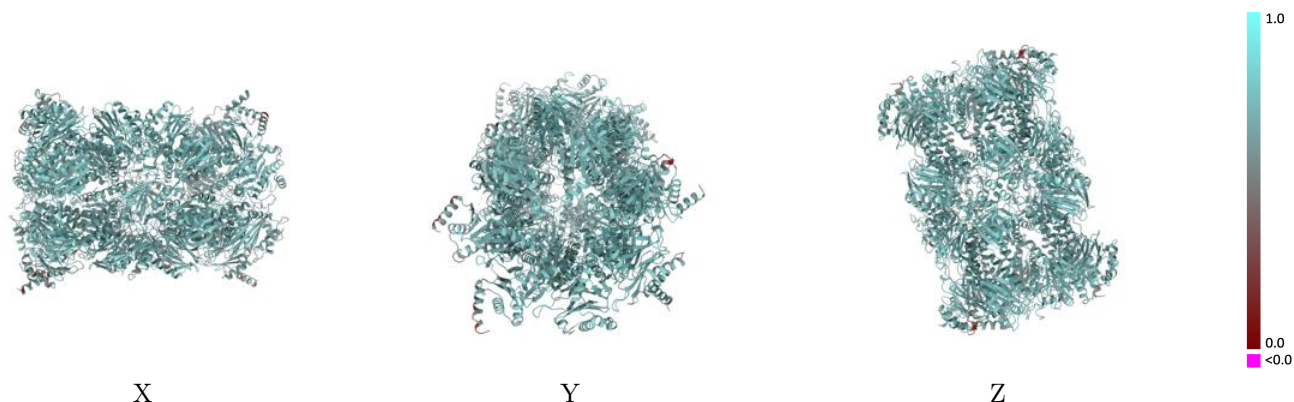
This section contains information regarding the fit between EMDB map EMD-41993 and PDB model 8U7U. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



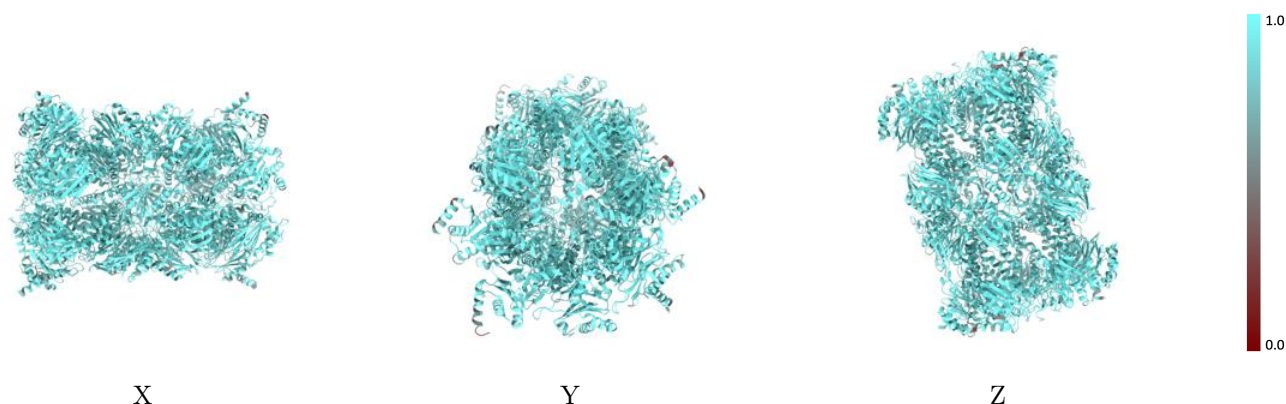
The images above show the 3D surface view of the map at the recommended contour level 0.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



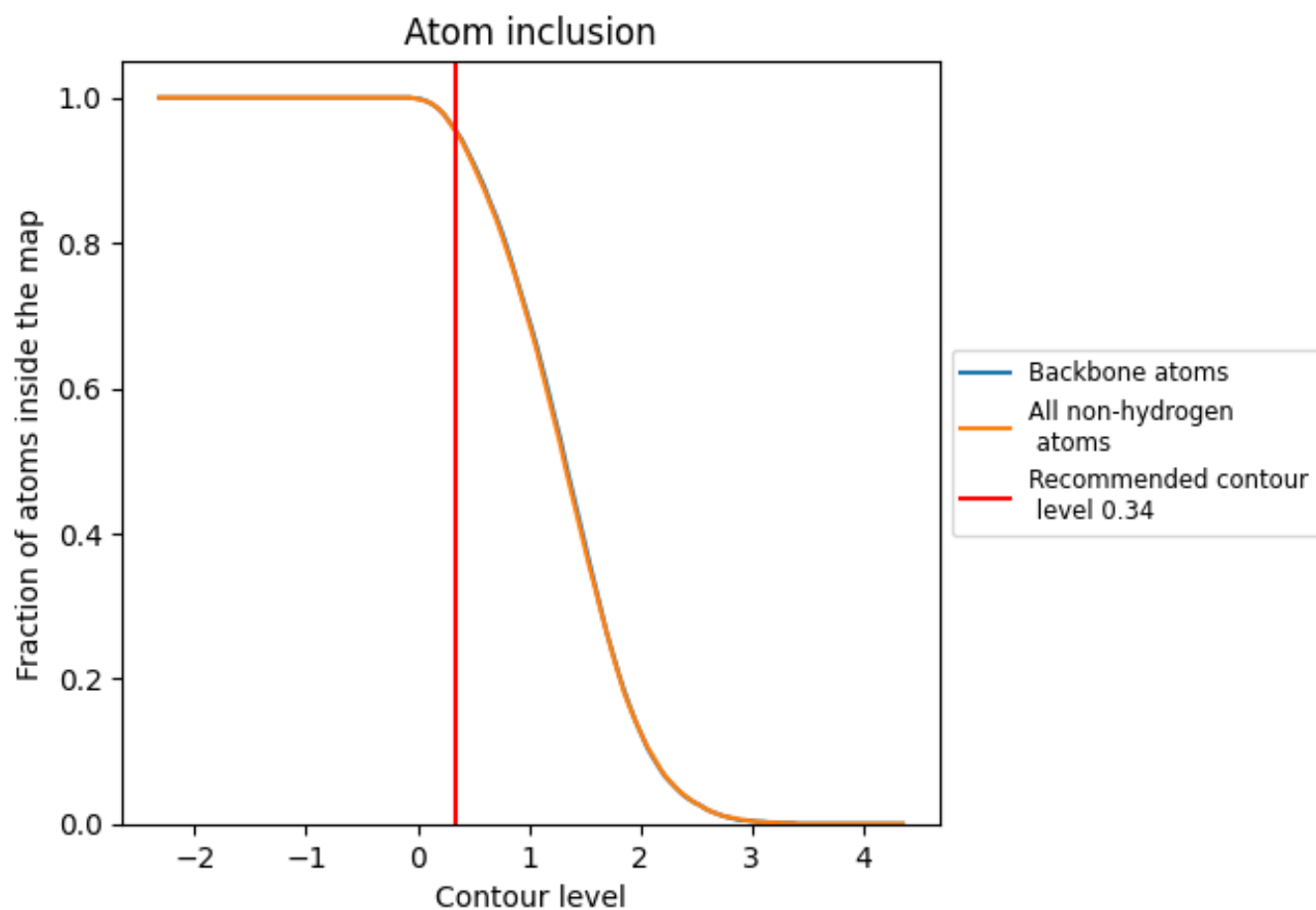
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.34).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9540	 0.6880
1	 0.9550	 0.6890
2	 0.9800	 0.7210
A	 0.9470	 0.6810
B	 0.9530	 0.6840
C	 0.9440	 0.6700
D	 0.9370	 0.6630
E	 0.9210	 0.6540
F	 0.9650	 0.6910
G	 0.9500	 0.6870
H	 0.9760	 0.7170
I	 0.9780	 0.7040
J	 0.9520	 0.6880
K	 0.9580	 0.6980
L	 0.9540	 0.6810
M	 0.9550	 0.6900
N	 0.9800	 0.7230
O	 0.9460	 0.6820
P	 0.9530	 0.6840
Q	 0.9440	 0.6700
R	 0.9350	 0.6640
S	 0.9200	 0.6550
T	 0.9650	 0.6920
U	 0.9500	 0.6880
V	 0.9760	 0.7180
W	 0.9780	 0.7050
X	 0.9520	 0.6900
Y	 0.9580	 0.6980
Z	 0.9540	 0.6800

