



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 07:20 pm GMT

PDB ID : 8QYM
EMDB ID : EMD-18758
Title : Human 20S proteasome assembly intermediate structure 3
Authors : Schulman, B.A.; Hanna, J.W.; Harper, J.W.; Adolf, F.; Du, J.; Rawson, S.D.;
Walsh Jr, R.M.; Goodall, E.A.
Deposited on : 2023-10-26
Resolution : 2.73 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
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

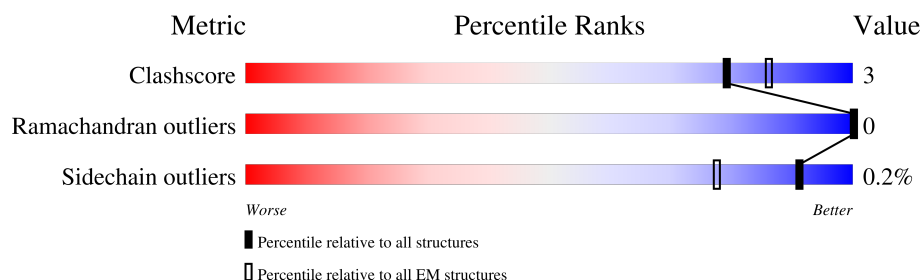
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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	234	
2	B	261	
3	C	248	
4	D	242	
5	E	264	
6	F	255	
7	G	246	
8	H	141	

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Mol	Chain	Length	Quality of chain
9	I	288	
10	J	265	
11	K	331	
12	L	205	
13	M	201	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22235 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1790	1146	305	333	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	249	Total	C	N	O	S	0	0
			1962	1241	338	373	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	237	Total	C	N	O	S	0	0
			1866	1172	331	358	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total	C	N	O	S	0	0
			1778	1124	295	347	12		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	240	Total	C	N	O	S	0	0
			1886	1182	340	352	12		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	240	Total	C	N	O	S	0	0
			1868	1184	319	354	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total	C	N	O	S	0	0
			1883	1195	315	360	13		

- Molecule 8 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	98	Total	C	N	O	S	0	0
			784	497	131	152	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	262	Total	C	N	O	S	0	0
			2082	1336	353	375	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	249	Total	C	N	O	S	0	0
			1929	1247	316	352	14		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	0	0
			1664	1058	289	307	10		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	237P	GLU	-	expression tag	UNP Q99436
K	237Q	ASP	-	expression tag	UNP Q99436
K	237R	LEU	-	expression tag	UNP Q99436
K	237S	TYR	-	expression tag	UNP Q99436
K	237T	PHE	-	expression tag	UNP Q99436
K	237U	GLN	-	expression tag	UNP Q99436
K	237V	SER	-	expression tag	UNP Q99436
K	237W	VAL	-	expression tag	UNP Q99436
K	237X	ASP	-	expression tag	UNP Q99436
K	237Y	SER	-	expression tag	UNP Q99436
K	237Z	ALA	-	expression tag	UNP Q99436
K	238A	TRP	-	expression tag	UNP Q99436
K	238B	SER	-	expression tag	UNP Q99436
K	238C	HIS	-	expression tag	UNP Q99436
K	238D	PRO	-	expression tag	UNP Q99436
K	238E	GLN	-	expression tag	UNP Q99436
K	238F	PHE	-	expression tag	UNP Q99436
K	238G	GLU	-	expression tag	UNP Q99436
K	238H	LYS	-	expression tag	UNP Q99436
K	238I	GLY	-	expression tag	UNP Q99436
K	238J	GLY	-	expression tag	UNP Q99436
K	238K	GLY	-	expression tag	UNP Q99436
K	238L	SER	-	expression tag	UNP Q99436
K	238M	GLY	-	expression tag	UNP Q99436
K	238N	GLY	-	expression tag	UNP Q99436
K	238O	GLY	-	expression tag	UNP Q99436
K	238P	SER	-	expression tag	UNP Q99436
K	238Q	GLY	-	expression tag	UNP Q99436
K	238R	GLY	-	expression tag	UNP Q99436
K	238S	SER	-	expression tag	UNP Q99436
K	238T	ALA	-	expression tag	UNP Q99436
K	238U	TRP	-	expression tag	UNP Q99436
K	238V	SER	-	expression tag	UNP Q99436
K	238W	HIS	-	expression tag	UNP Q99436
K	238X	PRO	-	expression tag	UNP Q99436
K	238Y	GLN	-	expression tag	UNP Q99436
K	238Z	PHE	-	expression tag	UNP Q99436
K	239A	GLU	-	expression tag	UNP Q99436
K	239B	LYS	-	expression tag	UNP Q99436
K	248	UNK	-	expression tag	UNP Q99436
K	249	UNK	-	expression tag	UNP Q99436
K	250	UNK	-	expression tag	UNP Q99436

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Chain	Residue	Modelled	Actual	Comment	Reference
K	251	UNK	-	expression tag	UNP Q99436
K	252	UNK	-	expression tag	UNP Q99436
K	253	UNK	-	expression tag	UNP Q99436
K	254	UNK	-	expression tag	UNP Q99436
K	255	UNK	-	expression tag	UNP Q99436
K	256	UNK	-	expression tag	UNP Q99436
K	257	UNK	-	expression tag	UNP Q99436
K	258	UNK	-	expression tag	UNP Q99436
K	259	UNK	-	expression tag	UNP Q99436
K	260	UNK	-	expression tag	UNP Q99436
K	261	UNK	-	expression tag	UNP Q99436
K	262	UNK	-	expression tag	UNP Q99436

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	179	Total	C	N	O	S	0	0
			1396	899	231	251	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	179	Total	C	N	O	S	0	0
			1347	865	235	240	7		

3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

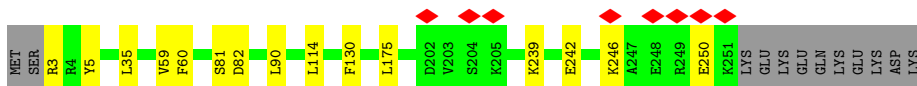
- Molecule 1: Proteasome subunit alpha type-2

Chain A: 




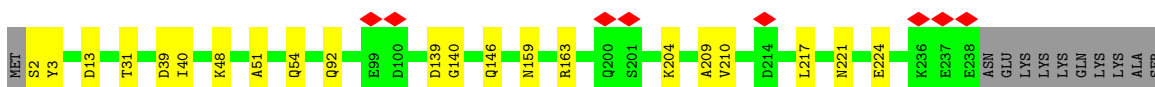
- Molecule 2: Proteasome subunit alpha type-4

Chain B: 




- Molecule 3: Proteasome subunit alpha type-7

Chain C: 




- Molecule 4: Proteasome subunit alpha type-5

Chain D: 




- Molecule 5: Proteasome subunit alpha type-1

Chain E: 




GLU
HIS

• Molecule 6: Proteasome subunit alpha type-3

Chain F:  91% 6%

MET SER SER ILE G5 L10 S35 I38 R66 M151 I152 V194 W216 V228 L244 LYS GLU GLU ASP GLU SER ASP ASP ASP ASN MET

• Molecule 7: Proteasome subunit alpha type-6

Chain G:  91% 7%


MET S2 R3 G4 S5 T13 T14 G20 A31 Q34 D46 D68 L61 T73 E74 D112 M113 D120 G158 F187 P212 E232 A243 GLU ARG ASP

• Molecule 8: Proteasome maturation protein

Chain H:  67% 30%


MET ASN ALA ARG GLY LEU GLY SER GLU LEU LYS ASP SER TLE PRO VAL THR GLU LEU SER ALA GLY SER PRO PHE GLU SER HIS ASP LEU ARG LYS GLY PHE SER CYS VAL LYS ASN ASP LEU LEU LEU P44 R68 K78 E82 R91 L141

• Molecule 9: Proteasome assembly chaperone 1

Chain I:  85% 6% 9%

MET A2 V9 T18 GLU ASP GLU GLU GLU GLU GLU GLU ARG ARG THR PRO E33 D34 R35 L39 V47 Q53 R107 THR THR ASP THR THR HIS LEU SER SER THR A119 K152 Y175 L189 R190 E207 D238 L242 L245 T246 V247
L254 V263 L273 K274 N280 T288

• Molecule 10: Proteasome assembly chaperone 2

Chain J:  88% 6% 6%

ACE0 M1 G14 F15 T16 M55 N74 C115 T137 R140 T144 P145 S146 R167 CYS ILE PRO GLU ILE ASP ASP SER GLU F177 E222 K232 S235 ASP ASP PRO THR VAL ALA S243 R244 F264

• Molecule 11: Proteasome subunit beta type-7

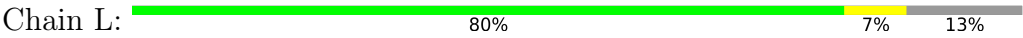
Chain K:  66% 31%

MET ALA ALA V4 S15 K31 R40 T44 D53 T61 ARG ALA THR GLU GLY MET VAL VAL ALA ASP LYS ASN CYS S75 K76 I77 H78 T99 T113 G114 R115 L206 PHE ASN ASP LEU GLY SER GLY S214 W236 LYS LYS GLY THR ARG LEU GLY ARG TYR

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

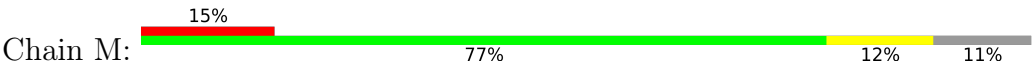
GLY SER ALA TRP SER HIS PRO PHE GLU LYS X248 X262

- Molecule 12: Proteasome subunit beta type-3



MET SER ILE MET SER Y6 R26 R27 F28 GLY ILE GLN ALA GLN MET VAL THR THR ASP F39 L49 L94 E97 K98 R99 G111 C122 S123 L124 D125 C129 D135 F136 A174 VAL ASP ARG ASP VAL SER GLY M183 G184 A202 ARG MET ASP

- Molecule 13: Proteasome subunit beta type-2



MET E2 I5 G9 Y12 A16 S17 D18 R19 VAL ALA ALA SER ASN VAL MET LYS ASP ASP HIS ASP K34 M35 L43 A50 L66 Y67 L75 S76 P77 T96 P97 N101 D108 G112 H132 G133 Y134 G135 A136 F137 L138 L143 D144

R145 Y146 Y147 T150 E154 R155 A156 L160 R161 L164 E165 E166 L167 Q168 K169 R170 F171 I172 L173 N174 L175 P176 T177 F178 S179 V180 I181 I182 D184 H189 D190 L191 D192 N193 I194 SER PHE PRO LYS GLY SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217491	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 ($e^-/\text{\AA}^2$)	66.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.283	Depositor
Minimum map value	-1.649	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	255.36, 255.36, 255.36	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8512, 0.8512, 0.8512	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/1829	0.48	0/2478
2	B	0.24	0/1992	0.46	0/2682
3	C	0.24	0/1892	0.49	0/2553
4	D	0.25	0/1803	0.47	0/2435
5	E	0.24	0/1919	0.51	0/2592
6	F	0.26	0/1903	0.48	0/2565
7	G	0.25	0/1917	0.46	0/2591
8	H	0.24	0/798	0.44	0/1074
9	I	0.24	0/2125	0.47	0/2879
10	J	0.25	0/1969	0.48	0/2667
11	K	0.25	0/1619	0.47	0/2194
12	L	0.24	0/1423	0.49	0/1920
13	M	0.25	0/1372	0.49	0/1862
All	All	0.25	0/22561	0.48	0/30492

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 [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	1790	0	1787	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1962	0	1985	8	0
3	C	1866	0	1889	13	0
4	D	1778	0	1772	16	0
5	E	1886	0	1876	13	0
6	F	1868	0	1843	6	0
7	G	1883	0	1892	13	0
8	H	784	0	782	2	0
9	I	2082	0	2115	11	0
10	J	1929	0	1968	8	0
11	K	1664	0	1614	6	0
12	L	1396	0	1406	9	0
13	M	1347	0	1316	14	0
All	All	22235	0	22245	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (117) 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)
3:C:146:GLN:OE1	3:C:159:ASN:ND2	2.23	0.72
13:M:108:ASP:HB2	13:M:112:GLY:H	1.55	0.72
4:D:210:LEU:HD11	4:D:215:ILE:HD13	1.73	0.70
10:J:14:GLY:HA2	10:J:115:CYS:HA	1.73	0.70
4:D:196:LYS:O	4:D:200:ILE:HD12	1.92	0.69
10:J:232:LYS:O	10:J:244:ARG:NH2	2.27	0.68
1:A:119:GLN:HG3	2:B:81:SER:HB2	1.78	0.65
11:K:44:THR:OG1	11:K:76:LYS:NZ	2.26	0.63
1:A:69:THR:HG22	1:A:70:LYS:H	1.64	0.61
11:K:78:HIS:HB3	11:K:99:THR:HG21	1.81	0.61
10:J:137:THR:O	10:J:140:ARG:NH1	2.35	0.59
3:C:209:ALA:HB1	3:C:217:LEU:HD11	1.84	0.58
7:G:212:PRO:HB2	7:G:232:GLU:HG3	1.86	0.58
1:A:119:GLN:OE1	8:H:91:ARG:NH2	2.37	0.58
5:E:207:THR:OG1	5:E:226:ASP:O	2.23	0.57
4:D:199:LEU:HB3	4:D:241:ILE:HD11	1.87	0.56
7:G:13:ILE:HG23	7:G:14:THR:HG23	1.87	0.56
1:A:84:ARG:NH1	7:G:120:ASP:OD1	2.40	0.54
13:M:77:PRO:HD2	13:M:108:ASP:OD1	2.08	0.54
3:C:31:THR:OG1	3:C:163:ARG:O	2.22	0.53
2:B:3:ARG:HG3	2:B:5:TYR:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:LYS:HD3	3:C:163:ARG:HH21	1.73	0.52
10:J:144:THR:HG22	10:J:146:SER:H	1.74	0.52
10:J:15:PHE:O	10:J:16:THR:OG1	2.25	0.52
12:L:122:CYS:SG	12:L:123:SER:N	2.82	0.52
12:L:135:ASP:OD1	12:L:136:PHE:N	2.39	0.52
2:B:35:LEU:HD11	2:B:175:LEU:HD11	1.92	0.52
4:D:184:VAL:HG12	4:D:185:TYR:N	2.24	0.52
4:D:156:MET:HB2	4:D:162:PHE:CE1	2.45	0.52
13:M:5:ILE:HD11	13:M:143:LEU:HD11	1.91	0.52
13:M:43:LEU:HD12	13:M:183:ILE:HD11	1.92	0.51
13:M:16:ALA:HB2	13:M:180:VAL:HG12	1.93	0.51
7:G:112:ASP:OD1	7:G:113:MET:N	2.44	0.50
3:C:51:ALA:HB3	3:C:54:GLN:HB2	1.92	0.50
5:E:100:ASP:N	5:E:100:ASP:OD1	2.45	0.50
6:F:35:SER:HB2	6:F:66:ARG:HH12	1.75	0.50
11:K:15:SER:HB3	12:L:98:LYS:HG2	1.93	0.50
11:K:53:ASP:N	11:K:53:ASP:OD1	2.43	0.50
9:I:238:ASP:OD1	9:I:238:ASP:N	2.42	0.49
9:I:47:VAL:O	9:I:152:LYS:NZ	2.46	0.49
4:D:41:GLN:NE2	4:D:151:PRO:O	2.45	0.49
9:I:247:VAL:HG11	9:I:273:LEU:HD11	1.93	0.49
4:D:28:ILE:O	4:D:31:ILE:HG12	2.13	0.49
10:J:243:SER:OG	10:J:244:ARG:N	2.46	0.49
4:D:184:VAL:HG12	4:D:185:TYR:H	1.77	0.49
9:I:189:LEU:O	9:I:190:ARG:NH1	2.43	0.49
9:I:254:LEU:HD22	9:I:263:VAL:HG21	1.93	0.49
2:B:90:LEU:HG	2:B:114:LEU:HD13	1.94	0.48
13:M:143:LEU:O	13:M:147:TYR:HB2	2.13	0.48
2:B:246:LYS:O	2:B:250:GLU:HG2	2.13	0.48
3:C:92:GLN:HG3	13:M:66:LEU:HB2	1.94	0.48
5:E:200:PRO:HG3	9:I:245:ILE:HD11	1.96	0.48
3:C:39:ASP:N	3:C:39:ASP:OD1	2.46	0.48
4:D:88:LEU:HD23	4:D:119:LEU:HD23	1.96	0.48
1:A:69:THR:HG22	1:A:70:LYS:N	2.29	0.47
6:F:38:ILE:HD11	6:F:194:VAL:HG13	1.96	0.47
7:G:58:ASP:HB3	7:G:61:LEU:HG	1.95	0.47
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.95	0.47
3:C:13:ASP:OD1	3:C:13:ASP:N	2.48	0.47
3:C:2:SER:OG	3:C:3:TYR:N	2.42	0.47
13:M:136:ALA:O	13:M:138:LEU:HD23	2.14	0.47
8:H:78:LYS:O	8:H:82:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:ARG:NH1	12:L:129:CYS:O	2.48	0.46
12:L:125:ASP:OD2	12:L:129:CYS:HB3	2.15	0.46
10:J:222:GLU:OE1	10:J:244:ARG:NH1	2.49	0.46
5:E:84:LEU:O	5:E:88:MET:HG3	2.17	0.45
9:I:175:TYR:OH	9:I:207:GLU:OE1	2.31	0.45
6:F:216:TRP:CZ3	6:F:228:VAL:HG22	2.51	0.45
3:C:221:ASN:HB2	3:C:224:GLU:HG3	1.98	0.45
4:D:41:GLN:HE21	4:D:151:PRO:HB2	1.82	0.45
1:A:182:LEU:HD11	1:A:186:ASP:HB2	1.98	0.45
12:L:49:LEU:HD12	12:L:111:GLY:HA3	1.99	0.45
7:G:73:THR:HG22	7:G:74:GLU:N	2.32	0.44
1:A:84:ARG:NH2	7:G:158:GLY:O	2.44	0.44
5:E:184:LEU:HD21	5:E:214:ILE:HG21	1.99	0.44
6:F:216:TRP:CE3	6:F:228:VAL:HG22	2.52	0.44
13:M:101:ASN:HB3	13:M:132:HIS:CE1	2.53	0.44
5:E:225:ASP:N	5:E:225:ASP:OD1	2.50	0.44
4:D:146:VAL:HG21	4:D:222:PRO:HG3	1.98	0.44
3:C:139:ASP:OD1	3:C:140:GLY:N	2.51	0.44
4:D:195:ILE:O	4:D:199:LEU:HD23	2.17	0.44
10:J:55:MET:HG3	10:J:74:ASN:HB3	1.99	0.44
5:E:200:PRO:HB2	5:E:203:GLN:OE1	2.18	0.44
13:M:9:GLY:HA3	13:M:12:TYR:CE1	2.53	0.43
1:A:28:ALA:HB2	7:G:20:GLY:HA3	2.01	0.43
4:D:184:VAL:O	4:D:185:TYR:HB3	2.19	0.43
6:F:10:LEU:O	7:G:3:ARG:NH2	2.51	0.43
9:I:35:ARG:HG2	9:I:39:LEU:HD23	2.01	0.43
11:K:113:THR:HG22	11:K:115:ARG:HE	1.83	0.43
6:F:151:MET:HG2	6:F:152:ILE:N	2.34	0.43
2:B:82:ASP:HB3	2:B:130:PHE:HD1	1.84	0.42
4:D:145:GLY:HA2	4:D:220:VAL:HG11	2.02	0.42
4:D:221:GLN:HG2	4:D:224:GLN:HG2	2.00	0.42
1:A:222:THR:OG1	1:A:225:GLU:OE1	2.37	0.41
2:B:239:LYS:O	2:B:242:GLU:HG3	2.20	0.41
5:E:128:TYR:O	5:E:149:PRO:HB3	2.20	0.41
13:M:17:SER:OG	13:M:18:ASP:N	2.53	0.41
5:E:203:GLN:O	5:E:239:ARG:NH1	2.54	0.41
7:G:73:THR:HG22	7:G:74:GLU:H	1.85	0.41
7:G:5:SER:HB2	9:I:9:VAL:HG22	2.02	0.41
7:G:31:ALA:HA	7:G:34:GLN:HG2	2.02	0.41
13:M:67:TYR:CD1	13:M:75:LEU:HG	2.55	0.41
1:A:130:PHE:O	1:A:151:PRO:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:LYS:HA	3:C:204:LYS:HD3	1.84	0.41
5:E:122:ARG:HG2	5:E:122:ARG:HH11	1.86	0.41
2:B:59:VAL:HG23	2:B:60:PHE:CD2	2.55	0.41
5:E:90:GLN:HA	5:E:90:GLN:NE2	2.36	0.41
9:I:242:LEU:HD12	9:I:242:LEU:HA	1.90	0.41
12:L:94:LEU:O	12:L:97:GLU:HG3	2.20	0.41
13:M:35:MET:SD	13:M:181:ARG:HD3	2.60	0.41
12:L:27:ARG:HH12	12:L:39:PHE:N	2.19	0.41
13:M:184:ASP:OD1	13:M:189:HIS:NE2	2.54	0.41
5:E:65:HIS:NE2	5:E:67:ASP:O	2.54	0.40
7:G:46:ASP:N	7:G:46:ASP:OD1	2.54	0.40
12:L:26:ARG:O	12:L:184:GLY:N	2.54	0.40
4:D:35:SER:HB2	4:D:51:GLU:HG3	2.04	0.40
5:E:202:GLU:HG2	9:I:274:LYS:HE3	2.03	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	228/234 (97%)	222 (97%)	6 (3%)	0	100	100
2	B	247/261 (95%)	243 (98%)	4 (2%)	0	100	100
3	C	235/248 (95%)	231 (98%)	4 (2%)	0	100	100
4	D	229/242 (95%)	224 (98%)	5 (2%)	0	100	100
5	E	238/264 (90%)	225 (94%)	13 (6%)	0	100	100
6	F	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
7	G	240/246 (98%)	238 (99%)	2 (1%)	0	100	100
8	H	96/141 (68%)	91 (95%)	5 (5%)	0	100	100
9	I	256/288 (89%)	251 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	243/265 (92%)	235 (97%)	8 (3%)	0	100	100
11	K	207/331 (62%)	205 (99%)	2 (1%)	0	100	100
12	L	173/205 (84%)	167 (96%)	6 (4%)	0	100	100
13	M	175/201 (87%)	172 (98%)	3 (2%)	0	100	100
All	All	2805/3181 (88%)	2739 (98%)	66 (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	A	187/191 (98%)	187 (100%)	0	100	100
2	B	208/221 (94%)	208 (100%)	0	100	100
3	C	200/211 (95%)	200 (100%)	0	100	100
4	D	194/203 (96%)	194 (100%)	0	100	100
5	E	204/224 (91%)	204 (100%)	0	100	100
6	F	195/212 (92%)	195 (100%)	0	100	100
7	G	206/210 (98%)	206 (100%)	0	100	100
8	H	91/128 (71%)	90 (99%)	1 (1%)	70	83
9	I	235/262 (90%)	235 (100%)	0	100	100
10	J	218/237 (92%)	217 (100%)	1 (0%)	86	92
11	K	167/257 (65%)	167 (100%)	0	100	100
12	L	149/174 (86%)	147 (99%)	2 (1%)	65	80
13	M	131/171 (77%)	131 (100%)	0	100	100
All	All	2385/2701 (88%)	2381 (100%)	4 (0%)	91	96

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

Mol	Chain	Res	Type
8	H	68	ARG
10	J	1	MET
12	L	27	ARG
12	L	99	ARG

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

Mol	Chain	Res	Type
3	C	116	GLN
4	D	41	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

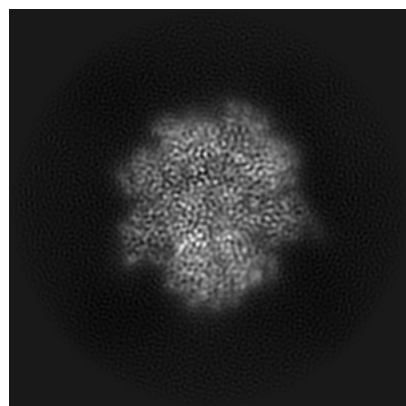
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18758. These allow visual inspection of the internal detail of the map and identification of artifacts.

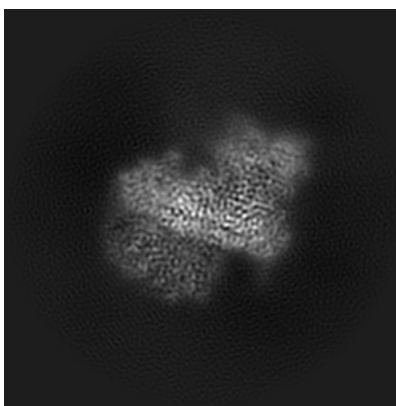
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

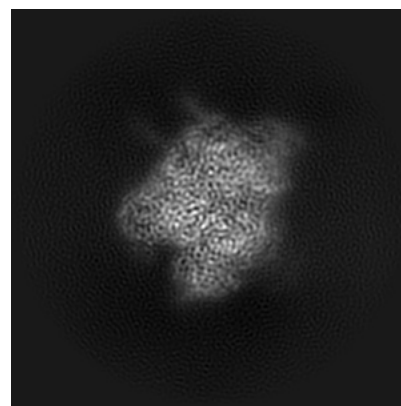
6.1.1 Primary map



X

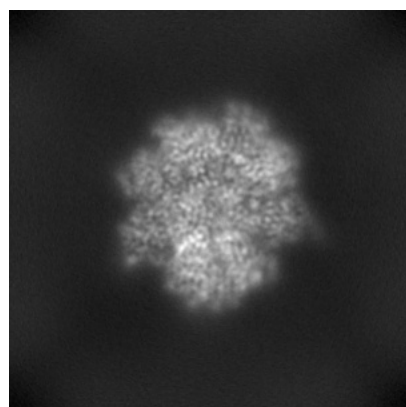


Y

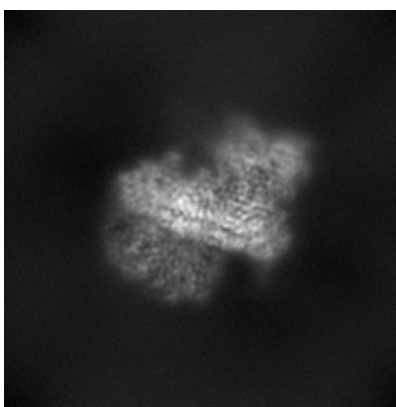


Z

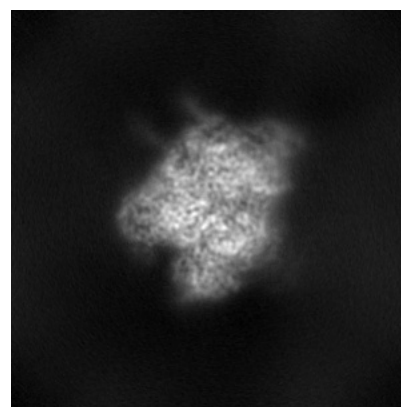
6.1.2 Raw map



X



Y

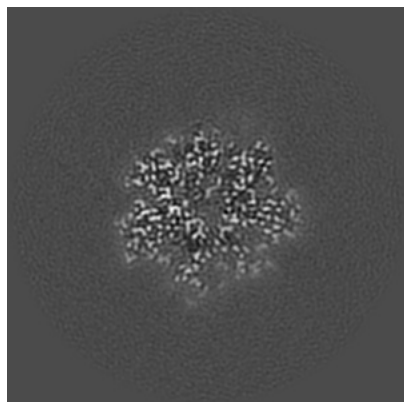


Z

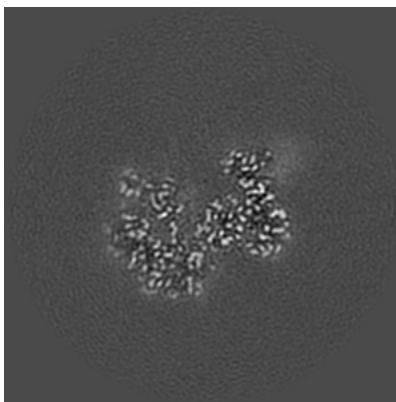
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

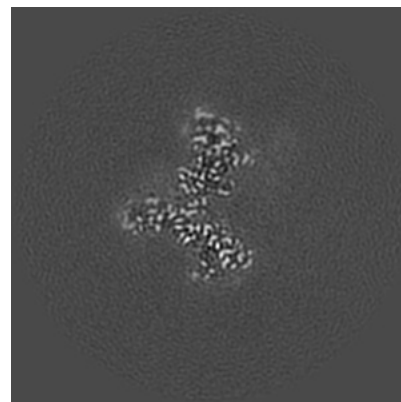
6.2.1 Primary map



X Index: 150

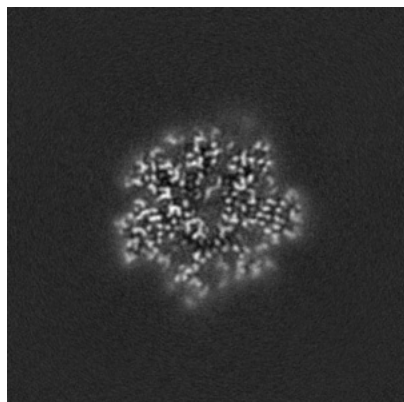


Y Index: 150

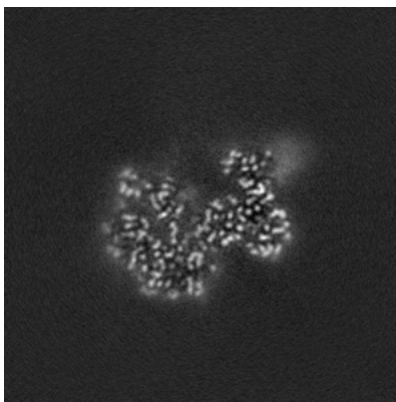


Z Index: 150

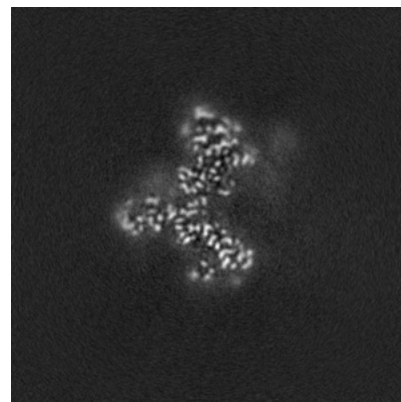
6.2.2 Raw map



X Index: 150



Y Index: 150

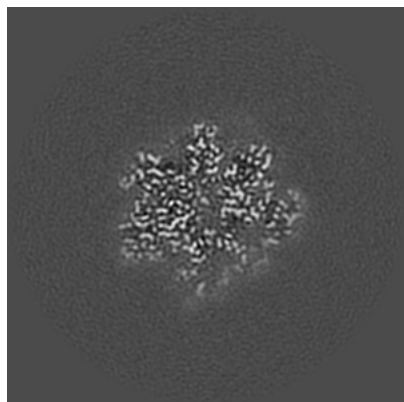


Z Index: 150

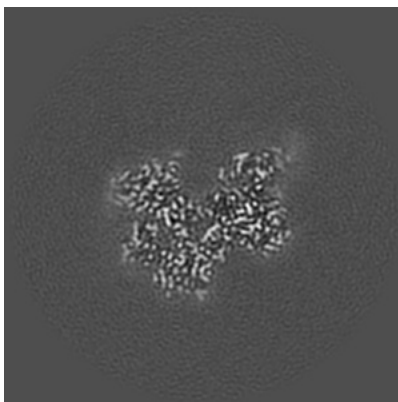
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

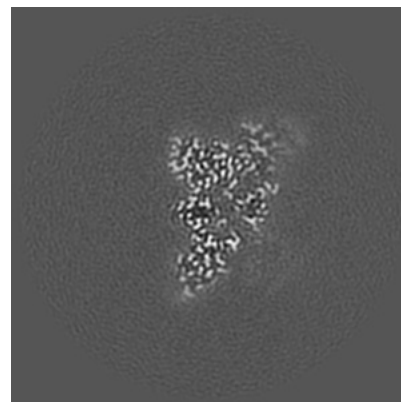
6.3.1 Primary map



X Index: 147

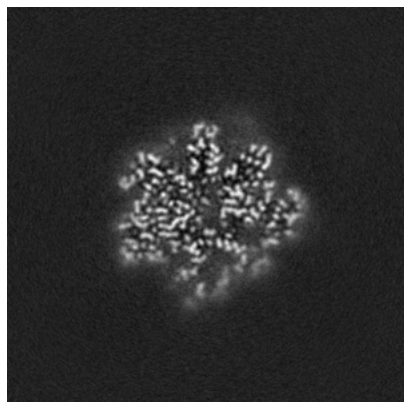


Y Index: 140

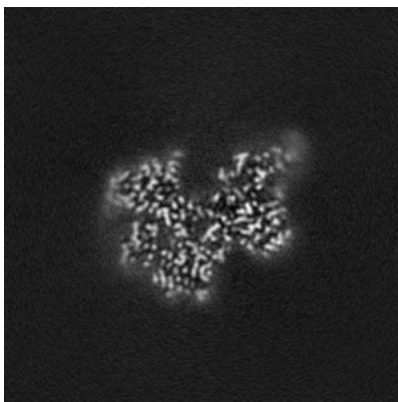


Z Index: 176

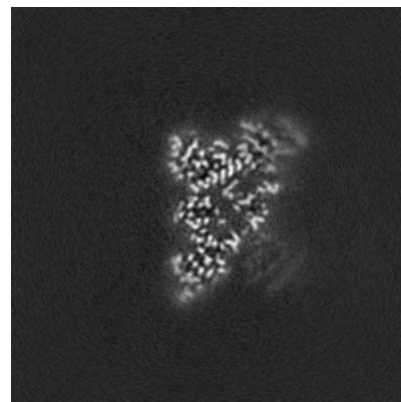
6.3.2 Raw map



X Index: 147



Y Index: 140

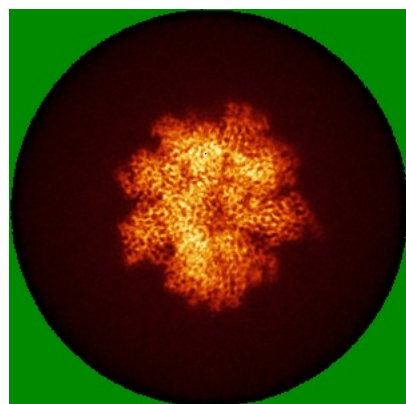


Z Index: 177

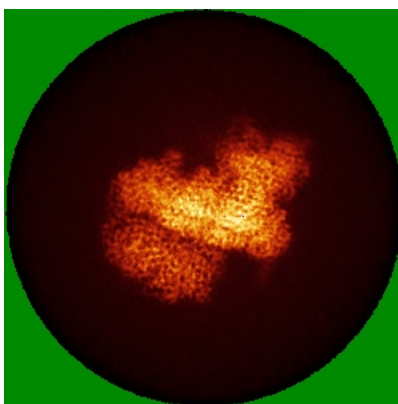
The images above show the largest variance slices of the map in three orthogonal directions.

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

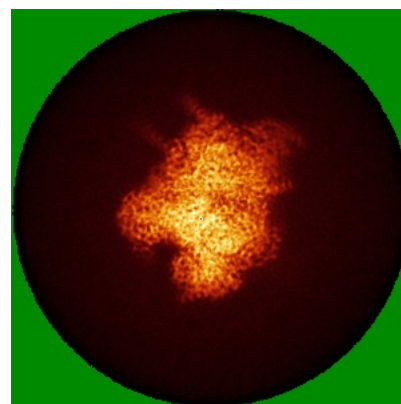
6.4.1 Primary map



X

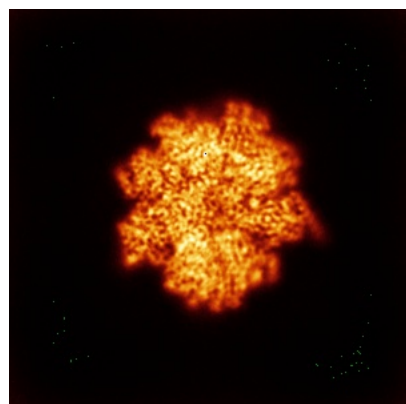


Y

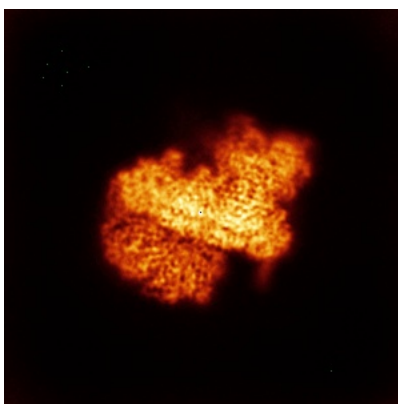


Z

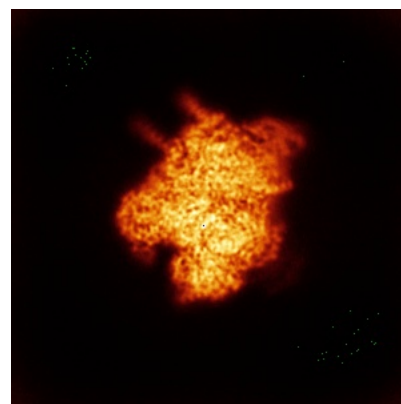
6.4.2 Raw map



X



Y

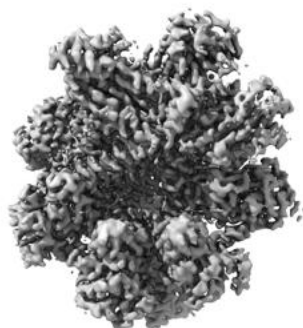


Z

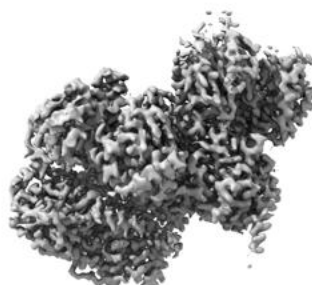
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

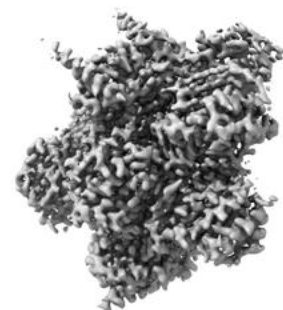
6.5.1 Primary map



X



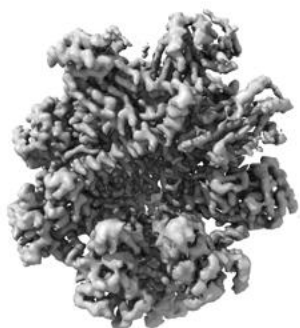
Y



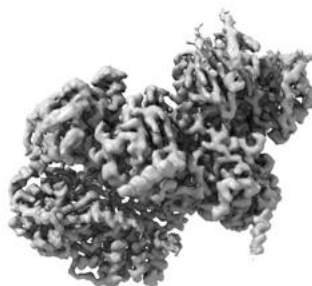
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

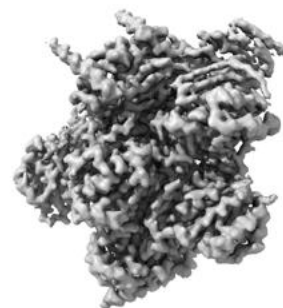
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

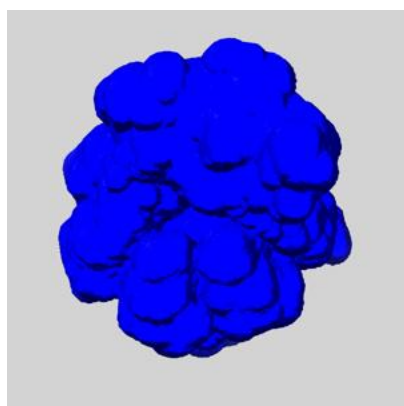
6.6 Mask visualisation [i](#)

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

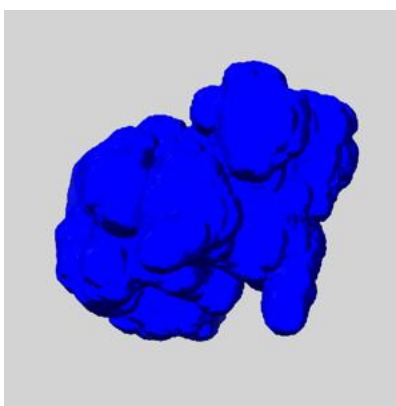
A mask typically either:

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

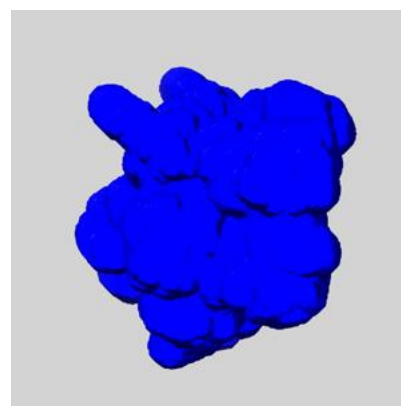
6.6.1 emd_18758_msk_1.map [i](#)



X



Y

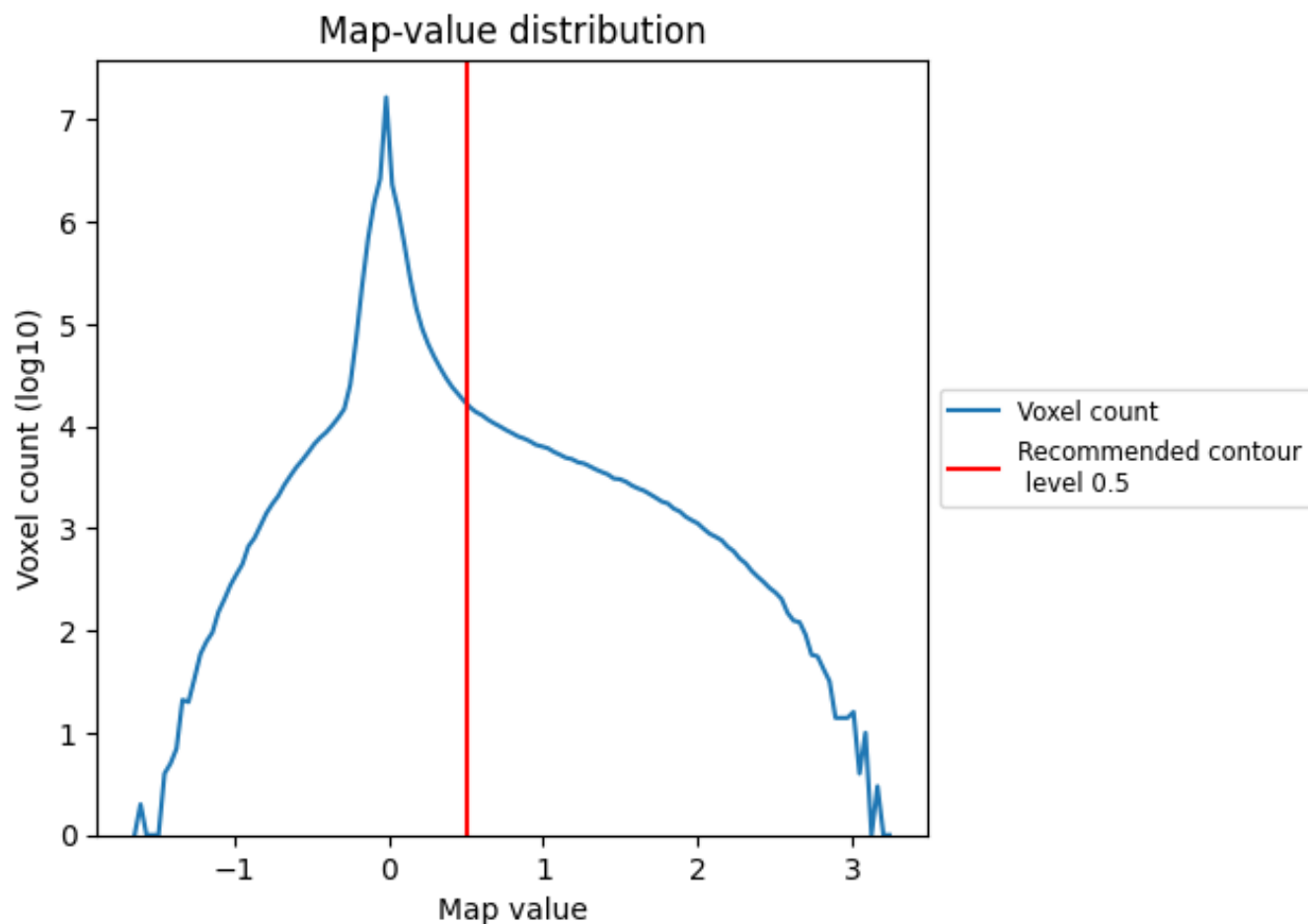


Z

7 Map analysis [i](#)

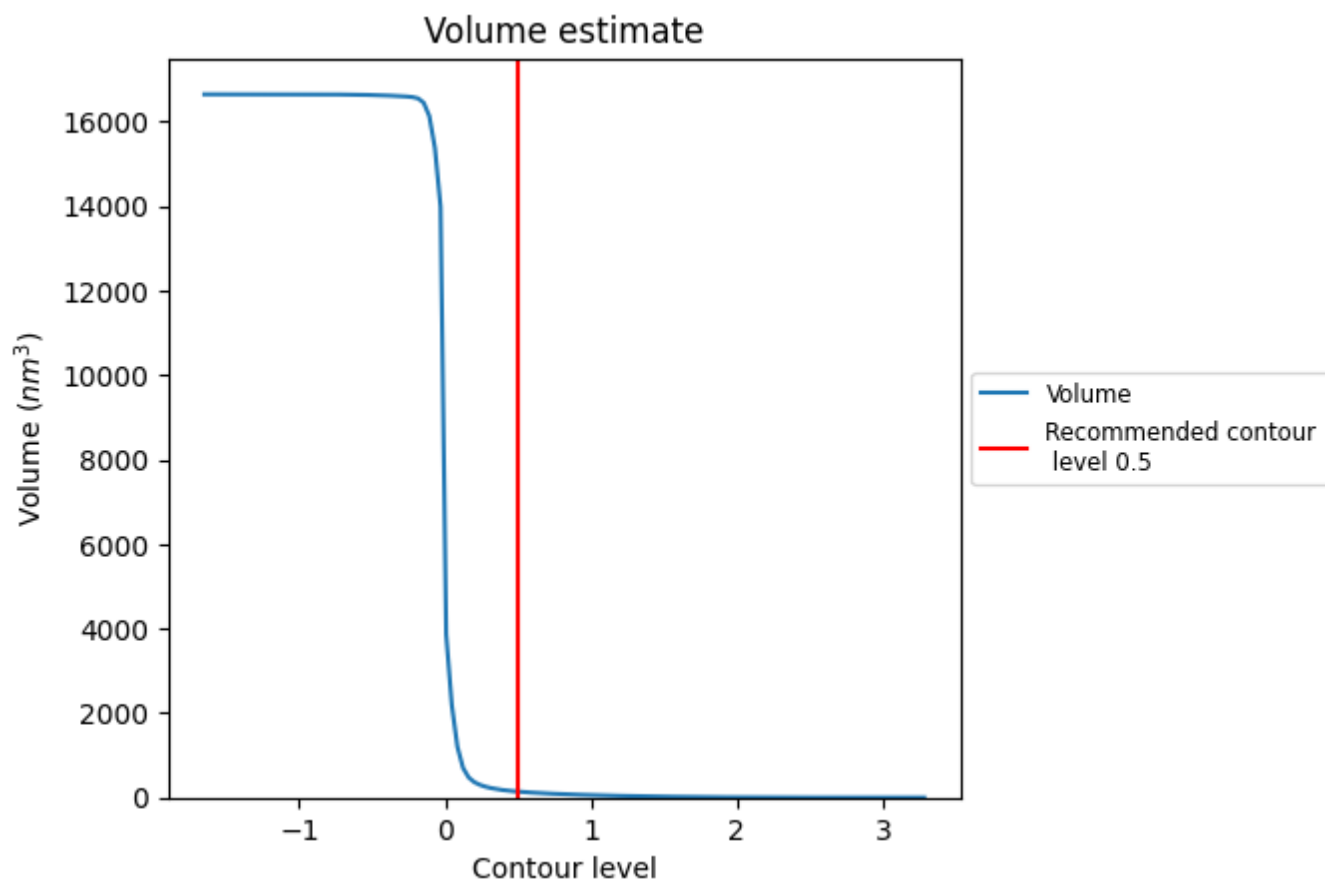
This section contains the results of statistical analysis of the map.

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.

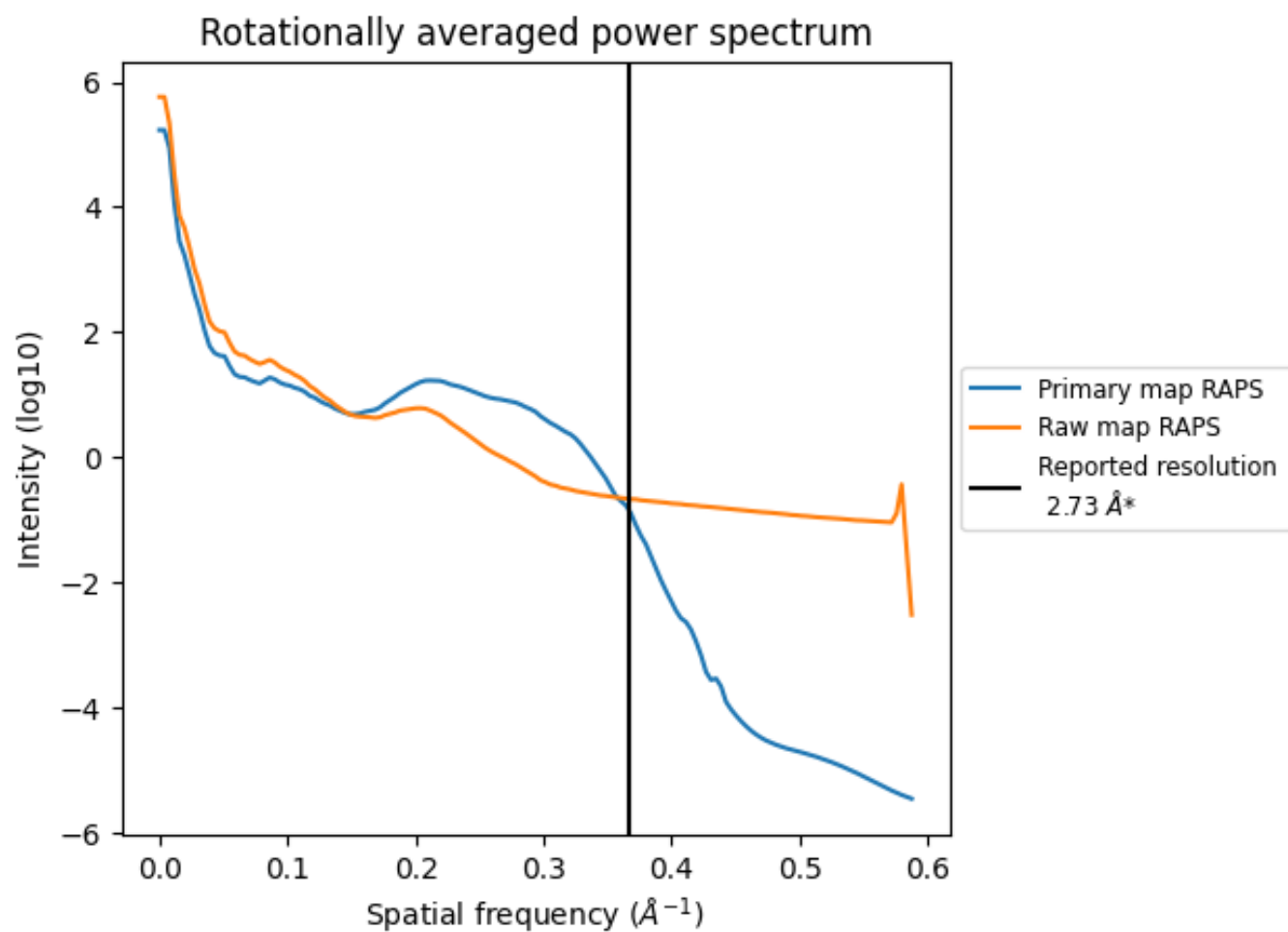
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 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 ⓘ

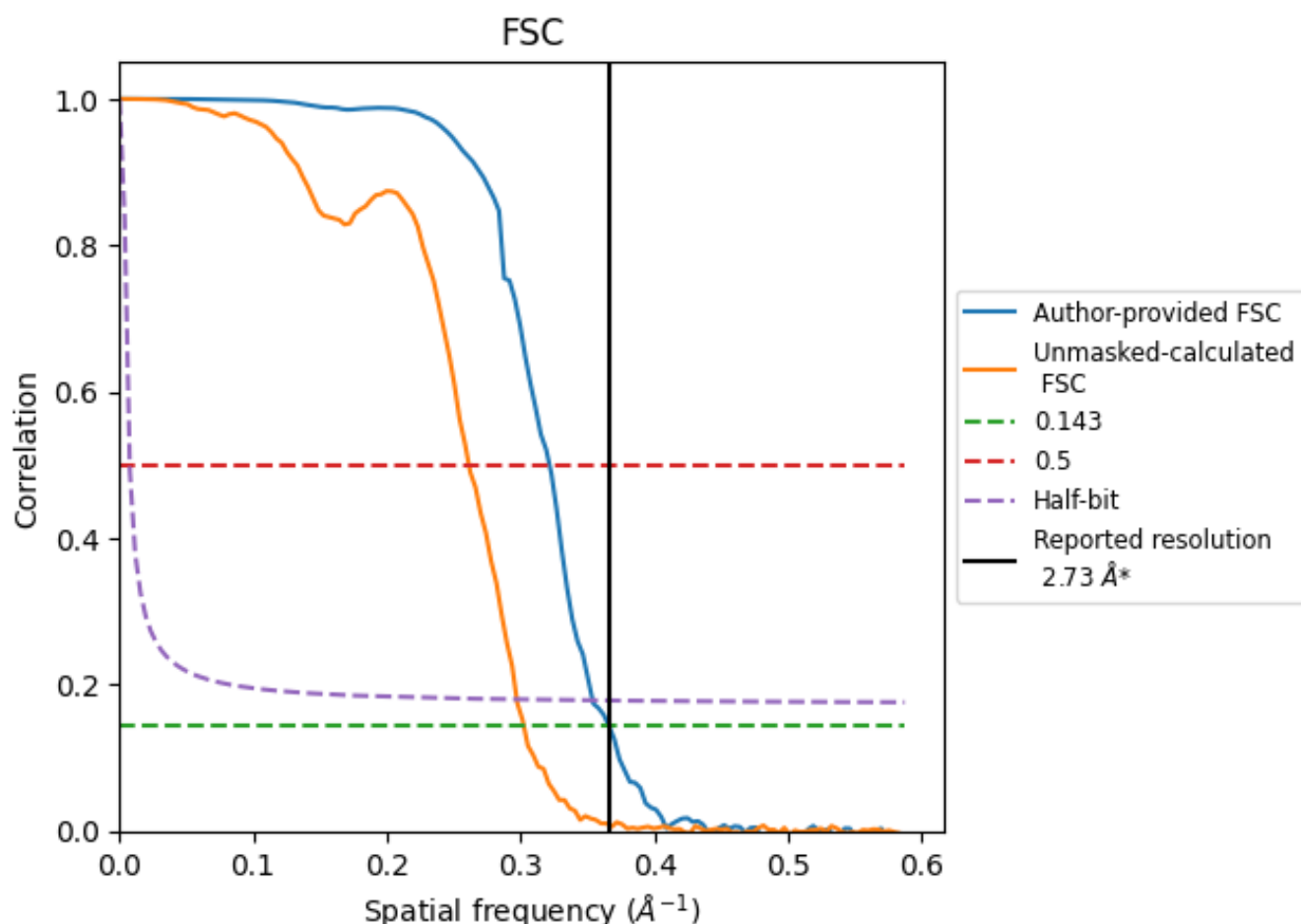


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 0.366 \AA^{-1}

8.2 Resolution estimates [i](#)

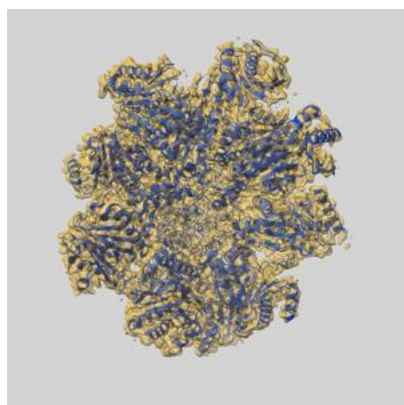
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.11	2.83
Unmasked-calculated*	3.31	3.83	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.73 by more than 10 %

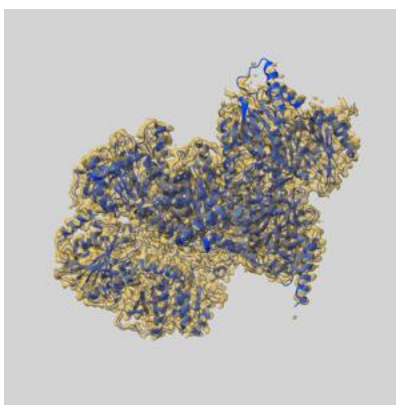
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18758 and PDB model 8QYM. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

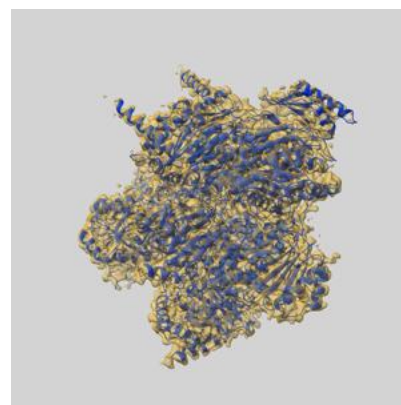
9.1 Map-model overlay [i](#)



X



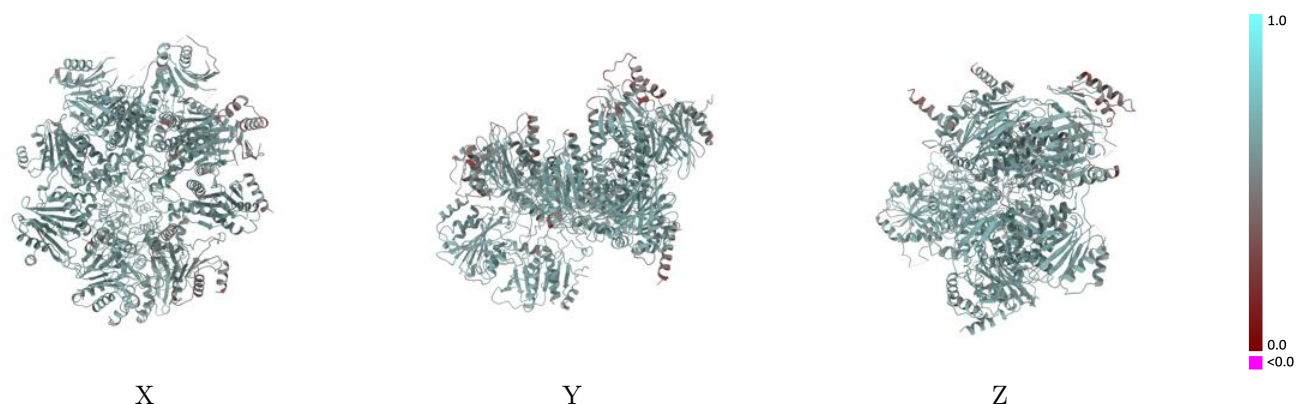
Y



Z

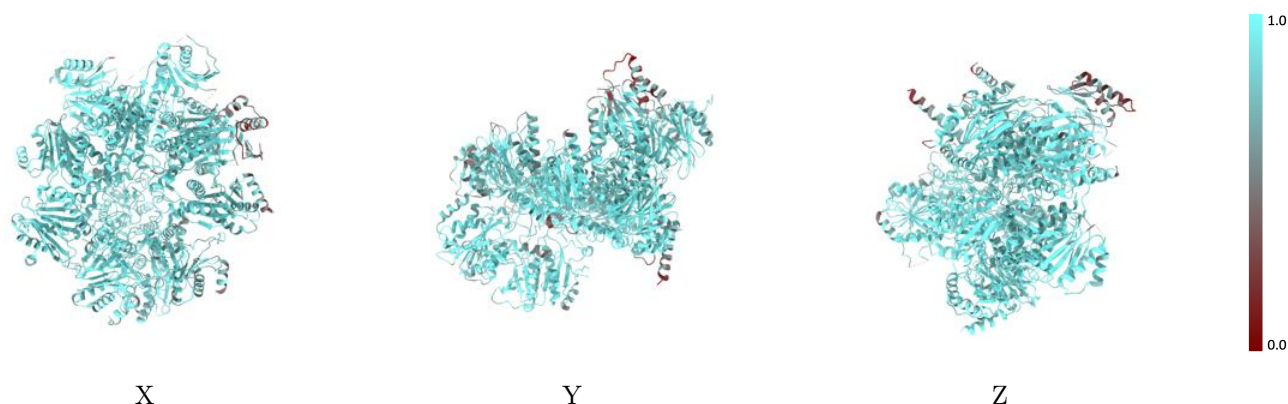
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



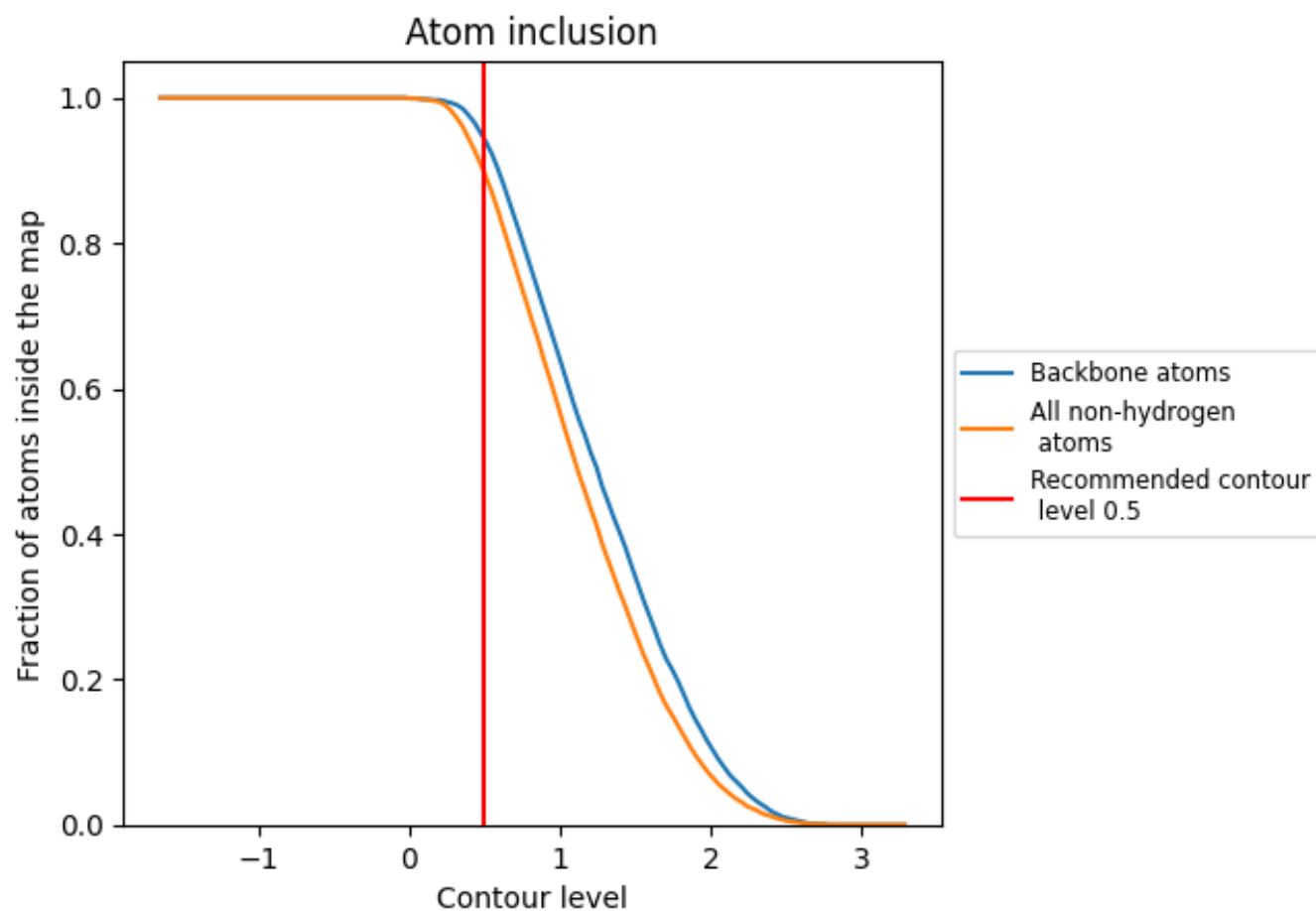
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.5950
A	 0.9540	 0.6220
B	 0.8920	 0.6000
C	 0.8900	 0.5920
D	 0.8310	 0.5450
E	 0.9120	 0.5900
F	 0.9290	 0.6110
G	 0.9430	 0.6180
H	 0.9160	 0.6130
I	 0.8830	 0.6030
J	 0.9270	 0.6120
K	 0.9110	 0.5970
L	 0.9000	 0.5920
M	 0.7240	 0.5290

