



Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 01:19 PM EDT

PDB ID : 8TM4 / pdb_00008tm4
EMDB ID : EMD-41378
Title : Human pre 13S proteasome assembly intermediate
Authors : Zhang, H.; Zhao, J.
Deposited on : 2023-07-28
Resolution : 3.00 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

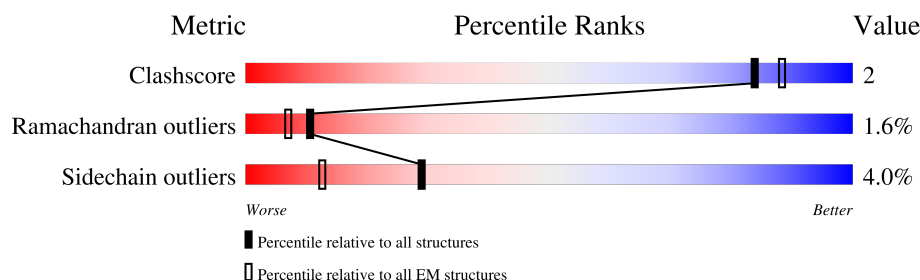
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	 91% 8%
2	B	261	 88% 7% .
3	C	248	 85% 11% .
4	D	241	 84% 11% . .
5	E	263	 83% 7% 10%
6	F	255	 86% 8% . 5%
7	G	246	 91% 8%
8	H	277	 66% 5% 28%

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Mol	Chain	Length	Quality of chain
9	I	205	<div><div><div></div><div></div><div></div></div><div>76%9%15%</div></div>
10	J	201	<div><div><div></div><div></div><div></div></div><div>14%48%11%39%</div></div>
11	c	288	<div><div><div></div><div></div><div></div></div><div>7%86%9%5%</div></div>
12	d	264	<div><div><div></div><div></div><div></div></div><div>83%9%7%</div></div>
13	e	141	<div><div><div></div><div></div><div></div></div><div>60%9%31%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21367 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	233	Total	C	N	O	S	0	0
			1813	1160	308	339	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	250	Total	C	N	O	S	0	0
			1901	1208	326	357	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	238	Total	C	N	O	S	0	0
			1819	1145	327	342	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1742	1104	291	335	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	238	Total	C	N	O	S	0	0
			1832	1156	331	333	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	243	Total	C	N	O	S	0	0
			1868	1186	320	351	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	245	Total	C	N	O	S	0	0
			1892	1203	318	359	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	199	Total	C	N	O	S	0	0
			1480	938	253	279	10		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	175	Total	C	N	O	S	0	0
			1342	863	224	240	15		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	123	Total	C	N	O	S	0	0
			904	581	156	161	6		

- Molecule 11 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	275	Total	C	N	O	S	0	0
			2100	1350	355	378	17		

- Molecule 12 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	246	Total	C	N	O	S	0	0
			1906	1230	312	351	13		

- Molecule 13 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	97	Total	C	N	O	S	0	0
			768	488	129	147	4		

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.

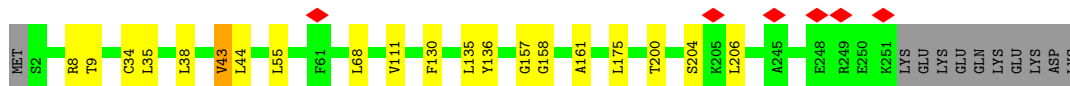
- Molecule 1: Proteasome subunit alpha type-2

Chain A: 




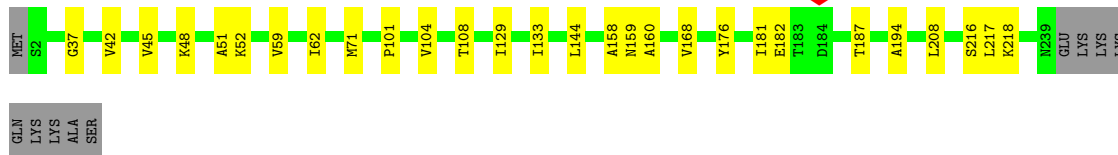
- Molecule 2: Proteasome subunit alpha type-4

Chain B: 




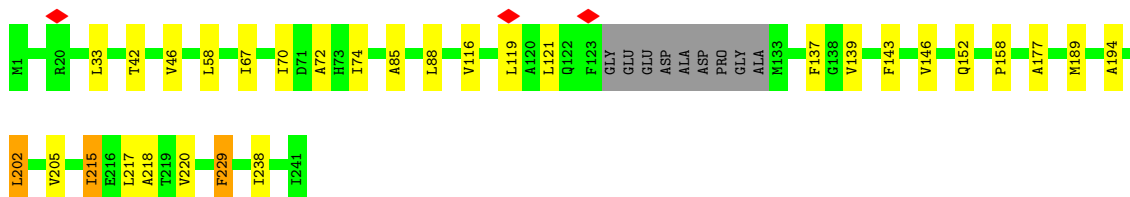
- Molecule 3: Proteasome subunit alpha type-7

Chain C: 




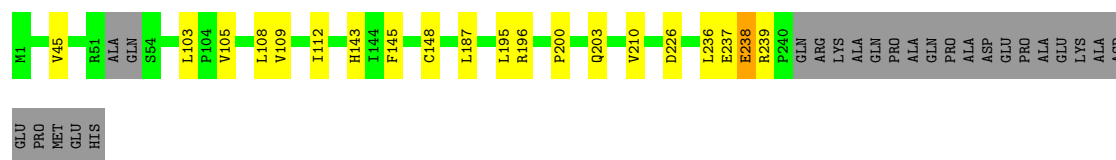
- Molecule 4: Proteasome subunit alpha type-5

Chain D: 




- Molecule 5: Proteasome subunit alpha type-1

Chain E:  83% 7% 10%



- Molecule 6: Proteasome subunit alpha type-3

Chain F:  86% 8% 5%



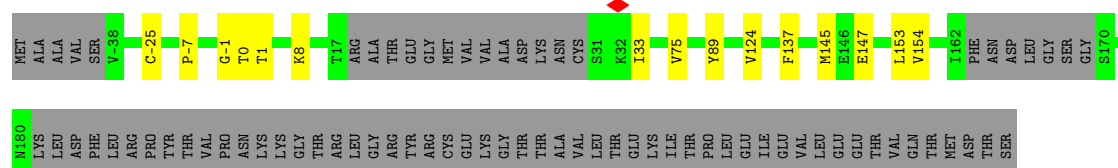
- Molecule 7: Proteasome subunit alpha type-6

Chain G:  91% 8%



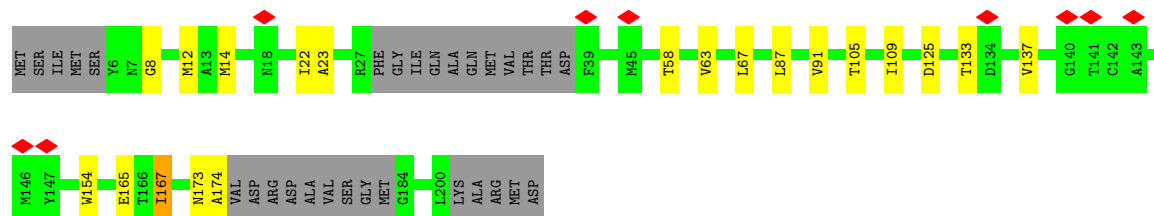
- Molecule 8: Proteasome subunit beta type-7

Chain H:  66% 5% 28%



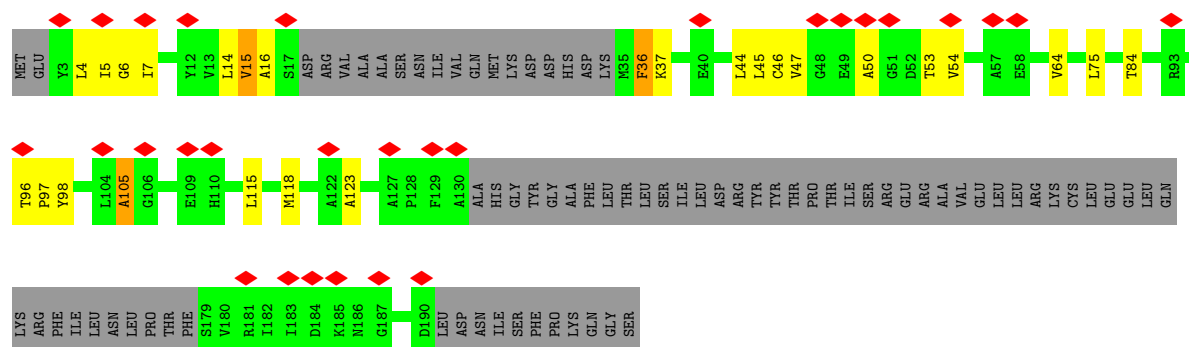
- Molecule 9: Proteasome subunit beta type-3

Chain I:  76% 9% 15%

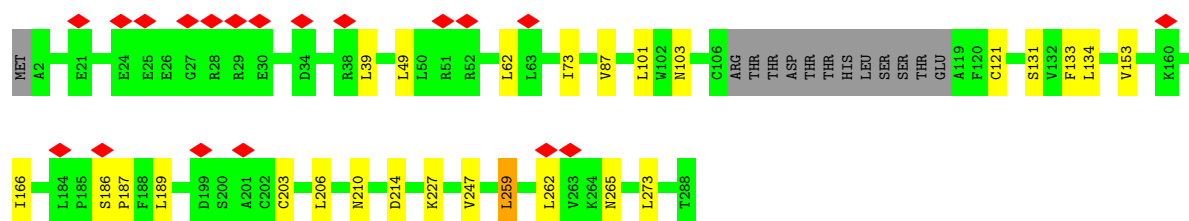
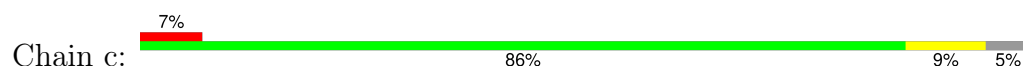


- Molecule 10: Proteasome subunit beta type-2

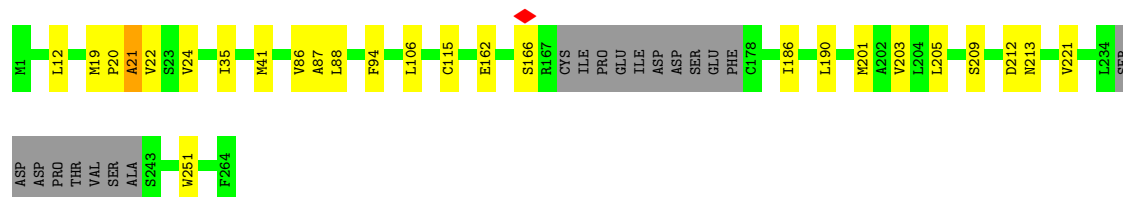
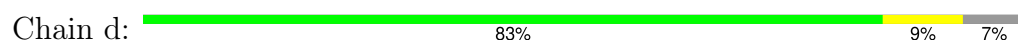
Chain J:  14% 48% 11% 39%



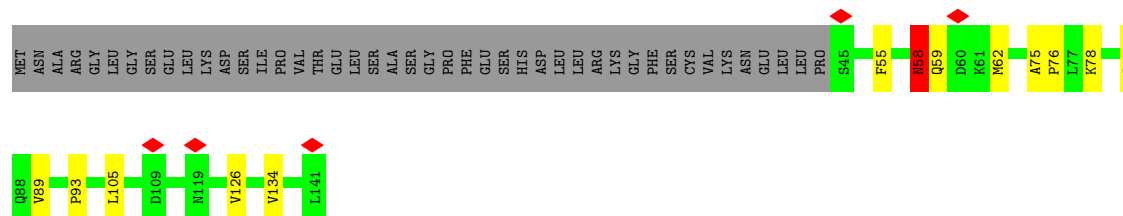
• Molecule 11: Proteasome assembly chaperone 1



• Molecule 12: Proteasome assembly chaperone 2



• Molecule 13: Proteasome maturation protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57026	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	37.005	Depositor
Minimum map value	-15.705	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	7	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.99	0/1852	1.49	1/2509 (0.0%)
2	B	0.99	0/1931	1.52	3/2613 (0.1%)
3	C	1.01	0/1845	1.53	0/2498
4	D	1.01	0/1769	1.51	0/2393
5	E	1.00	0/1867	1.48	0/2527
6	F	0.99	0/1903	1.53	0/2570
7	G	0.99	0/1926	1.52	0/2605
8	H	1.00	0/1506	1.54	0/2041
9	I	0.99	0/1367	1.51	0/1848
10	J	0.99	0/920	1.46	0/1251
11	c	1.01	0/2145	1.49	0/2918
12	d	0.97	0/1947	1.49	0/2641
13	e	0.97	0/781	1.55	1/1054 (0.1%)
All	All	0.99	0/21759	1.51	5/29468 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
4	D	0	1
5	E	0	2
6	F	0	1
7	G	0	1
8	H	0	2
11	c	0	1
13	e	0	1
All	All	0	11

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	157	GLY	CA-C-N	6.06	126.28	121.61
2	B	157	GLY	C-N-CA	6.06	126.28	121.61
13	e	58	ASN	N-CA-C	-5.36	107.29	112.97
1	A	43	GLY	CA-C-O	-5.17	117.92	122.16
2	B	158	GLY	CA-C-O	-5.11	117.12	121.57

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ILE	Peptide
3	C	101	PRO	Peptide
4	D	74	ILE	Peptide
5	E	143	HIS	Peptide
5	E	210	VAL	Peptide
6	F	167	GLY	Peptide
7	G	164	LYS	Peptide
8	H	0	THR	Peptide
8	H	89	TYR	Peptide
11	c	187	PRO	Peptide
13	e	87	GLN	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	1813	0	1806	6	0
2	B	1901	0	1862	6	0
3	C	1819	0	1791	12	0
4	D	1742	0	1709	9	0
5	E	1832	0	1799	11	0
6	F	1868	0	1813	6	0
7	G	1892	0	1888	3	0
8	H	1480	0	1469	1	0
9	I	1342	0	1342	15	0
10	J	904	0	870	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	c	2100	0	2055	6	0
12	d	1906	0	1925	9	0
13	e	768	0	758	6	0
All	All	21367	0	21087	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (95) 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)
5:E:200:PRO:HD2	5:E:203:GLN:OE1	1.68	0.94
9:I:23:ALA:HB2	9:I:167:ILE:HG12	1.61	0.82
9:I:14:MET:SD	9:I:167:ILE:HB	2.21	0.80
11:c:62:LEU:HD12	11:c:153:VAL:HG23	1.76	0.67
9:I:14:MET:HG3	9:I:167:ILE:HD12	1.77	0.66
13:e:55:PHE:O	13:e:59:GLN:HG2	1.98	0.64
5:E:196:ARG:NH1	5:E:236:LEU:HD22	2.11	0.64
4:D:177:ALA:HB2	4:D:205:VAL:HG21	1.81	0.63
10:J:64:VAL:HG12	10:J:75:LEU:HD12	1.82	0.62
9:I:23:ALA:CB	9:I:167:ILE:HG12	2.29	0.61
1:A:160:ALA:HB3	2:B:55:LEU:HD22	1.81	0.61
5:E:45:VAL:HG23	5:E:187:LEU:HD23	1.80	0.61
10:J:15:VAL:HG11	10:J:105:ALA:HB2	1.87	0.57
9:I:67:LEU:CD1	9:I:91:VAL:HG22	2.34	0.56
11:c:49:LEU:HD11	11:c:62:LEU:HD11	1.86	0.56
5:E:196:ARG:NH1	5:E:236:LEU:CD2	2.68	0.56
5:E:238:GLU:O	5:E:239:ARG:C	2.50	0.55
10:J:4:LEU:HD22	10:J:45:LEU:HB3	1.89	0.54
12:d:201:MET:HE3	12:d:203:VAL:CG2	2.38	0.54
10:J:7:ILE:HD12	10:J:14:LEU:HD22	1.91	0.53
6:F:113:ALA:HB1	6:F:152:ILE:HD11	1.91	0.52
3:C:158:ALA:HB2	3:C:176:TYR:CD1	2.44	0.52
4:D:116:VAL:HG21	4:D:143:PHE:CZ	2.45	0.52
3:C:176:TYR:CE1	3:C:181:ILE:HD11	2.46	0.51
1:A:39:LYS:HA	1:A:44:VAL:HG22	1.92	0.51
3:C:181:ILE:HD13	3:C:187:THR:HG22	1.92	0.51
9:I:87:LEU:O	9:I:91:VAL:HG23	2.11	0.51
10:J:36:PHE:CZ	10:J:54:VAL:HG12	2.47	0.50
6:F:191:VAL:HG21	6:F:228:VAL:HG21	1.94	0.50
3:C:168:VAL:HG13	3:C:194:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:212:ASP:C	12:d:213:ASN:HD22	2.19	0.49
4:D:217:LEU:HD23	4:D:218:ALA:N	2.27	0.49
5:E:109:VAL:HG21	5:E:145:PHE:CB	2.42	0.49
3:C:108:THR:HG22	3:C:133:ILE:HB	1.95	0.48
13:e:93:PRO:HD2	13:e:134:VAL:HG22	1.95	0.48
2:B:35:LEU:HD11	2:B:175:LEU:HD11	1.96	0.48
11:c:247:VAL:HG11	11:c:273:LEU:HD13	1.96	0.47
12:d:41:MET:HE2	12:d:87:ALA:HB2	1.96	0.47
10:J:84:THR:HG23	10:J:118:MET:HE1	1.96	0.47
4:D:202:LEU:HD13	4:D:215:ILE:HD11	1.96	0.47
9:I:12:MET:HE2	9:I:167:ILE:HG13	1.97	0.47
3:C:104:VAL:O	3:C:108:THR:HG23	2.15	0.46
7:G:40:VAL:HG13	7:G:179:LEU:HD11	1.96	0.46
9:I:14:MET:HE3	9:I:154:TRP:CD1	2.51	0.46
4:D:146:VAL:HG23	4:D:220:VAL:HG13	1.97	0.46
3:C:144:LEU:HD21	3:C:159:ASN:HB2	1.97	0.46
3:C:158:ALA:HB3	4:D:58:LEU:HD22	1.98	0.46
9:I:109:ILE:HD12	9:I:109:ILE:N	2.30	0.46
12:d:35:ILE:HD11	12:d:221:VAL:HG12	1.99	0.45
4:D:88:LEU:HD23	4:D:119:LEU:HD23	1.99	0.45
4:D:85:ALA:HB2	4:D:139:VAL:HG21	1.99	0.45
3:C:37:GLY:HA2	3:C:181:ILE:HD12	1.99	0.44
9:I:58:THR:HG22	10:J:123:ALA:HB2	1.98	0.44
3:C:42:VAL:CG1	3:C:208:LEU:HD21	2.47	0.44
5:E:200:PRO:CD	5:E:203:GLN:OE1	2.53	0.44
2:B:8:ARG:O	2:B:9:THR:HG22	2.17	0.44
6:F:109:LEU:HD11	6:F:138:LEU:HB3	1.98	0.44
12:d:12:LEU:HD22	12:d:86:VAL:HG11	2.00	0.44
2:B:161:ALA:HB1	2:B:175:LEU:HD13	1.99	0.44
7:G:171:LYS:O	7:G:172:GLN:C	2.60	0.44
11:c:206:LEU:HD22	11:c:210:ASN:HB3	2.00	0.44
2:B:38:LEU:HA	2:B:43:VAL:HG23	1.99	0.44
5:E:237:GLU:O	5:E:238:GLU:CB	2.66	0.44
1:A:160:ALA:HB1	1:A:174:LEU:HD21	2.01	0.43
6:F:216:TRP:CD2	6:F:228:VAL:HG22	2.53	0.43
11:c:259:LEU:HA	11:c:262:LEU:HD23	2.00	0.43
3:C:208:LEU:C	3:C:208:LEU:HD23	2.44	0.43
4:D:42:THR:CG2	4:D:194:ALA:HB2	2.49	0.43
8:H:137:PHE:HA	8:H:153:LEU:HD11	2.00	0.43
9:I:173:ASN:O	9:I:174:ALA:C	2.62	0.43
2:B:111:VAL:HG22	2:B:136:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:ILE:HD12	10:J:16:ALA:HB3	2.00	0.43
10:J:47:VAL:C	10:J:53:THR:HG22	2.44	0.43
12:d:19:MET:SD	12:d:190:LEU:HD21	2.59	0.43
11:c:87:VAL:CG2	11:c:259:LEU:HD11	2.49	0.42
12:d:19:MET:SD	12:d:106:LEU:HD21	2.59	0.42
13:e:58:ASN:O	13:e:62:MET:SD	2.77	0.42
5:E:105:VAL:O	5:E:109:VAL:HG23	2.19	0.42
9:I:23:ALA:CB	9:I:167:ILE:CG1	2.97	0.42
1:A:127:VAL:HB	13:e:89:VAL:HG11	2.01	0.42
7:G:124:VAL:HG11	13:e:105:LEU:HD11	2.02	0.41
1:A:69:THR:O	1:A:70:LYS:C	2.63	0.41
6:F:197:ILE:O	6:F:201:VAL:HG13	2.20	0.41
9:I:14:MET:HG3	9:I:167:ILE:CD1	2.47	0.41
12:d:20:PRO:O	12:d:21:ALA:C	2.63	0.41
13:e:75:ALA:HB3	13:e:76:PRO:HD3	2.01	0.41
9:I:63:VAL:HG11	9:I:105:THR:HG21	2.02	0.41
10:J:6:GLY:CA	10:J:115:LEU:HD21	2.50	0.41
5:E:103:LEU:HD23	5:E:108:LEU:HD13	2.02	0.41
6:F:69:ASN:O	6:F:70:VAL:C	2.63	0.41
12:d:94:PHE:CE2	12:d:186:ILE:HD13	2.55	0.41
1:A:47:ALA:HB3	1:A:191:ALA:HB1	2.03	0.41
3:C:216:SER:O	3:C:217:LEU:C	2.64	0.41
9:I:67:LEU:HD12	9:I:91:VAL:HG22	2.04	0.40
5:E:236:LEU:HD23	5:E:237:GLU:N	2.35	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	231/234 (99%)	212 (92%)	18 (8%)	1 (0%)	30 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	248/261 (95%)	222 (90%)	23 (9%)	3 (1%)	11	41
3	C	236/248 (95%)	208 (88%)	22 (9%)	6 (2%)	4	24
4	D	228/241 (95%)	197 (86%)	27 (12%)	4 (2%)	7	32
5	E	234/263 (89%)	214 (92%)	18 (8%)	2 (1%)	14	49
6	F	241/255 (94%)	214 (89%)	19 (8%)	8 (3%)	3	18
7	G	243/246 (99%)	228 (94%)	13 (5%)	2 (1%)	16	51
8	H	193/277 (70%)	171 (89%)	18 (9%)	4 (2%)	5	28
9	I	169/205 (82%)	142 (84%)	25 (15%)	2 (1%)	11	41
10	J	117/201 (58%)	93 (80%)	20 (17%)	4 (3%)	3	17
11	c	271/288 (94%)	236 (87%)	31 (11%)	4 (2%)	8	36
12	d	240/264 (91%)	221 (92%)	14 (6%)	5 (2%)	5	28
13	e	95/141 (67%)	88 (93%)	7 (7%)	0	100	100
All	All	2746/3124 (88%)	2446 (89%)	255 (9%)	45 (2%)	10	34

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	204	SER
5	E	238	GLU
6	F	70	VAL
7	G	172	GLN
8	H	-25	CYS
10	J	98	TYR
3	C	182	GLU
6	F	222	ASN
8	H	33	ILE
9	I	22	ILE
10	J	50	ALA
11	c	131	SER
11	c	214	ASP
11	c	265	ASN
12	d	21	ALA
12	d	24	VAL
2	B	130	PHE
3	C	51	ALA
3	C	160	ALA
3	C	218	LYS
4	D	72	ALA

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Mol	Chain	Res	Type
4	D	229	PHE
11	c	227	LYS
2	B	206	LEU
4	D	137	PHE
4	D	189	MET
5	E	226	ASP
6	F	35	SER
6	F	127	SER
6	F	163	GLY
7	G	209	ASP
12	d	251	TRP
1	A	215	GLU
3	C	48	LYS
3	C	52	LYS
6	F	80	GLY
6	F	209	ALA
8	H	8	LYS
10	J	105	ALA
12	d	166	SER
6	F	223	GLY
8	H	-1	GLY
12	d	22	VAL
10	J	97	PRO
9	I	8	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/191 (98%)	181 (96%)	7 (4%)	29	63
2	B	189/221 (86%)	183 (97%)	6 (3%)	34	67
3	C	183/211 (87%)	178 (97%)	5 (3%)	40	71
4	D	183/203 (90%)	172 (94%)	11 (6%)	16	47
5	E	191/224 (85%)	188 (98%)	3 (2%)	58	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	188/212 (89%)	182 (97%)	6 (3%)	34	67
7	G	202/210 (96%)	189 (94%)	13 (6%)	14	44
8	H	155/228 (68%)	148 (96%)	7 (4%)	23	57
9	I	141/174 (81%)	136 (96%)	5 (4%)	31	65
10	J	86/171 (50%)	80 (93%)	6 (7%)	12	41
11	c	222/262 (85%)	210 (95%)	12 (5%)	18	50
12	d	213/237 (90%)	208 (98%)	5 (2%)	45	75
13	e	87/128 (68%)	84 (97%)	3 (3%)	32	66
All	All	2228/2672 (83%)	2139 (96%)	89 (4%)	29	61

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	65	VAL
1	A	119	GLN
1	A	156	PHE
1	A	200	GLU
1	A	213	CYS
1	A	214	ASN
2	B	34	CYS
2	B	43	VAL
2	B	44	LEU
2	B	68	LEU
2	B	135	LEU
2	B	200	THR
3	C	45	VAL
3	C	59	VAL
3	C	62	ILE
3	C	71	MET
3	C	129	ILE
4	D	33	LEU
4	D	46	VAL
4	D	67	ILE
4	D	70	ILE
4	D	121	LEU
4	D	152	GLN
4	D	158	PRO
4	D	202	LEU

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Mol	Chain	Res	Type
4	D	215	ILE
4	D	229	PHE
4	D	238	ILE
5	E	112	ILE
5	E	148	CYS
5	E	195	LEU
6	F	4	ILE
6	F	36	THR
6	F	42	CYS
6	F	50	VAL
6	F	127	SER
6	F	191	VAL
7	G	12	HIS
7	G	23	TYR
7	G	50	ILE
7	G	56	VAL
7	G	66	VAL
7	G	73	THR
7	G	76	ILE
7	G	137	CYS
7	G	154	CYS
7	G	160	TYR
7	G	175	SER
7	G	200	THR
7	G	215	ILE
8	H	-7	PRO
8	H	1	THR
8	H	75	VAL
8	H	124	VAL
8	H	145	MET
8	H	147	GLU
8	H	154	VAL
9	I	125	ASP
9	I	133	THR
9	I	137	VAL
9	I	165	GLU
9	I	167	ILE
10	J	15	VAL
10	J	36	PHE
10	J	37	LYS
10	J	44	LEU
10	J	46	CYS

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Mol	Chain	Res	Type
10	J	96	THR
11	c	39	LEU
11	c	73	ILE
11	c	101	LEU
11	c	103	ASN
11	c	121	CYS
11	c	133	PHE
11	c	134	LEU
11	c	166	ILE
11	c	186	SER
11	c	189	LEU
11	c	203	CYS
11	c	259	LEU
12	d	88	LEU
12	d	115	CYS
12	d	162	GLU
12	d	205	LEU
12	d	209	SER
13	e	58	ASN
13	e	78	LYS
13	e	126	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	102	GLN
2	B	102	GLN
2	B	109	GLN
2	B	119	GLN
2	B	146	GLN
2	B	230	GLN
5	E	117	GLN
5	E	166	GLN
6	F	171	GLN
7	G	53	GLN
7	G	92	GLN
7	G	172	GLN
7	G	193	GLN
8	H	39	ASN
9	I	145	GLN
10	J	101	ASN

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Mol	Chain	Res	Type
11	c	103	ASN
11	c	146	GLN
11	c	208	GLN
12	d	59	ASN
12	d	67	ASN
12	d	213	ASN
13	e	56	GLN
13	e	87	GLN
13	e	99	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.

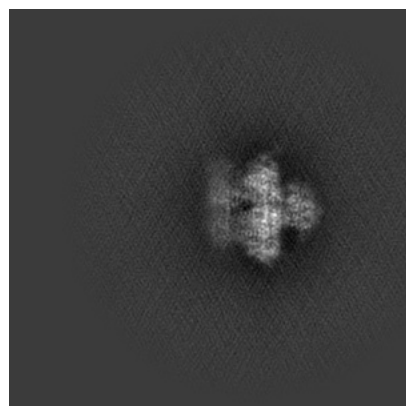
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41378. These allow visual inspection of the internal detail of the map and identification of artifacts.

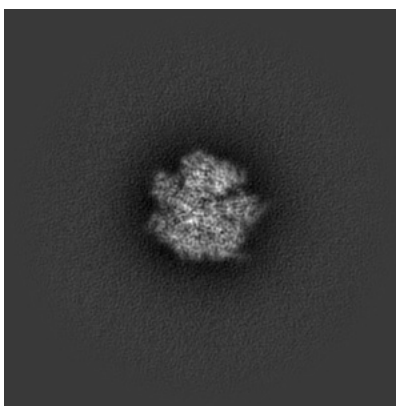
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

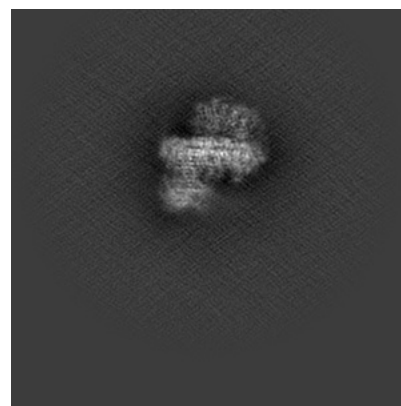
6.1.1 Primary map



X

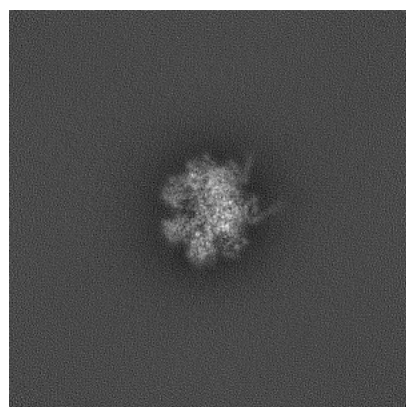


Y

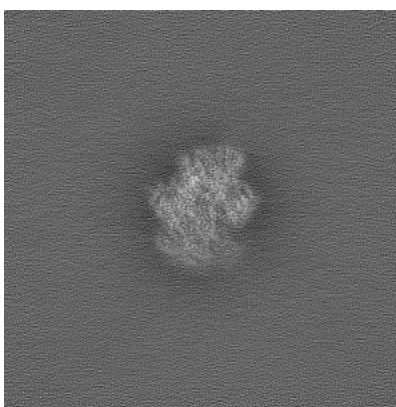


Z

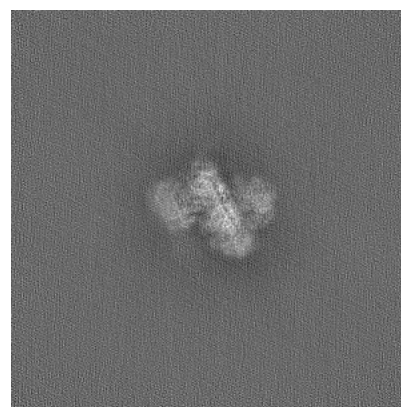
6.1.2 Raw map



X



Y

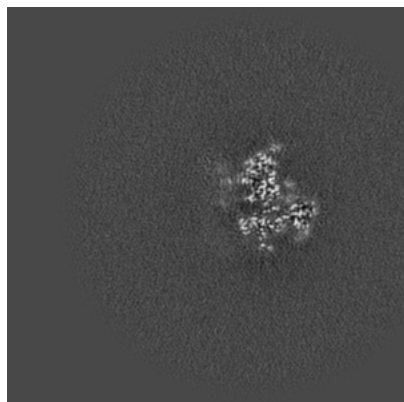


Z

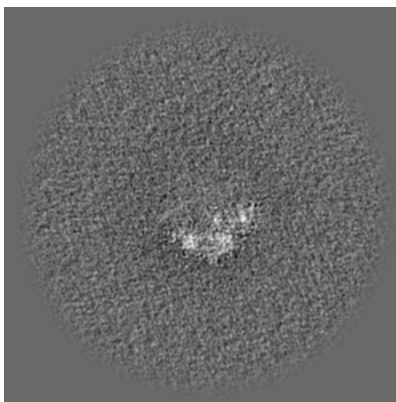
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

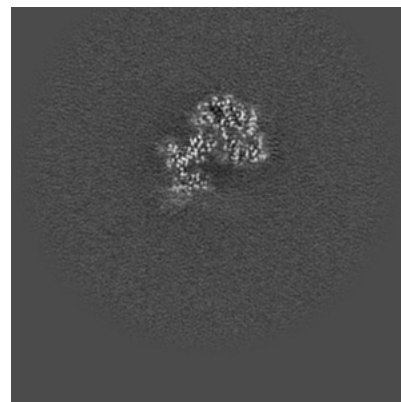
6.2.1 Primary map



X Index: 200

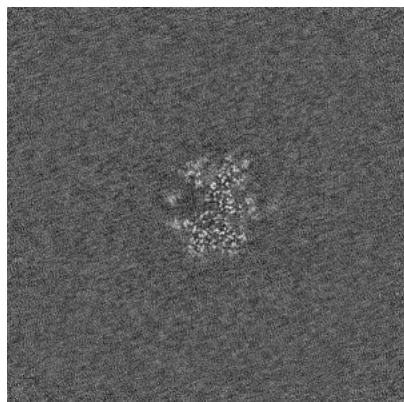


Y Index: 200

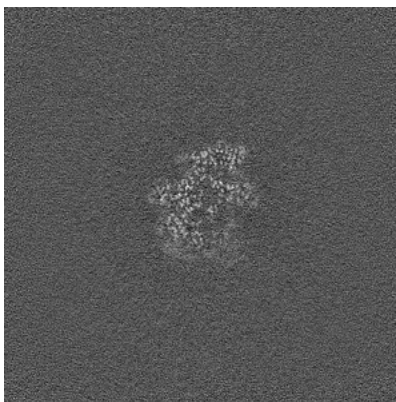


Z Index: 200

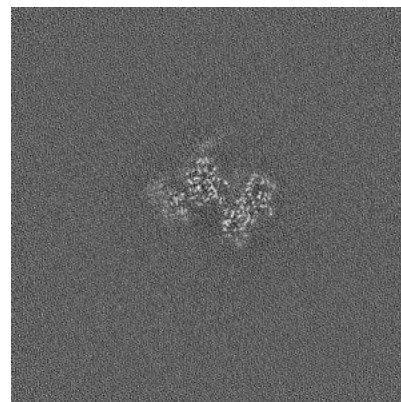
6.2.2 Raw map



X Index: 200



Y Index: 200

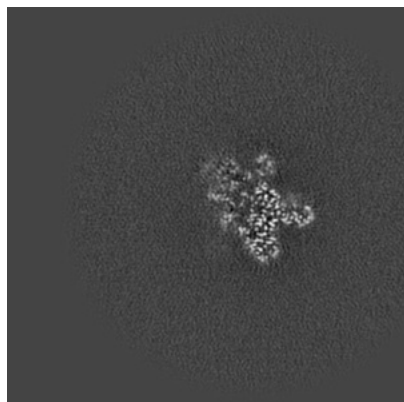


Z Index: 200

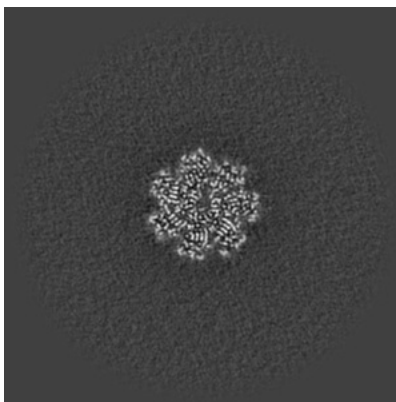
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

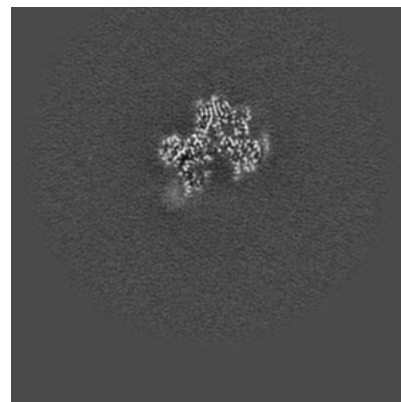
6.3.1 Primary map



X Index: 188

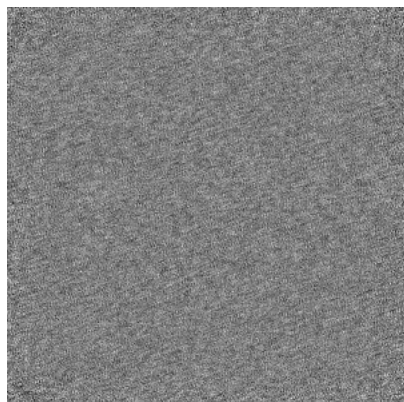


Y Index: 255

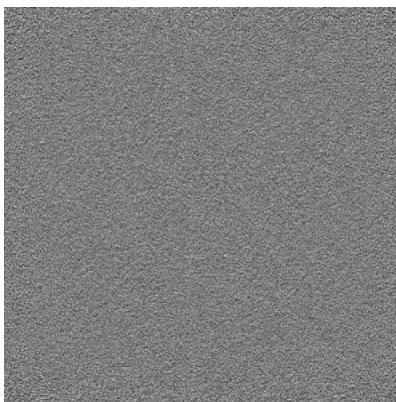


Z Index: 193

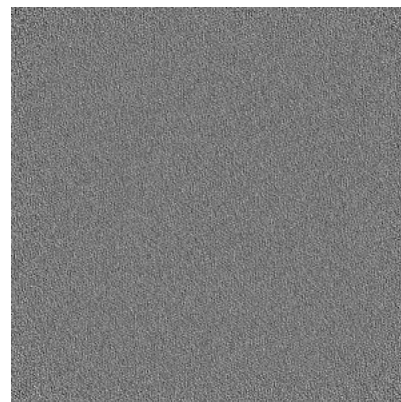
6.3.2 Raw map



X Index: 0



Y Index: 0

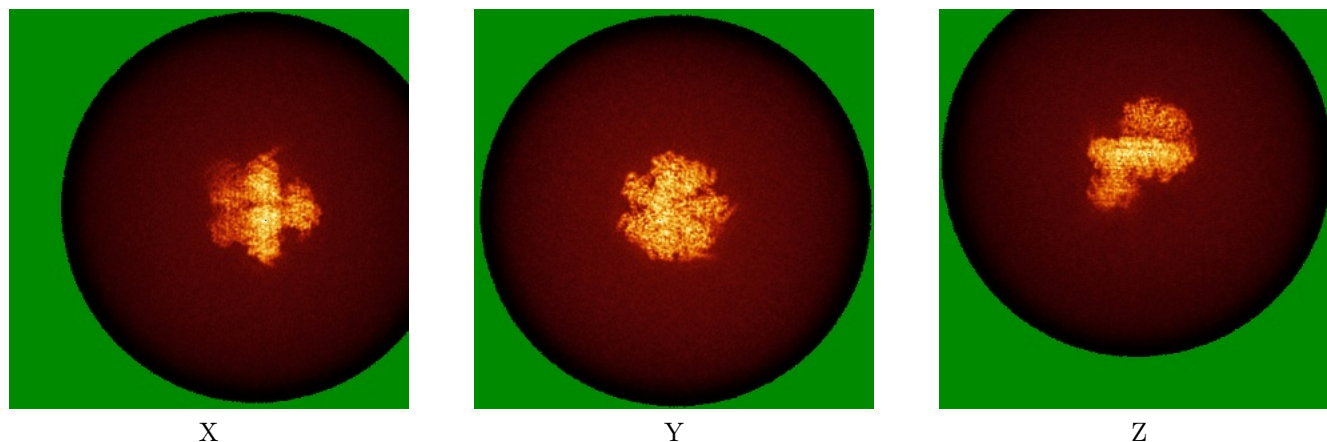


Z Index: 0

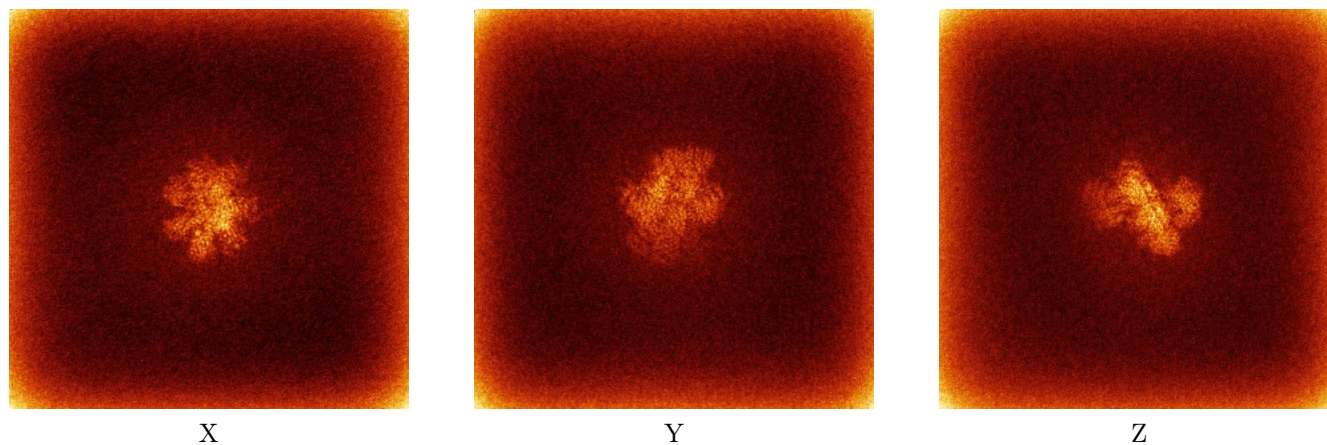
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



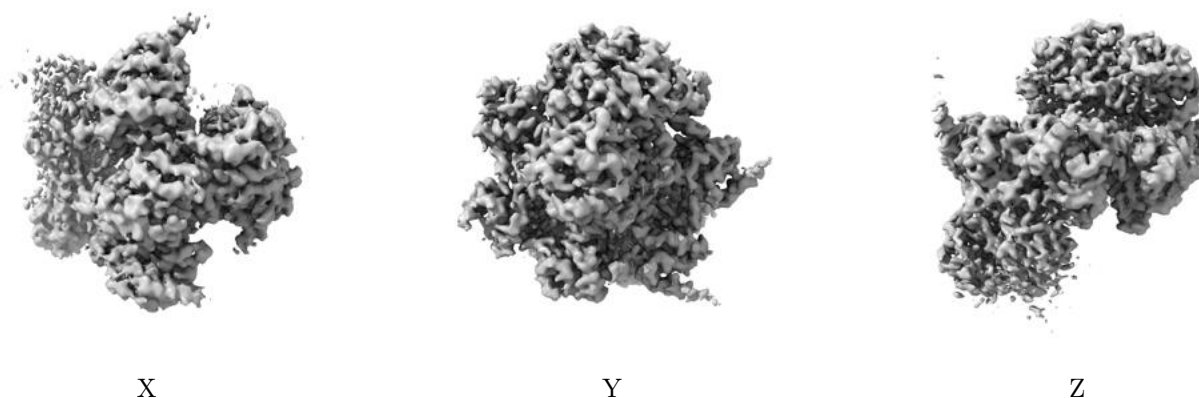
6.4.2 Raw map



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.

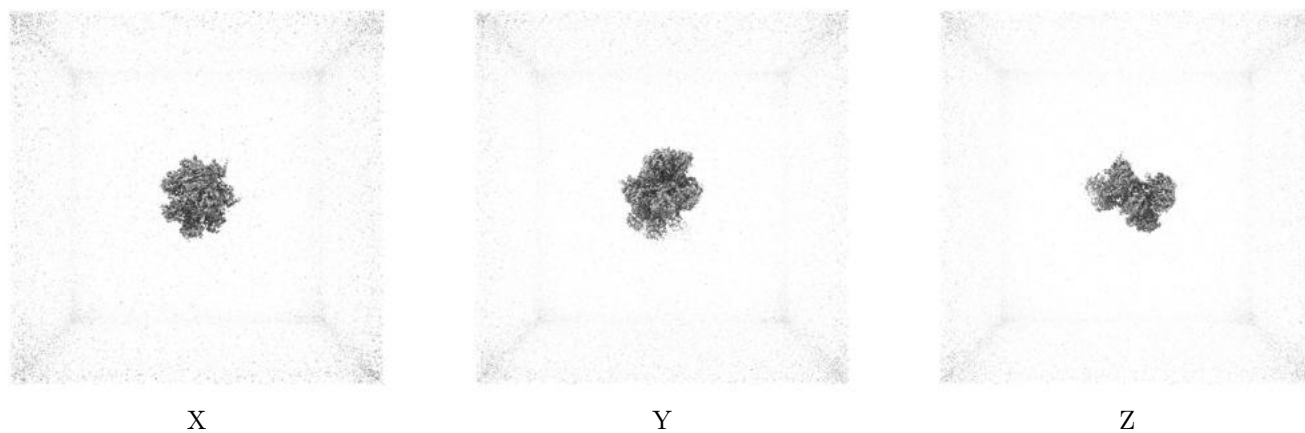
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. 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.

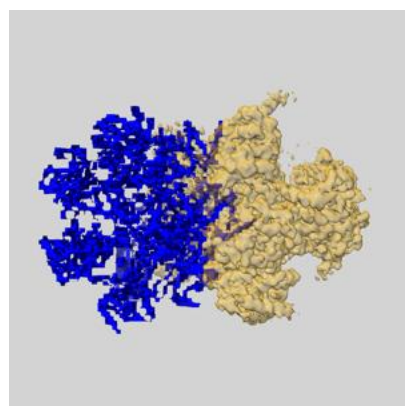
6.6 Mask visualisation [i](#)

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

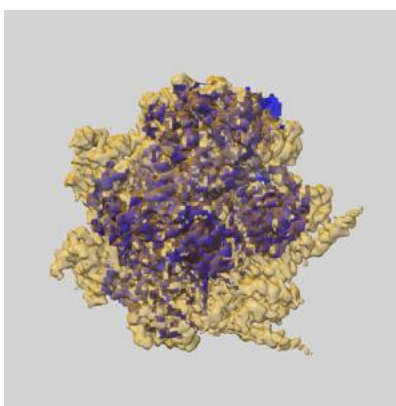
A mask typically either:

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

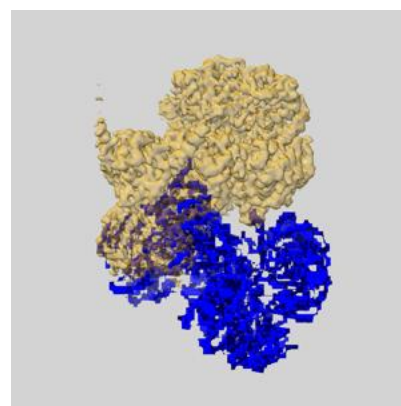
6.6.1 emd_41378_msk_1.map [i](#)



X



Y

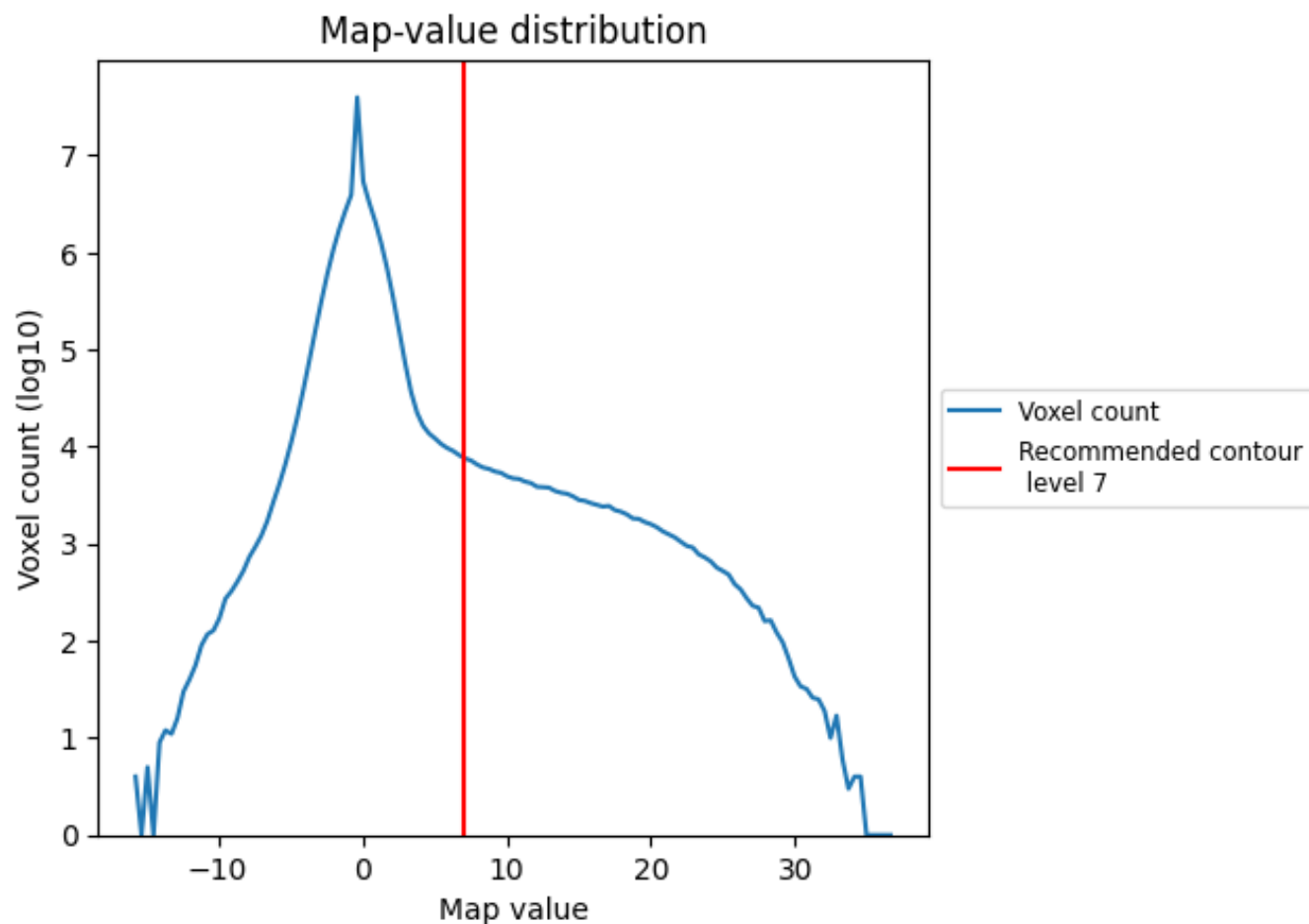


Z

7 Map analysis [i](#)

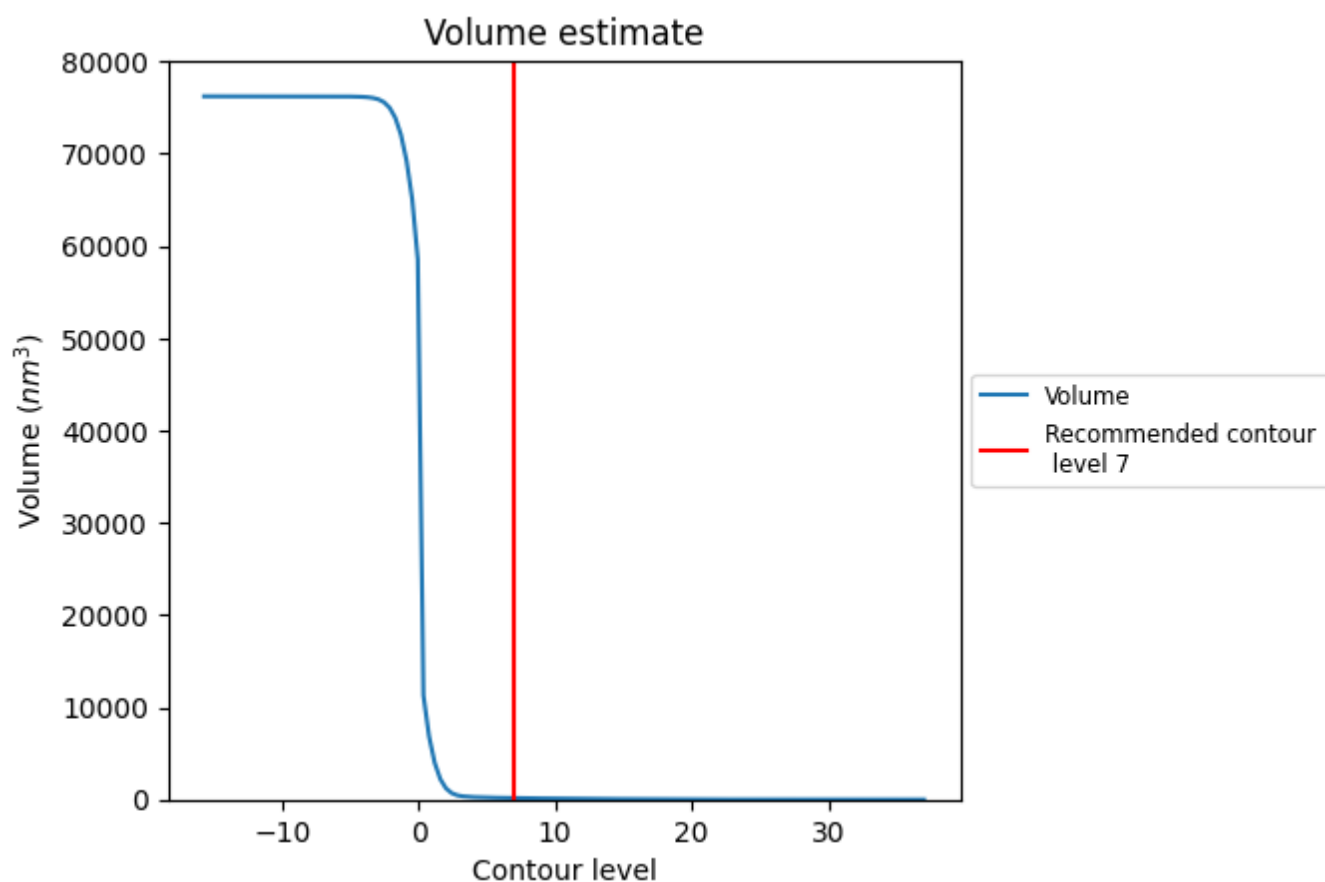
This section contains the results of statistical analysis of the map.

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.

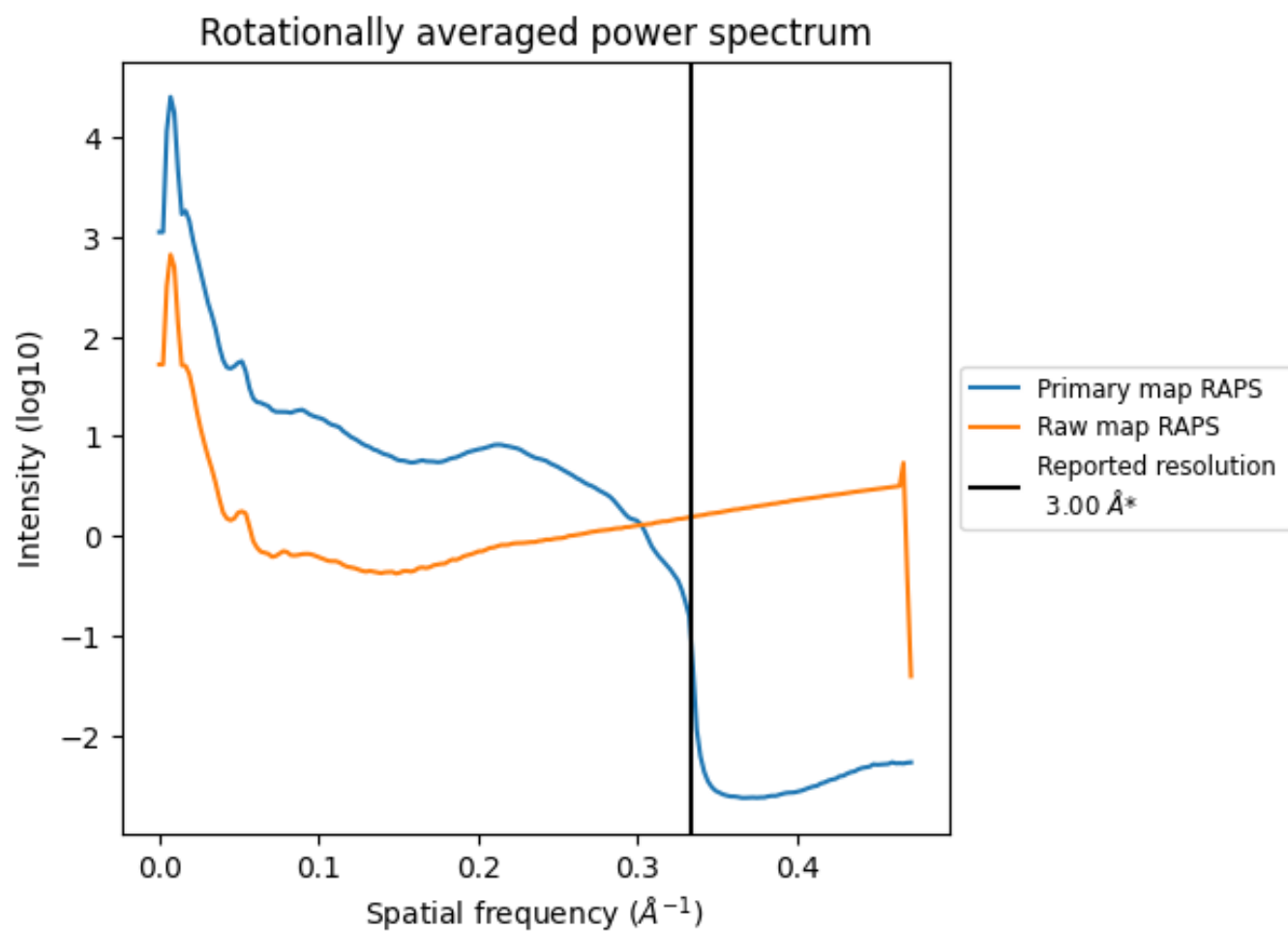
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 164 nm³; this corresponds to an approximate mass of 148 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 ⓘ

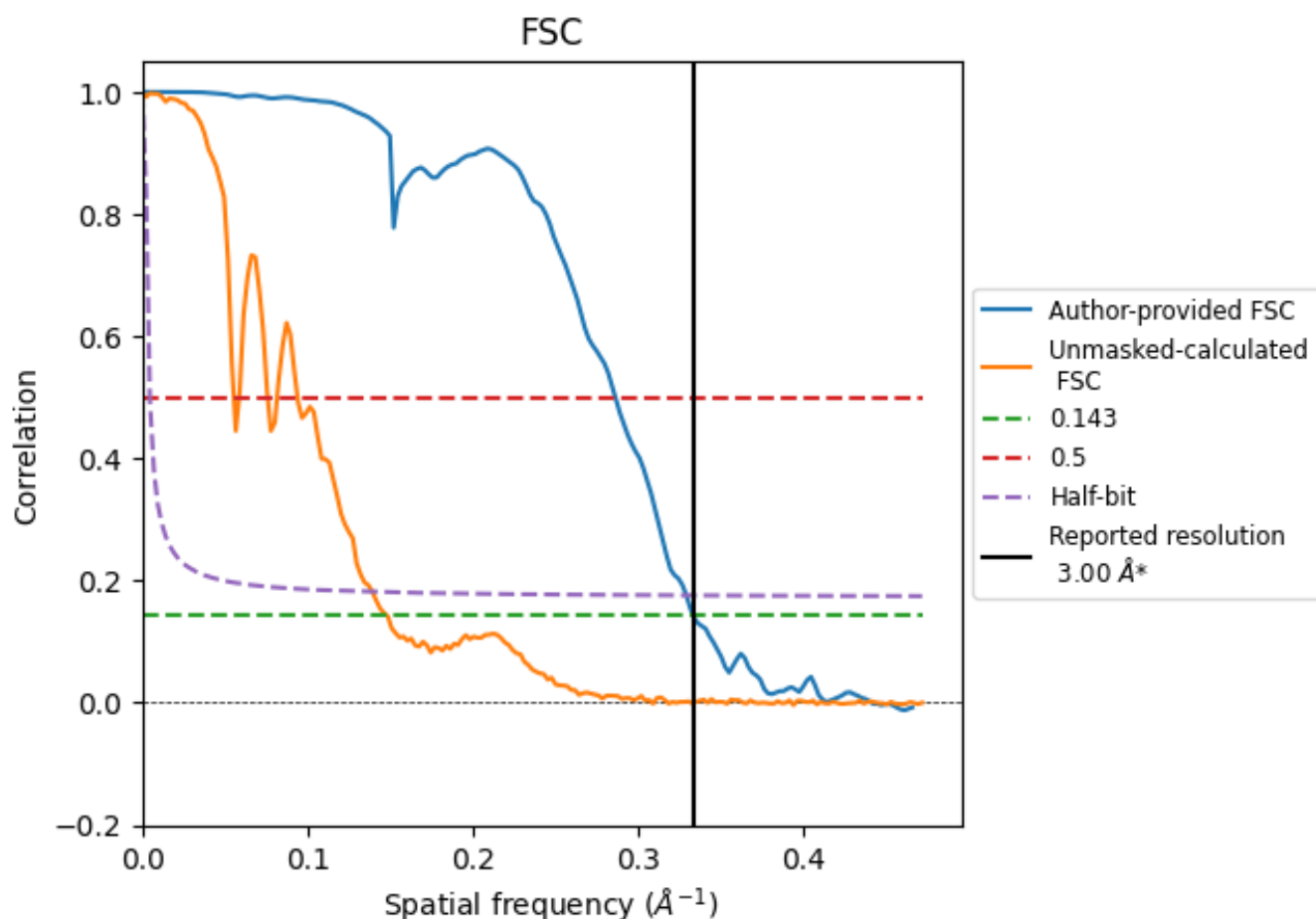


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

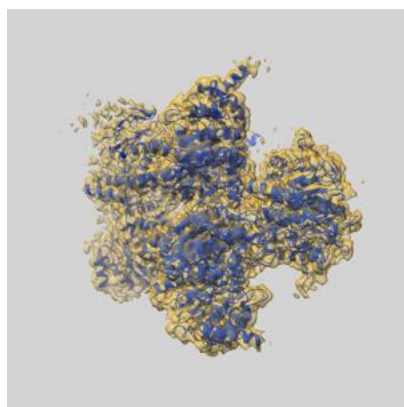
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.50	3.04
Unmasked-calculated*	6.76	18.05	7.18

*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 6.76 differs from the reported value 3.0 by more than 10 %

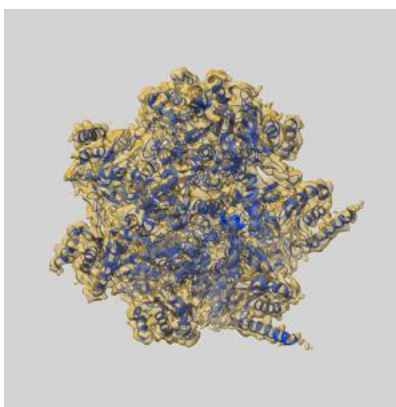
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41378 and PDB model 8TM4. Per-residue inclusion information can be found in section [3](#) on page [6](#).

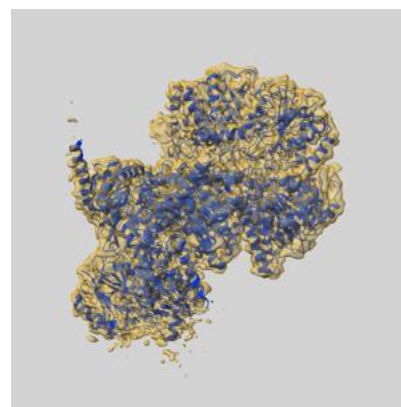
9.1 Map-model overlay [i](#)



X



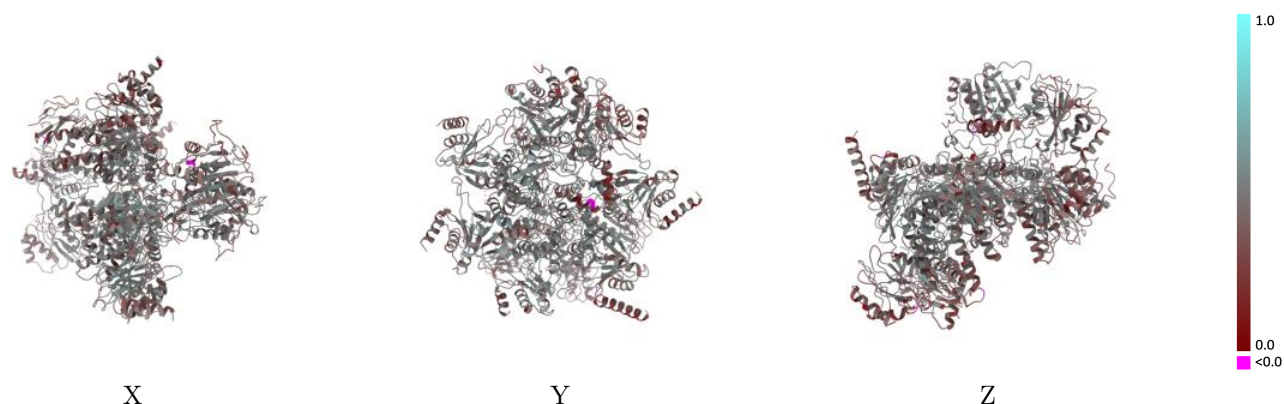
Y



Z

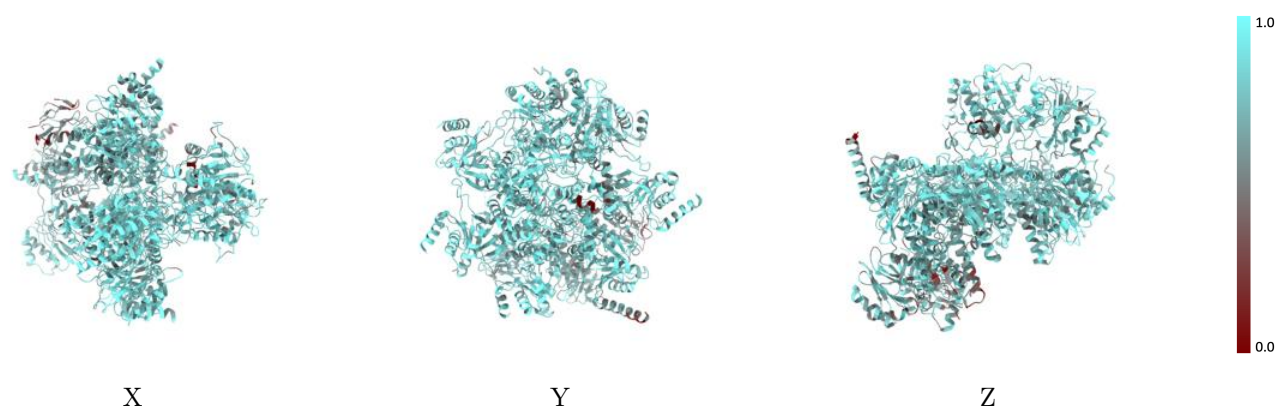
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



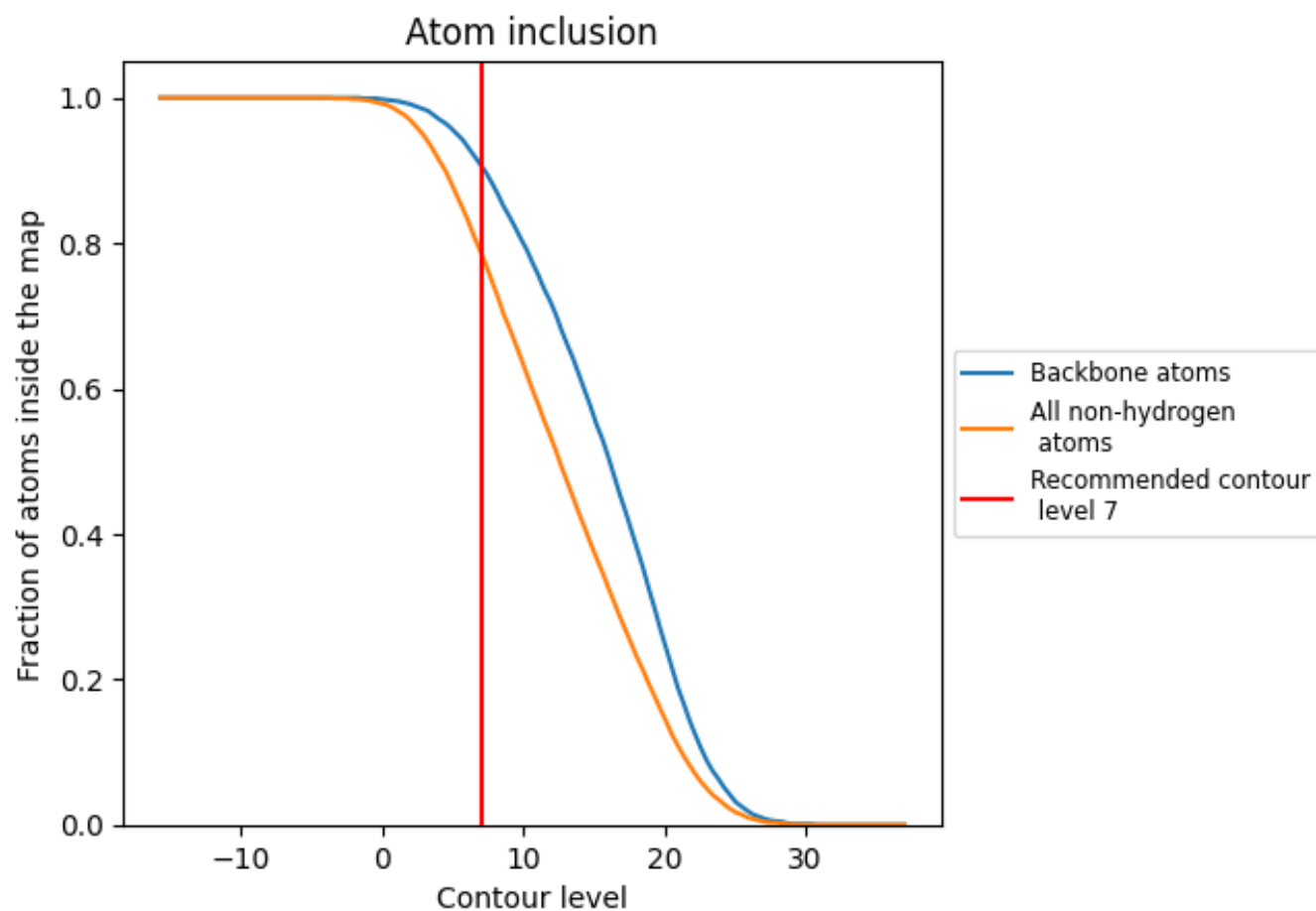
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 79% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7870	<div></div> 0.4290
A	<div></div> 0.8280	<div></div> 0.4620
B	<div></div> 0.8010	<div></div> 0.4480
C	<div></div> 0.8150	<div></div> 0.4240
D	<div></div> 0.7720	<div></div> 0.3920
E	<div></div> 0.8390	<div></div> 0.4500
F	<div></div> 0.8300	<div></div> 0.4440
G	<div></div> 0.8320	<div></div> 0.4590
H	<div></div> 0.7820	<div></div> 0.4070
I	<div></div> 0.7190	<div></div> 0.3980
J	<div></div> 0.5670	<div></div> 0.3790
c	<div></div> 0.7530	<div></div> 0.3930
d	<div></div> 0.8180	<div></div> 0.4480
e	<div></div> 0.6890	<div></div> 0.4590

1.0

0.0

<0.0