



Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 12:05 PM EDT

PDB ID : 8TM3 / pdb_00008tm3
EMDB ID : EMD-41377
Title : Human proteasome alpha ring 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

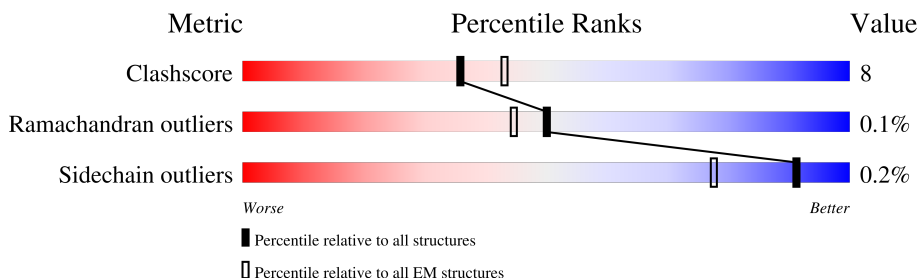
1 Overall quality at a glance

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	
2	B	261	
3	C	248	
4	D	241	
5	E	263	
6	F	255	
7	G	246	
8	c	288	

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Mol	Chain	Length	Quality of chain
9	d	264	 <div>79%16%5%</div>
10	i	122	 <div>72%24%</div>
11	j	123	 <div>84%8%8%</div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17562 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	228	Total	C	N	O	S	0	0
			1653	1066	279	303	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	239	Total	C	N	O	S	0	0
			1731	1099	299	325	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	231	Total	C	N	O	S	0	0
			1734	1096	314	319	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	241	Total	C	N	O	S	0	0
			1780	1128	299	341	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	239	Total	C	N	O	S	0	0
			1839	1161	332	335	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	242	Total	C	N	O	S	0	0
			1788	1138	306	334	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	241	Total	C	N	O	S	0	0
			1815	1159	304	339	13		

- Molecule 8 is a protein called Proteasome assembly chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	240	Total	C	N	O	S	0	0
			1777	1148	293	322	14		

- Molecule 9 is a protein called Proteasome assembly chaperone 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	250	Total	C	N	O	S	0	0
			1782	1153	296	323	10		

- Molecule 10 is a protein called Proteasome assembly chaperone 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	i	117	Total	C	N	O	S	0	0
			841	538	142	157	4		

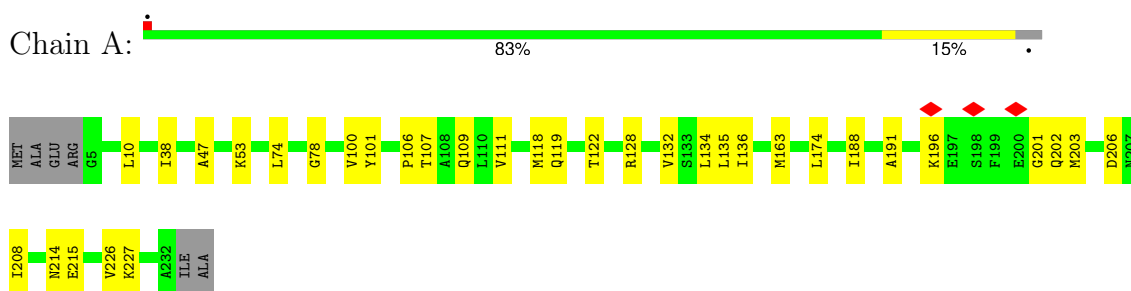
- Molecule 11 is a protein called Proteasome assembly chaperone 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	113	Total	C	N	O	S	0	0
			822	525	146	148	3		

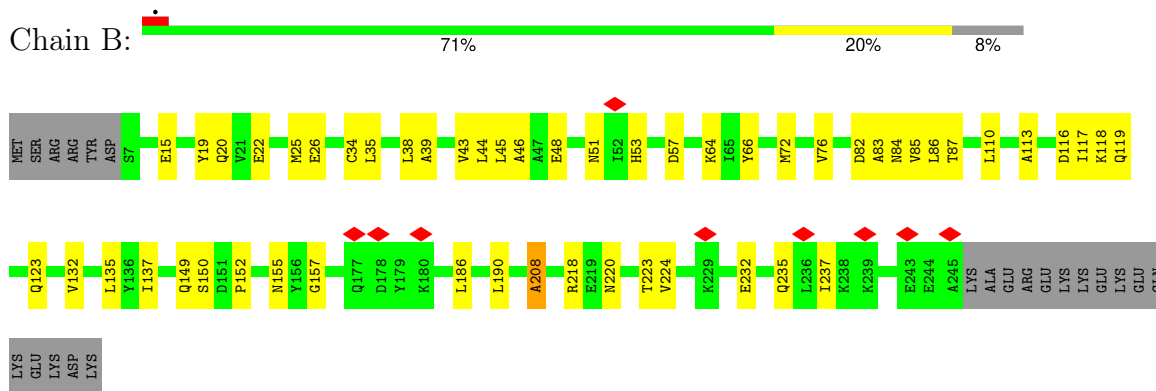
3 Residue-property plots

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.

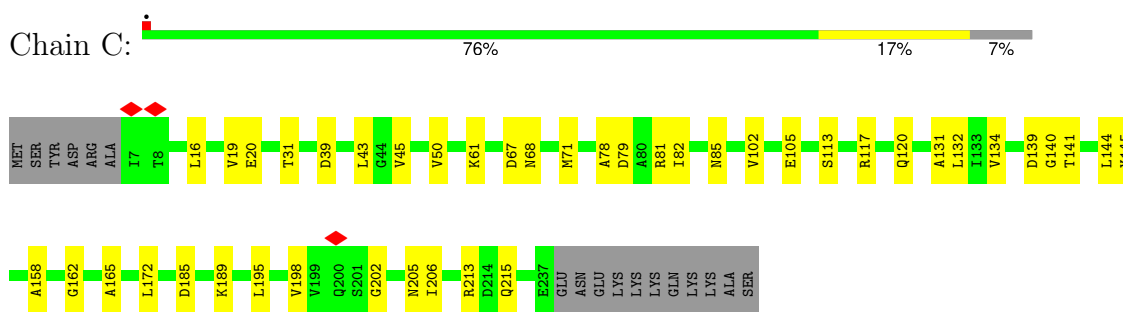
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-4



- Molecule 3: Proteasome subunit alpha type-7



- Molecule 4: Proteasome subunit alpha type-5

The chart displays the percentage of weeks with influenza activity in the United States during the 2019-2020 season. The y-axis represents the percentage of weeks with activity, ranging from 0 to 100. The x-axis shows the weeks of the year, from week 1 to week 52. The chart is divided into two main sections: 'Influenza A (H3N2) virus activity' (top) and 'Influenza A (H1N1) virus activity' (bottom). The top section shows a significant peak in activity around week 10, reaching nearly 100% for H3N2 and around 80% for H1N1. The bottom section shows a smaller peak around week 10, reaching about 40% for H3N2 and about 20% for H1N1. The chart also includes a legend for 'Influenza A (H3N2) virus activity' and 'Influenza A (H1N1) virus activity'.

- Chain E: 81% 9% 9%

GLU	M1
LYS	
ALA	P15
ASP	N26
GLU	
PRO	V29
MET	
GLU	A34
HIS	
	A44
	V45
	E55
	K62
	I72
	S73
	I74
	A75
	A81
	R82
	N86
	F87
	N88
	R89
	Q90
	E91
	I144
	A151
	N152
	M180
	L187
	V188
	I212
	R239
	GLN
	ARG
	LYS
	ALA
	GLN
	PRO
	ALA
	GLN
	PRO
	ALA
	ASP
	GLU
	PRO

- Chain F: 77% 18% 5%

[illegible]

- Chain G: 82% 16%

Diagram illustrating the locations of 100 genes across the human genome, showing the distribution of genes across chromosomes and the relative positions of specific genes (e.g., MET, G4, S5, T14, I15, R21, E26, F29, R30, A31, I32, G36, L37, R43, V49, P57, L61, D62, M80, M83, R88, Q92, C115, Q123, T126, M131, C154, Y159, Y160, C161, K164, A165, L179, E192, V195, V219, R228, T231, E232, A233, E234, H238, L242, A243, E244, ARG, ASP).

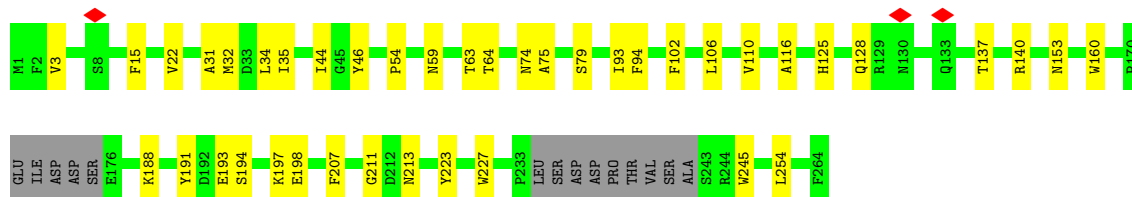
- Chain c:

[illegible]



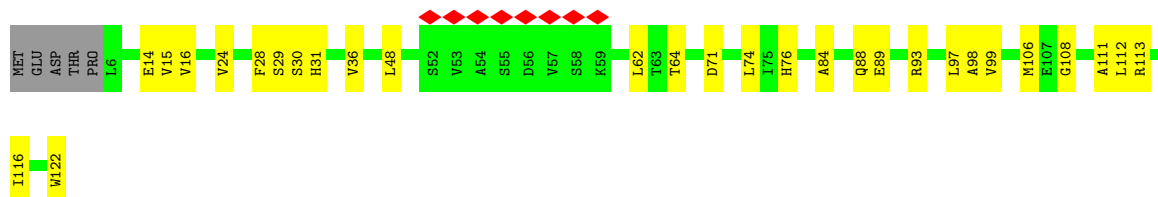
- Molecule 9: Proteasome assembly chaperone 2

Chain d: 79% 16% 5%



- Molecule 10: Proteasome assembly chaperone 3

Chain i: 7% 72% 24%



- Molecule 11: Proteasome assembly chaperone 4

Chain j: 84% 8% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111057	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	42.246	Depositor
Minimum map value	-19.073	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 [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	A	0.13	0/1690	0.33	0/2307
2	B	0.14	0/1758	0.36	0/2395
3	C	0.12	0/1759	0.27	0/2385
4	D	0.12	0/1808	0.28	0/2450
5	E	0.12	0/1874	0.27	0/2537
6	F	0.13	0/1823	0.28	0/2474
7	G	0.15	0/1849	0.36	1/2509 (0.0%)
8	c	0.12	0/1817	0.30	0/2487
9	d	0.13	0/1823	0.32	0/2494
10	i	0.15	0/852	0.33	0/1164
11	j	0.17	0/840	0.31	0/1149
All	All	0.13	0/17893	0.31	1/24351 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	57	PRO	CA-N-CD	-10.66	97.07	112.00

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	1653	0	1566	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1731	0	1621	42	0
3	C	1734	0	1703	29	0
4	D	1780	0	1723	25	0
5	E	1839	0	1808	17	0
6	F	1788	0	1670	28	0
7	G	1815	0	1777	26	0
8	c	1777	0	1663	23	0
9	d	1782	0	1661	33	0
10	i	841	0	846	22	0
11	j	822	0	746	7	0
All	All	17562	0	16784	262	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 8.

All (262) 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)
9:d:128:GLN:CB	9:d:207:PHE:CE1	2.34	1.10
3:C:120:GLN:NE2	4:D:133:MET:SD	2.42	0.93
9:d:128:GLN:CB	9:d:207:PHE:CD1	2.52	0.91
5:E:72:ILE:HG21	5:E:88:MET:HE1	1.54	0.89
5:E:15:PRO:O	6:F:29:LYS:NZ	2.09	0.85
10:i:29:SER:OG	11:j:45:PRO:O	1.96	0.81
4:D:114:GLN:OE1	5:E:82:ARG:NH1	2.16	0.78
11:j:32:ARG:NH1	11:j:121:GLU:O	2.18	0.76
2:B:15:GLU:OE1	2:B:15:GLU:N	2.19	0.75
4:D:233:GLU:O	4:D:237:VAL:HG23	1.85	0.75
2:B:118:LYS:NZ	2:B:150:SER:OG	2.20	0.74
2:B:45:LEU:HB2	2:B:137:ILE:HD13	1.71	0.73
3:C:140:GLY:O	3:C:213:ARG:NH1	2.21	0.72
2:B:51:ASN:OD1	2:B:53:HIS:N	2.23	0.71
10:i:64:THR:OG1	10:i:76:HIS:ND1	2.21	0.71
5:E:55:GLU:N	5:E:55:GLU:OE1	2.24	0.70
6:F:120:VAL:O	6:F:124:THR:HG23	1.91	0.70
6:F:20:ARG:NE	6:F:25:GLU:OE2	2.25	0.69
3:C:202:GLY:O	3:C:205:ASN:ND2	2.25	0.68
2:B:186:LEU:O	2:B:190:LEU:HD22	1.92	0.68
3:C:139:ASP:OD2	3:C:141:THR:OG1	2.11	0.68
5:E:180:MET:HE2	5:E:180:MET:HA	1.74	0.67
8:c:259:LEU:HA	8:c:262:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:208:GLN:NE2	9:d:59:ASN:O	2.28	0.67
2:B:43:VAL:HG22	2:B:137:ILE:HG22	1.76	0.66
9:d:211:GLY:O	9:d:213:ASN:ND2	2.29	0.65
7:G:192:GLU:OE1	7:G:192:GLU:N	2.29	0.65
2:B:218:ARG:NH1	2:B:223:THR:HG23	2.12	0.64
6:F:122:ALA:HA	6:F:125:LEU:HD12	1.80	0.64
6:F:40:ILE:HD11	6:F:177:ILE:HD12	1.80	0.64
2:B:48:GLU:O	2:B:64:LYS:NZ	2.23	0.64
1:A:38:ILE:HD11	1:A:174:LEU:HD12	1.80	0.63
2:B:116:ASP:OD1	3:C:81:ARG:NH1	2.32	0.63
9:d:63:THR:OG1	9:d:64:THR:N	2.28	0.63
10:i:28:PHE:O	10:i:93:ARG:NH1	2.31	0.62
4:D:195:ILE:HG23	4:D:217:LEU:HD11	1.80	0.62
1:A:214:ASN:OD1	1:A:215:GLU:N	2.33	0.62
1:A:188:ILE:HD12	1:A:188:ILE:H	1.65	0.62
7:G:43:ARG:N	7:G:164:LYS:O	2.32	0.62
9:d:102:PHE:CE1	9:d:106:LEU:HD12	2.34	0.62
7:G:231:THR:OG1	7:G:234:GLU:OE1	2.17	0.61
5:E:26:MET:O	5:E:29:VAL:HG12	2.01	0.60
1:A:109:GLN:N	1:A:109:GLN:OE1	2.29	0.60
10:i:89:GLU:HB2	10:i:122:TRP:HE1	1.67	0.60
1:A:74:LEU:HD22	1:A:134:LEU:HD12	1.84	0.60
1:A:119:GLN:NE2	2:B:82:ASP:OD1	2.35	0.60
1:A:119:GLN:HG2	2:B:85:VAL:HG21	1.84	0.59
4:D:147:ASP:OD1	4:D:149:LYS:N	2.34	0.59
9:d:106:LEU:HD23	9:d:106:LEU:O	2.03	0.59
6:F:182:MET:SD	6:F:182:MET:N	2.75	0.58
8:c:103:ASN:ND2	8:c:140:TYR:O	2.36	0.58
2:B:218:ARG:HH11	2:B:223:THR:HG23	1.68	0.58
6:F:109:LEU:HD13	6:F:140:SER:HB3	1.85	0.58
1:A:227:LYS:NZ	1:A:227:LYS:O	2.36	0.58
8:c:191:ALA:O	8:c:192:LEU:HD22	2.04	0.57
4:D:114:GLN:O	4:D:117:SER:OG	2.12	0.57
10:i:48:LEU:HB3	10:i:62:LEU:HD23	1.84	0.57
4:D:114:GLN:O	4:D:118:ASN:OD1	2.23	0.57
8:c:83:LEU:HD12	8:c:134:LEU:HD11	1.85	0.57
6:F:164:CYS:SG	6:F:165:ALA:N	2.77	0.57
1:A:196:LYS:NZ	1:A:201:GLY:O	2.38	0.57
7:G:228:ARG:NH2	7:G:234:GLU:OE2	2.37	0.56
9:d:22:VAL:HG23	9:d:22:VAL:O	2.06	0.56
9:d:128:GLN:CB	9:d:207:PHE:HE1	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:262:LEU:HD12	8:c:262:LEU:H	1.72	0.55
2:B:208:ALA:H	2:B:237:ILE:HG21	1.70	0.54
3:C:185:ASP:O	3:C:189:LYS:HG2	2.08	0.54
10:i:16:VAL:HG21	10:i:111:ALA:HB1	1.90	0.54
7:G:234:GLU:OE1	7:G:234:GLU:N	2.41	0.54
2:B:84:ASN:OD1	2:B:84:ASN:C	2.51	0.54
4:D:38:ILE:HD13	4:D:202:LEU:HD22	1.89	0.54
6:F:153:ASP:HB3	6:F:157:VAL:HG22	1.89	0.54
6:F:244:LEU:HD12	6:F:244:LEU:O	2.08	0.54
6:F:107:ILE:HD13	6:F:112:LEU:HD13	1.88	0.53
7:G:88:ARG:NH1	7:G:92:GLN:OE1	2.41	0.53
4:D:206:MET:HE1	4:D:215:ILE:HD13	1.91	0.53
3:C:134:VAL:HG12	3:C:144:LEU:HD13	1.90	0.53
10:i:106:MET:HE3	10:i:106:MET:HA	1.91	0.53
7:G:80:MET:HA	7:G:80:MET:HE3	1.90	0.53
2:B:34:CYS:SG	2:B:135:LEU:HD12	2.49	0.53
10:i:24:VAL:HG13	11:j:14:LEU:HD21	1.90	0.53
1:A:74:LEU:HD21	1:A:136:ILE:HD12	1.90	0.52
3:C:78:ALA:O	3:C:82:ILE:HG23	2.08	0.52
3:C:215:GLN:N	3:C:215:GLN:OE1	2.42	0.52
6:F:121:HIS:NE2	6:F:125:LEU:HD11	2.25	0.52
2:B:220:ASN:CG	2:B:220:ASN:O	2.52	0.52
8:c:163:GLN:OE1	8:c:163:GLN:N	2.42	0.52
8:c:277:MET:SD	8:c:277:MET:N	2.83	0.52
9:d:227:TRP:CD1	9:d:227:TRP:C	2.88	0.52
3:C:39:ASP:OD1	3:C:213:ARG:NH2	2.43	0.52
9:d:254:LEU:H	9:d:254:LEU:HD23	1.75	0.52
9:d:193:GLU:OE2	9:d:197:LYS:NZ	2.41	0.52
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.92	0.51
1:A:206:ASP:OD1	1:A:206:ASP:N	2.42	0.51
10:i:108:GLY:O	10:i:112:LEU:HG	2.11	0.51
9:d:102:PHE:HE1	9:d:106:LEU:HD12	1.74	0.51
4:D:11:GLY:O	4:D:14:THR:OG1	2.28	0.51
9:d:194:SER:O	9:d:198:GLU:N	2.44	0.51
8:c:223:CYS:SG	8:c:224:GLN:N	2.84	0.50
11:j:110:ASN:OD1	11:j:110:ASN:C	2.54	0.50
7:G:131:MET:SD	7:G:131:MET:N	2.84	0.50
8:c:280:ASN:C	8:c:280:ASN:OD1	2.55	0.50
10:i:106:MET:HE3	10:i:106:MET:CA	2.41	0.50
10:i:106:MET:HE3	10:i:106:MET:O	2.12	0.50
1:A:38:ILE:HD11	1:A:174:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:i:113:ARG:HA	10:i:116:ILE:HD12	1.93	0.50
4:D:7:GLU:N	4:D:7:GLU:OE1	2.44	0.50
2:B:232:GLU:O	2:B:235:GLN:NE2	2.44	0.50
9:d:34:LEU:HD11	9:d:245:TRP:HB3	1.94	0.50
2:B:72:MET:CE	2:B:110:LEU:HD23	2.42	0.50
2:B:66:TYR:CD2	2:B:87:THR:HG21	2.47	0.49
6:F:18:ASP:OD1	6:F:18:ASP:C	2.56	0.49
8:c:192:LEU:HD21	8:c:206:LEU:HB2	1.95	0.49
3:C:67:ASP:OD1	3:C:68:ASN:N	2.45	0.49
3:C:105:GLU:OE1	3:C:145:TYR:OH	2.22	0.49
1:A:74:LEU:CD2	1:A:136:ILE:HD12	2.43	0.49
1:A:196:LYS:HD2	1:A:203:MET:HE3	1.95	0.49
2:B:119:GLN:NE2	3:C:82:ILE:HD13	2.27	0.49
1:A:135:LEU:HG	1:A:163:MET:HE3	1.94	0.49
2:B:25:MET:HE1	2:B:152:PRO:HG2	1.93	0.49
4:D:65:GLU:OE2	4:D:65:GLU:HA	2.12	0.49
10:i:112:LEU:O	10:i:116:ILE:HG13	2.13	0.49
6:F:185:MET:HG3	6:F:190:ILE:HD11	1.94	0.49
7:G:165:ALA:HB1	7:G:179:LEU:CD2	2.43	0.49
2:B:149:GLN:C	2:B:149:GLN:OE1	2.56	0.48
3:C:132:LEU:HD21	3:C:144:LEU:HD11	1.95	0.48
7:G:10:ASP:OD1	7:G:10:ASP:N	2.41	0.48
7:G:238:HIS:O	7:G:242:LEU:HG	2.12	0.48
7:G:232:GLU:N	7:G:232:GLU:OE1	2.46	0.48
3:C:68:ASN:ND2	3:C:102:VAL:O	2.41	0.48
7:G:165:ALA:HB1	7:G:179:LEU:HD21	1.96	0.48
8:c:262:LEU:HD12	8:c:262:LEU:N	2.27	0.48
2:B:43:VAL:CG2	2:B:137:ILE:HG22	2.42	0.48
1:A:74:LEU:HD21	1:A:136:ILE:CD1	2.44	0.48
2:B:76:VAL:HG11	2:B:83:ALA:HB2	1.95	0.48
9:d:32:MET:HE3	9:d:32:MET:O	2.14	0.48
5:E:34:ALA:O	5:E:62:LYS:NZ	2.46	0.48
6:F:196:LYS:O	6:F:200:ILE:HG12	2.14	0.48
5:E:72:ILE:HG21	5:E:88:MET:CE	2.37	0.48
8:c:194:THR:OG1	8:c:224:GLN:OE1	2.29	0.48
4:D:68:VAL:HG11	4:D:89:ILE:HD13	1.95	0.47
5:E:45:VAL:HG23	5:E:187:LEU:HD23	1.96	0.47
3:C:79:ASP:OD1	3:C:79:ASP:N	2.44	0.47
9:d:93:ILE:HD12	9:d:94:PHE:H	1.79	0.47
1:A:53:LYS:NZ	1:A:53:LYS:O	2.47	0.47
2:B:72:MET:HE1	2:B:110:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:111:HIS:O	6:F:114:ASP:OD1	2.32	0.47
11:j:108:VAL:O	11:j:112:ILE:HG22	2.14	0.47
7:G:195:VAL:HG11	7:G:238:HIS:ND1	2.29	0.47
7:G:9:PHE:HA	7:G:15:ILE:HG23	1.97	0.47
2:B:86:LEU:HD22	2:B:132:VAL:HG21	1.97	0.47
2:B:113:ALA:O	2:B:117:ILE:HG13	2.14	0.47
6:F:181:GLN:NE2	6:F:183:LYS:O	2.48	0.47
5:E:74:ILE:HD12	5:E:81:ALA:HB1	1.97	0.47
9:d:34:LEU:HD12	9:d:34:LEU:O	2.15	0.47
4:D:198:SER:O	4:D:202:LEU:HD23	2.16	0.46
1:A:128:ARG:HB3	7:G:14:THR:HG23	1.98	0.46
3:C:113:SER:O	3:C:117:ARG:HG2	2.16	0.46
9:d:160:TRP:CG	9:d:223:TYR:HH	2.33	0.46
1:A:118:MET:O	1:A:122:THR:HG22	2.16	0.46
4:D:68:VAL:HG21	4:D:89:ILE:CD1	2.46	0.46
6:F:158:SER:O	6:F:158:SER:OG	2.28	0.46
10:i:14:GLU:C	10:i:14:GLU:OE2	2.59	0.46
3:C:158:ALA:HB1	3:C:172:LEU:HD21	1.96	0.46
6:F:193:GLU:O	6:F:197:ILE:HG12	2.16	0.46
9:d:191:TYR:CD1	9:d:191:TYR:C	2.93	0.46
2:B:66:TYR:N	2:B:66:TYR:CD1	2.82	0.46
4:D:71:ASP:OD2	4:D:73:HIS:ND1	2.47	0.46
4:D:183:GLU:C	4:D:183:GLU:OE2	2.59	0.46
8:c:198:LYS:HG3	8:c:198:LYS:O	2.16	0.45
4:D:24:VAL:O	4:D:28:ILE:HG12	2.15	0.45
3:C:71:MET:HE2	3:C:131:ALA:HB1	1.99	0.45
9:d:137:THR:O	9:d:140:ARG:NH1	2.50	0.45
3:C:31:THR:HG21	3:C:198:VAL:HG11	1.97	0.45
6:F:109:LEU:HD13	6:F:140:SER:CB	2.45	0.45
7:G:29:PHE:HA	7:G:32:ILE:HD12	1.99	0.45
7:G:31:ALA:HB1	7:G:83:MET:HE3	1.99	0.45
9:d:106:LEU:HD23	9:d:110:VAL:HG13	1.98	0.45
8:c:43:ARG:HD2	8:c:43:ARG:O	2.17	0.45
4:D:68:VAL:HG21	4:D:89:ILE:HD13	1.99	0.45
1:A:208:ILE:HD11	1:A:226:VAL:HG21	1.98	0.45
3:C:20:GLU:OE2	3:C:20:GLU:HA	2.17	0.45
6:F:175:THR:O	6:F:179:LYS:HG3	2.17	0.45
9:d:3:VAL:O	9:d:46:TYR:N	2.48	0.44
5:E:188:VAL:HG13	5:E:212:ILE:CD1	2.47	0.44
6:F:9:ASP:O	6:F:23:GLN:NE2	2.45	0.44
7:G:21:ARG:NH2	7:G:26:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:218:ALA:HB2	9:d:54:PRO:HG3	1.99	0.44
1:A:53:LYS:HZ2	1:A:53:LYS:C	2.25	0.44
3:C:16:LEU:HB2	3:C:19:VAL:HG22	2.00	0.44
9:d:125:HIS:O	9:d:207:PHE:HD1	2.00	0.44
4:D:1:MET:HE1	8:c:208:GLN:O	2.18	0.44
10:i:15:VAL:HG23	10:i:15:VAL:O	2.17	0.44
2:B:119:GLN:NE2	2:B:123:GLN:OE1	2.50	0.44
2:B:22:GLU:O	2:B:26:GLU:HG2	2.17	0.44
7:G:123:GLN:HA	7:G:126:THR:HG22	2.00	0.44
4:D:110:GLU:C	4:D:110:GLU:OE1	2.61	0.43
9:d:102:PHE:HD1	9:d:102:PHE:O	2.00	0.43
1:A:47:ALA:HB3	1:A:191:ALA:HB1	2.00	0.43
2:B:19:TYR:C	2:B:20:GLN:CD	2.87	0.43
2:B:66:TYR:HD2	2:B:87:THR:HG21	1.84	0.43
5:E:152:ASN:OD1	6:F:86:ARG:NH2	2.52	0.43
9:d:15:PHE:O	9:d:116:ALA:N	2.46	0.43
8:c:207:GLU:N	8:c:207:GLU:CD	2.76	0.43
9:d:102:PHE:C	9:d:102:PHE:CD1	2.96	0.43
5:E:29:VAL:HG23	5:E:75:ALA:O	2.17	0.43
2:B:155:ASN:OD1	2:B:155:ASN:N	2.51	0.43
7:G:61:LEU:HD23	7:G:62:ASP:N	2.34	0.43
10:i:84:ALA:O	10:i:88:GLN:HG3	2.18	0.43
3:C:81:ARG:O	3:C:85:ASN:ND2	2.49	0.43
10:i:97:LEU:HD11	10:i:99:VAL:HB	1.99	0.43
2:B:57:ASP:OD1	2:B:57:ASP:C	2.62	0.43
3:C:43:LEU:HD11	3:C:134:VAL:HG22	2.01	0.43
4:D:217:LEU:C	4:D:217:LEU:HD23	2.44	0.43
6:F:95:GLU:OE1	6:F:115:ARG:NH2	2.51	0.43
1:A:107:THR:O	1:A:111:VAL:HG23	2.19	0.42
2:B:35:LEU:O	2:B:46:ALA:N	2.50	0.42
7:G:115:CYS:O	7:G:154:CYS:SG	2.77	0.42
10:i:30:SER:OG	10:i:31:HIS:N	2.51	0.42
5:E:86:ASN:O	5:E:90:GLN:OE1	2.37	0.42
2:B:86:LEU:HD22	2:B:132:VAL:CG2	2.49	0.42
6:F:32:GLU:OE2	6:F:170:ARG:NH2	2.52	0.42
2:B:190:LEU:HD22	2:B:190:LEU:H	1.85	0.42
10:i:29:SER:N	11:j:45:PRO:O	2.48	0.42
1:A:106:PRO:HB2	1:A:109:GLN:OE1	2.20	0.42
3:C:45:VAL:HG21	3:C:61:LYS:HD2	2.01	0.42
9:d:32:MET:SD	9:d:35:ILE:HD11	2.59	0.42
11:j:59:ASP:OD1	11:j:60:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:HD23	2:B:39:ALA:N	2.35	0.42
7:G:49:VAL:HG12	7:G:219:VAL:HG23	2.02	0.42
8:c:144:ASP:N	8:c:144:ASP:OD1	2.50	0.42
9:d:44:ILE:HG21	9:d:79:SER:OG	2.20	0.42
9:d:74:ASN:OD1	9:d:75:ALA:N	2.52	0.42
5:E:87:PHE:O	5:E:91:GLU:HG2	2.19	0.42
1:A:10:LEU:HD12	7:G:14:THR:HG21	2.02	0.42
2:B:224:VAL:O	2:B:224:VAL:HG23	2.19	0.42
5:E:44:ALA:HB1	5:E:144:ILE:HD11	2.02	0.42
5:E:151:ALA:HB3	6:F:83:ALA:HB1	2.01	0.41
10:i:36:VAL:HG11	10:i:112:LEU:HD13	2.02	0.41
1:A:78:GLY:O	1:A:132:VAL:HG12	2.20	0.41
8:c:244:LEU:HA	8:c:247:VAL:HG22	2.01	0.41
10:i:71:ASP:OD1	10:i:71:ASP:C	2.63	0.41
4:D:147:ASP:OD1	4:D:147:ASP:C	2.63	0.41
1:A:100:VAL:HG12	1:A:101:TYR:CD1	2.55	0.41
4:D:31:ILE:HD11	4:D:139:VAL:C	2.45	0.41
9:d:31:ALA:O	9:d:35:ILE:HG23	2.21	0.41
1:A:119:GLN:OE1	1:A:119:GLN:HA	2.21	0.41
2:B:149:GLN:O	2:B:157:GLY:N	2.53	0.41
3:C:162:GLY:H	3:C:165:ALA:HB2	1.84	0.41
6:F:88:LEU:HD12	6:F:134:CYS:SG	2.60	0.41
6:F:110:LYS:O	6:F:114:ASP:OD1	2.39	0.41
8:c:210:ASN:N	8:c:210:ASN:OD1	2.54	0.41
8:c:250:PHE:O	8:c:253:ILE:HG13	2.21	0.41
3:C:195:LEU:HB3	3:C:206:ILE:HD12	2.03	0.41
7:G:36:GLY:C	7:G:37:LEU:HD23	2.46	0.41
9:d:188:LYS:HD2	9:d:188:LYS:O	2.22	0.40
10:i:97:LEU:HD12	10:i:98:ALA:N	2.36	0.40
2:B:155:ASN:H	3:C:78:ALA:HB2	1.86	0.40
1:A:202:GLN:OE1	1:A:202:GLN:C	2.64	0.40
3:C:134:VAL:HG12	3:C:144:LEU:CD1	2.50	0.40
4:D:3:LEU:HB3	8:c:211:ILE:HD11	2.03	0.40
7:G:159:TYR:CE1	7:G:161:CYS:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/234 (97%)	217 (96%)	9 (4%)	0	100	100
2	B	237/261 (91%)	219 (92%)	17 (7%)	1 (0%)	30	66
3	C	229/248 (92%)	221 (96%)	7 (3%)	1 (0%)	30	66
4	D	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
5	E	237/263 (90%)	229 (97%)	8 (3%)	0	100	100
6	F	240/255 (94%)	232 (97%)	8 (3%)	0	100	100
7	G	239/246 (97%)	234 (98%)	5 (2%)	0	100	100
8	c	234/288 (81%)	222 (95%)	12 (5%)	0	100	100
9	d	244/264 (92%)	232 (95%)	12 (5%)	0	100	100
10	i	115/122 (94%)	107 (93%)	8 (7%)	0	100	100
11	j	111/123 (90%)	102 (92%)	9 (8%)	0	100	100
All	All	2351/2545 (92%)	2246 (96%)	103 (4%)	2 (0%)	50	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	50	VAL
2	B	208	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/191 (81%)	154 (100%)	0	100	100
2	B	159/221 (72%)	159 (100%)	0	100	100
3	C	170/211 (81%)	170 (100%)	0	100	100
4	D	180/203 (89%)	180 (100%)	0	100	100
5	E	190/224 (85%)	189 (100%)	1 (0%)	86	94
6	F	168/212 (79%)	168 (100%)	0	100	100
7	G	187/210 (89%)	187 (100%)	0	100	100
8	c	180/262 (69%)	180 (100%)	0	100	100
9	d	172/237 (73%)	171 (99%)	1 (1%)	84	93
10	i	90/107 (84%)	89 (99%)	1 (1%)	70	87
11	j	77/107 (72%)	76 (99%)	1 (1%)	65	85
All	All	1727/2185 (79%)	1723 (100%)	4 (0%)	91	97

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

Mol	Chain	Res	Type
5	E	72	ILE
9	d	153	ASN
10	i	74	LEU
11	j	74	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	GLN
4	D	178	GLN
4	D	186	HIS
5	E	5	GLN
5	E	16	GLN
7	G	33	ASN
8	c	146	GLN

5.3.3 RNA ⓘ

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.

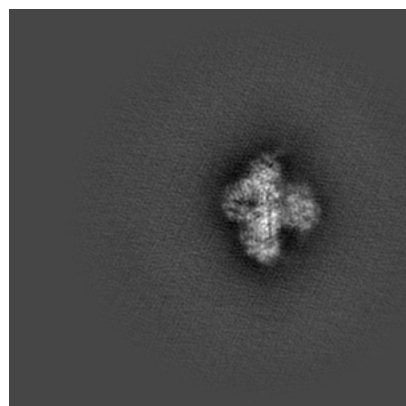
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41377. These allow visual inspection of the internal detail of the map and identification of artifacts.

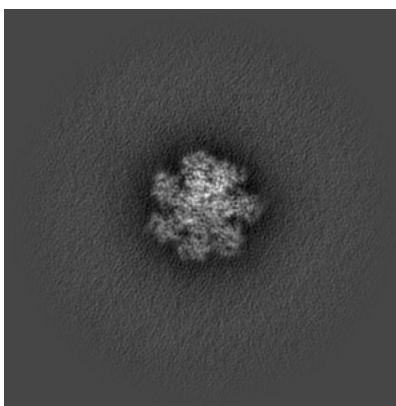
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

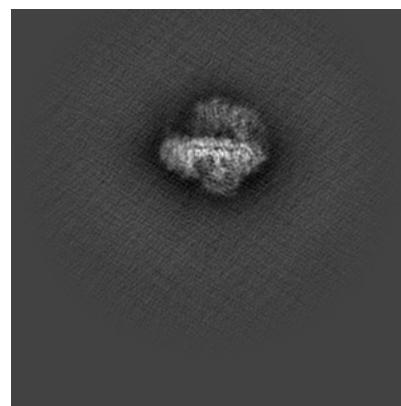
6.1.1 Primary map



X

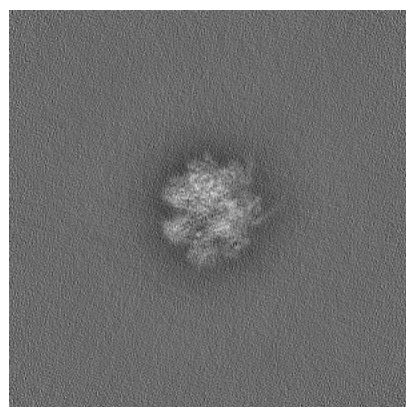


Y

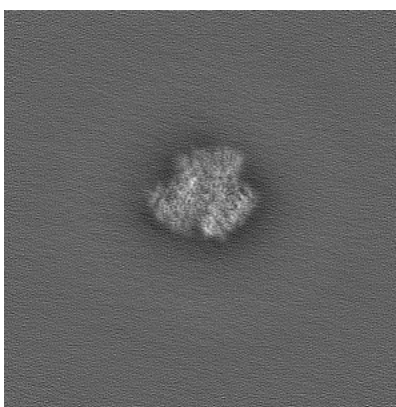


Z

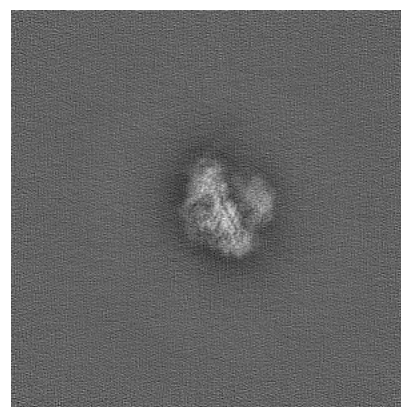
6.1.2 Raw map



X



Y

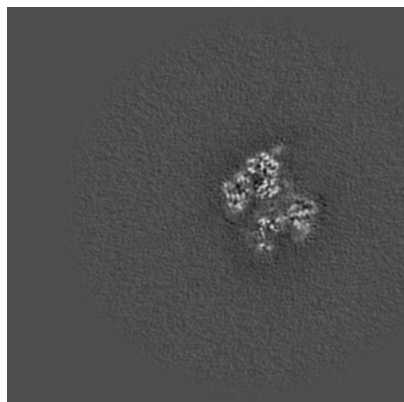


Z

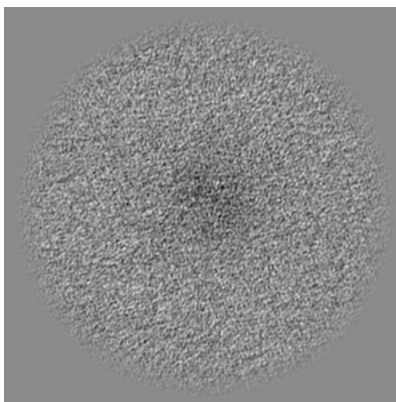
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

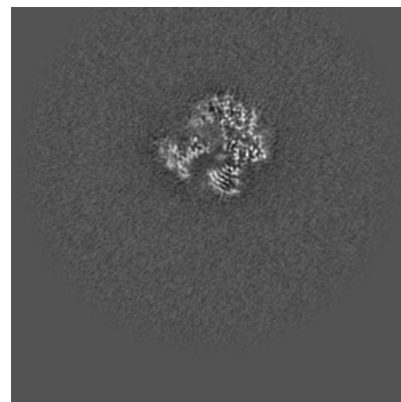
6.2.1 Primary map



X Index: 200

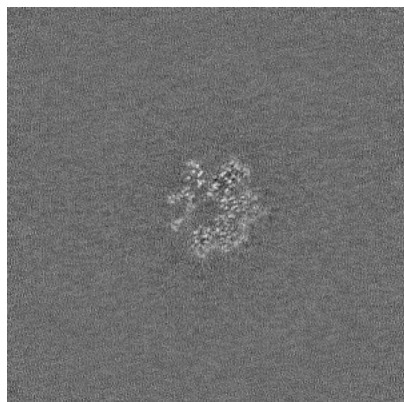


Y Index: 200

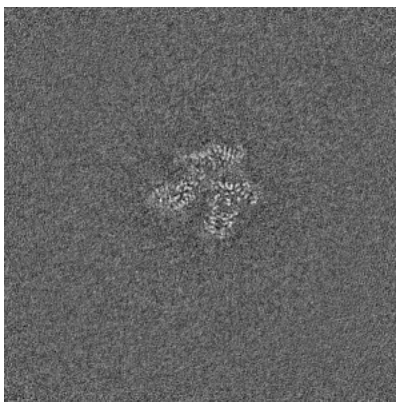


Z Index: 200

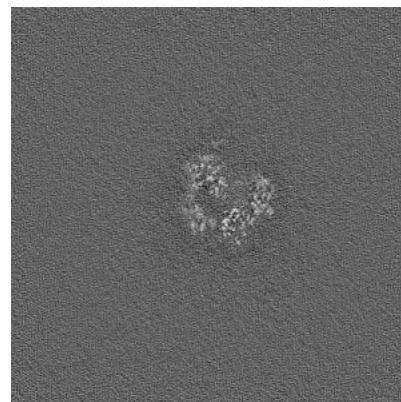
6.2.2 Raw map



X Index: 200



Y Index: 200

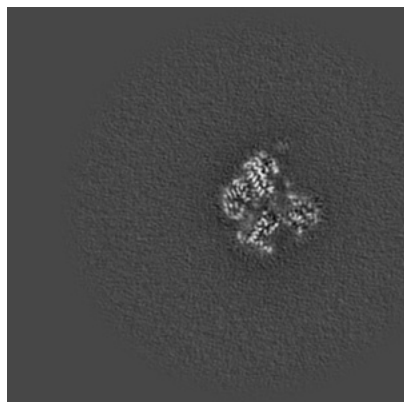


Z Index: 200

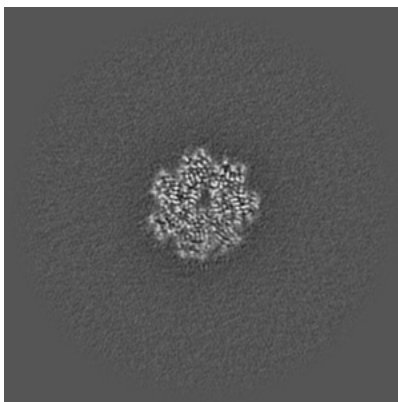
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

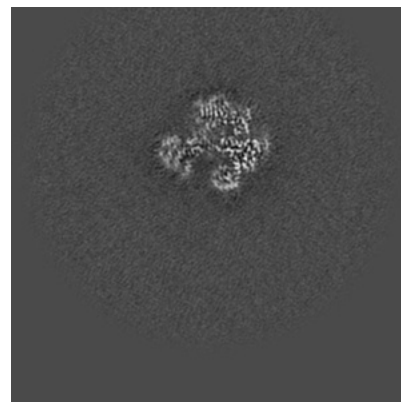
6.3.1 Primary map



X Index: 207

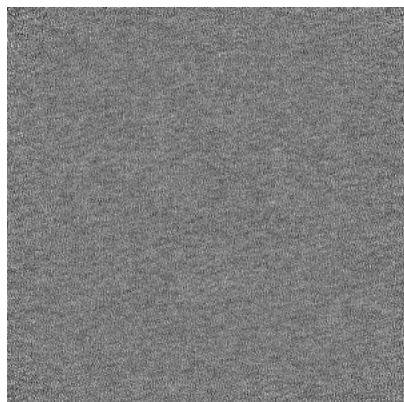


Y Index: 255

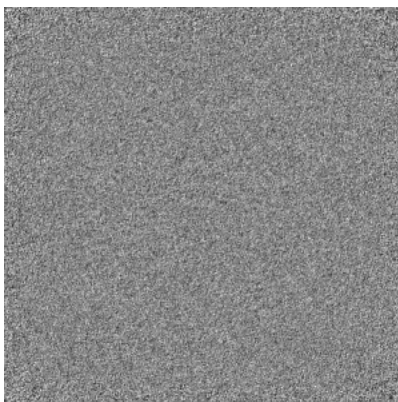


Z Index: 194

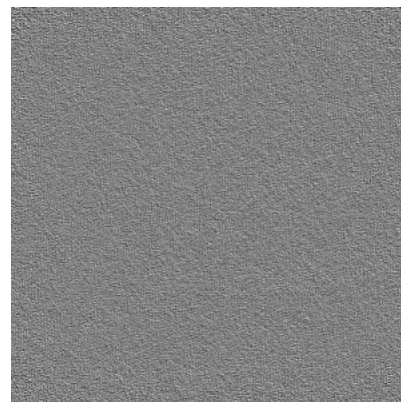
6.3.2 Raw map



X Index: 0



Y Index: 0

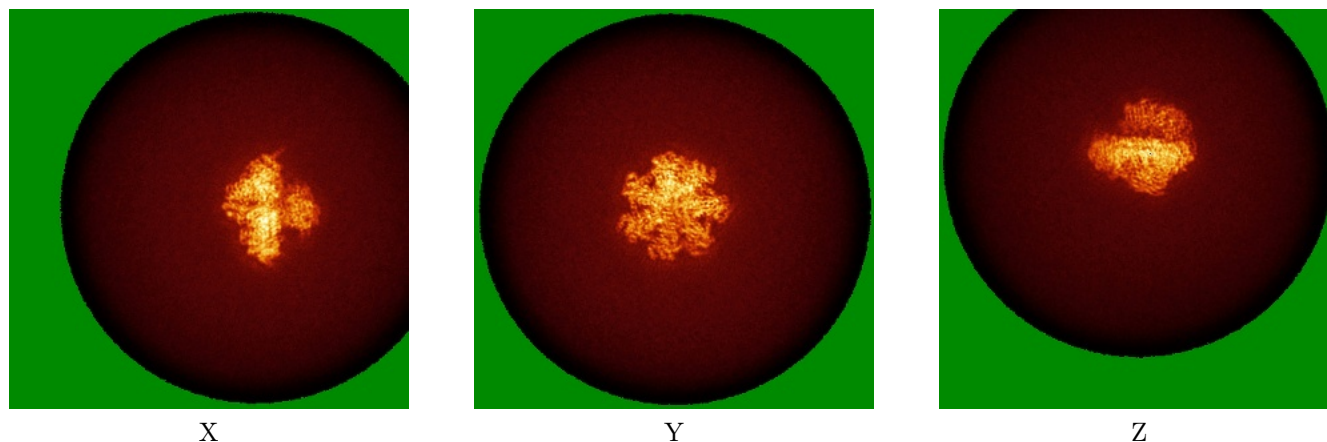


Z Index: 0

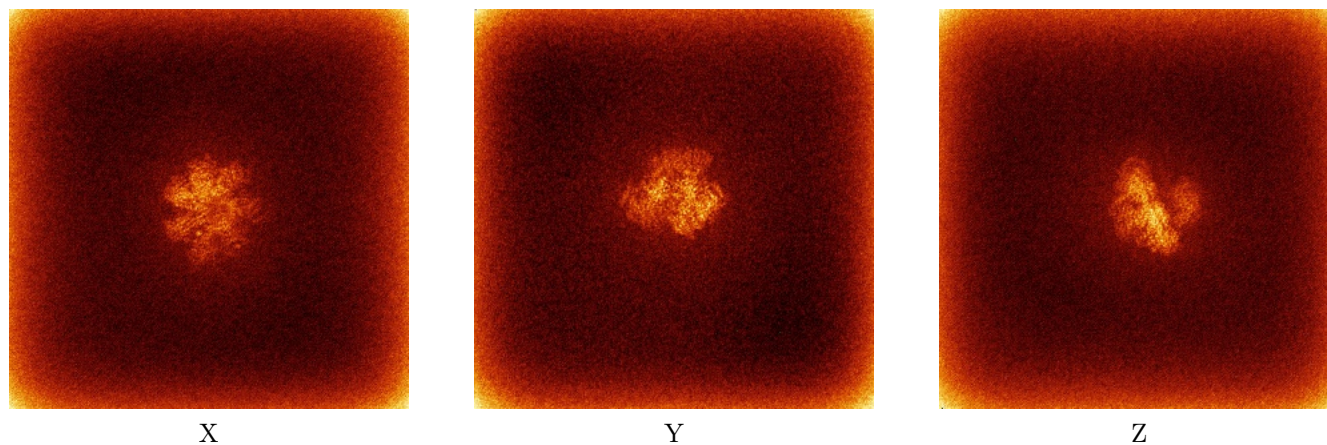
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



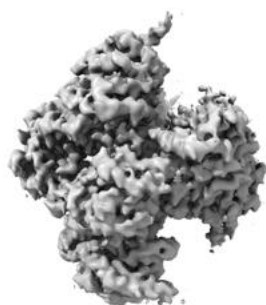
6.4.2 Raw map



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



X



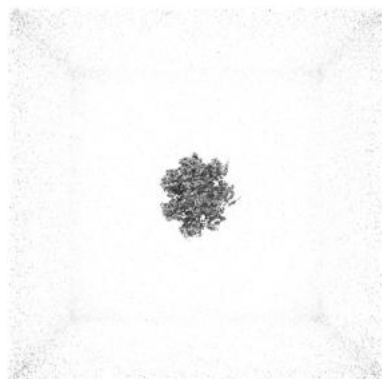
Y



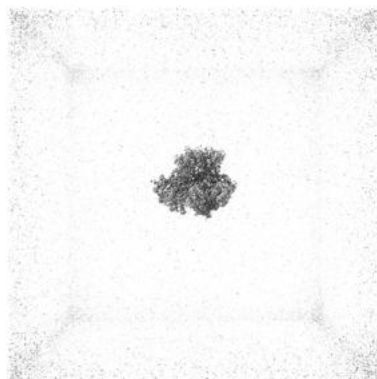
Z

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.

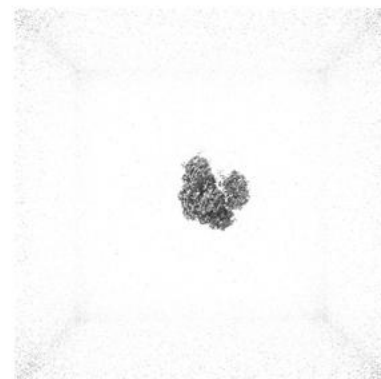
6.5.2 Raw map



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.

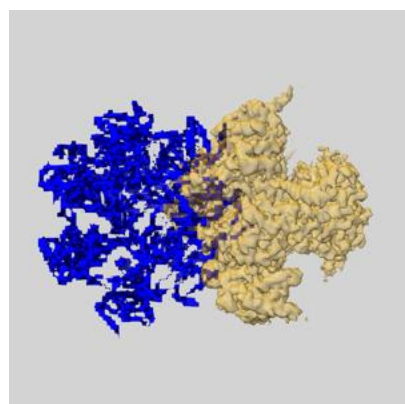
6.6 Mask visualisation [i](#)

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

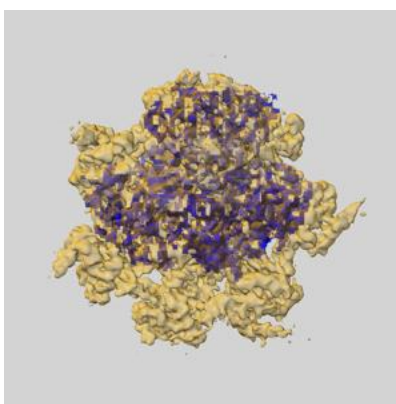
A mask typically either:

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

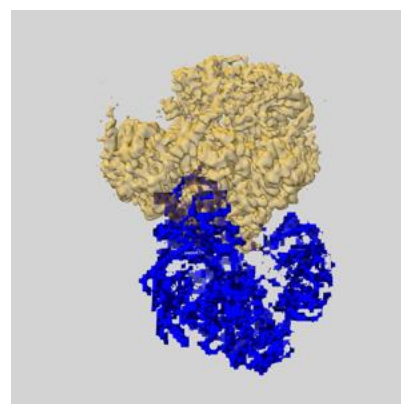
6.6.1 emd_41377_msk_1.map [i](#)



X



Y

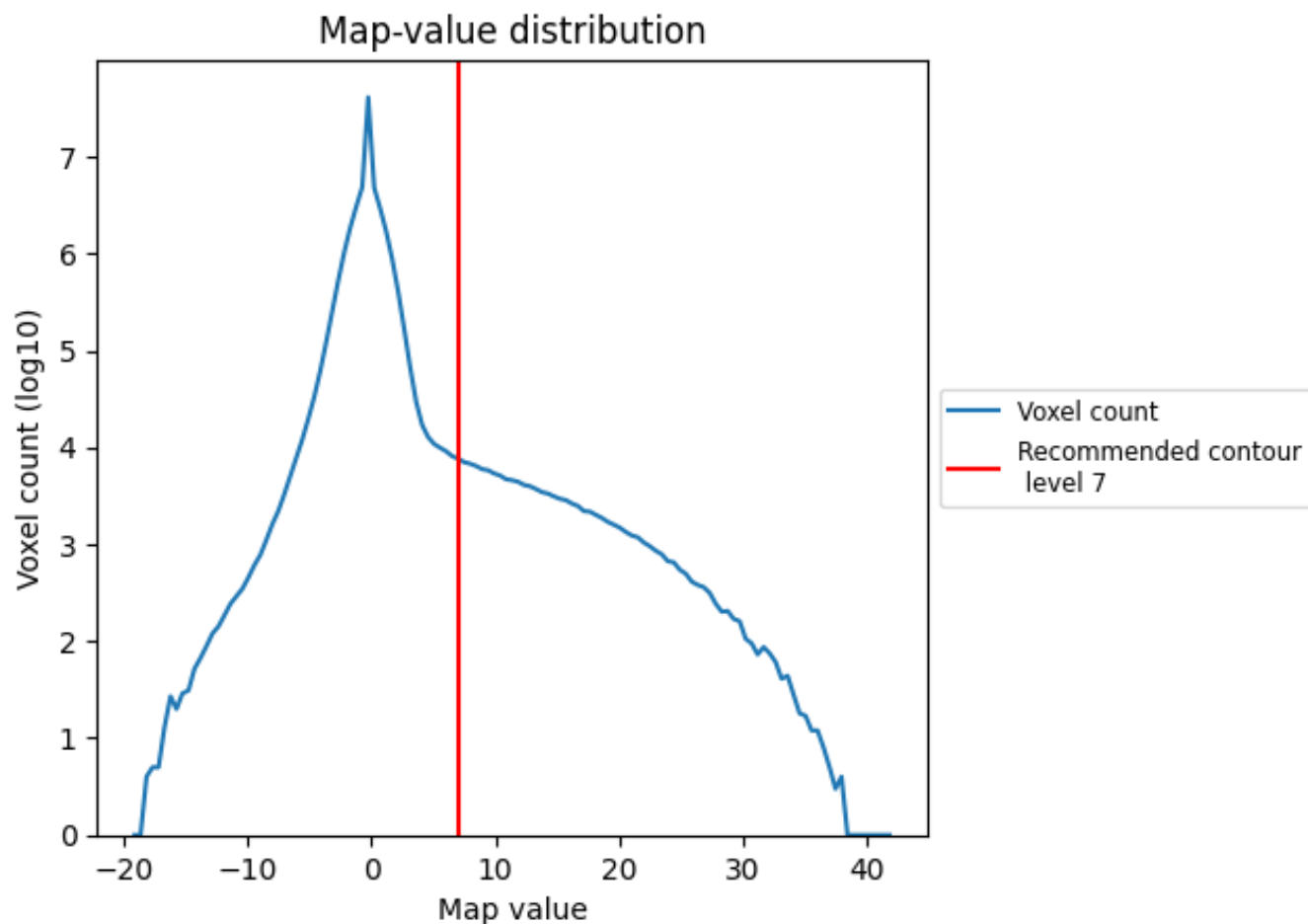


Z

7 Map analysis [i](#)

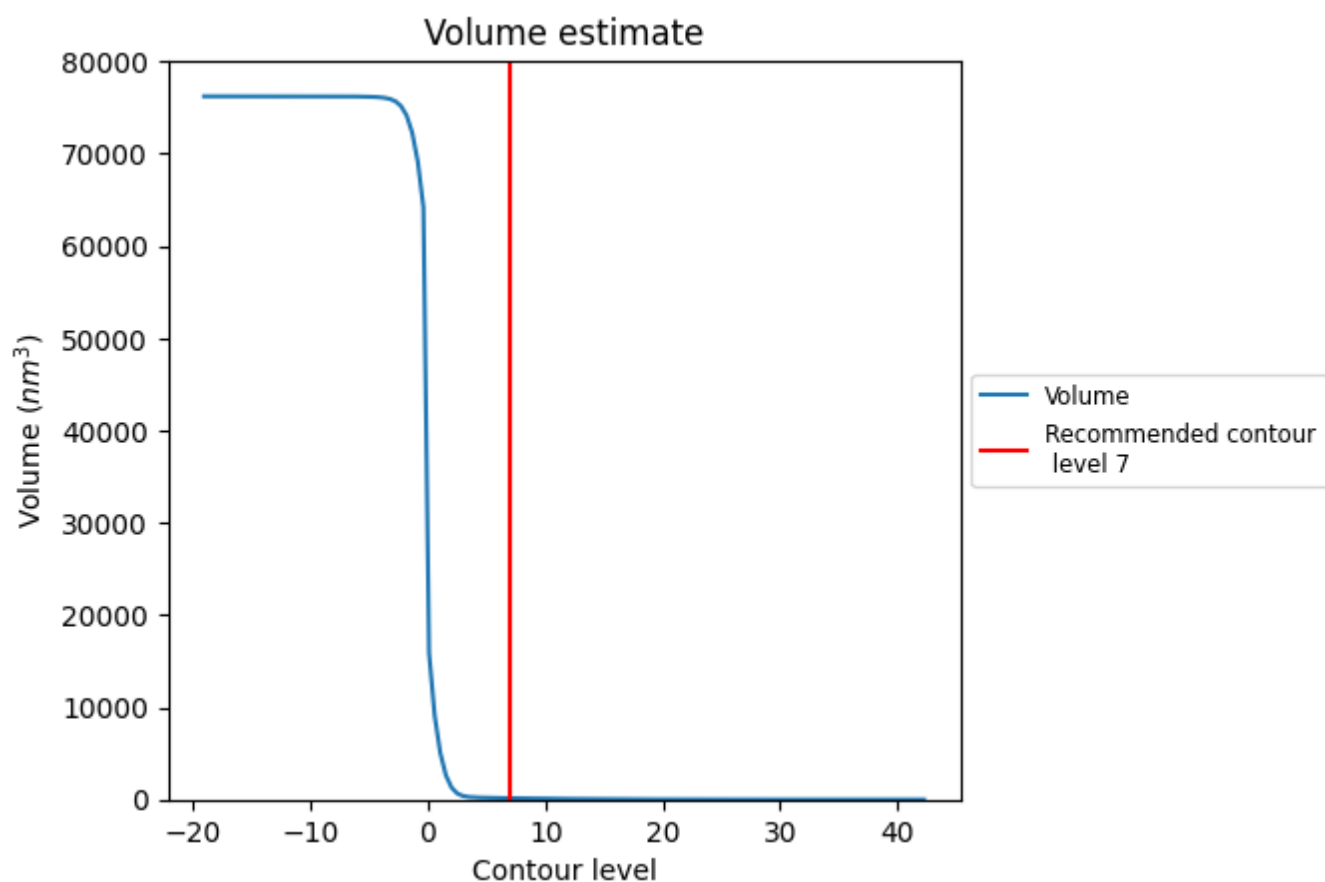
This section contains the results of statistical analysis of the map.

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.

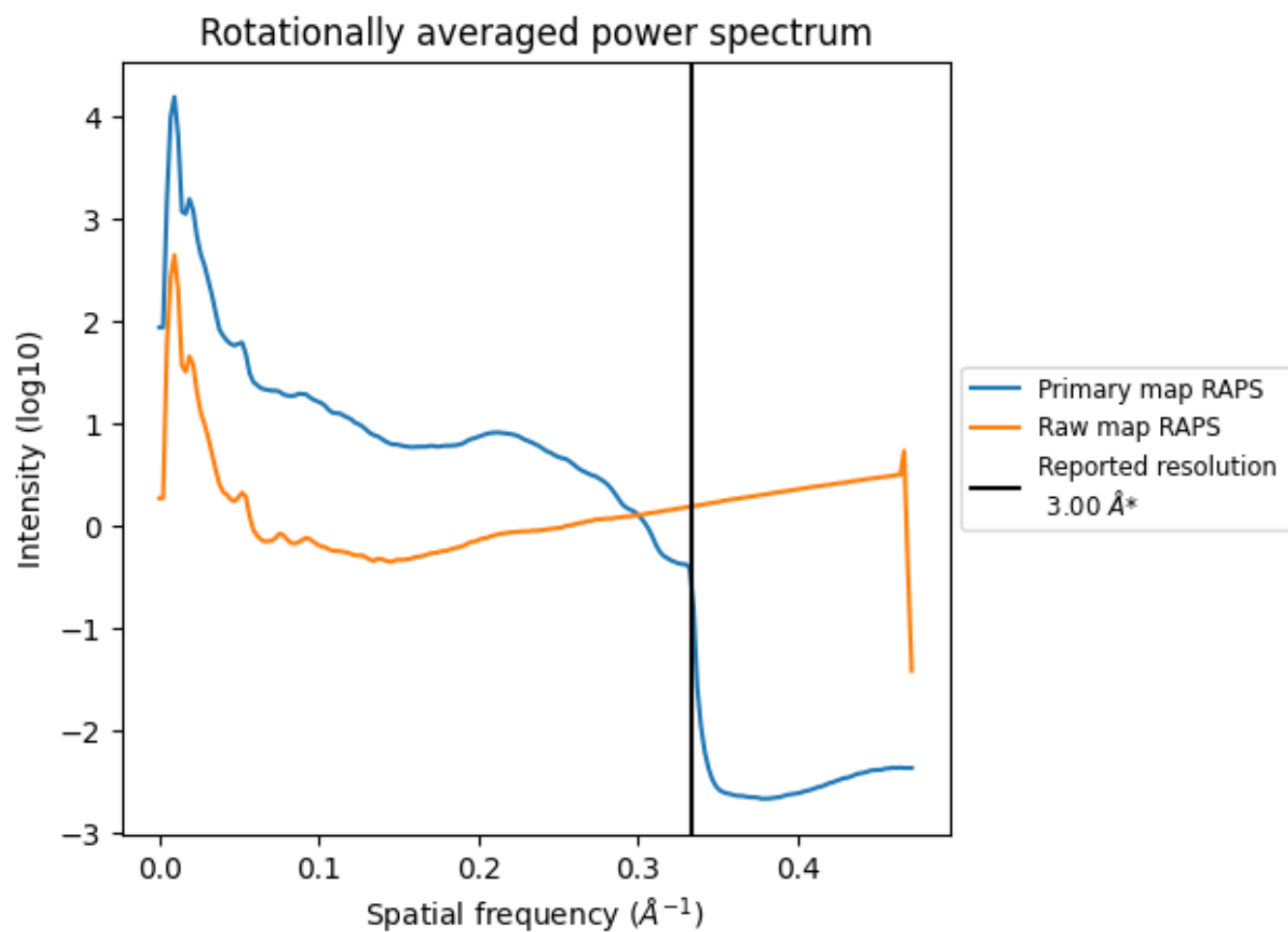
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 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 ⓘ

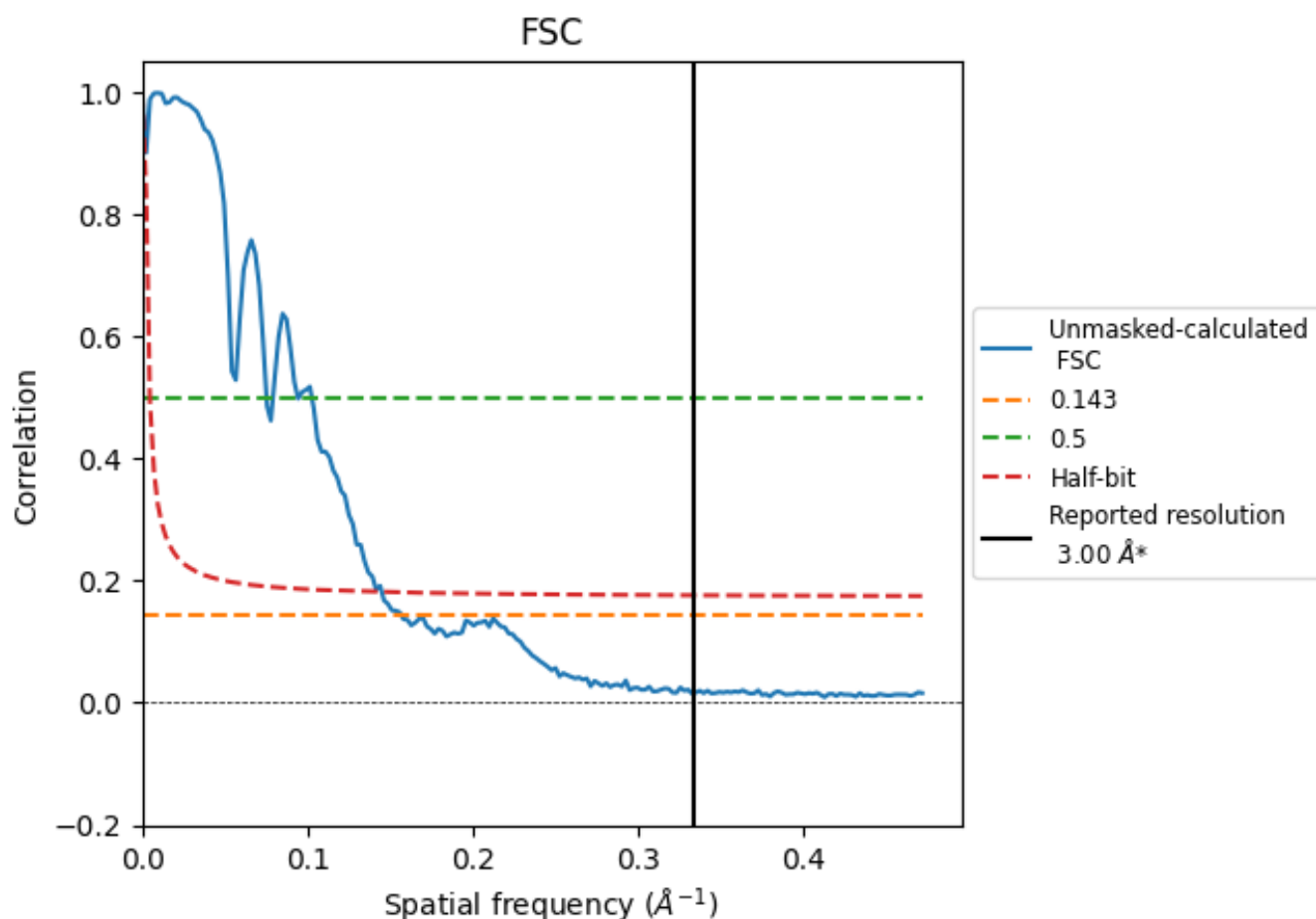


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

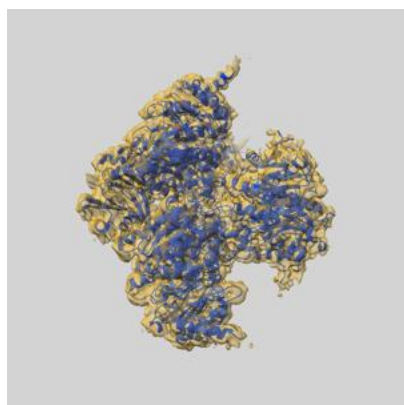
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.38	13.32	6.90

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

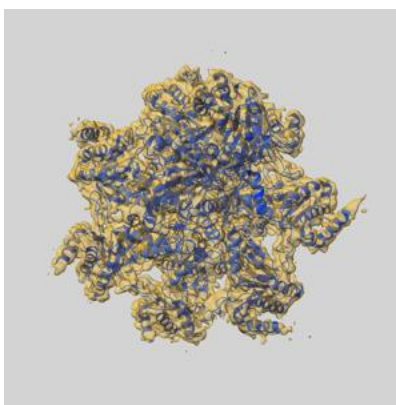
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41377 and PDB model 8TM3. Per-residue inclusion information can be found in section [3](#) on page [6](#).

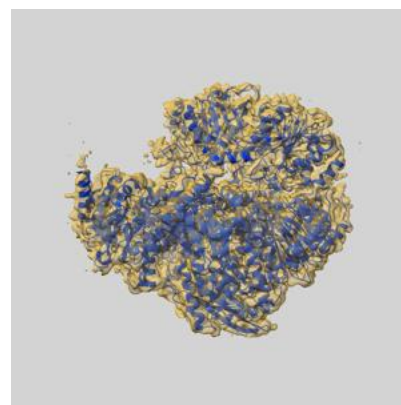
9.1 Map-model overlay [i](#)



X



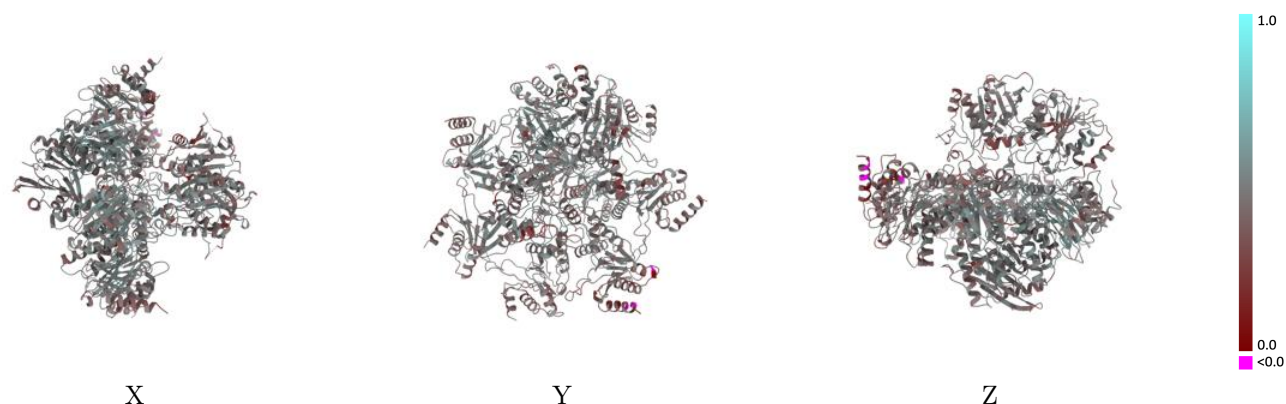
Y



Z

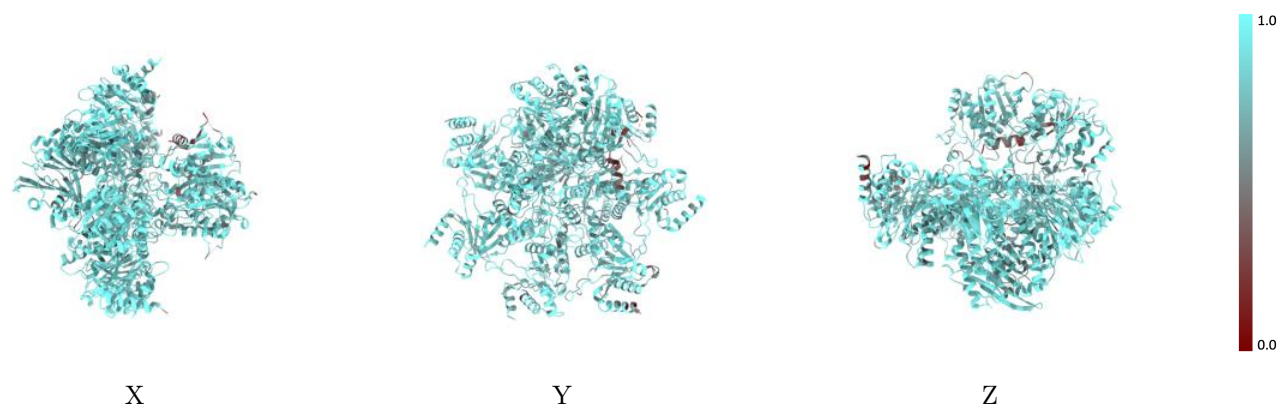
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



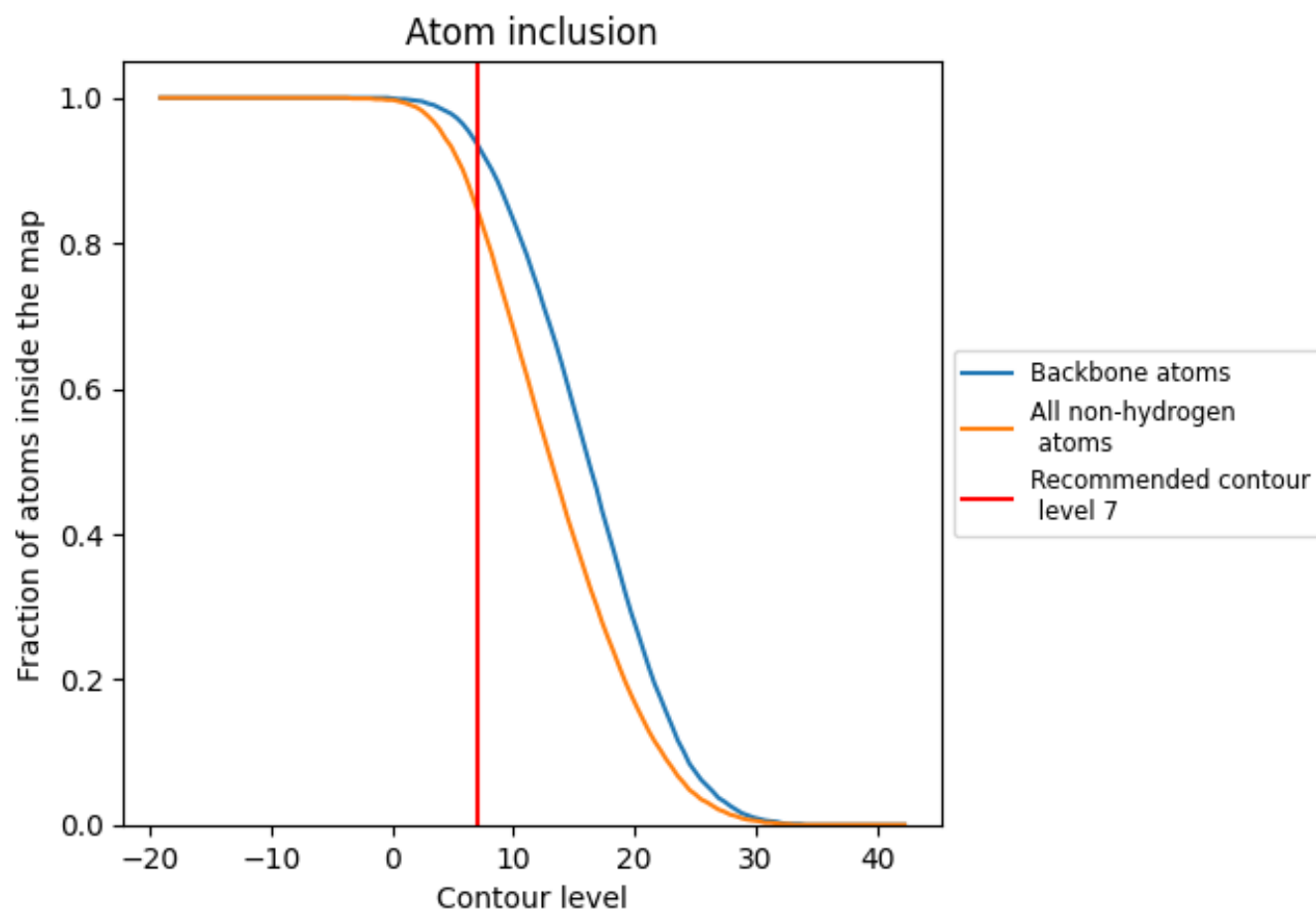
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

























9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% 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	 0.8470	 0.4530
A	 0.8300	 0.4270
B	 0.8060	 0.4080
C	 0.8840	 0.4650
D	 0.8540	 0.4860
E	 0.8920	 0.4940
F	 0.9030	 0.4650
G	 0.8620	 0.4490
c	 0.7850	 0.4470
d	 0.8300	 0.4370
i	 0.7850	 0.4380
j	 0.8610	 0.4530

