



Full wwPDB EM Validation Report ⓘ

Apr 11, 2024 – 04:26 pm BST

PDB ID : 8QYJ
EMDB ID : EMD-18755
Title : Human 20S proteasome assembly structure 1
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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

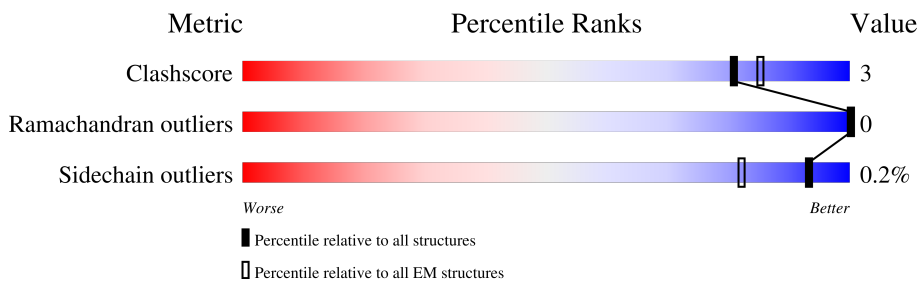
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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	<p>9% 79% 6% 16%</p>
10	J	265	<p>9% 88% 5% 6%</p>
11	K	316	<p>9% 20% 78%</p>
12	L	122	<p>9% 94% 5% 6%</p>
13	M	123	<p>7% 80% 12% 8%</p>

2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 19402 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
			Total	C	N	O	S		
1	A	228	1766	1131	297	332	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	236	1841	1171	310	350	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	236	1847	1159	327	356	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	242	1848	1163	305	368	12	0	0

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
			Total	C	N	O	S		
5	E	240	1886	1182	340	352	12	0	0

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
			Total	C	N	O	S		
6	F	240	1872	1187	320	354	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	235	1787	1140	300	334	13	0	0

- Molecule 8 is a protein called Proteasome maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	52	408	258	72	76	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	243	1933	1243	326	348	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	248	1909	1234	310	351	14	0	0

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
			Total	C	N	O	S		
11	K	70	512	325	91	92	4	0	0

There are 39 discrepancies between the modelled and reference sequences:

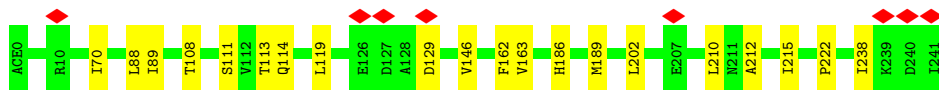
Chain	Residue	Modelled	Actual	Comment	Reference
K	278	GLU	-	expression tag	UNP Q99436
K	279	ASP	-	expression tag	UNP Q99436
K	280	LEU	-	expression tag	UNP Q99436
K	281	TYR	-	expression tag	UNP Q99436
K	282	PHE	-	expression tag	UNP Q99436
K	283	GLN	-	expression tag	UNP Q99436
K	284	SER	-	expression tag	UNP Q99436
K	285	VAL	-	expression tag	UNP Q99436
K	286	ASP	-	expression tag	UNP Q99436
K	287	SER	-	expression tag	UNP Q99436
K	288	ALA	-	expression tag	UNP Q99436
K	289	TRP	-	expression tag	UNP Q99436
K	290	SER	-	expression tag	UNP Q99436
K	291	HIS	-	expression tag	UNP Q99436
K	292	PRO	-	expression tag	UNP Q99436
K	293	GLN	-	expression tag	UNP Q99436
K	294	PHE	-	expression tag	UNP Q99436
K	295	GLU	-	expression tag	UNP Q99436
K	296	LYS	-	expression tag	UNP Q99436
K	297	GLY	-	expression tag	UNP Q99436
K	298	GLY	-	expression tag	UNP Q99436
K	299	GLY	-	expression tag	UNP Q99436
K	300	SER	-	expression tag	UNP Q99436
K	301	GLY	-	expression tag	UNP Q99436
K	302	GLY	-	expression tag	UNP Q99436
K	303	GLY	-	expression tag	UNP Q99436
K	304	SER	-	expression tag	UNP Q99436
K	305	GLY	-	expression tag	UNP Q99436
K	306	GLY	-	expression tag	UNP Q99436
K	307	SER	-	expression tag	UNP Q99436
K	308	ALA	-	expression tag	UNP Q99436
K	309	TRP	-	expression tag	UNP Q99436
K	310	SER	-	expression tag	UNP Q99436
K	311	HIS	-	expression tag	UNP Q99436
K	312	PRO	-	expression tag	UNP Q99436
K	313	GLN	-	expression tag	UNP Q99436
K	314	PHE	-	expression tag	UNP Q99436
K	315	GLU	-	expression tag	UNP Q99436
K	316	LYS	-	expression tag	UNP Q99436

- Molecule 12 is a protein called Proteasome assembly chaperone 3.

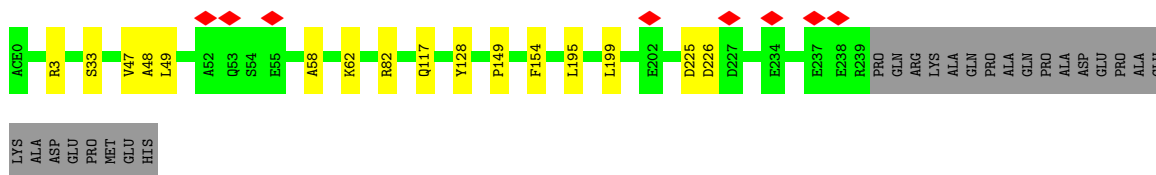
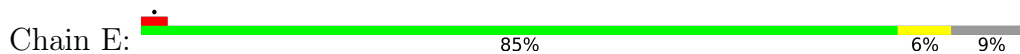
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	118	885	569	149	162	5	0	0

- Molecule 13 is a protein called Proteasome assembly chaperone 4.

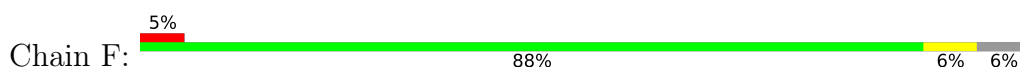
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	113	908	574	159	171	4	0	0



- Molecule 5: Proteasome subunit alpha type-1



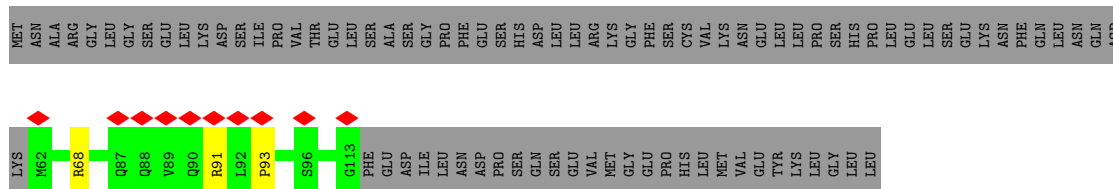
- Molecule 6: Proteasome subunit alpha type-3



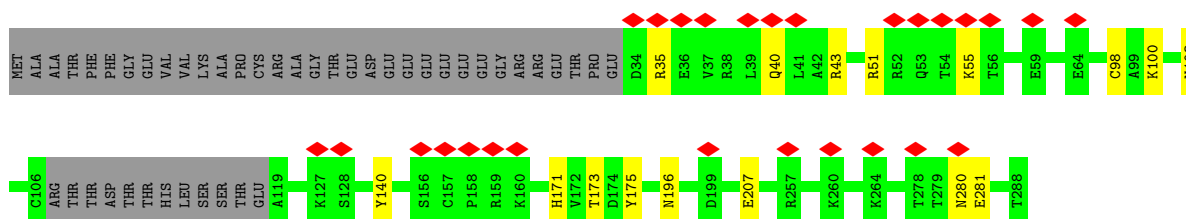
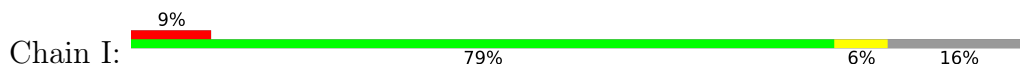
- Molecule 7: Proteasome subunit alpha type-6



- Molecule 8: Proteasome maturation protein



- Molecule 9: Proteasome assembly chaperone 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	318973	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	3.897	Depositor
Minimum map value	-2.037	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.129	Depositor
Recommended contour level	0.8	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	0.24	0/1804	0.45	0/2446
2	B	0.24	0/1869	0.45	0/2518
3	C	0.24	0/1872	0.49	0/2528
4	D	0.25	0/1875	0.46	0/2533
5	E	0.24	0/1919	0.50	0/2592
6	F	0.25	0/1907	0.46	0/2569
7	G	0.25	0/1819	0.45	0/2467
8	H	0.25	0/413	0.50	0/555
9	I	0.24	0/1974	0.47	0/2679
10	J	0.24	0/1949	0.46	0/2645
11	K	0.23	0/517	0.47	0/699
12	L	0.24	0/897	0.45	0/1217
13	M	0.25	0/927	0.51	0/1256
All	All	0.24	0/19742	0.47	0/26704

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	1766	0	1757	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1841	0	1860	13	0
3	C	1847	0	1861	13	0
4	D	1848	0	1833	12	0
5	E	1886	0	1876	12	0
6	F	1872	0	1854	12	0
7	G	1787	0	1772	6	0
8	H	408	0	413	1	0
9	I	1933	0	1959	8	0
10	J	1909	0	1925	8	0
11	K	512	0	510	6	0
12	L	885	0	948	2	0
13	M	908	0	893	10	0
All	All	19402	0	19461	99	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 (99) 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)
8:H:91:ARG:HG3	8:H:93:PRO:HD2	1.67	0.76
11:K:124:ARG:HG3	11:K:128:GLN:HE22	1.52	0.72
6:F:35:SER:HB3	6:F:66:ARG:HH12	1.54	0.72
11:K:124:ARG:O	11:K:128:GLN:NE2	2.23	0.70
5:E:33:SER:OG	5:E:62:LYS:NZ	2.24	0.70
10:J:33:ASP:OD1	10:J:89:GLN:NE2	2.27	0.68
1:A:119:GLN:HG3	2:B:81:SER:HB2	1.75	0.68
13:M:97:LEU:HD13	13:M:104:PHE:HE2	1.61	0.66
2:B:140:ASP:OD1	2:B:146:GLN:NE2	2.29	0.66
10:J:144:THR:HG22	10:J:146:SER:H	1.64	0.62
1:A:143:ARG:NH1	1:A:144:PRO:O	2.32	0.62
3:C:146:GLN:OE1	3:C:159:ASN:ND2	2.32	0.62
3:C:221:ASN:ND2	3:C:224:GLU:OE1	2.33	0.61
13:M:19:ALA:HB2	13:M:111:ARG:HE	1.67	0.60
13:M:33:LEU:HB2	13:M:36:SER:HB2	1.84	0.60
2:B:90:LEU:HG	2:B:114:LEU:HD13	1.86	0.57
10:J:55:MET:HG3	10:J:74:ASN:HB3	1.88	0.56
4:D:210:LEU:HD11	4:D:215:ILE:HD13	1.87	0.55
9:I:40:GLN:OE1	9:I:43:ARG:NH2	2.38	0.55
9:I:175:TYR:OH	9:I:207:GLU:OE1	2.25	0.54
6:F:231:ASP:OD1	6:F:231:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:ILE:HG22	3:C:8:THR:HG23	1.90	0.53
3:C:208:LEU:HD23	3:C:220:LEU:HD12	1.90	0.53
5:E:33:SER:HG	5:E:62:LYS:NZ	2.07	0.52
11:K:124:ARG:HG3	11:K:128:GLN:NE2	2.23	0.52
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.90	0.52
2:B:76:VAL:HG11	2:B:83:ALA:HB2	1.91	0.52
4:D:146:VAL:HG11	4:D:222:PRO:HA	1.91	0.52
6:F:52:LYS:NZ	6:F:63:SER:O	2.37	0.50
7:G:71:LYS:HE2	7:G:74:GLU:HA	1.94	0.49
1:A:65:VAL:O	1:A:220:ARG:NH1	2.46	0.48
4:D:163:VAL:HG11	5:E:58:ALA:HB1	1.96	0.48
5:E:117:GLN:HG3	6:F:83:ALA:HB1	1.96	0.48
12:L:79:ALA:O	12:L:83:VAL:HG22	2.14	0.48
9:I:280:ASN:OD1	9:I:281:GLU:N	2.45	0.48
4:D:212:ALA:HB2	4:D:238:ILE:HD12	1.95	0.48
4:D:88:LEU:HD23	4:D:119:LEU:HD23	1.96	0.47
2:B:236:LEU:HD23	2:B:239:LYS:HZ1	1.79	0.47
3:C:195:LEU:HD23	3:C:206:ILE:HG23	1.96	0.47
7:G:13:ILE:HG23	7:G:14:THR:HG23	1.97	0.47
1:A:222:THR:HG22	1:A:224:THR:H	1.79	0.47
5:E:225:ASP:OD1	5:E:226:ASP:N	2.47	0.47
3:C:178:ASP:N	3:C:178:ASP:OD1	2.46	0.47
4:D:129:ASP:OD1	4:D:129:ASP:N	2.48	0.47
5:E:154:PHE:HD2	6:F:64:ASN:HD21	1.62	0.47
6:F:216:TRP:CZ3	6:F:228:VAL:HG22	2.50	0.46
2:B:175:LEU:O	2:B:179:TYR:HB2	2.16	0.46
9:I:103:ASN:ND2	9:I:140:TYR:O	2.49	0.46
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.98	0.46
6:F:168:LYS:HB3	6:F:168:LYS:HE2	1.76	0.46
2:B:160:LYS:NZ	3:C:55:ASP:OD1	2.49	0.45
6:F:216:TRP:HZ3	6:F:228:VAL:HG13	1.80	0.45
13:M:112:ILE:O	13:M:116:MET:HG3	2.15	0.45
2:B:241:GLU:O	2:B:244:GLU:HG3	2.16	0.45
3:C:97:THR:OG1	13:M:109:GLU:OE2	2.29	0.45
4:D:113:THR:HG23	4:D:162:PHE:CG	2.51	0.45
9:I:98:CYS:SG	9:I:100:LYS:NZ	2.89	0.45
13:M:97:LEU:HD13	13:M:104:PHE:CE2	2.47	0.45
5:E:3:ARG:HH21	10:J:256:GLY:HA3	1.82	0.45
5:E:49:LEU:HD21	5:E:199:LEU:HD21	1.98	0.45
6:F:36:THR:HA	6:F:167:GLY:HA3	1.98	0.44
9:I:171:HIS:CE1	9:I:173:THR:HG1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:THR:HG23	10:J:66:GLY:H	1.83	0.44
11:K:98:THR:O	11:K:102:ILE:HG12	2.18	0.44
4:D:114:GLN:OE1	5:E:82:ARG:NH2	2.34	0.44
5:E:128:TYR:O	5:E:149:PRO:HB3	2.18	0.43
6:F:216:TRP:CE3	6:F:228:VAL:HG22	2.53	0.43
12:L:6:LEU:HG	13:M:45:PRO:HG3	1.99	0.43
5:E:48:ALA:HB1	5:E:62:LYS:HG2	2.01	0.43
13:M:113:LYS:O	13:M:117:GLU:OE1	2.36	0.43
4:D:70:ILE:HD11	4:D:89:ILE:HD12	2.00	0.43
3:C:39:ASP:OD1	3:C:39:ASP:N	2.50	0.43
11:K:97:MET:HG3	11:K:99:THR:H	1.84	0.42
9:I:51:ARG:O	9:I:55:LYS:N	2.50	0.42
13:M:48:ARG:NH2	13:M:96:ASN:O	2.52	0.42
4:D:108:THR:HG1	4:D:111:SER:HG	1.60	0.42
10:J:0:ACE:H3	10:J:105:LYS:HD3	2.01	0.42
2:B:41:ASP:OD1	2:B:41:ASP:N	2.52	0.42
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.91	0.42
2:B:35:LEU:HD23	2:B:163:CYS:HB2	2.02	0.41
3:C:42:VAL:HB	3:C:191:VAL:HG21	2.02	0.41
7:G:174:GLU:OE2	7:G:174:GLU:N	2.49	0.41
2:B:197:LEU:HD12	2:B:197:LEU:HA	1.93	0.41
6:F:142:SER:HB3	6:F:145:ASP:HB2	2.03	0.41
3:C:233:GLU:O	3:C:237:GLU:OE1	2.38	0.41
7:G:43:ARG:HH21	7:G:164:LYS:HG2	1.86	0.41
2:B:76:VAL:HG13	2:B:132:VAL:HG13	2.02	0.41
3:C:107:ILE:HD12	3:C:107:ILE:HA	1.95	0.41
4:D:186:HIS:NE2	4:D:189:MET:HB3	2.36	0.41
10:J:76:GLU:OE2	10:J:91:ARG:NH1	2.47	0.41
7:G:73:THR:HG22	7:G:74:GLU:N	2.36	0.41
7:G:112:ASP:OD1	7:G:113:MET:N	2.54	0.41
4:D:202:LEU:HD23	4:D:202:LEU:HA	1.93	0.40
9:I:196:ASN:OD1	9:I:196:ASN:N	2.54	0.40
10:J:231:LEU:HD23	10:J:231:LEU:HA	1.95	0.40
11:K:111:LEU:HD23	11:K:111:LEU:HA	1.98	0.40
1:A:68:ILE:HG12	1:A:74:LEU:HD22	2.02	0.40
6:F:81:LEU:HD23	6:F:81:LEU:HA	1.95	0.40
13:M:106:LEU:HD23	13:M:106:LEU:HA	1.99	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	226/234 (97%)	220 (97%)	6 (3%)	0	100	100
2	B	232/261 (89%)	228 (98%)	4 (2%)	0	100	100
3	C	234/248 (94%)	231 (99%)	3 (1%)	0	100	100
4	D	240/242 (99%)	238 (99%)	2 (1%)	0	100	100
5	E	238/264 (90%)	233 (98%)	5 (2%)	0	100	100
6	F	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
7	G	231/246 (94%)	229 (99%)	2 (1%)	0	100	100
8	H	50/141 (36%)	47 (94%)	3 (6%)	0	100	100
9	I	239/288 (83%)	235 (98%)	4 (2%)	0	100	100
10	J	242/265 (91%)	230 (95%)	12 (5%)	0	100	100
11	K	62/316 (20%)	61 (98%)	1 (2%)	0	100	100
12	L	116/122 (95%)	114 (98%)	2 (2%)	0	100	100
13	M	111/123 (90%)	110 (99%)	1 (1%)	0	100	100
All	All	2459/3005 (82%)	2409 (98%)	50 (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	185/191 (97%)	184 (100%)	1 (0%)	88	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/221 (88%)	194 (100%)	0	100	100
3	C	197/211 (93%)	197 (100%)	0	100	100
4	D	202/203 (100%)	202 (100%)	0	100	100
5	E	204/224 (91%)	204 (100%)	0	100	100
6	F	196/212 (92%)	195 (100%)	1 (0%)	88	92
7	G	188/210 (90%)	188 (100%)	0	100	100
8	H	46/128 (36%)	45 (98%)	1 (2%)	52	71
9	I	219/262 (84%)	218 (100%)	1 (0%)	88	92
10	J	214/237 (90%)	214 (100%)	0	100	100
11	K	56/257 (22%)	56 (100%)	0	100	100
12	L	103/107 (96%)	103 (100%)	0	100	100
13	M	102/107 (95%)	102 (100%)	0	100	100
All	All	2106/2570 (82%)	2102 (100%)	4 (0%)	93	96

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

Mol	Chain	Res	Type
1	A	143	ARG
6	F	182	MET
8	H	68	ARG
9	I	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
11	K	128	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

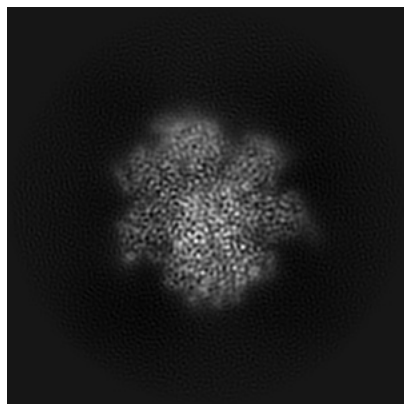
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18755. These allow visual inspection of the internal detail of the map and identification of artifacts.

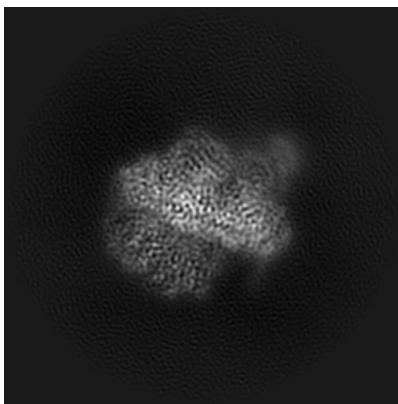
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

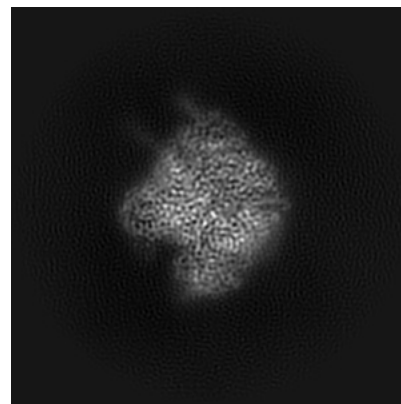
6.1.1 Primary map



X

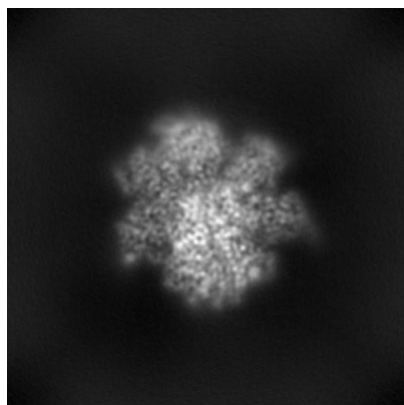


Y

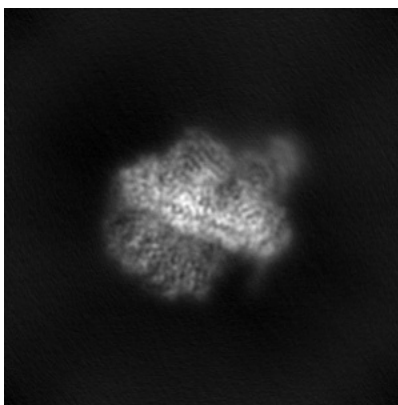


Z

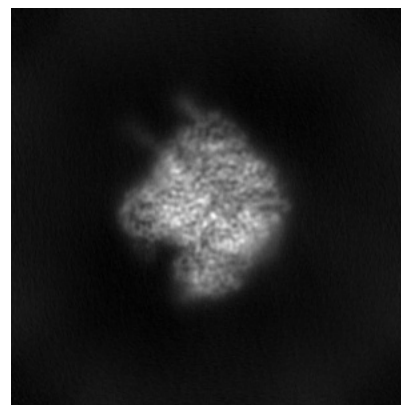
6.1.2 Raw map



X



Y

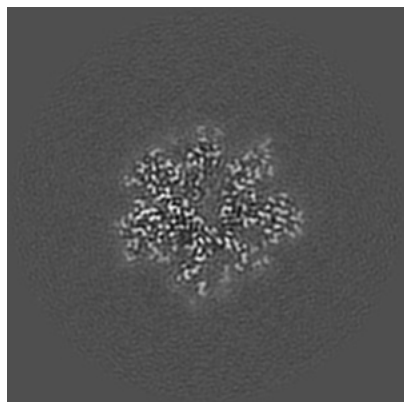


Z

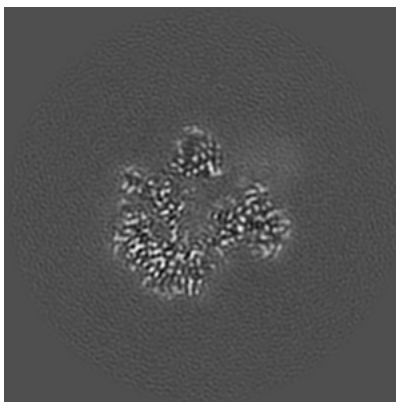
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

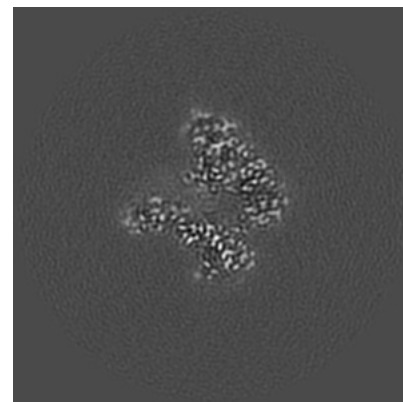
6.2.1 Primary map



X Index: 150

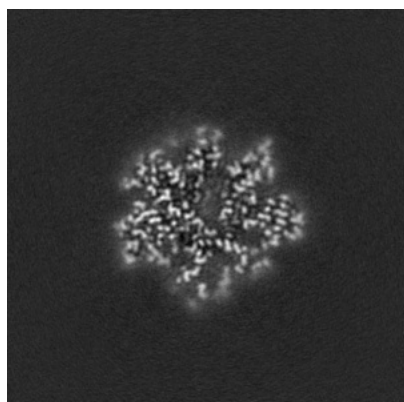


Y Index: 150

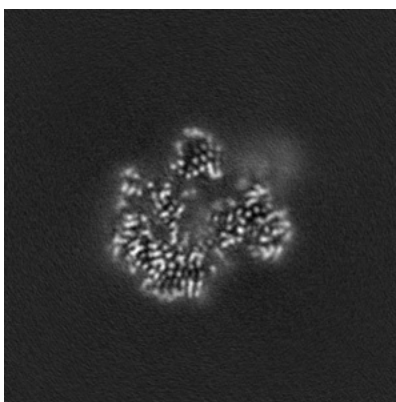


Z Index: 150

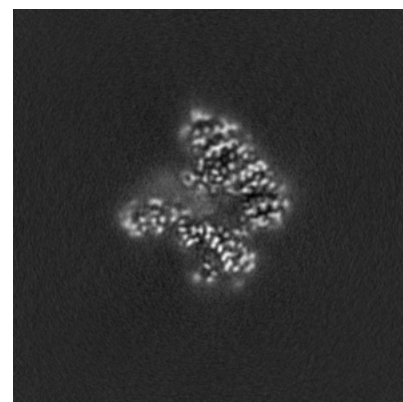
6.2.2 Raw map



X Index: 150



Y Index: 150

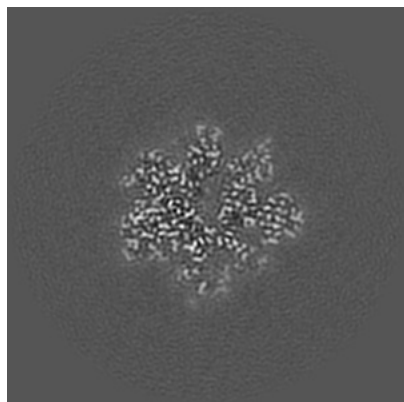


Z Index: 150

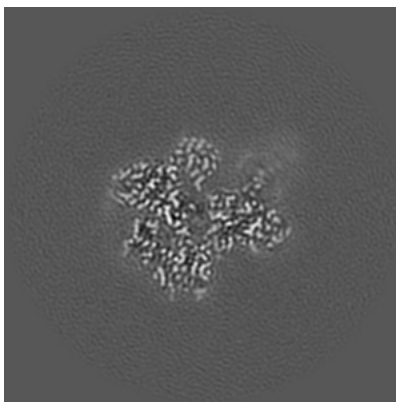
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

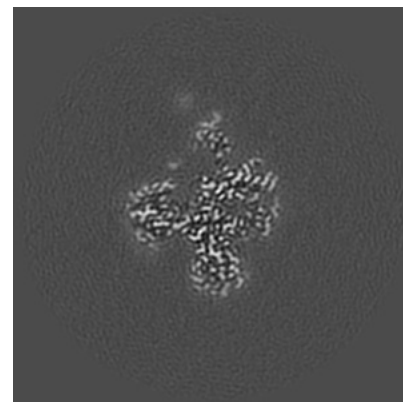
6.3.1 Primary map



X Index: 149

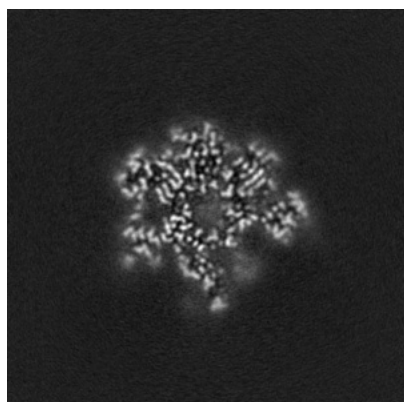


Y Index: 141

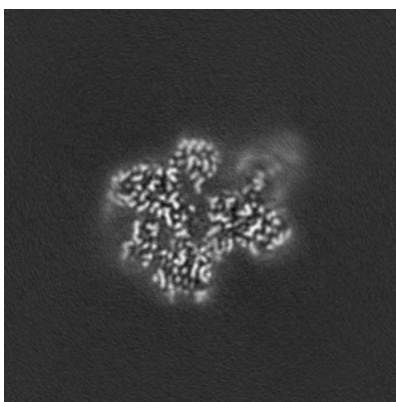


Z Index: 130

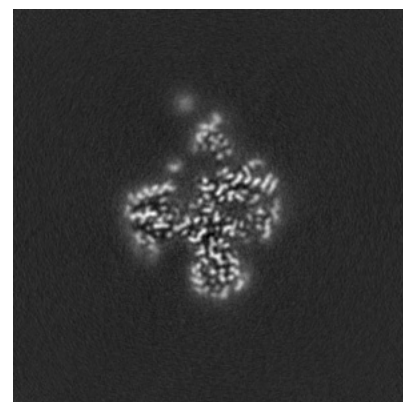
6.3.2 Raw map



X Index: 139



Y Index: 141

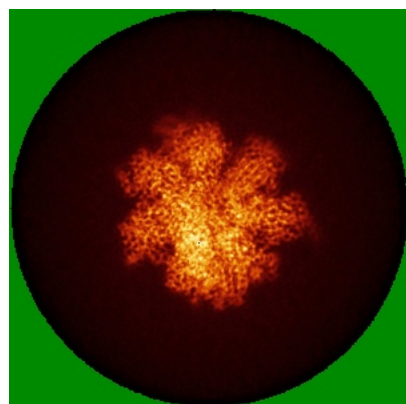


Z Index: 130

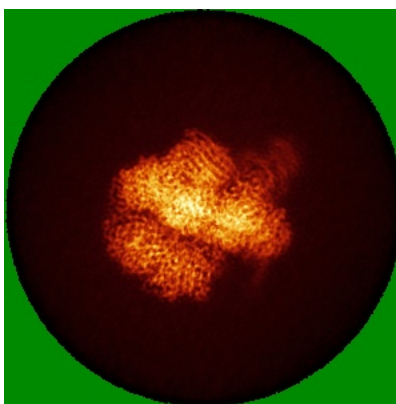
The images above show the largest variance slices of the map in three orthogonal directions.

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

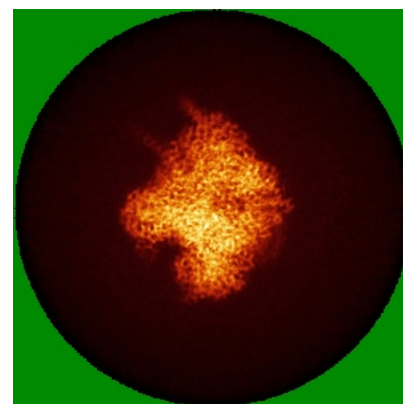
6.4.1 Primary map



X

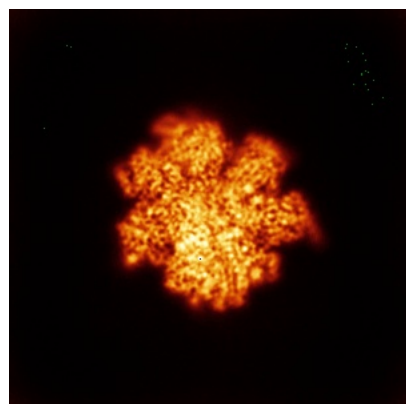


Y

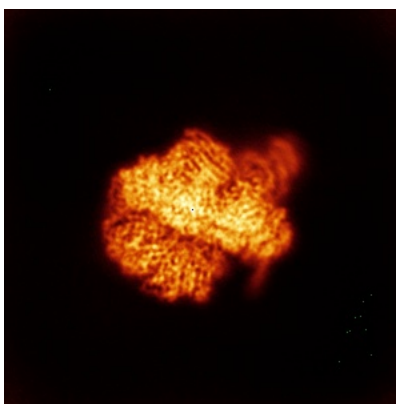


Z

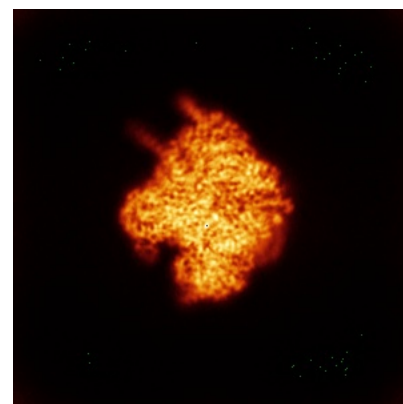
6.4.2 Raw map



X



Y

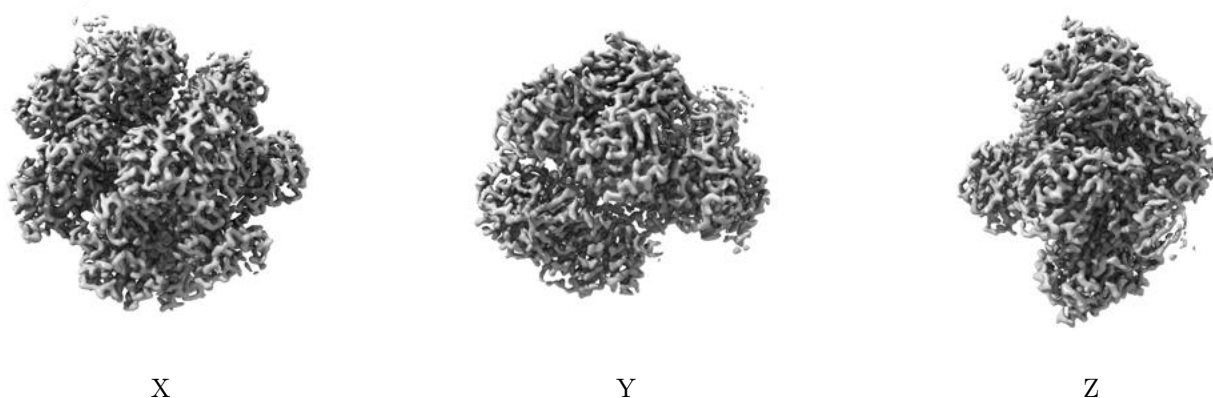


Z

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

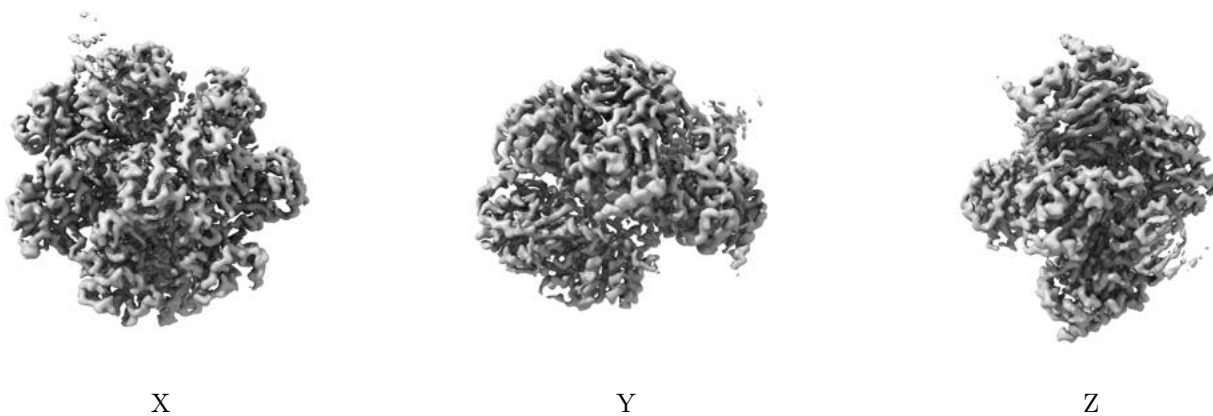
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

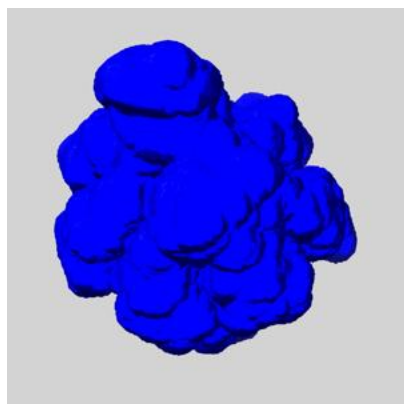
6.6 Mask visualisation [i](#)

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

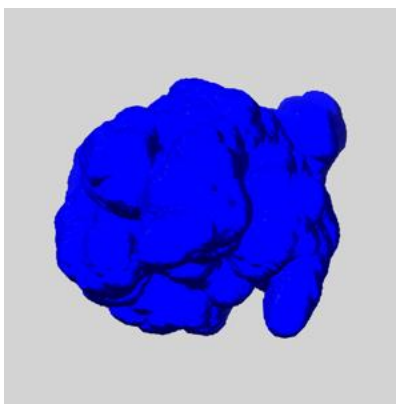
A mask typically either:

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

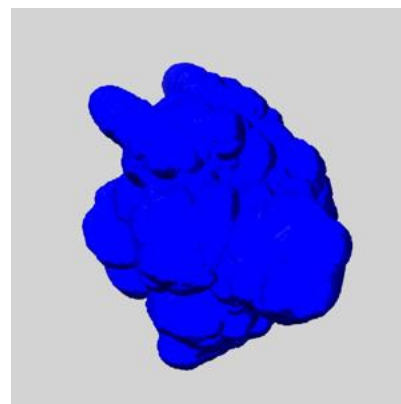
6.6.1 emd_18755_msk_1.map [i](#)



X



Y

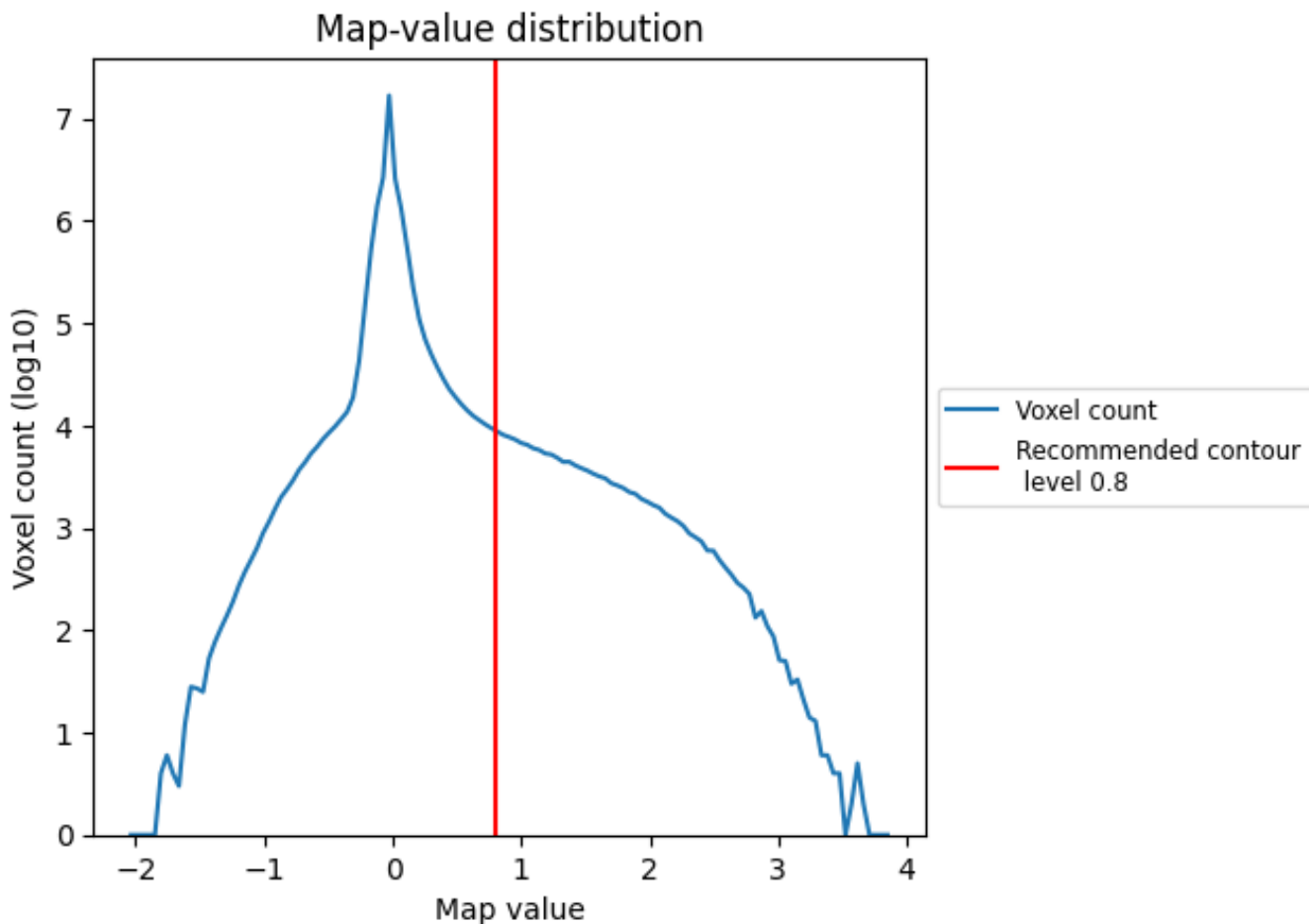


Z

7 Map analysis [i](#)

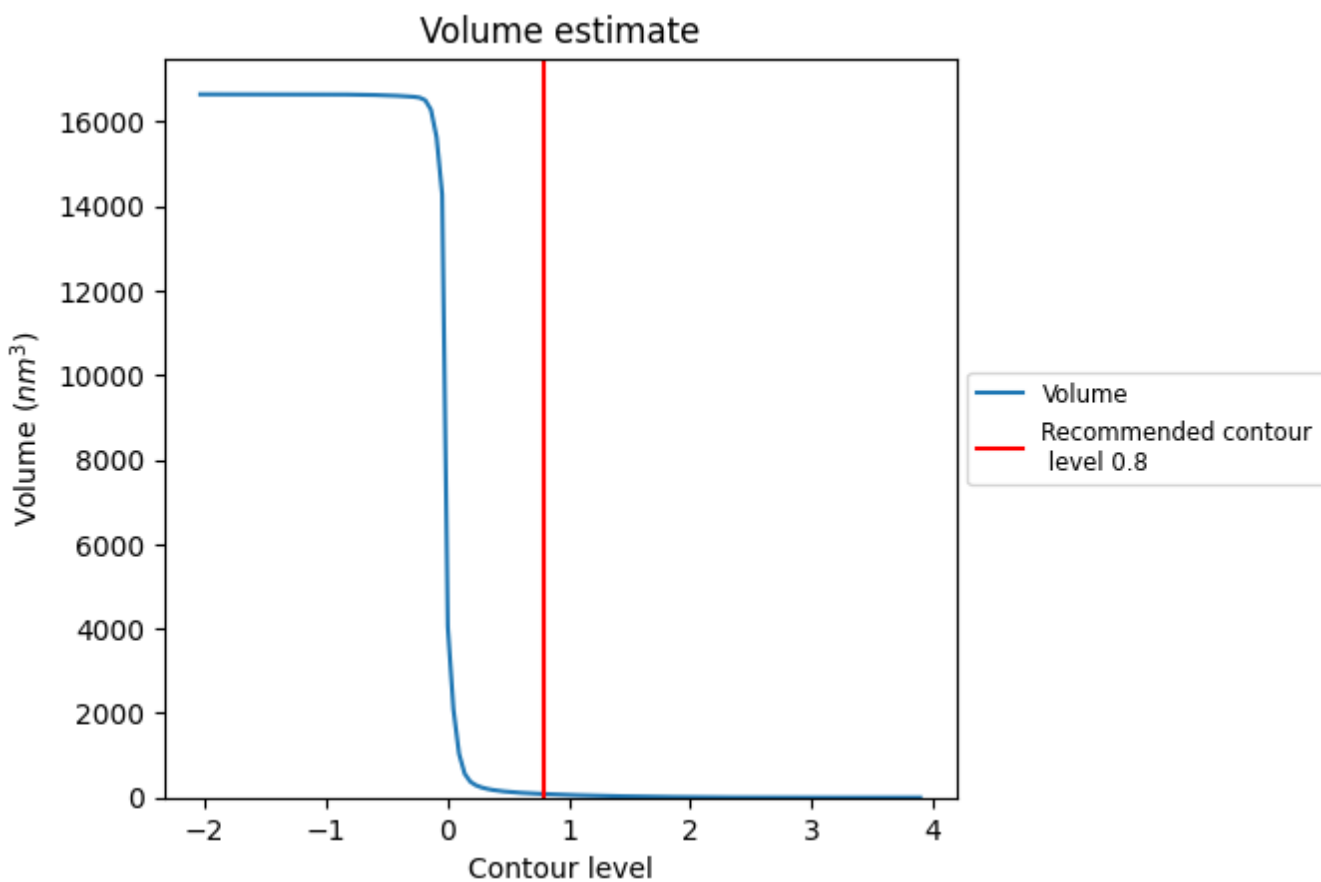
This section contains the results of statistical analysis of the map.

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.

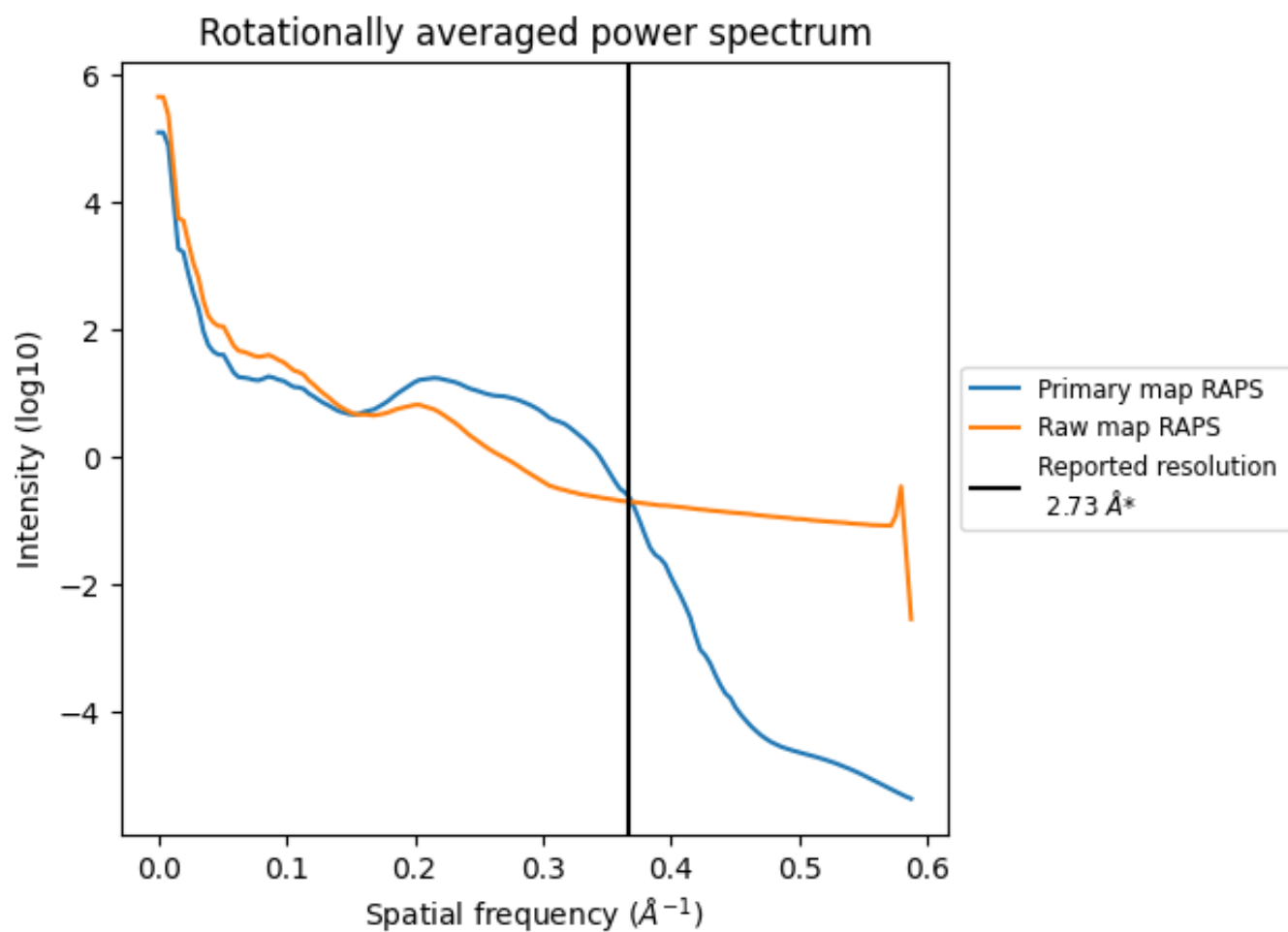
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

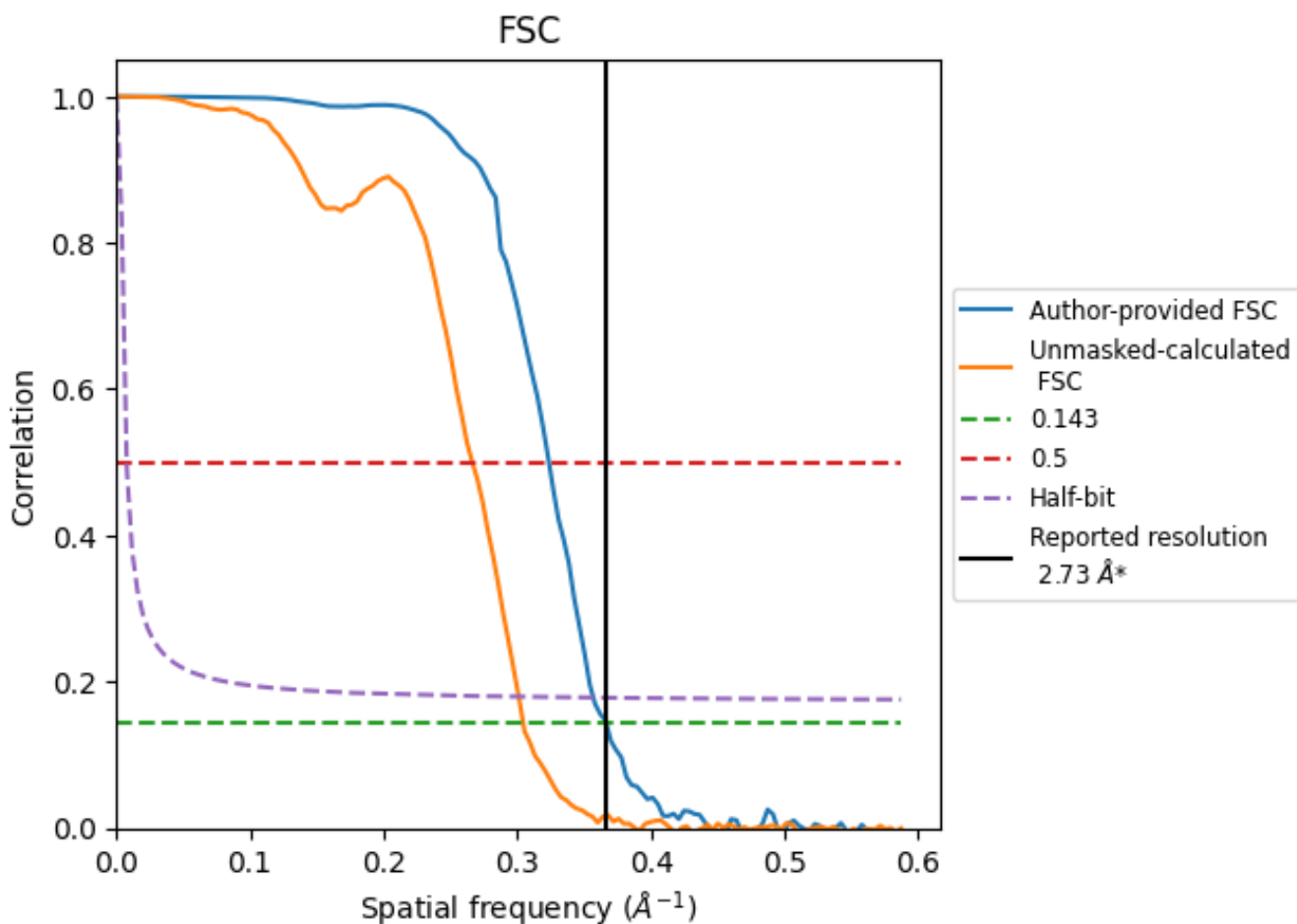


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

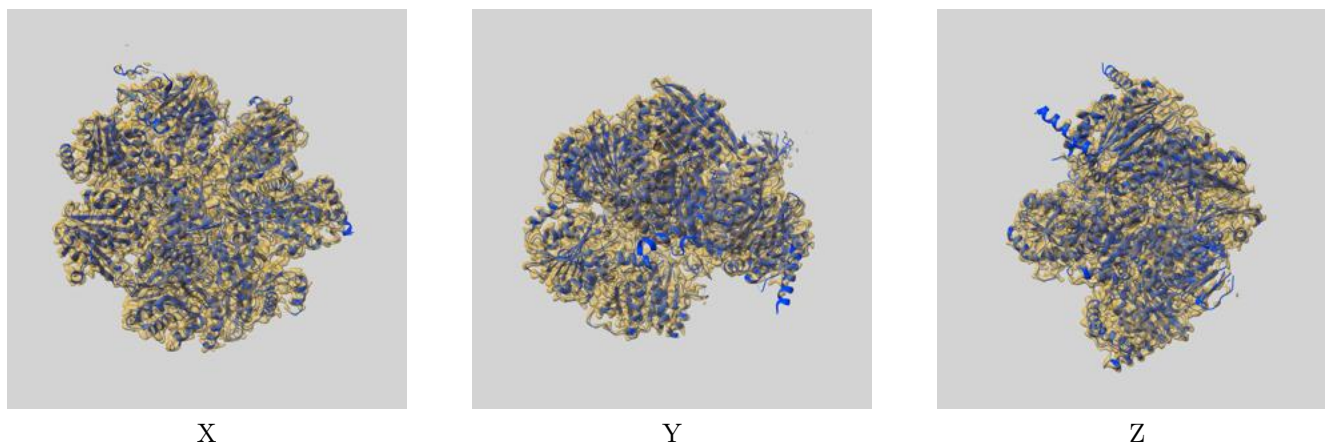
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.09	2.80
Unmasked-calculated*	3.28	3.75	3.32

*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 3.28 differs from the reported value 2.73 by more than 10 %

9 Map-model fit [i](#)

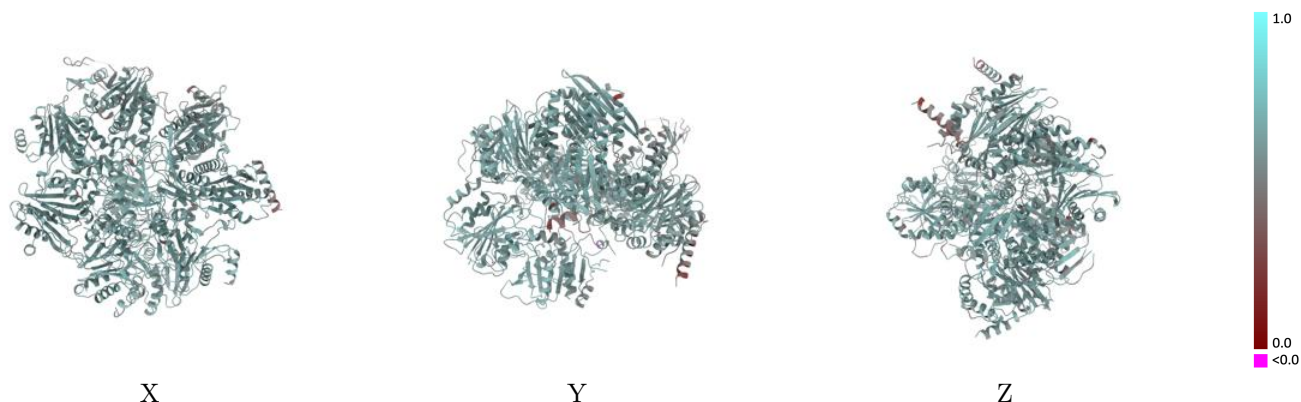
This section contains information regarding the fit between EMDB map EMD-18755 and PDB model 8QYJ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



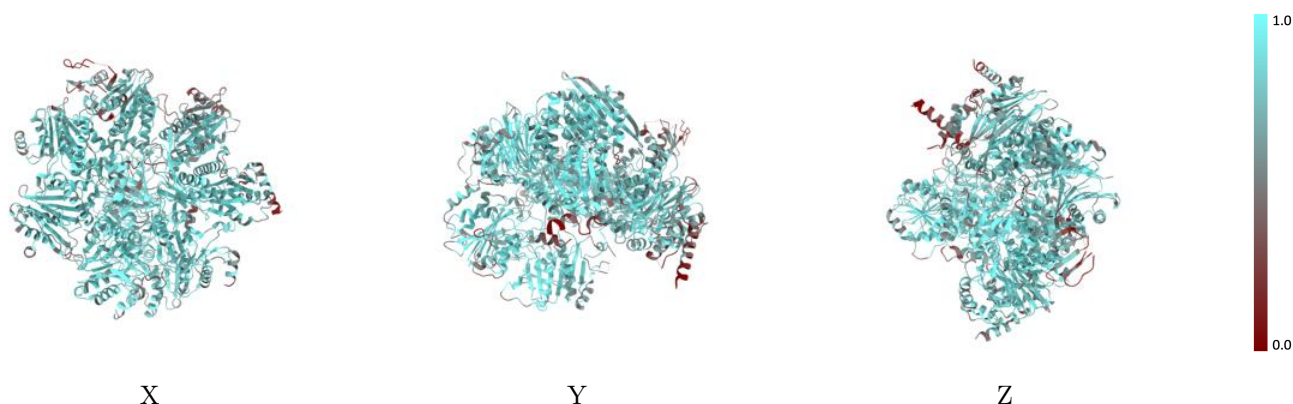
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



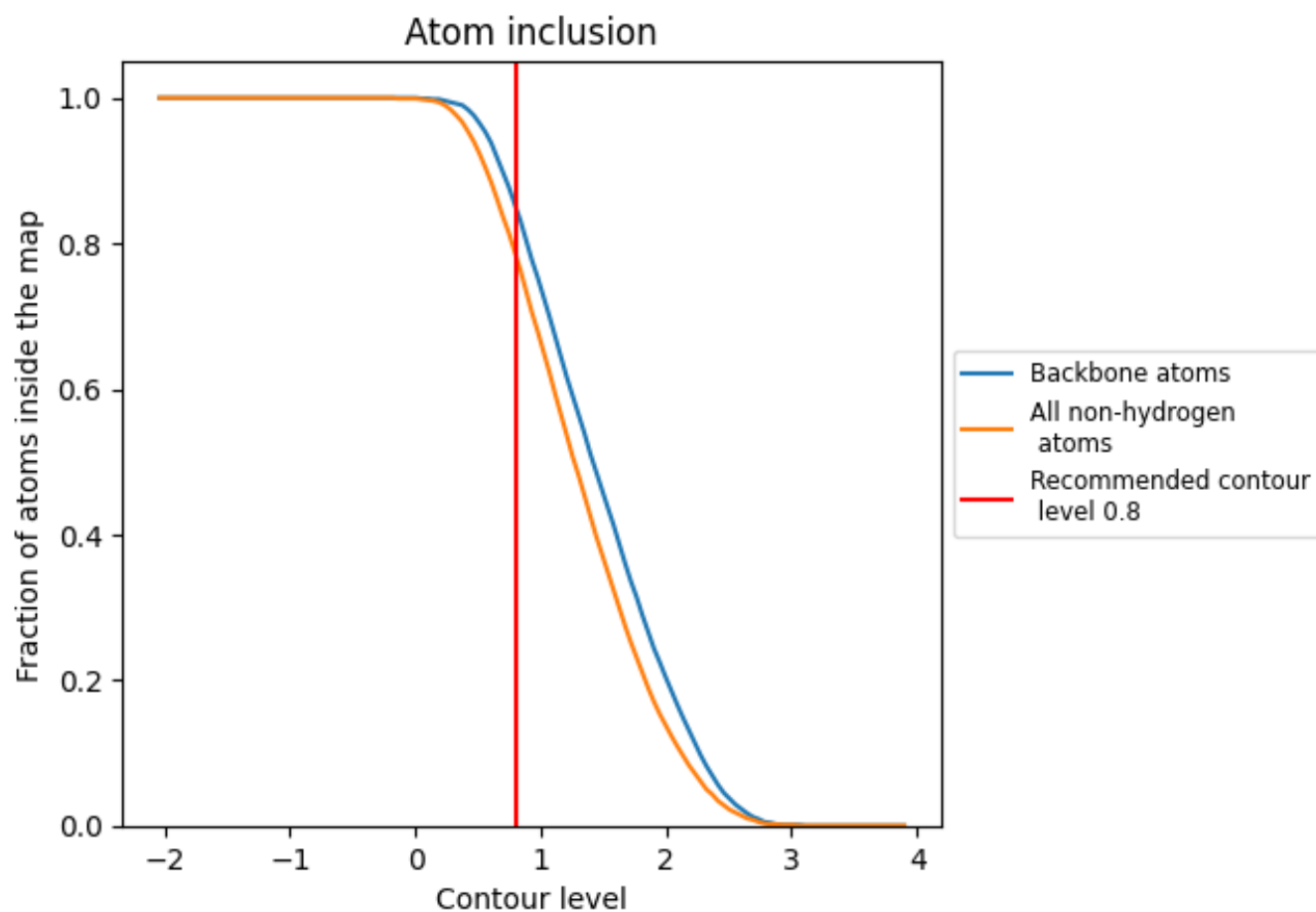
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.6020
A	 0.8000	 0.6020
B	 0.6510	 0.5600
C	 0.7640	 0.5970
D	 0.8230	 0.6140
E	 0.8640	 0.6200
F	 0.8140	 0.6100
G	 0.8400	 0.6130
H	 0.6790	 0.5850
I	 0.7670	 0.6060
J	 0.8320	 0.6100
K	 0.5040	 0.5440
L	 0.7840	 0.6150
M	 0.8140	 0.6060

