



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:59 AM UTC

PDB ID : 8R3M / pdb_00008r3m
EMDB ID : EMD-18873
Title : Mycobacterium smegmatis RNA polymerase transcription initiation complex with SigmaA, RbpA, HelD N-terminal, CO and PCh loop domain, and an upstream-fork promoter fragment; State III conformation
Authors : Koval, T.; Krasny, L.; Dohnalek, J.; Kouba, T.
Deposited on : 2023-11-09
Resolution : 3.49 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:

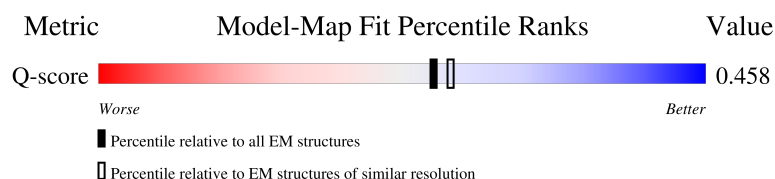
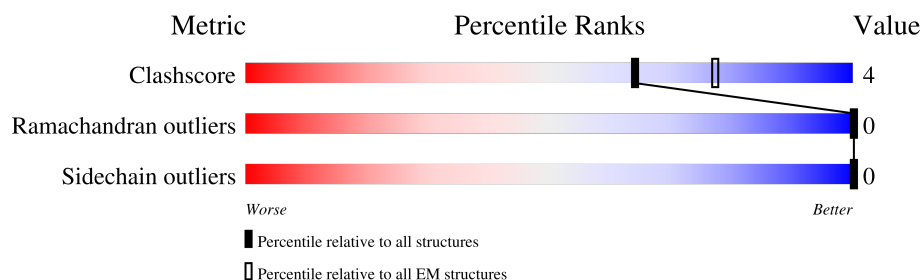
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.49 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.



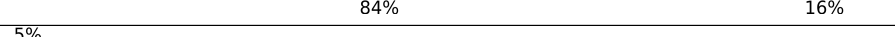
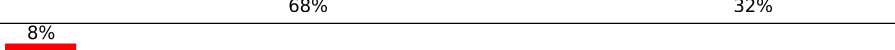
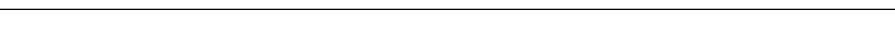
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13600 (2.99 - 3.99)

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	350	
1	B	350	
2	C	1169	
3	D	1317	

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Mol	Chain	Length	Quality of chain
4	E	107	
5	F	466	
6	J	114	
7	O	31	
8	P	22	
9	H	736	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 29417 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1716	1080	296	337	3		
1	B	239	Total	C	N	O	S	0	0
			1808	1136	311	358	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1109	Total	C	N	O	S	0	0
			8594	5377	1505	1677	35		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1280	Total	C	N	O	S	0	0
			9998	6258	1812	1887	41		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	84	Total	C	N	O	0	0
			656	416	109	131		

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	302	Total	C	N	O	S	0	0
			2423	1517	437	462	7		

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	104	Total	C	N	O	S	0	0
			842	525	153	162	2		

- Molecule 7 is a DNA chain called DNA 31-MER.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	31	Total	C	N	O	P	0	0
			635	306	114	185	30		

- Molecule 8 is a DNA chain called DNA 22-MER.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	22	Total	C	N	O	P	0	0
			443	215	76	131	21		

- Molecule 9 is a protein called Helicase.

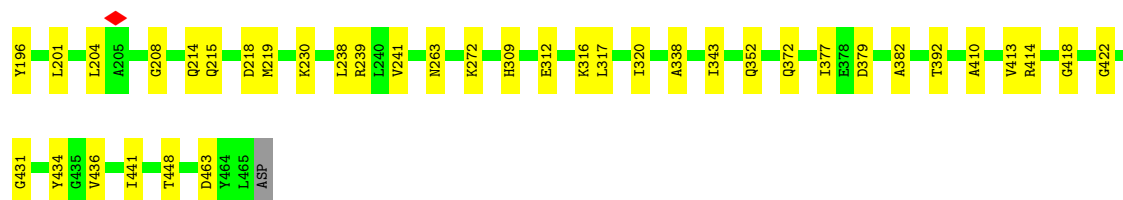
Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	338	Total	C	N	O	S	0	0
			2299	1397	438	459	5		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

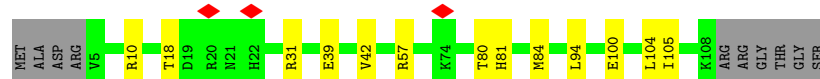
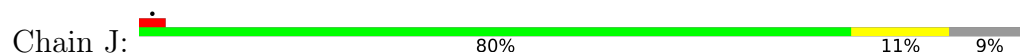
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

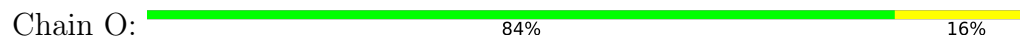
Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Mg	0
			1	1	



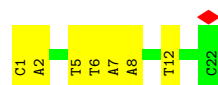
• Molecule 6: RNA polymerase-binding protein RbpA



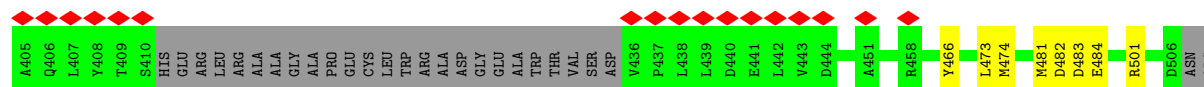
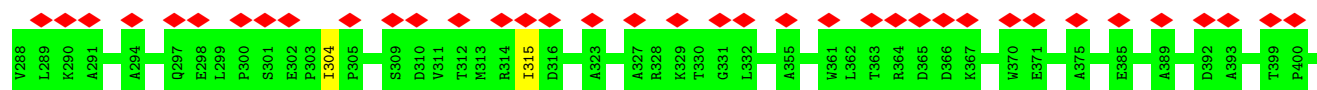
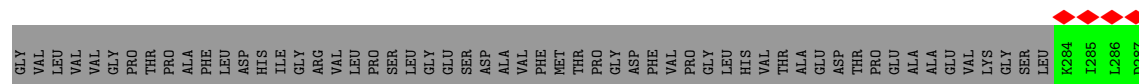
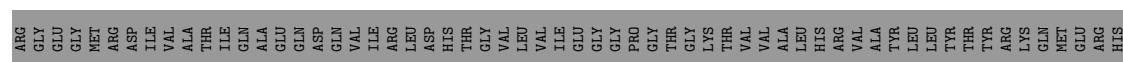
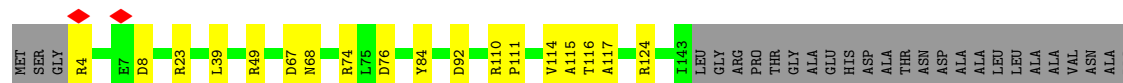
• Molecule 7: DNA 31-MER



• Molecule 8: DNA 22-MER



• Molecule 9: Helicase



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.691	Depositor
Minimum map value	-0.225	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	300.096, 300.096, 300.096	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83360004, 0.83360004, 0.83360004	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.11	0/1742	0.24	0/2370
1	B	0.10	0/1837	0.28	0/2501
2	C	0.11	0/8747	0.29	0/11853
3	D	0.10	0/10160	0.26	0/13730
4	E	0.09	0/669	0.27	0/909
5	F	0.10	0/2454	0.28	0/3307
6	J	0.09	0/858	0.26	0/1160
7	O	0.16	0/712	0.43	0/1098
8	P	0.20	0/495	0.47	0/761
9	H	0.08	0/2319	0.22	0/3155
All	All	0.11	0/29993	0.28	0/40844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1716	0	1759	4	0
1	B	1808	0	1841	10	0
2	C	8594	0	8544	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9998	0	10117	96	0
4	E	656	0	648	8	0
5	F	2423	0	2468	35	0
6	J	842	0	833	10	0
7	O	635	0	354	4	0
8	P	443	0	252	4	0
9	H	2299	0	1851	25	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
All	All	29417	0	28667	236	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 4.

All (236) 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)
2:C:1118:GLU:OE1	3:D:412:ARG:NH2	1.95	0.99
5:F:392:THR:HG22	6:J:18:THR:HG21	1.57	0.87
3:D:320:ILE:O	3:D:325:ARG:NH1	2.09	0.86
3:D:383:ASP:OD1	3:D:403:SER:OG	1.97	0.82
3:D:1223:SER:OG	3:D:1251:GLU:OE1	2.03	0.77
3:D:323:GLU:OE1	6:J:10:ARG:NH1	2.19	0.75
3:D:1031:ARG:NH1	3:D:1034:GLU:OE1	2.20	0.75
2:C:1119:LEU:HD23	2:C:1126:VAL:HG21	1.69	0.75
2:C:180:GLU:OE1	2:C:191:HIS:NE2	2.22	0.73
1:B:55:ARG:NH2	1:B:158:GLU:OE2	2.22	0.72
2:C:758:GLU:OE1	2:C:796:LYS:NZ	2.22	0.71
3:D:501:ALA:H	9:H:481:MET:CE	2.04	0.71
5:F:176:VAL:O	5:F:239:ARG:NH2	2.25	0.69
1:A:224:GLU:O	1:A:226:ASN:ND2	2.25	0.69
1:B:18:ARG:NH2	1:B:195:ASP:OD2	2.26	0.69
2:C:736:ASP:OD1	2:C:869:LYS:NZ	2.26	0.69
3:D:874:ARG:HD2	9:H:473:LEU:HD22	1.74	0.69
9:H:114:VAL:HG12	9:H:114:VAL:O	1.93	0.68
2:C:183:ASP:OD2	2:C:185:SER:OG	2.09	0.67
1:B:89:ASP:OD1	1:B:90:ASP:N	2.28	0.67
2:C:548:ASP:OD1	2:C:549:ARG:N	2.28	0.66
2:C:710:LEU:HD12	2:C:1021:ILE:HD11	1.75	0.66
3:D:501:ALA:H	9:H:481:MET:HE3	1.62	0.64
3:D:923:THR:HG22	3:D:942:ASP:OD1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1267:ARG:NE	4:E:105:GLU:OE2	2.30	0.64
2:C:532:VAL:HG12	2:C:569:TYR:HB2	1.79	0.64
3:D:169:ASP:OD2	3:D:208:LEU:HD23	1.98	0.64
2:C:880:HIS:NE2	2:C:924:GLU:OE1	2.32	0.63
3:D:756:GLU:OE1	3:D:769:ARG:NH1	2.32	0.63
5:F:182:GLU:O	5:F:186:GLU:OE1	2.17	0.63
1:B:149:ALA:N	1:B:165:ASP:OD1	2.32	0.62
3:D:384:ASN:ND2	3:D:399:LEU:O	2.33	0.61
3:D:1168:ILE:O	3:D:1179:GLY:N	2.33	0.61
9:H:4:ARG:NH1	9:H:8:ASP:OD1	2.34	0.60
3:D:868:ASP:OD2	9:H:501:ARG:NH1	2.35	0.59
5:F:413:VAL:HG21	5:F:448:THR:HG21	1.82	0.59
3:D:83:THR:HG22	3:D:84:ARG:H	1.66	0.59
2:C:163:GLU:OE1	2:C:433:GLN:NE2	2.34	0.59
3:D:81:GLU:OE2	3:D:91:ARG:NH2	2.30	0.59
2:C:724:ASP:OD2	2:C:916:ARG:NH2	2.35	0.58
3:D:17:ALA:O	3:D:21:ARG:NE	2.36	0.58
3:D:327:MET:HG3	3:D:337:THR:HG22	1.86	0.58
3:D:1101:SER:N	3:D:1104:ASP:OD2	2.35	0.57
3:D:1273:VAL:HG13	4:E:53:TYR:CE1	2.40	0.57
5:F:272:LYS:HG3	6:J:84:MET:HE2	1.86	0.57
5:F:214:GLN:NE2	5:F:218:ASP:OD2	2.35	0.56
3:D:24:SER:O	6:J:57:ARG:NH1	2.39	0.56
3:D:1273:VAL:HG13	4:E:53:TYR:HE1	1.70	0.56
9:H:23:ARG:NH2	9:H:92:ASP:OD1	2.36	0.56
9:H:39:LEU:O	9:H:49:ARG:NH2	2.39	0.56
2:C:394:ARG:NH2	2:C:407:THR:O	2.38	0.56
3:D:540:GLN:HB2	9:H:481:MET:HB2	1.88	0.55
2:C:398:GLN:CB	2:C:403:ILE:HD11	2.36	0.55
3:D:874:ARG:HA	3:D:877:VAL:HG12	1.89	0.55
1:B:111:VAL:O	1:B:111:VAL:HG13	2.06	0.55
3:D:848:TYR:O	3:D:852:THR:HG23	2.06	0.55
2:C:392:ARG:O	2:C:396:THR:HG23	2.07	0.55
2:C:285:THR:HG22	2:C:289:ASN:ND2	2.22	0.55
2:C:1082:ILE:HG23	2:C:1093:VAL:HG21	1.88	0.54
2:C:1082:ILE:CG2	2:C:1093:VAL:HG21	2.37	0.54
3:D:204:GLU:O	3:D:208:LEU:HD13	2.07	0.54
2:C:179:ASP:OD1	2:C:192:SER:OG	2.18	0.54
3:D:400:LYS:NZ	5:F:372:GLN:OE1	2.39	0.54
3:D:529:CYS:O	3:D:533:ASN:N	2.40	0.54
5:F:309:HIS:NE2	7:O:21:DT:OP2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:482:ASP:OD1	9:H:483:ASP:N	2.39	0.53
3:D:604:LYS:O	3:D:605:ASP:OD1	2.25	0.53
2:C:148:PHE:CE1	2:C:380:ILE:HD11	2.43	0.53
3:D:16:THR:O	3:D:16:THR:HG22	2.07	0.53
5:F:316:LYS:O	5:F:320:ILE:HD12	2.08	0.53
3:D:376:GLU:OE2	5:F:165:SER:OG	2.21	0.53
9:H:76:ASP:O	9:H:124:ARG:N	2.40	0.52
1:B:56:ILE:HD13	1:B:136:VAL:HG23	1.90	0.52
5:F:201:LEU:HD12	5:F:219:MET:HE1	1.91	0.52
2:C:23:VAL:HG21	2:C:623:LEU:HD21	1.91	0.52
2:C:387:MET:O	2:C:391:VAL:HG23	2.09	0.52
3:D:74:ILE:HD12	6:J:42:VAL:HG23	1.91	0.52
3:D:1079:ASP:OD1	3:D:1079:ASP:N	2.42	0.52
2:C:23:VAL:CG2	2:C:623:LEU:HD21	2.39	0.51
2:C:711:LEU:HD12	2:C:1017:GLY:O	2.10	0.51
3:D:1277:GLU:OE1	3:D:1277:GLU:N	2.39	0.51
2:C:437:LEU:HB2	2:C:704:MET:HE1	1.91	0.51
2:C:398:GLN:HB3	2:C:403:ILE:HD11	1.93	0.51
2:C:394:ARG:HA	2:C:397:THR:HG22	1.92	0.51
3:D:447:MET:O	3:D:451:LEU:HD13	2.10	0.51
2:C:131:ILE:HD12	2:C:138:ILE:HG22	1.93	0.51
3:D:1186:GLU:N	3:D:1186:GLU:OE1	2.44	0.51
3:D:74:ILE:HG12	3:D:81:GLU:HB3	1.94	0.50
5:F:241:VAL:HG11	5:F:263:ASN:OD1	2.10	0.50
2:C:344:THR:HG22	2:C:344:THR:O	2.12	0.50
2:C:299:LEU:HD23	2:C:303:GLY:C	2.36	0.50
2:C:335:TYR:CE2	2:C:356:VAL:HG22	2.47	0.50
3:D:114:LEU:O	3:D:118:LEU:HD23	2.11	0.50
2:C:148:PHE:HE1	2:C:380:ILE:HD11	1.77	0.50
2:C:910:THR:HG21	3:D:728:VAL:HG12	1.94	0.50
2:C:806:THR:HG23	2:C:809:GLU:H	1.77	0.49
3:D:814:ARG:O	3:D:818:GLY:N	2.37	0.49
1:B:150:VAL:O	1:B:150:VAL:HG13	2.12	0.49
3:D:748:HIS:CG	3:D:780:ALA:HB2	2.47	0.49
2:C:731:ARG:NH1	2:C:735:GLU:OE1	2.44	0.49
3:D:929:VAL:CG1	3:D:935:VAL:HG12	2.43	0.49
6:J:100:GLU:OE2	6:J:104:LEU:HD21	2.12	0.49
3:D:1096:THR:HG22	3:D:1096:THR:O	2.13	0.48
2:C:248:ILE:O	2:C:252:THR:HG23	2.14	0.48
3:D:874:ARG:NH1	9:H:466:TYR:CE1	2.81	0.48
4:E:35:PRO:HG2	4:E:40:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1056:GLY:O	3:D:421:ARG:NH1	2.46	0.48
5:F:317:LEU:HD21	5:F:352:GLN:OE1	2.13	0.48
2:C:611:ARG:O	2:C:708:LYS:NZ	2.42	0.48
4:E:73:LEU:HD23	4:E:73:LEU:H	1.79	0.48
2:C:485:ILE:HD11	3:D:859:LEU:HD23	1.96	0.47
2:C:965:THR:HG23	2:C:965:THR:O	2.14	0.47
3:D:1037:GLU:OE1	3:D:1212:THR:HG23	2.14	0.47
1:A:2:LEU:HD23	1:A:2:LEU:H	1.79	0.47
3:D:360:LEU:HD23	3:D:360:LEU:H	1.78	0.47
3:D:1027:GLY:O	3:D:1146:GLN:NE2	2.47	0.47
2:C:1119:LEU:CD2	2:C:1126:VAL:HG21	2.41	0.47
2:C:939:VAL:HG22	2:C:939:VAL:O	2.14	0.47
9:H:116:THR:HG22	9:H:117:ALA:N	2.29	0.47
1:B:56:ILE:HD13	1:B:136:VAL:CG2	2.45	0.47
5:F:183:GLU:OE1	5:F:183:GLU:N	2.45	0.47
1:B:79:ASN:OD1	3:D:636:ARG:NH1	2.35	0.47
2:C:1042:MET:N	5:F:377:ILE:O	2.46	0.47
2:C:1118:GLU:OE2	3:D:405:LEU:HB2	2.14	0.47
3:D:83:THR:HG22	3:D:84:ARG:N	2.28	0.47
2:C:1098:VAL:HG11	3:D:469:ILE:CD1	2.44	0.47
3:D:430:ILE:HG21	3:D:541:MET:HG3	1.96	0.47
3:D:202:GLU:O	3:D:206:ARG:HG2	2.15	0.46
4:E:63:ASP:O	4:E:67:GLN:N	2.36	0.46
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.97	0.46
3:D:645:ASP:OD1	3:D:645:ASP:N	2.47	0.46
3:D:1171:SER:OG	3:D:1176:PHE:O	2.34	0.46
6:J:80:THR:HG22	6:J:81:HIS:N	2.31	0.46
2:C:131:ILE:CD1	2:C:138:ILE:HG22	2.46	0.46
3:D:1020:THR:HG22	3:D:1022:GLY:H	1.80	0.46
6:J:31:ARG:NH2	6:J:39:GLU:OE1	2.48	0.46
2:C:606:ALA:HB2	2:C:1022:LEU:HD13	1.99	0.45
5:F:379:ASP:CG	5:F:382:ALA:HB2	2.41	0.45
7:O:12:DG:C2'	7:O:13:DT:H72	2.47	0.45
1:A:69:VAL:HG22	1:A:128:LEU:HD22	1.98	0.45
5:F:191:ILE:HD11	5:F:230:LYS:HA	1.98	0.45
9:H:67:ASP:OD1	9:H:68:ASN:N	2.50	0.45
3:D:346:ARG:NH2	3:D:391:VAL:HG11	2.32	0.45
3:D:365:ILE:HD12	3:D:365:ILE:H	1.82	0.45
3:D:400:LYS:HE2	3:D:405:LEU:HD21	1.98	0.45
5:F:431:GLY:HA2	5:F:441:ILE:HD11	1.98	0.45
2:C:588:LEU:HB3	2:C:967:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:964:VAL:HG13	3:D:973:VAL:HG11	1.99	0.45
5:F:215:GLN:OE1	5:F:215:GLN:N	2.50	0.45
2:C:265:LEU:HD13	2:C:284:GLN:HB2	1.98	0.45
9:H:114:VAL:O	9:H:114:VAL:CG1	2.64	0.45
2:C:224:PRO:HB2	2:C:227:VAL:HG23	1.99	0.44
5:F:204:LEU:O	5:F:208:GLY:N	2.50	0.44
5:F:187:LEU:O	5:F:191:ILE:HG13	2.17	0.44
2:C:209:LYS:O	2:C:209:LYS:HG2	2.18	0.44
3:D:1198:GLY:O	3:D:1200:GLU:N	2.46	0.44
2:C:369:LEU:HD11	2:C:446:LEU:HD22	2.00	0.44
3:D:1075:GLU:N	3:D:1075:GLU:OE1	2.51	0.44
2:C:304:ARG:NH2	2:C:325:THR:OG1	2.51	0.44
3:D:35:ASN:OD1	3:D:36:TYR:N	2.48	0.44
3:D:87:VAL:HG12	3:D:87:VAL:O	2.17	0.44
3:D:432:VAL:O	3:D:432:VAL:HG13	2.18	0.44
3:D:875:ARG:NH1	9:H:466:TYR:CE2	2.86	0.44
3:D:1162:MET:C	3:D:1163:LEU:HD22	2.43	0.44
2:C:1126:VAL:HG13	3:D:10:LEU:HD21	1.98	0.44
2:C:1127:GLU:OE2	3:D:11:ARG:NE	2.44	0.44
5:F:434:TYR:HB2	5:F:436:VAL:HG23	1.98	0.44
2:C:412:ARG:N	2:C:413:PRO:HD2	2.33	0.44
3:D:867:ALA:HA	9:H:474:MET:HE1	2.00	0.43
2:C:534:GLN:NE2	2:C:536:ASN:OD1	2.49	0.43
2:C:1102:ASN:ND2	4:E:63:ASP:OD1	2.51	0.43
3:D:814:ARG:NH1	3:D:819:MET:O	2.51	0.43
7:O:12:DG:N2	8:P:12:DT:C2	2.86	0.43
2:C:165:VAL:HG23	2:C:431:MET:HB2	1.99	0.43
2:C:704:MET:CE	2:C:706:LEU:HD21	2.49	0.43
3:D:16:THR:O	3:D:17:ALA:HB3	2.17	0.43
3:D:1166:VAL:HG23	3:D:1205:ARG:C	2.43	0.43
5:F:218:ASP:HB3	6:J:105:ILE:HD13	1.99	0.43
2:C:53:GLU:HA	2:C:53:GLU:OE1	2.18	0.43
3:D:1060:ASP:OD1	3:D:1060:ASP:N	2.52	0.43
5:F:312:GLU:HA	5:F:312:GLU:OE1	2.18	0.43
3:D:1111:GLN:NE2	3:D:1113:MET:O	2.48	0.43
2:C:193:VAL:HG13	2:C:193:VAL:O	2.18	0.43
5:F:173:ILE:HG22	5:F:238:LEU:HD23	2.00	0.43
2:C:227:VAL:HG12	2:C:268:ILE:HD11	2.01	0.42
3:D:471:SER:N	5:F:463:ASP:OD2	2.52	0.42
3:D:875:ARG:HD3	9:H:466:TYR:CE2	2.53	0.42
2:C:173:SER:O	2:C:177:TYR:OH	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:369:LEU:HD23	2:C:497:VAL:HG21	2.01	0.42
2:C:723:GLU:HB2	3:D:536:PHE:HD2	1.84	0.42
2:C:1001:LEU:HD12	2:C:1014:VAL:HG21	2.01	0.42
1:B:70:LYS:HE2	1:B:127:THR:HG21	2.02	0.42
2:C:477:ILE:HD11	2:C:593:ALA:O	2.18	0.42
3:D:1050:VAL:O	3:D:1067:ILE:HG21	2.20	0.42
8:P:7:DA:H2''	8:P:8:DA:O5'	2.20	0.42
3:D:509:ILE:O	3:D:509:ILE:HG23	2.18	0.42
9:H:111:PRO:O	9:H:115:ALA:HB3	2.20	0.42
2:C:334:GLU:O	2:C:338:ARG:HG2	2.20	0.42
3:D:550:GLU:O	3:D:554:GLU:HG3	2.20	0.42
2:C:715:MET:HE1	2:C:1010:PHE:CE2	2.55	0.41
2:C:1084:SER:O	2:C:1085:ASP:OD1	2.38	0.41
5:F:180:ASN:HB2	5:F:183:GLU:OE1	2.19	0.41
3:D:560:LEU:O	3:D:564:ASN:ND2	2.53	0.41
8:P:1:DC:H2''	8:P:2:DA:C8	2.56	0.41
3:D:87:VAL:HG11	3:D:91:ARG:NE	2.35	0.41
3:D:920:PHE:O	3:D:921:ALA:HB3	2.20	0.41
3:D:1090:ILE:N	3:D:1098:GLY:O	2.44	0.41
5:F:196:TYR:HB2	6:J:94:LEU:HD12	2.02	0.41
5:F:219:MET:HE3	5:F:219:MET:HB3	1.96	0.41
5:F:379:ASP:OD1	5:F:379:ASP:N	2.53	0.41
3:D:364:GLU:N	3:D:364:GLU:OE1	2.54	0.41
8:P:5:DT:H2'	8:P:6:DT:H72	2.03	0.41
9:H:483:ASP:OD1	9:H:484:GLU:N	2.53	0.41
2:C:132:ASN:O	2:C:136:GLY:N	2.54	0.41
2:C:178:PHE:CE1	2:C:193:VAL:HG21	2.55	0.41
4:E:43:ARG:HH11	4:E:43:ARG:HG3	1.86	0.41
3:D:477:GLU:OE1	3:D:478:ARG:HD2	2.21	0.41
9:H:74:ARG:NH1	9:H:84:TYR:OH	2.54	0.41
3:D:429:VAL:HG22	3:D:430:ILE:N	2.36	0.41
3:D:920:PHE:O	3:D:1151:HIS:NE2	2.45	0.41
5:F:338:ALA:HB1	5:F:343:ILE:O	2.21	0.41
5:F:410:ALA:HB1	5:F:414:ARG:NH2	2.36	0.41
5:F:418:GLY:O	5:F:422:GLY:N	2.54	0.41
5:F:463:ASP:O	5:F:463:ASP:OD1	2.39	0.41
2:C:579:SER:OG	2:C:580:VAL:N	2.54	0.40
2:C:1089:GLY:O	2:C:1093:VAL:HG23	2.21	0.40
3:D:357:LEU:CD2	3:D:366:ILE:HG22	2.51	0.40
5:F:201:LEU:HD23	5:F:201:LEU:C	2.46	0.40
2:C:93:SER:O	2:C:133:ASN:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:498:ASN:O	2:C:501:GLY:N	2.55	0.40
3:D:501:ALA:HB3	9:H:481:MET:HE2	2.01	0.40
3:D:501:ALA:N	9:H:481:MET:HE3	2.34	0.40
7:O:19:DA:C8	7:O:20:DT:H72	2.56	0.40
9:H:110:ARG:N	9:H:111:PRO:HD2	2.37	0.40
2:C:323:THR:OG1	2:C:324:LEU:N	2.55	0.40
9:H:304:ILE:O	9:H:315:ILE:N	2.49	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	224/350 (64%)	219 (98%)	5 (2%)	0	100	100
1	B	237/350 (68%)	228 (96%)	9 (4%)	0	100	100
2	C	1107/1169 (95%)	1072 (97%)	35 (3%)	0	100	100
3	D	1278/1317 (97%)	1240 (97%)	38 (3%)	0	100	100
4	E	82/107 (77%)	80 (98%)	2 (2%)	0	100	100
5	F	300/466 (64%)	292 (97%)	8 (3%)	0	100	100
6	J	102/114 (90%)	98 (96%)	4 (4%)	0	100	100
9	H	332/736 (45%)	322 (97%)	10 (3%)	0	100	100
All	All	3662/4609 (80%)	3551 (97%)	111 (3%)	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	193/297 (65%)	193 (100%)	0	100	100
1	B	203/297 (68%)	203 (100%)	0	100	100
2	C	937/984 (95%)	937 (100%)	0	100	100
3	D	1064/1095 (97%)	1064 (100%)	0	100	100
4	E	70/86 (81%)	70 (100%)	0	100	100
5	F	259/379 (68%)	259 (100%)	0	100	100
6	J	91/98 (93%)	91 (100%)	0	100	100
9	H	159/583 (27%)	159 (100%)	0	100	100
All	All	2976/3819 (78%)	2976 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	GLN
1	B	61	HIS
2	C	398	GLN
2	C	470	HIS
2	C	921	GLN
2	C	1120	GLN
3	D	22	ASN
3	D	103	HIS
3	D	375	GLN
3	D	851	ASN
3	D	1000	GLN
3	D	1154	HIS
4	E	66	ASN
4	E	85	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

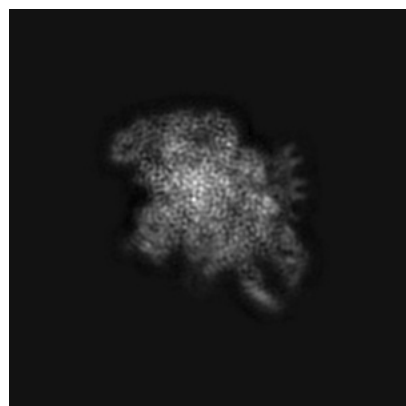
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18873. These allow visual inspection of the internal detail of the map and identification of artifacts.

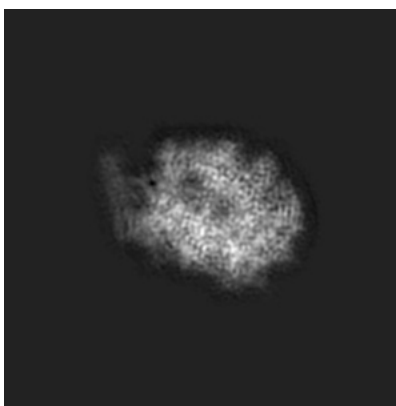
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

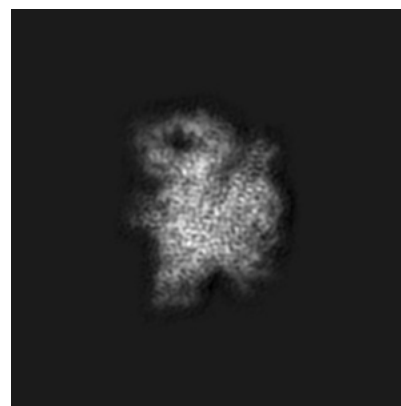
6.1.1 Primary map



X

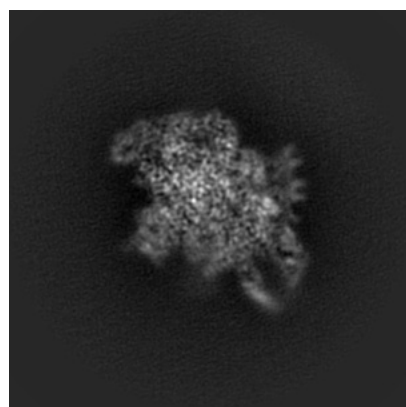


Y

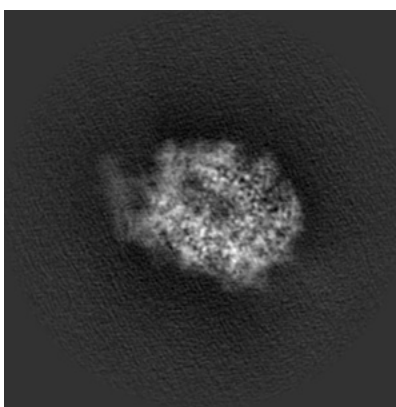


Z

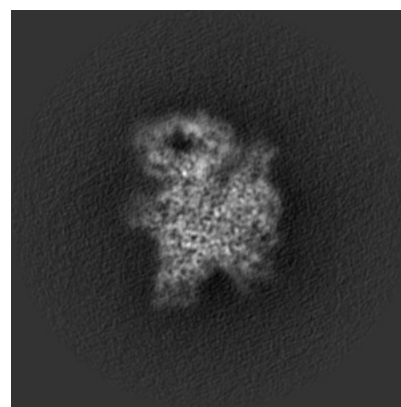
6.1.2 Raw map



X



Y

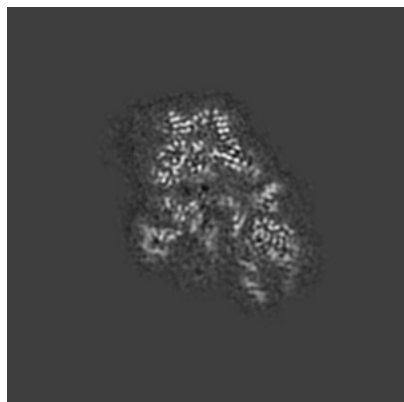


Z

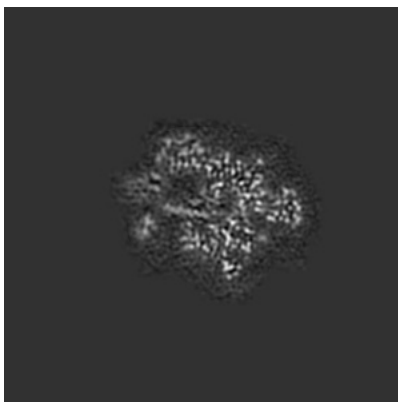
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

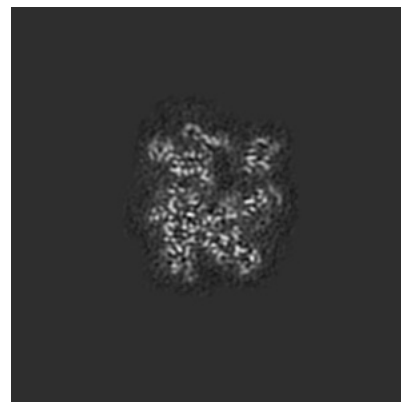
6.2.1 Primary map



X Index: 180

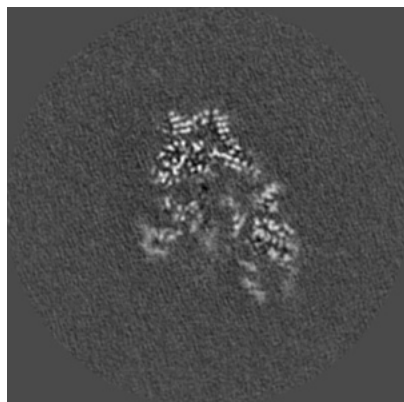


Y Index: 180

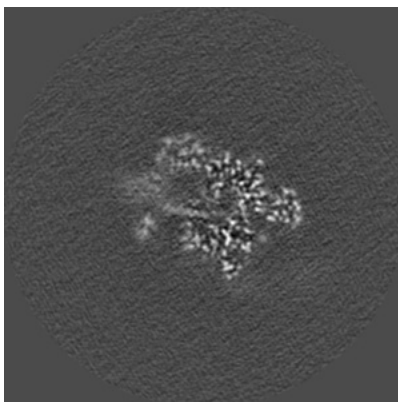


Z Index: 180

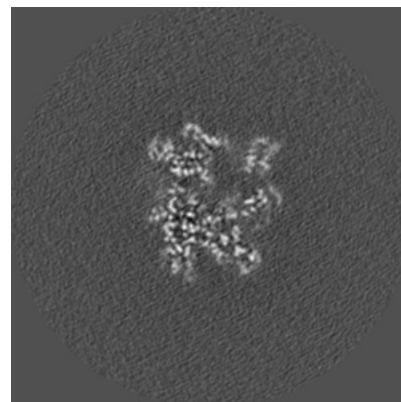
6.2.2 Raw map



X Index: 180



Y Index: 180

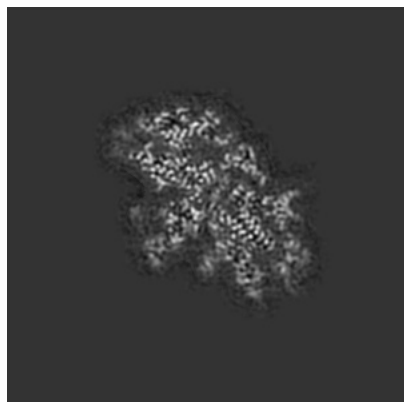


Z Index: 180

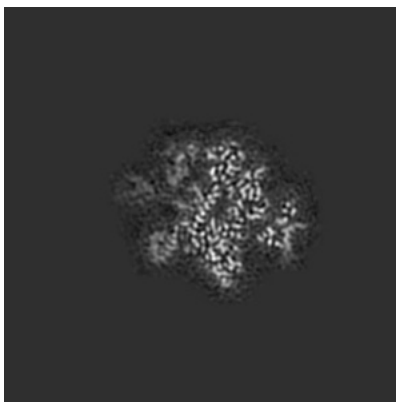
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

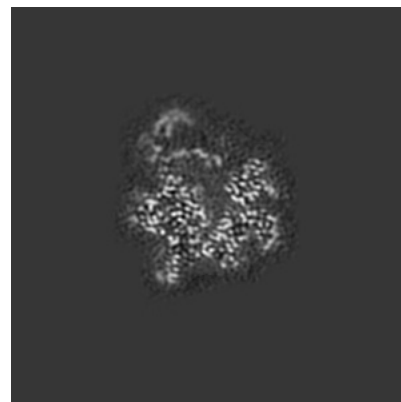
6.3.1 Primary map



X Index: 167

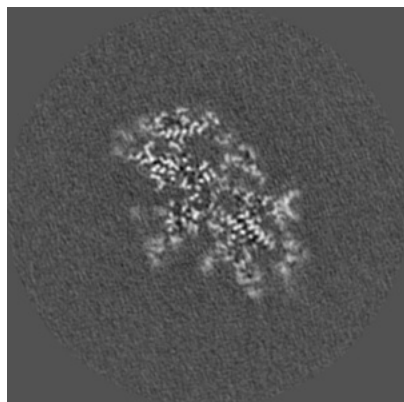


Y Index: 166

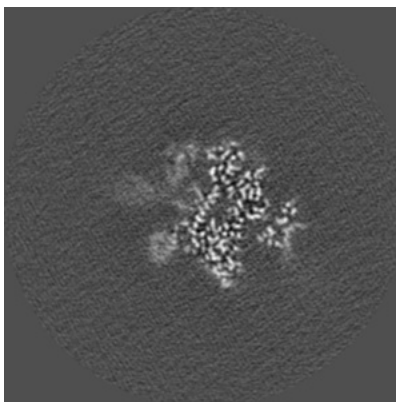


Z Index: 204

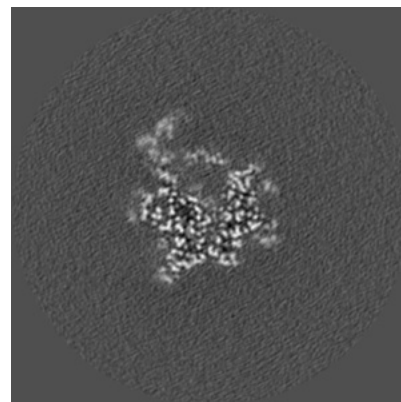
6.3.2 Raw map



X Index: 166



Y Index: 166

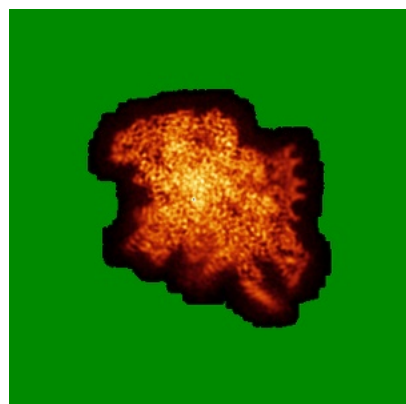


Z Index: 208

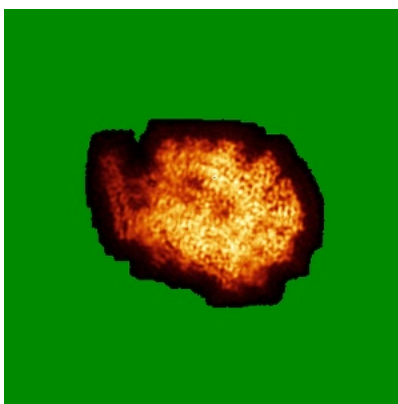
The images above show the largest variance slices of the map in three orthogonal directions.

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

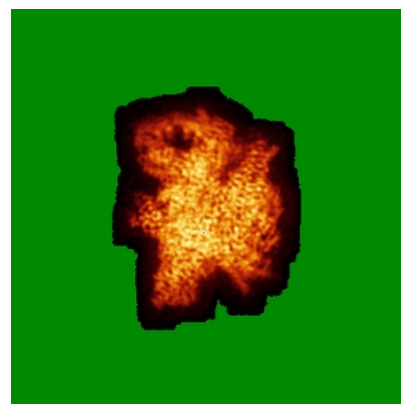
6.4.1 Primary map



X

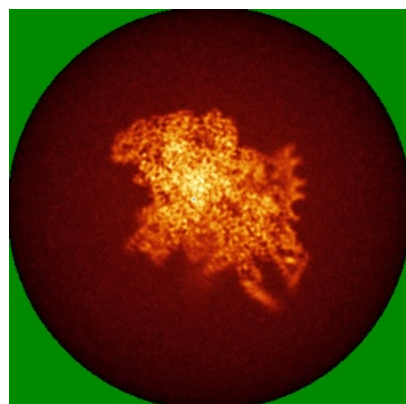


Y

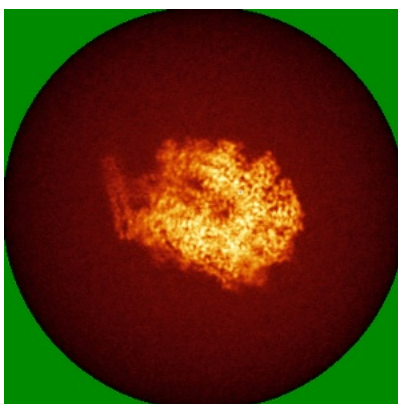


Z

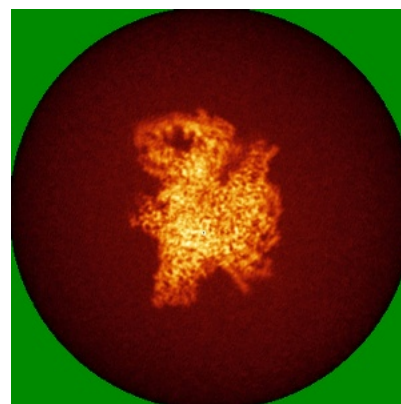
6.4.2 Raw map



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.

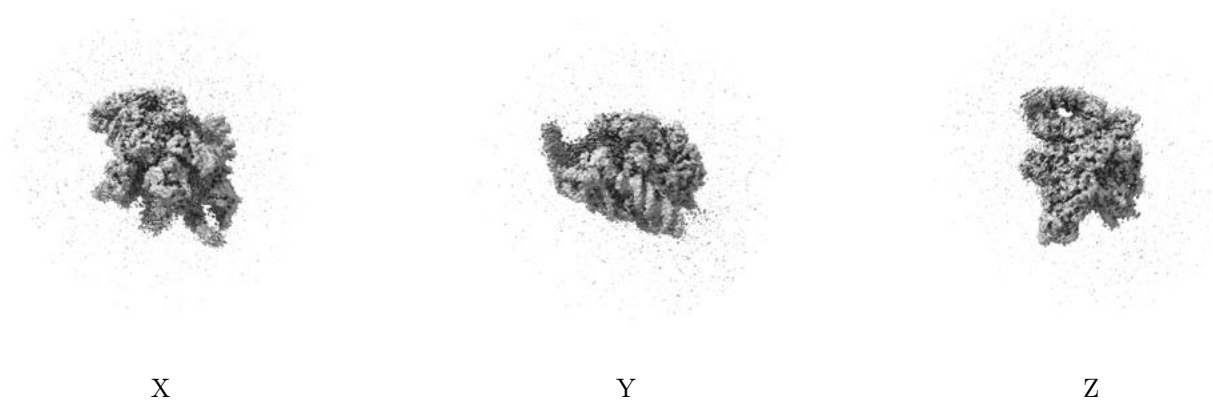
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

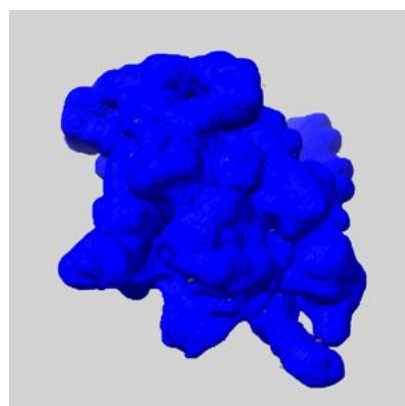
6.6 Mask visualisation [i](#)

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

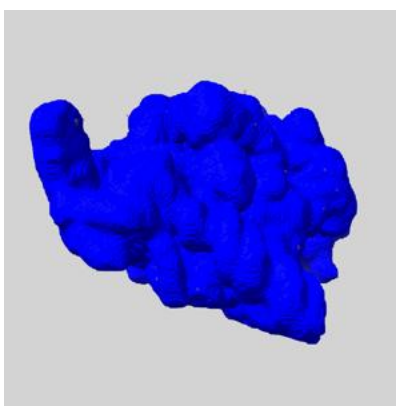
A mask typically either:

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

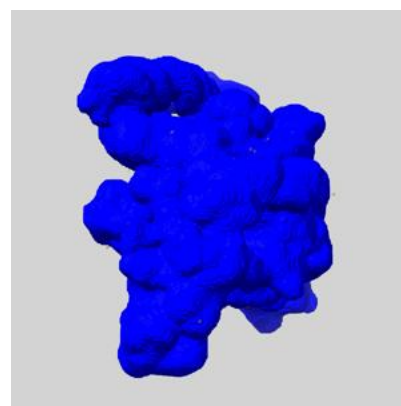
6.6.1 emd_18873_msk_1.map [i](#)



X



Y

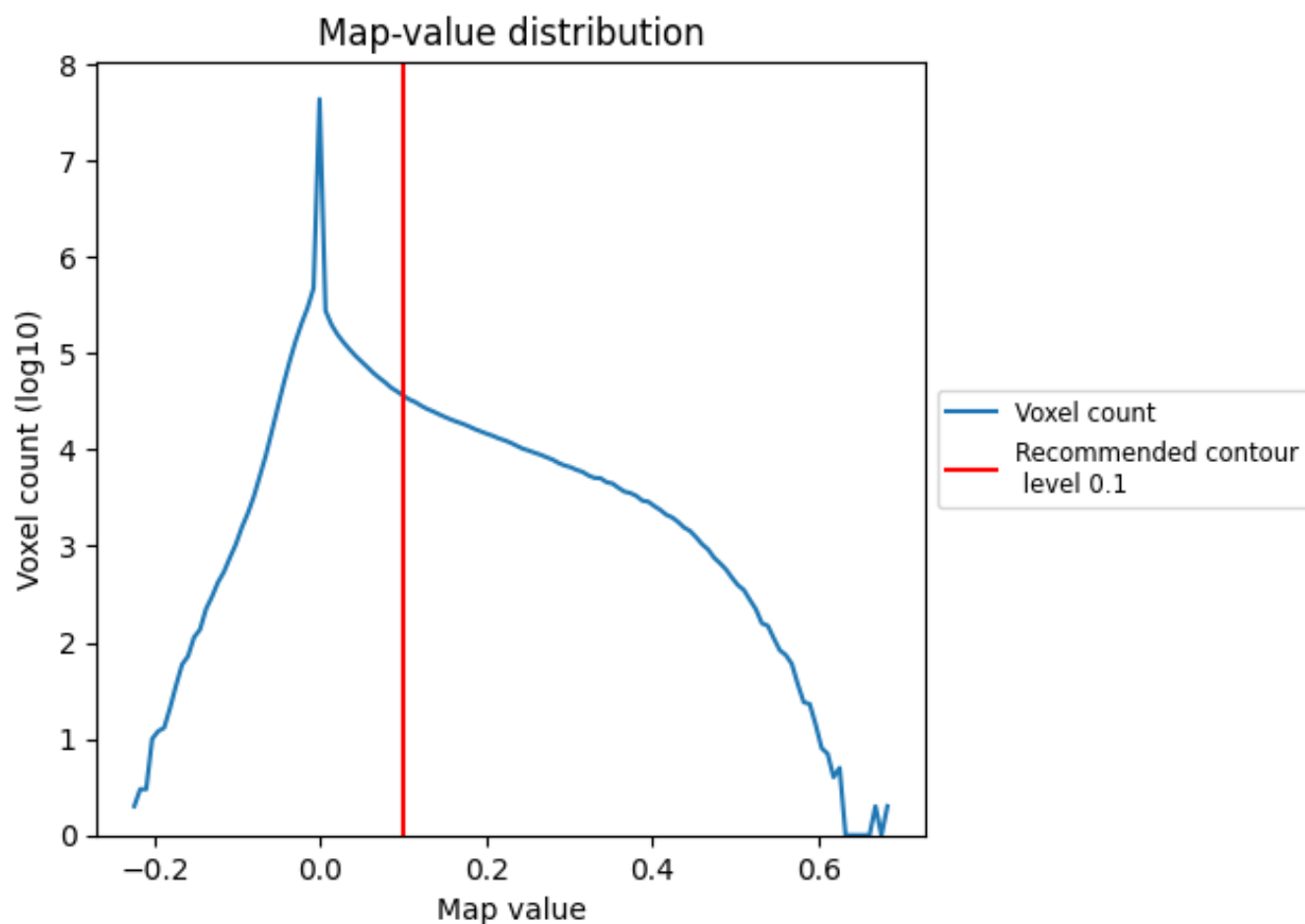


Z

7 Map analysis [i](#)

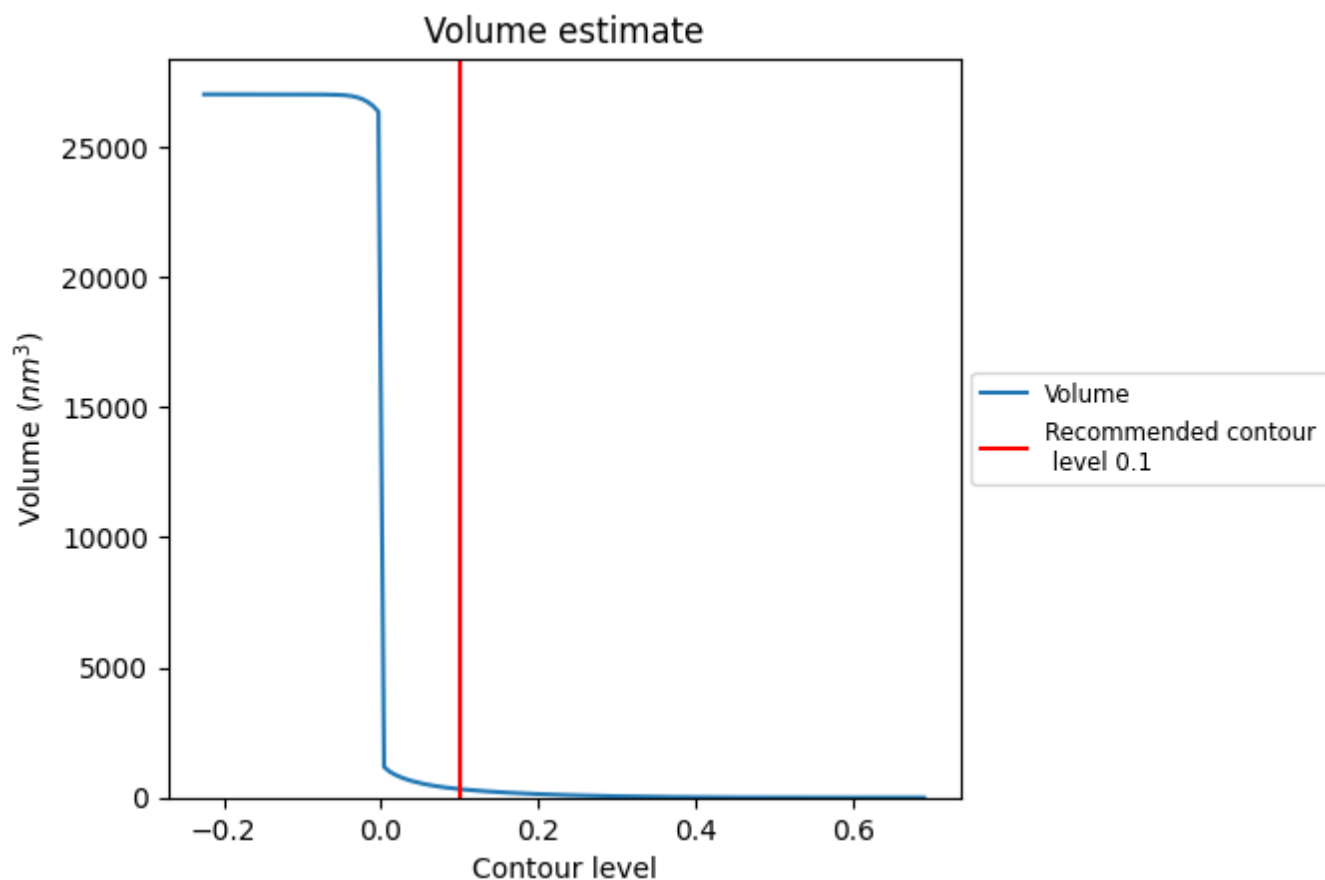
This section contains the results of statistical analysis of the map.

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.

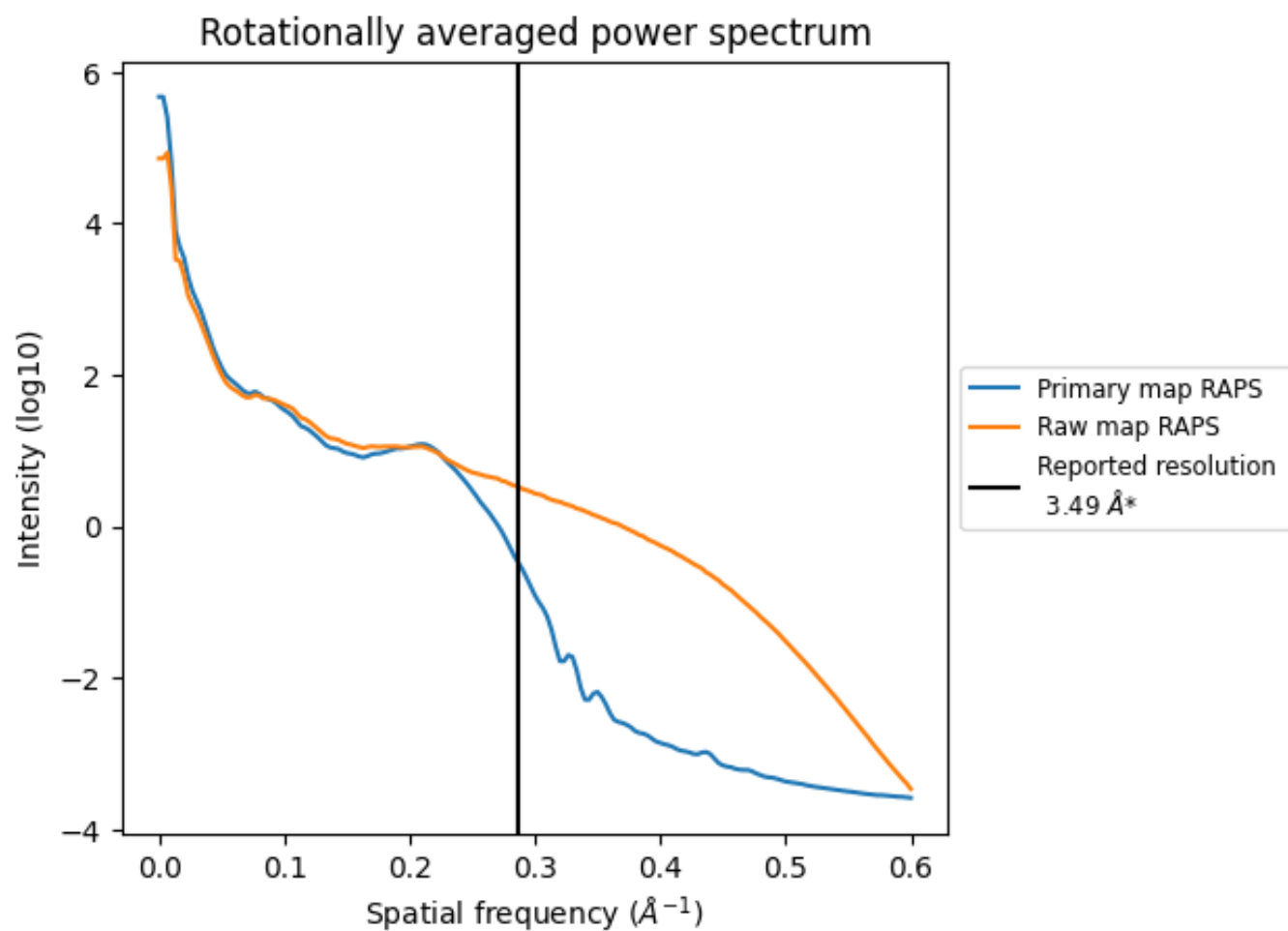
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm^3 ; this corresponds to an approximate mass of 294 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 ⓘ

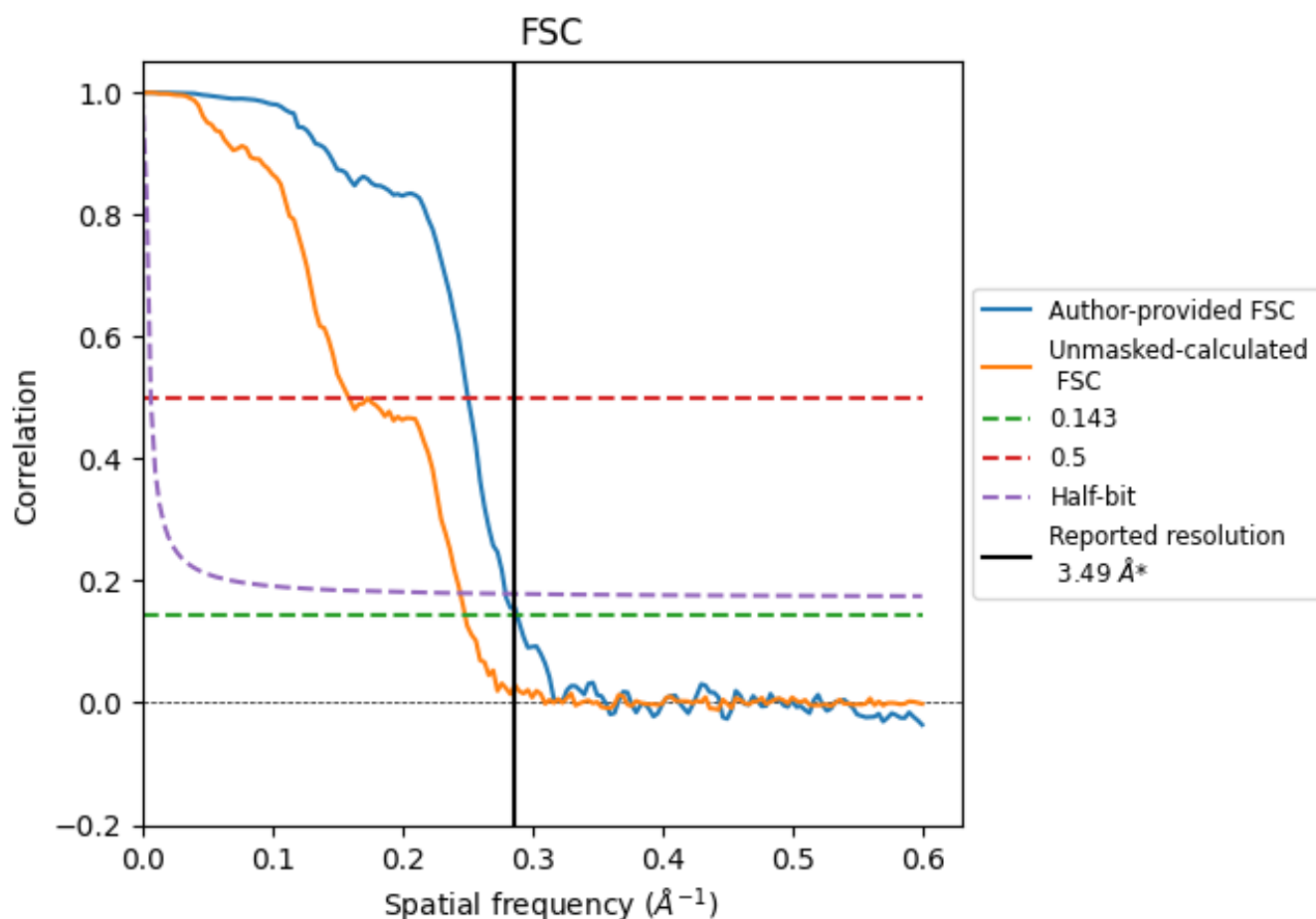


*Reported resolution corresponds to spatial frequency of $0.287 \text{ \AA}^{-1}$

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 0.287 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

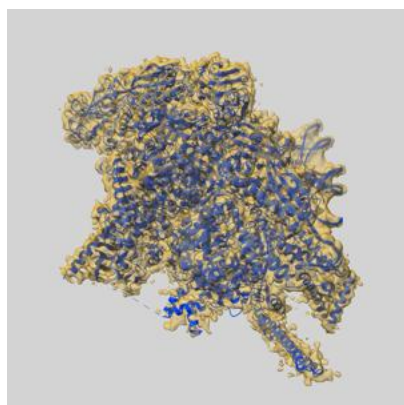
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.47	3.99	3.58
Unmasked-calculated*	4.03	6.29	4.09

*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 4.03 differs from the reported value 3.49 by more than 10 %

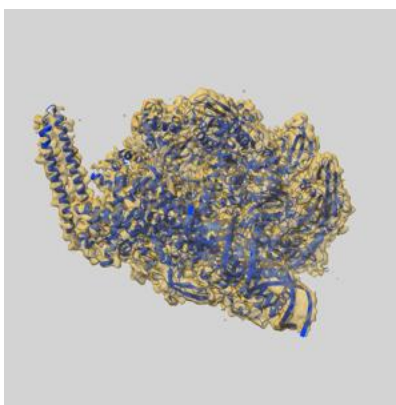
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18873 and PDB model 8R3M. Per-residue inclusion information can be found in section [3](#) on page [6](#).

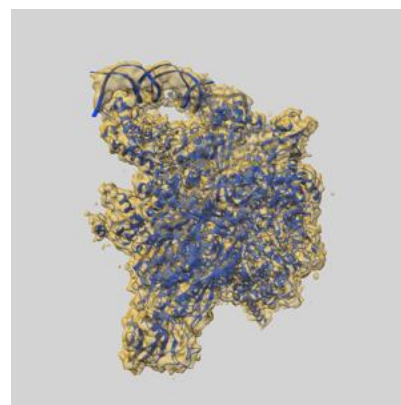
9.1 Map-model overlay [i](#)



X



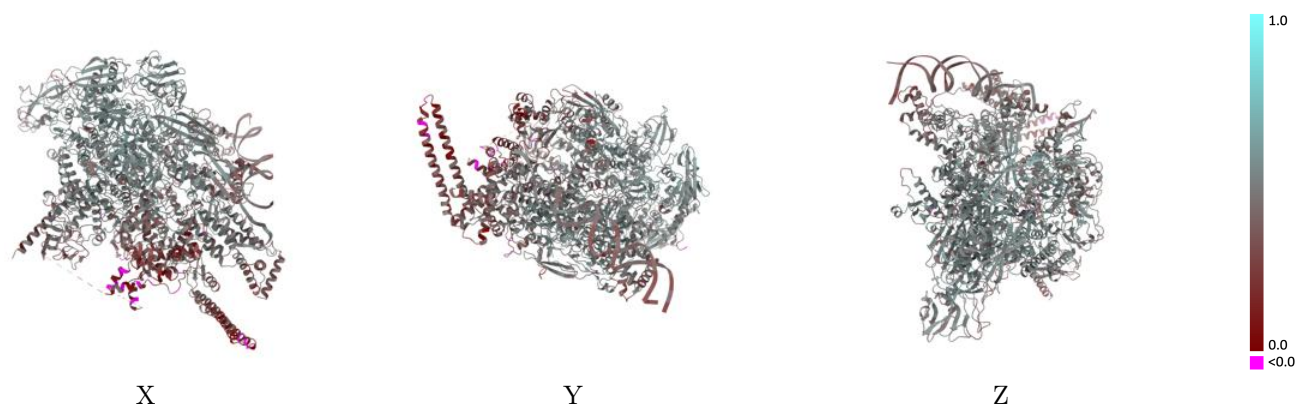
Y



Z

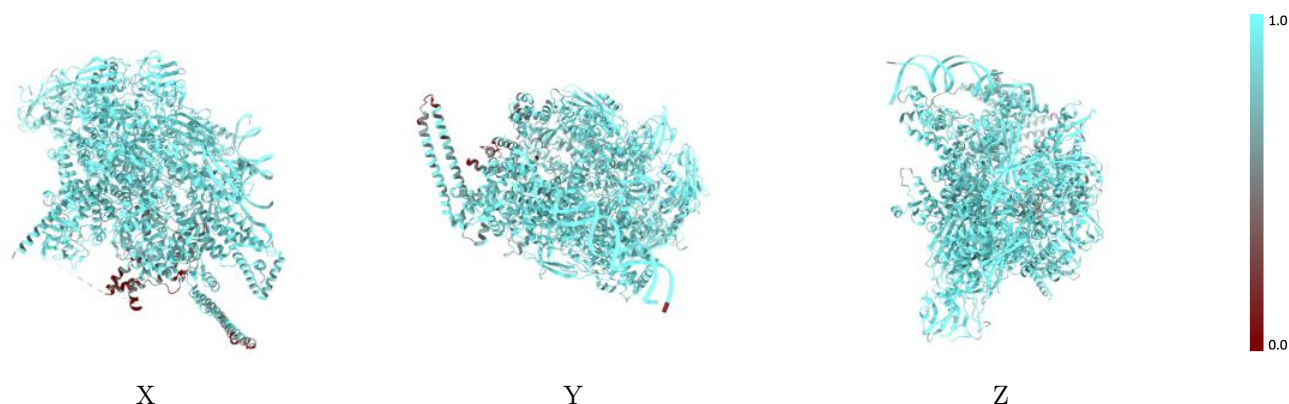
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



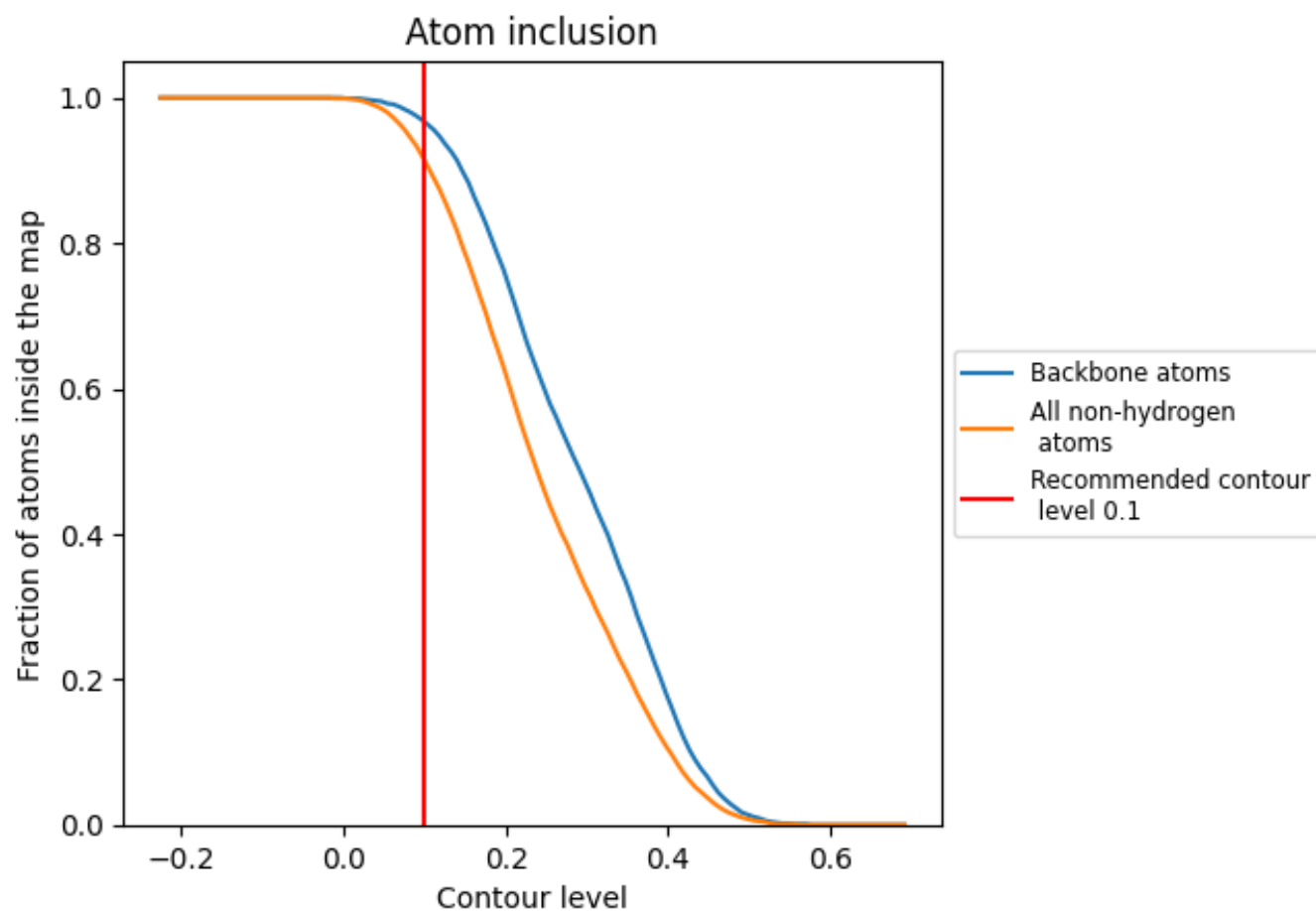
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.4580
A	0.9670	0.5120
B	0.9370	0.4890
C	0.9340	0.4820
D	0.9230	0.4650
E	0.9280	0.4900
F	0.9000	0.4190
H	0.7800	0.3560
J	0.8140	0.4020
O	0.9420	0.4000
P	0.9160	0.3800

1.0

0.0

<0.0