



Full wwPDB EM Validation Report ⓘ

Jun 16, 2026 – 06:29 PM EDT

PDB ID : 10MF / pdb_000010mf
EMDB ID : EMD-75284
Title : CBR9379 bound Open1 Eco-ePEC: Cryo-EM structure of Eco RNAP his-
elemental paused elongation complex with an open active site (open TL, SI3
and RH-FL)
Authors : Dhingra, Y.; Darst, S.A.
Deposited on : 2026-01-27
Resolution : 2.80 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:

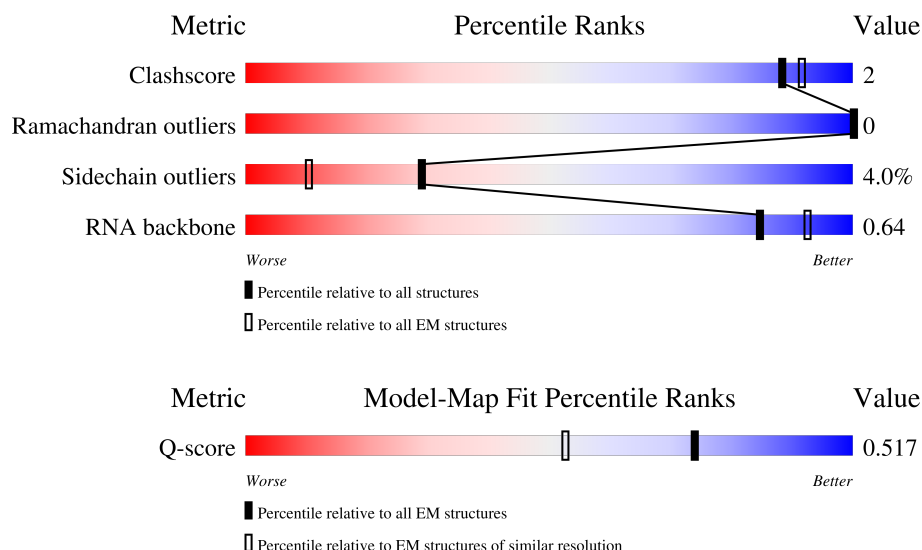
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	B	32	
2	K	91	
3	R	19	

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Mol	Chain	Length	Quality of chain
4	A	32	
5	G	329	
5	H	329	
6	I	1342	
7	J	1407	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 52809 atoms, of which 25841 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 DNA chain called template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	30	Total	C	H	N	O	P	0	0
			945	290	337	109	179	30		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	K	79	Total	C	H	N	O	S	0	0
			1261	382	634	118	126	1		

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	R	10	Total	C	H	N	O	P	0	0
			320	95	106	36	73	10		

- Molecule 4 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	23	Total	C	H	N	O	P	0	0
			729	225	259	87	136	22		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	218	Total	C	H	N	O	S	0	0
			3396	1051	1717	297	325	6		
5	H	218	Total	C	H	N	O	S	0	0
			3395	1050	1714	297	328	6		

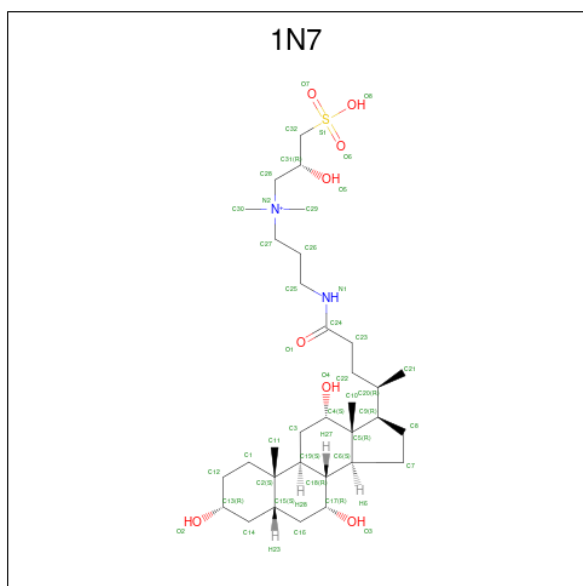
- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	1316	Total	C	H	N	O	S	0	0
			20773	6514	10392	1810	2014	43		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	1337	Total	C	H	N	O	S	0	0
			21031	6536	10628	1856	1961	50		

- Molecule 8 is CHAPSO (CCD ID: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



Mol	Chain	Residues	Atoms				AltConf
8	I	1	Total	C	H	O	0
			66	24	39	3	

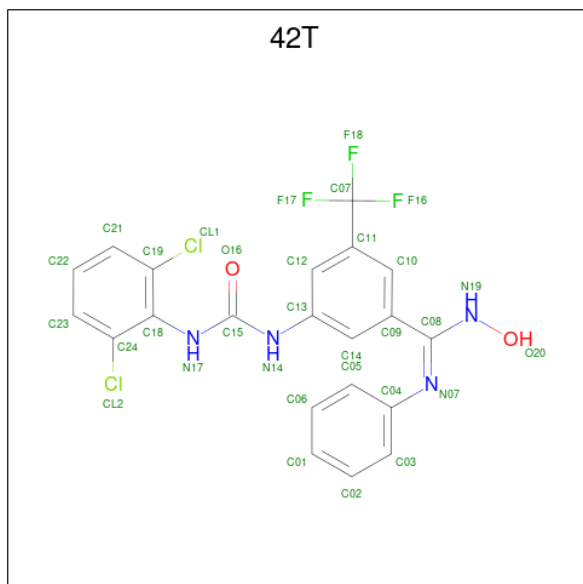
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total	Mg	0
			1	1	

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

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

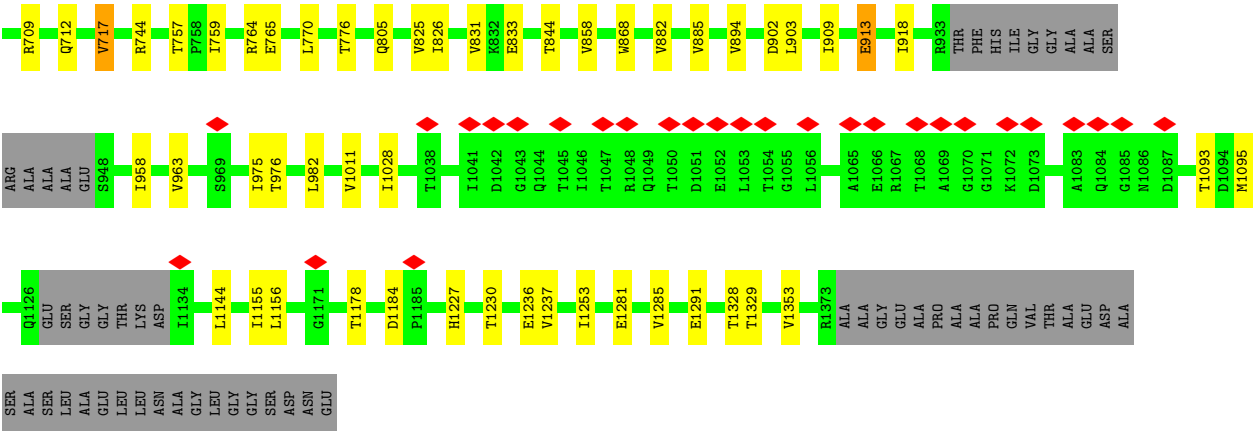
- Molecule 11 is 3-[[[(2,6-dichlorophenyl)carbamoyl]amino}-N-hydroxy-N'-phenyl-5-(trifluoromethyl)benzenecarboximidamide (CCD ID: 42T) (formula: C₂₁H₁₅Cl₂F₃N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
			Total	C	Cl	F	H	N	O	
11	J	1	47	21	2	3	15	4	2	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	B	20	Total	O	0
			20	20	
12	K	15	Total	O	0
			15	15	
12	R	23	Total	O	0
			23	23	
12	A	5	Total	O	0
			5	5	
12	G	55	Total	O	0
			55	55	
12	H	44	Total	O	0
			44	44	
12	I	385	Total	O	0
			385	385	
12	J	296	Total	O	0
			296	296	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.459	Depositor
Minimum map value	-0.327	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	259.58398, 259.58398, 259.58398	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.67599994, 0.67599994, 0.67599994	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: 1N7, 42T, MG, ZN

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	B	0.23	0/680	0.46	0/1045
2	K	0.13	0/629	0.27	0/847
3	R	0.21	0/238	0.34	0/369
4	A	0.20	0/526	0.40	0/808
5	G	0.19	0/1699	0.34	0/2302
5	H	0.17	0/1700	0.35	0/2304
6	I	0.21	0/10547	0.36	0/14232
7	J	0.20	0/10560	0.36	0/14257
All	All	0.20	0/26579	0.36	0/36164

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	B	608	337	338	7	0
2	K	627	634	634	0	0
3	R	214	106	106	1	0
4	A	470	259	262	3	0
5	G	1679	1717	1717	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1681	1714	1714	8	0
6	I	10381	10392	10392	33	0
7	J	10403	10628	10628	45	0
8	I	27	39	39	0	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
11	J	32	15	15	0	0
12	A	5	0	0	0	0
12	B	20	0	0	0	0
12	G	55	0	0	0	0
12	H	44	0	0	0	0
12	I	385	0	0	0	0
12	J	296	0	0	1	0
12	K	15	0	0	0	0
12	R	23	0	0	0	0
All	All	26968	25841	25845	100	0

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

All (100) 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)
7:J:572:THR:HG21	7:J:589:TYR:OH	1.83	0.77
6:I:521:LEU:O	6:I:525:THR:HG22	1.85	0.76
6:I:1273:MET:HE2	7:J:428:THR:O	1.90	0.72
6:I:560:PRO:HB2	7:J:776:THR:HG21	1.73	0.70
5:G:45:ARG:HE	5:H:38:THR:HG22	1.61	0.65
6:I:600:THR:HG22	6:I:601:ASP:H	1.62	0.64
1:B:11:DC:H2''	1:B:12:DT:H71	1.79	0.64
6:I:114:VAL:HG21	6:I:117:ILE:HB	1.82	0.61
6:I:888:THR:HG23	6:I:890:LYS:HG3	1.83	0.60
7:J:858:VAL:HG12	7:J:868:TRP:CZ3	2.38	0.59
6:I:22:LEU:HD13	6:I:603:ILE:HD13	1.84	0.59
5:H:29:GLU:HB3	5:H:30:PRO:CD	2.32	0.59
7:J:426:ALA:HB3	7:J:427:PRO:HD3	1.85	0.58
7:J:201:LEU:HD11	7:J:220:ARG:HH11	1.68	0.57
7:J:1178:THR:HG22	7:J:1184:ASP:HB3	1.87	0.57
6:I:666:SER:O	6:I:702:THR:HG21	2.06	0.56
7:J:268:LEU:CD2	7:J:316:ILE:HD11	2.35	0.56
6:I:309:LEU:H	6:I:309:LEU:HD23	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:1237:VAL:CG2	7:J:1253:ILE:HD13	2.36	0.56
5:G:208:ASN:OD1	5:G:210:THR:HG22	2.06	0.55
6:I:878:THR:HG22	6:I:879:GLY:H	1.72	0.55
6:I:283:LYS:HG3	6:I:284:LEU:HD12	1.88	0.55
7:J:549:LYS:HB3	7:J:569:LEU:HD11	1.89	0.54
5:H:29:GLU:HB3	5:H:30:PRO:HD2	1.90	0.53
7:J:1093:THR:HG22	7:J:1095:MET:H	1.74	0.52
7:J:515:ARG:NH2	7:J:717:VAL:HG13	2.24	0.52
1:B:9:DC:H2'	1:B:10:DT:H71	1.92	0.52
5:H:208:ASN:OD1	5:H:210:THR:HG22	2.10	0.52
6:I:757:THR:HG22	6:I:758:ARG:N	2.25	0.51
6:I:75:LEU:HD21	6:I:127:ILE:HD11	1.93	0.51
6:I:1313:HIS:HB2	7:J:474:LEU:HD13	1.92	0.50
6:I:672:GLU:OE1	6:I:1186:VAL:O	2.30	0.49
7:J:331:ILE:HG22	7:J:1328:THR:HG21	1.95	0.49
7:J:268:LEU:HD21	7:J:316:ILE:HD11	1.95	0.49
7:J:357:VAL:O	7:J:449:LEU:O	2.30	0.49
7:J:487:THR:HG22	7:J:487:THR:O	2.13	0.48
6:I:948:ILE:HG23	6:I:951:MET:HE2	1.95	0.48
6:I:878:THR:HG22	6:I:879:GLY:N	2.28	0.48
1:B:20:DC:H2'	1:B:21:DA:C8	2.49	0.47
6:I:888:THR:HG23	6:I:890:LYS:CG	2.43	0.47
7:J:1237:VAL:HG21	7:J:1253:ILE:HD13	1.96	0.47
7:J:958:ILE:HG23	7:J:982:LEU:HD11	1.95	0.47
6:I:691:PRO:O	6:I:830:THR:HG22	2.13	0.47
7:J:826:ILE:HG22	7:J:831:VAL:HG12	1.96	0.47
6:I:921:PRO:O	6:I:924:VAL:HG12	2.14	0.47
7:J:416:ILE:O	7:J:416:ILE:HG23	2.15	0.47
6:I:1043:ALA:O	6:I:1046:VAL:HG12	2.14	0.46
6:I:946:LEU:HD12	6:I:947:GLU:N	2.30	0.46
7:J:1155:ILE:C	7:J:1156:LEU:HD12	2.39	0.46
7:J:825:VAL:HG12	7:J:833:GLU:HB3	1.98	0.46
4:A:6:DC:H2''	4:A:7:DT:O4'	2.16	0.46
7:J:902:ASP:OD2	7:J:909:ILE:HD12	2.16	0.45
7:J:976:THR:HG22	7:J:1028:ILE:HD11	1.97	0.45
3:R:10:G:O2'	3:R:11:A:P	2.75	0.45
5:H:65:LEU:H	5:H:65:LEU:HD23	1.82	0.45
6:I:204:LEU:N	6:I:204:LEU:HD23	2.32	0.45
7:J:80:HIS:O	7:J:83:VAL:HG22	2.17	0.45
5:G:28:LEU:HD12	5:G:28:LEU:N	2.31	0.45
7:J:601:ILE:HG21	12:J:1723:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:24:LEU:HD21	7:J:116:PHE:CZ	2.51	0.44
7:J:126:LEU:HD23	7:J:223:LEU:HD22	2.00	0.44
7:J:963:VAL:HG23	7:J:975:ILE:HD13	1.99	0.44
7:J:744:ARG:HB3	7:J:759:ILE:HB	2.01	0.43
5:H:90:VAL:HG22	5:H:91:ARG:N	2.34	0.43
7:J:831:VAL:HG23	7:J:831:VAL:O	2.19	0.43
6:I:306:THR:HG23	6:I:308:GLU:H	1.84	0.43
7:J:858:VAL:HG12	7:J:868:TRP:CE3	2.53	0.43
4:A:20:DA:H2''	4:A:21:DA:H5'	2.01	0.42
1:B:9:DC:C2'	1:B:10:DT:H71	2.49	0.42
5:H:198:LEU:HD22	5:H:198:LEU:N	2.34	0.42
7:J:1227:HIS:HA	7:J:1230:THR:HG22	2.00	0.42
6:I:525:THR:HG21	6:I:687:ARG:HD2	2.01	0.42
6:I:834:GLN:OE1	6:I:924:VAL:HG21	2.20	0.42
6:I:832:HIS:CD2	6:I:1058:ARG:HG3	2.55	0.42
6:I:1289:GLU:O	6:I:1294:LYS:HG2	2.20	0.42
7:J:492:SER:O	7:J:495:ASN:O	2.38	0.42
5:H:171:LEU:HD12	5:H:171:LEU:N	2.35	0.41
7:J:490:ILE:HD11	7:J:609:TYR:CE1	2.54	0.41
6:I:1002:LEU:HD23	6:I:1002:LEU:H	1.84	0.41
7:J:268:LEU:HD23	7:J:316:ILE:HD11	2.01	0.41
7:J:902:ASP:O	7:J:903:LEU:HB2	2.19	0.41
5:G:29:GLU:HB3	5:G:30:PRO:HD3	2.03	0.41
6:I:26:TYR:HE2	6:I:32:LEU:HD12	1.85	0.41
7:J:201:LEU:HD11	7:J:220:ARG:NH1	2.36	0.41
7:J:201:LEU:HD12	7:J:224:LEU:HD12	2.03	0.41
7:J:1281:GLU:O	7:J:1285:VAL:HG23	2.20	0.41
4:A:6:DC:H2'	4:A:7:DT:C6	2.55	0.41
5:G:29:GLU:O	5:G:199:ASP:O	2.39	0.41
6:I:255:ILE:HB	6:I:263:VAL:HG21	2.02	0.41
7:J:909:ILE:HD11	7:J:913:GLU:HG2	2.03	0.41
1:B:11:DC:H4'	1:B:12:DT:OP1	2.21	0.40
5:G:210:THR:O	5:G:210:THR:HG23	2.21	0.40
1:B:21:DA:H2'	1:B:22:DC:C6	2.56	0.40
6:I:189:ASP:CG	6:I:190:PRO:HD2	2.46	0.40
7:J:510:LEU:HD23	7:J:513:MET:CE	2.52	0.40
1:B:9:DC:H5'	1:B:9:DC:H6	1.87	0.40
7:J:405:GLU:O	7:J:408:VAL:HG22	2.21	0.40
5:G:65:LEU:HD22	5:G:168:ILE:HD12	2.02	0.40
6:I:400:VAL:HG22	6:I:584:TYR:HD1	1.85	0.40
7:J:119:SER:O	7:J:120:LEU:C	2.65	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	
2	K	77/91 (85%)	72 (94%)	5 (6%)	0	100	100
5	G	214/329 (65%)	209 (98%)	5 (2%)	0	100	100
5	H	214/329 (65%)	205 (96%)	9 (4%)	0	100	100
6	I	1312/1342 (98%)	1266 (96%)	46 (4%)	0	100	100
7	J	1331/1407 (95%)	1279 (96%)	52 (4%)	0	100	100
All	All	3148/3498 (90%)	3031 (96%)	117 (4%)	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	
2	K	67/75 (89%)	65 (97%)	2 (3%)	36	72
5	G	185/286 (65%)	177 (96%)	8 (4%)	26	60
5	H	186/286 (65%)	178 (96%)	8 (4%)	26	60
6	I	1135/1157 (98%)	1087 (96%)	48 (4%)	26	61
7	J	1122/1168 (96%)	1080 (96%)	42 (4%)	30	65
All	All	2695/2972 (91%)	2587 (96%)	108 (4%)	29	63

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	59	ILE
2	K	76	GLU
5	G	26	VAL
5	G	74	VAL
5	G	92	VAL
5	G	129	VAL
5	G	173	VAL
5	G	180	VAL
5	G	203	ILE
5	G	228	LEU
5	H	7	GLU
5	H	16	ILE
5	H	27	THR
5	H	31	LEU
5	H	32	GLU
5	H	38	THR
5	H	191	ARG
5	H	206	GLU
6	I	11	ILE
6	I	18	ARG
6	I	30	ILE
6	I	65	ASN
6	I	142	GLU
6	I	204	LEU
6	I	261	VAL
6	I	378	ARG
6	I	403	MET
6	I	456	VAL
6	I	472	GLU
6	I	524	ILE
6	I	538	LEU
6	I	541	GLU
6	I	547	VAL
6	I	550	VAL
6	I	561	ILE
6	I	562	GLU
6	I	574	SER
6	I	581	THR
6	I	598	VAL
6	I	615	VAL
6	I	650	VAL
6	I	651	ASP

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Mol	Chain	Res	Type
6	I	655	VAL
6	I	697	LYS
6	I	702	THR
6	I	711	ASP
6	I	727	VAL
6	I	791	LEU
6	I	811	ASN
6	I	888	THR
6	I	890	LYS
6	I	943	LYS
6	I	979	LEU
6	I	1046	VAL
6	I	1056	VAL
6	I	1064	ASP
6	I	1079	ILE
6	I	1092	THR
6	I	1094	VAL
6	I	1159	VAL
6	I	1201	LEU
6	I	1233	LEU
6	I	1265	PHE
6	I	1293	VAL
6	I	1309	VAL
6	I	1327	LEU
7	J	86	GLU
7	J	92	VAL
7	J	252	LEU
7	J	299	LEU
7	J	316	ILE
7	J	342	LEU
7	J	347	VAL
7	J	361	LEU
7	J	363	LEU
7	J	368	LEU
7	J	408	VAL
7	J	430	HIS
7	J	435	GLN
7	J	460	ASP
7	J	474	LEU
7	J	505	ASP
7	J	507	VAL
7	J	518	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	J	553	THR
7	J	569	LEU
7	J	572	THR
7	J	701	LEU
7	J	709	ARG
7	J	712	GLN
7	J	717	VAL
7	J	757	THR
7	J	764	ARG
7	J	765	GLU
7	J	770	LEU
7	J	805	GLN
7	J	844	THR
7	J	882	VAL
7	J	885	VAL
7	J	894	VAL
7	J	913	GLU
7	J	918	ILE
7	J	1011	VAL
7	J	1144	LEU
7	J	1236	GLU
7	J	1291	GLU
7	J	1329	THR
7	J	1353	VAL

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

Mol	Chain	Res	Type
6	I	510	GLN
6	I	620	ASN
6	I	677	ASN
6	I	832	HIS
6	I	1136	GLN
6	I	1220	GLN
6	I	1244	HIS
7	J	435	GLN
7	J	700	ASN
7	J	720	ASN
7	J	771	GLN
7	J	1086	ASN
7	J	1249	ASN
7	J	1295	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	10/19 (52%)	1 (10%)	1 (10%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	11	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	R	10	G

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	42T	J	1504	-	34,34,34	0.65	0	47,48,48	1.13	5 (10%)
8	1N7	I	1401	-	30,30,46	0.43	0	47,48,72	0.87	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	42T	J	1504	-	-	0/23/24/24	0/3/3/3
8	1N7	I	1401	-	-	0/7/72/92	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	1504	42T	C04-N07-C08	3.14	127.33	120.49
11	J	1504	42T	C14-C13-N14	2.92	129.61	120.13
11	J	1504	42T	C12-C13-N14	-2.82	110.97	120.13
11	J	1504	42T	C09-C08-N19	-2.18	111.10	114.61
11	J	1504	42T	C13-N14-C15	2.14	130.97	126.61
8	I	1401	1N7	C11-C2-C1	-2.02	105.09	108.31

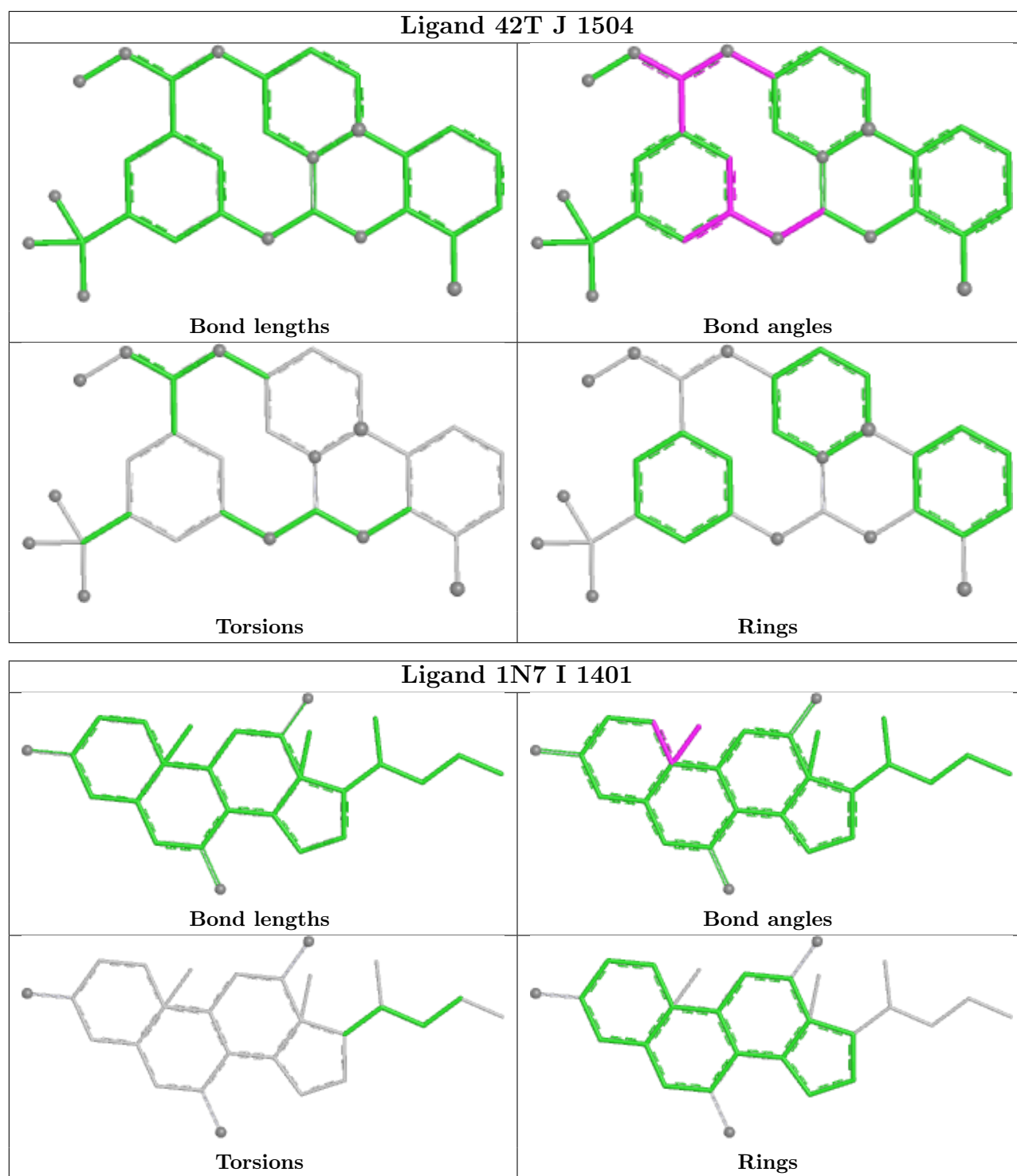
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

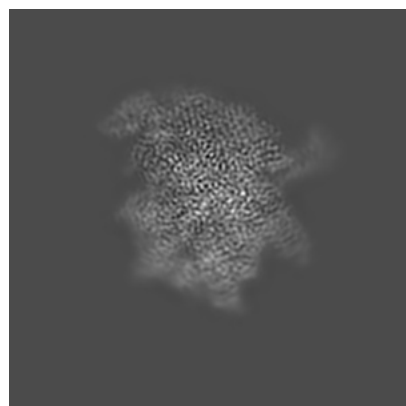
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75284. These allow visual inspection of the internal detail of the map and identification of artifacts.

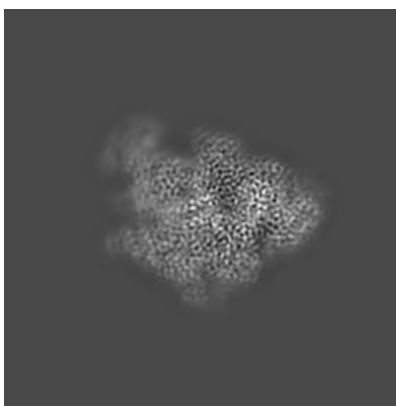
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

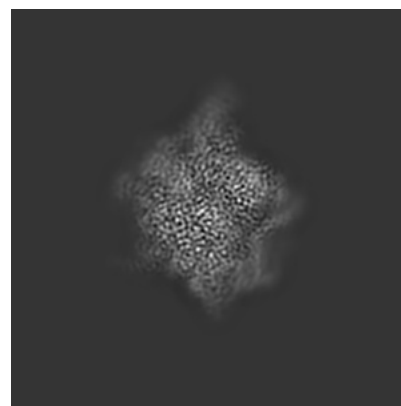
6.1.1 Primary map



X

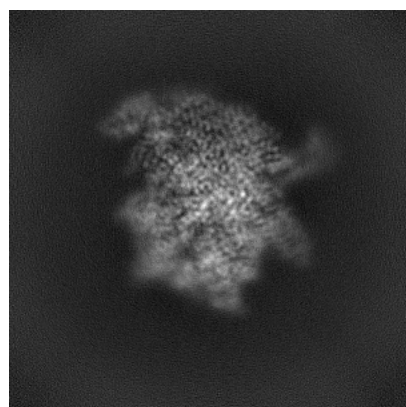


Y

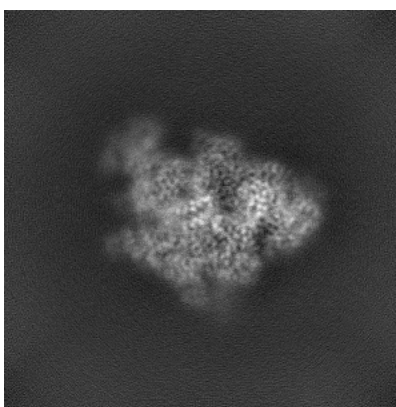


Z

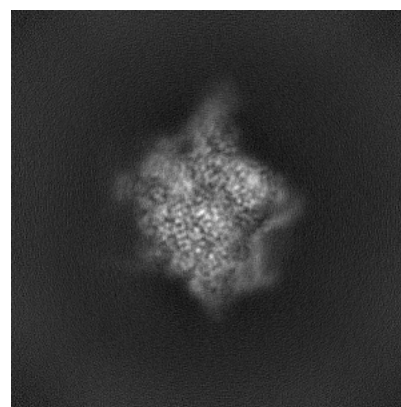
6.1.2 Raw map



X



Y

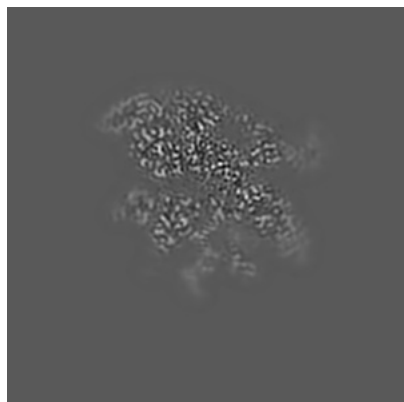


Z

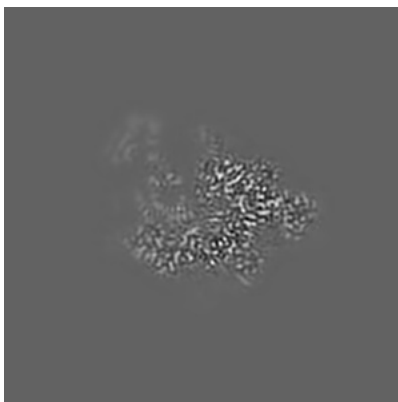
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

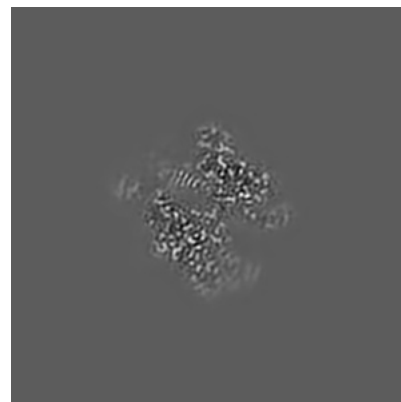
6.2.1 Primary map



X Index: 192

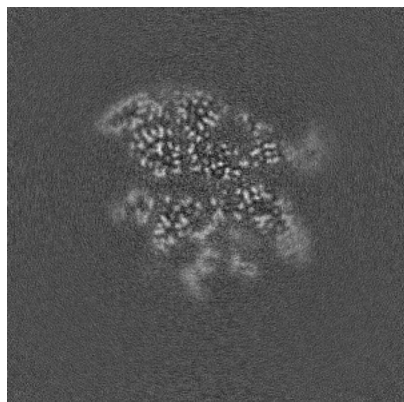


Y Index: 192

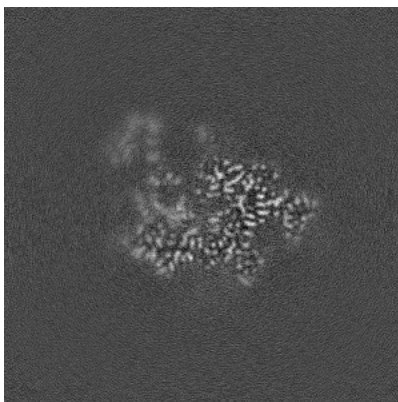


Z Index: 192

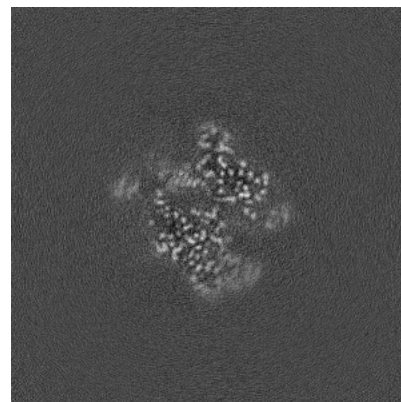
6.2.2 Raw map



X Index: 192



Y Index: 192

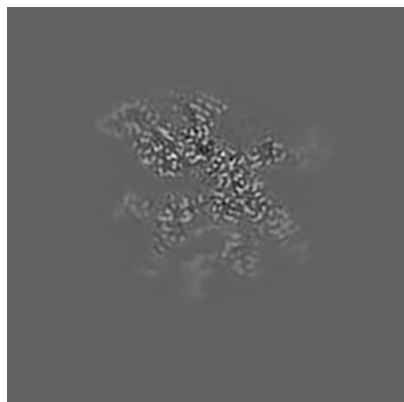


Z Index: 192

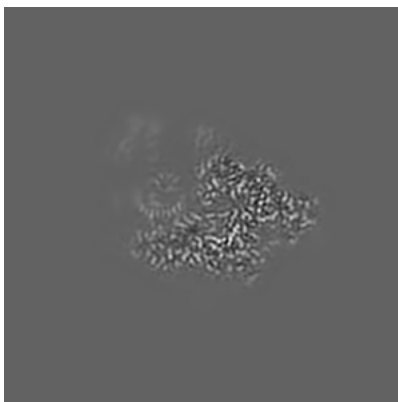
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

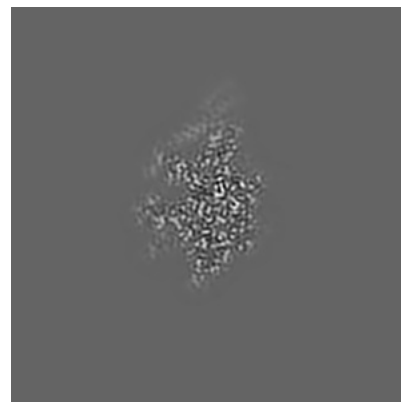
6.3.1 Primary map



X Index: 198

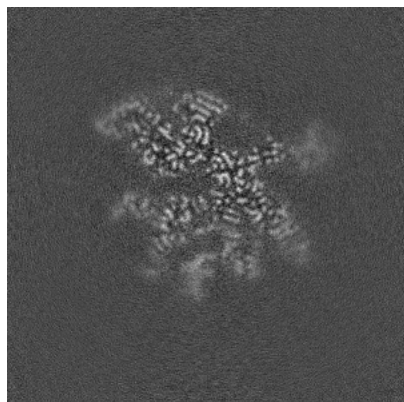


Y Index: 189

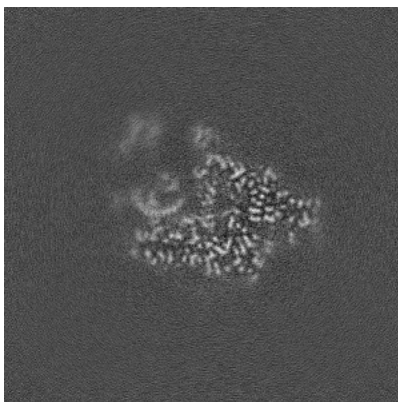


Z Index: 237

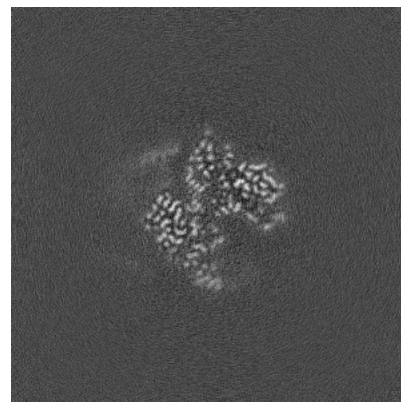
6.3.2 Raw map



X Index: 197



Y Index: 187

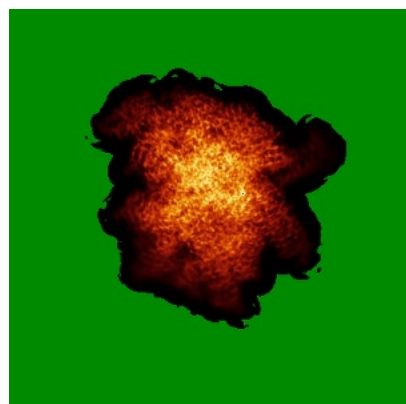


Z Index: 201

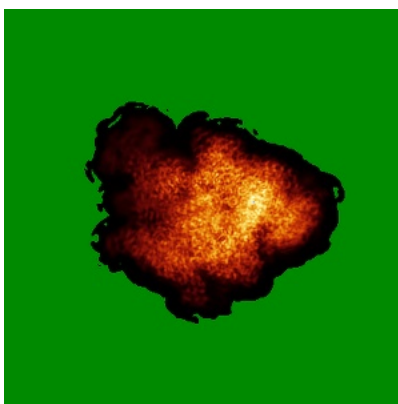
The images above show the largest variance slices of the map in three orthogonal directions.

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

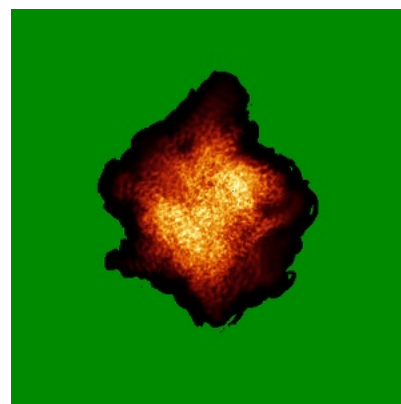
6.4.1 Primary map



X

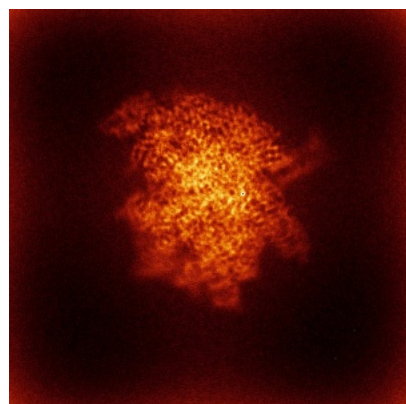


Y

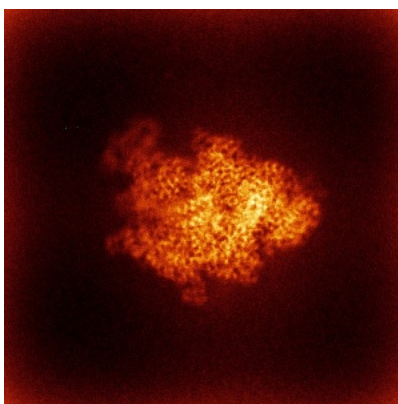


Z

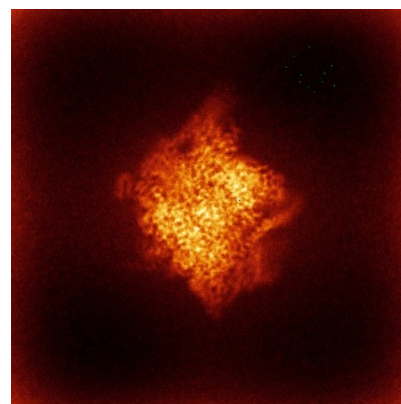
6.4.2 Raw map



X



Y

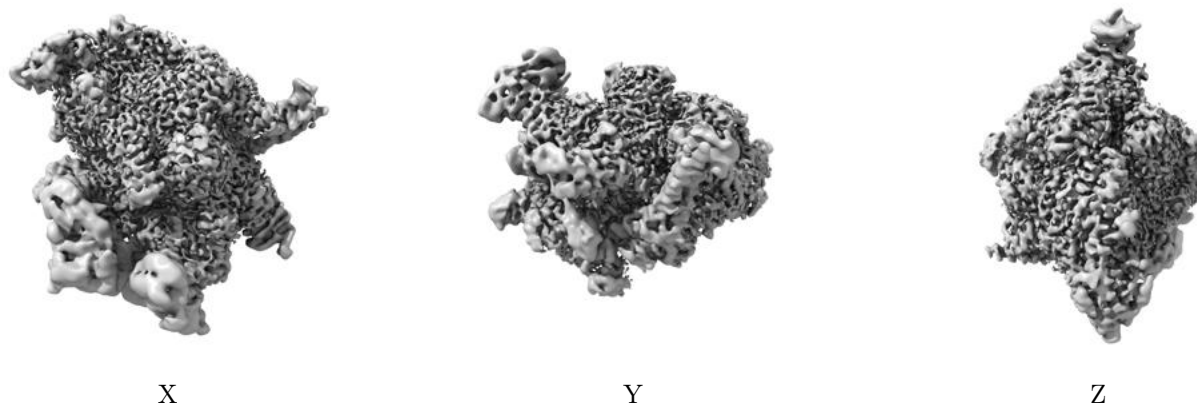


Z

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.

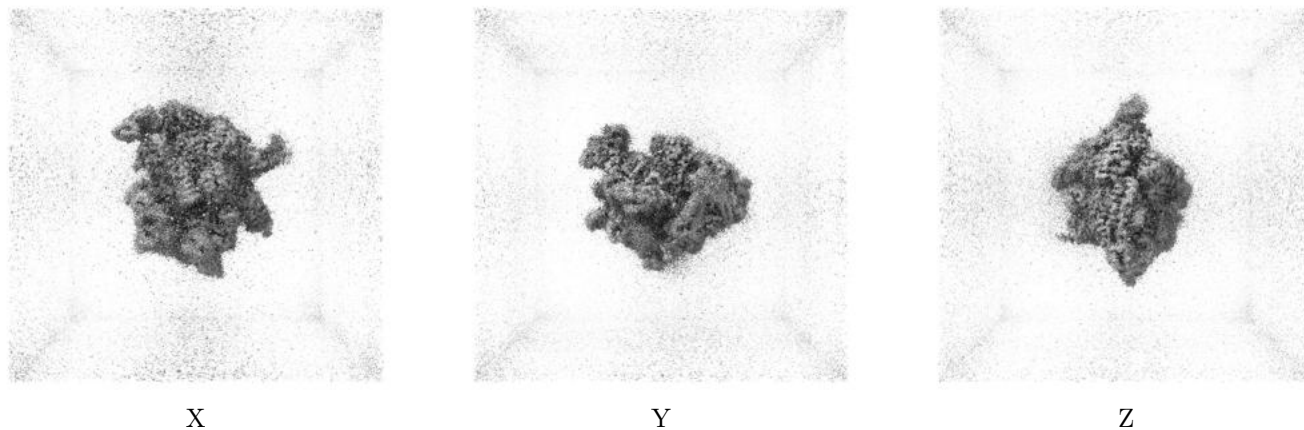
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

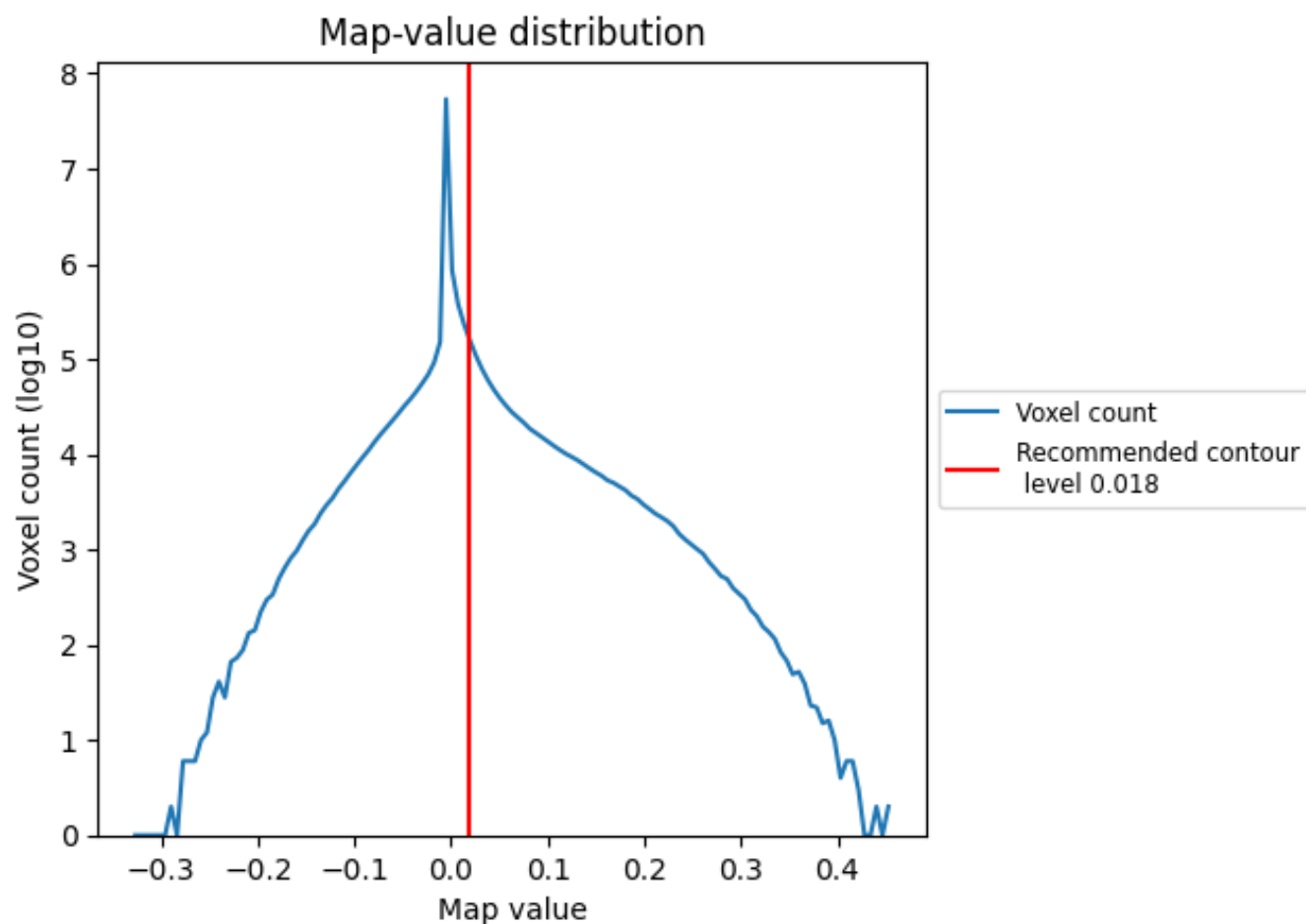
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

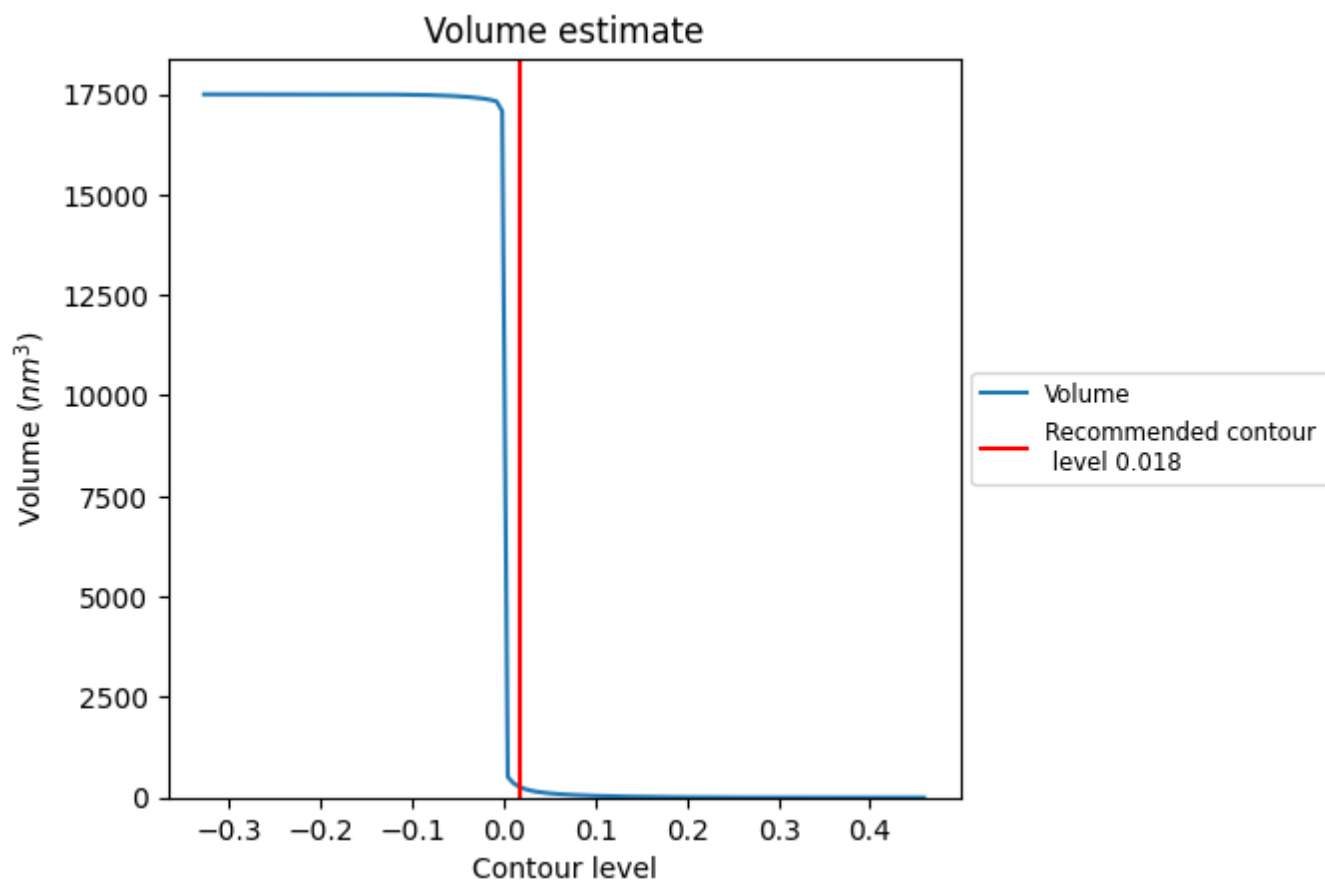
This section contains the results of statistical analysis of the map.

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.

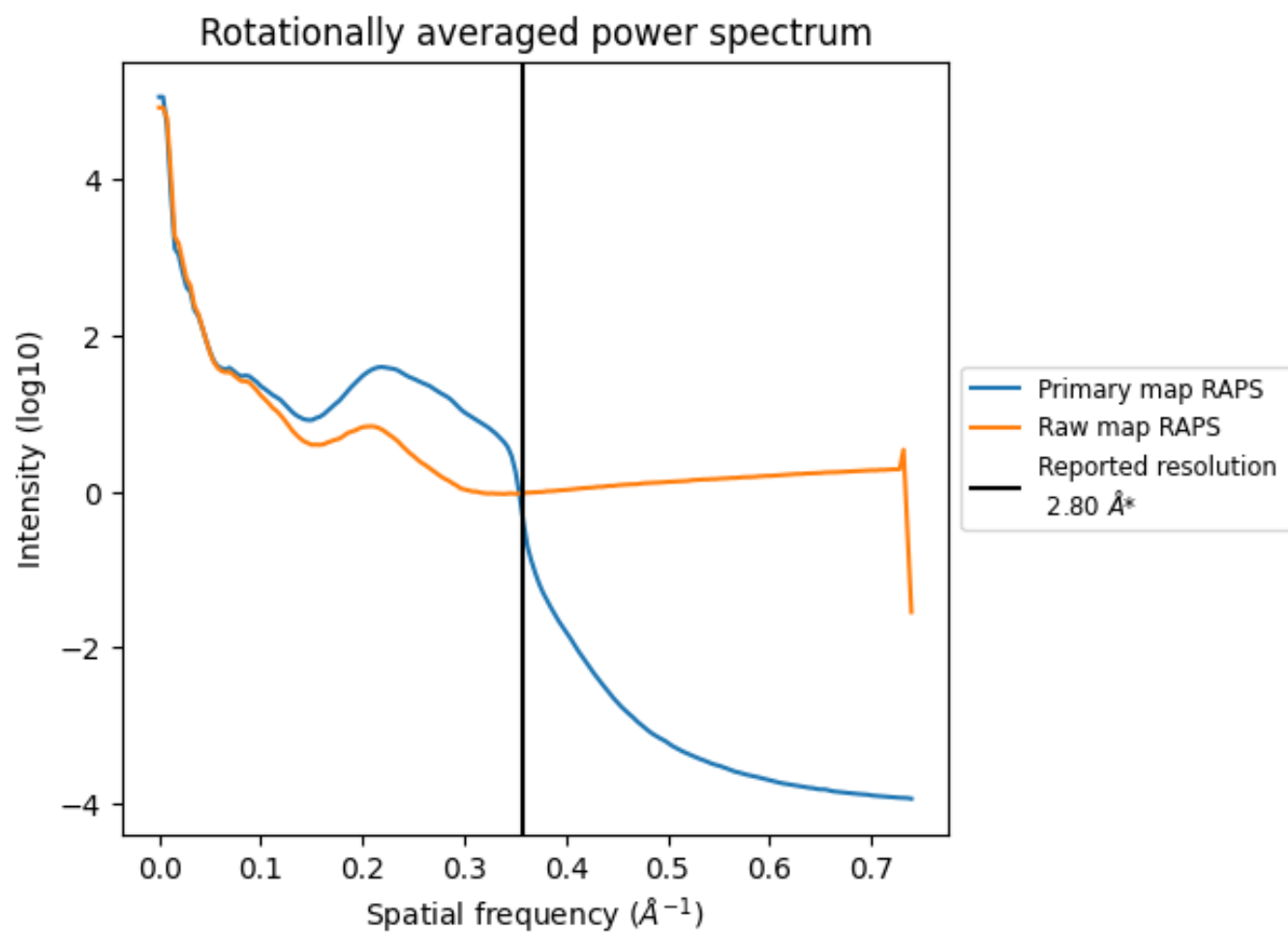
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm³; this corresponds to an approximate mass of 236 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 ⓘ

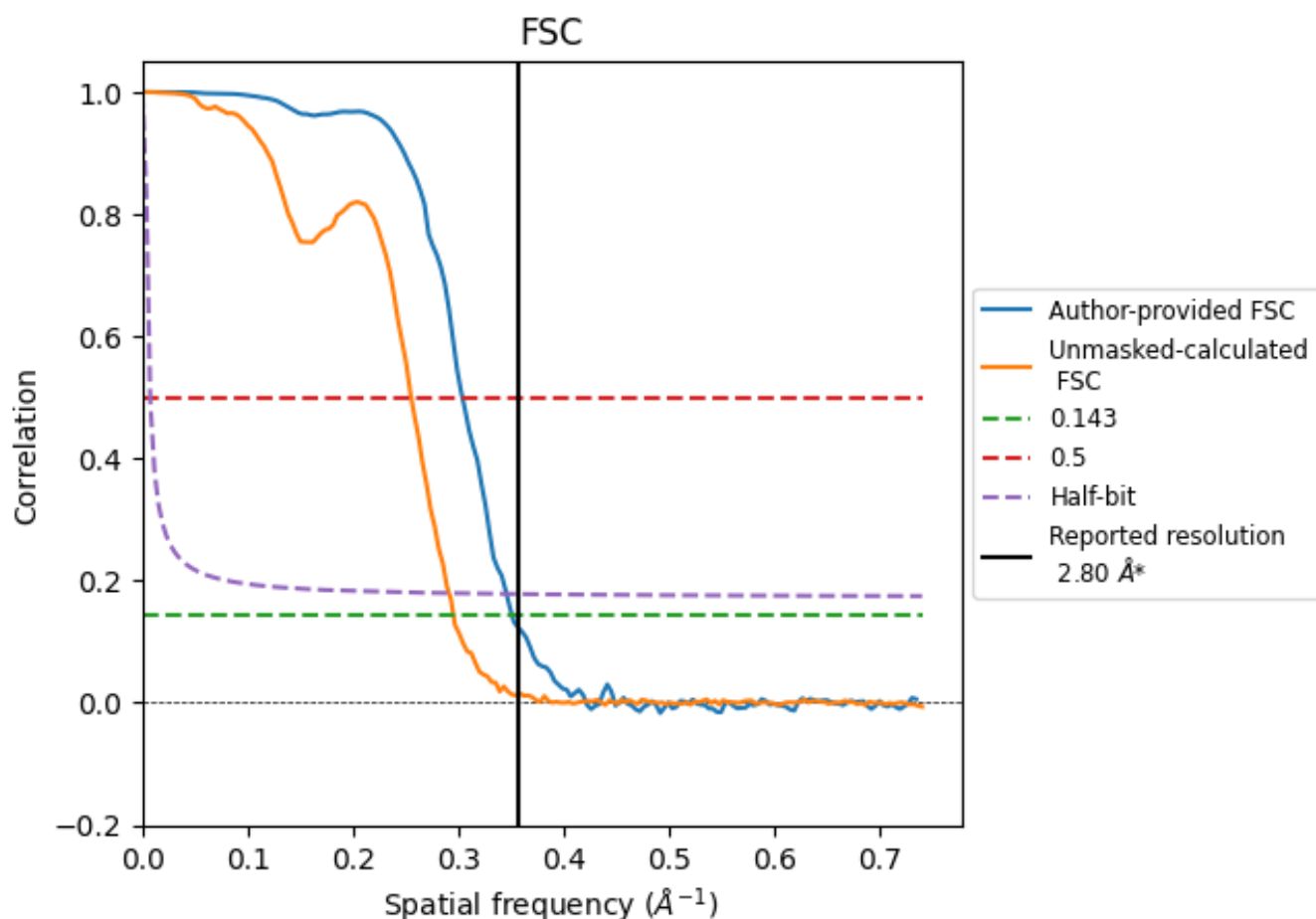


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

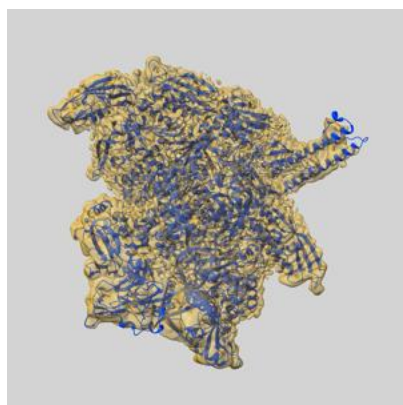
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.85	3.29	2.89
Unmasked-calculated*	3.39	3.92	3.44

*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 3.39 differs from the reported value 2.8 by more than 10 %

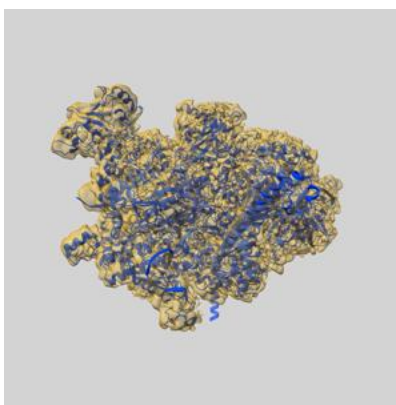
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75284 and PDB model 10MF. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

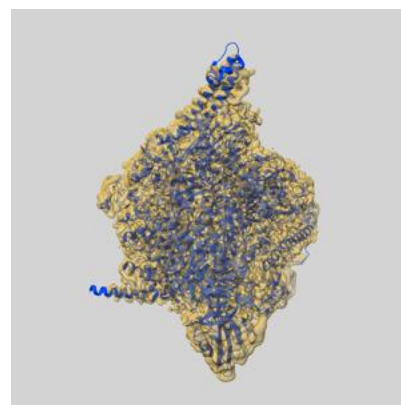
9.1 Map-model overlay [i](#)



X



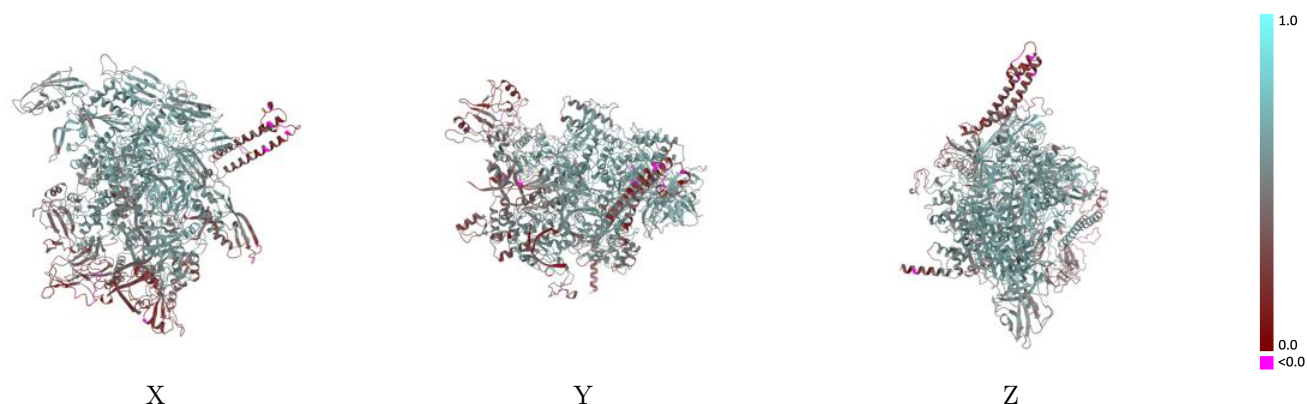
Y



Z

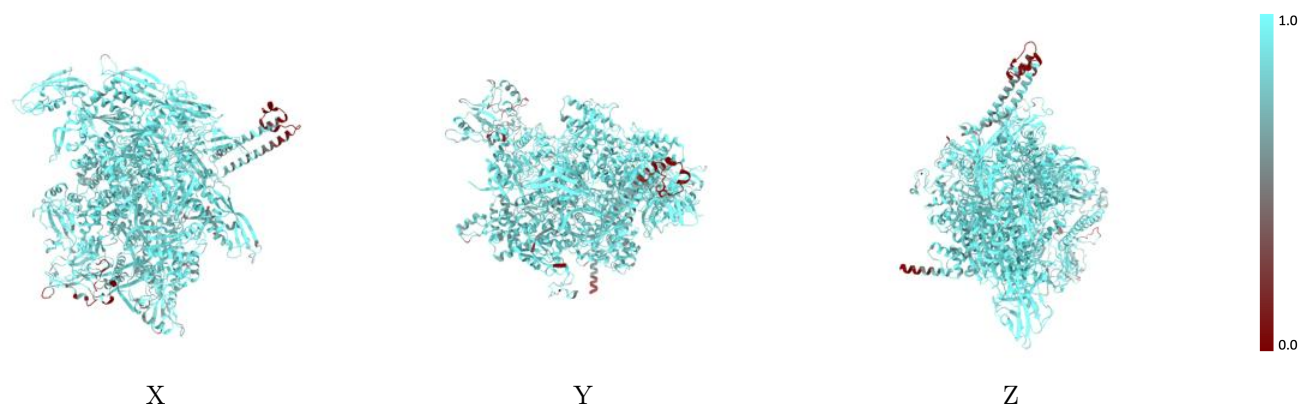
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



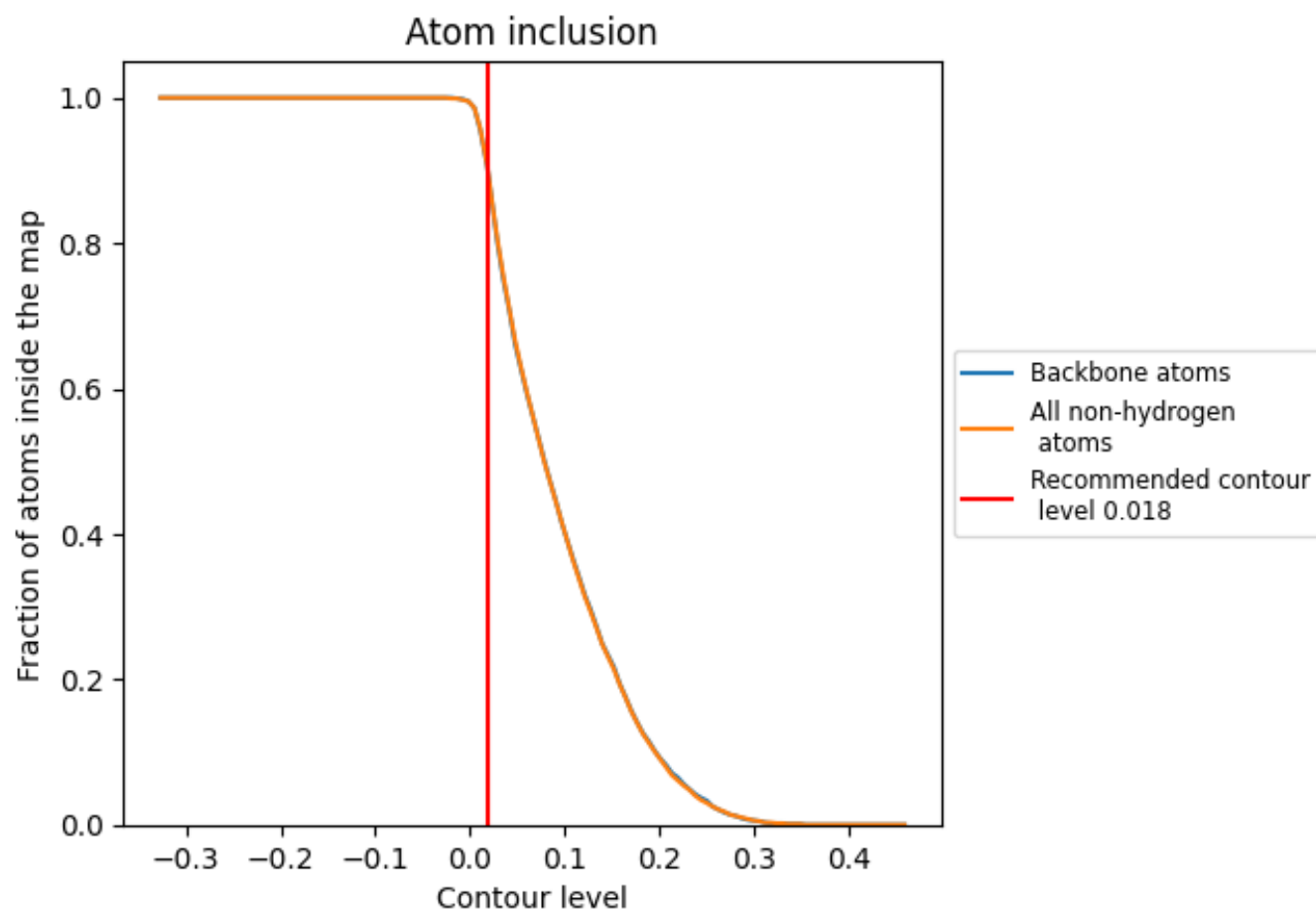
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9080	<div></div> 0.5170
A	<div></div> 0.9000	<div></div> 0.3840
B	<div></div> 0.8850	<div></div> 0.4110
G	<div></div> 0.9560	<div></div> 0.5850
H	<div></div> 0.9280	<div></div> 0.5260
I	<div></div> 0.9050	<div></div> 0.5250
J	<div></div> 0.9040	<div></div> 0.5100
K	<div></div> 0.7500	<div></div> 0.4550
R	<div></div> 0.9810	<div></div> 0.5880

1.0

0.0

<0.0