



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:40 PM UTC

PDB ID : 8P4E / pdb_00008p4e
EMDB ID : EMD-17407
Title : Structural insights into human co-transcriptional capping - structure 5
Authors : Garg, G.; Dienemann, C.; Farnung, L.; Schwarz, J.; Linden, A.; Urlaub, H.; Cramer, P.
Deposited on : 2023-05-20
Resolution : 3.90 Å(reported)

This is a wwPDB EM Validation Summary 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:

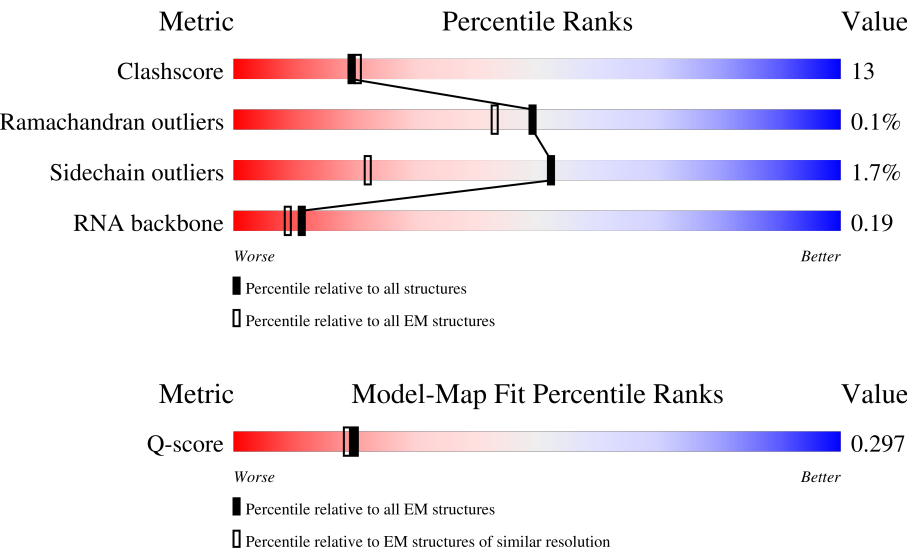
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.90 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	8855 (3.40 - 4.40)

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	Z	1087	<div><div></div><div>95%</div></div>
2	M	597	<div><div>48%</div><div>27%</div><div>24%</div><div>45%</div></div>
3	A	1970	<div><div>57%</div><div>14%</div><div>29%</div></div>

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Mol	Chain	Length	Quality of chain
4	B	1174	
5	C	275	
6	E	210	
7	F	127	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	D	142	
14	G	172	
15	O	835	
16	P	21	
17	N	26	
18	T	35	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 41213 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 Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	52	Total	C	N	O	S	0	0
			397	243	73	80	1		

- Molecule 2 is a protein called mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	329	Total	C	N	O	S	0	0
			2649	1689	456	483	21		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1407	Total	C	N	O	S	0	0
			11142	7014	1997	2063	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1116	Total	C	N	O	S	0	0
			8928	5652	1568	1644	64		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	258	Total	C	N	O	S	0	0
			2071	1301	353	411	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	82	Total	C	N	O	S	0	0
			658	418	113	122	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 13 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	129	Total	C	N	O	S	0	1
			998	629	170	195	4		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	171	Total	C	N	O	S	0	0
			1305	852	205	240	8		

- Molecule 15 is a protein called Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	695	Total	C	N	O	S	0	0
			5643	3606	962	1040	35		

- Molecule 16 is a RNA chain called RNA (5'-D(*(MGT))-R(P*GP*AP*CP*AP*UP*AP*C P*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	21	Total	C	N	O	P	0	0
			462	204	89	146	23		

- Molecule 17 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	26	Total	C	N	O	P	0	0
			538	257	100	155	26		

- Molecule 18 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	35	Total	C	N	O	P	0	0
			714	342	126	211	35		

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	

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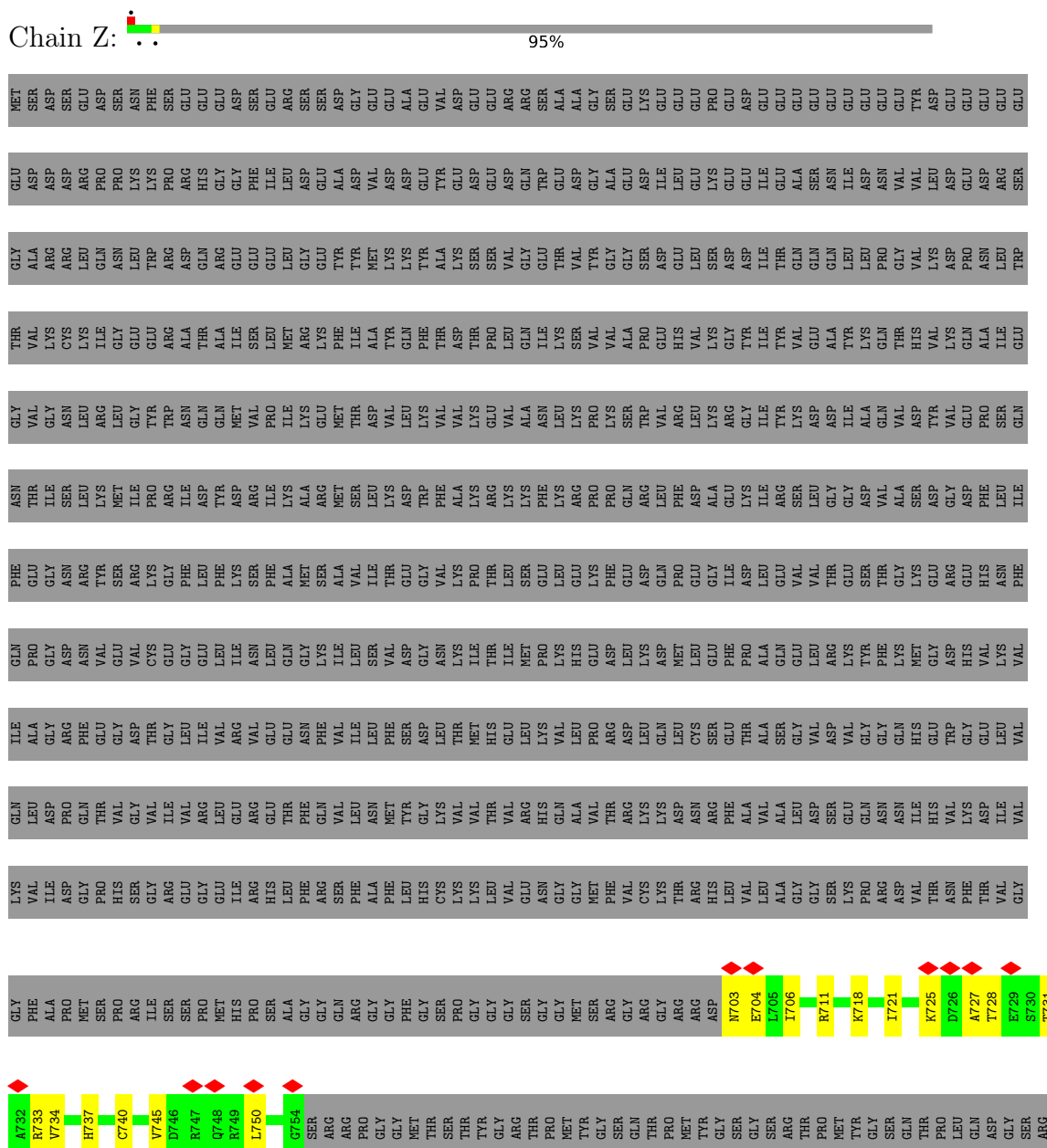
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Mol	Chain	Residues	Atoms		AltConf
20	C	1	Total 1	Zn 1	0
20	I	2	Total 2	Zn 2	0
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0

3 Residue-property plots

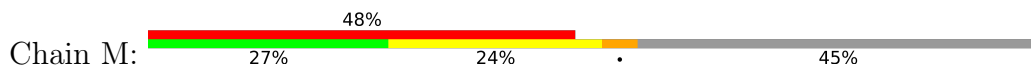
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transcription elongation factor SPT5



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

- Molecule 2: mRNA-capping enzyme

[illegible][illegible]

- Molecule 3: DNA-directed RNA polymerase II subunit RPB1





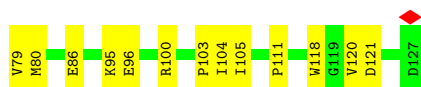
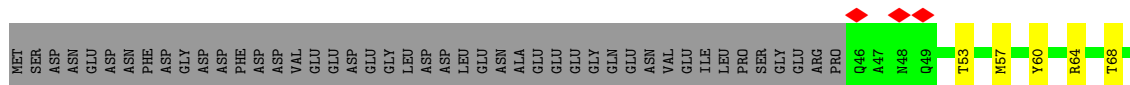
- Molecule 6: DNA-directed RNA polymerase II subunit E

Chain E: 77% 22%



- Molecule 7: DNA-directed RNA polymerase II subunit F

Chain F: 50% 14% 35%



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 77% 21%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 72% 22% 6%



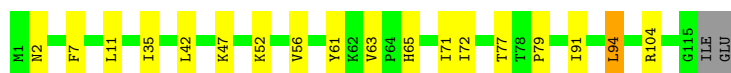
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 90% 10%



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 83% 15% ..



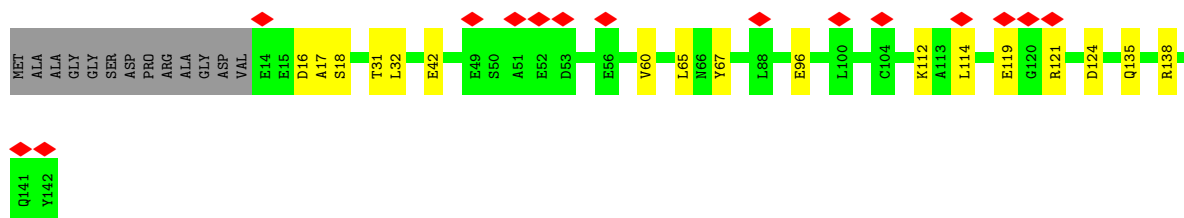
- Molecule 12: RNA polymerase II subunit K

Chain L: 66% 14% 21%



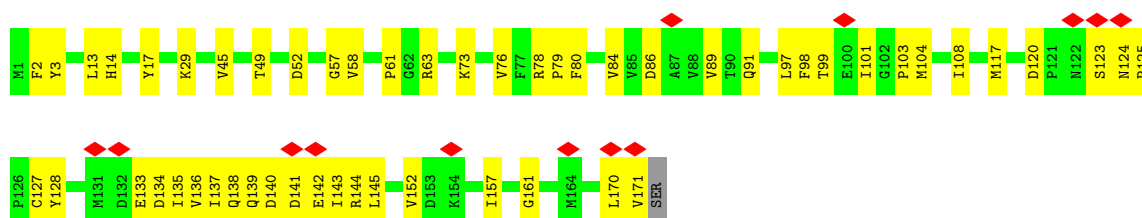
- Molecule 13: RNA polymerase II subunit D

Chain D: 11% 79% 12% 9%



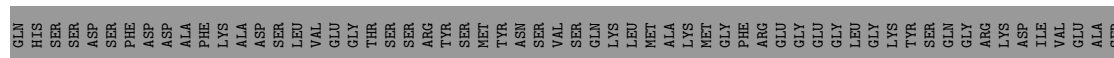
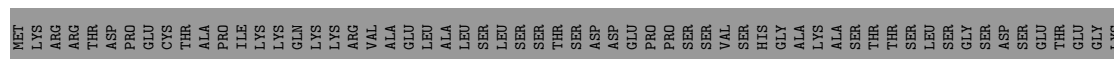
- Molecule 14: DNA-directed RNA polymerase II subunit RPB7

Chain G: 8% 68% 31%

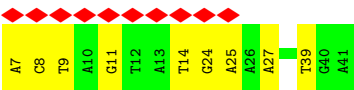


- Molecule 15: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase 1

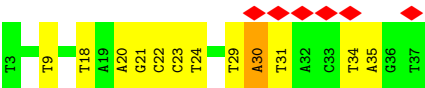
Chain O: 62% 73% 7% 17%







• Molecule 18: DNA (35-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48148	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0221	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: ZN, MG, MGT

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	Z	0.30	0/400	0.46	0/541
2	M	0.70	0/2706	1.12	13/3646 (0.4%)
3	A	0.36	0/11345	0.61	0/15315
4	B	0.39	0/9105	0.60	0/12290
5	C	0.39	0/2114	0.59	2/2873 (0.1%)
6	E	0.33	0/1752	0.58	0/2366
7	F	0.33	0/668	0.49	0/901
8	H	0.36	0/1207	0.59	0/1628
9	I	0.28	0/973	0.51	0/1316
10	J	0.40	0/542	0.54	0/730
11	K	0.41	0/939	0.56	2/1271 (0.2%)
12	L	0.37	0/395	0.59	0/524
13	D	0.17	0/1012	0.43	0/1366
14	G	0.22	0/1336	0.46	0/1820
15	O	2.30	4/5775 (0.1%)	1.47	10/7785 (0.1%)
16	P	0.49	0/482	1.17	4/749 (0.5%)
17	N	0.33	0/603	0.78	0/927
18	T	0.44	0/799	0.73	1/1230 (0.1%)
All	All	0.93	4/42153 (0.0%)	0.82	32/57278 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	5
4	B	0	1
14	G	0	1
15	O	0	1
16	P	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	1	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	659	HIS	CE1-NE2	120.55	2.53	1.32
15	O	659	HIS	ND1-CE1	83.32	2.15	1.32
15	O	659	HIS	CD2-NE2	69.86	2.14	1.37
15	O	549	PRO	C-N	23.94	1.66	1.33

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	549	PRO	O-C-N	39.14	165.65	122.98
15	O	549	PRO	CA-C-N	-30.38	76.05	121.31
15	O	549	PRO	C-N-CA	-30.38	76.05	121.31
15	O	659	HIS	ND1-CE1-NE2	-23.43	84.97	108.40
15	O	659	HIS	CG-CD2-NE2	21.59	128.79	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	P	40	A	C4'

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1108	HIS	Peptide
3	A	1112	VAL	Peptide
3	A	1467	GLY	Peptide
3	A	412	GLN	Peptide
3	A	910	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	397	0	403	31	0
2	M	2649	0	2658	195	0
3	A	11142	0	11286	222	0
4	B	8928	0	8946	225	0
5	C	2071	0	2016	42	0
6	E	1721	0	1737	43	0
7	F	658	0	684	18	0
8	H	1186	0	1147	26	0
9	I	950	0	880	20	0
10	J	533	0	553	7	0
11	K	920	0	942	14	0
12	L	389	0	395	11	0
13	D	998	0	953	14	0
14	G	1305	0	1264	157	0
15	O	5643	0	5592	223	0
16	P	462	0	234	39	0
17	N	538	0	296	33	0
18	T	714	0	397	47	0
19	A	1	0	0	0	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
All	All	41213	0	40383	1031	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 13.

The worst 5 of 1031 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)
14:G:125:PRO:HG3	15:O:655:ILE:CG1	1.18	1.60
14:G:170:LEU:CD2	15:O:650:LYS:HA	1.36	1.53
14:G:170:LEU:HD23	15:O:650:LYS:CA	1.32	1.53
6:E:112:PRO:CG	18:T:9:DT:H5''	1.47	1.45
14:G:137:ILE:HA	15:O:725:LYS:NZ	1.11	1.38

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	50/1087 (5%)	48 (96%)	2 (4%)	0	100	100
2	M	325/597 (54%)	308 (95%)	17 (5%)	0	100	100
3	A	1395/1970 (71%)	1298 (93%)	96 (7%)	1 (0%)	48	80
4	B	1102/1174 (94%)	1030 (94%)	72 (6%)	0	100	100
5	C	254/275 (92%)	242 (95%)	12 (5%)	0	100	100
6	E	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
7	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
8	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
9	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	D	127/142 (89%)	120 (94%)	7 (6%)	0	100	100
14	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
15	O	693/835 (83%)	666 (96%)	25 (4%)	2 (0%)	36	69
All	All	4885/7106 (69%)	4611 (94%)	271 (6%)	3 (0%)	49	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	O	294	HIS
3	A	1108	HIS
15	O	230	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	45/940 (5%)	45 (100%)	0	100	100
2	M	297/534 (56%)	264 (89%)	33 (11%)	6	23
3	A	1238/1749 (71%)	1228 (99%)	10 (1%)	73	77
4	B	979/1027 (95%)	977 (100%)	2 (0%)	87	87
5	C	235/252 (93%)	234 (100%)	1 (0%)	84	83
6	E	191/192 (100%)	190 (100%)	1 (0%)	81	82
7	F	71/111 (64%)	71 (100%)	0	100	100
8	H	129/131 (98%)	127 (98%)	2 (2%)	55	69
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	103 (99%)	1 (1%)	68	75
12	L	43/55 (78%)	43 (100%)	0	100	100
13	D	104/126 (82%)	104 (100%)	0	100	100
14	G	138/153 (90%)	138 (100%)	0	100	100
15	O	623/741 (84%)	598 (96%)	25 (4%)	28	51
All	All	4358/6285 (69%)	4283 (98%)	75 (2%)	52	68

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	352	ASN
15	O	682	LEU
15	O	642	VAL
15	O	654	LYS
2	M	484	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	22	ASN
15	O	372	GLN
11	K	2	ASN
13	D	48	ASN
15	O	681	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	19/21 (90%)	12 (63%)	7 (36%)

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	32	A
16	P	33	C
16	P	34	A
16	P	35	U
16	P	36	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	37	C
16	P	39	U
16	P	42	A
16	P	40	A
16	P	36	A

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 9 ligands modelled in this entry, 9 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	P	1
17	N	1
15	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	101:MGT	O3'	31:G	P	51.64
1	N	14:DT	O3'	24:DG	P	27.51
1	O	549:PRO	C	550:SER	N	1.66

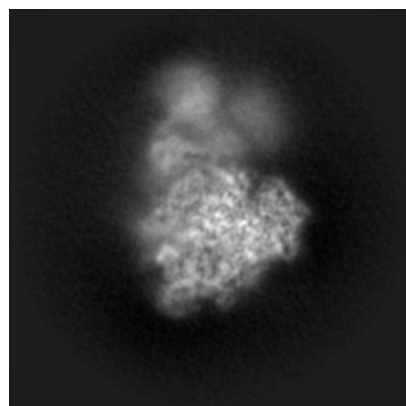
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17407. These allow visual inspection of the internal detail of the map and identification of artifacts.

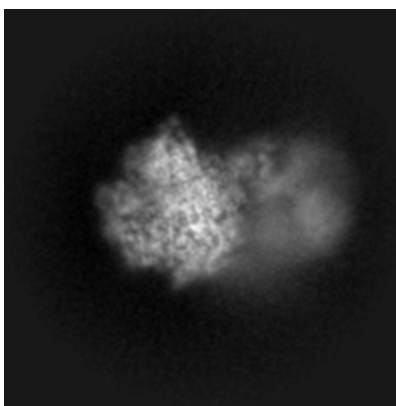
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

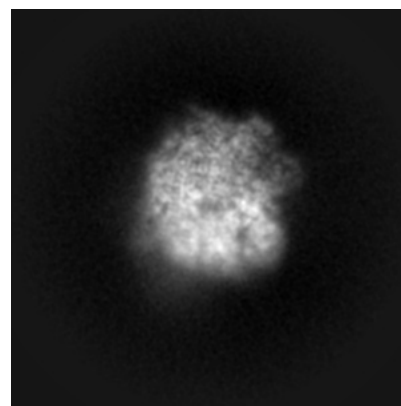
6.1.1 Primary map



X

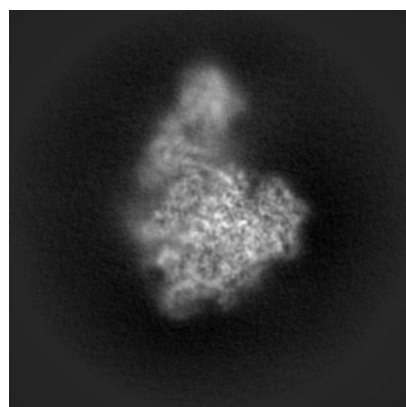


Y

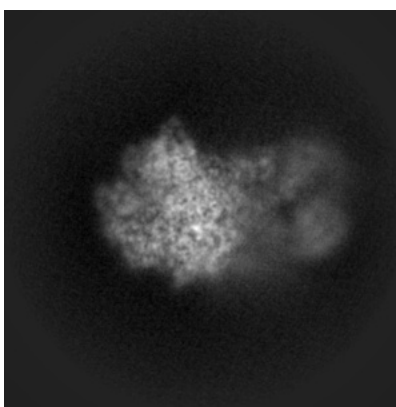


Z

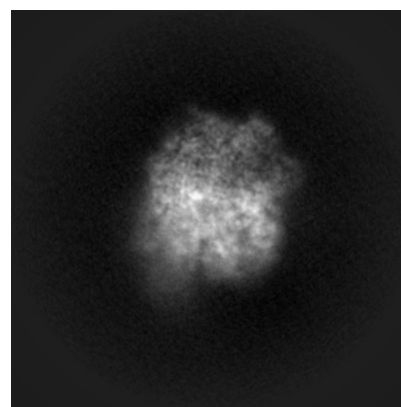
6.1.2 Raw map



X



Y

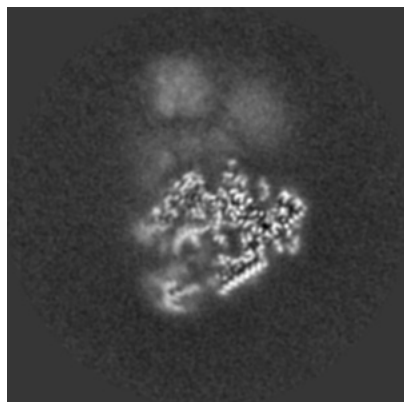


Z

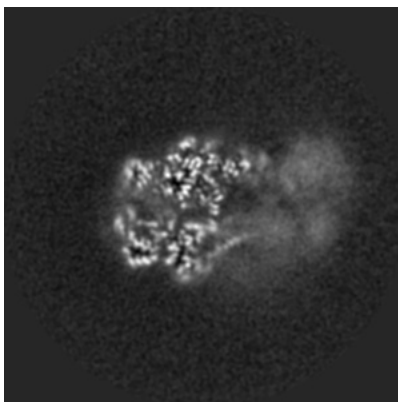
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

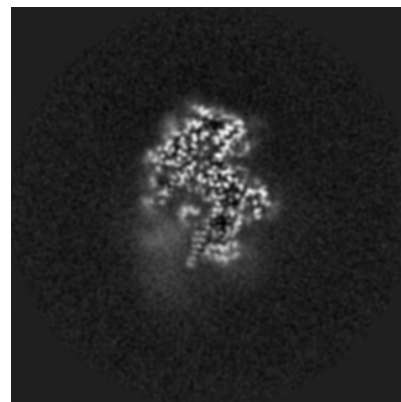
6.2.1 Primary map



X Index: 150

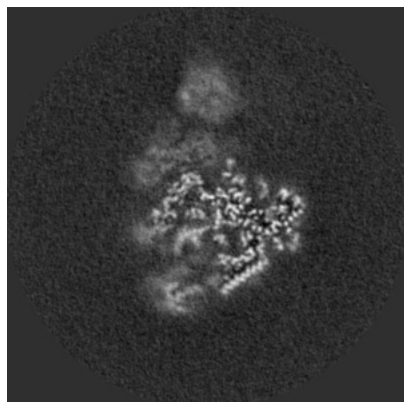


Y Index: 150

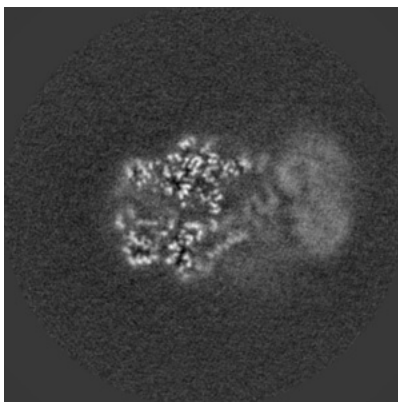


Z Index: 150

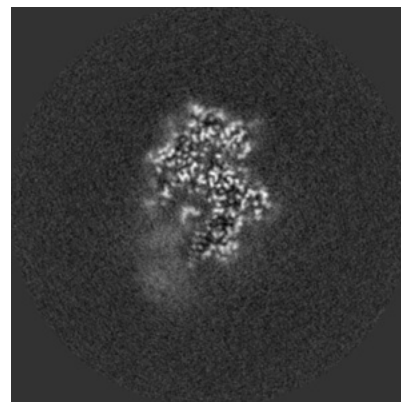
6.2.2 Raw map



X Index: 150



Y Index: 150

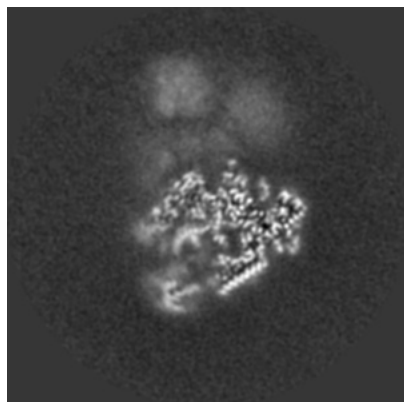


Z Index: 150

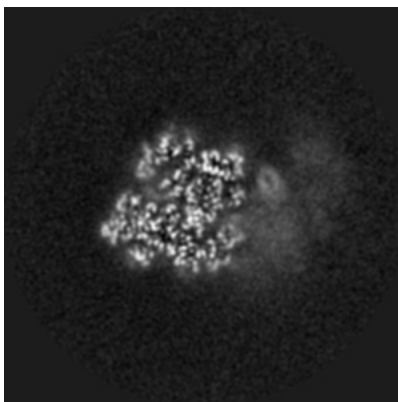
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

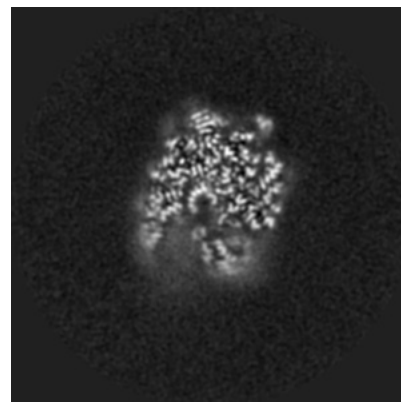
6.3.1 Primary map



X Index: 150

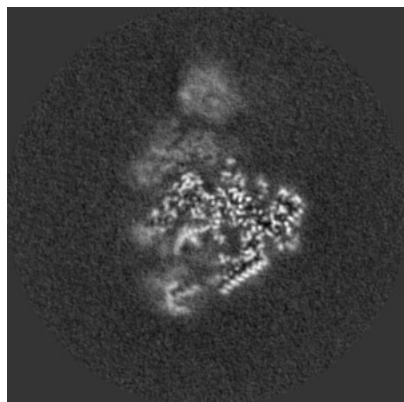


Y Index: 161

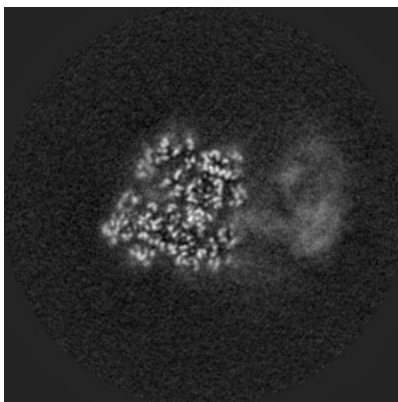


Z Index: 139

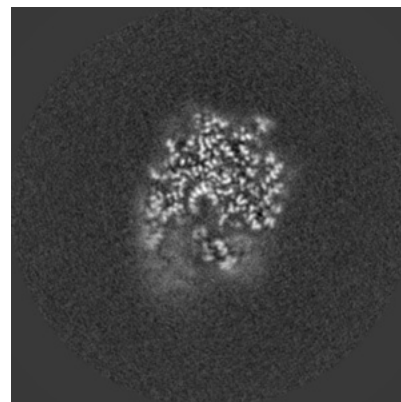
6.3.2 Raw map



X Index: 151



Y Index: 161

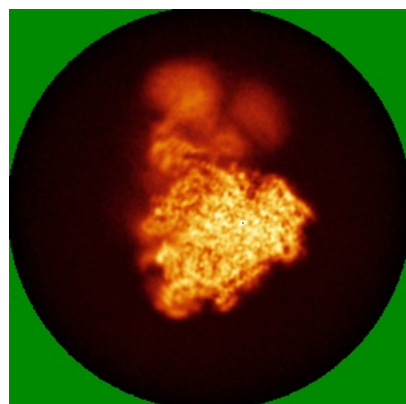


Z Index: 139

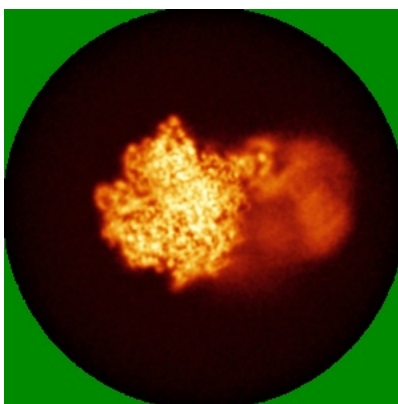
The images above show the largest variance slices of the map in three orthogonal directions.

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

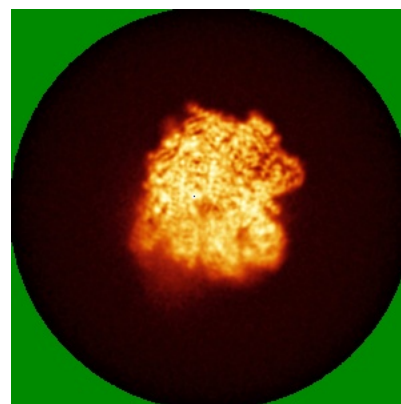
6.4.1 Primary map



X



Y

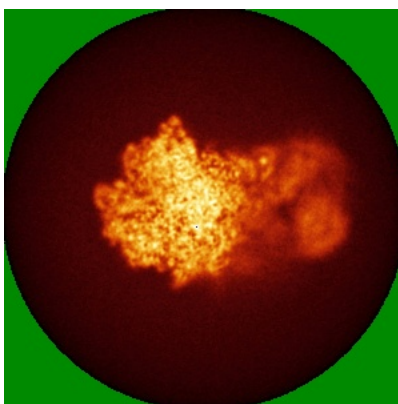


Z

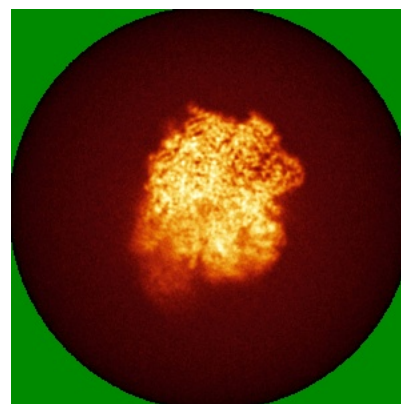
6.4.2 Raw map



X



Y

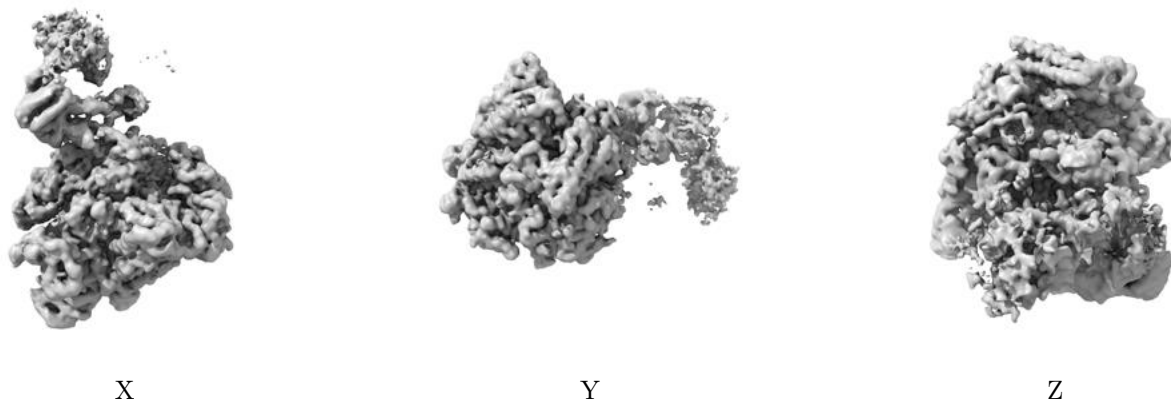


Z

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.

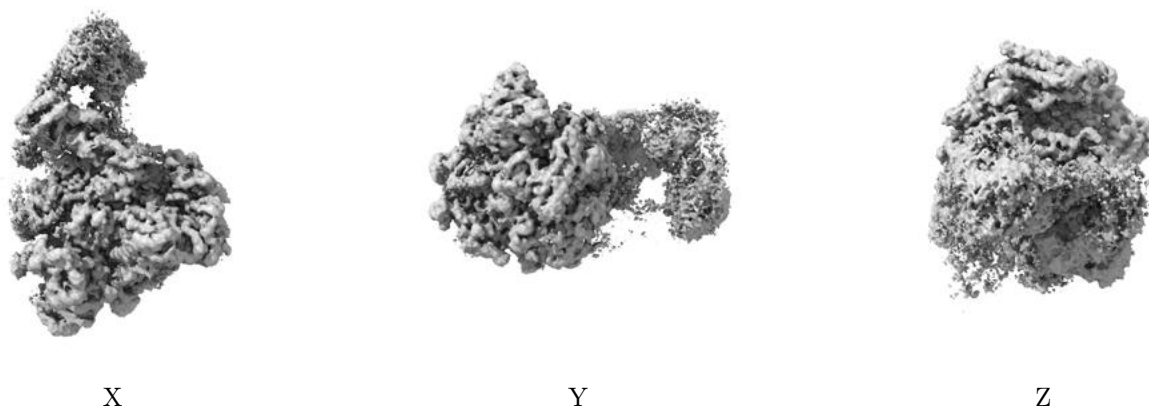
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0221. 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.

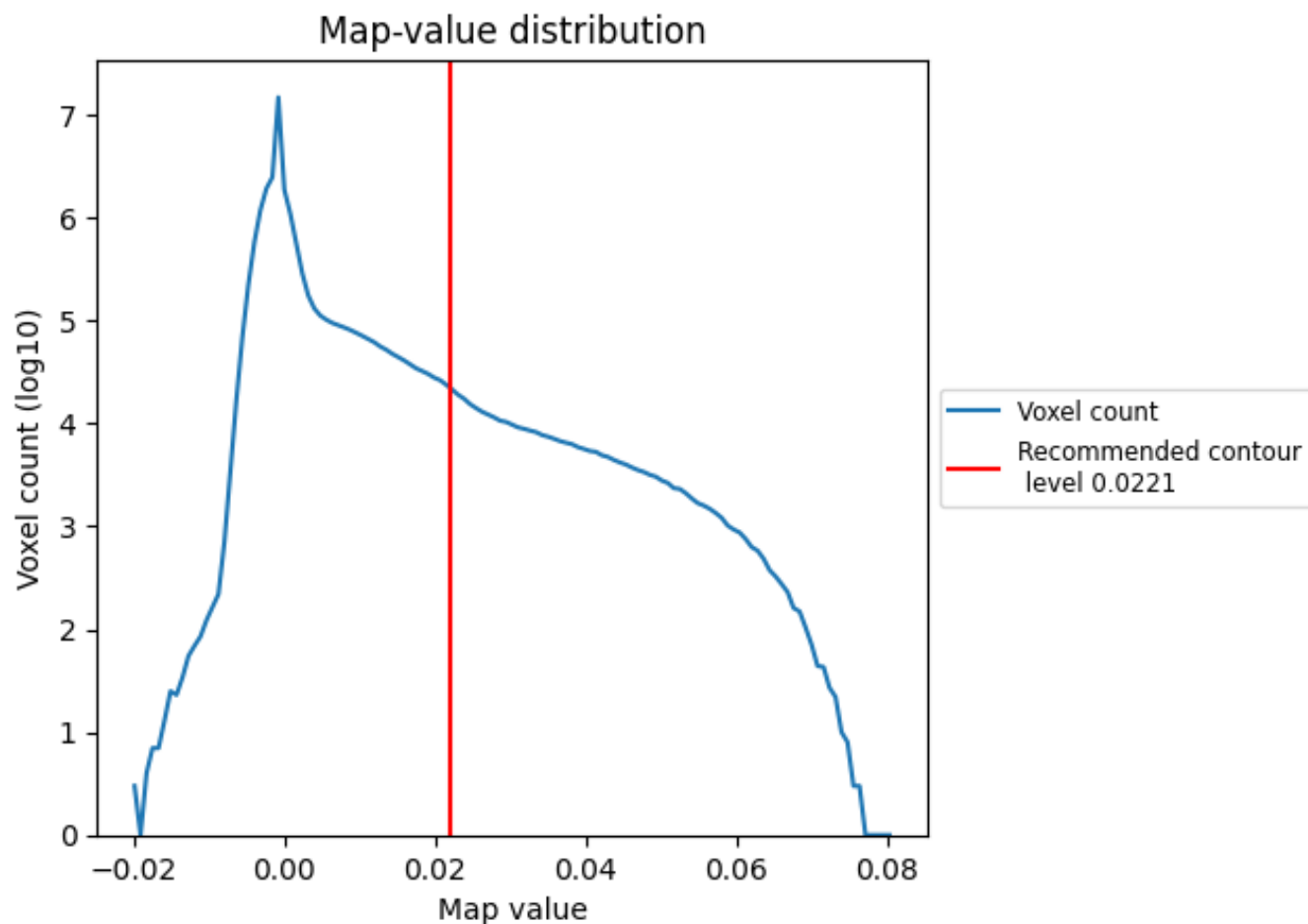
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

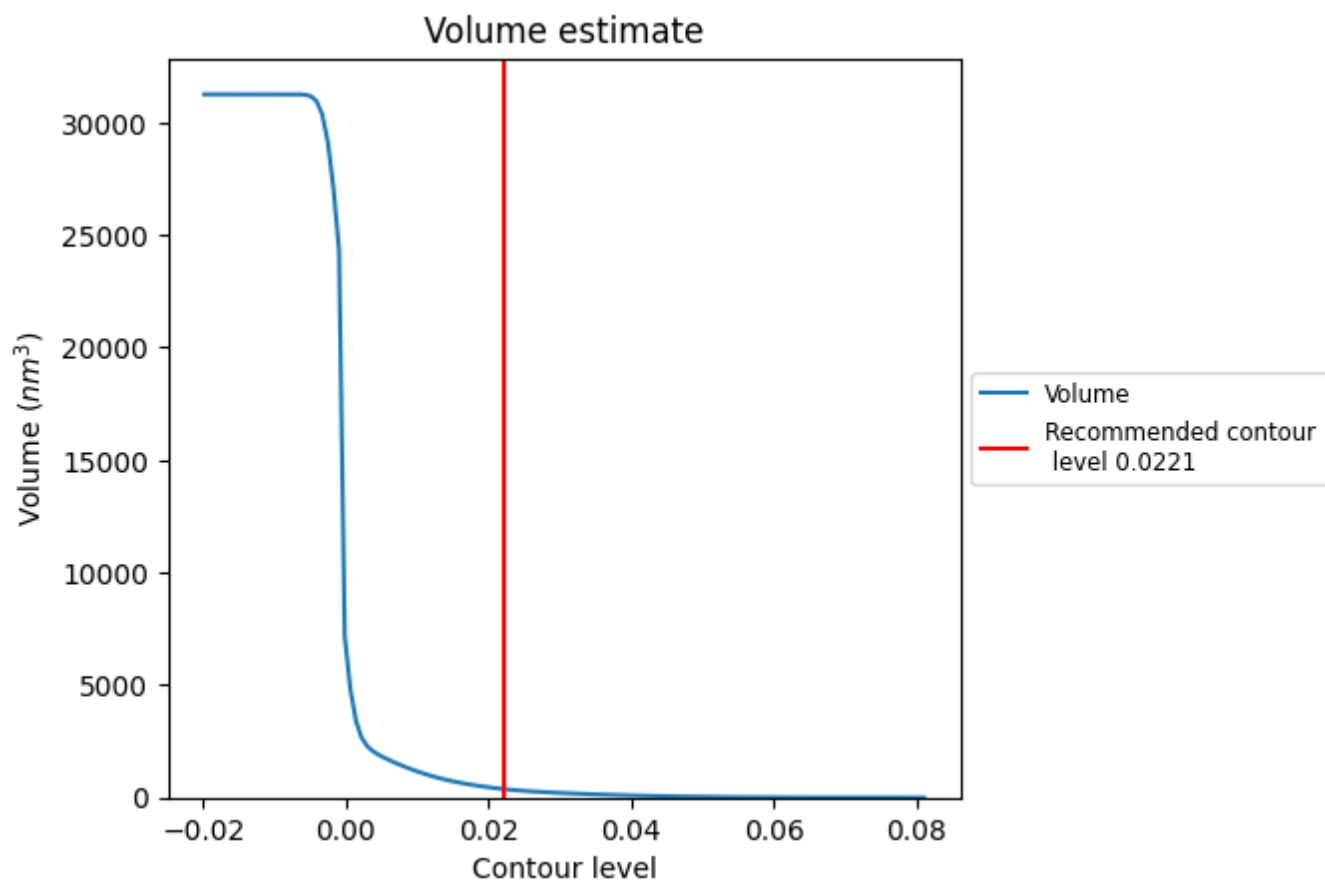
This section contains the results of statistical analysis of the map.

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.

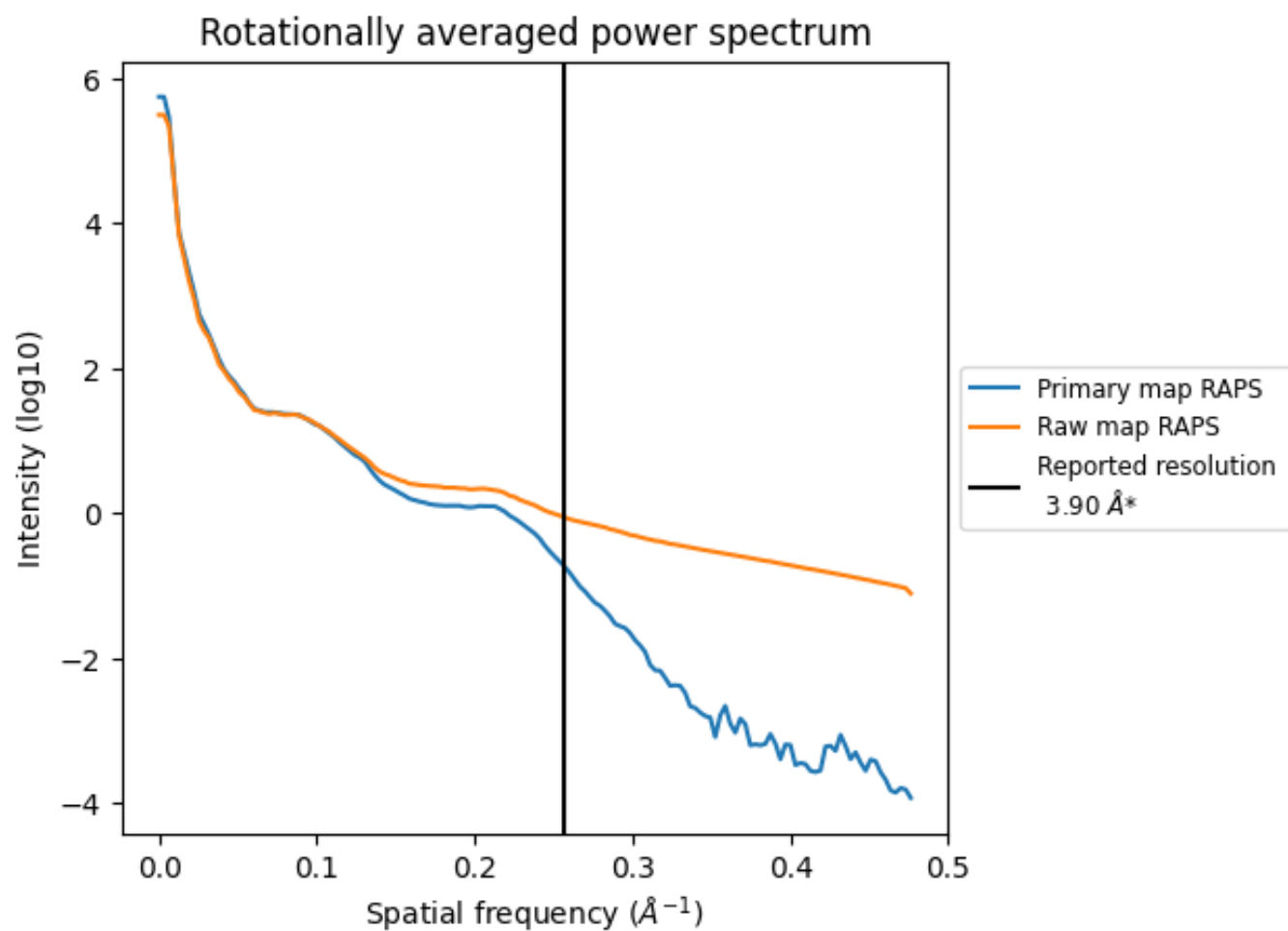
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 379 nm³; this corresponds to an approximate mass of 342 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 ⓘ

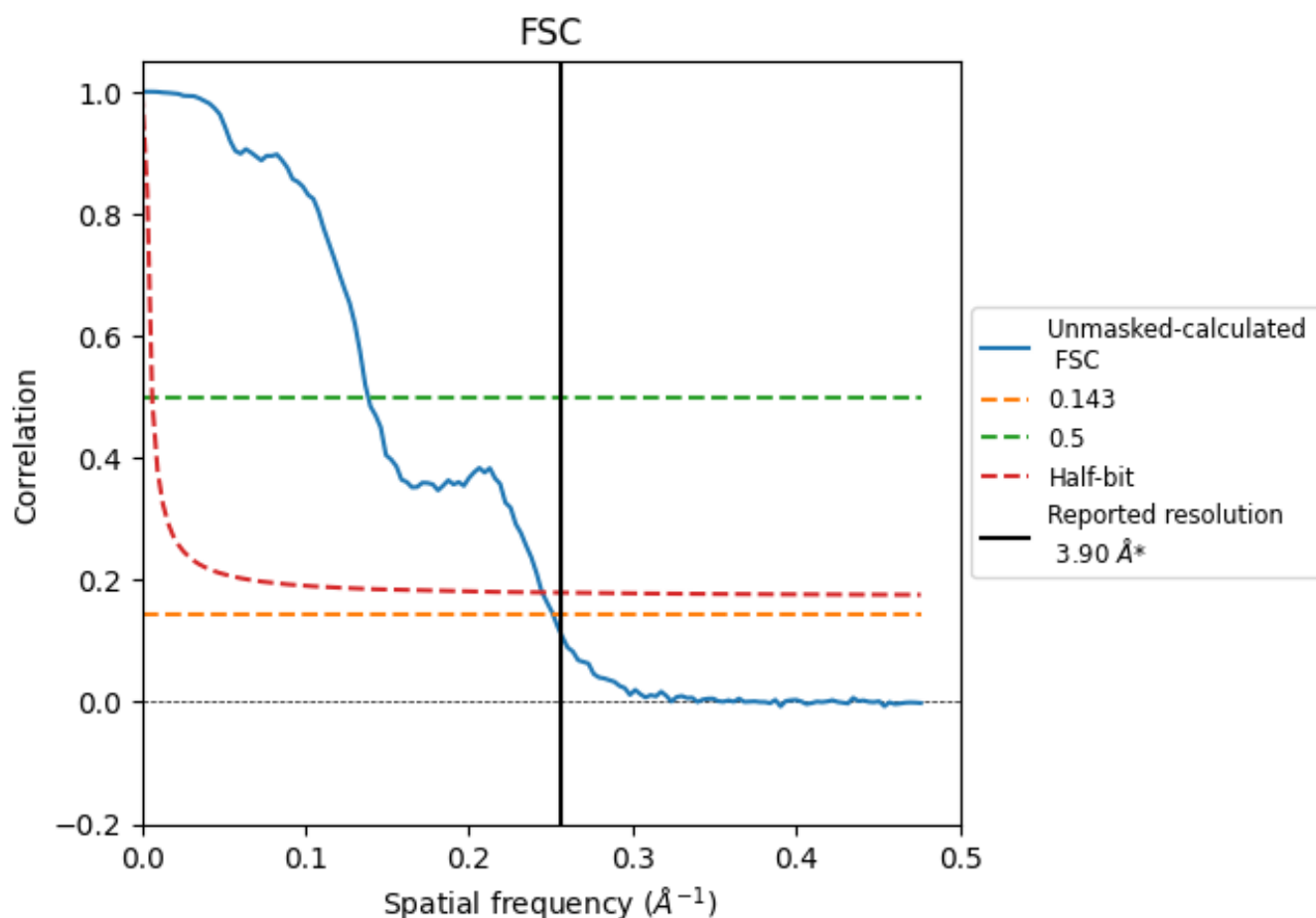


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

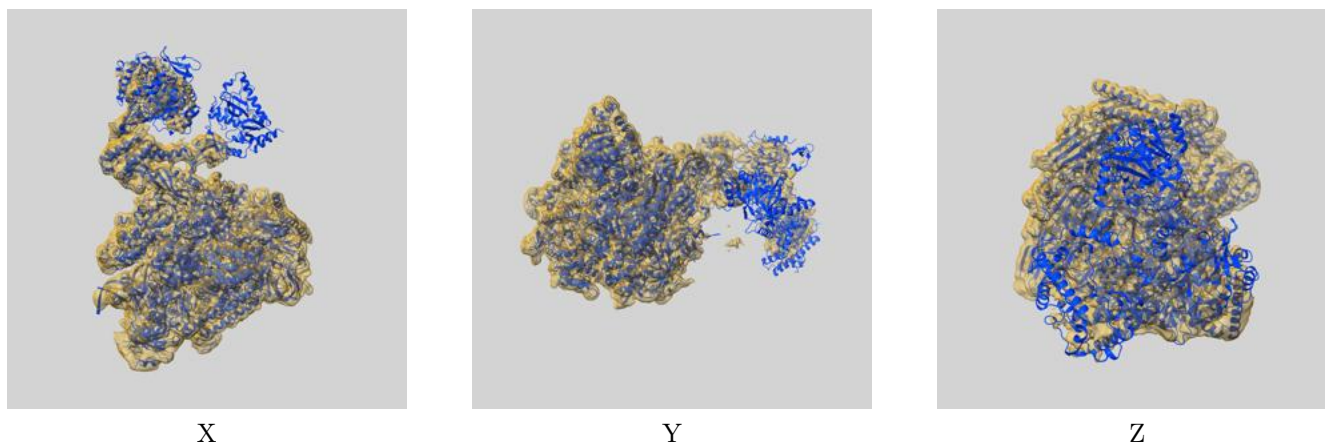
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	7.23	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

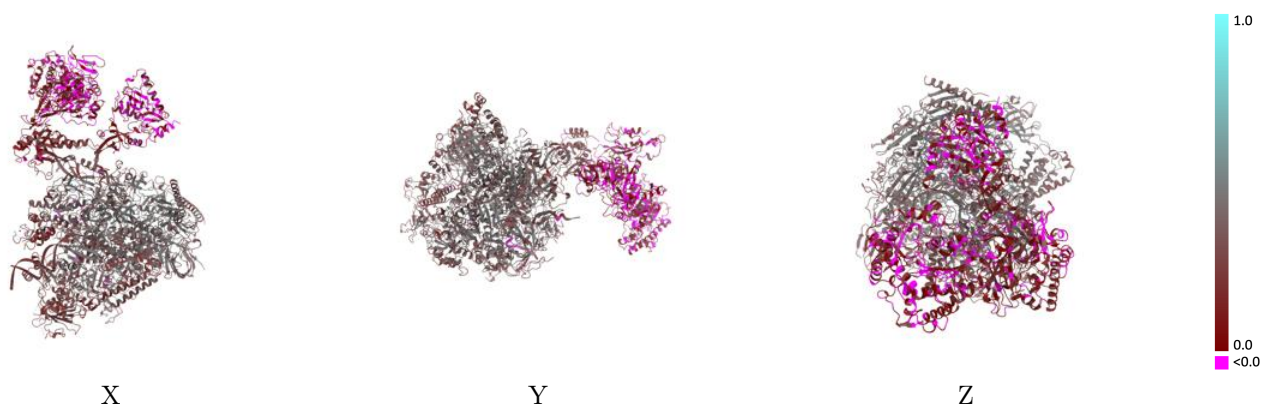
This section contains information regarding the fit between EMDB map EMD-17407 and PDB model 8P4E. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



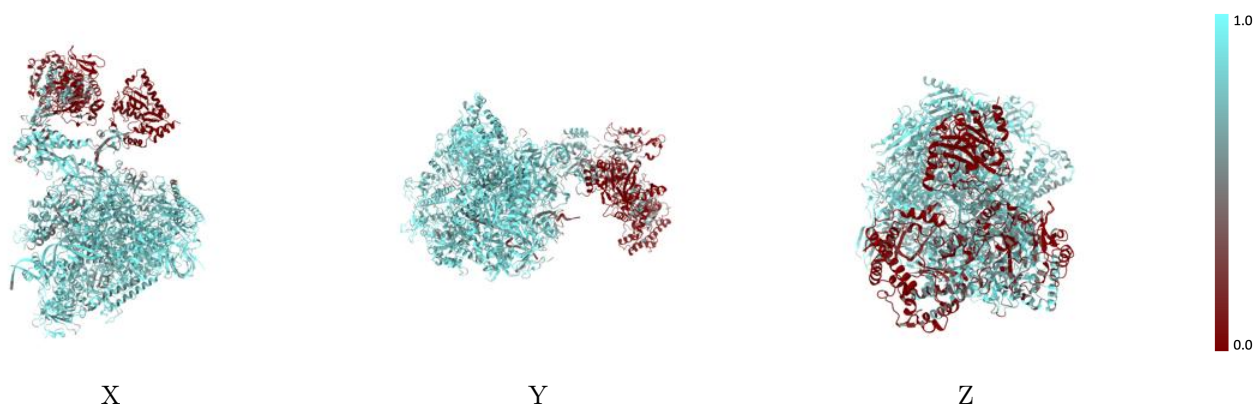
The images above show the 3D surface view of the map at the recommended contour level 0.0221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



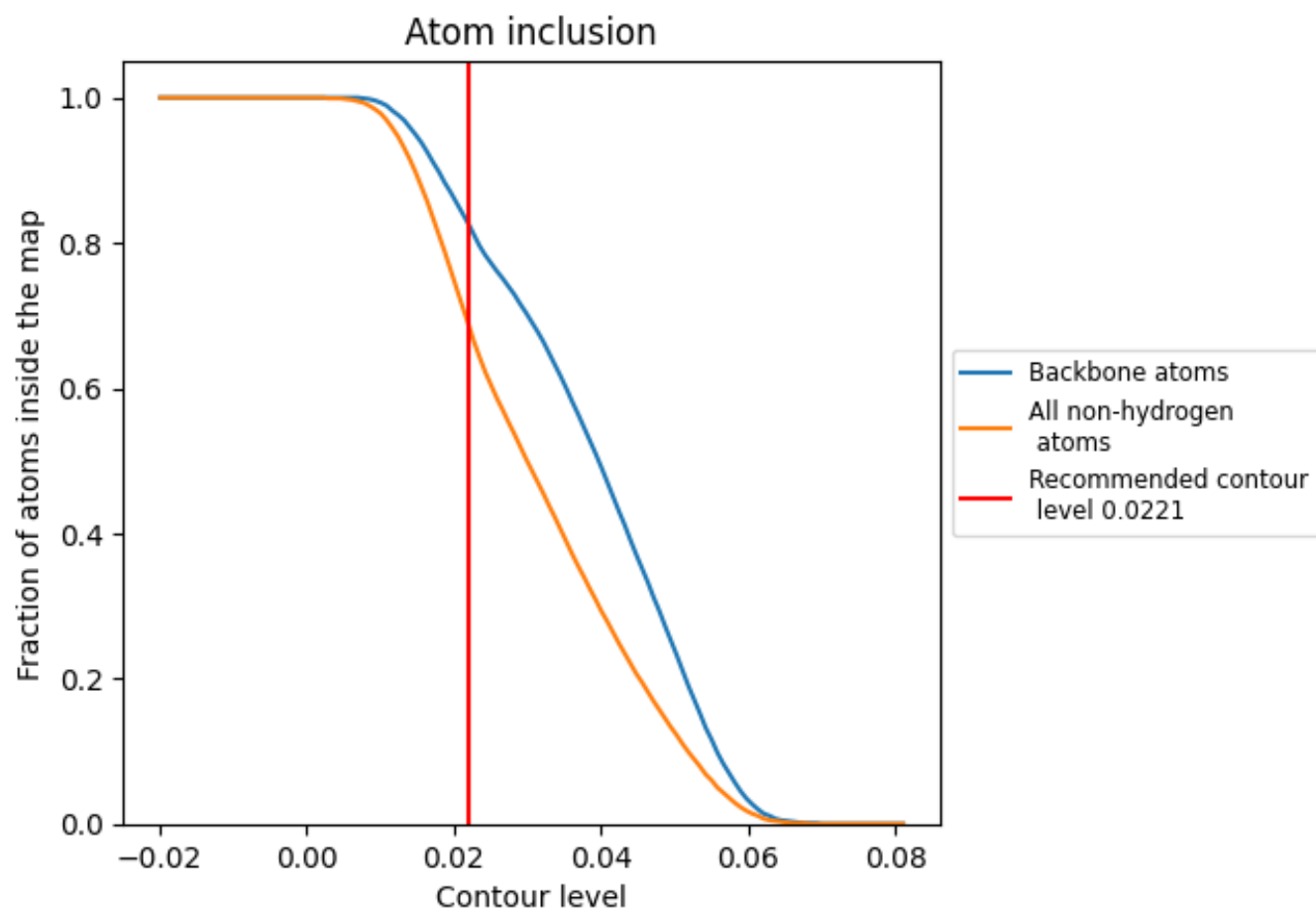
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0221).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.0221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6860	 0.2970
A	 0.8160	 0.3630
B	 0.8340	 0.3820
C	 0.8530	 0.4020
D	 0.7220	 0.1970
E	 0.8360	 0.3340
F	 0.8190	 0.3890
G	 0.7440	 0.2530
H	 0.8340	 0.3920
I	 0.8280	 0.3200
J	 0.8580	 0.4020
K	 0.8490	 0.4020
L	 0.8100	 0.3500
M	 0.1100	 0.0650
N	 0.6130	 0.2020
O	 0.2200	 0.0600
P	 0.7040	 0.2650
T	 0.7590	 0.2700
Z	 0.5740	 0.4180

