



Full wwPDB EM Validation Report ⓘ

Jun 1, 2025 – 10:23 PM JST

PDB ID : 8XRM / pdb_00008xrm
EMDB ID : EMD-38607
Title : RNA polymerase II elongation complex with DSIF, SPT6, and ELOF1 transcribing genomic DNA extracted from human nuclei
Authors : Kujirai, T.; Kato, J.; Yamamoto, K.; Hirai, S.; Negishi, L.; Ogasawara, M.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2024-01-07
Resolution : 3.13 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

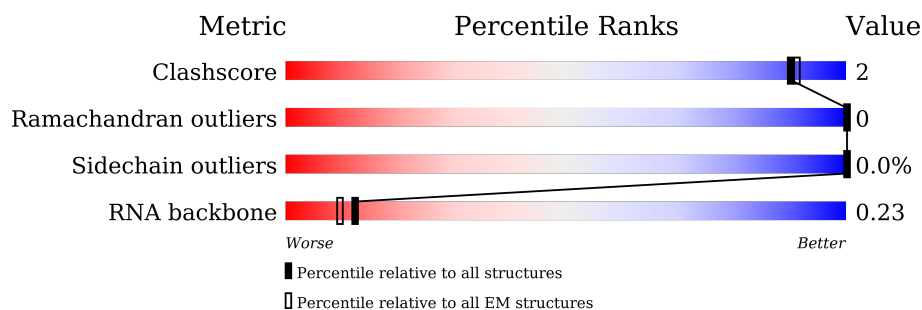
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



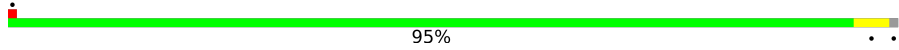

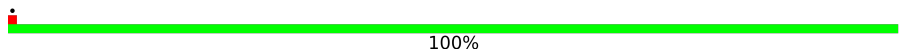
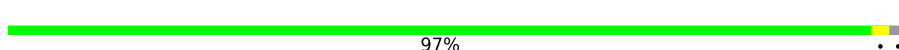

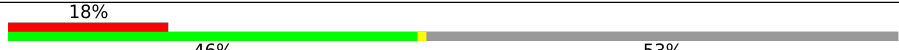
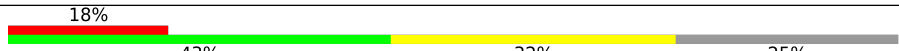
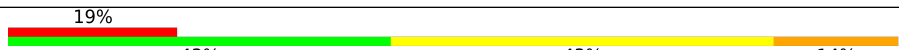
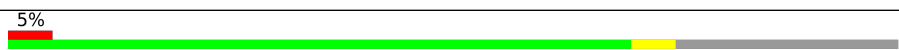

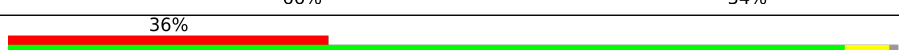
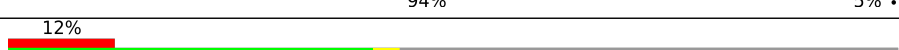
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1970	
2	B	1174	
3	C	292	
4	D	142	
5	E	210	
6	F	127	
7	G	172	

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1726	
14	N	44	
15	P	21	
16	Q	83	
17	T	44	
18	Y	117	
19	Z	1087	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 44872 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1400	Total	C	N	O	S	0	0
			11088	6978	1988	2053	69		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1133	Total	C	N	O	S	0	0
			9061	5731	1594	1672	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	259	Total	C	N	O	S	0	0
			2082	1307	357	412	6		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P19387
C	-15	HIS	-	expression tag	UNP P19387
C	-14	HIS	-	expression tag	UNP P19387
C	-13	HIS	-	expression tag	UNP P19387
C	-12	HIS	-	expression tag	UNP P19387
C	-11	HIS	-	expression tag	UNP P19387
C	-10	HIS	-	expression tag	UNP P19387
C	-9	ASP	-	expression tag	UNP P19387
C	-8	TYR	-	expression tag	UNP P19387
C	-7	LYS	-	expression tag	UNP P19387
C	-6	ASP	-	expression tag	UNP P19387
C	-5	ASP	-	expression tag	UNP P19387
C	-4	ASP	-	expression tag	UNP P19387
C	-3	ASP	-	expression tag	UNP P19387
C	-2	LYS	-	expression tag	UNP P19387

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P19387
C	0	HIS	-	expression tag	UNP P19387

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	127	Total	C	N	O	S	0	0
			1015	639	171	201	4		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	79	Total	C	N	O	S	0	0
			636	407	108	116	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- 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	113	Total	C	N	O	S	0	0
			918	566	165	176	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 DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	818	Total	C	N	O	S	0	0
			6742	4279	1172	1258	33		

- Molecule 14 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	33	Total	C	N	O	P	0	0
			694	323	145	193	33		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	21	Total	C	N	O	P	0	0
			452	202	88	141	21		

- Molecule 16 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	62	Total	C	N	O	S	0	0
			488	301	79	101	7		

- Molecule 17 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	44	Total	C	N	O	P	0	0
			889	422	151	272	44		

- Molecule 18 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

- Molecule 19 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	478	Total	C	N	O	S	0	0
			3810	2425	669	699	17		

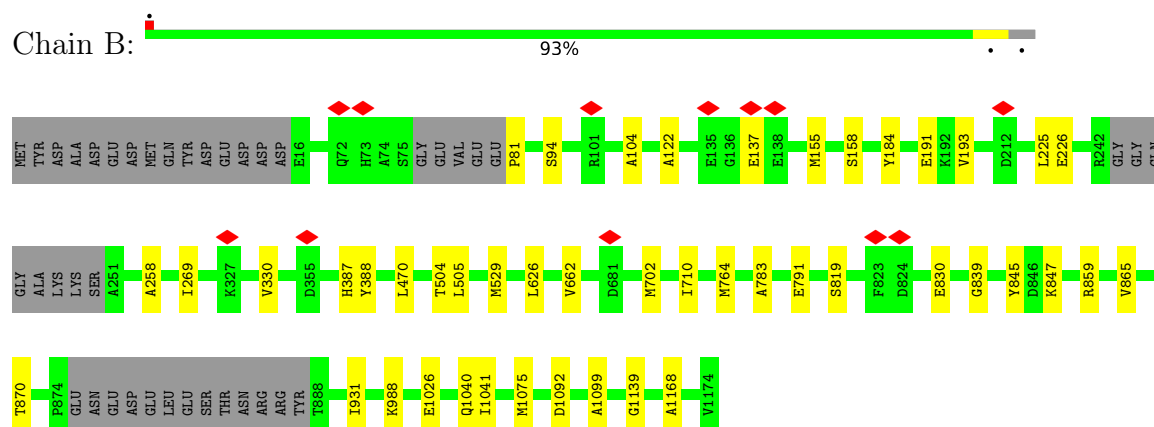
- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	C	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	
20	Q	1	Total	Zn	0
			1	1	
20	Y	1	Total	Zn	0
			1	1	

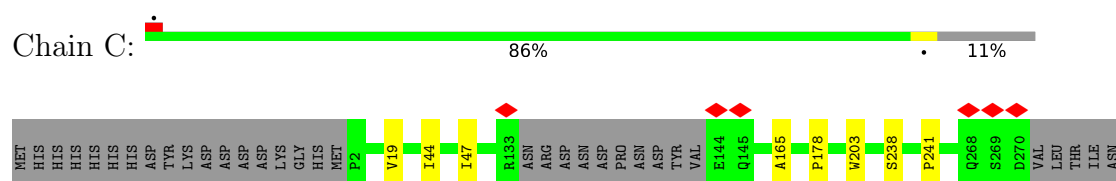
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

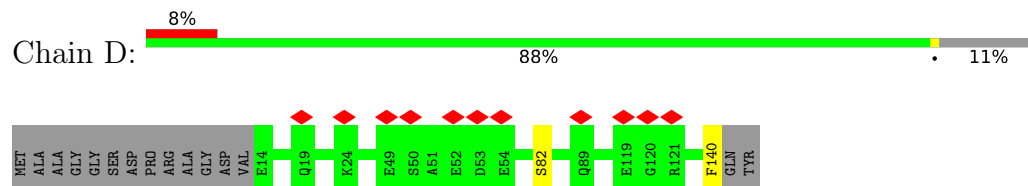
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2



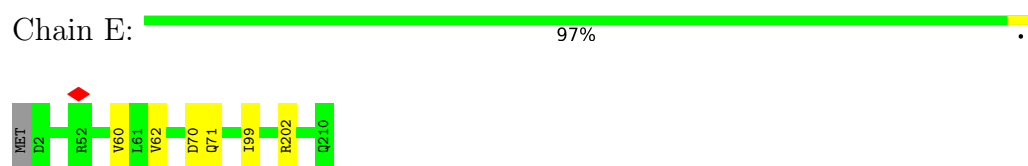
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



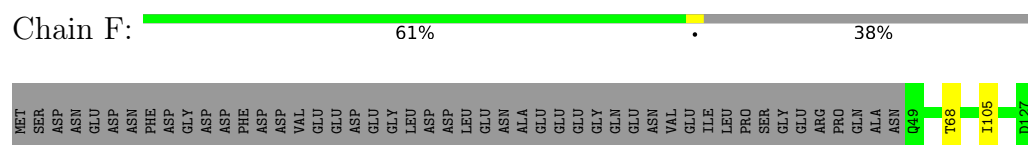
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



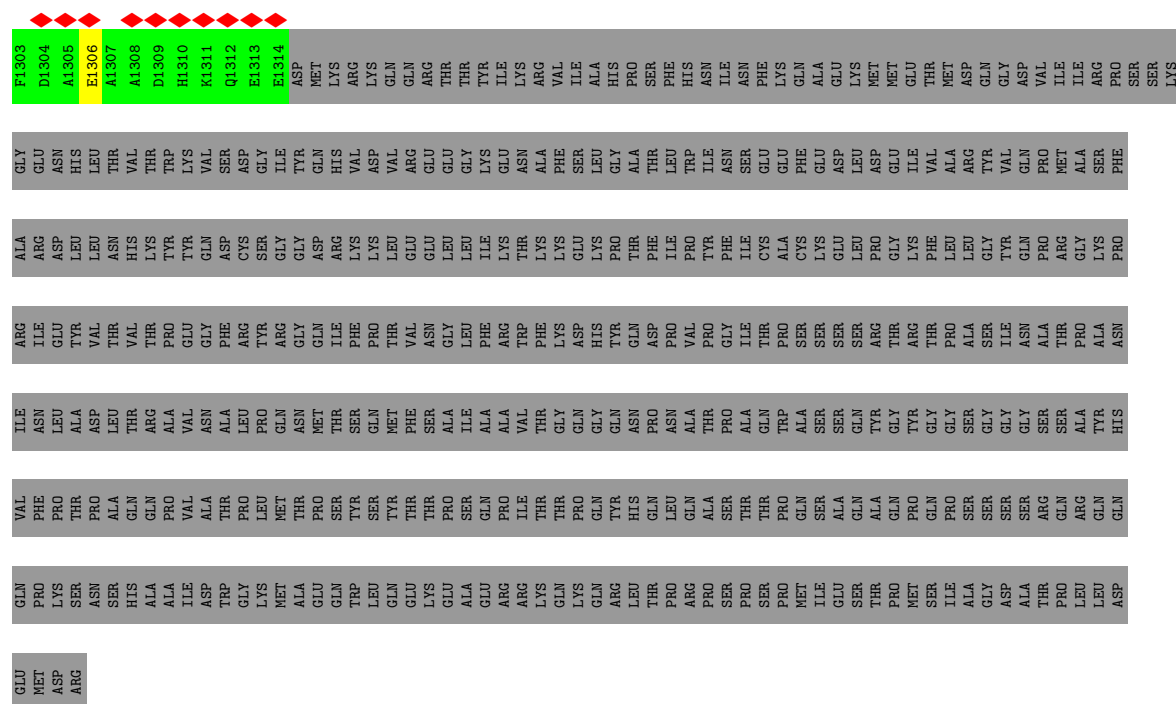
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



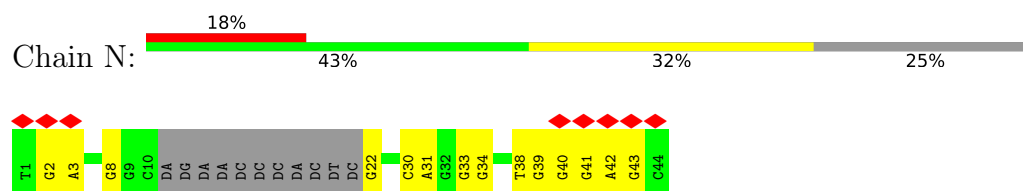
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



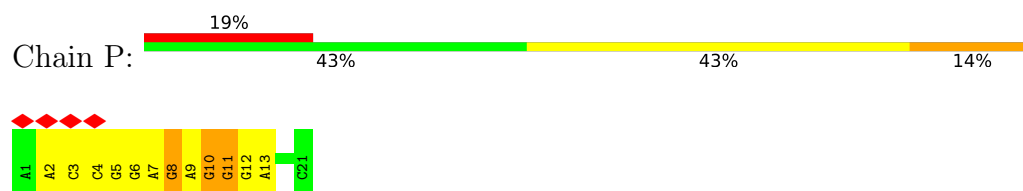




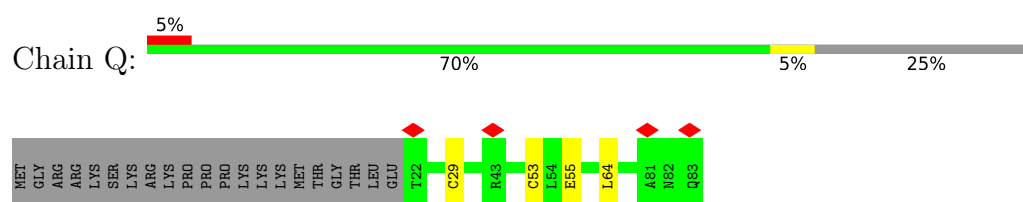
- Molecule 14: DNA



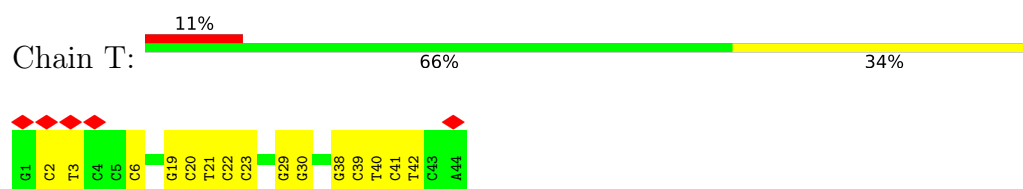
- Molecule 15: RNA



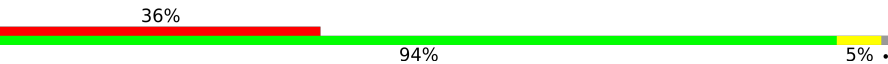
- Molecule 16: Transcription elongation factor 1 homolog

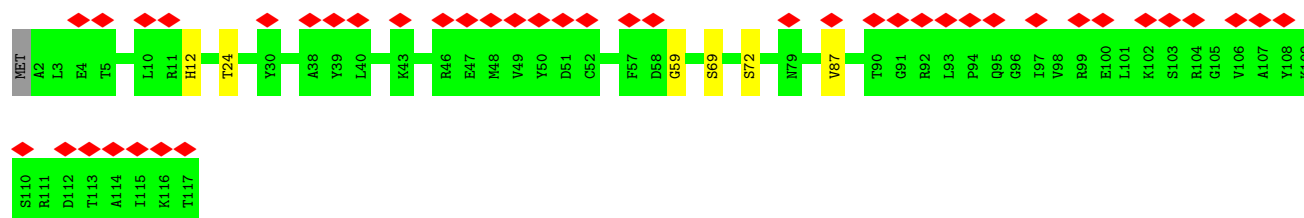


- Molecule 17: DNA



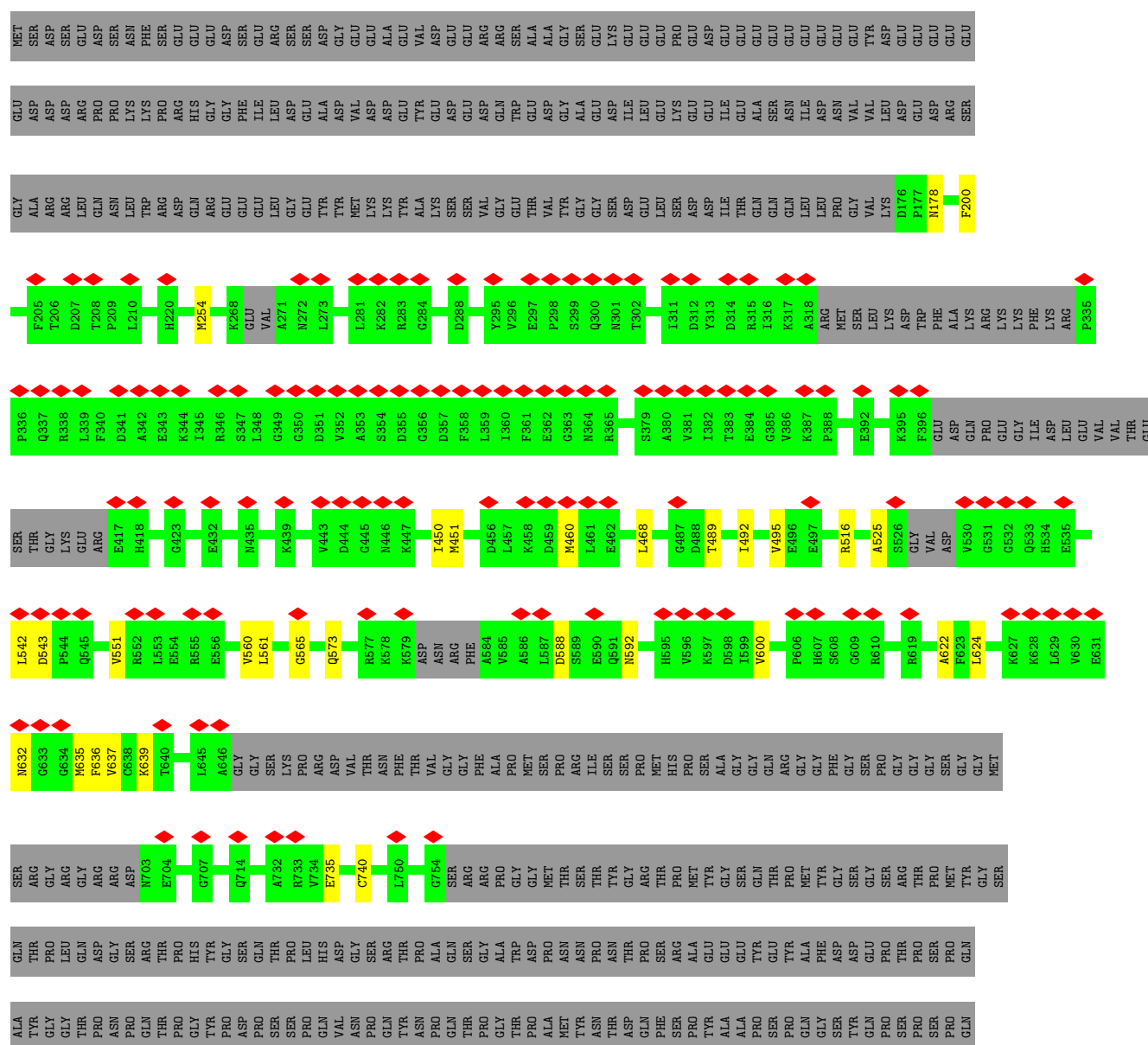
• Molecule 18: Transcription elongation factor SPT4

Chain Y: 



• Molecule 19: Transcription elongation factor SPT5

Chain Z: 



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132687	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00864	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.46	0/11287	0.76	10/15233 (0.1%)
2	B	0.47	0/9242	0.76	6/12476 (0.0%)
3	C	0.43	0/2125	0.69	0/2886
4	D	0.46	0/1029	0.76	2/1384 (0.1%)
5	E	0.45	0/1745	0.72	0/2358
6	F	0.50	0/646	0.84	0/873
7	G	0.52	0/1364	0.92	0/1853
8	H	0.40	0/1207	0.64	0/1628
9	I	0.61	0/939	0.90	2/1272 (0.2%)
10	J	0.46	0/542	0.77	0/730
11	K	0.41	0/939	0.57	0/1271
12	L	0.74	0/394	1.04	0/524
13	M	0.44	0/6869	0.72	1/9252 (0.0%)
14	N	0.28	0/782	0.45	0/1206
15	P	0.55	0/506	0.70	0/787
16	Q	0.37	0/498	0.72	0/677
17	T	0.30	0/991	0.50	0/1525
18	Y	0.46	0/927	0.81	0/1250
19	Z	0.51	0/3875	0.81	2/5216 (0.0%)
All	All	0.46	0/45907	0.75	23/62401 (0.0%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	330	VAL	N-CA-C	9.01	118.74	111.62
2	B	81	PRO	CA-C-N	7.99	127.88	120.21
2	B	81	PRO	C-N-CA	7.99	127.88	120.21
1	A	297	GLY	N-CA-C	-7.27	103.70	112.49
1	A	480	SER	N-CA-C	6.67	121.09	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	979	LEU	CA-C-N	6.51	126.28	119.05
1	A	979	LEU	C-N-CA	6.51	126.28	119.05
1	A	521	VAL	CB-CA-C	-6.34	107.67	113.70
1	A	521	VAL	N-CA-CB	5.95	114.51	110.52
19	Z	639	LYS	CA-C-N	5.75	128.30	120.54
19	Z	639	LYS	C-N-CA	5.75	128.30	120.54
1	A	1302	GLU	N-CA-C	5.41	118.00	111.40
1	A	343	LEU	CA-C-N	5.29	128.59	120.82
1	A	343	LEU	C-N-CA	5.29	128.59	120.82
1	A	980	PRO	N-CA-C	5.28	120.87	113.53
9	I	29	ASP	CA-C-N	5.23	127.29	120.28
9	I	29	ASP	C-N-CA	5.23	127.29	120.28
2	B	819	SER	N-CA-C	5.22	122.14	113.89
4	D	82	SER	CA-C-N	5.21	127.21	120.70
4	D	82	SER	C-N-CA	5.21	127.21	120.70
13	M	888	GLU	N-CA-C	5.12	117.25	111.11
2	B	104	ALA	CA-C-N	5.12	125.03	119.76
2	B	104	ALA	C-N-CA	5.12	125.03	119.76

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	11088	0	11244	39	0
2	B	9061	0	9094	30	0
3	C	2082	0	2029	6	0
4	D	1015	0	989	2	0
5	E	1715	0	1733	4	0
6	F	636	0	667	4	0
7	G	1333	0	1321	3	0
8	H	1186	0	1147	4	0
9	I	918	0	854	1	0
10	J	533	0	554	0	0
11	K	920	0	942	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	388	0	394	1	0
13	M	6742	0	6704	14	0
14	N	694	0	367	11	0
15	P	452	0	231	3	0
16	Q	488	0	446	3	0
17	T	889	0	496	11	0
18	Y	911	0	905	4	0
19	Z	3810	0	3878	26	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
20	Q	1	0	0	0	0
20	Y	1	0	0	0	0
21	A	1	0	0	0	0
All	All	44872	0	43995	142	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 (142) 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)
19:Z:551:VAL:HG11	19:Z:632:ASN:O	1.79	0.82
1:A:686:THR:HG21	2:B:1041:ILE:HA	1.69	0.74
18:Y:12:HIS:CE1	18:Y:24:THR:HB	2.24	0.72
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.70	0.72
16:Q:64:LEU:HD23	16:Q:64:LEU:O	1.89	0.71
19:Z:450:ILE:HD12	19:Z:468:LEU:HD13	1.77	0.67
1:A:26:LEU:HG	2:B:1168:ALA:HB2	1.76	0.67
19:Z:551:VAL:CG1	19:Z:632:ASN:O	2.44	0.65
18:Y:12:HIS:HE1	18:Y:24:THR:HB	1.61	0.64
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.79	0.64
13:M:848:VAL:HB	13:M:882:VAL:HG12	1.80	0.63
1:A:470:MET:HE3	1:A:521:VAL:HG22	1.80	0.63
1:A:340:LYS:HE3	1:A:1436:VAL:HG21	1.81	0.61
13:M:855:ARG:NH1	13:M:1235:GLY:O	2.33	0.61
19:Z:178:ASN:HB3	19:Z:254:MET:HE1	1.82	0.61
1:A:471:GLY:O	1:A:521:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:71:GLN:HB2	5:E:99:ILE:HG22	1.85	0.58
4:D:140:PHE:CD1	13:M:526:ILE:HD13	2.38	0.58
13:M:379:TYR:OH	13:M:1033:GLY:O	2.21	0.57
2:B:710:ILE:HB	2:B:764:MET:HE3	1.87	0.57
7:G:119:PHE:CE2	7:G:121:PRO:HB3	2.40	0.56
19:Z:561:LEU:HD11	19:Z:565:GLY:HA2	1.88	0.56
1:A:514:GLU:OE2	2:B:1099:ALA:HB1	2.06	0.56
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.87	0.56
19:Z:450:ILE:HD12	19:Z:468:LEU:CD1	2.36	0.56
1:A:983:LEU:HD13	1:A:1048:THR:HG21	1.88	0.55
4:D:140:PHE:CE1	13:M:526:ILE:HG21	2.41	0.54
14:N:42:DA:H2''	14:N:43:DG:H5''	1.90	0.54
1:A:1473:LEU:HD23	6:F:68:THR:HG21	1.91	0.53
1:A:865:ILE:HD13	2:B:1092:ASP:OD2	2.09	0.53
19:Z:600:VAL:CG2	19:Z:624:LEU:HD21	2.38	0.53
2:B:847:LYS:NZ	19:Z:735:GLU:OE2	2.22	0.52
5:E:70:ASP:OD1	5:E:70:ASP:N	2.41	0.52
13:M:756:ALA:HB3	13:M:1140:ALA:HA	1.92	0.52
2:B:783:ALA:HB2	2:B:1041:ILE:HG23	1.92	0.52
13:M:593:ALA:HA	13:M:716:ALA:HB2	1.92	0.51
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.92	0.50
1:A:1036:ASN:OD1	5:E:202:ARG:NH1	2.44	0.50
5:E:60:VAL:HG12	5:E:62:VAL:HG13	1.92	0.50
1:A:1476:ASP:CB	6:F:105:ILE:HD11	2.42	0.50
2:B:839:GLY:HA3	15:P:8:G:H5'	1.93	0.50
3:C:47:ILE:HA	3:C:165:ALA:HA	1.94	0.50
19:Z:551:VAL:HG13	19:Z:635:MET:HB2	1.94	0.50
19:Z:561:LEU:HD21	19:Z:636:PHE:C	2.37	0.49
1:A:1163:HIS:CD2	1:A:1302:GLU:HA	2.47	0.49
17:T:20:DC:H2''	17:T:21:DT:H71	1.95	0.49
19:Z:600:VAL:HG23	19:Z:624:LEU:HD21	1.95	0.49
19:Z:489:THR:HG23	19:Z:525:ALA:HB2	1.95	0.49
1:A:1476:ASP:HB2	6:F:105:ILE:HD11	1.96	0.48
12:L:48:ARG:HH22	12:L:53:VAL:HG21	1.77	0.48
1:A:479:TRP:HB2	2:B:931:ILE:HD11	1.95	0.48
8:H:32:SER:HB3	8:H:37:MET:H	1.78	0.48
1:A:141:LEU:HD13	1:A:1445:HIS:HE1	1.78	0.48
2:B:845:TYR:HA	2:B:865:VAL:HG21	1.95	0.48
2:B:1075:MET:HE1	15:P:11:G:H5''	1.96	0.48
3:C:44:ILE:HD12	3:C:178:PRO:HB3	1.95	0.48
1:A:876:ASP:HB2	1:A:878:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:8:DG:C2	17:T:38:DG:N2	2.81	0.48
2:B:859:ARG:NH2	19:Z:740:CYS:HA	2.29	0.48
17:T:41:DC:H2'	17:T:42:DT:H72	1.95	0.47
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.97	0.47
14:N:33:DG:H2''	14:N:34:DG:C8	2.50	0.47
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.96	0.47
3:C:44:ILE:HD11	3:C:238:SER:HB3	1.95	0.47
19:Z:561:LEU:HD11	19:Z:565:GLY:CA	2.45	0.47
19:Z:551:VAL:HG13	19:Z:635:MET:CB	2.44	0.46
1:A:1481:LYS:HA	7:G:20:PRO:HA	1.96	0.46
1:A:983:LEU:HD12	1:A:1044:HIS:CE1	2.50	0.46
14:N:30:DC:H2''	14:N:31:DA:H8	1.80	0.46
1:A:804:HIS:NE2	9:I:100:HIS:CD2	2.84	0.45
17:T:2:DC:H2'	17:T:3:DT:H71	1.98	0.45
17:T:20:DC:C2'	17:T:21:DT:H71	2.46	0.45
19:Z:542:LEU:HD21	19:Z:560:VAL:HG11	1.99	0.45
14:N:30:DC:H2''	14:N:31:DA:C8	2.52	0.45
1:A:1130:ILE:HD13	1:A:1411:LEU:HD22	1.98	0.45
1:A:540:ASP:OD1	1:A:540:ASP:C	2.59	0.45
15:P:10:G:O3'	15:P:11:G:H8	2.00	0.45
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.99	0.44
13:M:904:ARG:O	13:M:904:ARG:NE	2.51	0.44
16:Q:53:CYS:SG	16:Q:55:GLU:HG2	2.57	0.44
17:T:39:DC:H2''	17:T:40:DT:C6	2.52	0.44
1:A:1476:ASP:CA	6:F:105:ILE:HD11	2.48	0.44
14:N:2:DG:H2''	14:N:3:DA:C8	2.53	0.44
1:A:918:LYS:O	1:A:1052:ARG:NH2	2.50	0.44
2:B:387:HIS:CD2	2:B:504:THR:HG21	2.53	0.44
2:B:155:MET:O	2:B:158:SER:HB3	2.18	0.44
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.52	0.44
19:Z:622:ALA:O	19:Z:637:VAL:HG23	2.17	0.44
17:T:38:DG:H2''	17:T:39:DC:C6	2.52	0.43
19:Z:451:MET:HE3	19:Z:460:MET:HB3	1.99	0.43
19:Z:516:ARG:HG2	19:Z:516:ARG:HH11	1.83	0.43
2:B:94:SER:O	2:B:122:ALA:HB1	2.18	0.43
8:H:116:VAL:CG1	8:H:123:MET:HE2	2.48	0.43
19:Z:543:ASP:OD1	19:Z:543:ASP:C	2.60	0.43
1:A:983:LEU:HD12	1:A:1044:HIS:ND1	2.32	0.43
1:A:1189:ASP:HA	1:A:1192:TRP:CD2	2.53	0.43
2:B:988:LYS:NZ	2:B:1026:GLU:OE2	2.32	0.43
11:K:39:ASP:O	11:K:71:ILE:HD11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:39:DG:H2''	14:N:40:DG:C8	2.54	0.43
13:M:664:LEU:HD12	13:M:664:LEU:O	2.19	0.43
2:B:258:ALA:HB2	2:B:269:ILE:CD1	2.49	0.42
2:B:137:GLU:O	2:B:137:GLU:HG2	2.19	0.42
2:B:388:TYR:CE1	2:B:505:LEU:HD21	2.54	0.42
2:B:226:GLU:O	2:B:226:GLU:CD	2.62	0.42
1:A:878:THR:HG21	1:A:880:ARG:HE	1.83	0.42
19:Z:588:ASP:OD1	19:Z:592:ASN:N	2.50	0.42
19:Z:492:ILE:HD12	19:Z:495:VAL:CG2	2.49	0.42
19:Z:561:LEU:CD1	19:Z:565:GLY:HA2	2.49	0.42
1:A:33:ARG:HG2	2:B:1139:GLY:HA2	2.02	0.42
14:N:22:DG:H5'	14:N:22:DG:C8	2.54	0.42
17:T:22:DC:H2'	17:T:23:DC:C6	2.55	0.42
8:H:37:MET:HE3	8:H:127:GLY:HA3	2.00	0.42
14:N:42:DA:C8	14:N:42:DA:H5'	2.55	0.42
19:Z:561:LEU:HD21	19:Z:637:VAL:HG12	2.01	0.42
1:A:865:ILE:HG21	2:B:1092:ASP:OD2	2.19	0.41
3:C:44:ILE:HD11	3:C:238:SER:CB	2.49	0.41
18:Y:59:GLY:HA3	18:Y:87:VAL:HG23	2.02	0.41
14:N:40:DG:H2''	14:N:41:DG:C8	2.55	0.41
1:A:1180:ASN:O	1:A:1183:SER:OG	2.35	0.41
19:Z:200:PHE:CD1	19:Z:200:PHE:C	2.97	0.41
1:A:1374:VAL:CG1	1:A:1411:LEU:HD21	2.49	0.41
2:B:184:TYR:CE1	2:B:191:GLU:HG2	2.55	0.41
14:N:38:DT:O4	17:T:6:DC:N4	2.53	0.41
1:A:539:GLN:HG3	2:B:791:GLU:HG2	2.02	0.41
13:M:444:ASP:OD1	13:M:444:ASP:N	2.54	0.41
2:B:529:MET:HE2	2:B:702:MET:HG3	2.02	0.41
2:B:830:GLU:OE2	2:B:870:THR:OG1	2.38	0.41
13:M:322:ARG:HA	13:M:326:ALA:HB3	2.03	0.41
13:M:548:GLU:HA	13:M:551:ARG:HE	1.85	0.41
17:T:19:DG:H2''	17:T:20:DC:C5	2.56	0.41
18:Y:69:SER:O	18:Y:72:SER:OG	2.31	0.41
1:A:1007:ILE:HD12	1:A:1007:ILE:HA	1.98	0.40
13:M:569:LEU:HD22	13:M:569:LEU:N	2.36	0.40
2:B:225:LEU:HD12	2:B:225:LEU:HA	1.96	0.40
8:H:10:PHE:CE1	8:H:32:SER:HB2	2.56	0.40
13:M:895:ASN:HB3	19:Z:573:GLN:HB3	2.04	0.40
1:A:365:THR:HG22	1:A:482:PHE:CE2	2.57	0.40
1:A:530:SER:O	1:A:532:ARG:HG3	2.22	0.40
1:A:872:MET:HE2	1:A:1084:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:626:LEU:HD23	2:B:662:VAL:HG12	2.04	0.40
16:Q:29:CYS:HB3	16:Q:53:CYS:HB3	2.02	0.40
17:T:29:DG:H2'	17:T:30:DG:C8	2.56	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	1386/1970 (70%)	1334 (96%)	52 (4%)	0	100	100
2	B	1125/1174 (96%)	1070 (95%)	55 (5%)	0	100	100
3	C	255/292 (87%)	248 (97%)	7 (3%)	0	100	100
4	D	125/142 (88%)	122 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	77/127 (61%)	74 (96%)	3 (4%)	0	100	100
7	G	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	111/125 (89%)	107 (96%)	4 (4%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	37 (84%)	7 (16%)	0	100	100
13	M	794/1726 (46%)	758 (96%)	36 (4%)	0	100	100
16	Q	60/83 (72%)	58 (97%)	2 (3%)	0	100	100
18	Y	114/117 (97%)	114 (100%)	0	0	100	100
19	Z	464/1087 (43%)	449 (97%)	15 (3%)	0	100	100
All	All	5255/7617 (69%)	5055 (96%)	200 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1233/1748 (70%)	1233 (100%)	0	100	100
2	B	993/1028 (97%)	993 (100%)	0	100	100
3	C	236/268 (88%)	236 (100%)	0	100	100
4	D	110/126 (87%)	110 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	69/111 (62%)	69 (100%)	0	100	100
7	G	146/153 (95%)	146 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	102/112 (91%)	102 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	735/1522 (48%)	733 (100%)	2 (0%)	91	95
16	Q	57/76 (75%)	57 (100%)	0	100	100
18	Y	102/103 (99%)	102 (100%)	0	100	100
19	Z	420/940 (45%)	420 (100%)	0	100	100
All	All	4726/6727 (70%)	4724 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	283	THR
13	M	1306	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	311	GLN
1	A	353	ASN
1	A	711	GLN
1	A	757	GLN
1	A	935	GLN
1	A	995	HIS
1	A	1093	GLN
1	A	1417	HIS
2	B	56	GLN
2	B	144	HIS
2	B	344	GLN
2	B	387	HIS
2	B	471	ASN
2	B	1145	GLN
5	E	30	GLN
5	E	148	HIS
7	G	28	GLN
9	I	22	ASN
9	I	100	HIS
11	K	55	GLN
13	M	281	HIS
13	M	370	HIS
13	M	389	HIS
13	M	427	GLN
13	M	604	GLN
13	M	895	ASN
13	M	912	GLN
13	M	929	GLN
13	M	1151	ASN
18	Y	75	GLN
19	Z	616	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/21 (95%)	11 (55%)	3 (15%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	2	A

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Mol	Chain	Res	Type
15	P	3	C
15	P	4	C
15	P	5	G
15	P	6	G
15	P	7	A
15	P	8	G
15	P	9	A
15	P	10	G
15	P	11	G
15	P	13	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	2	A
15	P	4	C
15	P	12	G

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 11 ligands modelled in this entry, 11 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.

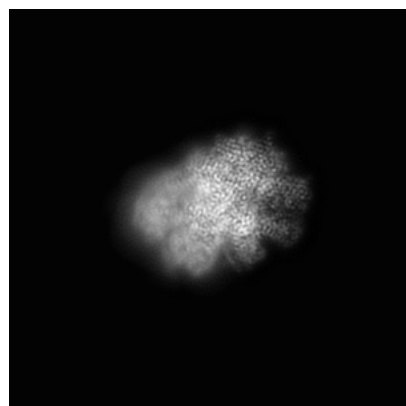
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38607. These allow visual inspection of the internal detail of the map and identification of artifacts.

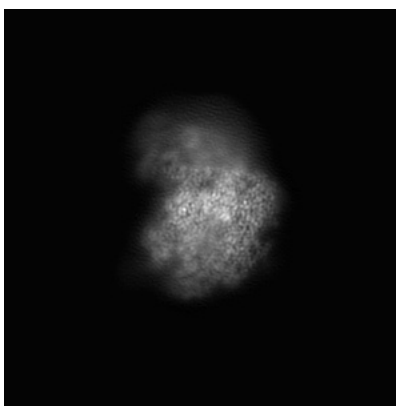
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

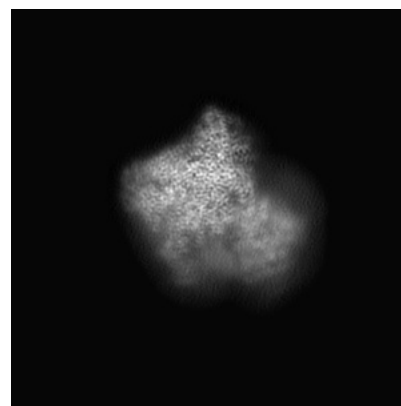
6.1.1 Primary map



X

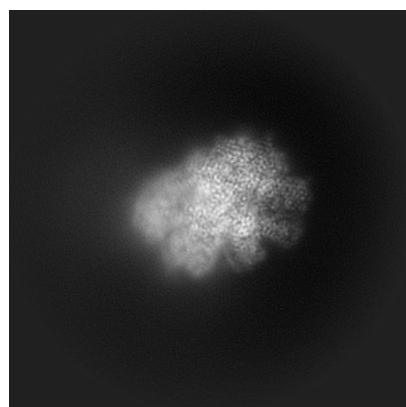


Y

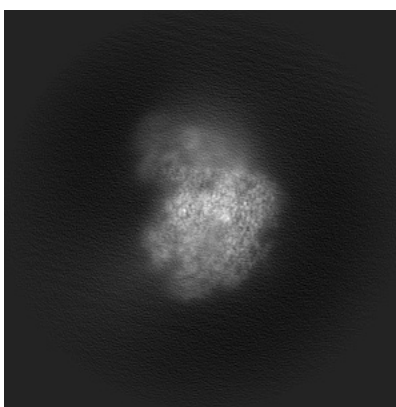


Z

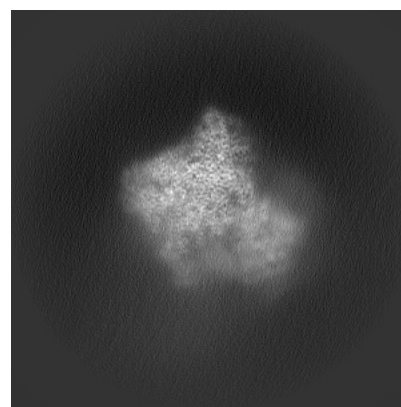
6.1.2 Raw map



X



Y

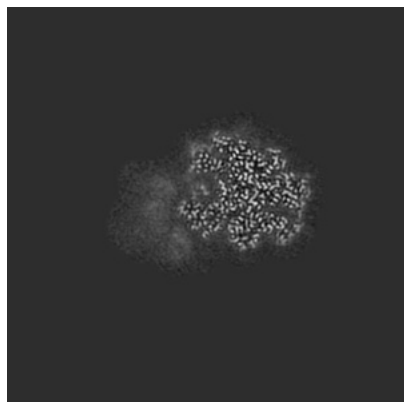


Z

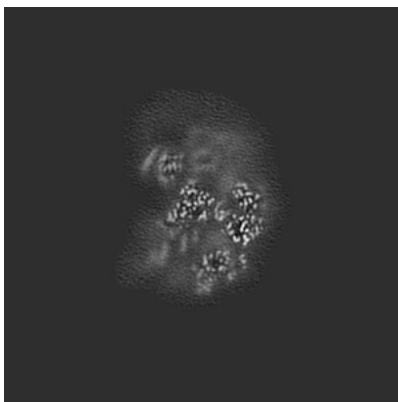
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

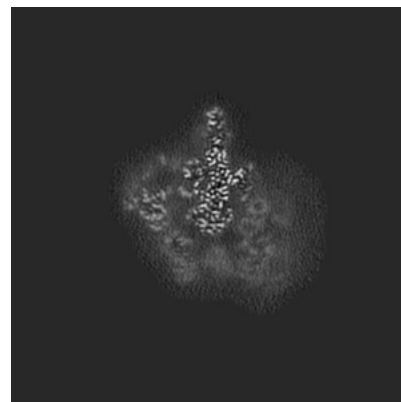
6.2.1 Primary map



X Index: 180

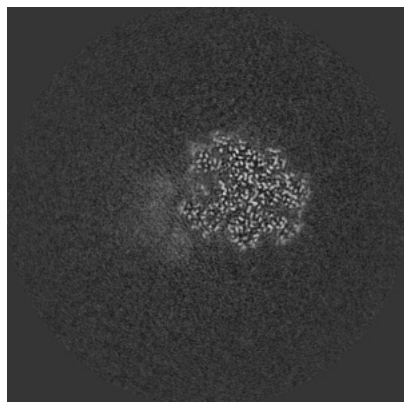


Y Index: 180

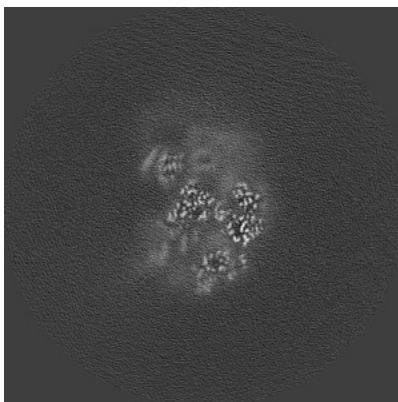


Z Index: 180

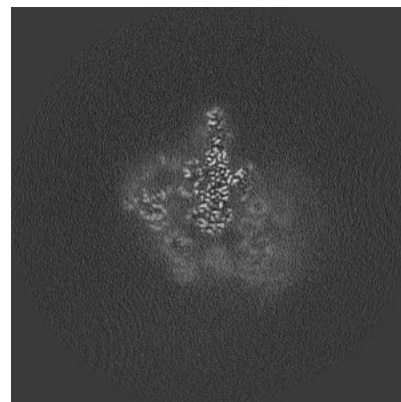
6.2.2 Raw map



X Index: 180



Y Index: 180

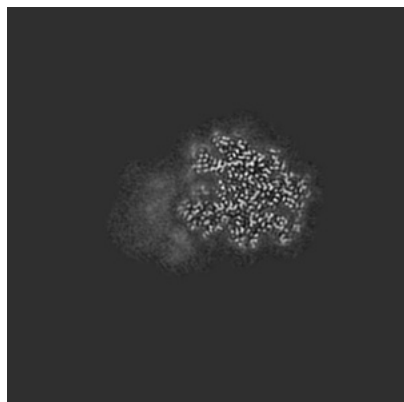


Z Index: 180

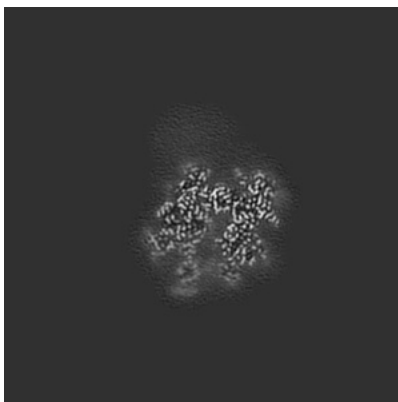
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

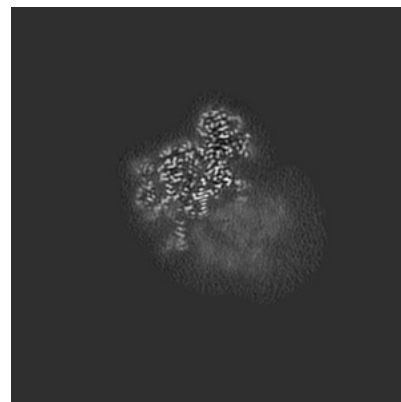
6.3.1 Primary map



X Index: 181

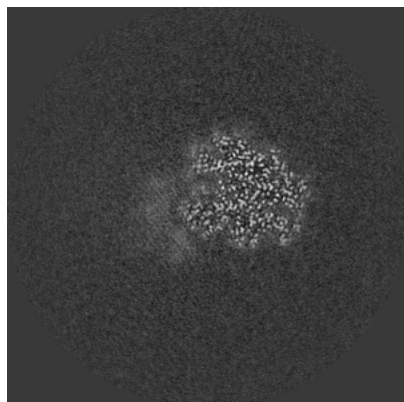


Y Index: 211

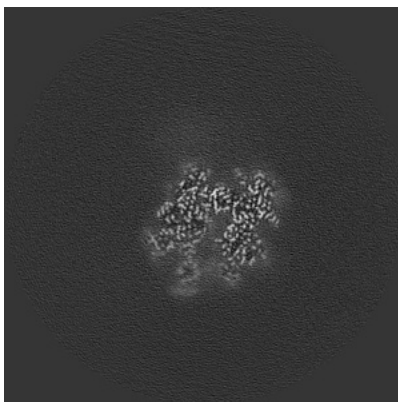


Z Index: 201

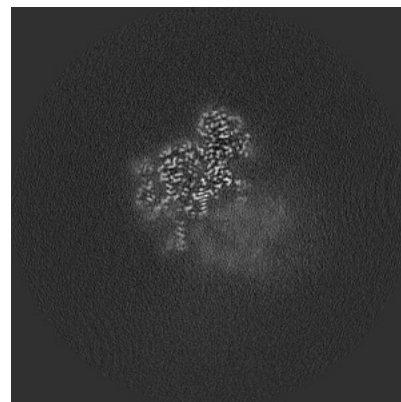
6.3.2 Raw map



X Index: 181



Y Index: 211

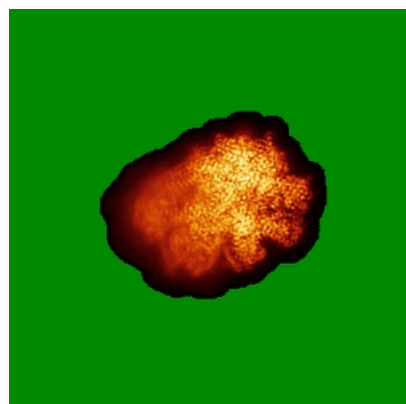


Z Index: 201

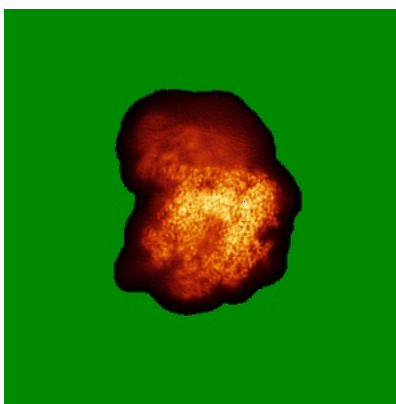
The images above show the largest variance slices of the map in three orthogonal directions.

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

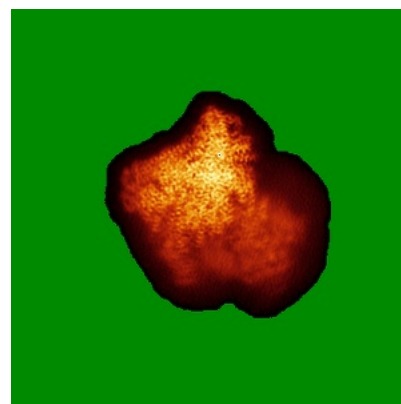
6.4.1 Primary map



X

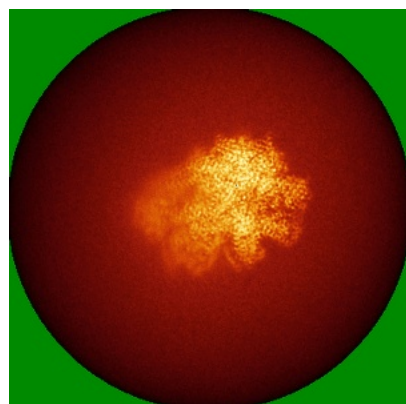


Y

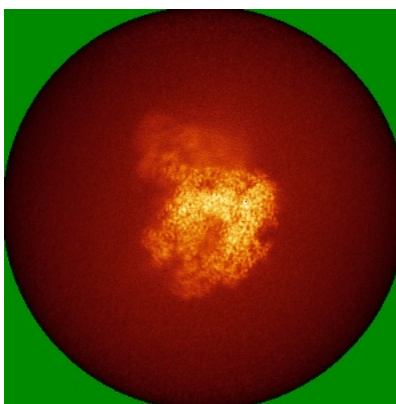


Z

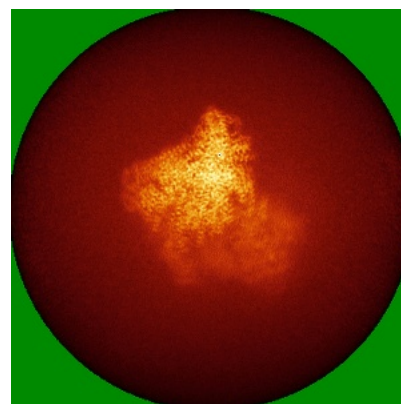
6.4.2 Raw map



X



Y

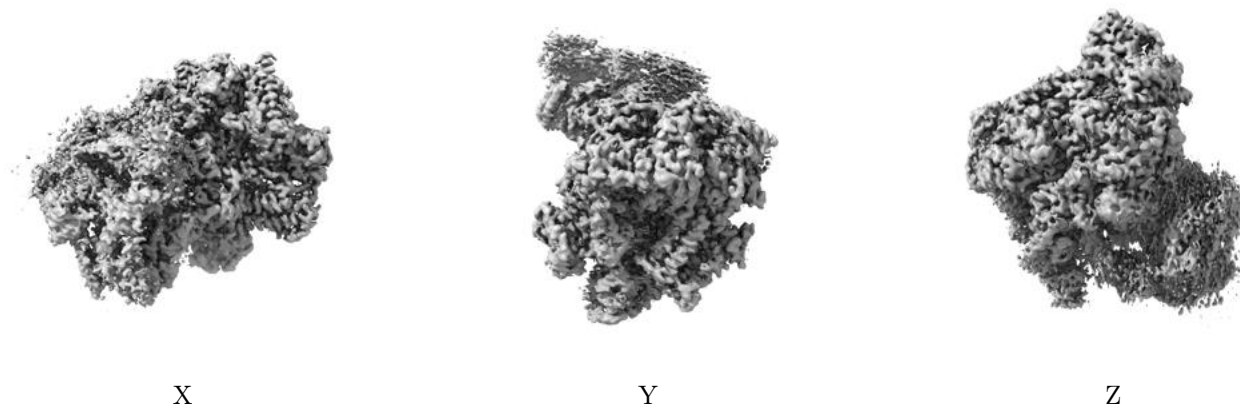


Z

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.

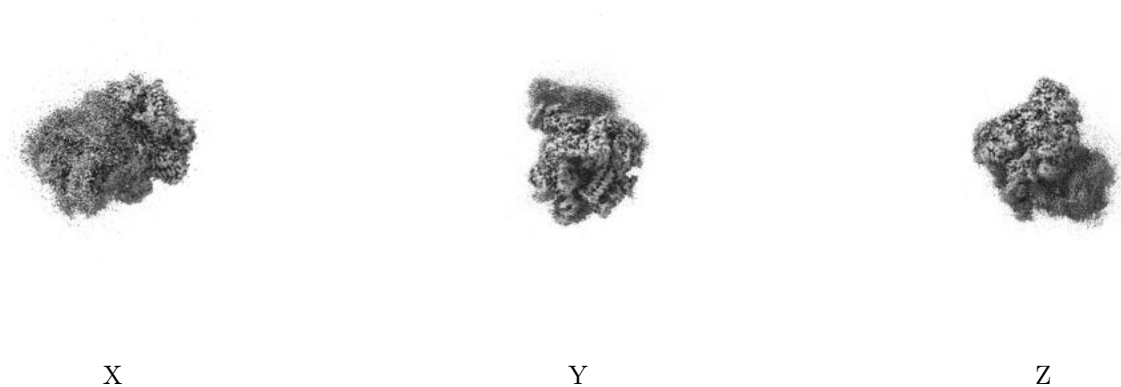
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00864. 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.

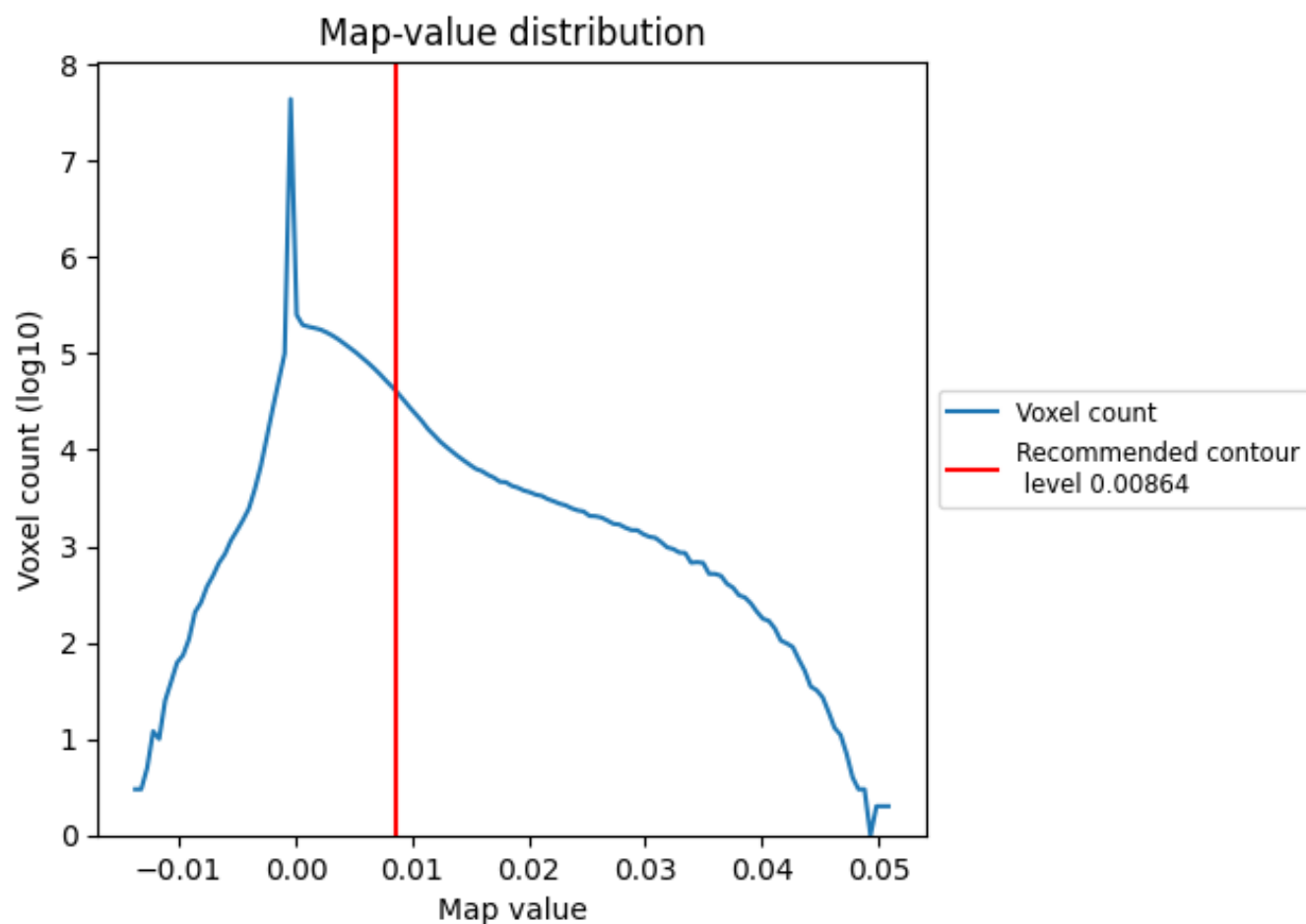
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

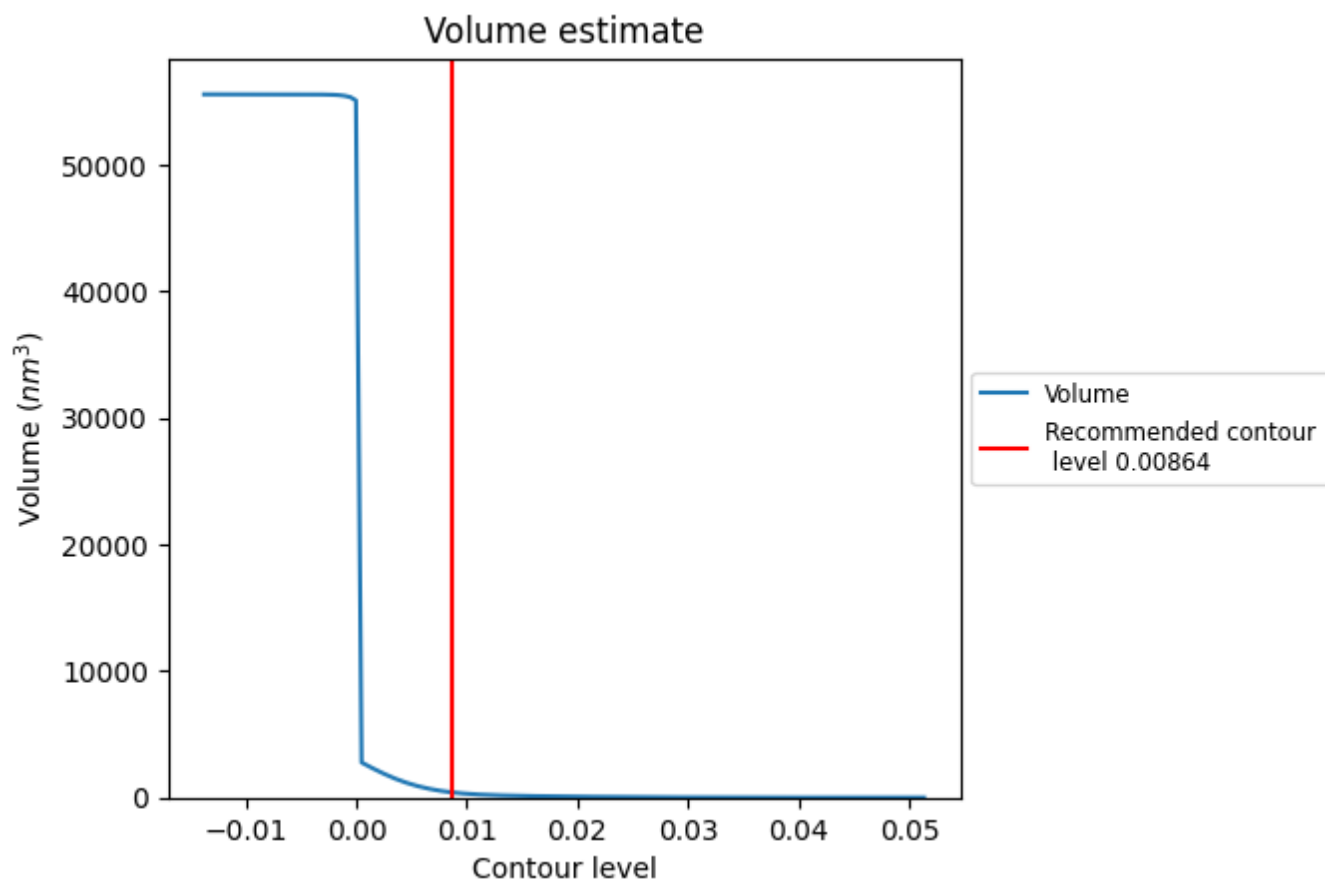
This section contains the results of statistical analysis of the map.

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.

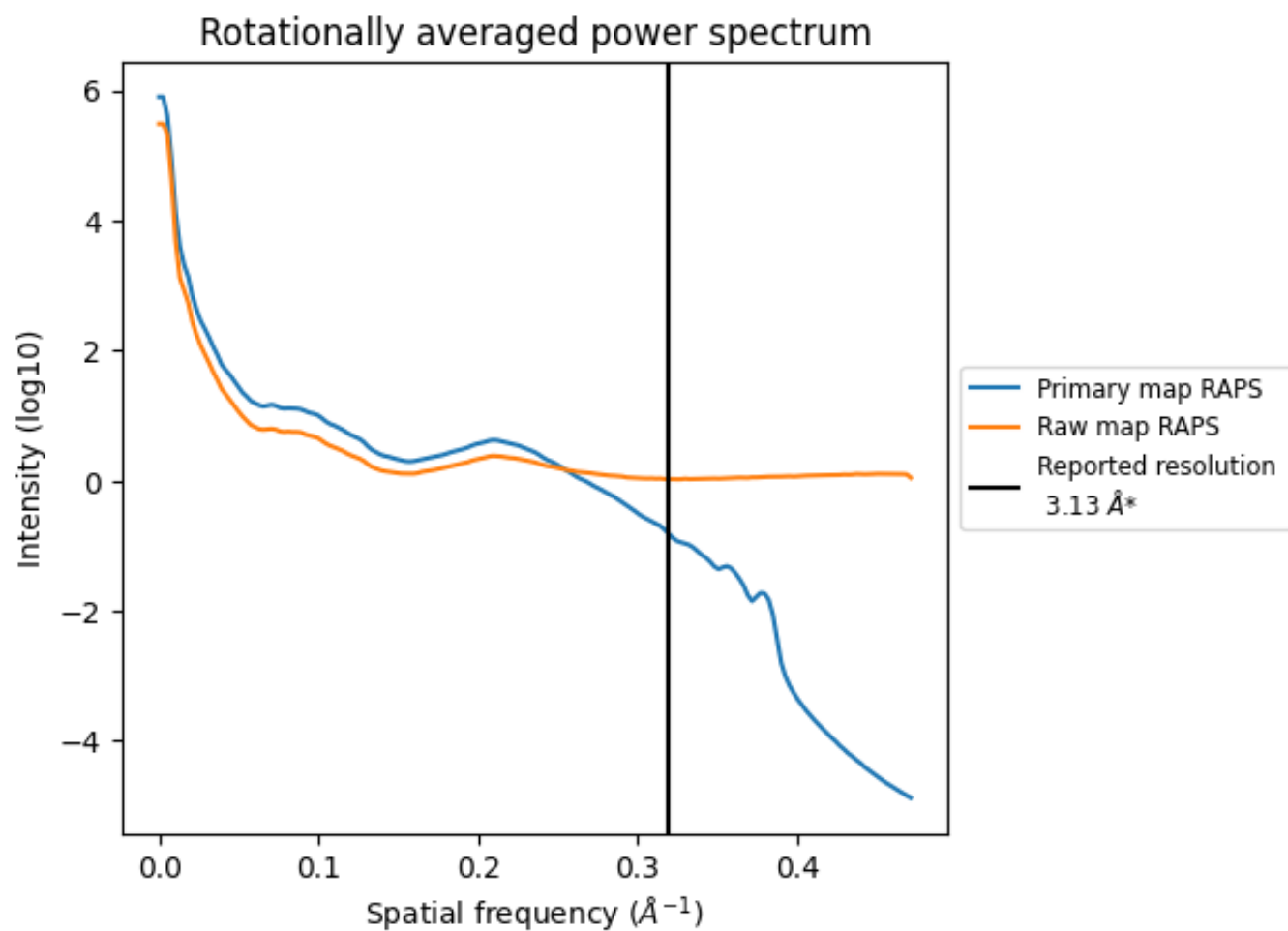
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm³; this corresponds to an approximate mass of 373 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 ⓘ

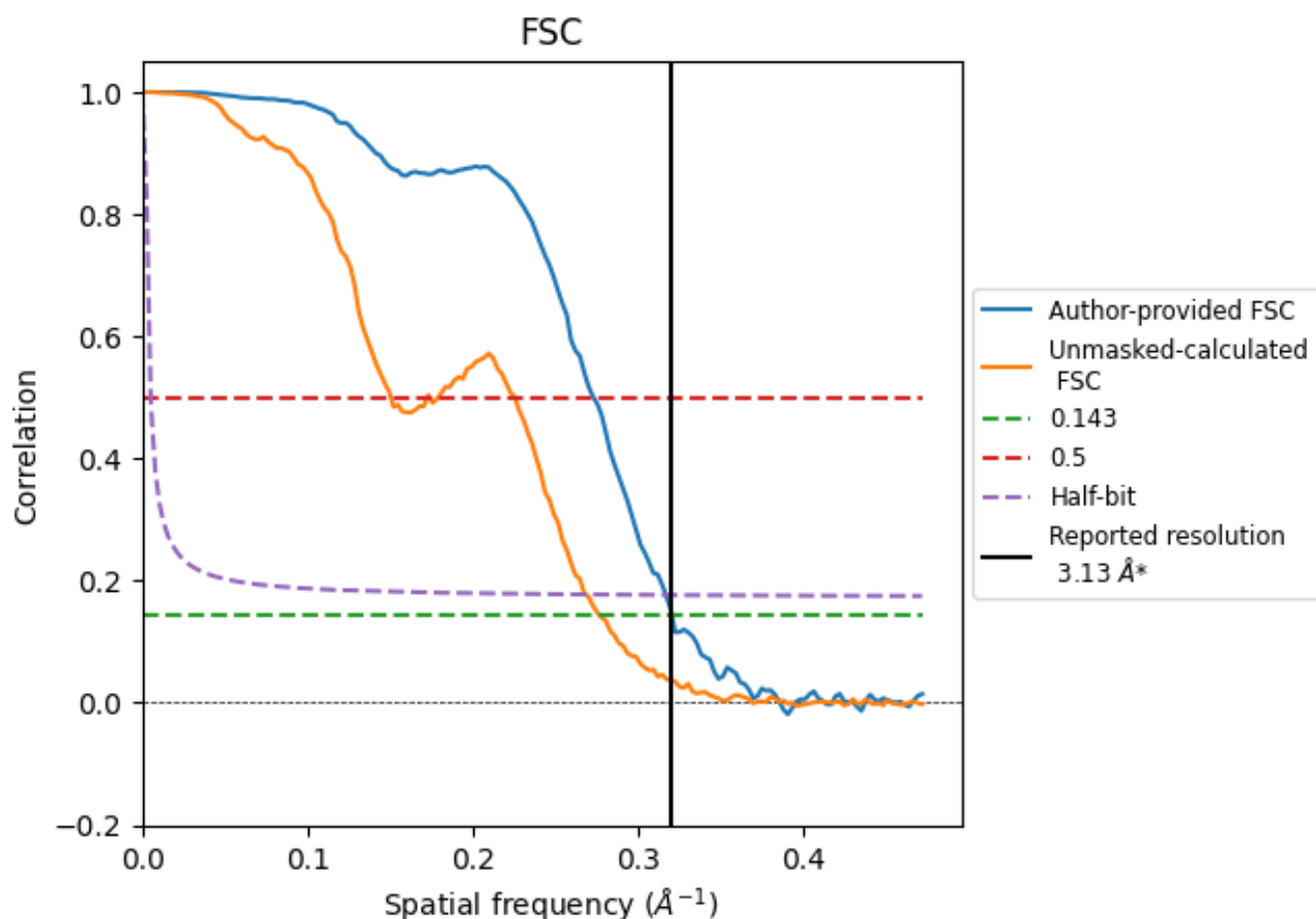


*Reported resolution corresponds to spatial frequency of 0.319 \AA^{-1}

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 0.319 \AA^{-1}

8.2 Resolution estimates [i](#)

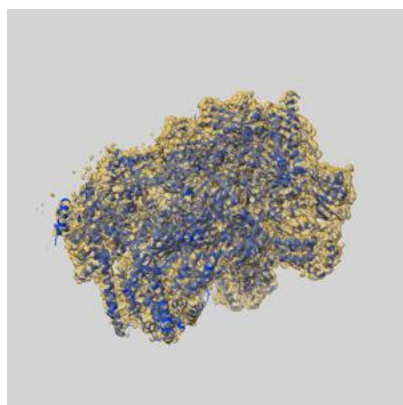
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.12	3.66	3.16
Unmasked-calculated*	3.61	6.65	3.73

*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 3.61 differs from the reported value 3.13 by more than 10 %

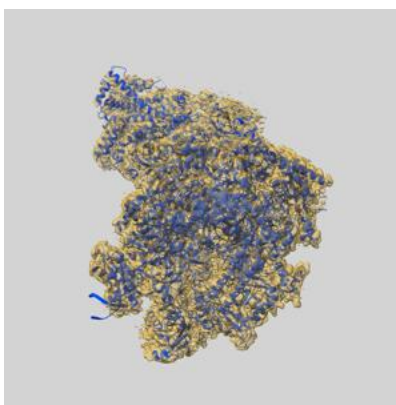
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38607 and PDB model 8XRM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

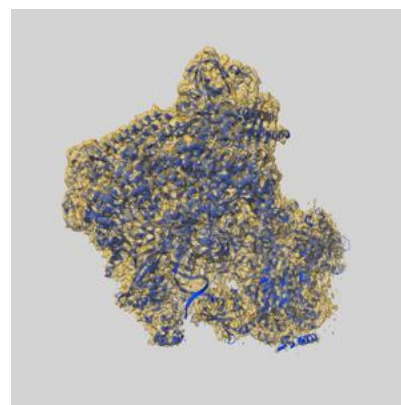
9.1 Map-model overlay [i](#)



X



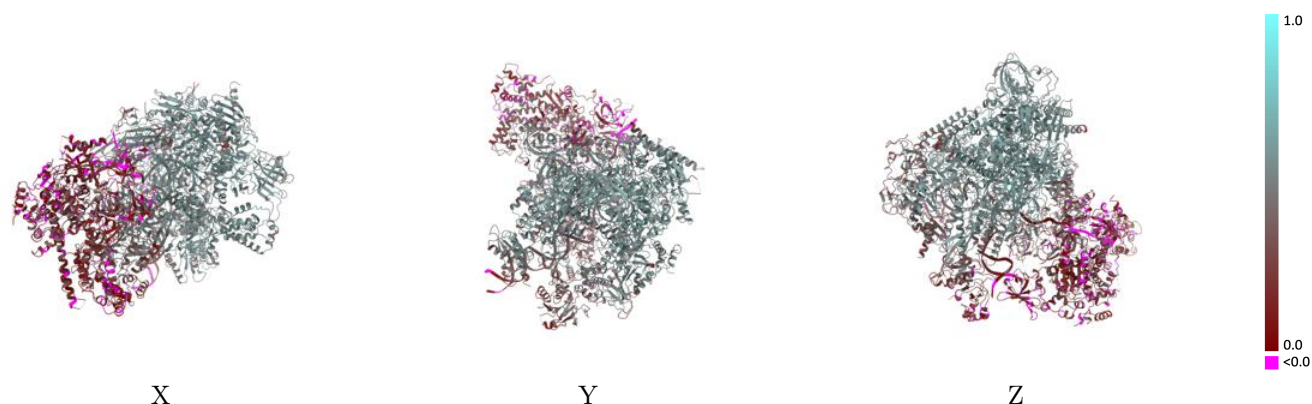
Y



Z

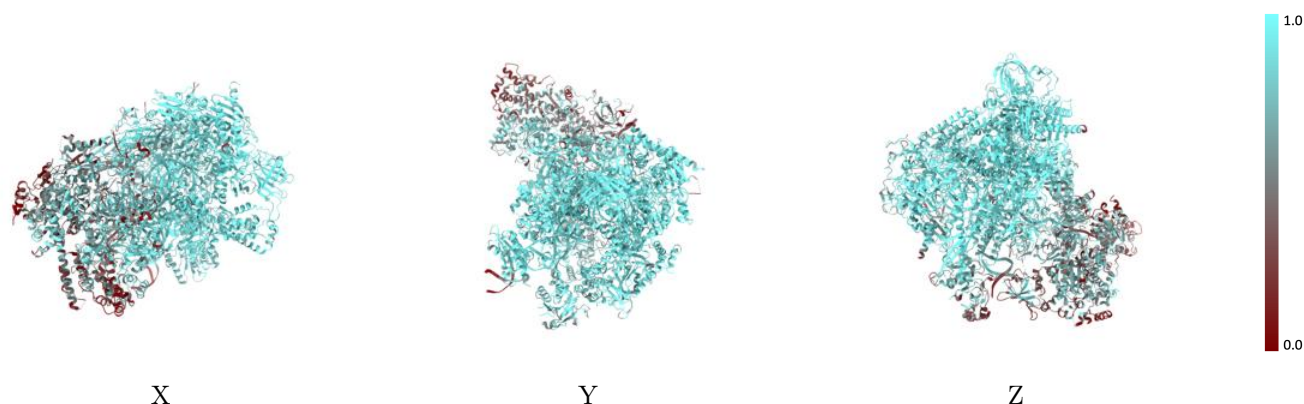
The images above show the 3D surface view of the map at the recommended contour level 0.00864 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



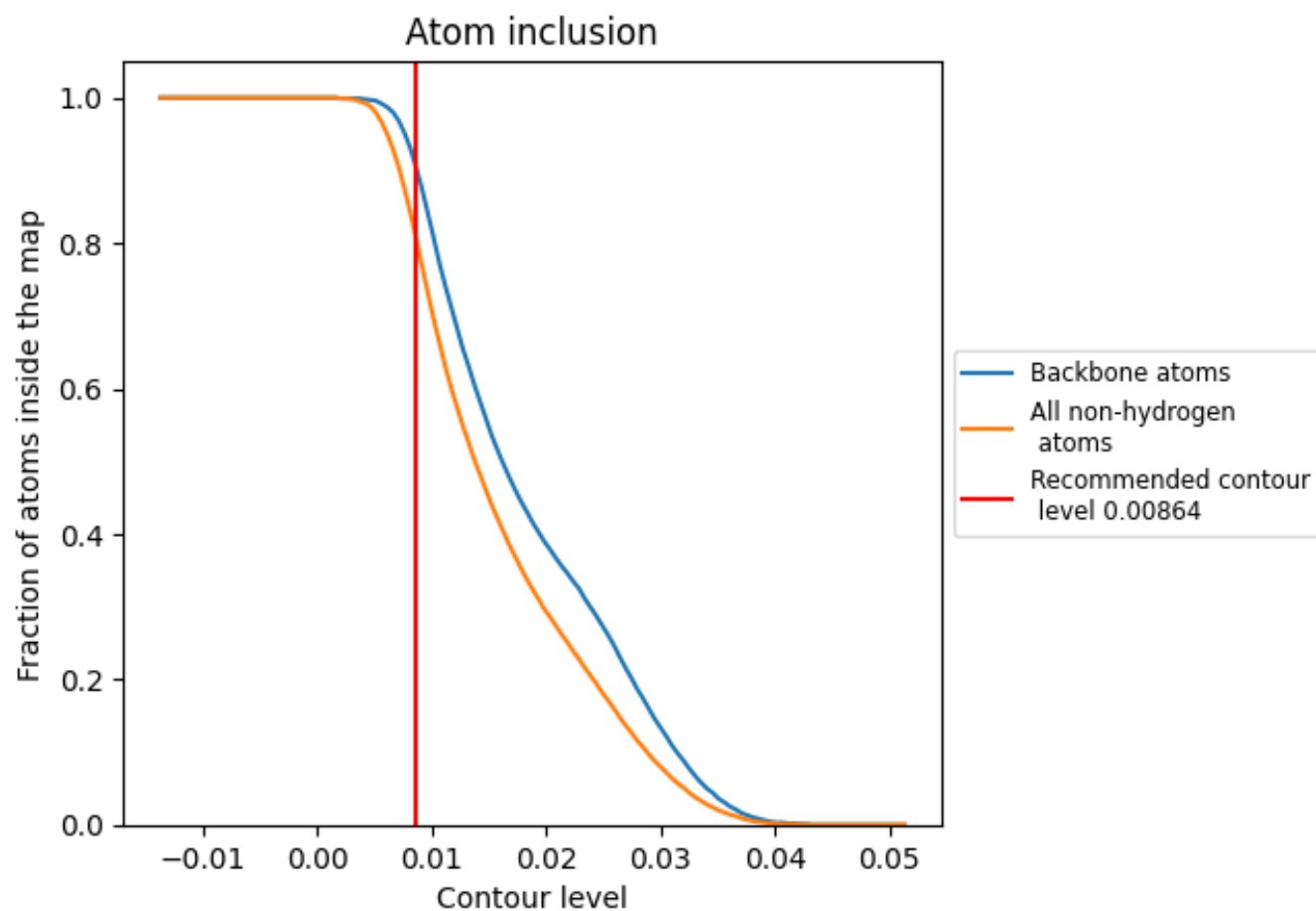
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00864).









































9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.00864) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.4110
A	 0.9260	 0.5170
B	 0.9350	 0.5260
C	 0.9240	 0.5380
D	 0.7110	 0.3140
E	 0.8970	 0.4940
F	 0.9470	 0.5600
G	 0.8480	 0.4430
H	 0.9240	 0.5310
I	 0.7640	 0.3710
J	 0.9560	 0.5650
K	 0.9520	 0.5550
L	 0.8010	 0.4440
M	 0.4990	 0.1600
N	 0.6950	 0.2430
P	 0.7920	 0.2870
Q	 0.7610	 0.3480
T	 0.8140	 0.3350
Y	 0.5310	 0.1970
Z	 0.5680	 0.1890

