



wwPDB EM Validation Summary Report ⓘ

Jun 11, 2025 – 01:03 AM JST

PDB ID : 9J0O / pdb_00009j0o
EMDB ID : EMD-61059
Title : Arrested elongation complex of mammalian RNA polymerase II with nucleosome (AEC1-nuc)
Authors : Naganuma, M.; Kujirai, T.; Ehara, H.; Uejima, T.; Ito, T.; Goto, M.; Aoki, M.; Henmi, M.; Miyamoto-Kohno, S.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2024-08-02
Resolution : 3.30 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.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

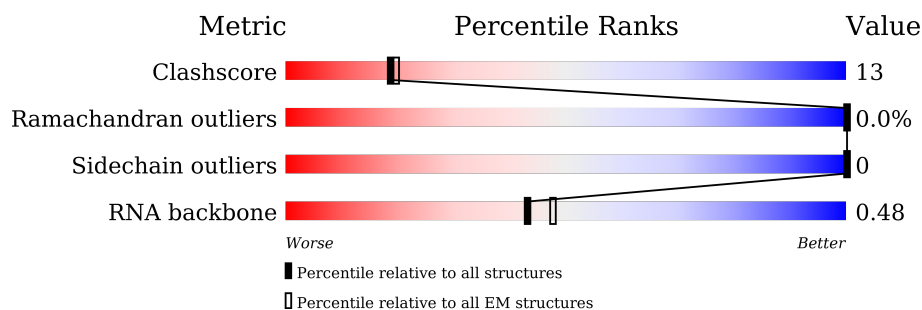
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.















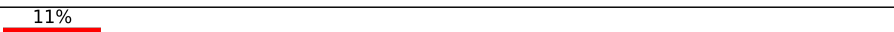

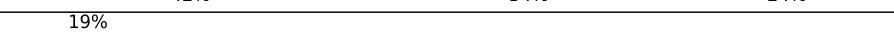

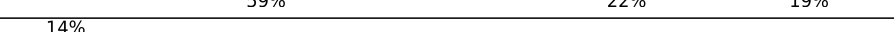





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	271	
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	Y	118	
14	Z	1107	
15	N	198	
16	P	16	
17	T	198	
18	a	136	
18	e	136	
19	b	103	
19	f	103	
20	c	130	
20	g	130	
21	d	126	
21	h	126	
22	U	528	
23	W	611	
24	V	580	
25	X	404	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 59777 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0
			11050	6952	1982	2047	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1121	Total	C	N	O	S	0	0
			8971	5679	1575	1653	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			1004	630	170	200	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			626	401	106	114	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	149	Total	C	N	O	S	0	0
			1197	759	195	238	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			942	582	168	181	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 RPB12.

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 Transcription elongation factor SPT4.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	0	SER	-	expression tag	UNP P63272

- Molecule 14 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	480	Total	C	N	O	S	0	0
			3837	2439	676	705	17		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1088	LYS	-	expression tag	UNP O00267
Z	1089	GLU	-	expression tag	UNP O00267
Z	1090	THR	-	expression tag	UNP O00267
Z	1091	ALA	-	expression tag	UNP O00267
Z	1092	ALA	-	expression tag	UNP O00267
Z	1093	ALA	-	expression tag	UNP O00267
Z	1094	LYS	-	expression tag	UNP O00267
Z	1095	PHE	-	expression tag	UNP O00267
Z	1096	GLU	-	expression tag	UNP O00267
Z	1097	ARG	-	expression tag	UNP O00267
Z	1098	GLN	-	expression tag	UNP O00267
Z	1099	HIS	-	expression tag	UNP O00267
Z	1100	MET	-	expression tag	UNP O00267
Z	1101	ASP	-	expression tag	UNP O00267
Z	1102	SER	-	expression tag	UNP O00267
Z	1103	SER	-	expression tag	UNP O00267
Z	1104	THR	-	expression tag	UNP O00267
Z	1105	SER	-	expression tag	UNP O00267
Z	1106	ALA	-	expression tag	UNP O00267
Z	1107	ALA	-	expression tag	UNP O00267

- Molecule 15 is a DNA chain called NON-TEMPLATE DNA (180-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	180	Total	C	N	O	P	0	0
			3706	1762	647	1117	180		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	16	Total	C	N	O	P	0	0
			335	150	52	117	16		

- Molecule 17 is a DNA chain called TEMPLATE DNA (191-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	191	Total	C	N	O	P	0	0
			3899	1848	756	1105	190		

- Molecule 18 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
18	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

- Molecule 19 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
19	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 20 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	c	103	Total	C	N	O	0	0
			796	502	155	139		
20	g	105	Total	C	N	O	0	0
			810	511	158	141		

- Molecule 21 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
21	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 22 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	183	Total	C	N	O	S	0	0
			1410	895	239	269	7		

- Molecule 23 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	543	Total	C	N	O	S	0	0
			4308	2753	721	810	24		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	591	GLY	-	expression tag	UNP Q8IXH7
W	592	SER	-	expression tag	UNP Q8IXH7
W	593	SER	-	expression tag	UNP Q8IXH7
W	594	GLY	-	expression tag	UNP Q8IXH7
W	595	SER	-	expression tag	UNP Q8IXH7
W	596	SER	-	expression tag	UNP Q8IXH7
W	597	GLY	-	expression tag	UNP Q8IXH7
W	598	LEU	-	expression tag	UNP Q8IXH7
W	599	GLU	-	expression tag	UNP Q8IXH7
W	600	VAL	-	expression tag	UNP Q8IXH7
W	601	LEU	-	expression tag	UNP Q8IXH7
W	602	PHE	-	expression tag	UNP Q8IXH7
W	603	GLN	-	expression tag	UNP Q8IXH7
W	604	GLY	-	expression tag	UNP Q8IXH7
W	605	PRO	-	expression tag	UNP Q8IXH7
W	606	HIS	-	expression tag	UNP Q8IXH7
W	607	HIS	-	expression tag	UNP Q8IXH7
W	608	HIS	-	expression tag	UNP Q8IXH7
W	609	HIS	-	expression tag	UNP Q8IXH7
W	610	HIS	-	expression tag	UNP Q8IXH7
W	611	HIS	-	expression tag	UNP Q8IXH7

- Molecule 24 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	548	Total	C	N	O	S	0	0
			4396	2818	749	804	25		

- Molecule 25 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	35	Total	C	N	O	S	0	0
			281	185	48	47	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-23	MET	-	initiating methionine	UNP P18615
X	-22	ASP	-	expression tag	UNP P18615
X	-21	TYR	-	expression tag	UNP P18615
X	-20	LYS	-	expression tag	UNP P18615
X	-19	ASP	-	expression tag	UNP P18615
X	-18	ASP	-	expression tag	UNP P18615
X	-17	ASP	-	expression tag	UNP P18615
X	-16	ASP	-	expression tag	UNP P18615
X	-15	LYS	-	expression tag	UNP P18615
X	-14	LEU	-	expression tag	UNP P18615
X	-13	GLU	-	expression tag	UNP P18615
X	-12	VAL	-	expression tag	UNP P18615
X	-11	LEU	-	expression tag	UNP P18615
X	-10	PHE	-	expression tag	UNP P18615
X	-9	GLN	-	expression tag	UNP P18615
X	-8	GLY	-	expression tag	UNP P18615
X	-7	PRO	-	expression tag	UNP P18615
X	-6	GLY	-	expression tag	UNP P18615
X	-5	SER	-	expression tag	UNP P18615
X	-4	SER	-	expression tag	UNP P18615
X	-3	GLY	-	expression tag	UNP P18615
X	-2	SER	-	expression tag	UNP P18615
X	-1	SER	-	expression tag	UNP P18615
X	0	GLY	-	expression tag	UNP P18615

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	C	1	Total	Zn	0
			1	1	
26	I	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total 1	Zn 1	0
26	L	1	Total 1	Zn 1	0
26	Y	1	Total 1	Zn 1	0

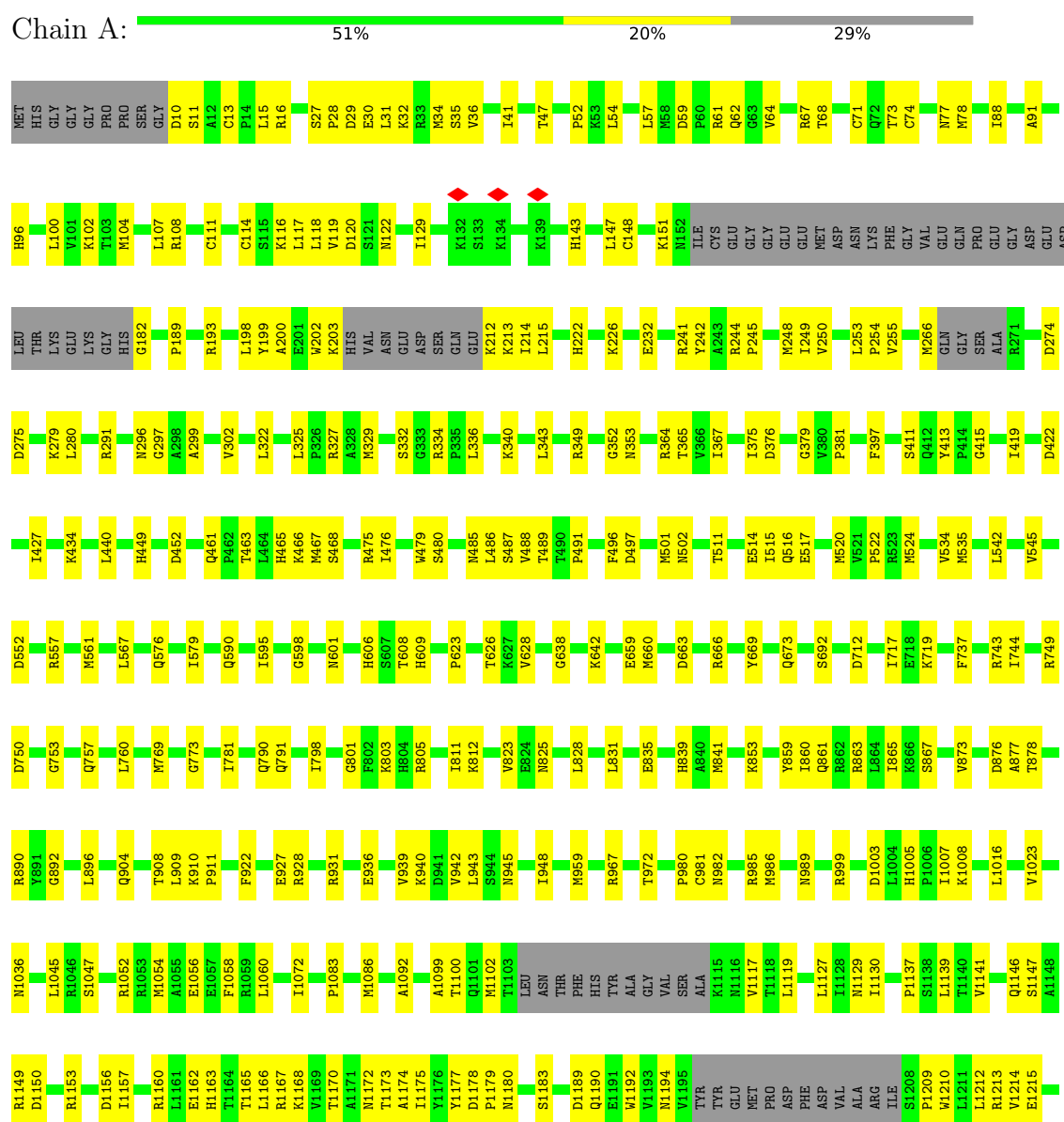
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

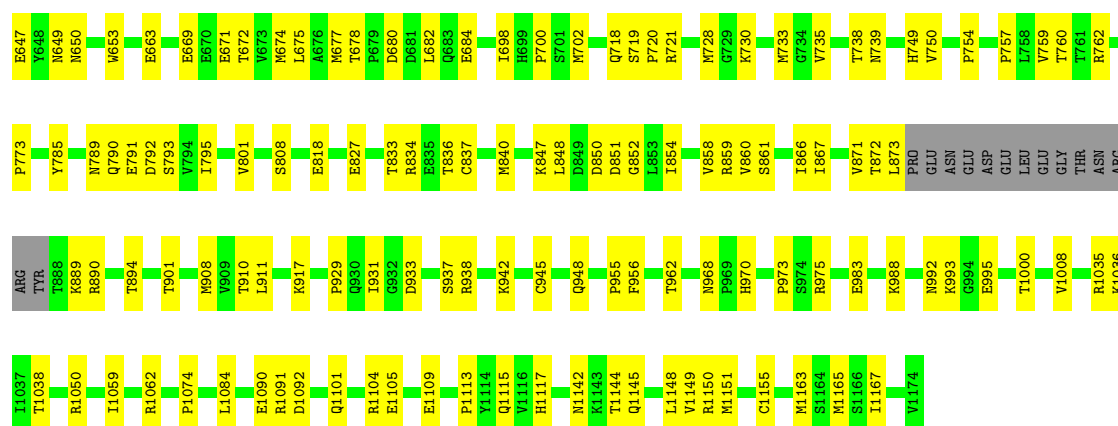
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total 1	Mg 1	0

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.

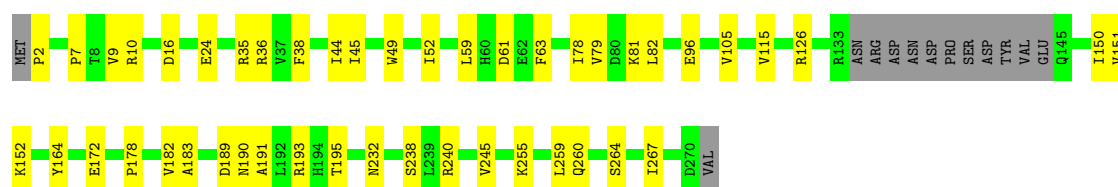
• Molecule 1: DNA-directed RNA polymerase subunit





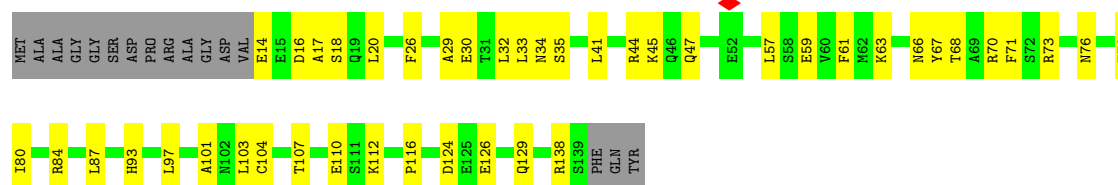
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 78% 17% 5%



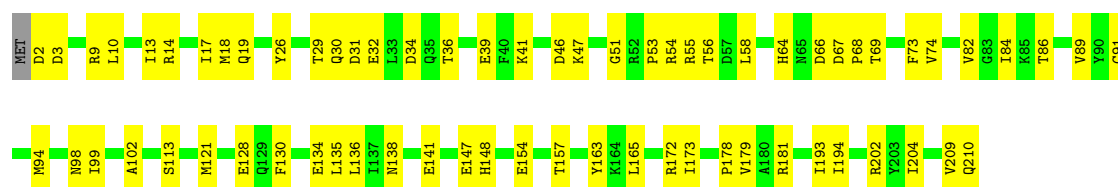
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 58% 31% 11%



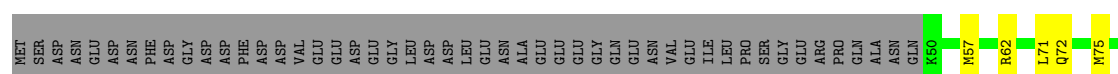
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 67% 32%



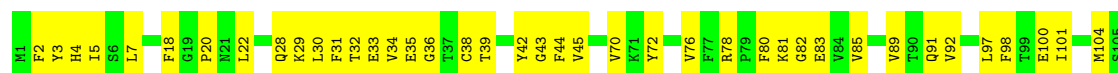
• Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 50% 11% 39%

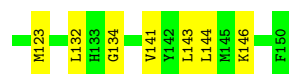




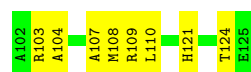
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



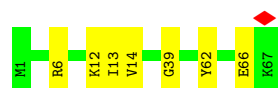
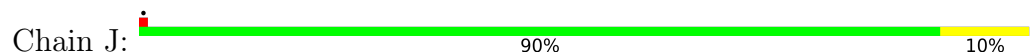
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



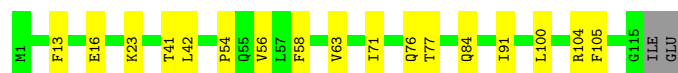
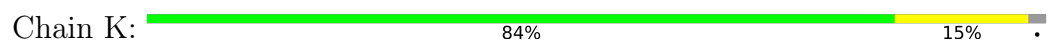
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



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



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



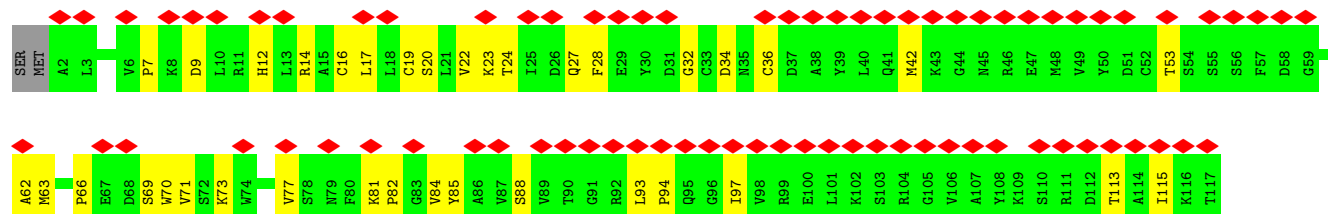
- Molecule 12: RPB12

Chain L: 




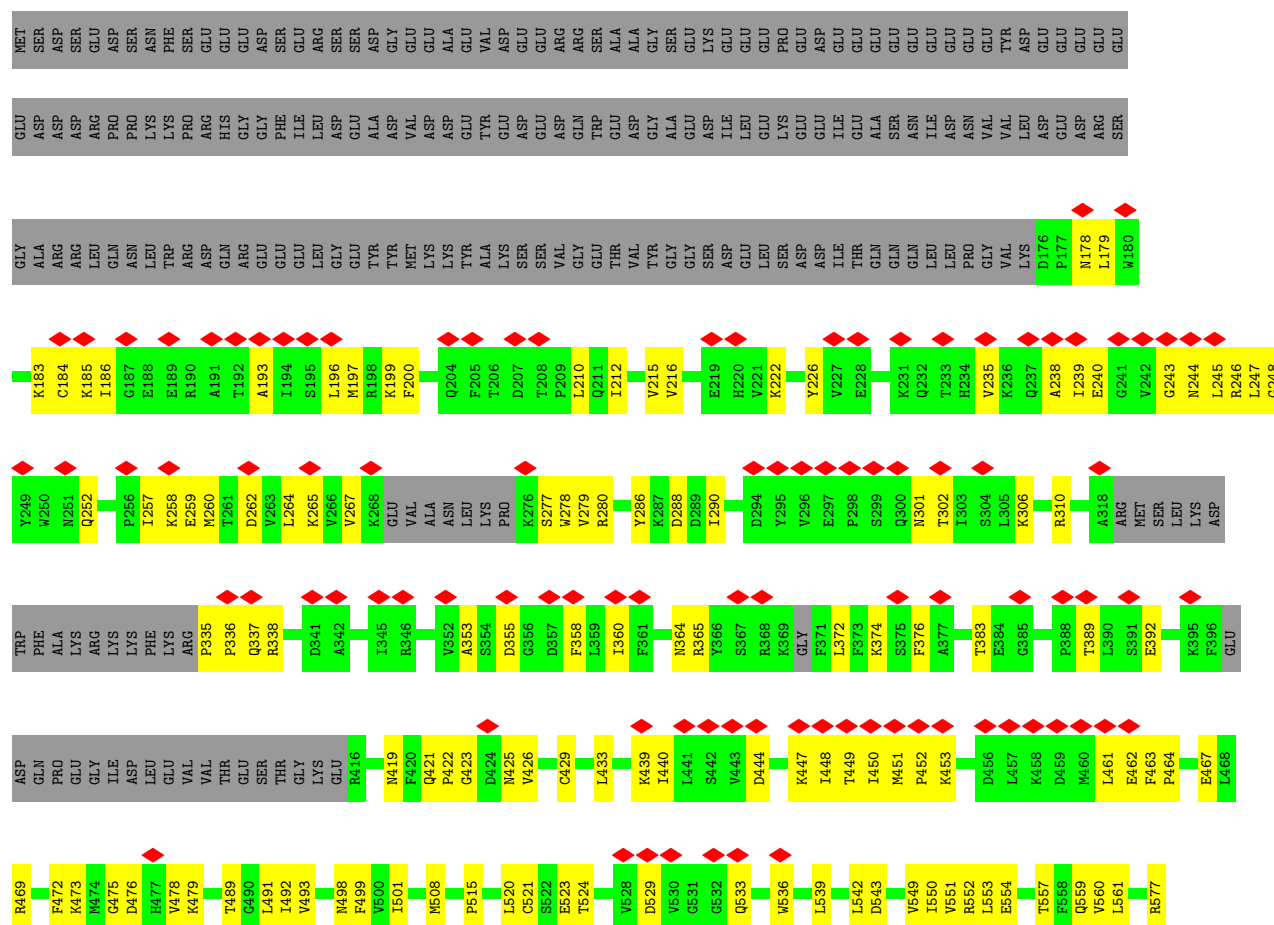
- Molecule 13: Transcription elongation factor SPT4

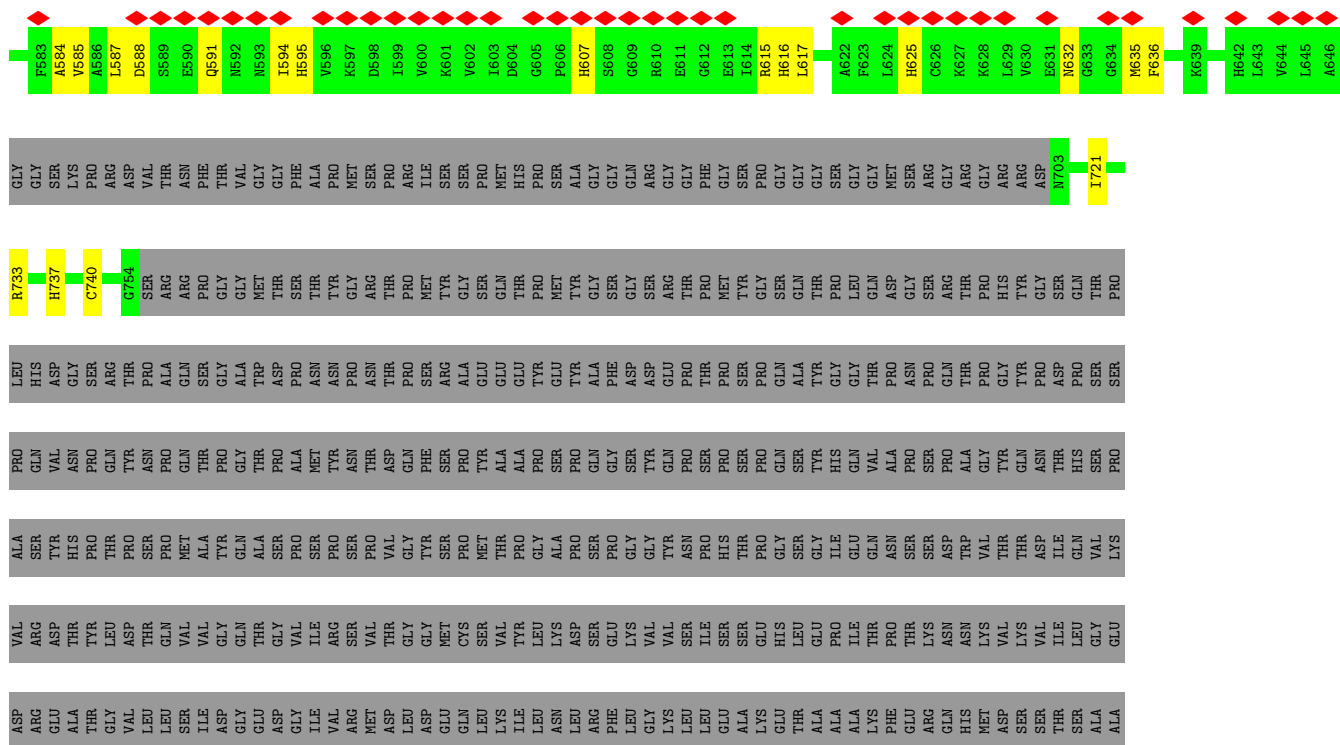
Chain Y: 



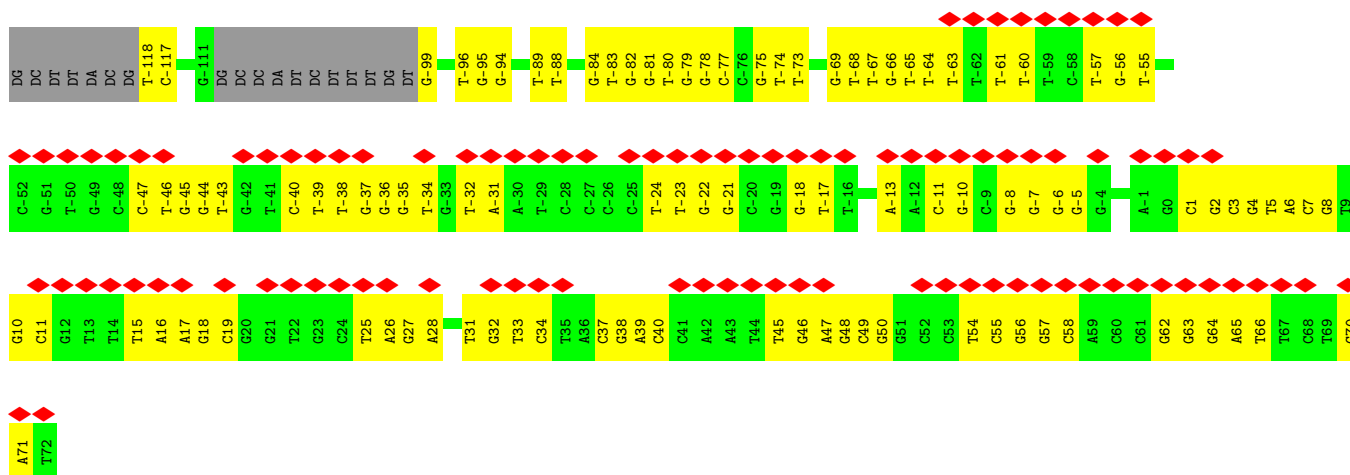
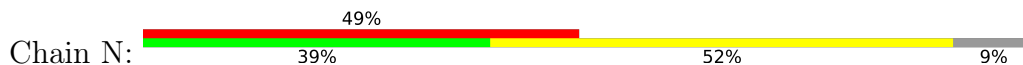
- Molecule 14: Transcription elongation factor SPT5

Chain Z: 

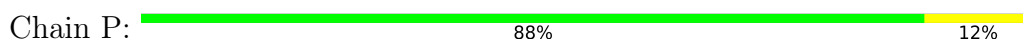




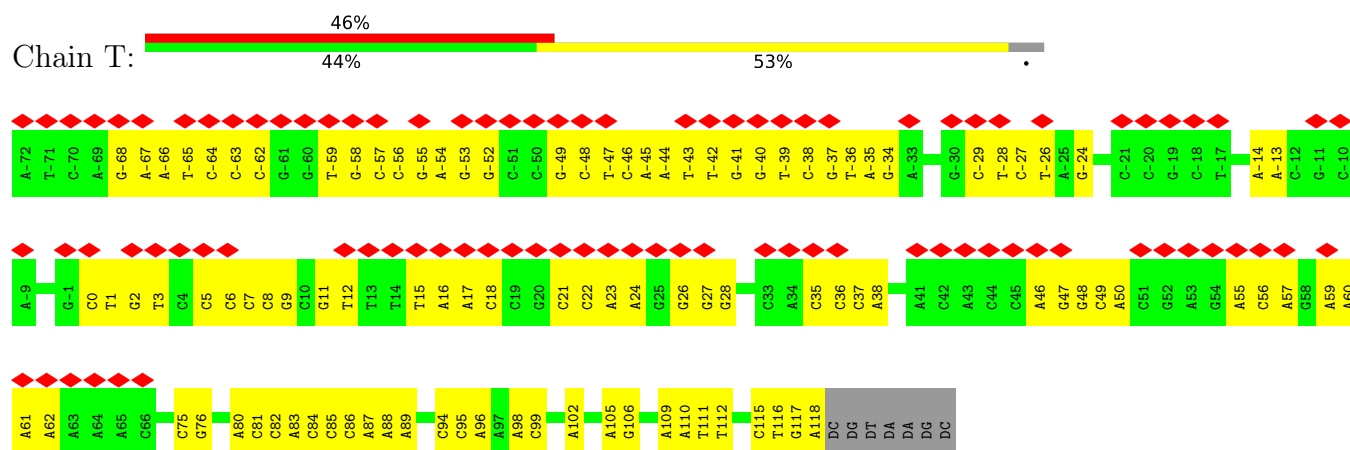
- Molecule 15: NON-TEMPLATE DNA (180-MER)



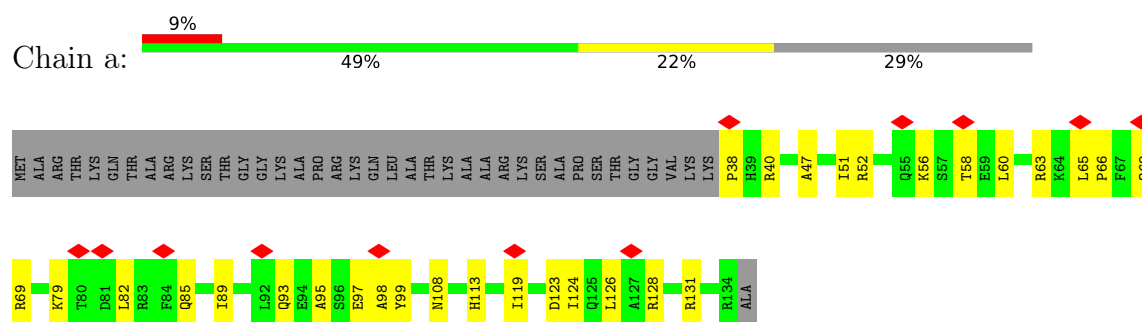
- Molecule 16: RNA (5'-R(P*AP*AP*UP*UP*AP*GP*CP*UP*CP*UP*UP*GP*UP*GP*UP*U)-3')



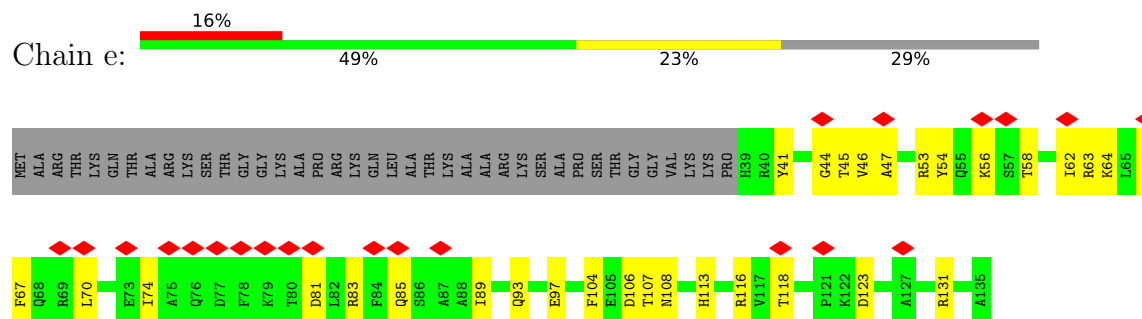
- Molecule 17: TEMPLATE DNA (191-MER)



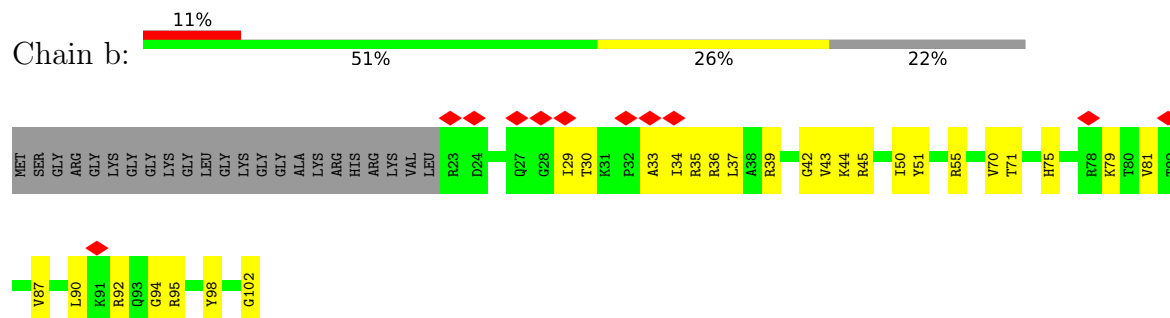
- Molecule 18: Histone H3.3



- Molecule 18: Histone H3.3

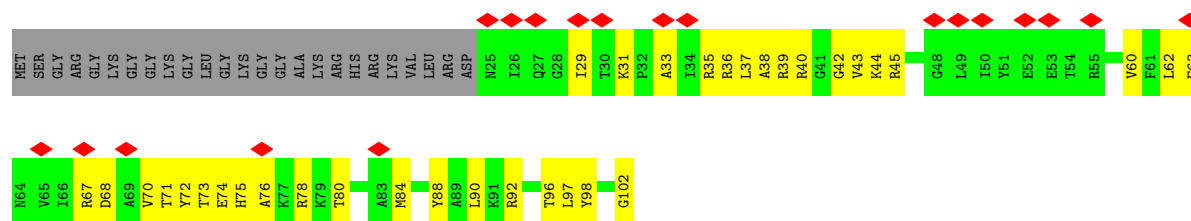


- Molecule 19: Histone H4

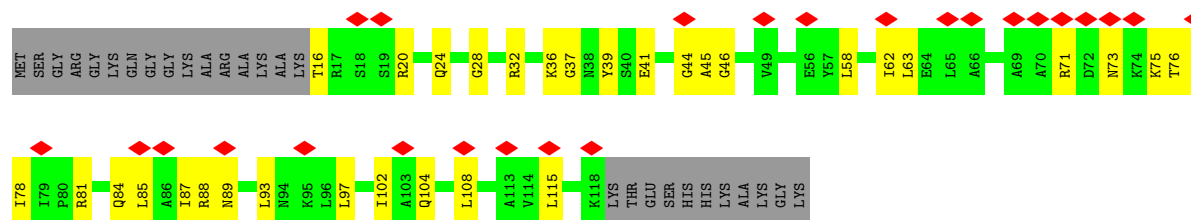


- Molecule 19: Histone H4

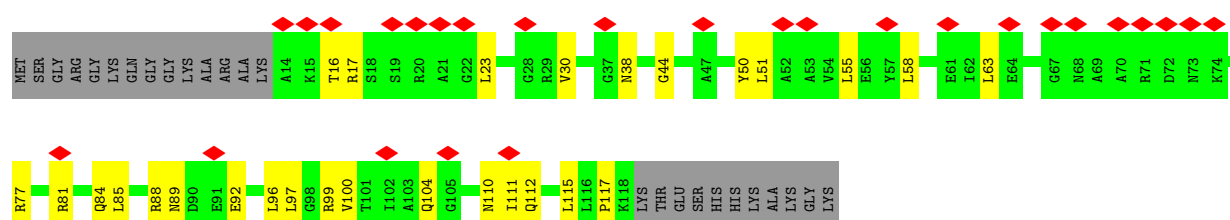




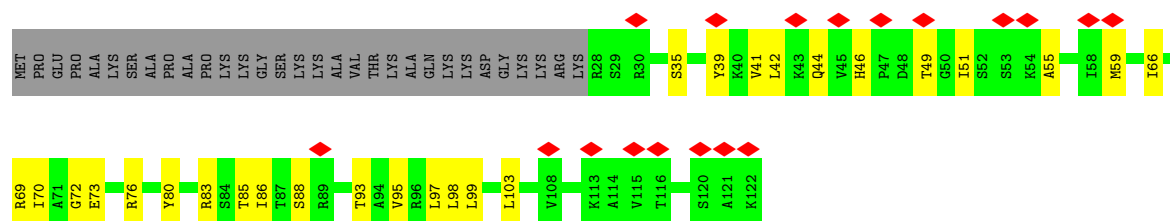
• Molecule 20: Histone H2A type 1-B/E



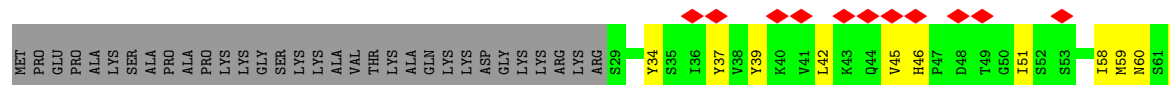
• Molecule 20: Histone H2A type 1-B/E



• Molecule 21: Histone H2B type 1-J

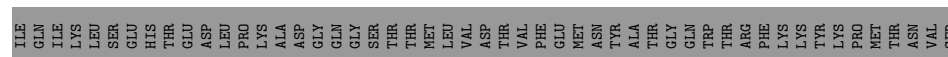
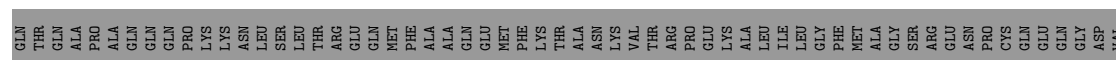
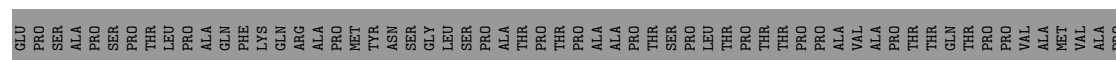
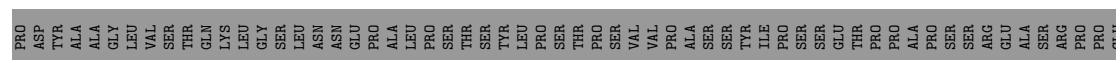
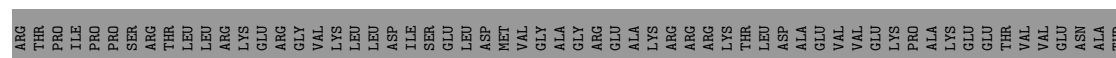
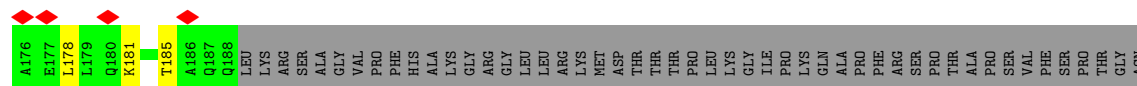


• Molecule 21: Histone H2B type 1-J

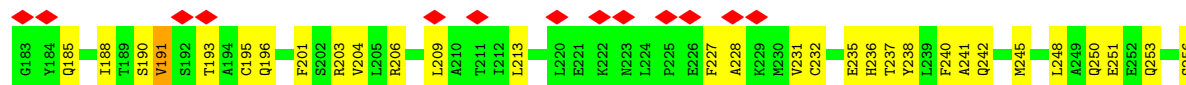
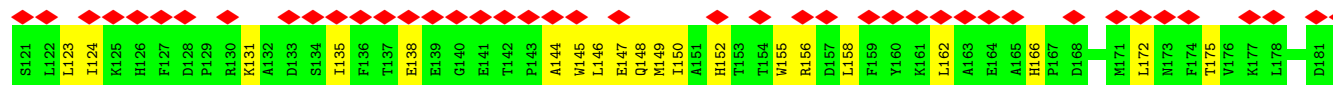
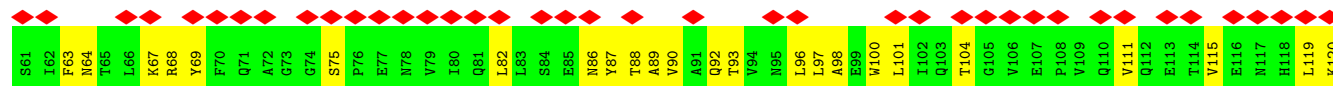
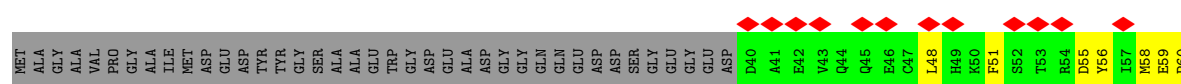


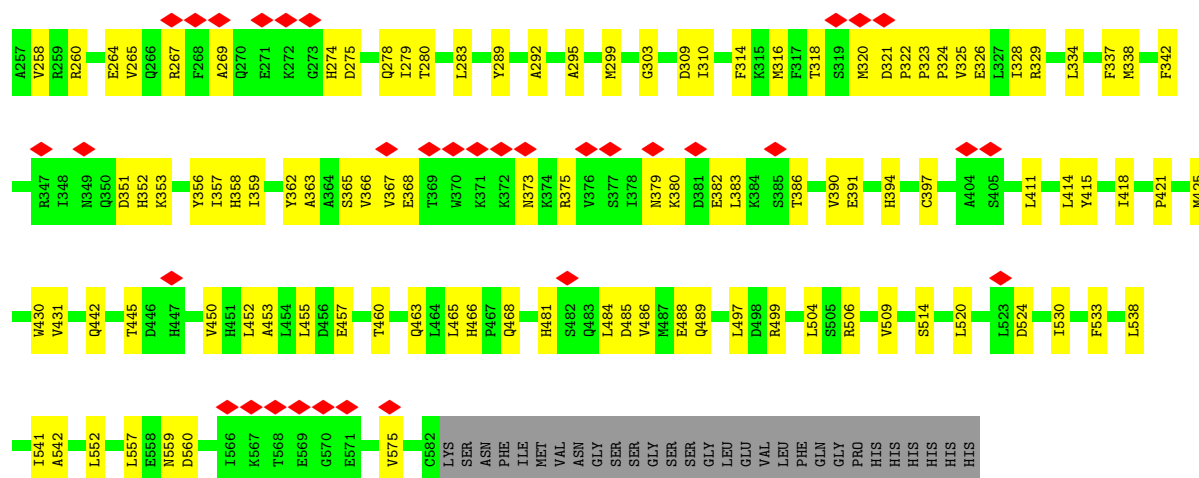


• Molecule 22: Negative elongation factor A

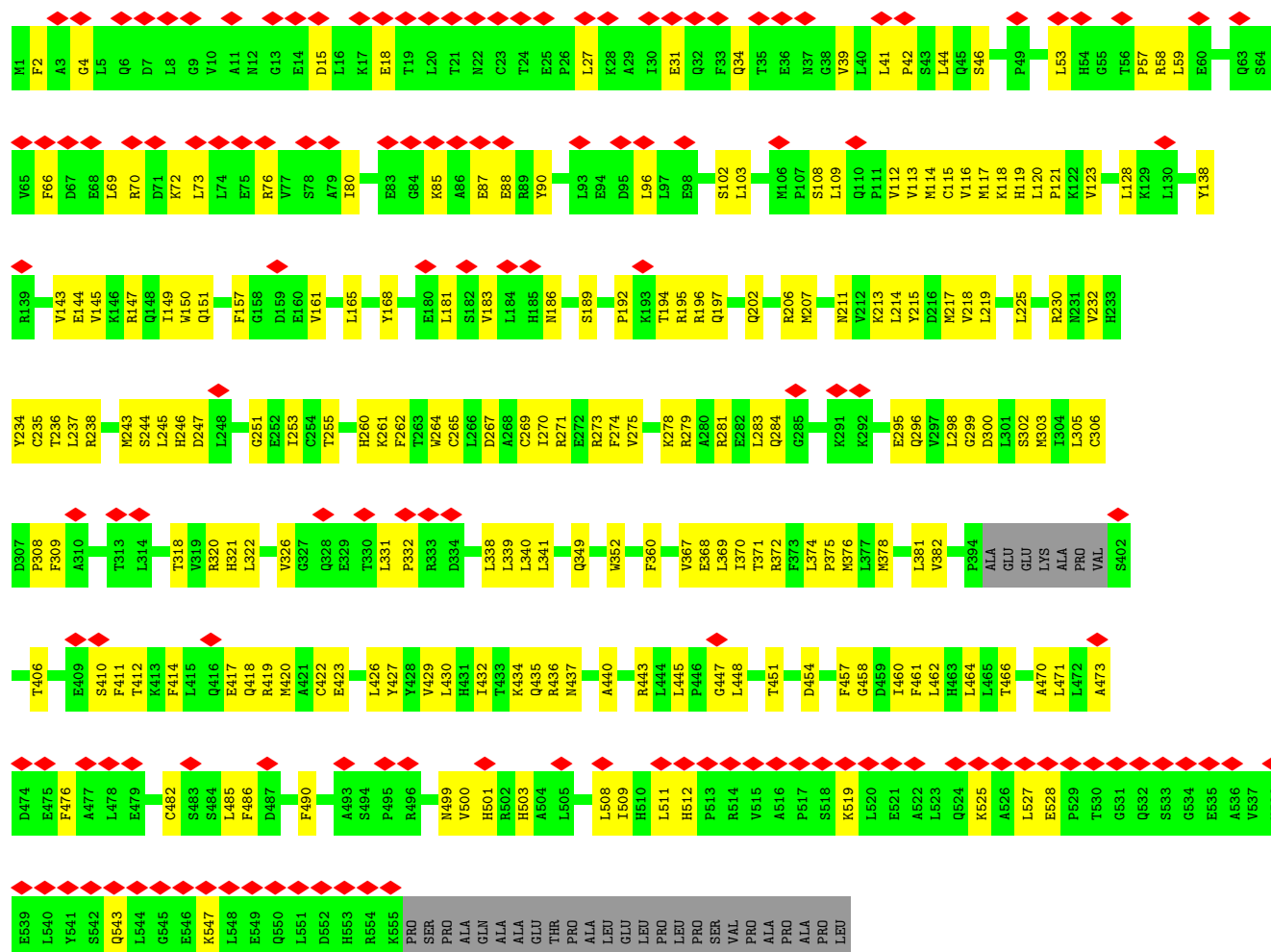


• Molecule 23: Negative elongation factor C/D





• Molecule 24: Negative elongation factor B



• Molecule 25: Negative elongation factor E

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24102	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 ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.272, 1.272, 1.272	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	0.22	0/11248	0.36	0/15179
2	B	0.24	0/9149	0.38	0/12348
3	C	0.26	0/2115	0.36	0/2873
4	D	0.12	0/1017	0.34	0/1368
5	E	0.21	0/1751	0.38	0/2366
6	F	0.24	0/636	0.35	0/859
7	G	0.18	0/1364	0.41	0/1853
8	H	0.24	0/1219	0.39	0/1644
9	I	0.14	0/964	0.37	0/1305
10	J	0.26	0/542	0.40	1/730 (0.1%)
11	K	0.27	0/939	0.37	0/1271
12	L	0.23	0/395	0.44	0/524
13	Y	0.18	0/927	0.38	0/1250
14	Z	0.12	0/3903	0.33	0/5254
15	N	0.18	0/4147	0.37	0/6407
16	P	0.18	0/372	0.24	0/576
17	T	0.19	0/4384	0.34	0/6754
18	a	0.12	0/809	0.28	0/1085
18	e	0.11	0/807	0.30	0/1081
19	b	0.13	0/645	0.31	0/862
19	f	0.13	0/626	0.34	0/837
20	c	0.11	0/806	0.29	0/1089
20	g	0.12	0/820	0.32	0/1107
21	d	0.11	0/757	0.32	0/1015
21	h	0.11	0/736	0.29	0/990
22	U	0.13	0/1434	0.33	0/1948
23	W	0.13	0/4400	0.34	0/5977
24	V	0.13	0/4480	0.32	0/6049
25	X	0.12	0/283	0.27	0/372
All	All	0.19	0/61675	0.35	1/84973 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	14	VAL	N-CA-C	-6.36	106.93	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	910	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11050	0	11200	282	0
2	B	8971	0	9013	200	0
3	C	2072	0	2019	37	0
4	D	1004	0	980	37	0
5	E	1720	0	1737	53	0
6	F	626	0	657	13	0
7	G	1333	0	1321	53	0
8	H	1197	0	1156	35	0
9	I	942	0	871	31	0
10	J	533	0	553	4	0
11	K	920	0	942	14	0
12	L	389	0	393	16	0
13	Y	911	0	904	26	0
14	Z	3837	0	3895	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	3706	0	2041	107	0
16	P	335	0	169	0	0
17	T	3899	0	2128	98	0
18	a	797	0	835	29	0
18	e	796	0	832	31	0
19	b	638	0	676	33	0
19	f	619	0	659	35	0
20	c	796	0	848	35	0
20	g	810	0	866	24	0
21	d	746	0	771	26	0
21	h	725	0	745	29	0
22	U	1410	0	1455	58	0
23	W	4308	0	4306	157	0
24	V	4396	0	4491	173	0
25	X	281	0	330	8	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	C	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	Y	1	0	0	0	0
27	A	1	0	0	0	0
All	All	59777	0	56793	1472	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 1472 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)
23:W:149:MET:HE3	24:V:46:SER:HB2	1.41	1.02
15:N:-82:DG:H1	17:T:82:DC:H42	1.10	0.99
13:Y:63:MET:HE1	13:Y:69:SER:HB3	1.55	0.88
1:A:111:CYS:SG	1:A:114:CYS:HB3	2.14	0.86
15:N:-21:DG:N2	17:T:21:DC:O2	2.10	0.84

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	A	1381/1970 (70%)	1298 (94%)	83 (6%)	0	100	100
2	B	1111/1174 (95%)	1042 (94%)	69 (6%)	0	100	100
3	C	254/271 (94%)	238 (94%)	16 (6%)	0	100	100
4	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	76 (100%)	0	0	100	100
7	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
8	H	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
9	I	114/125 (91%)	111 (97%)	3 (3%)	0	100	100
10	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	39 (89%)	5 (11%)	0	100	100
13	Y	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
14	Z	468/1107 (42%)	441 (94%)	27 (6%)	0	100	100
18	a	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
18	e	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
19	b	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
19	f	76/103 (74%)	72 (95%)	4 (5%)	0	100	100
20	c	101/130 (78%)	100 (99%)	1 (1%)	0	100	100
20	g	103/130 (79%)	97 (94%)	6 (6%)	0	100	100
21	d	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
21	h	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
22	U	181/528 (34%)	178 (98%)	3 (2%)	0	100	100
23	W	541/611 (88%)	508 (94%)	32 (6%)	1 (0%)	44	71
24	V	544/580 (94%)	535 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	X	33/404 (8%)	33 (100%)	0	0	100	100
All	All	6418/8921 (72%)	6116 (95%)	301 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	W	191	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	A	1229/1749 (70%)	1229 (100%)	0	100	100
2	B	985/1027 (96%)	985 (100%)	0	100	100
3	C	235/248 (95%)	235 (100%)	0	100	100
4	D	109/126 (86%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	146/153 (95%)	146 (100%)	0	100	100
8	H	130/131 (99%)	130 (100%)	0	100	100
9	I	104/112 (93%)	104 (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	Y	102/104 (98%)	102 (100%)	0	100	100
14	Z	423/955 (44%)	423 (100%)	0	100	100
18	a	83/110 (76%)	83 (100%)	0	100	100
18	e	82/110 (74%)	82 (100%)	0	100	100
19	b	65/79 (82%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	f	63/79 (80%)	63 (100%)	0	100	100
20	c	82/100 (82%)	82 (100%)	0	100	100
20	g	83/100 (83%)	83 (100%)	0	100	100
21	d	81/105 (77%)	81 (100%)	0	100	100
21	h	79/105 (75%)	79 (100%)	0	100	100
22	U	158/451 (35%)	158 (100%)	0	100	100
23	W	479/530 (90%)	479 (100%)	0	100	100
24	V	491/515 (95%)	491 (100%)	0	100	100
25	X	31/351 (9%)	31 (100%)	0	100	100
All	All	5702/7760 (74%)	5702 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
14	Z	632	ASN
19	f	27	GLN
24	V	296	GLN
14	Z	737	HIS
20	c	84	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	15/16 (93%)	2 (13%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	3	U
16	P	5	A

There are no RNA pucker outliers to report.

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 10 ligands modelled in this entry, 10 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.

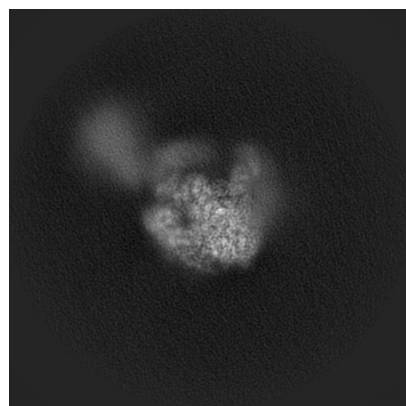
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61059. These allow visual inspection of the internal detail of the map and identification of artifacts.

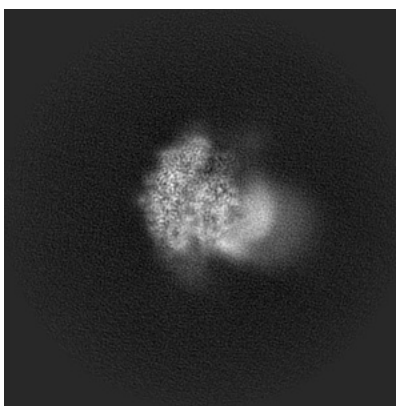
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

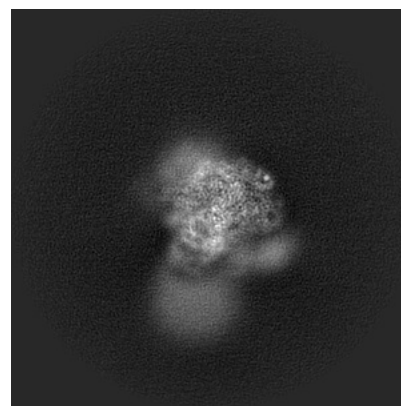
6.1.1 Primary map



X

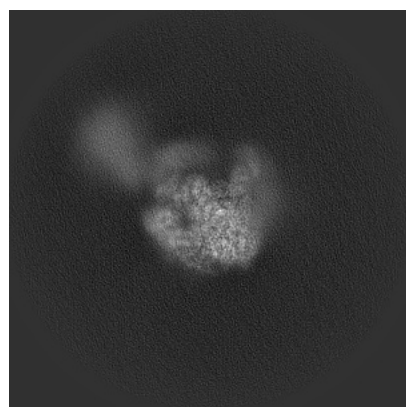


Y

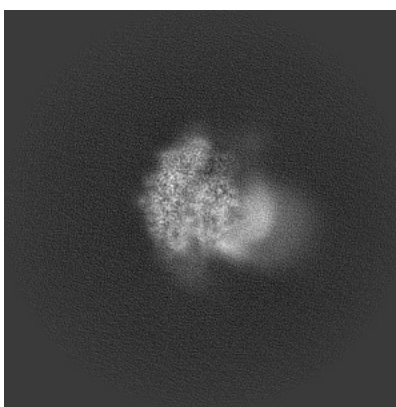


Z

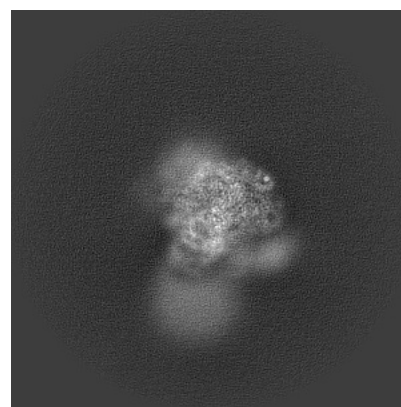
6.1.2 Raw map



X



Y

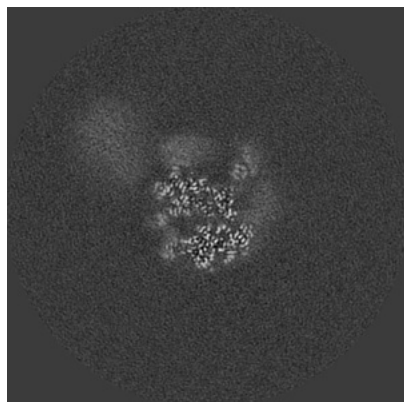


Z

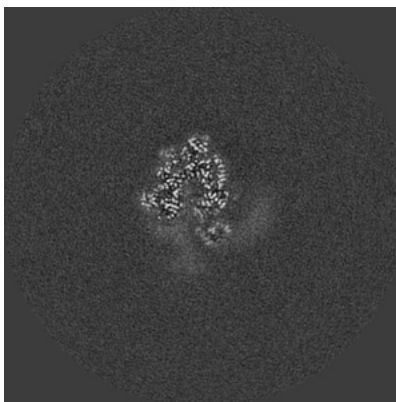
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

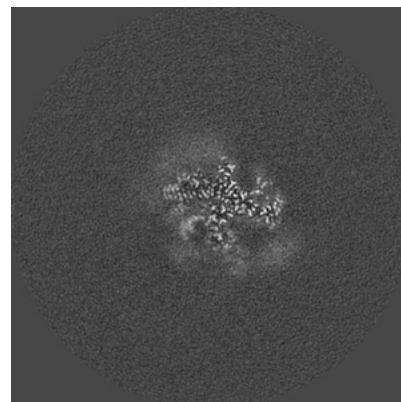
6.2.1 Primary map



X Index: 175

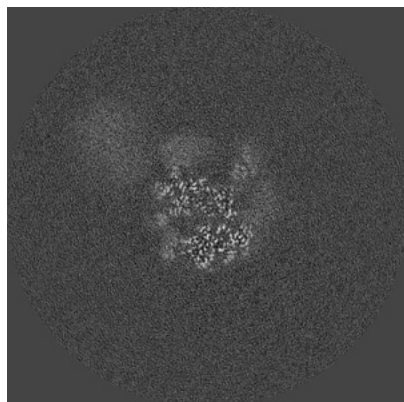


Y Index: 175

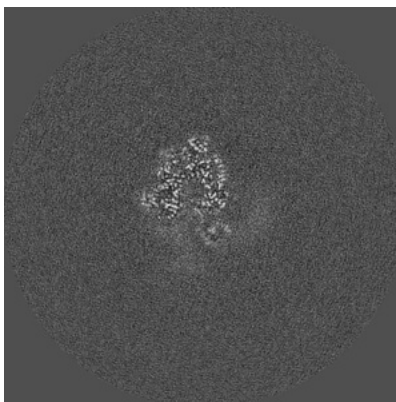


Z Index: 175

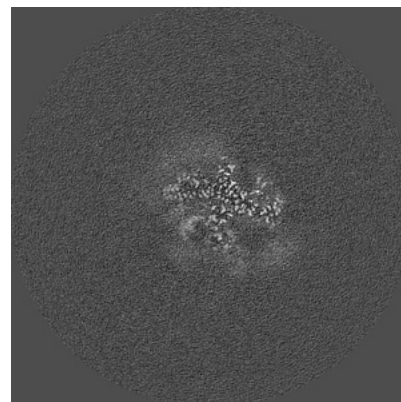
6.2.2 Raw map



X Index: 175



Y Index: 175

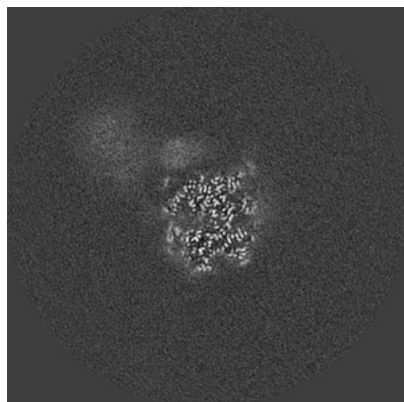


Z Index: 175

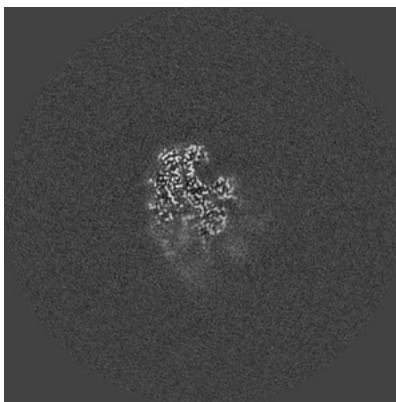
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

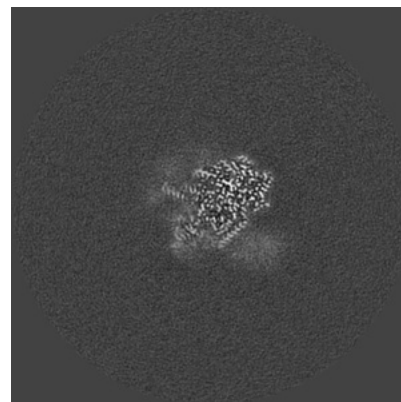
6.3.1 Primary map



X Index: 184

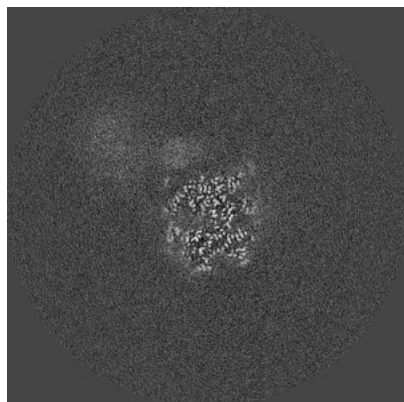


Y Index: 194

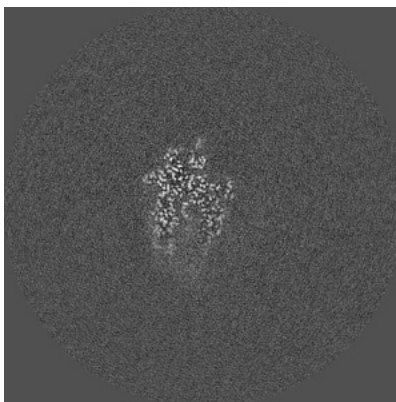


Z Index: 147

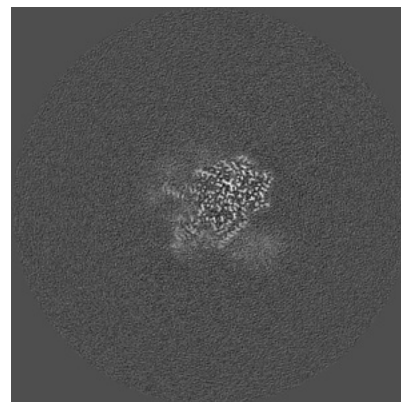
6.3.2 Raw map



X Index: 184



Y Index: 188

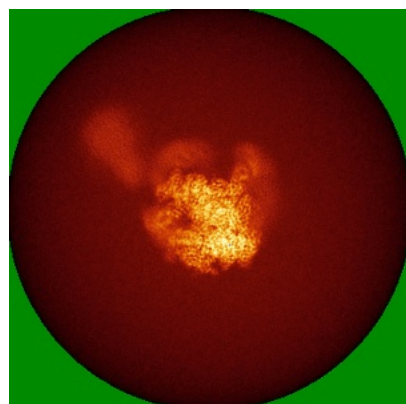


Z Index: 147

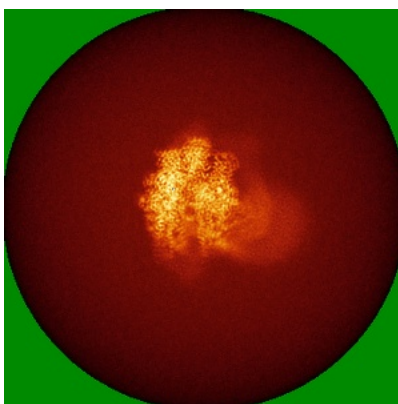
The images above show the largest variance slices of the map in three orthogonal directions.

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

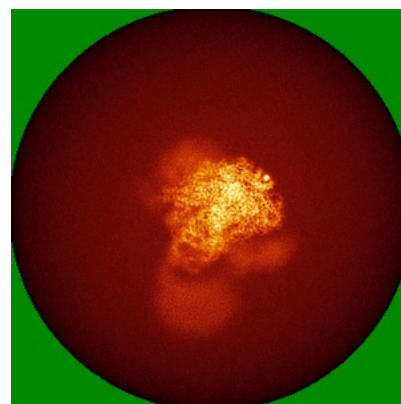
6.4.1 Primary map



X

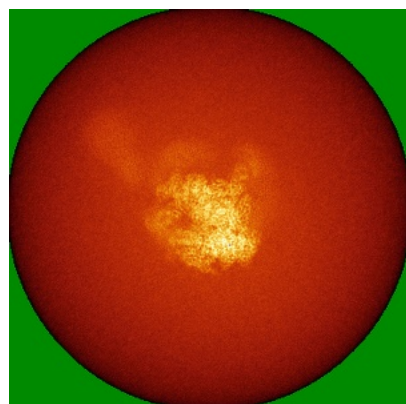


Y

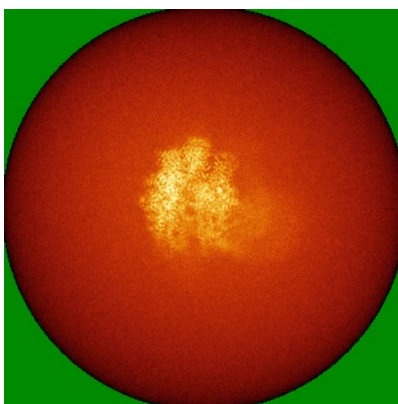


Z

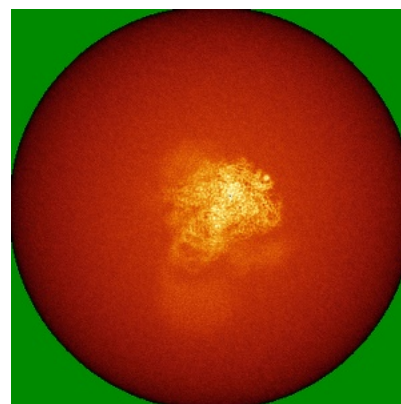
6.4.2 Raw map



X



Y

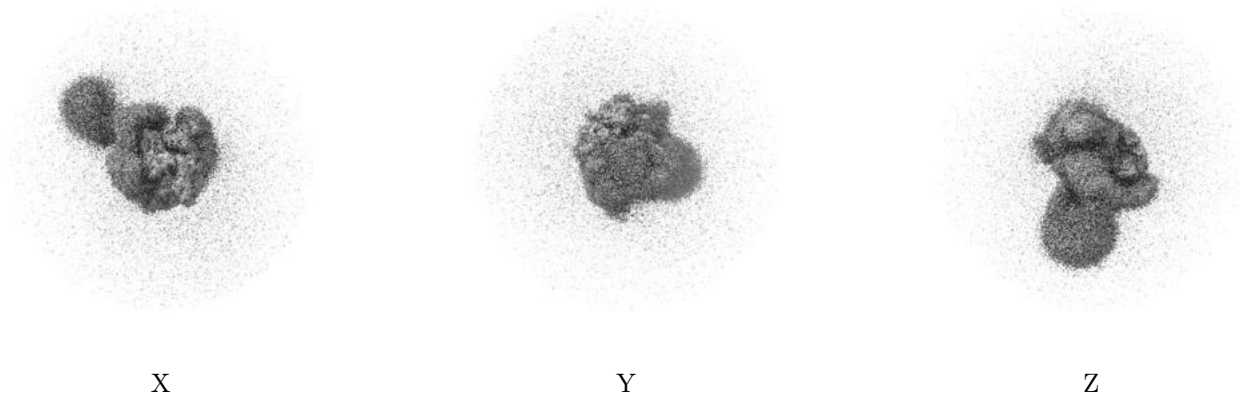


Z

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.

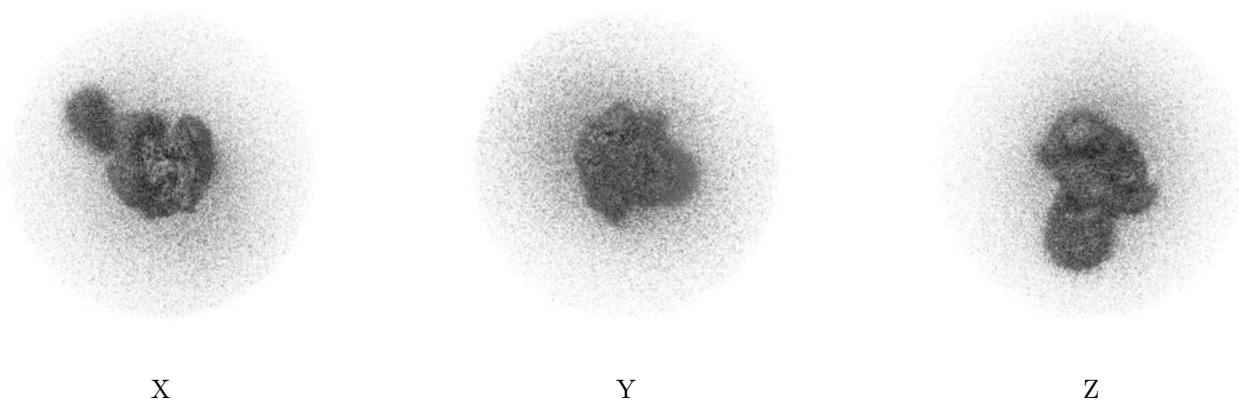
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

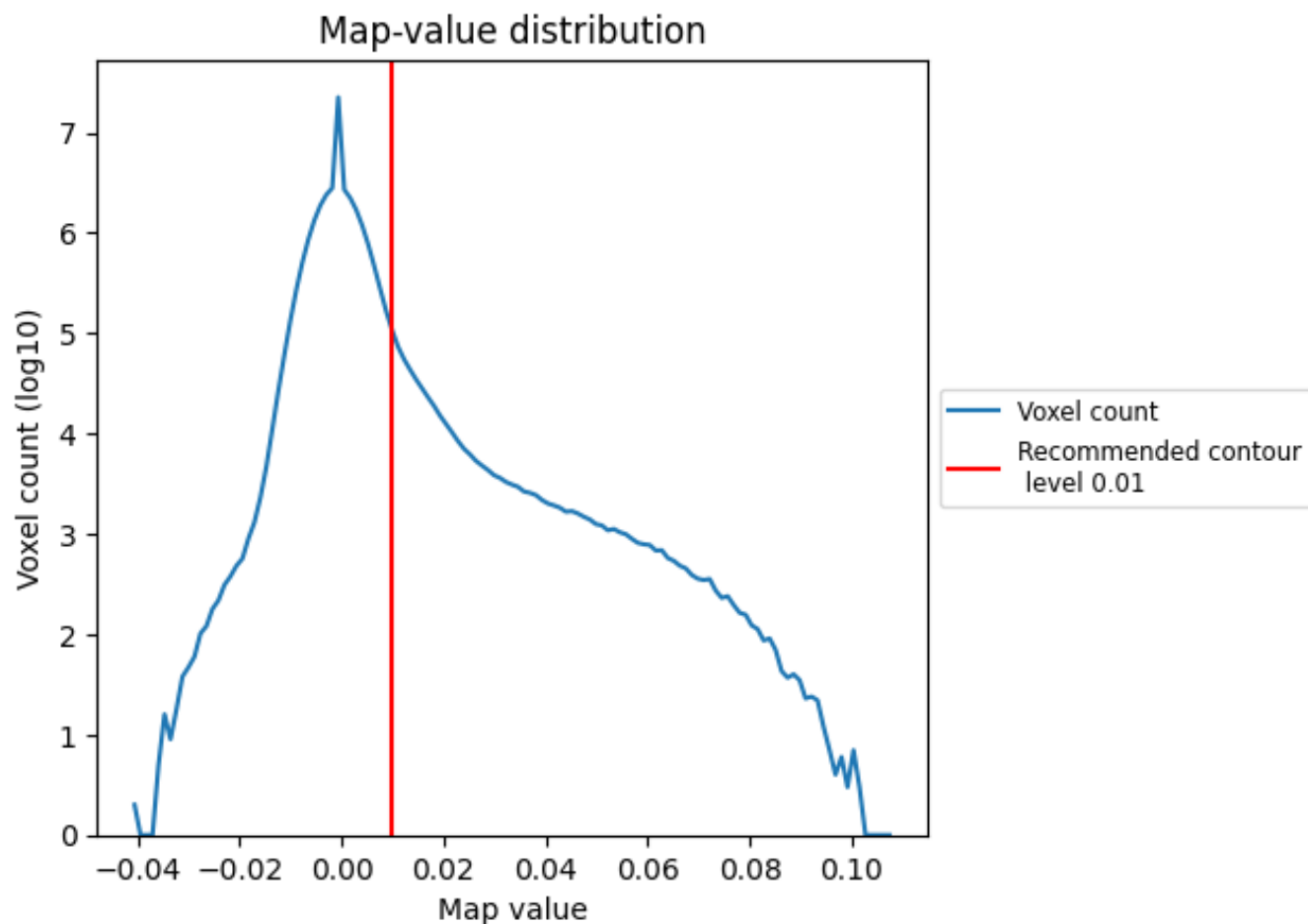
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

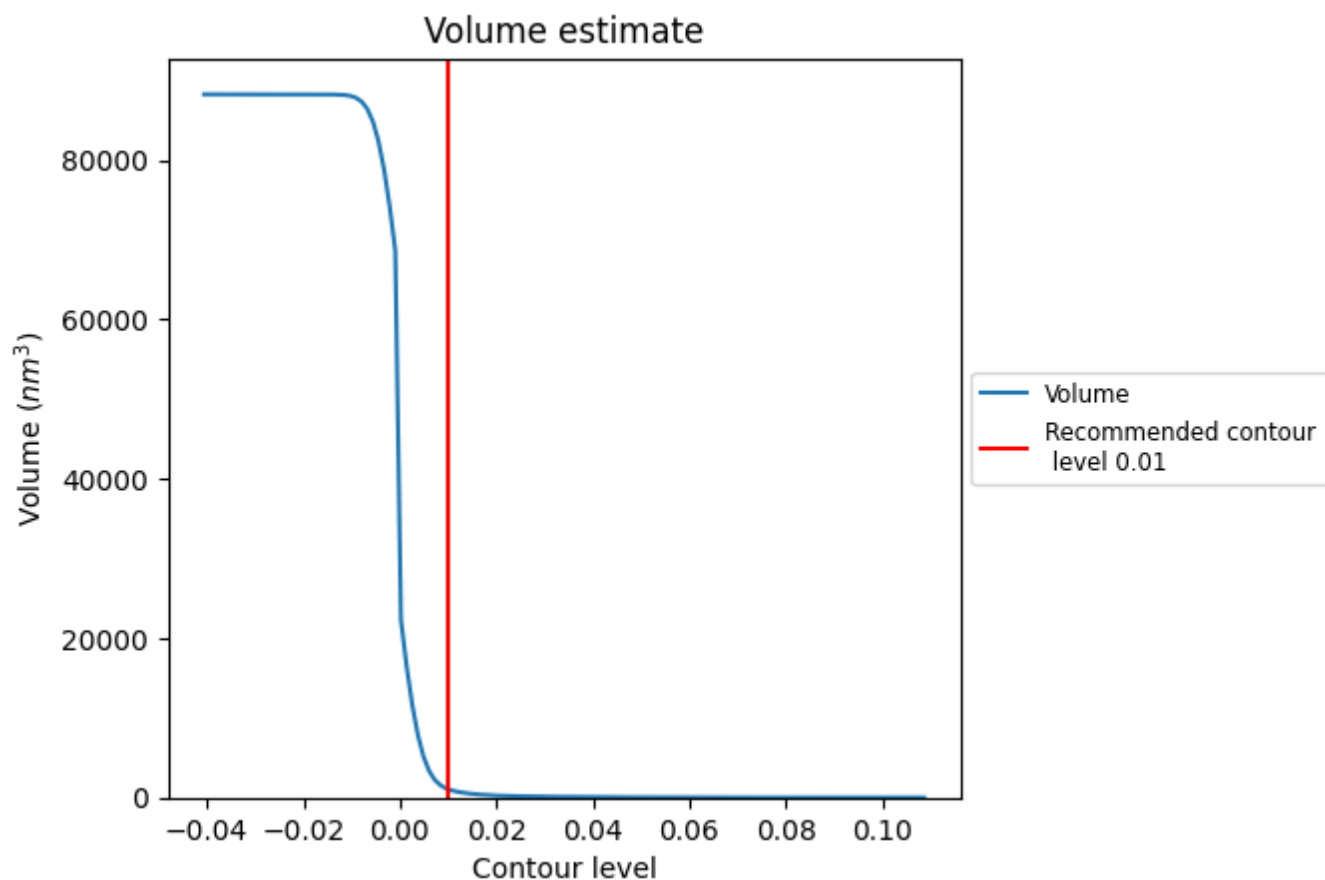
This section contains the results of statistical analysis of the map.

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.

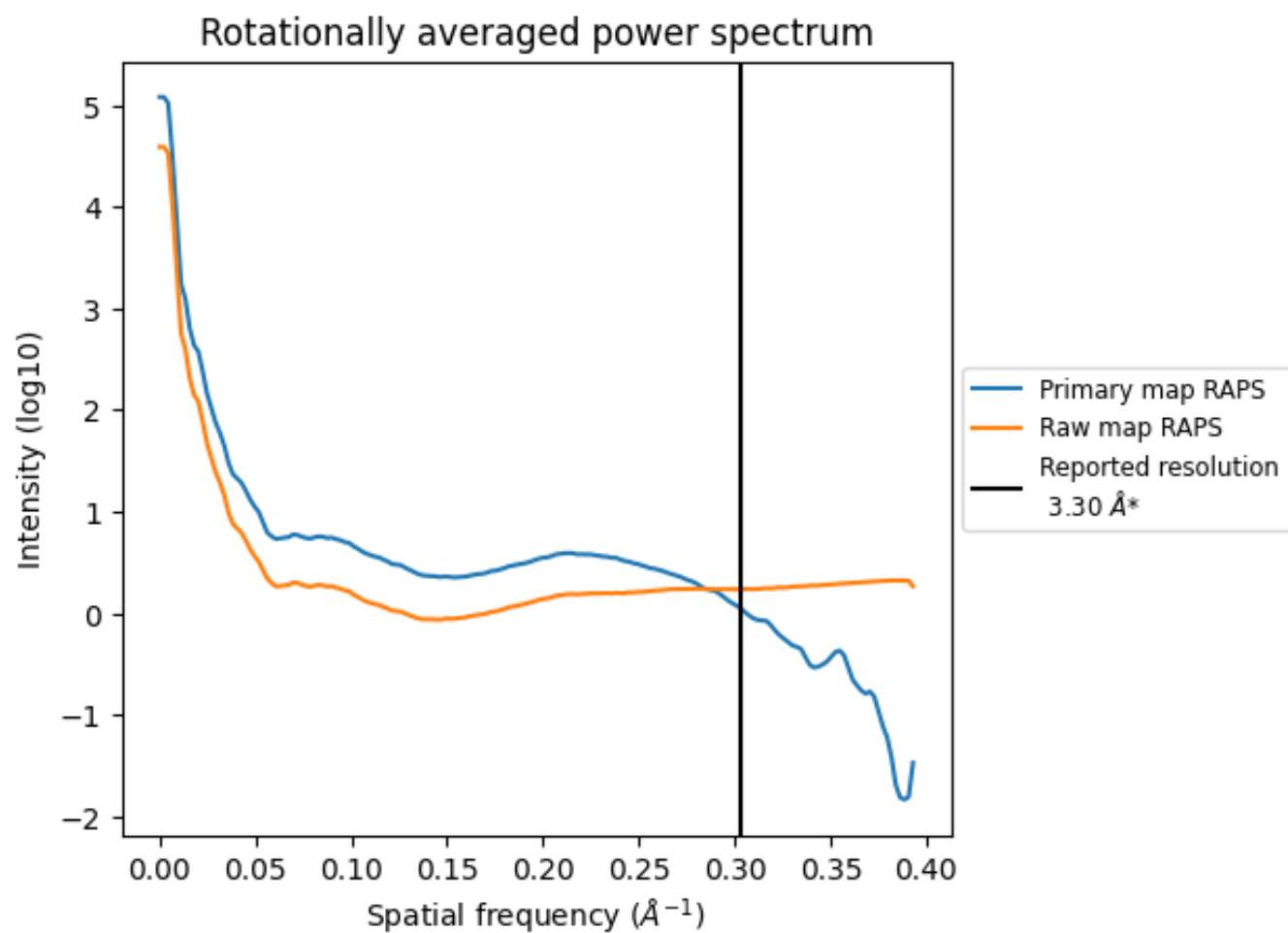
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1058 nm³; this corresponds to an approximate mass of 956 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 ⓘ

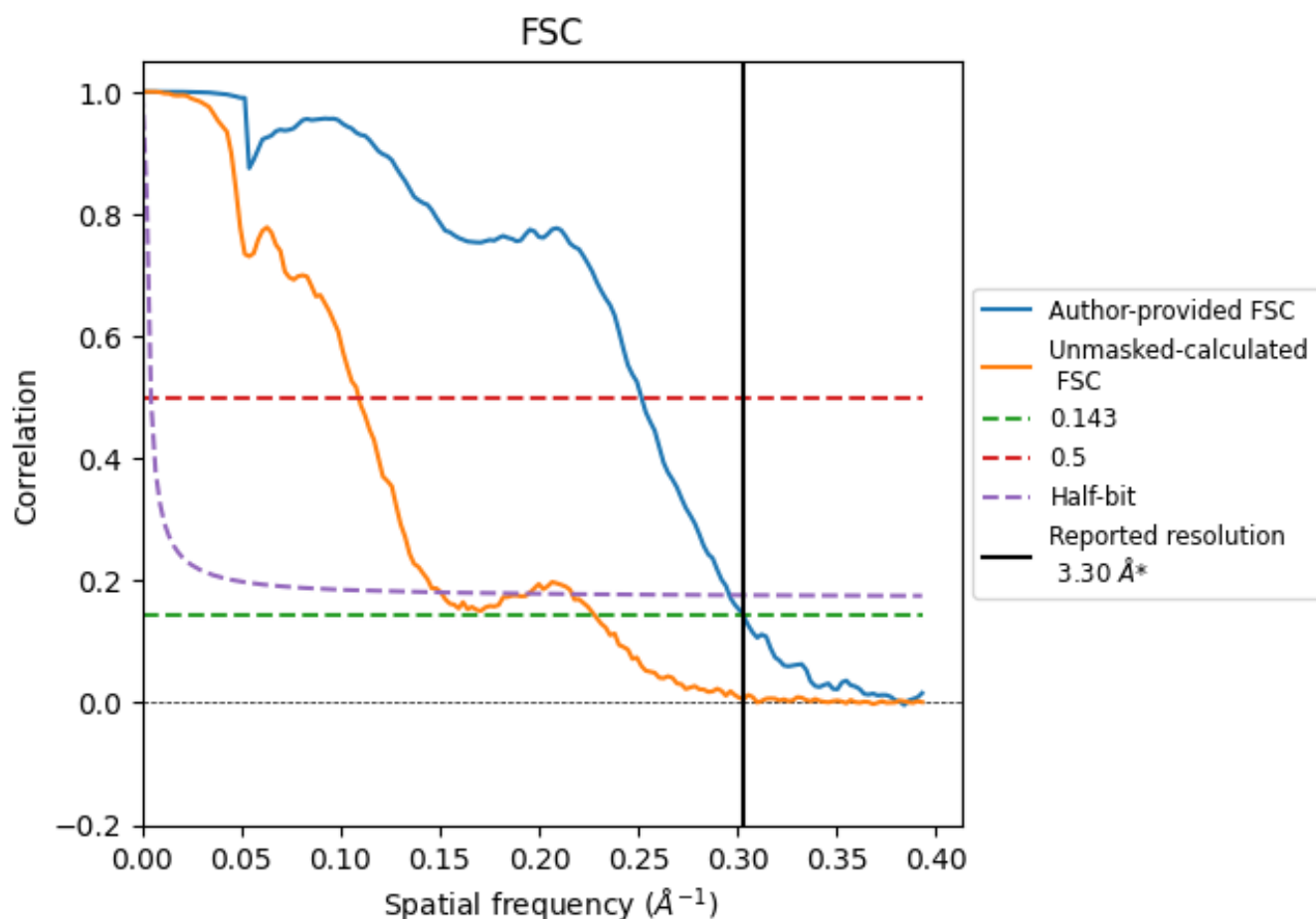


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

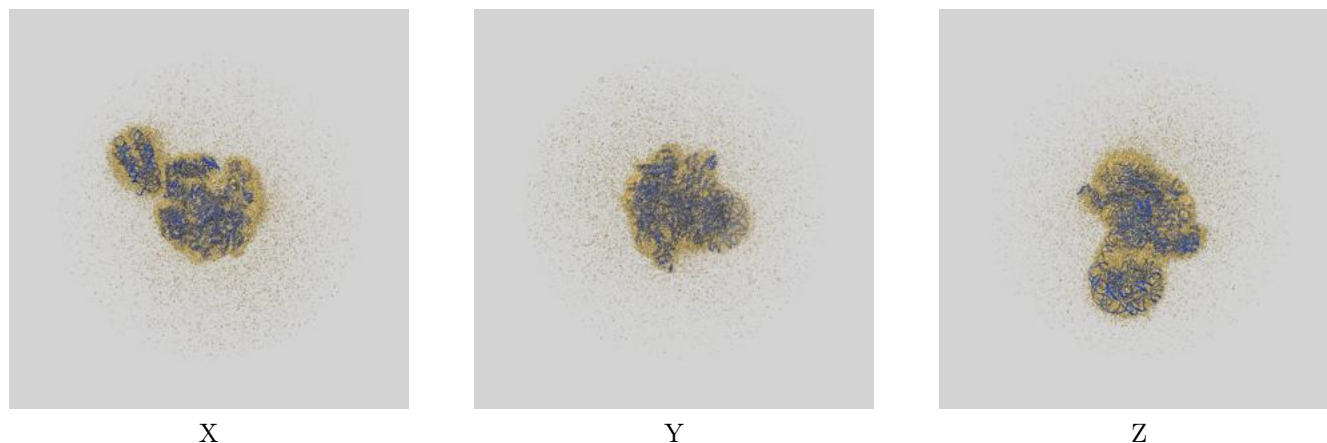
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.97	3.38
Unmasked-calculated*	4.39	9.17	6.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

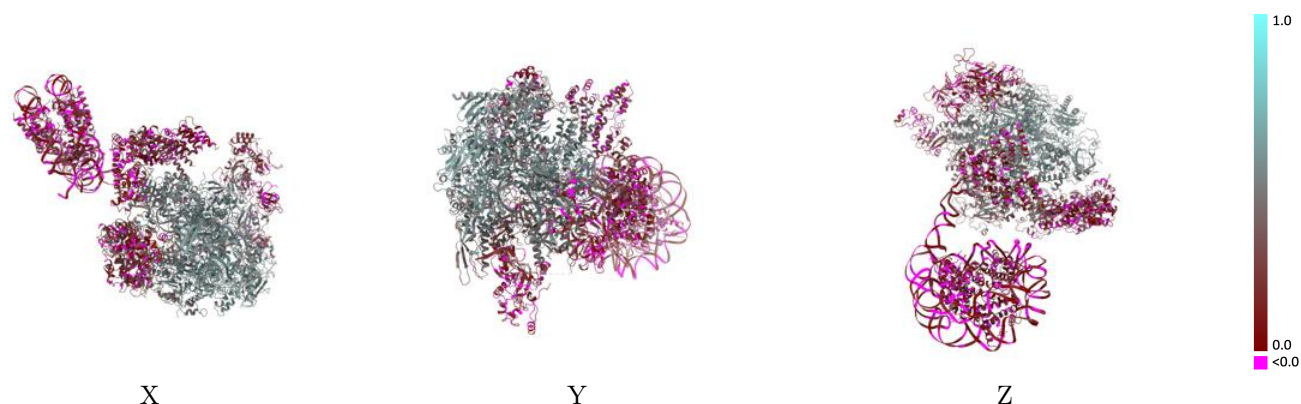
This section contains information regarding the fit between EMDB map EMD-61059 and PDB model 9J0O. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



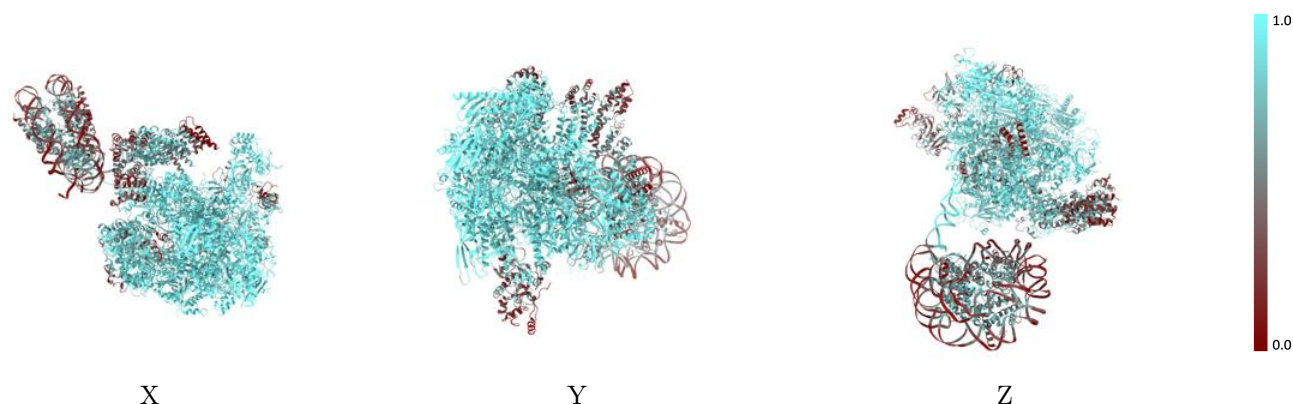
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



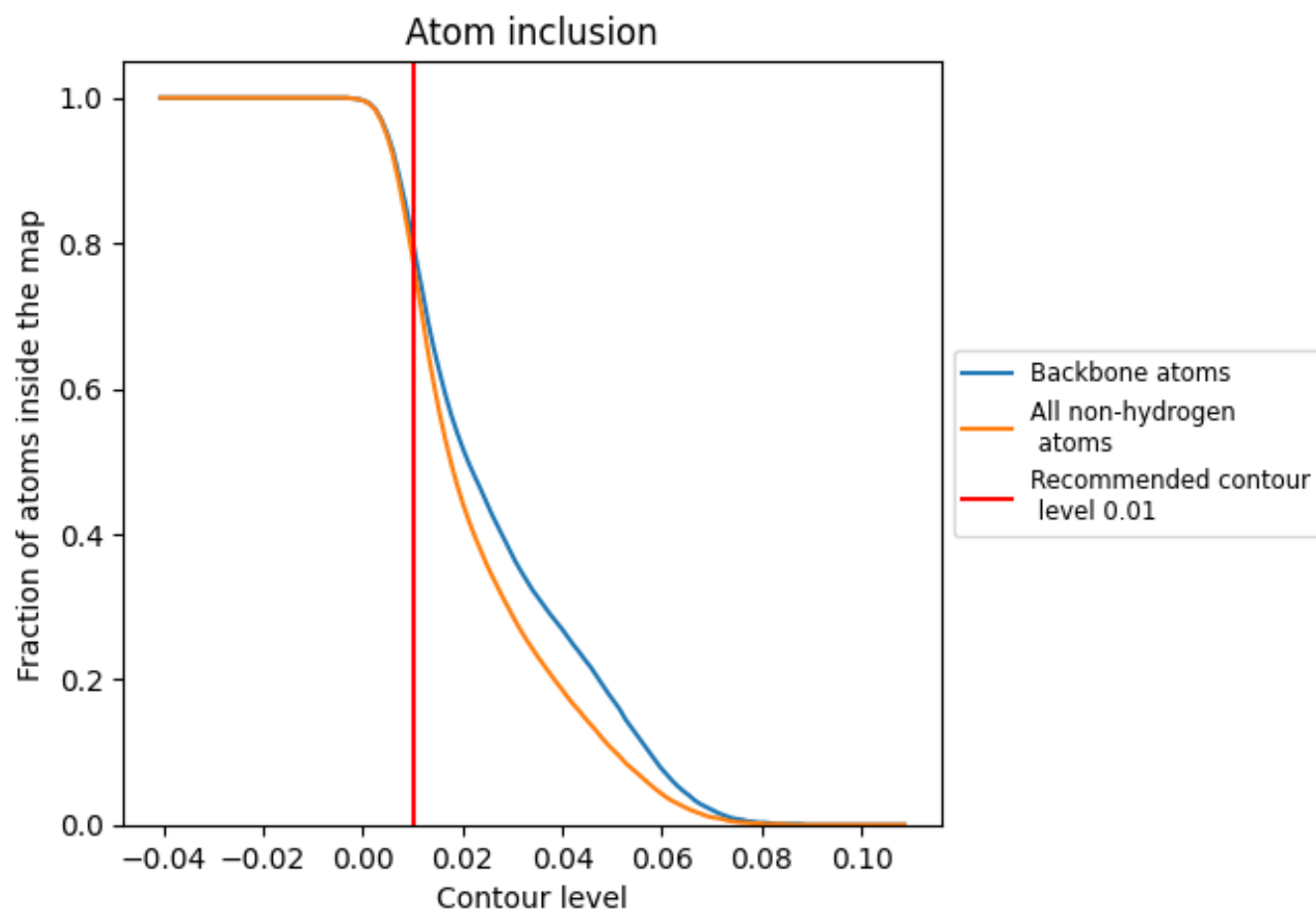
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.3130
A	 0.9750	 0.5000
B	 0.9780	 0.4970
C	 0.9910	 0.5420
D	 0.9500	 0.2010
E	 0.9760	 0.4770
F	 0.9870	 0.5350
G	 0.9600	 0.2810
H	 0.9820	 0.5170
I	 0.9430	 0.3490
J	 0.9870	 0.5520
K	 0.9900	 0.5420
L	 0.9840	 0.4710
N	 0.4420	 0.1010
P	 0.9220	 0.4290
T	 0.4810	 0.1190
U	 0.6740	 0.1610
V	 0.6330	 0.1330
W	 0.6410	 0.1780
X	 0.4340	 0.1040
Y	 0.2940	 0.0770
Z	 0.6000	 0.1750
a	 0.6720	 0.1070
b	 0.6650	 0.1180
c	 0.5990	 0.1060
d	 0.6270	 0.1070
e	 0.5940	 0.1420
f	 0.5610	 0.1150
g	 0.5830	 0.0940
h	 0.5340	 0.0760

