



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2025 – 12:55 PM JST

PDB ID : 9J0P
EMDB ID : EMD-61060
Title : Arrested elongation complex of mammalian RNA polymerase II with nucleosome (AEC2-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.dev117
MolProbity : 4.02b-467
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) : 2.41.2

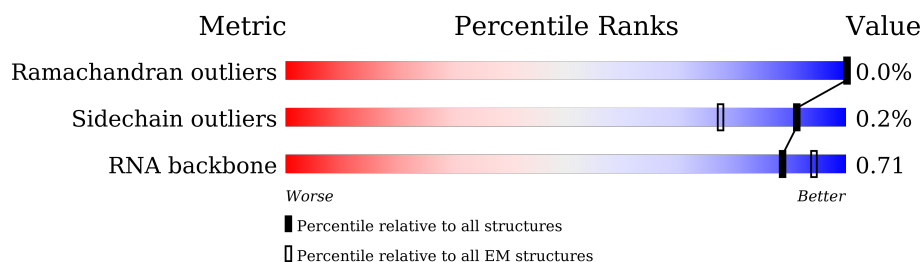
1 Overall quality at a glance

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.



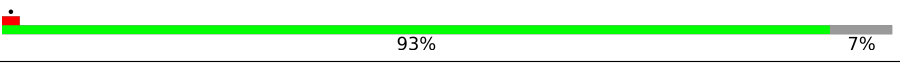
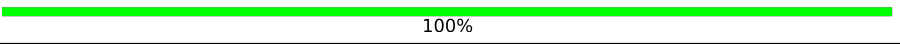
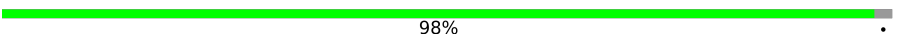

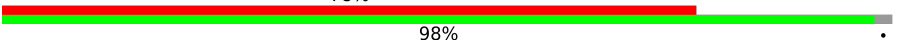

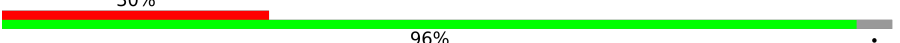




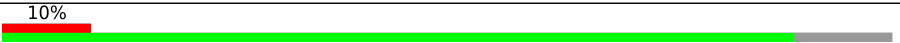




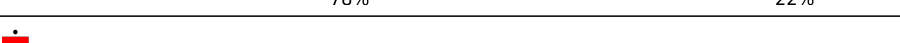
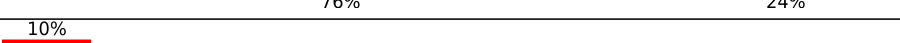
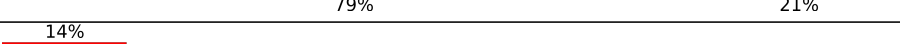
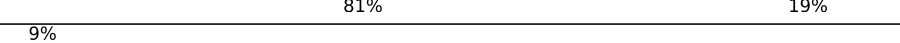

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	71% 29%
2	B	1174	95% 5%
3	C	271	95% 5%
4	D	142	89% 11%
5	E	210	99%
6	F	127	61% 39%
7	G	172	99% .
8	H	150	99% .

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	Y	118	
14	Z	1107	
15	T	198	
16	N	198	
17	P	16	
18	U	528	
19	V	580	
20	W	611	
21	X	404	
22	a	136	
22	e	136	
23	b	103	
23	f	103	
24	c	130	
24	g	130	
25	d	126	
25	h	126	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 59755 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 TEMPLATE DNA (191-MER).

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

- Molecule 16 is a DNA chain called NON-TEMPLATE DNA (180-MER).

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

- Molecule 17 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
17	P	16	Total	C	N	O	P	0	0
			335	150	52	117	16		

- Molecule 18 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	187	Total	C	N	O	S	0	0
			1439	912	245	273	9		

- Molecule 19 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	542	Total	C	N	O	S	0	0
			4341	2785	736	795	25		

- Molecule 20 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	543	Total	C	N	O	S	0	0
			4312	2755	722	811	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 21 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	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 22 is a protein called Histone H3.3.

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

- Molecule 23 is a protein called Histone H4.

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

- Molecule 24 is a protein called Histone H2A type 1-B/E.

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

- Molecule 25 is a protein called Histone H2B type 1-J.

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

- Molecule 26 is ZINC ION (three-letter code: 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	
26	J	1	Total	Zn	0
			1	1	

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

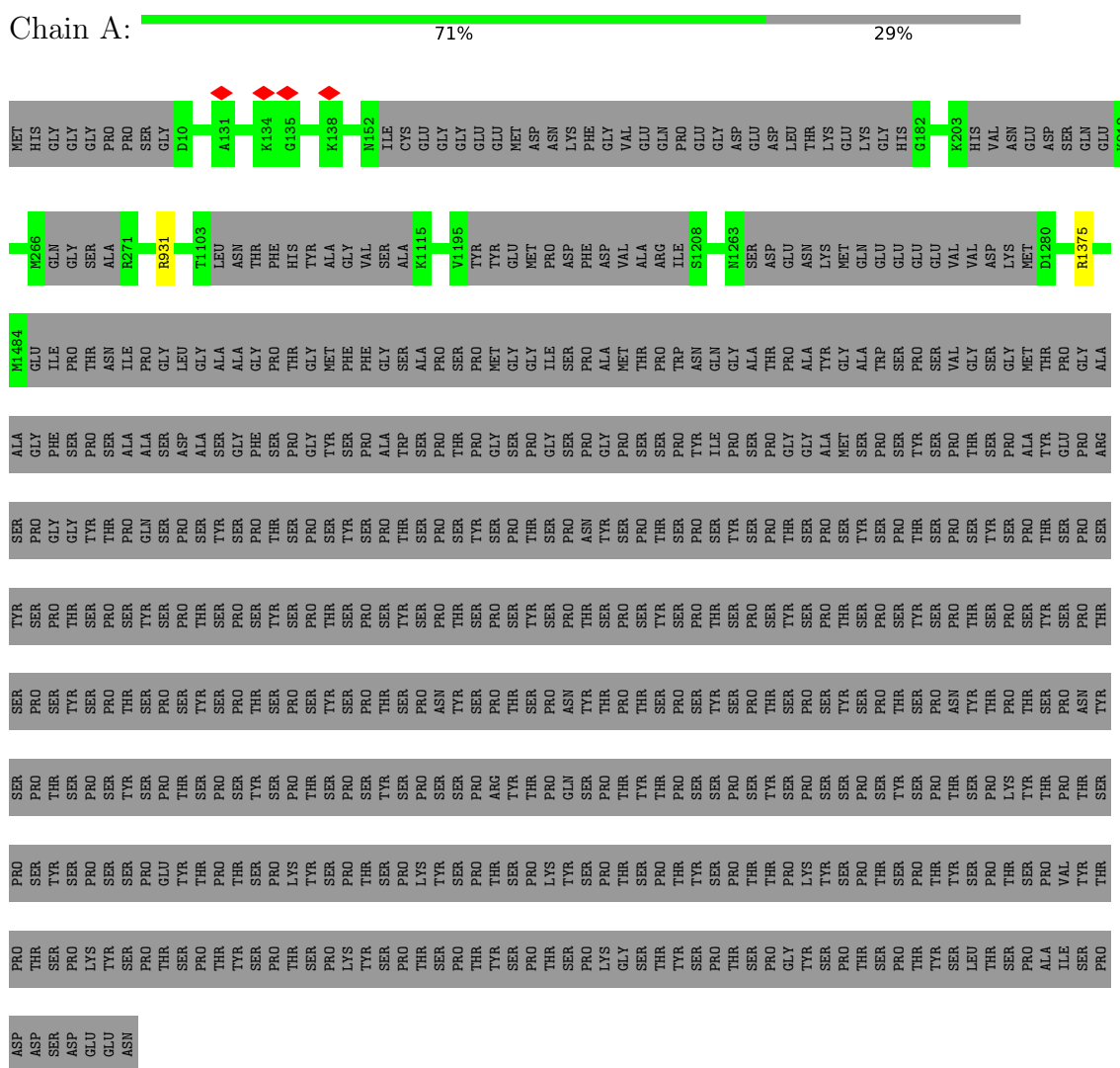
- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

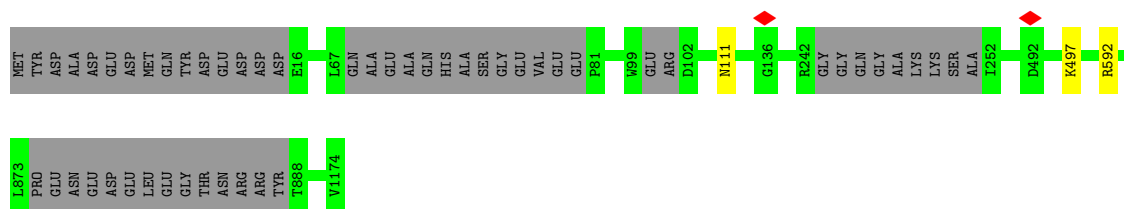
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



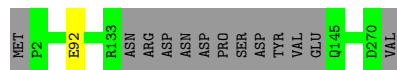
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:  95%  5%



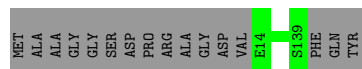
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 95% 5%



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

Chain D: 89% 11%



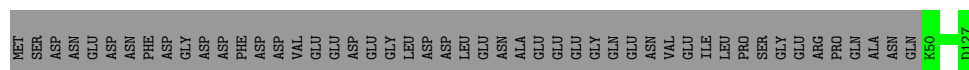
- Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E: 99%



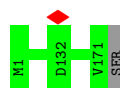
- Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F: 61% 39%



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

Chain G: 99%

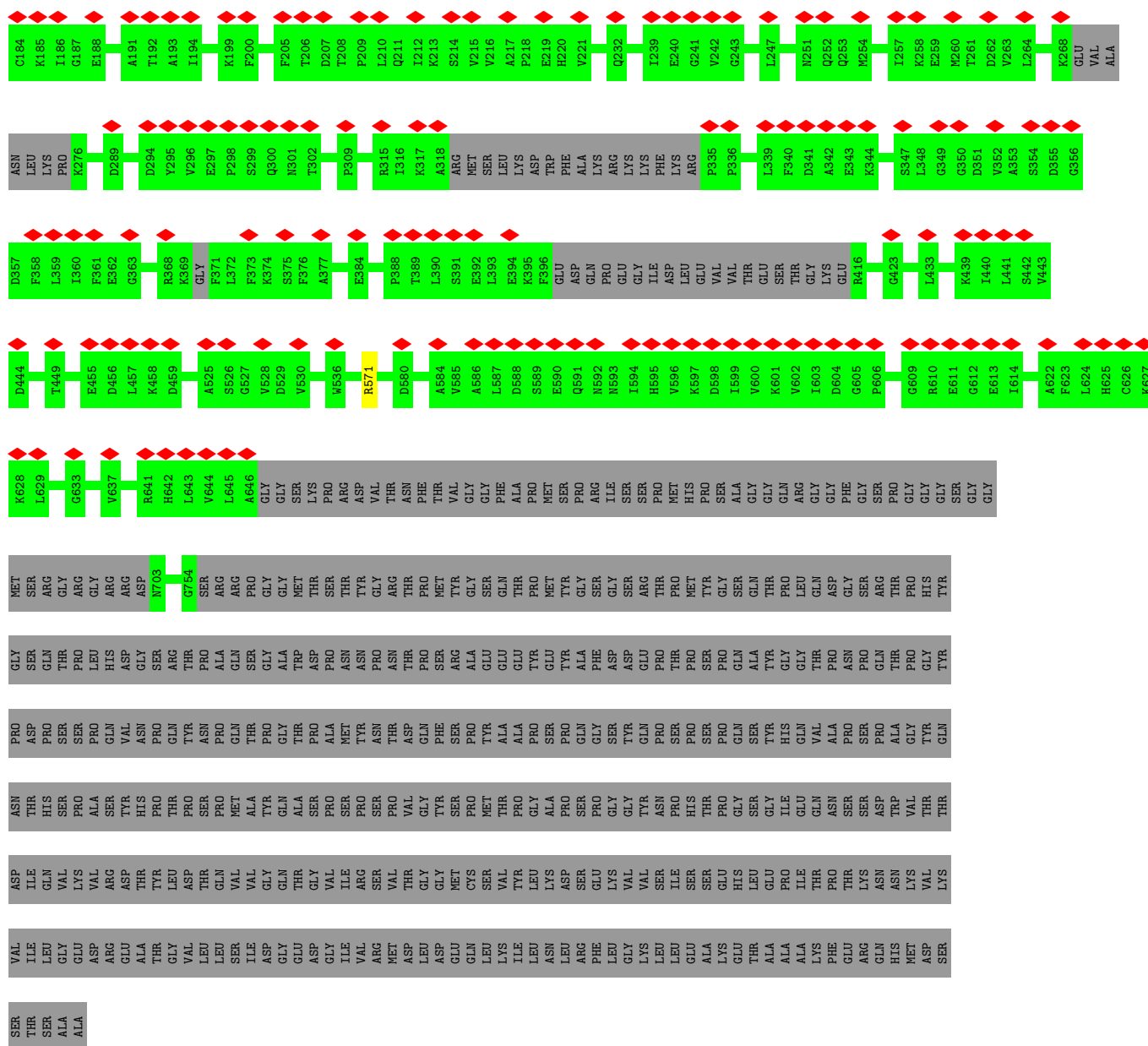


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

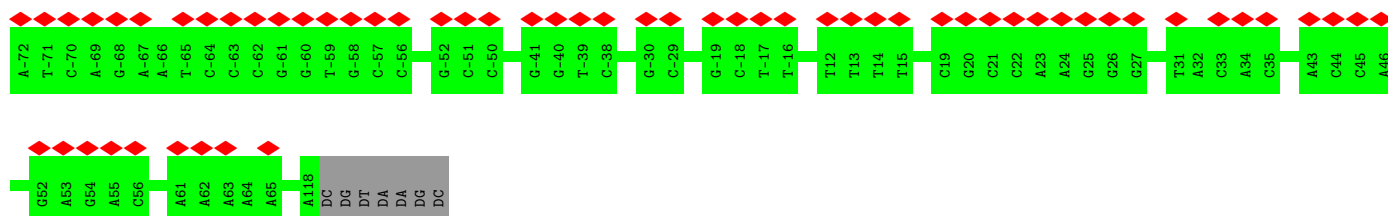
Chain H: 99%



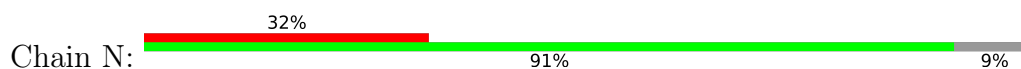
- [illegible]

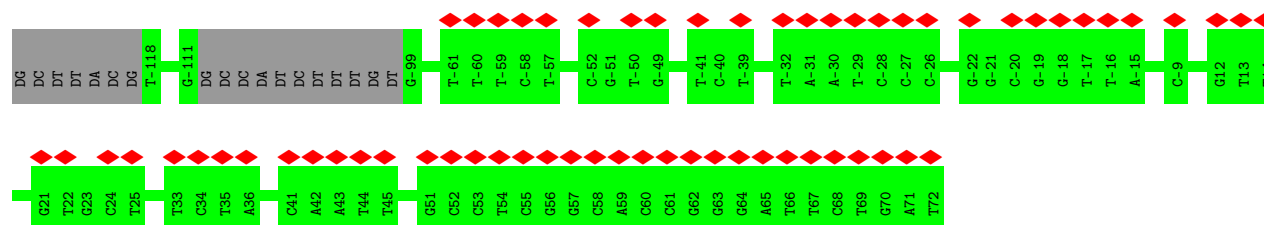


• Molecule 15: TEMPLATE DNA (191-MER)



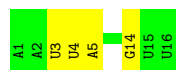
• Molecule 16: NON-TEMPLATE DNA (180-MER)





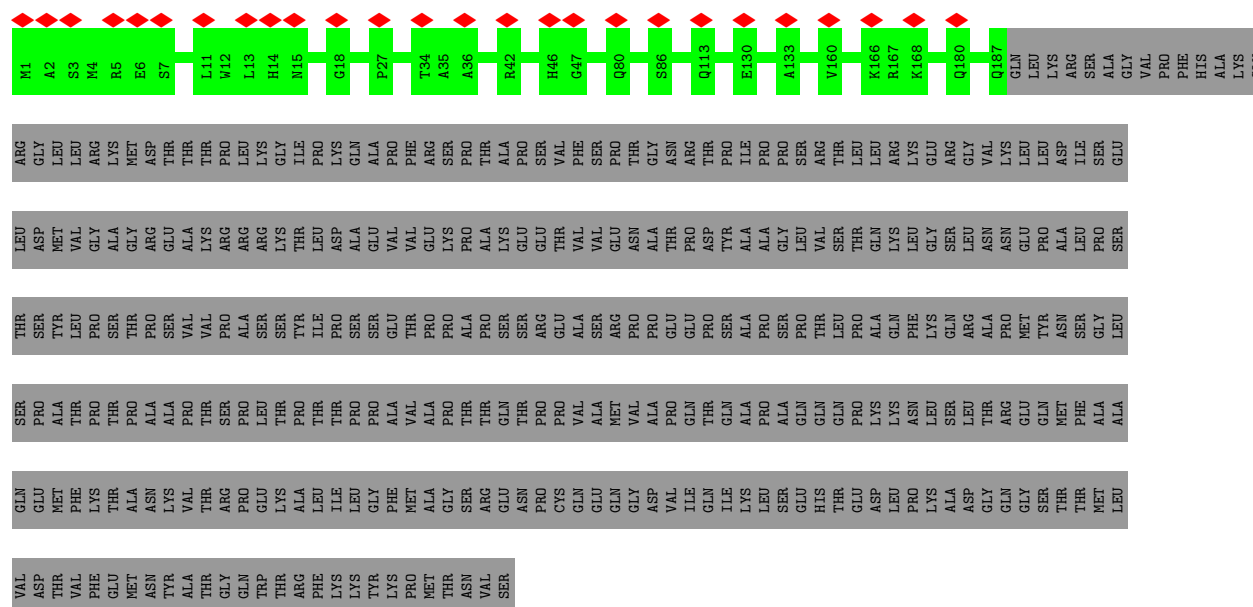
- Molecule 17: RNA (5'-R(P*AP*AP*UP*UP*AP*GP*CP*UP*CP*UP*UP*GP*UP*GP*UP*U)-3')

Chain P: 75% 25%



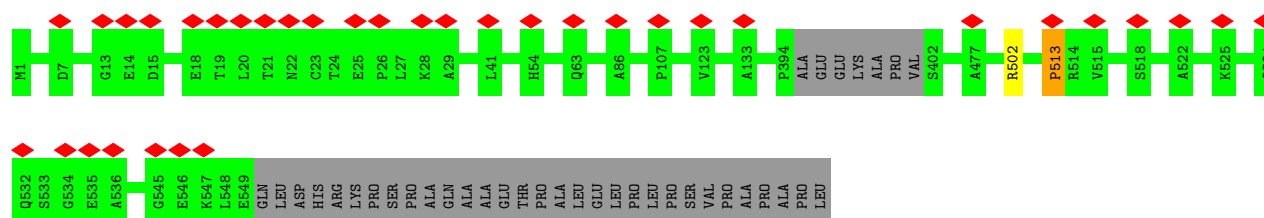
- Molecule 18: Negative elongation factor A

Chain U: 5% 35% 65%

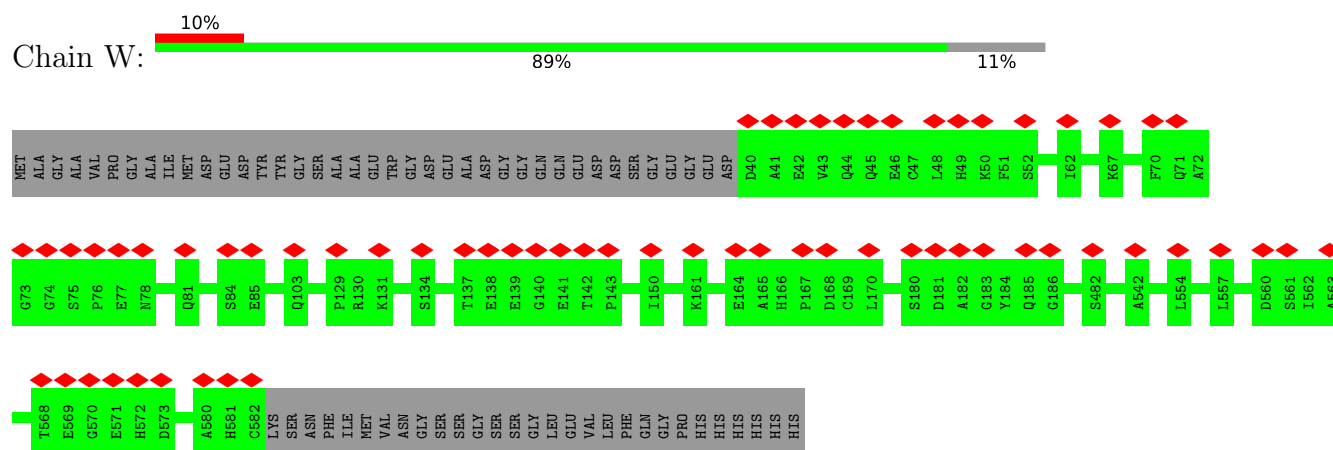


- Molecule 19: Negative elongation factor B

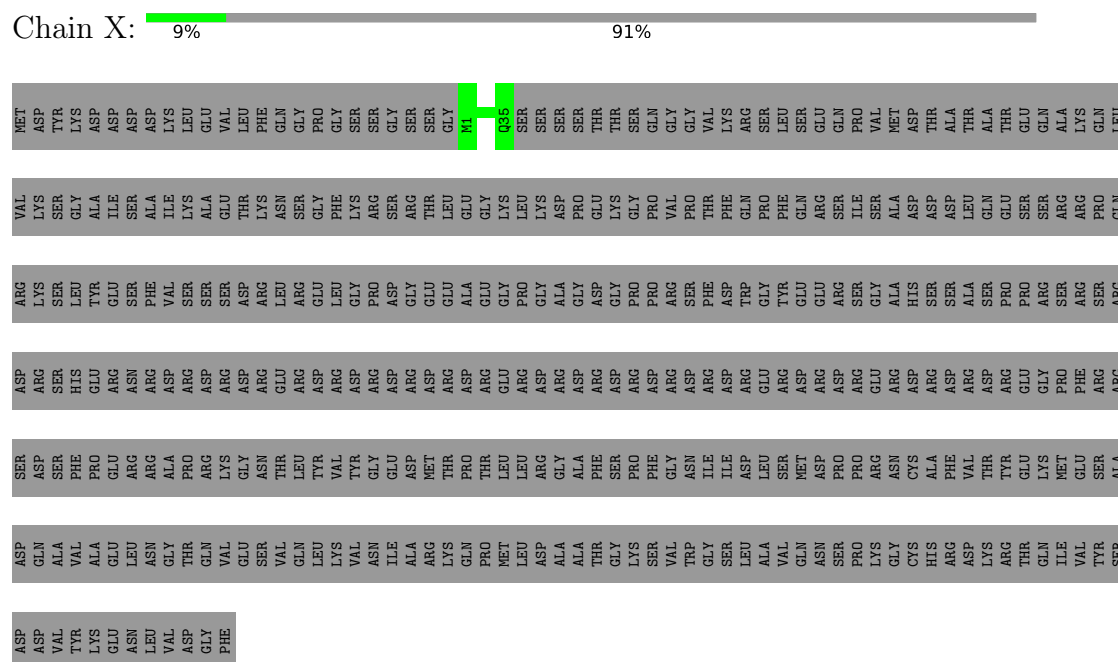
Chain V: 6% 93% 7%



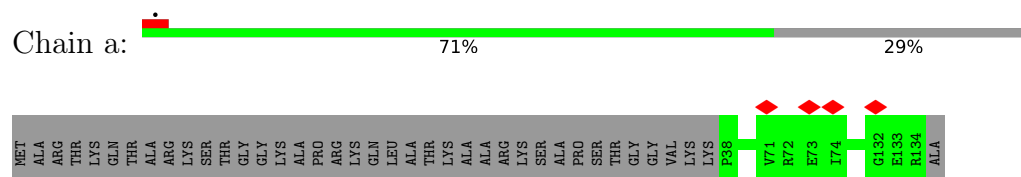
- Molecule 20: Negative elongation factor C/D



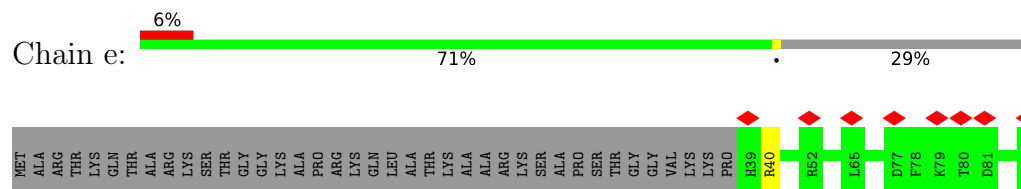
- Molecule 21: Negative elongation factor E




- Molecule 22: Histone H3.3

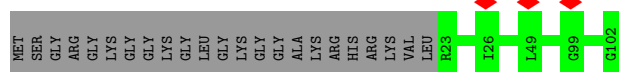


- Molecule 22: Histone H3.3




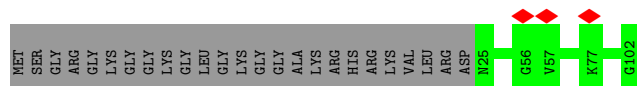
- Molecule 23: Histone H4

Chain b:  78% 22%




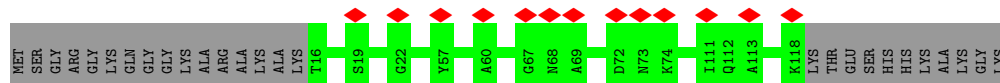
- Molecule 23: Histone H4

Chain f:  76% 24%




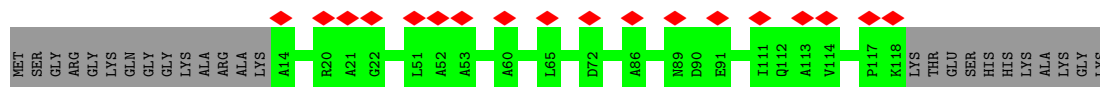
- Molecule 24: Histone H2A type 1-B/E

Chain c:  10% 79% 21%




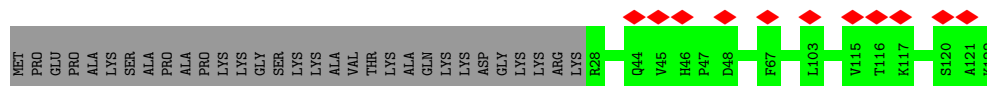
- Molecule 24: Histone H2A type 1-B/E

Chain g:  14% 81% 19%




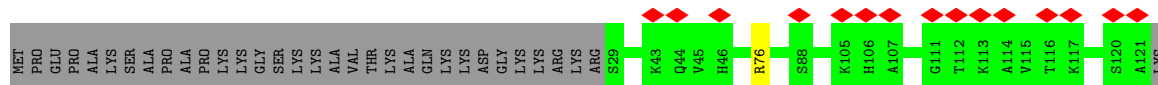
- Molecule 25: Histone H2B type 1-J

Chain d:  9% 75% 25%



- Molecule 25: Histone H2B type 1-J

Chain h:  12% 73% 26%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22970	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	0.114	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: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/11248	0.50	0/15179
2	B	0.27	0/9149	0.51	0/12348
3	C	0.27	0/2115	0.49	0/2873
4	D	0.24	0/1017	0.46	0/1368
5	E	0.26	0/1751	0.51	0/2366
6	F	0.26	0/636	0.50	0/859
7	G	0.26	0/1364	0.49	0/1853
8	H	0.28	0/1219	0.51	0/1644
9	I	0.24	0/964	0.50	0/1305
10	J	0.28	0/542	0.46	0/730
11	K	0.28	0/939	0.49	0/1271
12	L	0.28	0/395	0.61	0/524
13	Y	0.23	0/927	0.48	0/1250
14	Z	0.25	0/3903	0.51	0/5254
15	T	0.51	0/4384	0.84	0/6754
16	N	0.50	0/4147	0.96	0/6407
17	P	0.21	0/372	0.76	0/576
18	U	0.24	0/1463	0.48	0/1985
19	V	0.25	0/4424	0.47	1/5975 (0.0%)
20	W	0.25	0/4404	0.44	0/5982
21	X	0.25	0/283	0.34	0/372
22	a	0.24	0/809	0.52	0/1085
22	e	0.24	0/807	0.53	0/1081
23	b	0.24	0/645	0.53	0/862
23	f	0.24	0/626	0.54	0/837
24	c	0.24	0/806	0.52	0/1089
24	g	0.23	0/820	0.53	0/1107
25	d	0.23	0/757	0.47	0/1015
25	h	0.24	0/736	0.47	0/990
All	All	0.30	0/61652	0.58	1/84941 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	513	PRO	CA-N-CD	-5.18	104.25	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1381/1970 (70%)	1314 (95%)	67 (5%)	0	100	100
2	B	1111/1174 (95%)	1046 (94%)	65 (6%)	0	100	100
3	C	254/271 (94%)	240 (94%)	13 (5%)	1 (0%)	30	61
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
6	F	76/127 (60%)	75 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
8	H	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
9	I	114/125 (91%)	113 (99%)	1 (1%)	0	100	100
10	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	Y	114/118 (97%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	Z	468/1107 (42%)	446 (95%)	22 (5%)	0	100	100
18	U	185/528 (35%)	179 (97%)	6 (3%)	0	100	100
19	V	538/580 (93%)	531 (99%)	7 (1%)	0	100	100
20	W	541/611 (88%)	531 (98%)	10 (2%)	0	100	100
21	X	33/404 (8%)	33 (100%)	0	0	100	100
22	a	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
22	e	95/136 (70%)	95 (100%)	0	0	100	100
23	b	78/103 (76%)	78 (100%)	0	0	100	100
23	f	76/103 (74%)	76 (100%)	0	0	100	100
24	c	101/130 (78%)	100 (99%)	1 (1%)	0	100	100
24	g	103/130 (79%)	101 (98%)	2 (2%)	0	100	100
25	d	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
25	h	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
All	All	6416/8921 (72%)	6178 (96%)	237 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	92	GLU

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%)	1227 (100%)	2 (0%)	92	95
2	B	985/1027 (96%)	982 (100%)	3 (0%)	91	94
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%)	190 (100%)	1 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	422 (100%)	1 (0%)	92	95
18	U	161/451 (36%)	161 (100%)	0	100	100
19	V	485/515 (94%)	483 (100%)	2 (0%)	89	93
20	W	480/530 (91%)	480 (100%)	0	100	100
21	X	31/351 (9%)	31 (100%)	0	100	100
22	a	83/110 (76%)	83 (100%)	0	100	100
22	e	82/110 (74%)	81 (99%)	1 (1%)	67	80
23	b	65/79 (82%)	65 (100%)	0	100	100
23	f	63/79 (80%)	63 (100%)	0	100	100
24	c	82/100 (82%)	82 (100%)	0	100	100
24	g	83/100 (83%)	83 (100%)	0	100	100
25	d	81/105 (77%)	81 (100%)	0	100	100
25	h	79/105 (75%)	78 (99%)	1 (1%)	65	79
All	All	5700/7760 (74%)	5689 (100%)	11 (0%)	91	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	V	502	ARG
19	V	513	PRO
25	h	76	ARG
22	e	40	ARG
2	B	592	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
20	W	401	ASN
22	a	108	ASN
24	g	110	ASN
8	H	131	ASN
12	L	26	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	P	15/16 (93%)	3 (20%)	1 (6%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	P	3	U
17	P	5	A
17	P	14	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	P	4	U

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

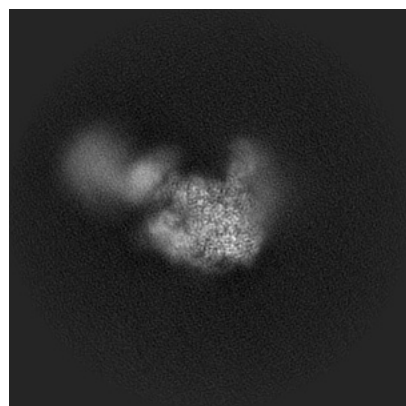
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61060. These allow visual inspection of the internal detail of the map and identification of artifacts.

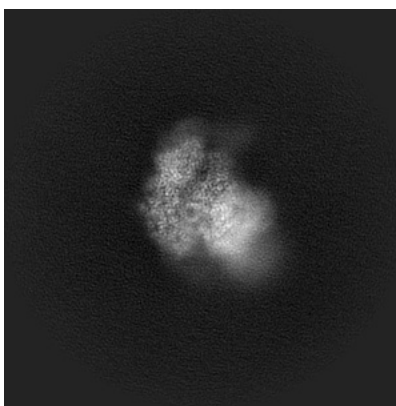
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

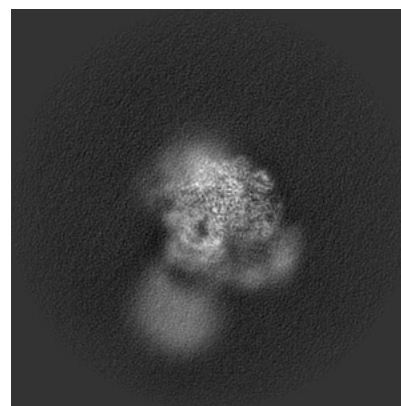
6.1.1 Primary map



X

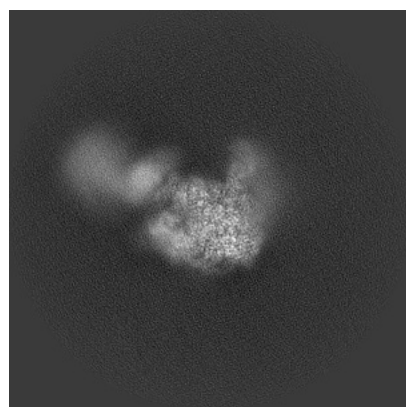


Y

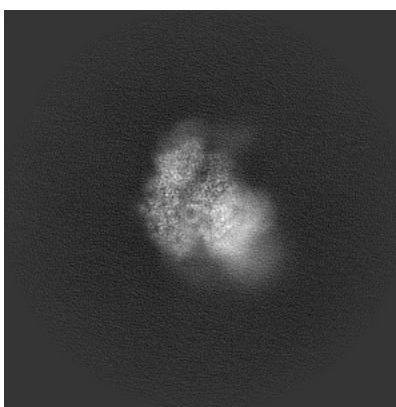


Z

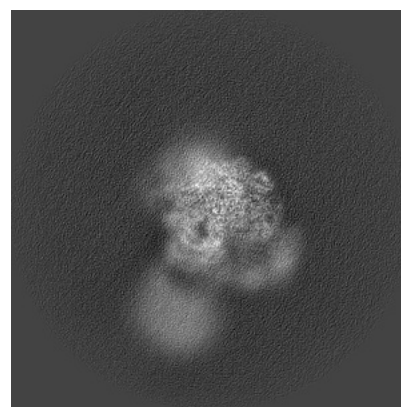
6.1.2 Raw map



X



Y

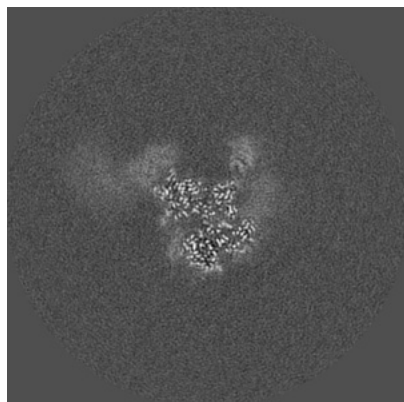


Z

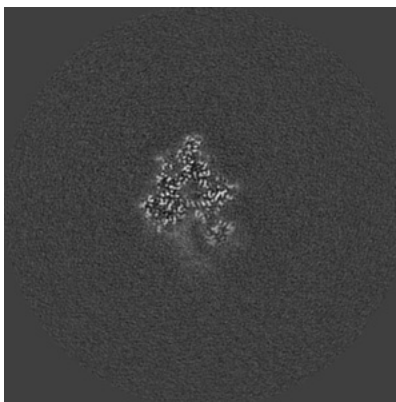
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

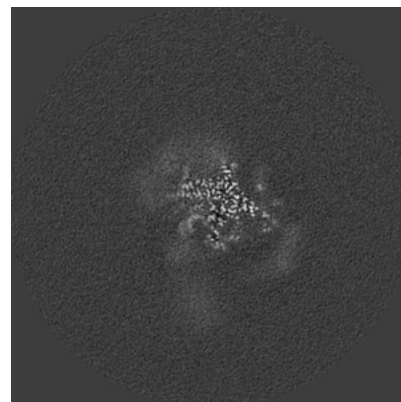
6.2.1 Primary map



X Index: 175

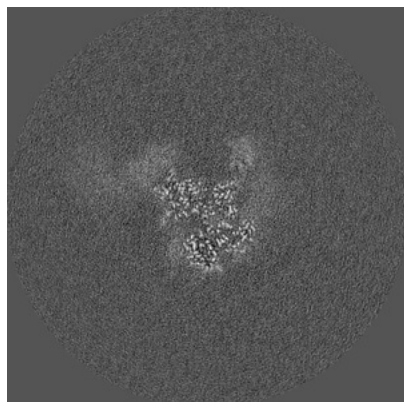


Y Index: 175

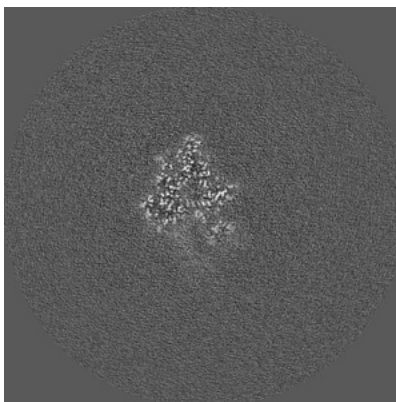


Z Index: 175

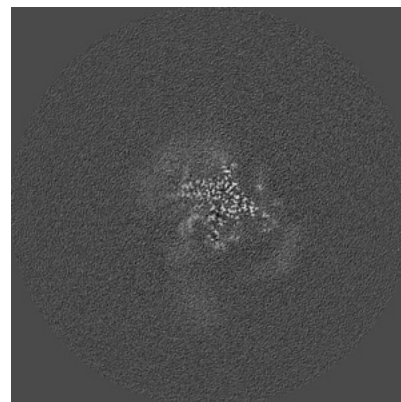
6.2.2 Raw map



X Index: 175



Y Index: 175

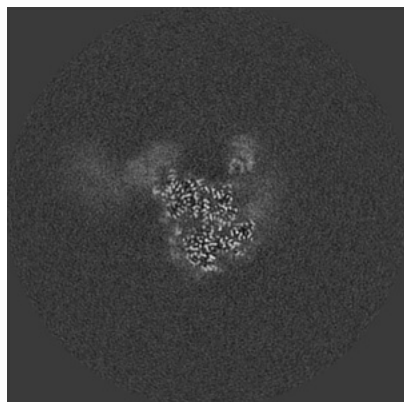


Z Index: 175

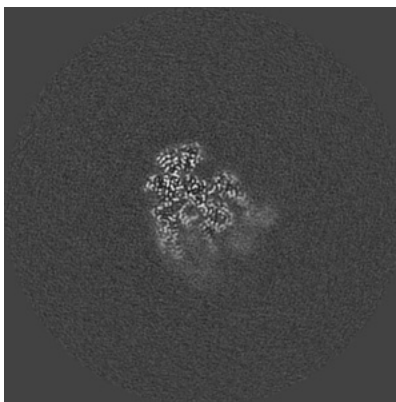
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

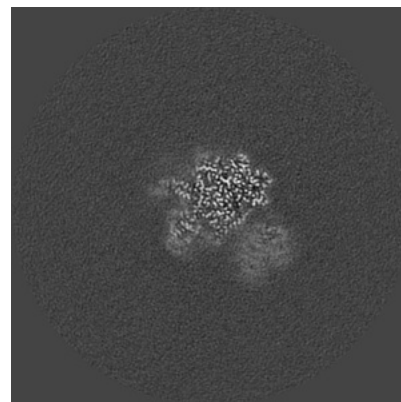
6.3.1 Primary map



X Index: 177

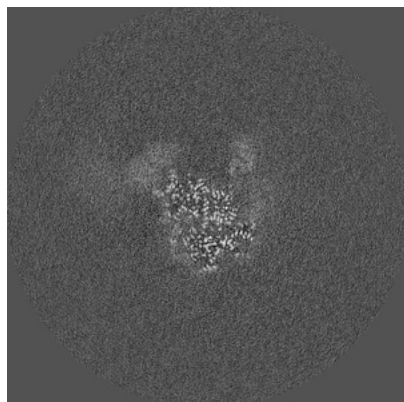


Y Index: 195

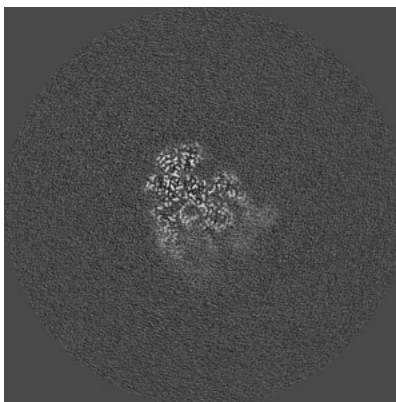


Z Index: 148

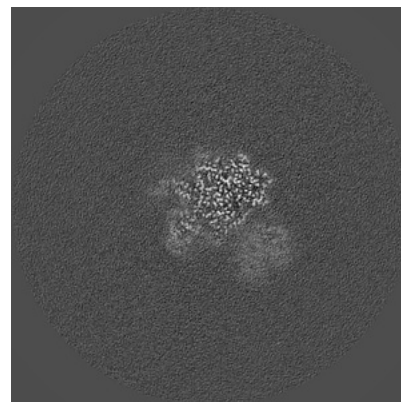
6.3.2 Raw map



X Index: 178



Y Index: 195

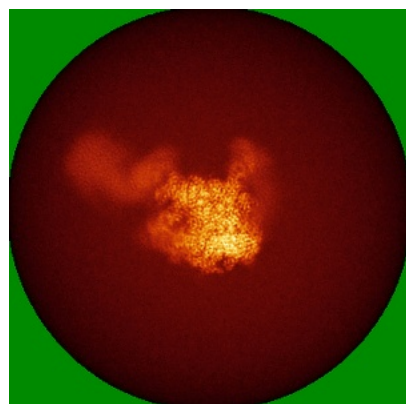


Z Index: 148

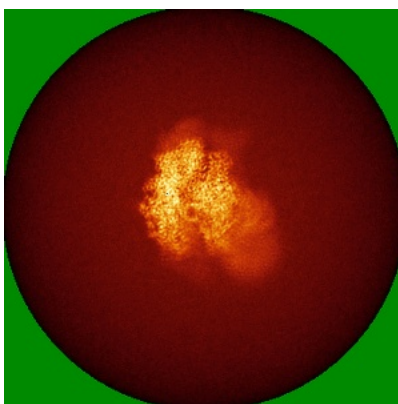
The images above show the largest variance slices of the map in three orthogonal directions.

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

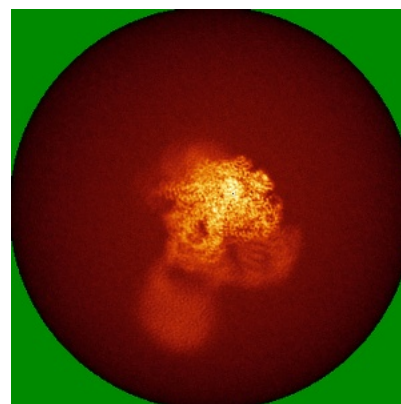
6.4.1 Primary map



X

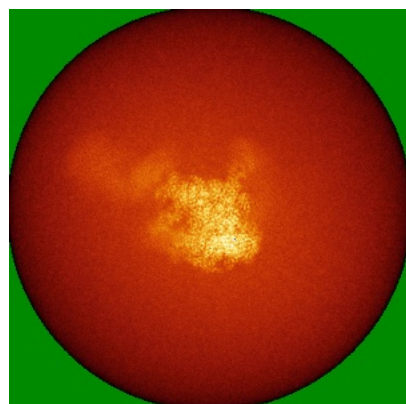


Y

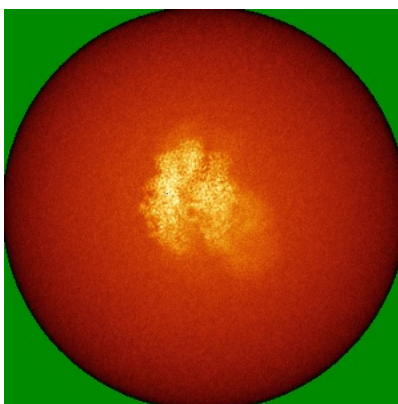


Z

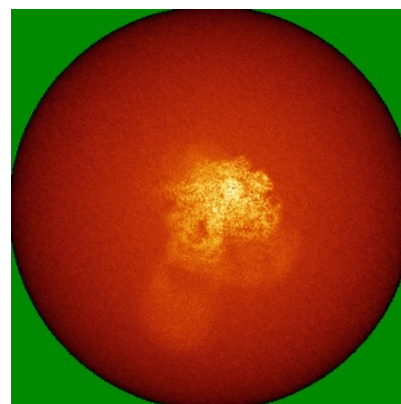
6.4.2 Raw map



X



Y

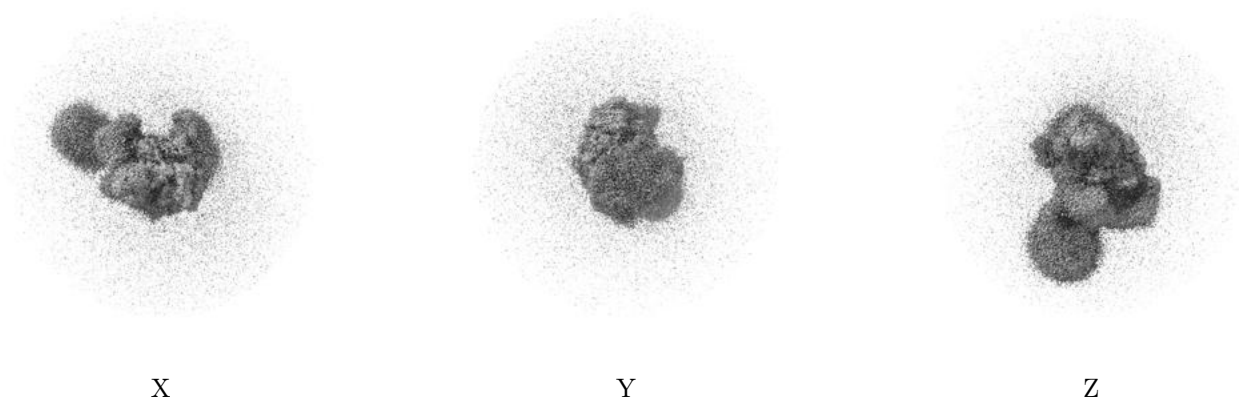


Z

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.

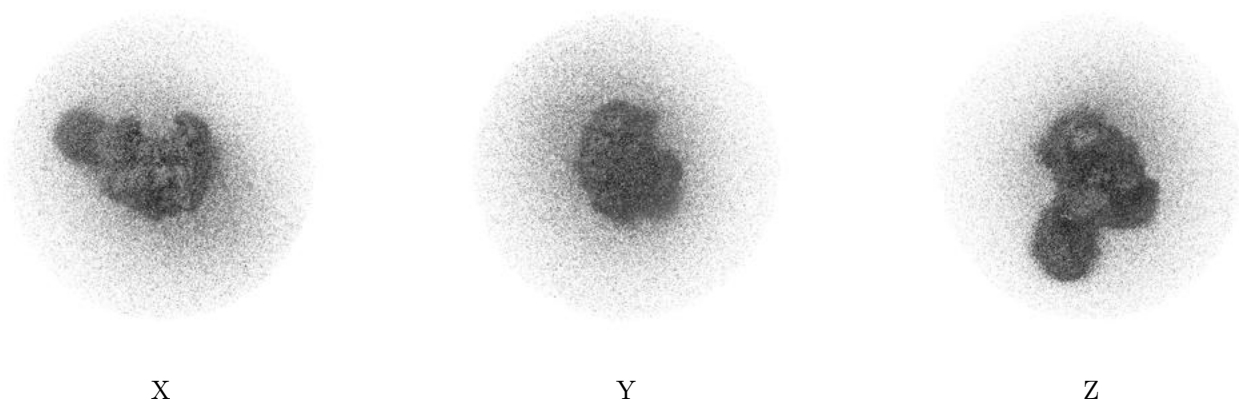
6.5 Orthogonal surface views [i](#)

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.

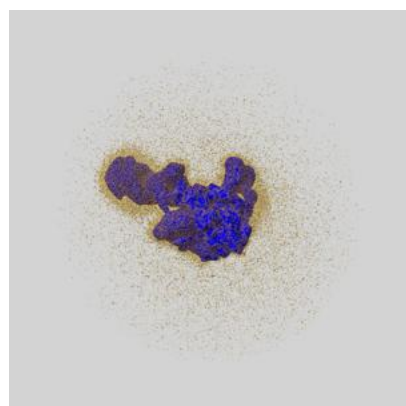
6.6 Mask visualisation [i](#)

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

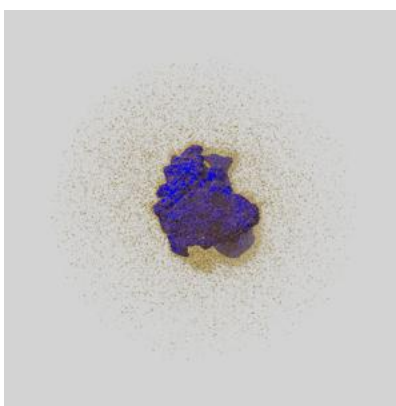
A mask typically either:

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

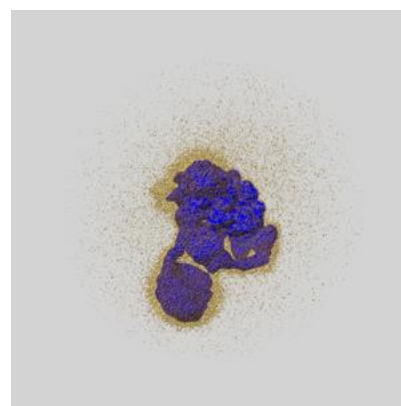
6.6.1 emd_61060_msk_1.map [i](#)



X



Y

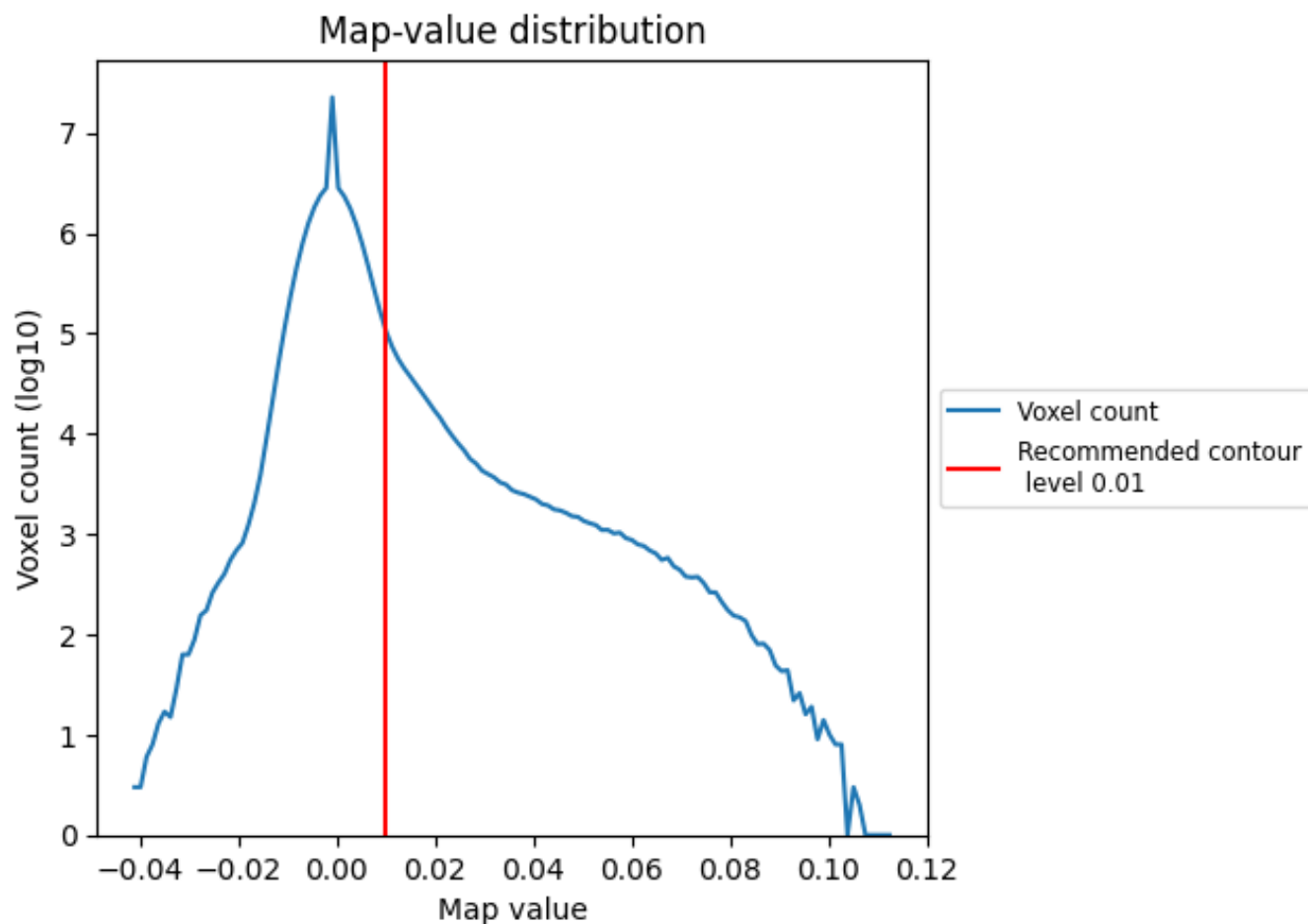


Z

7 Map analysis [i](#)

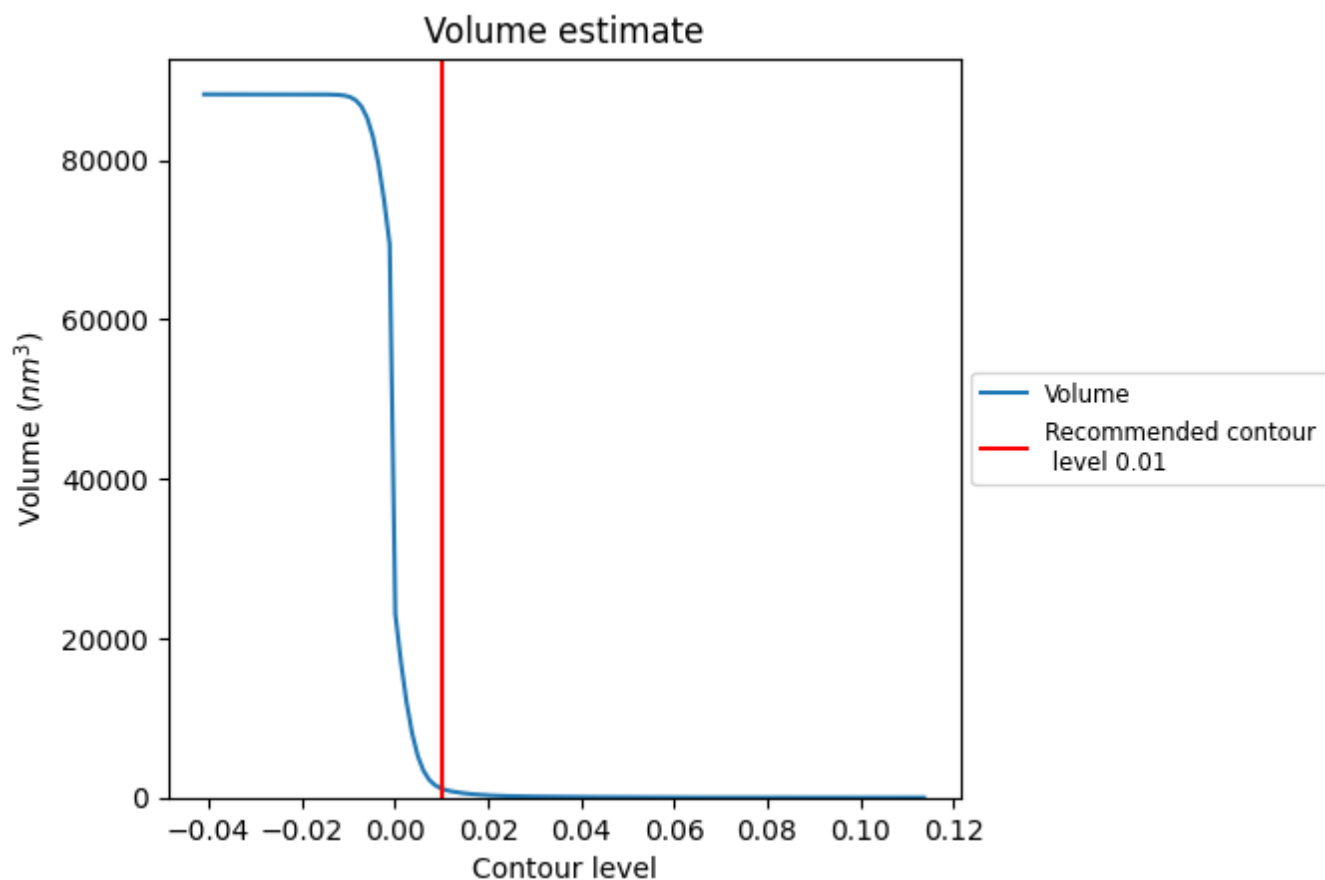
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

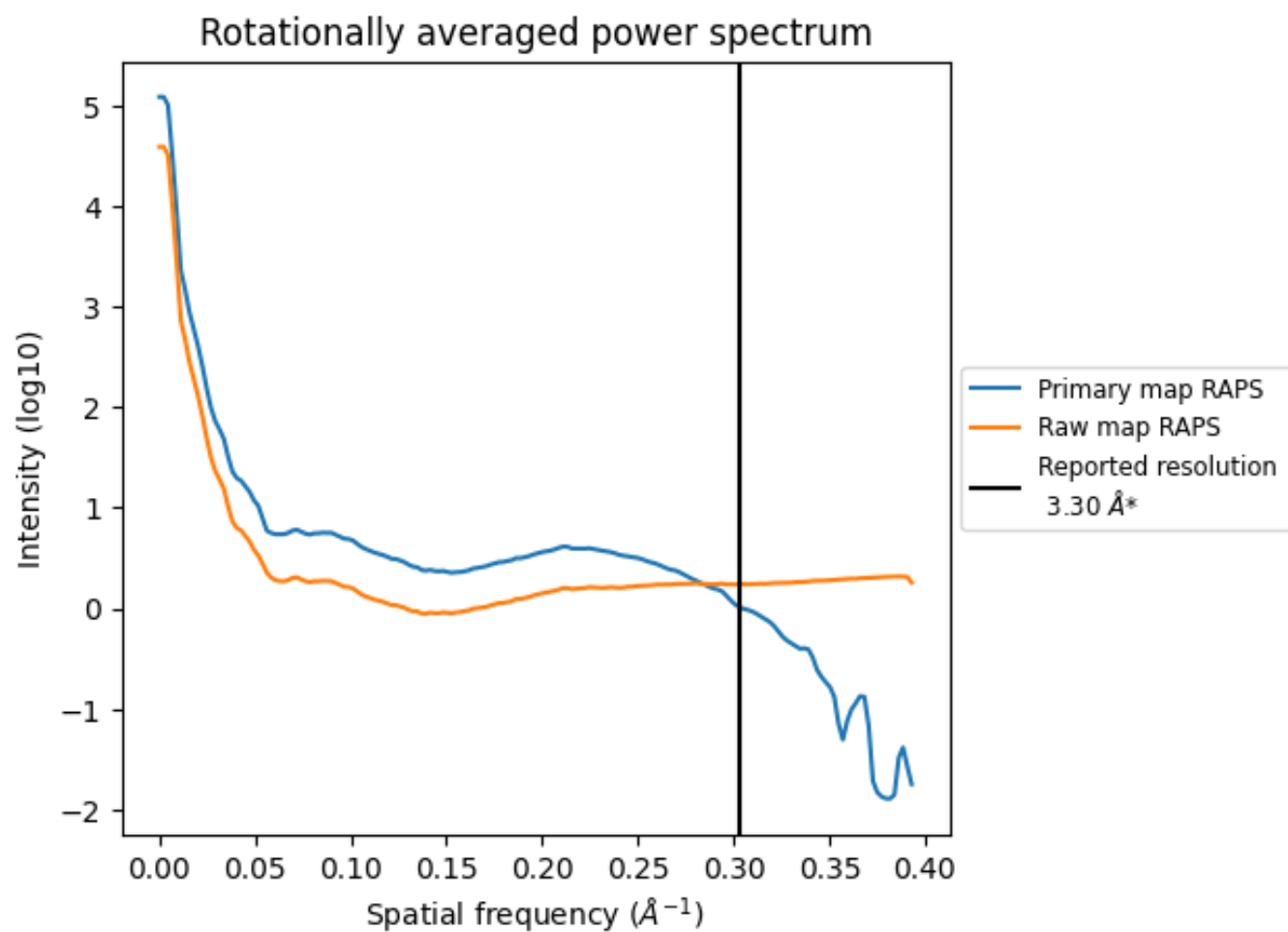
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1141 nm³; this corresponds to an approximate mass of 1030 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 ⓘ

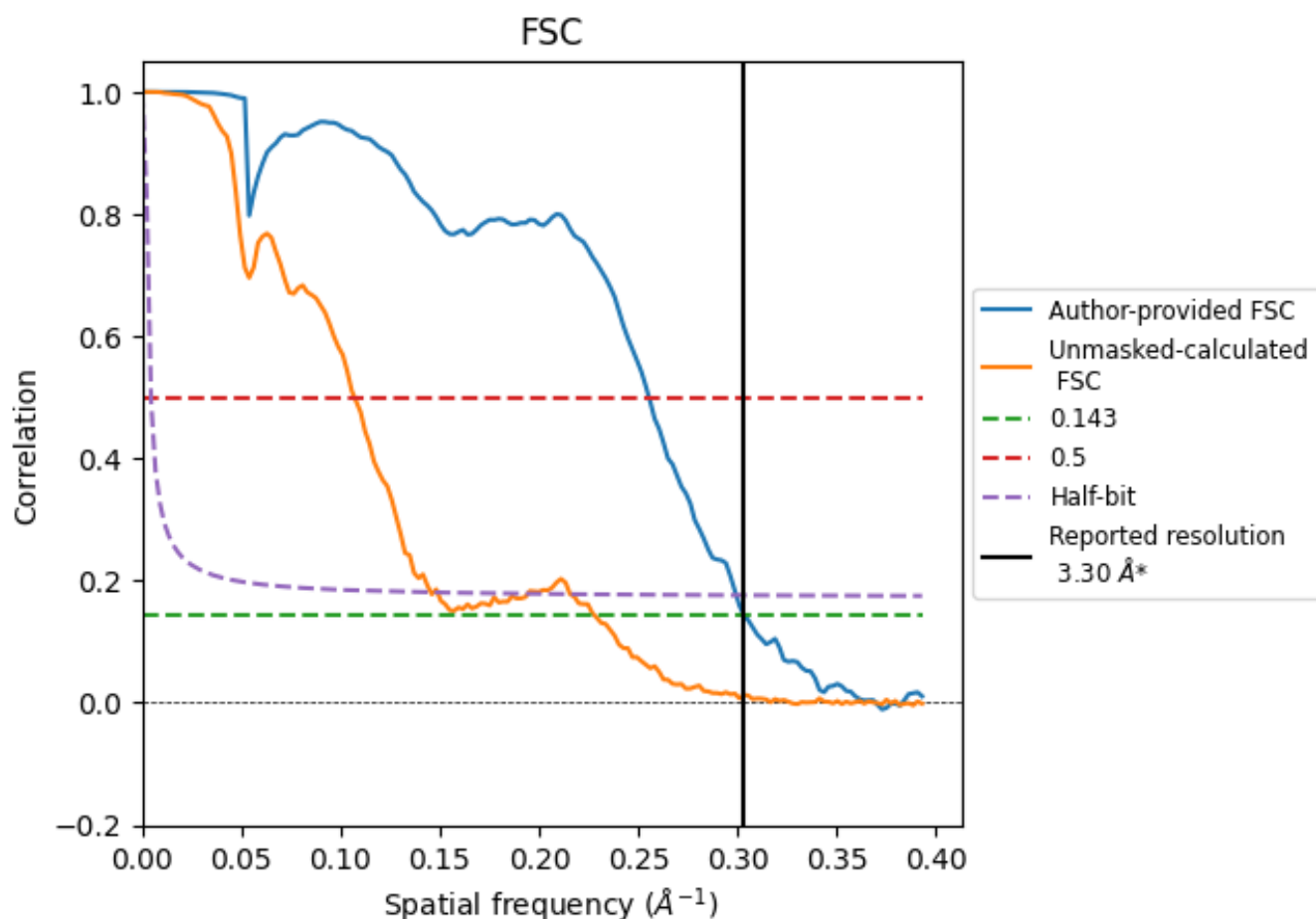


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 Å⁻¹

8.2 Resolution estimates [i](#)

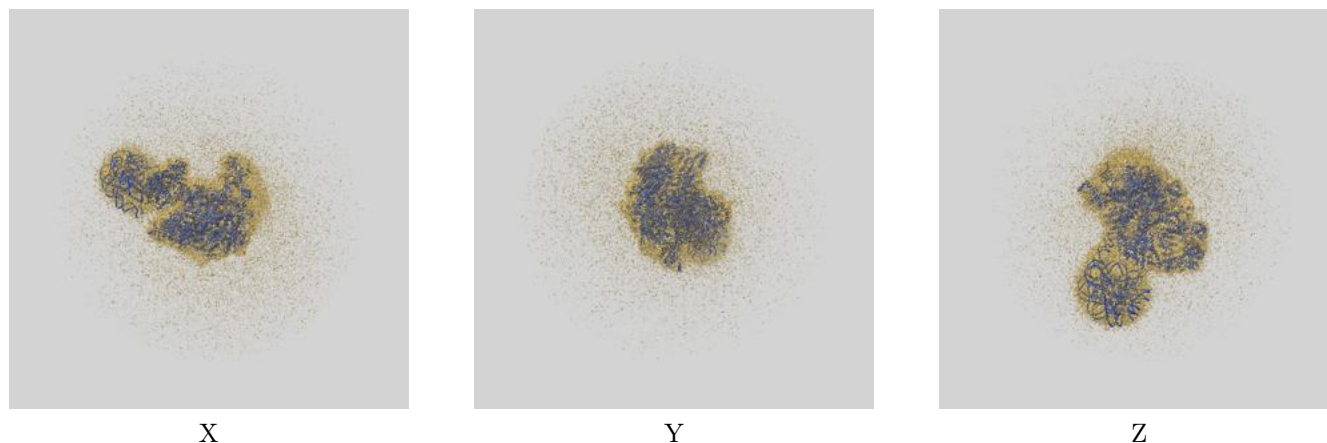
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.92	3.34
Unmasked-calculated*	4.39	9.35	6.87

*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](#)

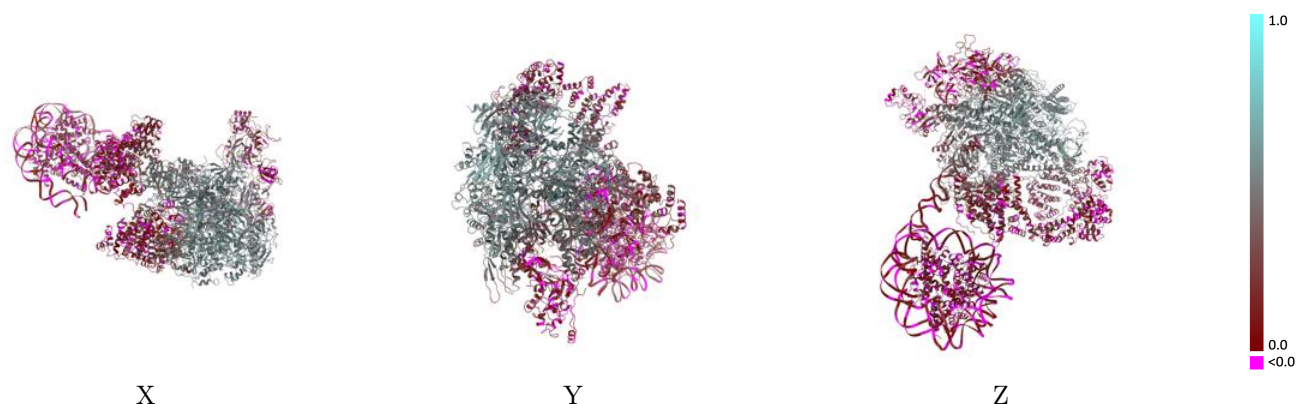
This section contains information regarding the fit between EMDB map EMD-61060 and PDB model 9J0P. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



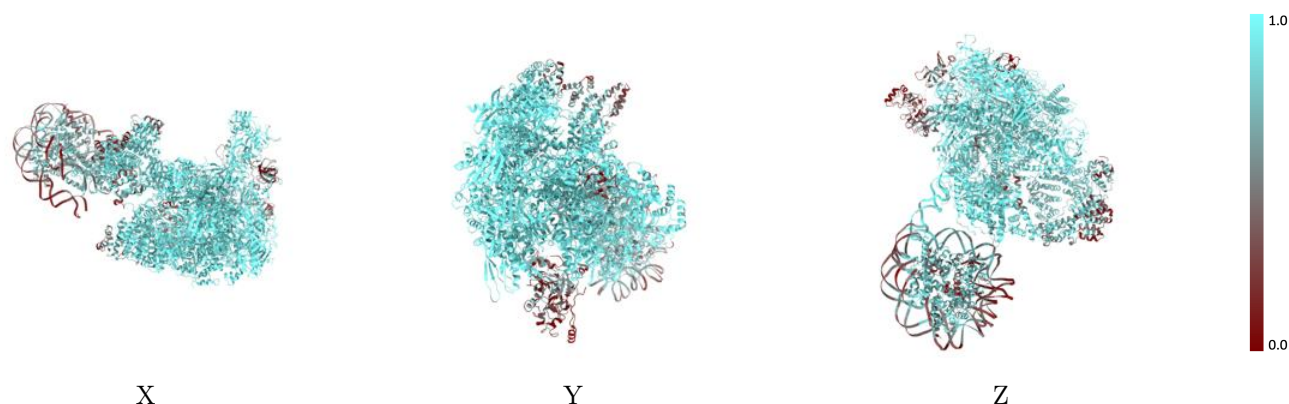
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



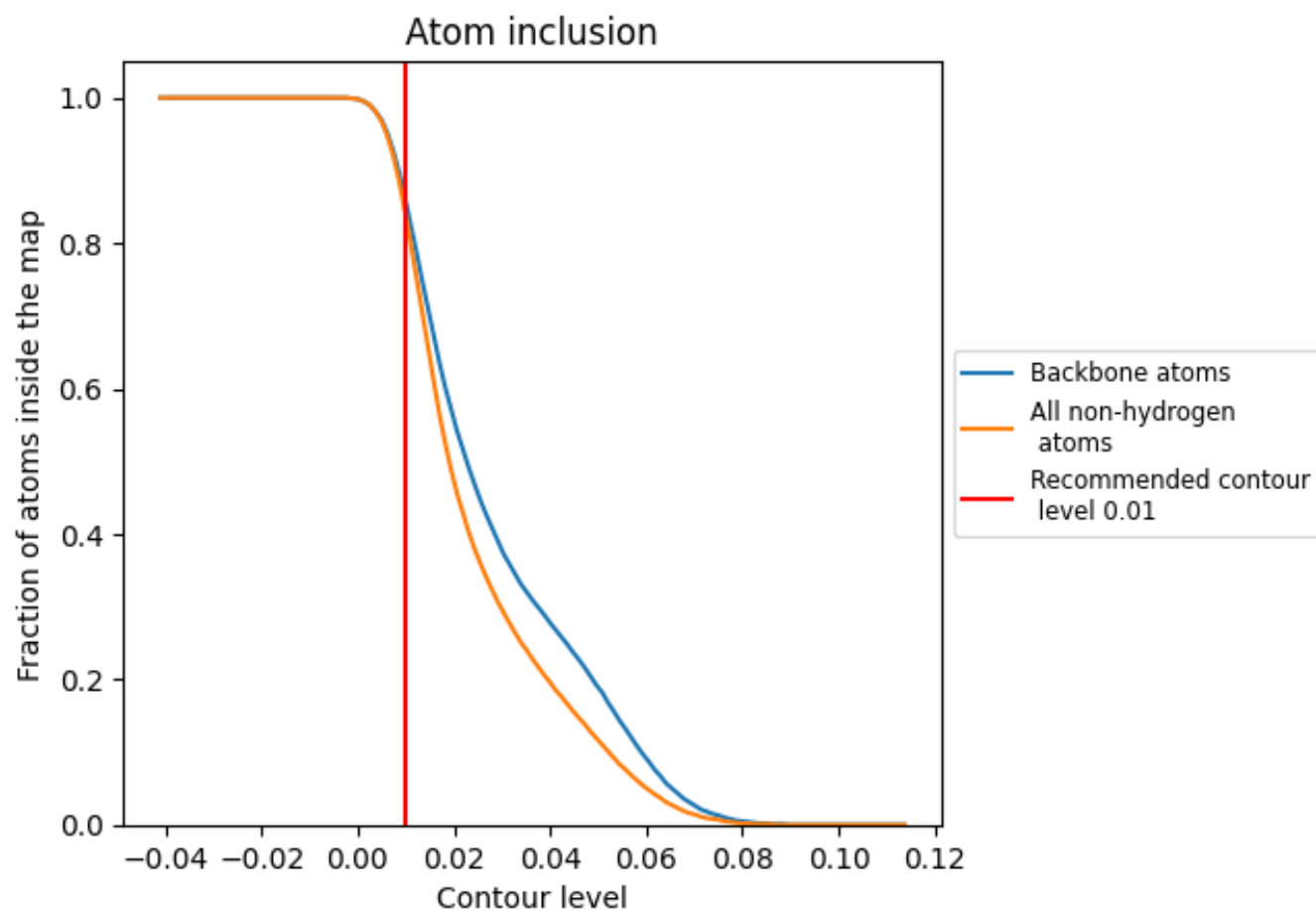
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 84% 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	 0.8370	 0.3110
A	 0.9740	 0.4890
B	 0.9810	 0.4970
C	 0.9870	 0.5370
D	 0.9380	 0.2150
E	 0.9760	 0.4800
F	 0.9850	 0.5360
G	 0.9570	 0.2930
H	 0.9780	 0.5250
I	 0.9230	 0.3220
J	 0.9870	 0.5560
K	 0.9920	 0.5450
L	 0.9920	 0.4710
N	 0.5830	 0.0970
P	 0.9610	 0.4770
T	 0.6100	 0.1280
U	 0.7350	 0.1500
V	 0.8410	 0.1520
W	 0.7830	 0.1600
X	 0.9360	 0.2100
Y	 0.2330	 0.0950
Z	 0.5750	 0.1510
a	 0.8460	 0.1030
b	 0.8170	 0.0870
c	 0.7200	 0.0960
d	 0.7130	 0.0820
e	 0.7710	 0.1420
f	 0.7980	 0.1090
g	 0.6840	 0.1030
h	 0.6650	 0.0870

