



## wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 12:11 PM JST

PDB ID : 6J4X  
EMDB ID : EMD-0672  
Title : RNA polymerase II elongation complex bound with Elf1 and Spt4/5, stalled at SHL(-1) of the nucleosome (+1A)  
Authors : Ehara, H.; Kujirai, T.; Fujino, Y.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.  
Deposited on : 2019-01-10  
Resolution : 4.30 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](mailto: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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

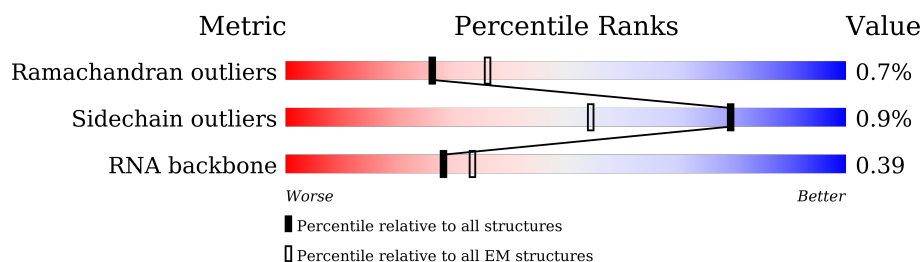
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	1743	 8% 80% 19%
2	B	1227	 7% 92% 6%
3	C	304	 1% 85% 13%
4	D	186	 76% 87% 10%
5	E	214	 5% 98% 2%
6	F	155	 1% 54% 46%
7	G	171	 55% 99% 1%
8	H	145	 1% 90% 8%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	16	
14	T	198	
15	N	198	
16	M	113	
17	V	108	
18	W	911	
19	a	139	
19	e	139	
20	b	106	
20	f	106	
21	c	133	
21	g	133	
22	d	129	
22	h	129	

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 46185 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	1411	Total	C	N	O	S	0	0
			11116	7009	1937	2100	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9228	5816	1630	1724	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a RNA chain called RNA (5'-R(P\*CP\*CP\*UP\*GP\*GP\*UP\*GP\*UP\*CP\*UP\*UP\*GP\*GP\*GP\*UP\*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	16	Total	C	N	O	P	0	0
			341	151	56	118	16		

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	127	Total	C	N	O	P	0	0
			2589	1227	486	750	126		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	122	Total	C	N	O	P	0	0
			2509	1188	459	740	122		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	64	Total	C	N	O	S	0	0
			505	318	82	99	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 17 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	102	Total	C	N	O	S	0	0
			792	492	143	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	initiating methionine	UNP C4R0E6

- Molecule 18 is a protein called Protein that forms a complex with Spt4p.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	275	Total	C	N	O	S	0	0
			2226	1425	397	403	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	GLY	-	expression tag	UNP C4R370
W	-1	PRO	-	expression tag	UNP C4R370
W	0	GLY	-	expression tag	UNP C4R370

- Molecule 19 is a protein called Histone H3.3.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 20 is a protein called Histone H4.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 21 is a protein called Histone H2A type 1-B/E.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 22 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
22	h	91	Total	C	N	O	S	0	0
			708	447	125	134	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

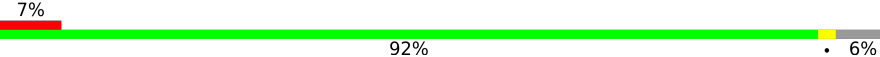


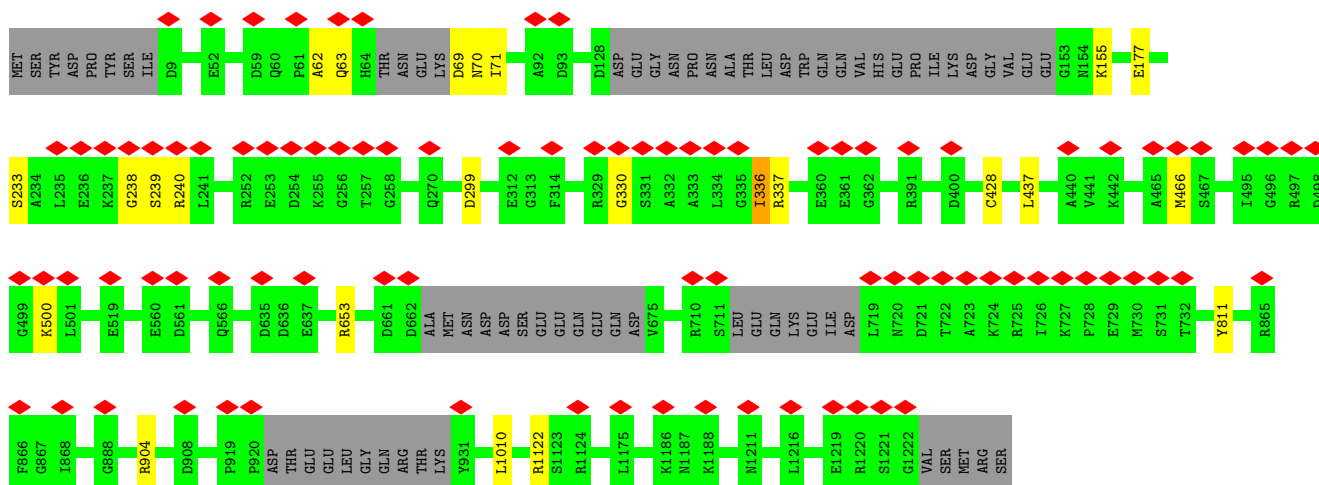
Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total 2	Zn 2	0
23	B	1	Total 1	Zn 1	0
23	C	1	Total 1	Zn 1	0
23	I	2	Total 2	Zn 2	0
23	J	1	Total 1	Zn 1	0
23	L	1	Total 1	Zn 1	0
23	M	1	Total 1	Zn 1	0
23	V	1	Total 1	Zn 1	0

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).


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

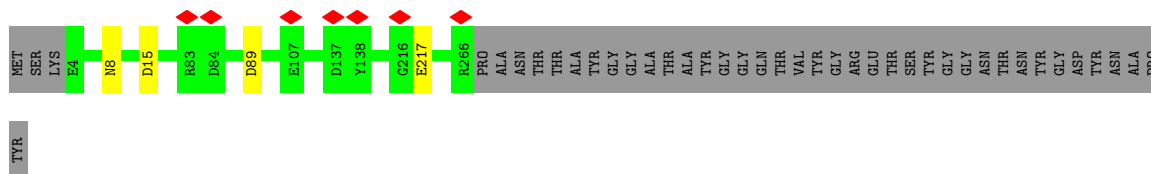


Chain B: 




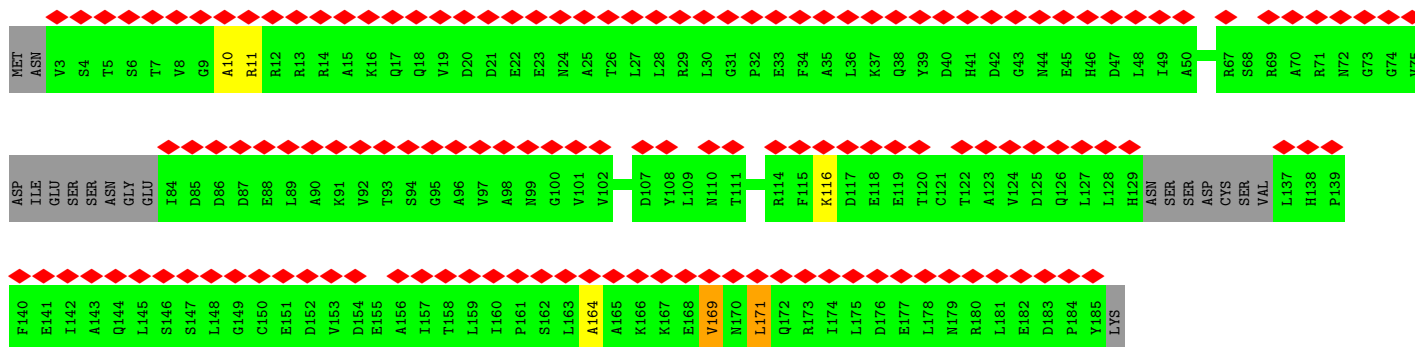
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C: 



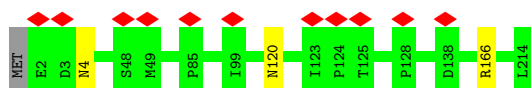
- Molecule 4: RNA polymerase II subunit B32

Chain D: 



- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

Chain E: 



- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F:  54% 46%

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

ILE LYS ALA HIS ARG LYS ARG SER ASN LYS E71 L72 I111 D154 ASN


- Molecule 7: RNA polymerase II subunit

Chain G:  55% 99%

W1 K5 D33 V34 E35 G36 T37 G40 Q41 F42 G43 Y44 M52 N53 K83 G84 E85 V86 V87 D88 A89 I90 V91 S92 N93 V94 S95 P96 I97 G98 F99 F100 A101 D102 V103 G104 P105 L106 N107 V108 F109 V110 S111 T112 R113 L114 I115 P116 D117 N118 L119 V120 Y121 N122 P123


S124 N125 S126 P127 A129 Y130 M131 S132 M133 D134 E135 L136 I137 T138 K139 G140 S141 K142 V143 L144 L145 K146 V147 V148 G149 T150 R151 T152 D153 V154 N155 E156 I157 Y158 A159 I160 G161 S162 I163 K164 E165 D166 F167 A170 I171

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

Chain H:  90% 8%

MET SER S3 G18 L65 ASP GLY GLU ASP GLU SER ALA ASN PHE SER K76 E108 R145


- Molecule 9: DNA-directed RNA polymerase subunit

Chain I:  50% 94%

MET ALA S3 F4 R5 L6 E9 D19 R20 E21 N22 Q23 R24 D33 L37 A38 E39 D40 E47 L48 I49 T50 N51 S52 E53 E54 T55 A56 S57 S58 V59 D60 D61 I62 G63 D64 D65 S71 D72 K73 E74 C75 P76 E77 C78 H79 S80 R81 D82 C83 V84 F85 F86

Q89 Q90 R91 R92 K93 D94 C103 L104 N105 C106 K107 Q108 T109 E113 SER GLU

- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J:  90% 8%

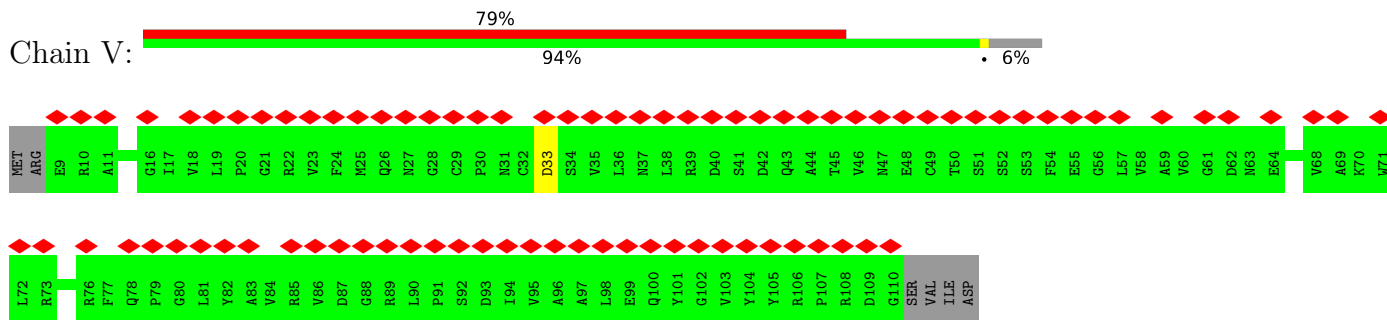
W1 P64 L65 E66 LYS LYS ASP PHE ASP SER

- Molecule 11: RNA polymerase II subunit B12.5

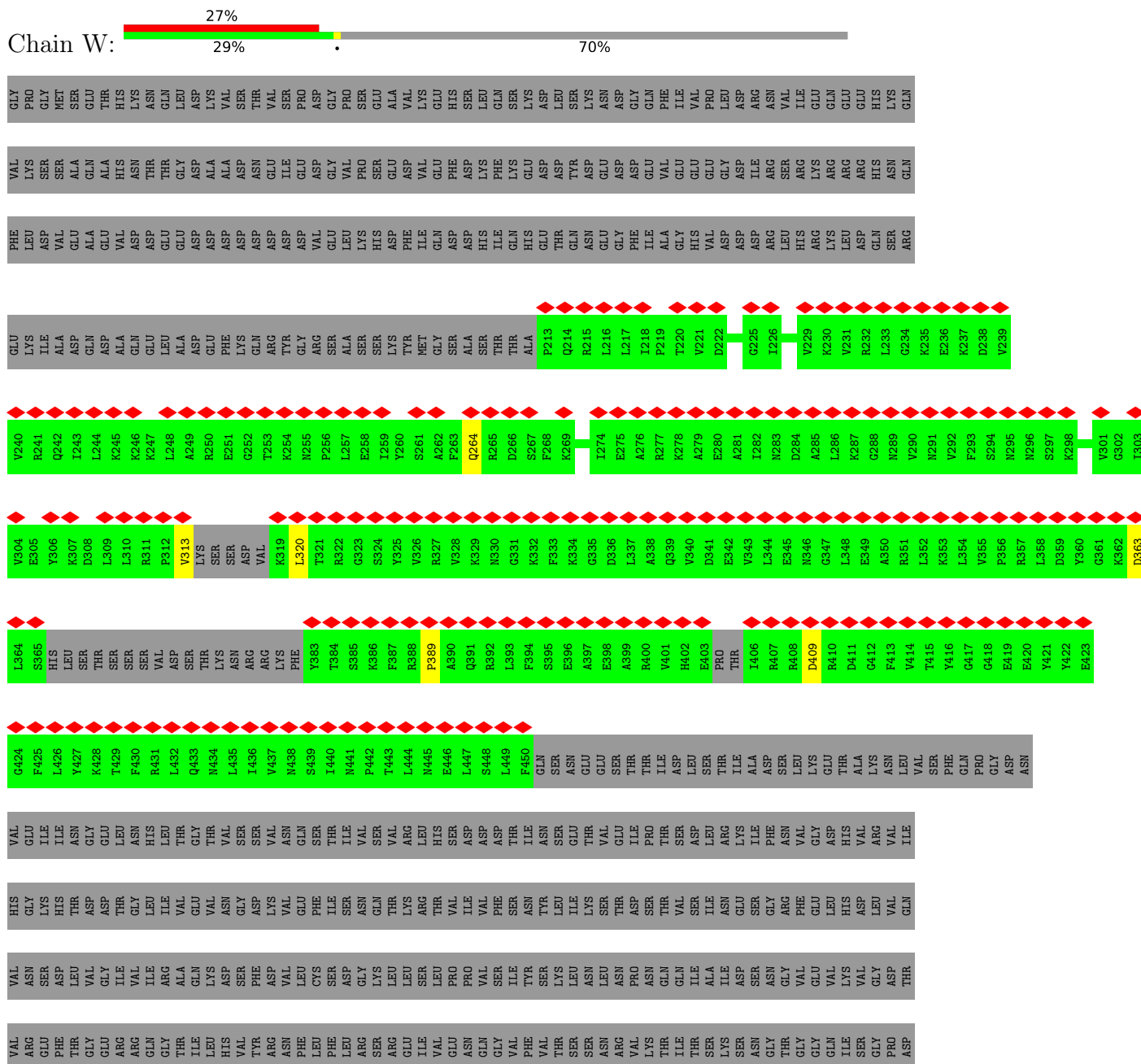
Chain K:  9% 96%

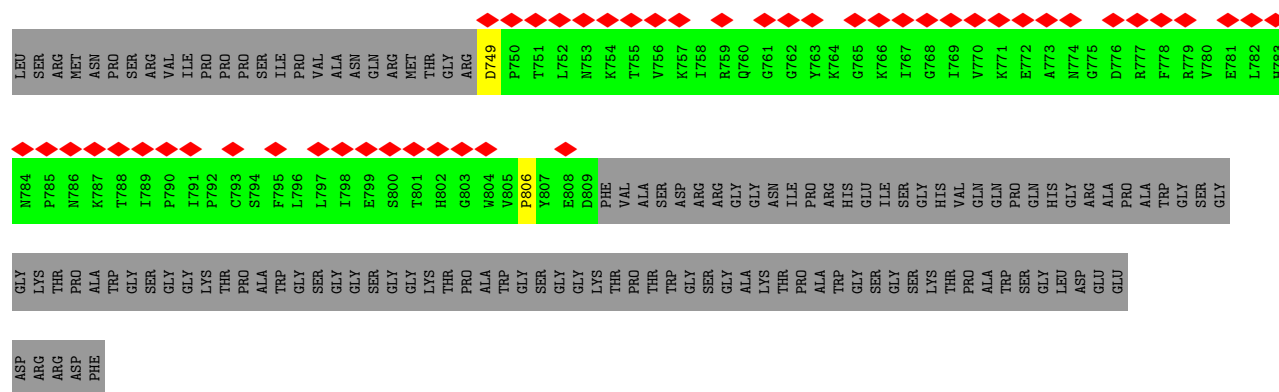


Chain V:

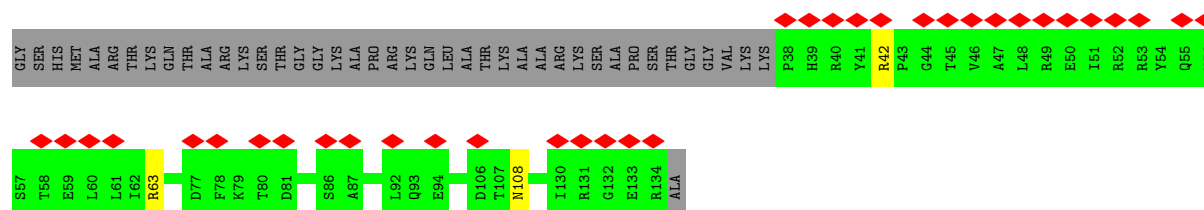


## Chain W:

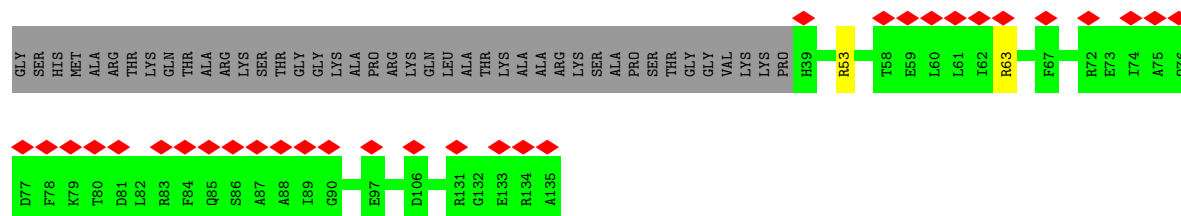




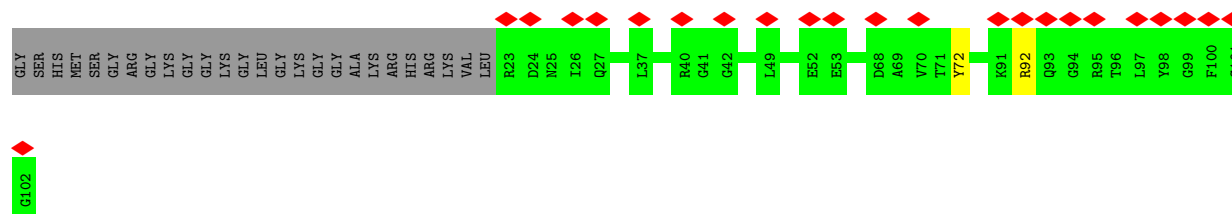
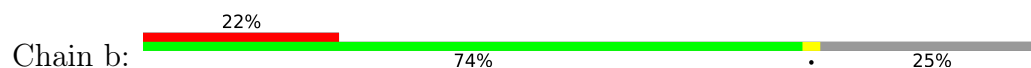
- Molecule 19: Histone H3.3



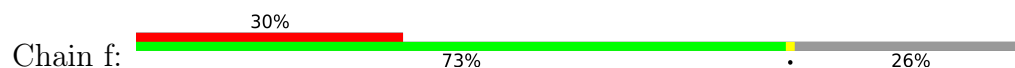
- Molecule 19: Histone H3.3

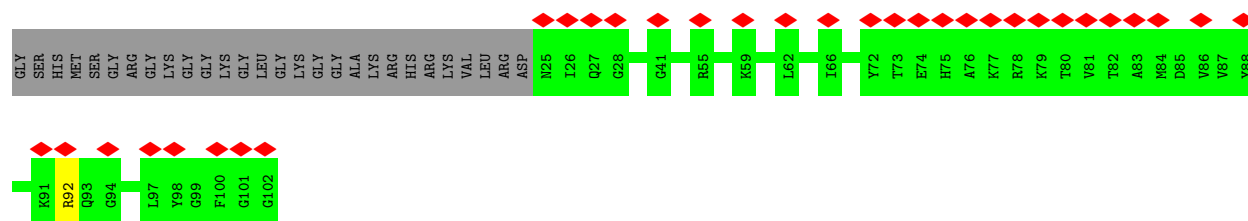


- Molecule 20: Histone H4

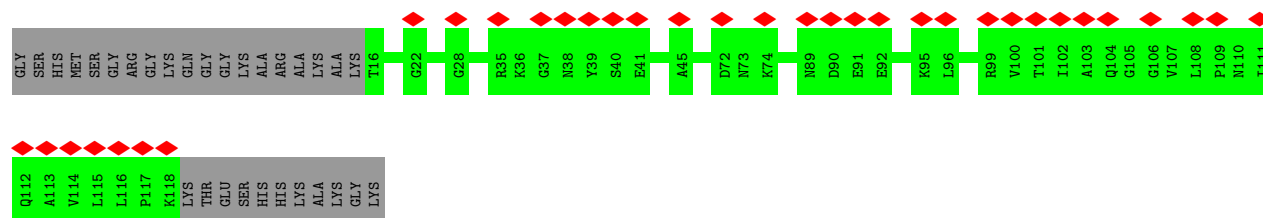
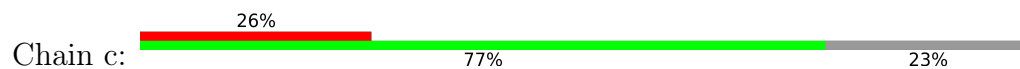


- Molecule 20: Histone H4

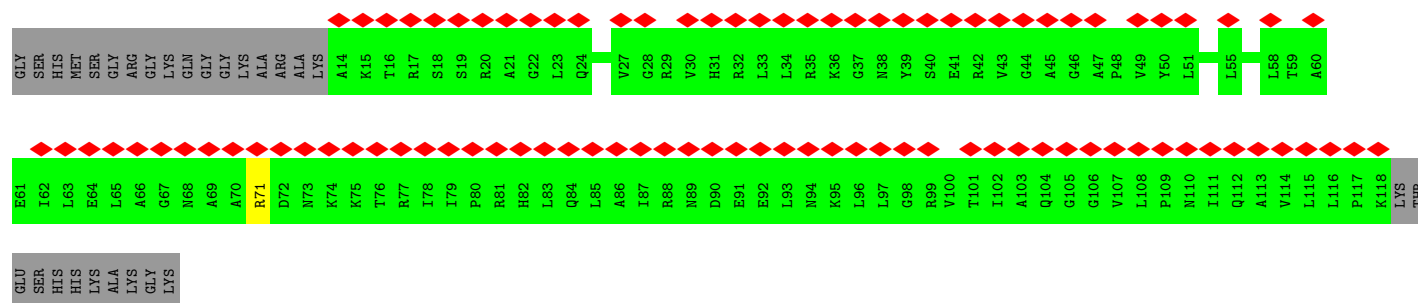
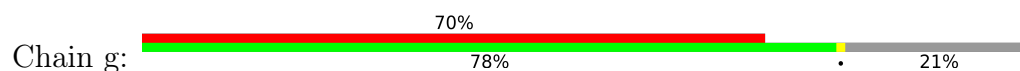




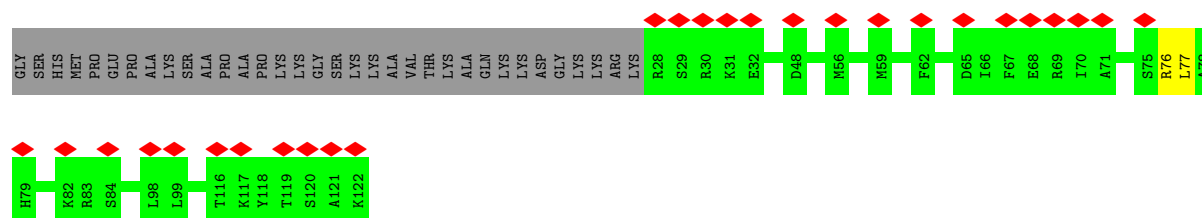
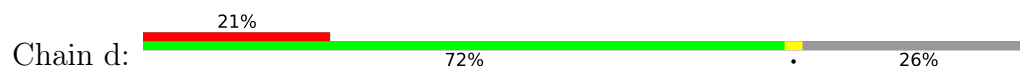
• Molecule 21: Histone H2A type 1-B/E



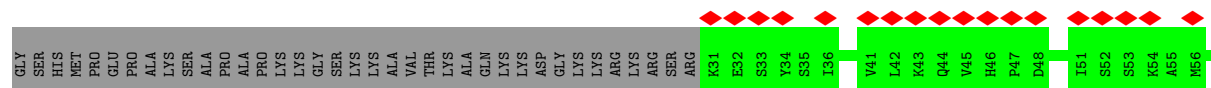
• Molecule 21: Histone H2A type 1-B/E



• Molecule 22: Histone H2B type 1-J



• Molecule 22: Histone H2B type 1-J





M60	S61	F62	V63	N64	D65	I66	F67	E68	R69	I70	A71	S75	R76	L77	A78	H79	Y80	N81	K82	R83	S84	T85	I86	T87	S88	R89	E90	I91	R96	L97	L98	L99	P100	G101	E102	L103	A107	V108	S109	E110	G111	T112	K113	A114	V115	T116	K117	Y118	T119	S120	A121	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size ( $\text{\AA}$ )	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.49, 1.49, 1.49	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	0.44	0/11322	0.67	6/15300 (0.0%)
2	B	0.48	0/9407	0.71	6/12685 (0.0%)
3	C	0.46	0/2139	0.72	1/2895 (0.0%)
4	D	0.32	0/1326	0.68	1/1788 (0.1%)
5	E	0.42	0/1772	0.64	0/2385
6	F	0.45	0/687	0.64	0/931
7	G	0.36	0/1353	0.71	0/1837
8	H	0.42	0/1069	0.67	0/1444
9	I	0.35	0/934	0.80	2/1257 (0.2%)
10	J	0.57	0/554	0.75	0/742
11	K	0.44	0/953	0.65	0/1291
12	L	0.46	0/365	0.76	0/484
13	P	1.11	3/379 (0.8%)	1.29	4/589 (0.7%)
14	T	1.07	2/2905 (0.1%)	1.08	3/4477 (0.1%)
15	N	1.13	10/2812 (0.4%)	1.09	0/4339
16	M	0.26	0/513	0.45	0/693
17	V	0.46	0/808	0.60	0/1097
18	W	0.40	0/2267	0.68	4/3048 (0.1%)
19	a	0.42	0/809	0.62	0/1085
19	e	0.45	0/807	0.55	0/1081
20	b	0.44	0/645	0.64	0/862
20	f	0.43	0/626	0.61	0/837
21	c	0.40	0/806	0.58	0/1089
21	g	0.36	0/820	0.55	0/1107
22	d	0.46	0/757	0.56	0/1015
22	h	0.41	0/719	0.56	0/968
All	All	0.57	15/47554 (0.0%)	0.75	27/65326 (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
2	B	0	1
19	a	0	2
19	e	0	1
All	All	0	4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	-2	G	C1'-N9	-7.33	1.36	1.46
13	P	-1	G	C1'-N9	-7.31	1.36	1.46
15	N	-37	DG	C1'-N9	-6.94	1.37	1.47
13	P	4	U	C1'-N1	6.65	1.58	1.48
15	N	-19	DG	C1'-N9	-6.59	1.38	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	389	PRO	CA-N-CD	-8.57	99.51	111.50
1	A	473	LEU	CA-CB-CG	-8.22	96.40	115.30
2	B	63	GLN	N-CA-CB	-7.67	96.80	110.60
2	B	63	GLN	N-CA-C	-6.91	92.33	111.00
14	T	-26	DT	O4'-C4'-C3'	-6.71	101.81	104.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	336	ILE	Mainchain
19	a	42	ARG	Peptide
19	a	63	ARG	Peptide
19	e	63	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

## 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	1399/1743 (80%)	1342 (96%)	47 (3%)	10 (1%)	22	62
2	B	1145/1227 (93%)	1082 (94%)	55 (5%)	8 (1%)	22	62
3	C	261/304 (86%)	253 (97%)	6 (2%)	2 (1%)	19	60
4	D	162/186 (87%)	149 (92%)	9 (6%)	4 (2%)	5	35
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	13	50
8	H	129/145 (89%)	125 (97%)	2 (2%)	2 (2%)	9	45
9	I	109/115 (95%)	102 (94%)	6 (6%)	1 (1%)	17	56
10	J	64/72 (89%)	61 (95%)	2 (3%)	1 (2%)	9	45
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	42 (98%)	0	1 (2%)	6	37
16	M	62/113 (55%)	58 (94%)	4 (6%)	0	100	100
17	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
18	W	265/911 (29%)	246 (93%)	17 (6%)	2 (1%)	19	60
19	a	95/139 (68%)	85 (90%)	10 (10%)	0	100	100
19	e	95/139 (68%)	89 (94%)	6 (6%)	0	100	100
20	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
20	f	76/106 (72%)	69 (91%)	7 (9%)	0	100	100
21	c	101/133 (76%)	92 (91%)	9 (9%)	0	100	100
21	g	103/133 (77%)	94 (91%)	9 (9%)	0	100	100
22	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
22	h	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	5042/6668 (76%)	4794 (95%)	215 (4%)	33 (1%)	26	62

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	287	GLN
1	A	960	VAL
1	A	1109	VAL
2	B	155	LYS

### 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	1224/1528 (80%)	1217 (99%)	7 (1%)	86	92
2	B	1012/1077 (94%)	1001 (99%)	11 (1%)	73	85
3	C	236/264 (89%)	235 (100%)	1 (0%)	91	94
4	D	143/160 (89%)	140 (98%)	3 (2%)	53	72
5	E	196/197 (100%)	193 (98%)	3 (2%)	65	80
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	105 (99%)	1 (1%)	78	88
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	37 (97%)	1 (3%)	46	67
16	M	61/99 (62%)	61 (100%)	0	100	100
17	V	86/92 (94%)	85 (99%)	1 (1%)	71	84
18	W	241/796 (30%)	239 (99%)	2 (1%)	81	89
19	a	83/112 (74%)	82 (99%)	1 (1%)	71	84
19	e	82/112 (73%)	81 (99%)	1 (1%)	71	84
20	b	65/81 (80%)	63 (97%)	2 (3%)	40	63
20	f	63/81 (78%)	62 (98%)	1 (2%)	62	79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	c	82/102 (80%)	82 (100%)	0	100	100
21	g	83/102 (81%)	82 (99%)	1 (1%)	71	84
22	d	81/107 (76%)	79 (98%)	2 (2%)	47	68
22	h	77/107 (72%)	75 (97%)	2 (3%)	46	67
All	All	4466/5772 (77%)	4426 (99%)	40 (1%)	79	88

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	W	264	GLN
19	e	53	ARG
18	W	313	VAL
20	b	92	ARG
21	g	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
21	g	31	HIS
21	g	110	ASN
5	E	4	ASN
3	C	242	GLN
21	g	112	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	15/16 (93%)	6 (40%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	-4	C
13	P	-3	U
13	P	-1	G
13	P	0	U
13	P	1	G

There are no RNA pucker outliers to report.

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

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

#### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

#### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



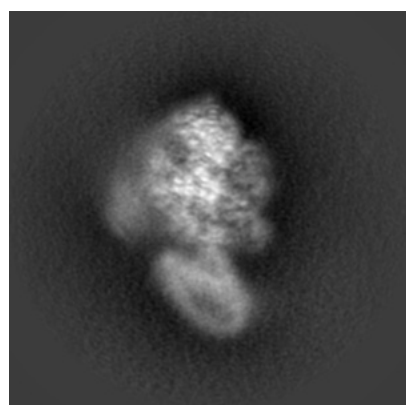
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0672. These allow visual inspection of the internal detail of the map and identification of artifacts.

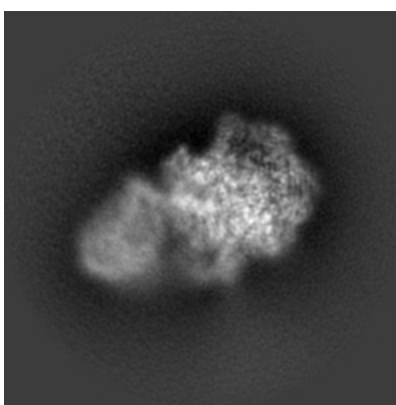
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

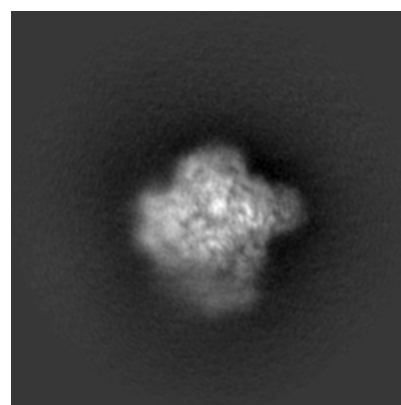
#### 6.1.1 Primary map



X



Y

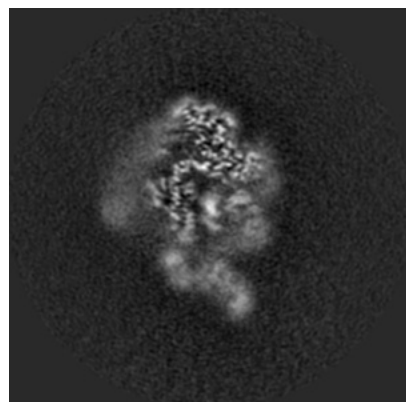


Z

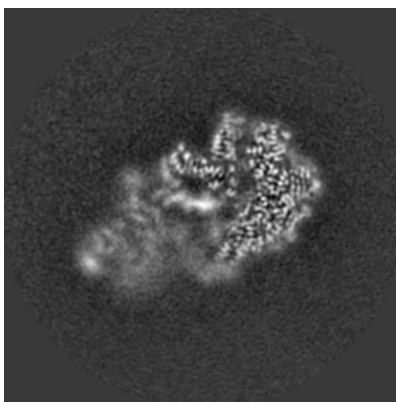
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

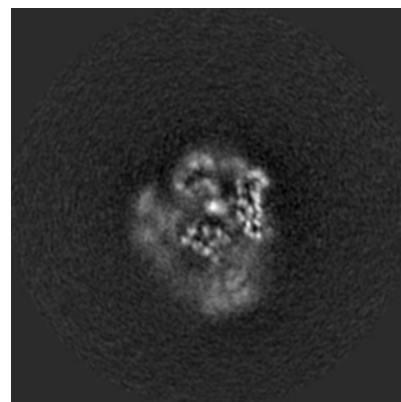
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

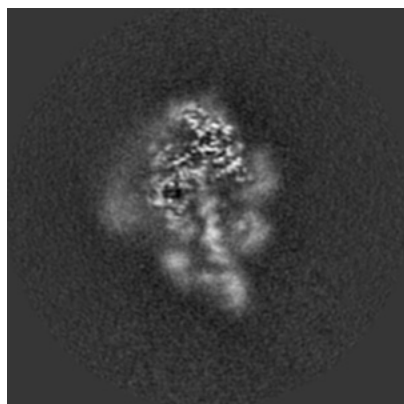


Z Index: 120

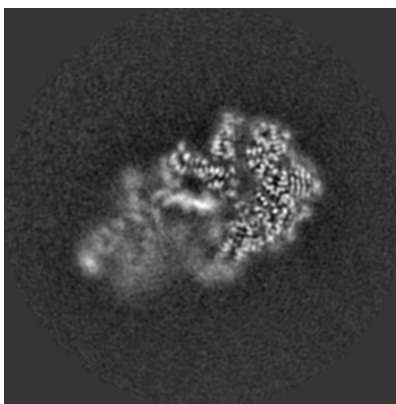
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

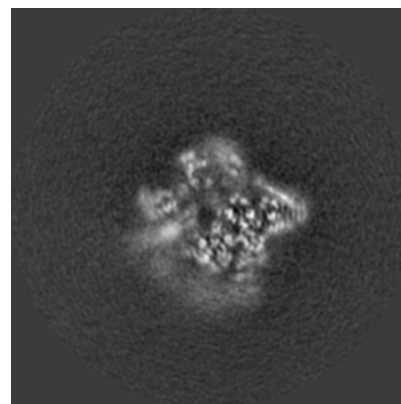
### 6.3.1 Primary map



X Index: 125



Y Index: 121



Z Index: 132

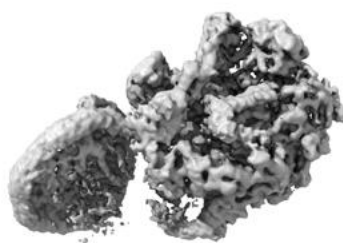
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

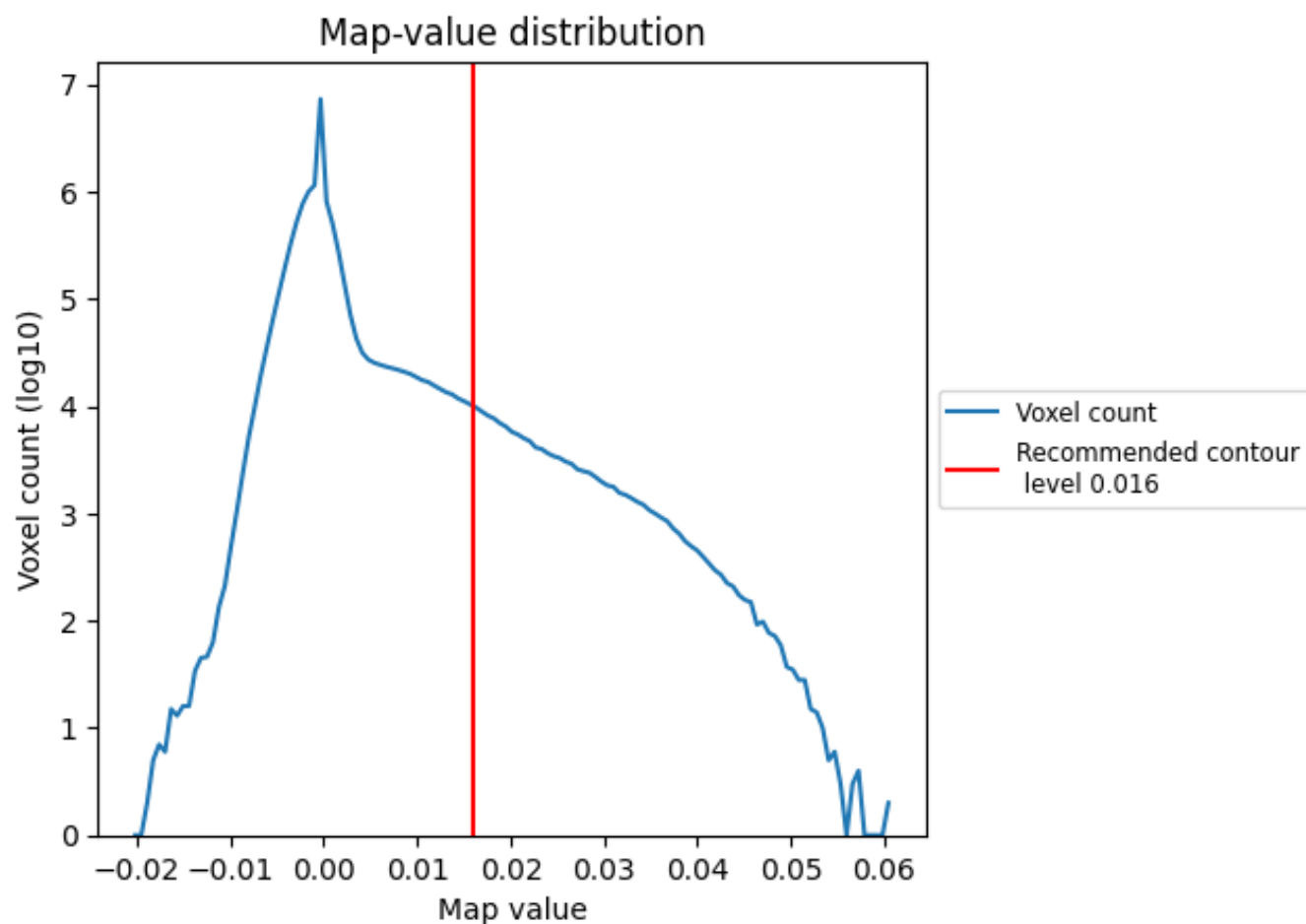
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

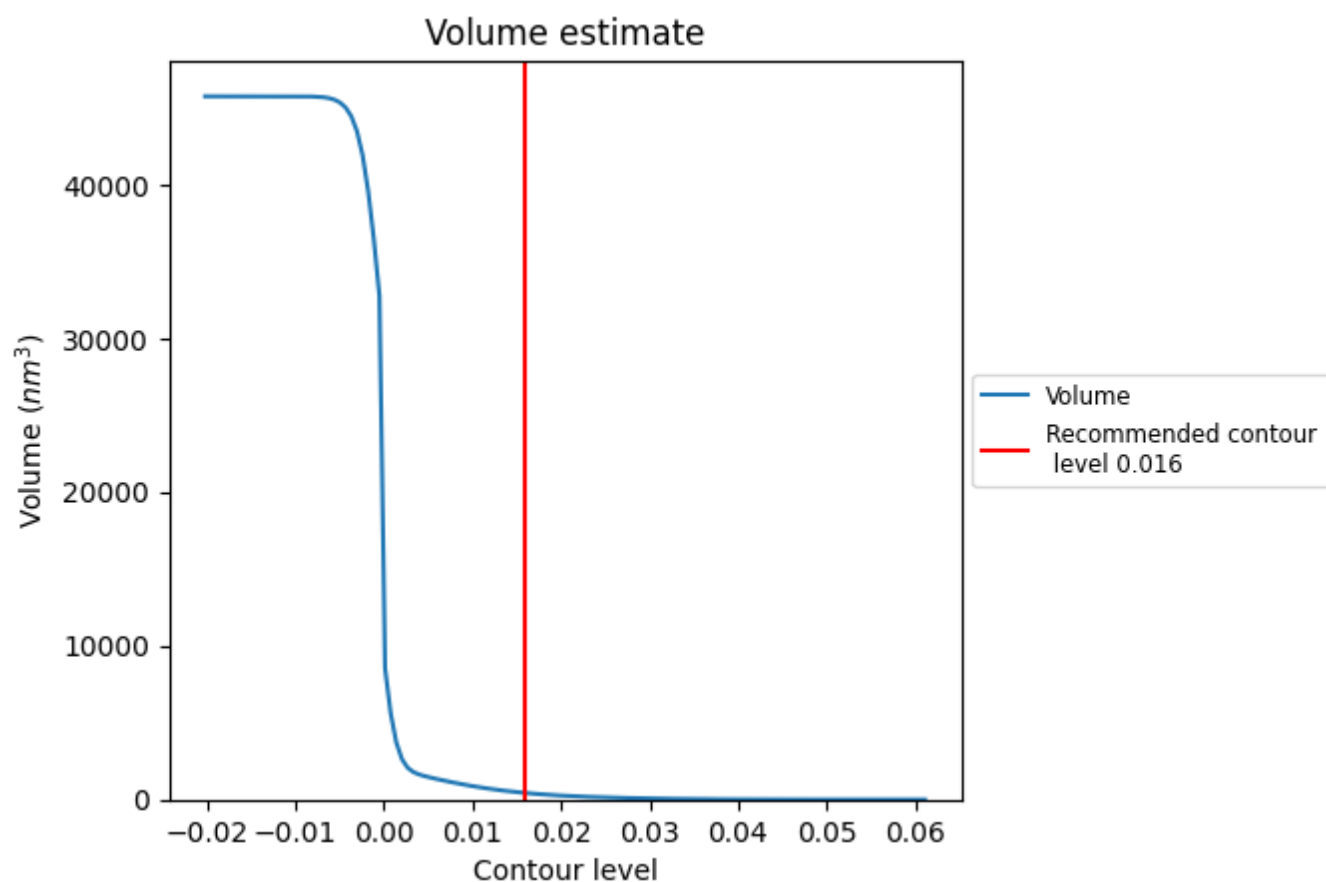
This section contains the results of statistical analysis of the map.

### 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.

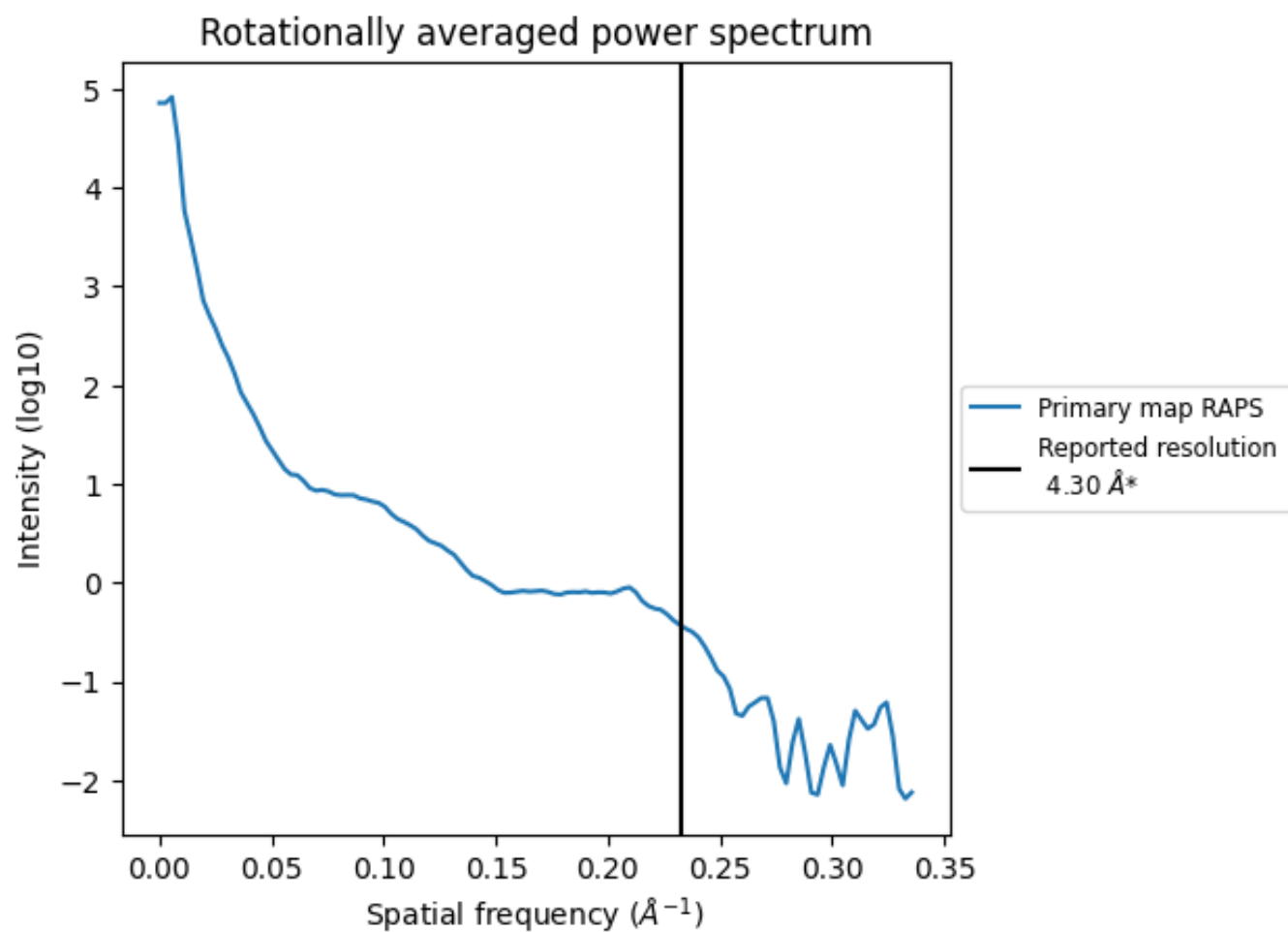
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 428 nm<sup>3</sup>; this corresponds to an approximate mass of 387 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 ⓘ

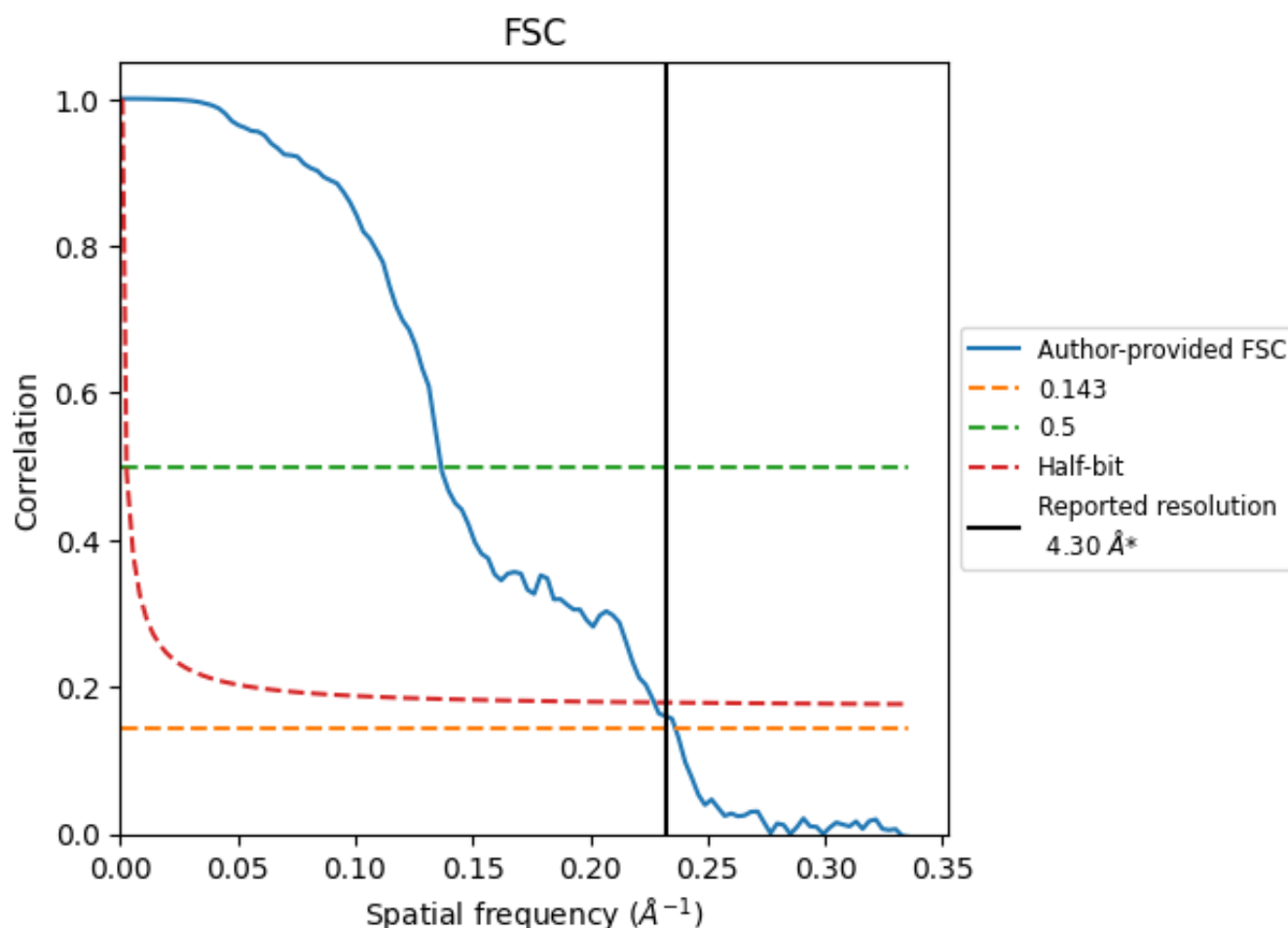


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.23	7.32	4.40
Unmasked-calculated*	-	-	-

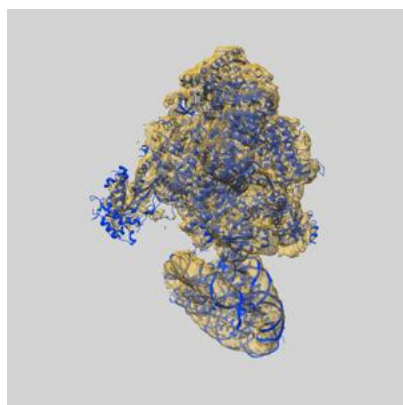
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



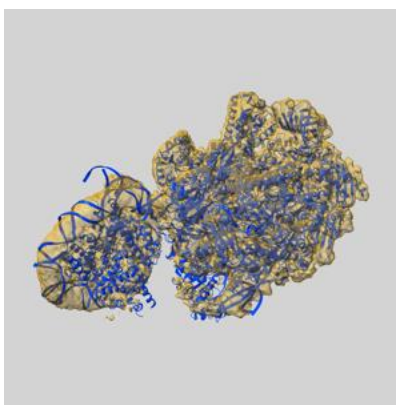
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0672 and PDB model 6J4X. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

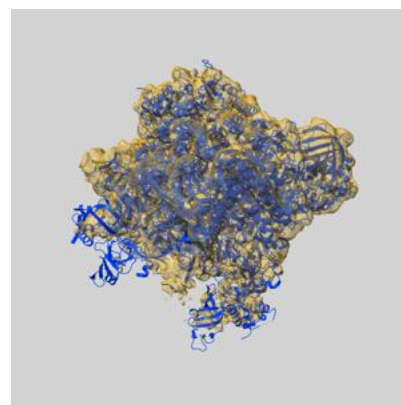
### 9.1 Map-model overlay [i](#)



X



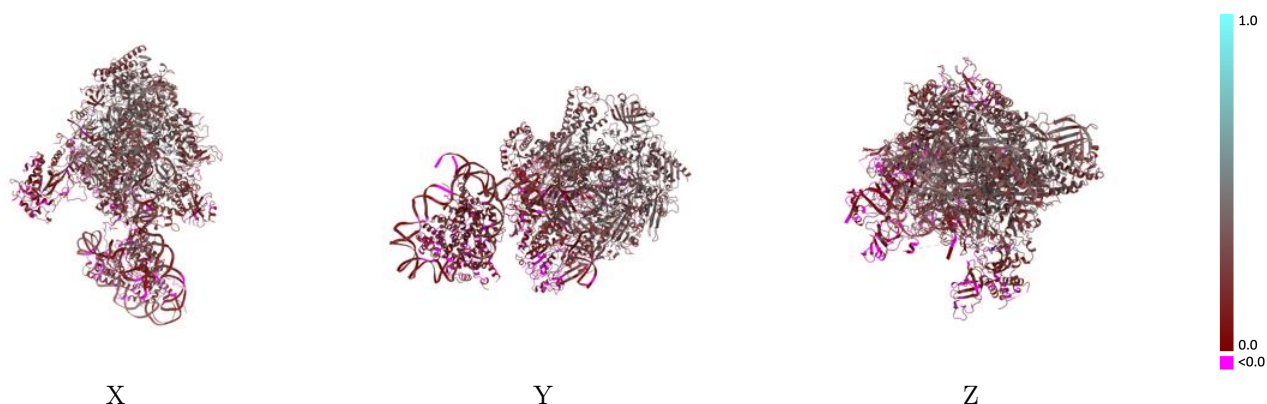
Y



Z

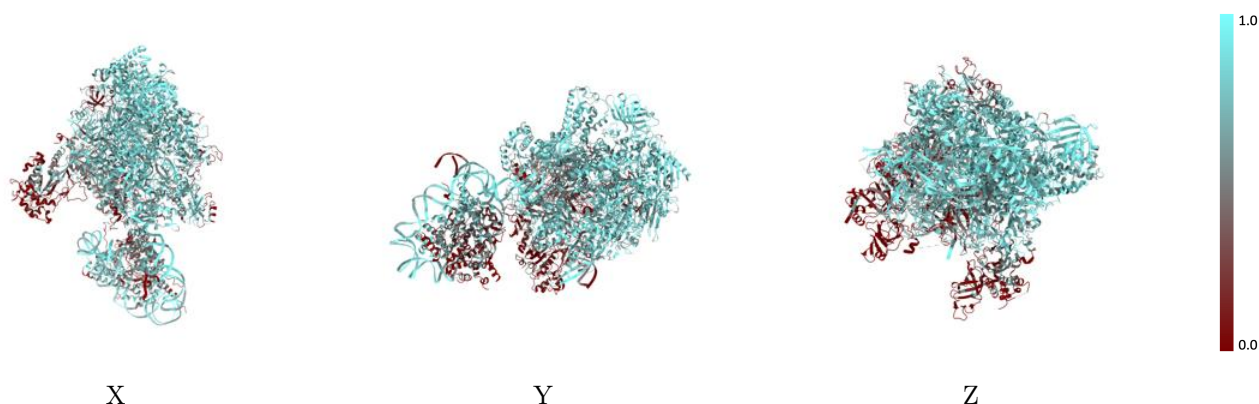
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



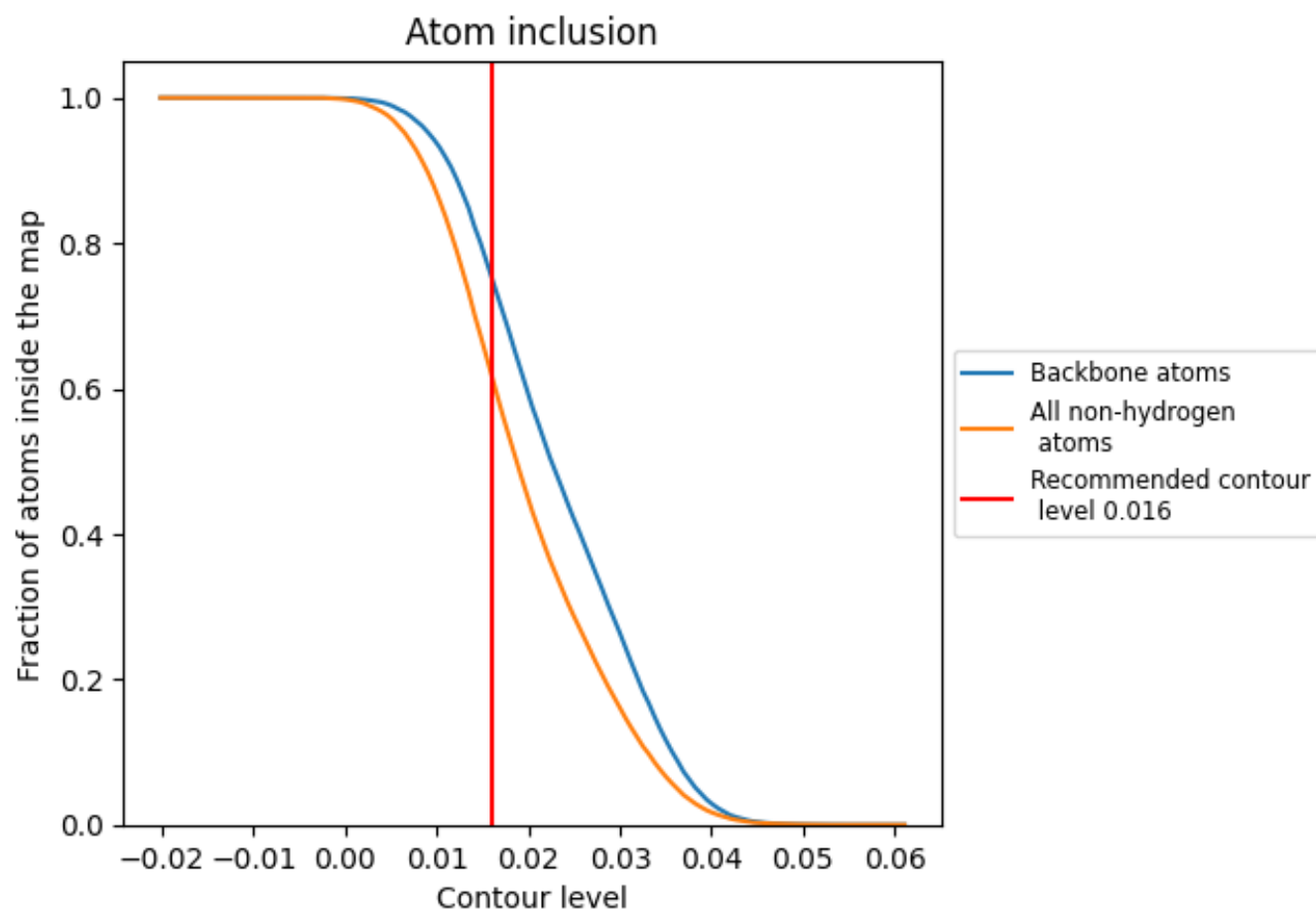
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 62% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6169	 0.2330
A	 0.6977	 0.3030
B	 0.7265	 0.3140
C	 0.8100	 0.3350
D	 0.1463	 0.0970
E	 0.7702	 0.2820
F	 0.7736	 0.3200
G	 0.3543	 0.1600
H	 0.8453	 0.3240
I	 0.4319	 0.1430
J	 0.8000	 0.3250
K	 0.7541	 0.3270
L	 0.7155	 0.2720
M	 0.0893	 0.1220
N	 0.7286	 0.1300
P	 0.7771	 0.2300
T	 0.7489	 0.1470
V	 0.1560	 0.0210
W	 0.1074	 0.0840
a	 0.5183	 0.1150
b	 0.5964	 0.1050
c	 0.5642	 0.0990
d	 0.5791	 0.0960
e	 0.5425	 0.1580
f	 0.4807	 0.1320
g	 0.1083	 0.0620
h	 0.2323	 0.0980

