



## Full wwPDB EM Validation Report ⓘ

Feb 1, 2025 – 01:07 PM EST

PDB ID : 9EGY  
EMDB ID : EMD-48040  
Title : RNA polymerase II-DSIF-SPT6-PAF1c-TFIIS-IWS1-nucleosome, bp +27  
Authors : Markert, J.; Farnung, L.  
Deposited on : 2024-11-21  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.40

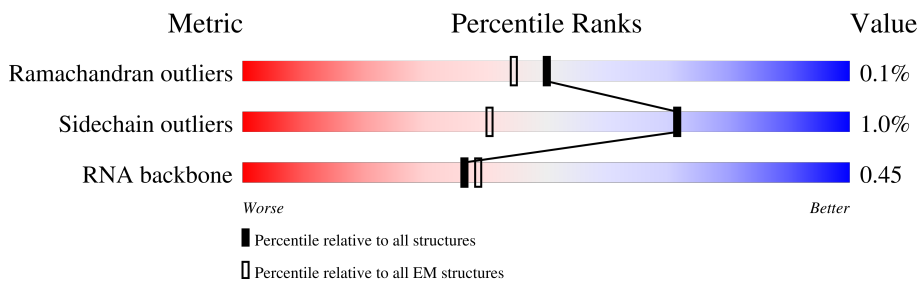
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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




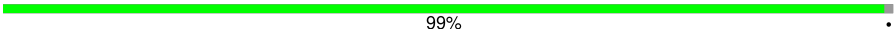
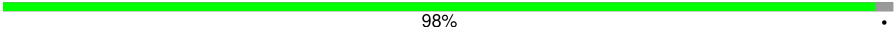








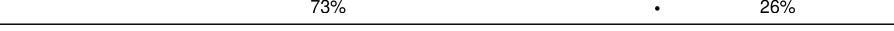


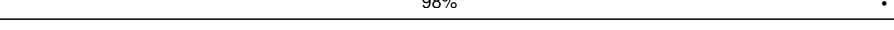

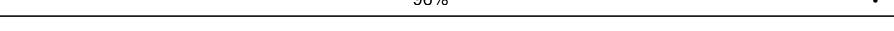


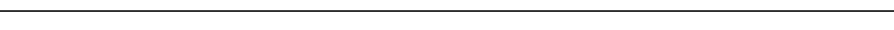

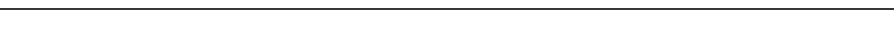
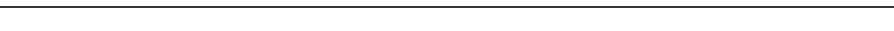


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	1984	
2	B	1251	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	206	
15	O	821	
16	P	21	
17	Q	1179	
18	R	713	
19	S	304	
20	T	215	
21	U	666	
22	V	531	
23	W	305	
24	X	531	
25	Y	121	
26	Z	1087	
27	a	136	
27	e	136	
28	b	103	
28	f	103	
29	c	130	
29	g	130	
30	d	123	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
30	h	123	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 72%, a yellow segment representing 2%, and a grey segment representing 24%. A small black dot is located at the end of the yellow segment.

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 66649 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	1426	Total	C	N	O	P	S	0	0
			11210	7040	2013	2086	2	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1122	Total	C	N	O	S	0	0
			8980	5684	1576	1656	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 RNA polymerase Rpb4/RPC9 core domain-containing protein.

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 polymerases I, II, and III subunit RPABC2.

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	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	47	Total	C	N	O	S	0	0
			397	246	77	68	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	1002	Total	C	N	O	0	0
			4309	2295	1003	1011		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	149	Total	C	N	O	P	0	0
			3070	1456	560	905	149		

- Molecule 15 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	132	Total	C	N	O	0	0
			656	392	132	132		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	SER	-	expression tag	UNP Q96ST2
O	0	ASN	-	expression tag	UNP Q96ST2
O	1	ALA	-	expression tag	UNP Q96ST2

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	21	Total	C	N	O	P	0	0
			432	193	59	159	21		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	N	O	S	0	0
			6427	4026	1164	1218	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	244	Total	C	N	O	S	0	0
			1428	866	281	280	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	161	Total	C	N	O	0	0
			657	334	161	162		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP P23193
S	-1	ASN	-	expression tag	UNP P23193
S	0	ALA	-	expression tag	UNP P23193

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	160	Total	C	N	O	P	0	0
			3264	1549	611	945	159		

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	125	Total	C	N	O	0	0
			617	367	125	125		



- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	244	Total	C	N	O	S	0	0
			1378	842	267	267	2		

- Molecule 23 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	300	Total	C	N	O	S	0	0
			2333	1483	392	454	4		

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	43	Total	C	N	O	0	0
			353	220	69	64		

- Molecule 25 is a protein called Transcription elongation factor SPT4.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	510	Total	C	N	O	P	S	0	0
			4025	2552	709	745	1	18		

- Molecule 27 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	92	Total	C	N	O	S	0	0
			751	474	142	132	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	97	Total	C	N	O	S	0	0
			801	504	155	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	36	MET	LYS	engineered mutation	UNP A0A310TTQ1
e	36	MET	LYS	engineered mutation	UNP A0A310TTQ1

- Molecule 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
28	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 29 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	103	Total	C	N	O		0	0
			795	501	155	139			
29	g	98	Total	C	N	O		0	0
			755	474	149	132			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	99	ARG	GLY	conflict	UNP P06897
c	123	SER	ALA	conflict	UNP P06897
g	99	ARG	GLY	conflict	UNP P06897
g	123	SER	ALA	conflict	UNP P06897

- Molecule 30 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	95	Total	C	N	O	S	0	0
			745	469	134	140	2		
30	h	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

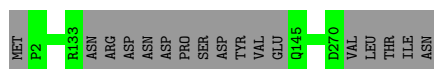
Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total 2	Zn 2	0
31	B	1	Total 1	Zn 1	0
31	C	1	Total 1	Zn 1	0
31	I	2	Total 2	Zn 2	0
31	J	1	Total 1	Zn 1	0
31	L	1	Total 1	Zn 1	0
31	Y	1	Total 1	Zn 1	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

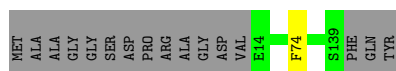
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total 1	Mg 1	0



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



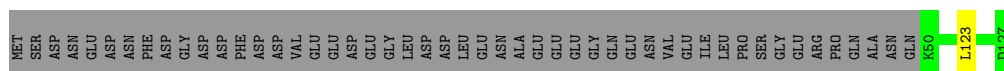
- Molecule 4: RNA polymerase Rpb4/RPC9 core domain-containing protein



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



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



- 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

Chain I:  92% • 7%

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

Chain J:  99%

- Molecule 11: RNA polymerase II subunit J

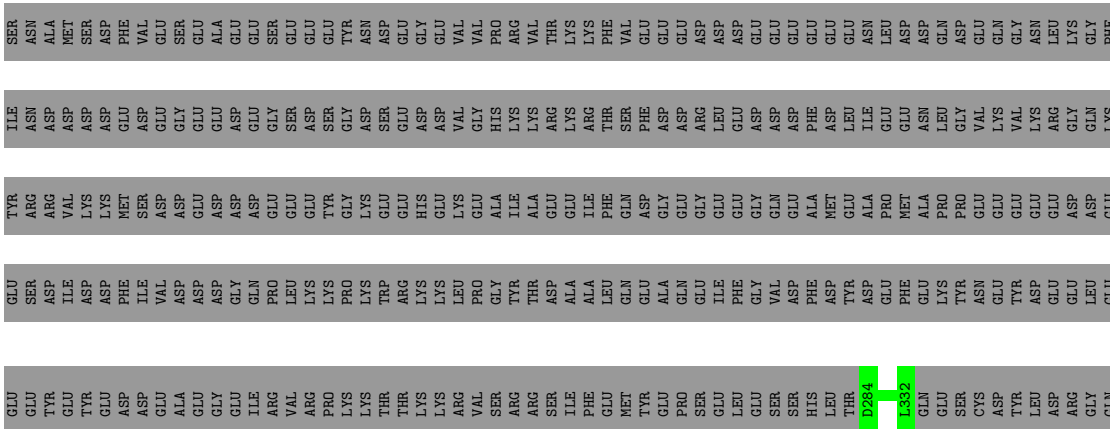
Chain K:  98%

- Molecule 12: RNA polymerase II subunit K

Chain L:  79% • 19%

- Molecule 13: Transcription elongation factor SPT6

Chain M: 

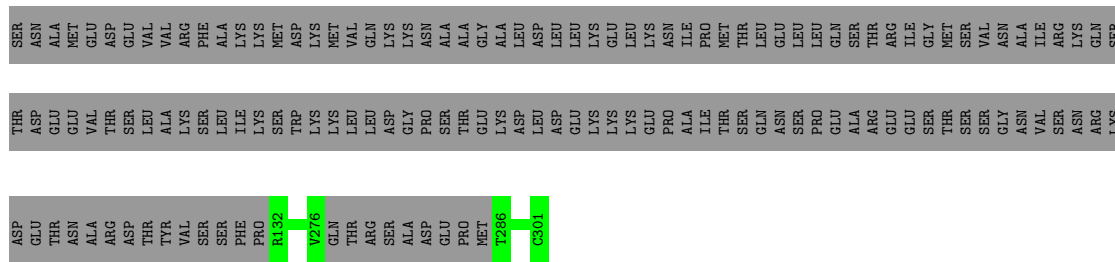




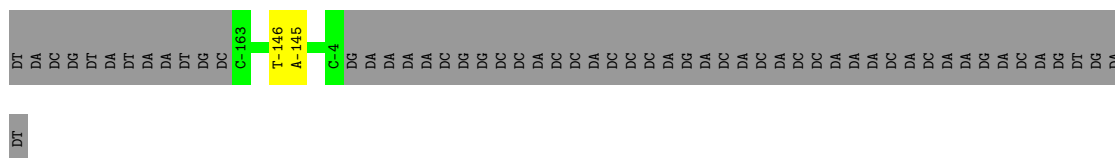




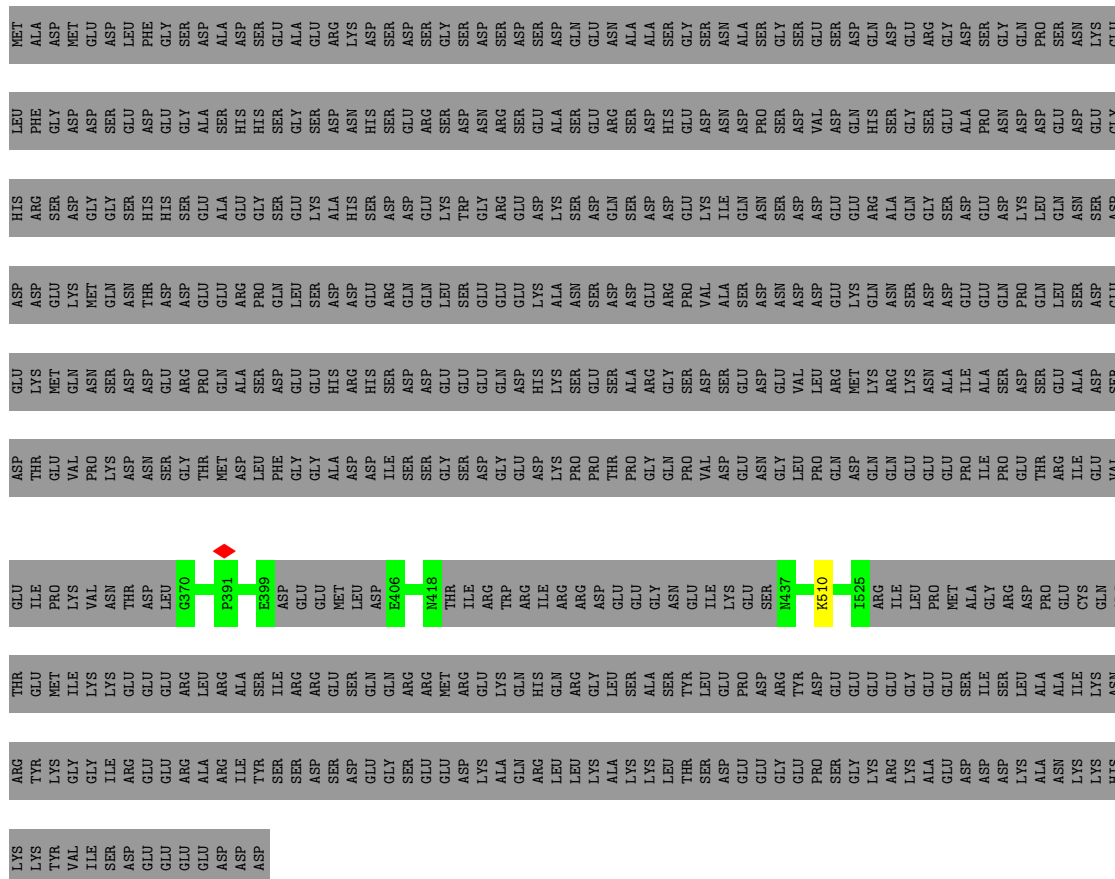




- Molecule 20: Template DNA



- Molecule 21: RNA polymerase-associated protein LEO1

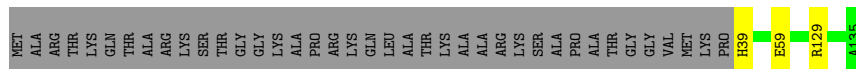


- Molecule 22: RNA polymerase II-associated factor 1 homolog


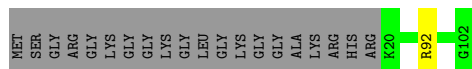




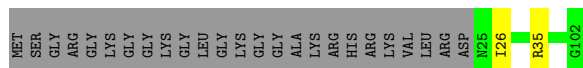
## ● Molecule 27: Histone H3

Chain e:  69% 29%

## ● Molecule 28: Histone H4

Chain b:  80% 19%

## ● Molecule 28: Histone H4

Chain f:  74% 24%

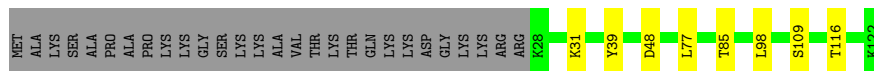
## ● Molecule 29: Histone H2A type 1

Chain c:  75% 21%

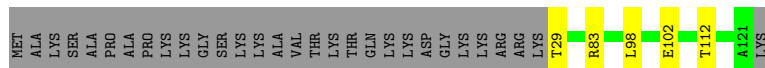
## ● Molecule 29: Histone H2A type 1

Chain g:  72% 25%

## ● Molecule 30: Histone H2B 1.1

Chain d:  71% 7% 23%

## ● Molecule 30: Histone H2B 1.1

Chain h:  72% 24%

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1139653	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.746	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	549.46, 549.46, 549.46	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09892, 1.09892, 1.09892	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, TPO, SEP, 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	0.26	0/11384	0.51	0/15361
2	B	0.26	0/9158	0.51	0/12360
3	C	0.26	0/2115	0.49	0/2873
4	D	0.25	0/1017	0.48	0/1368
5	E	0.26	0/1751	0.53	0/2366
6	F	0.25	0/636	0.51	0/859
7	G	0.26	0/1364	0.51	0/1853
8	H	0.26	0/1219	0.53	0/1644
9	I	0.25	0/964	0.50	0/1305
10	J	0.26	0/533	0.48	0/719
11	K	0.26	0/939	0.45	0/1271
12	L	0.27	0/403	0.61	0/536
13	M	0.23	0/4330	0.42	0/5591
14	N	0.56	0/3442	0.93	3/5314 (0.1%)
15	O	0.23	0/655	0.36	0/913
16	P	0.18	0/477	0.76	0/738
17	Q	0.25	0/6531	0.46	1/8861 (0.0%)
18	R	0.24	0/1437	0.44	0/1972
19	S	0.22	0/659	0.40	0/827
20	T	0.54	0/3663	0.86	2/5646 (0.0%)
21	U	0.24	0/613	0.45	0/847
22	V	0.24	0/1386	0.47	0/1909
23	W	0.24	0/2392	0.46	0/3257
24	X	0.23	0/356	0.57	0/478
25	Y	0.24	0/927	0.52	0/1250
26	Z	0.24	0/4084	0.50	0/5498
27	a	0.25	0/760	0.51	0/1019
27	e	0.25	0/812	0.53	0/1088
28	b	0.25	0/669	0.55	0/894
28	f	0.27	0/626	0.55	0/837
29	c	0.25	0/805	0.52	0/1088
29	g	0.24	0/764	0.52	0/1031

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
30	d	0.25	0/756	0.48	0/1015
30	h	0.24	0/737	0.46	0/993
All	All	0.29	0/68364	0.56	6/93581 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	146	DA	OP1-P-OP2	-6.68	109.58	119.60
20	T	-145	DA	OP1-P-OP2	-6.64	109.64	119.60
14	N	153	DG	OP1-P-OP2	-6.59	109.72	119.60
14	N	145	DT	OP1-P-O3'	5.96	118.30	105.20
20	T	-146	DT	OP2-P-O3'	5.13	116.49	105.20
17	Q	772	GLU	C-N-CA	5.05	134.33	121.70

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	1408/1984 (71%)	1286 (91%)	121 (9%)	1 (0%)	48	77
2	B	1112/1251 (89%)	1009 (91%)	102 (9%)	1 (0%)	48	77
3	C	254/275 (92%)	229 (90%)	25 (10%)	0	100	100
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	207/210 (99%)	194 (94%)	13 (6%)	0	100	100
6	F	76/127 (60%)	72 (95%)	4 (5%)	0	100	100
7	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
8	H	147/150 (98%)	133 (90%)	14 (10%)	0	100	100
9	I	114/125 (91%)	103 (90%)	11 (10%)	0	100	100
10	J	64/67 (96%)	57 (89%)	7 (11%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	45/58 (78%)	41 (91%)	3 (7%)	1 (2%)	5	21
13	M	976/1729 (56%)	910 (93%)	65 (7%)	1 (0%)	48	77
15	O	130/821 (16%)	125 (96%)	4 (3%)	1 (1%)	16	45
17	Q	888/1179 (75%)	851 (96%)	37 (4%)	0	100	100
18	R	240/713 (34%)	228 (95%)	12 (5%)	0	100	100
19	S	157/304 (52%)	153 (98%)	4 (2%)	0	100	100
21	U	117/666 (18%)	101 (86%)	15 (13%)	1 (1%)	14	43
22	V	234/531 (44%)	214 (92%)	20 (8%)	0	100	100
23	W	298/305 (98%)	284 (95%)	14 (5%)	0	100	100
24	X	41/531 (8%)	40 (98%)	1 (2%)	0	100	100
25	Y	114/121 (94%)	106 (93%)	8 (7%)	0	100	100
26	Z	497/1087 (46%)	451 (91%)	46 (9%)	0	100	100
27	a	90/136 (66%)	88 (98%)	2 (2%)	0	100	100
27	e	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
28	b	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
28	f	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
29	c	101/130 (78%)	99 (98%)	2 (2%)	0	100	100
29	g	96/130 (74%)	92 (96%)	4 (4%)	0	100	100
30	d	93/123 (76%)	90 (97%)	3 (3%)	0	100	100
30	h	91/123 (74%)	89 (98%)	2 (2%)	0	100	100
All	All	8248/13649 (60%)	7680 (93%)	562 (7%)	6 (0%)	50	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	39	CYS

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
13	M	700	HIS
1	A	1343	LEU
21	U	510	LYS
2	B	684	GLU
15	O	645	PRO

### 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	1229/1761 (70%)	1226 (100%)	3 (0%)	92	98
2	B	986/1084 (91%)	981 (100%)	5 (0%)	86	96
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/126 (86%)	108 (99%)	1 (1%)	75	92
5	E	191/192 (100%)	190 (100%)	1 (0%)	86	96
6	F	68/111 (61%)	67 (98%)	1 (2%)	60	85
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%)	103 (99%)	1 (1%)	73	91
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	44/55 (80%)	44 (100%)	0	100	100
13	M	41/1524 (3%)	41 (100%)	0	100	100
17	Q	533/1011 (53%)	526 (99%)	7 (1%)	65	88
18	R	57/625 (9%)	56 (98%)	1 (2%)	54	82
19	S	4/268 (2%)	4 (100%)	0	100	100
22	V	46/462 (10%)	46 (100%)	0	100	100
23	W	255/260 (98%)	254 (100%)	1 (0%)	89	97
24	X	40/467 (9%)	40 (100%)	0	100	100
25	Y	102/105 (97%)	102 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	Z	435/939 (46%)	432 (99%)	3 (1%)	81 94
27	a	80/111 (72%)	75 (94%)	5 (6%)	15 42
27	e	84/111 (76%)	81 (96%)	3 (4%)	30 65
28	b	68/79 (86%)	67 (98%)	1 (2%)	60 85
28	f	63/79 (80%)	61 (97%)	2 (3%)	34 69
29	c	82/102 (80%)	77 (94%)	5 (6%)	15 43
29	g	76/102 (74%)	72 (95%)	4 (5%)	19 49
30	d	81/103 (79%)	73 (90%)	8 (10%)	6 21
30	h	79/103 (77%)	74 (94%)	5 (6%)	15 42
All	All	5527/10590 (52%)	5470 (99%)	57 (1%)	71 91

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	VAL
1	A	567	LEU
1	A	931	ARG
2	B	610	ARG
2	B	650	ASN
2	B	768	ARG
2	B	848	LEU
2	B	1080	ARG
4	D	74	PHE
5	E	18	MET
6	F	123	LEU
9	I	56	ASN
17	Q	377	THR
17	Q	697	TYR
17	Q	707	CYS
17	Q	813	GLU
17	Q	817	CYS
17	Q	820	LEU
17	Q	858	LYS
18	R	576	GLU
23	W	231	HIS
26	Z	429	CYS
26	Z	484	ARG
26	Z	778	TYR
27	a	48	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
27	a	63	ARG
27	a	115	LYS
27	a	117	VAL
27	a	129	ARG
28	b	92	ARG
29	c	29	ARG
29	c	81	ARG
29	c	101	THR
29	c	114	VAL
29	c	118	LYS
30	d	31	LYS
30	d	39	TYR
30	d	48	ASP
30	d	77	LEU
30	d	85	THR
30	d	98	LEU
30	d	109	SER
30	d	116	THR
27	e	39	HIS
27	e	59	GLU
27	e	129	ARG
28	f	26	ILE
28	f	35	ARG
29	g	50	TYR
29	g	74	LYS
29	g	81	ARG
29	g	84	GLN
30	h	29	THR
30	h	83	ARG
30	h	98	LEU
30	h	102	GLU
30	h	112	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	188	GLN
1	A	288	ASN
1	A	372	ASN
1	A	387	ASN
1	A	539	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	700	GLN
1	A	780	ASN
1	A	790	GLN
1	A	791	GLN
1	A	991	GLN
1	A	1036	ASN
1	A	1044	HIS
1	A	1194	ASN
1	A	1332	GLN
1	A	1457	ASN
1	A	1462	GLN
2	B	197	GLN
2	B	227	ASN
2	B	420	GLN
2	B	471	ASN
2	B	582	GLN
2	B	725	GLN
3	C	111	GLN
8	H	29	HIS
9	I	56	ASN
12	L	13	GLN
12	L	26	ASN
17	Q	466	ASN
17	Q	527	HIS
17	Q	616	HIS
17	Q	714	HIS
17	Q	860	GLN
22	V	69	GLN
22	V	72	HIS
23	W	27	ASN
23	W	173	ASN
23	W	223	ASN
23	W	273	HIS
26	Z	244	ASN
26	Z	272	ASN
27	a	108	ASN
29	c	112	GLN
30	d	64	ASN
27	e	108	ASN
29	g	84	GLN
30	h	60	ASN
30	h	64	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	20/21 (95%)	7 (35%)	3 (15%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	8	U
16	P	9	U
16	P	10	U
16	P	11	U
16	P	16	U
16	P	17	G
16	P	19	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	8	U
16	P	16	U
16	P	18	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SEP	A	1547	1	8,9,10	1.62	1 (12%)	7,12,14	1.44	1 (14%)
1	TPO	A	1525	1	8,10,11	1.11	0	10,14,16	2.08	1 (10%)
26	TPO	Z	775	26	8,10,11	1.14	0	10,14,16	1.77	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	1547	1	-	0/6/8/10	-
1	TPO	A	1525	1	-	0/9/11/13	-
26	TPO	Z	775	26	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.54	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	P-OG1-CB	-5.92	107.23	123.33
26	Z	775	TPO	P-OG1-CB	-4.89	110.03	123.33
1	A	1547	SEP	OG-CB-CA	3.21	111.27	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	Z	775	TPO	C-CA-CB-CG2
26	Z	775	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	1
22	V	1
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	27.14
1	V	299:GLU	C	310:ASN	N	12.59
1	M	1334:ASN	C	1338:ILE	N	5.53



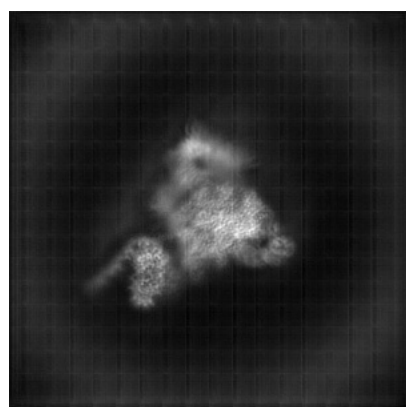
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48040. These allow visual inspection of the internal detail of the map and identification of artifacts.

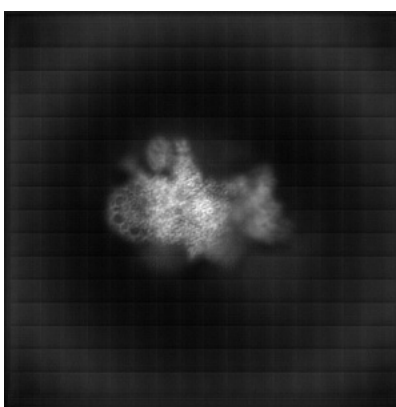
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

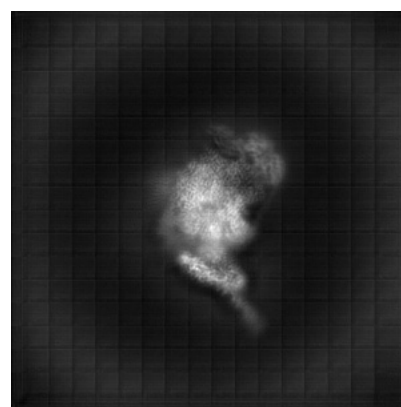
#### 6.1.1 Primary map



X



Y

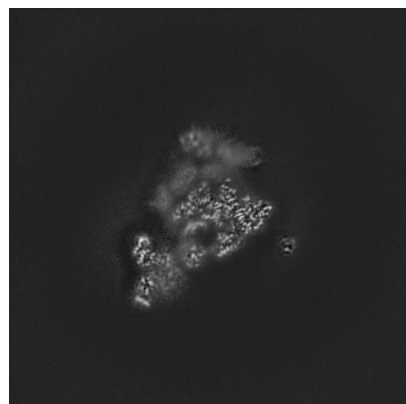


Z

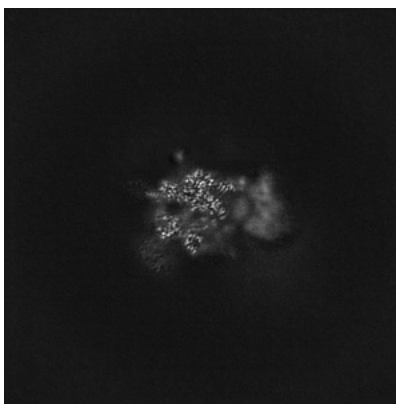
The images above show the map projected in three orthogonal directions.

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

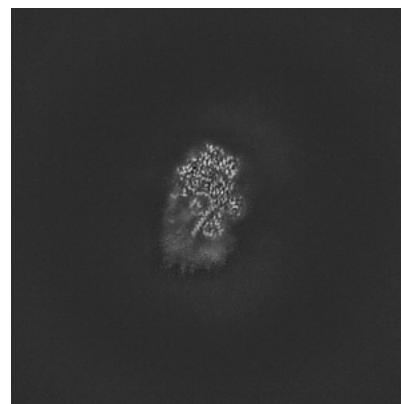
#### 6.2.1 Primary map



X Index: 250



Y Index: 250

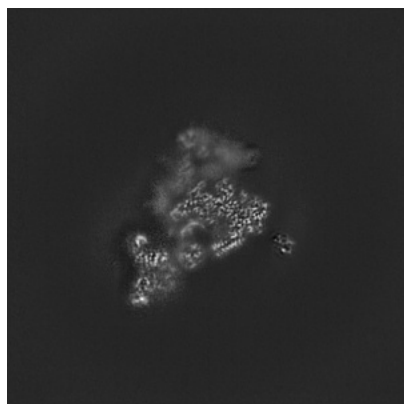


Z Index: 250

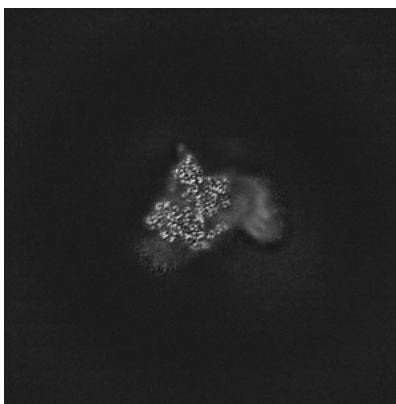
The images above show central slices of the map in three orthogonal directions.

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

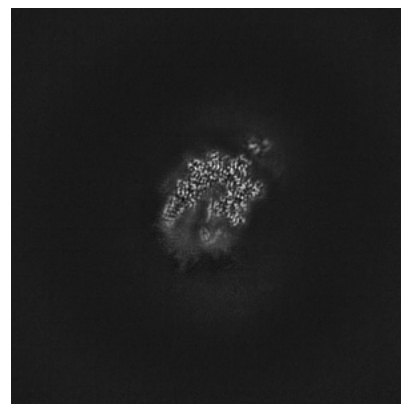
### 6.3.1 Primary map



X Index: 253



Y Index: 264

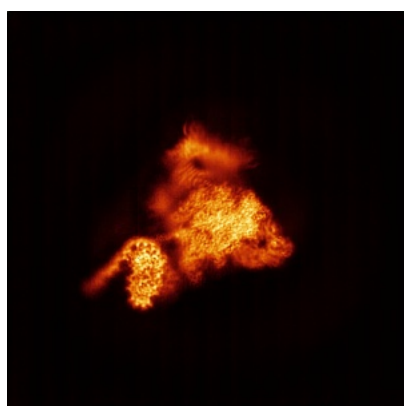


Z Index: 236

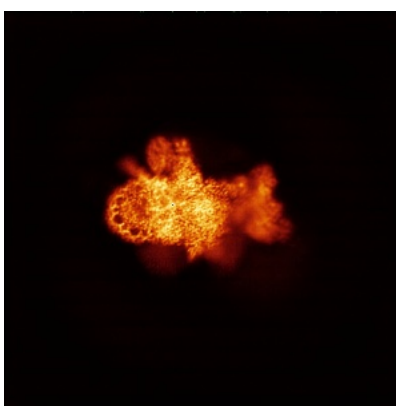
The images above show the largest variance slices of the map in three orthogonal directions.

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

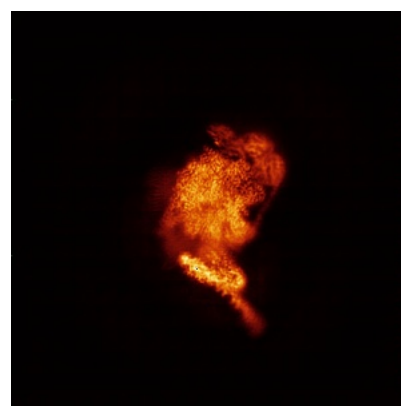
### 6.4.1 Primary map



X



Y

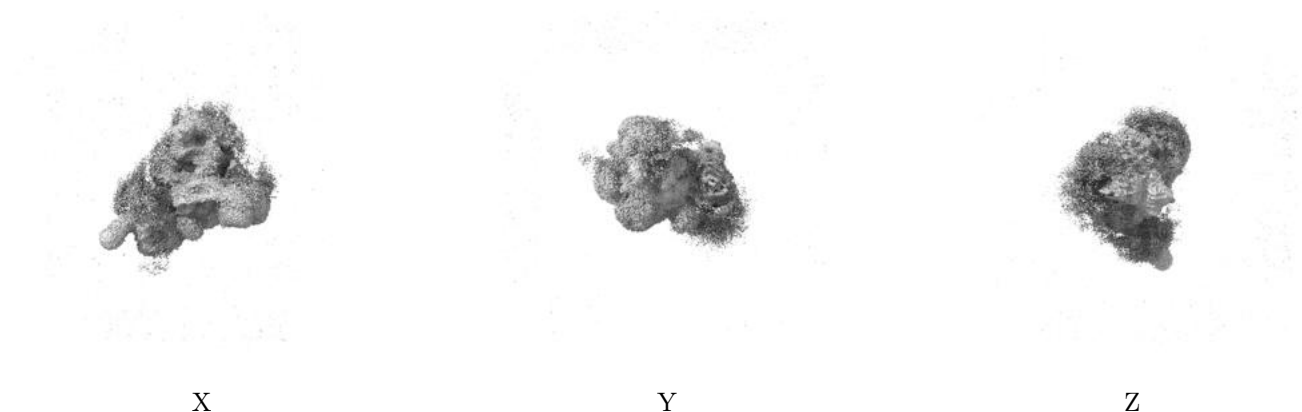


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

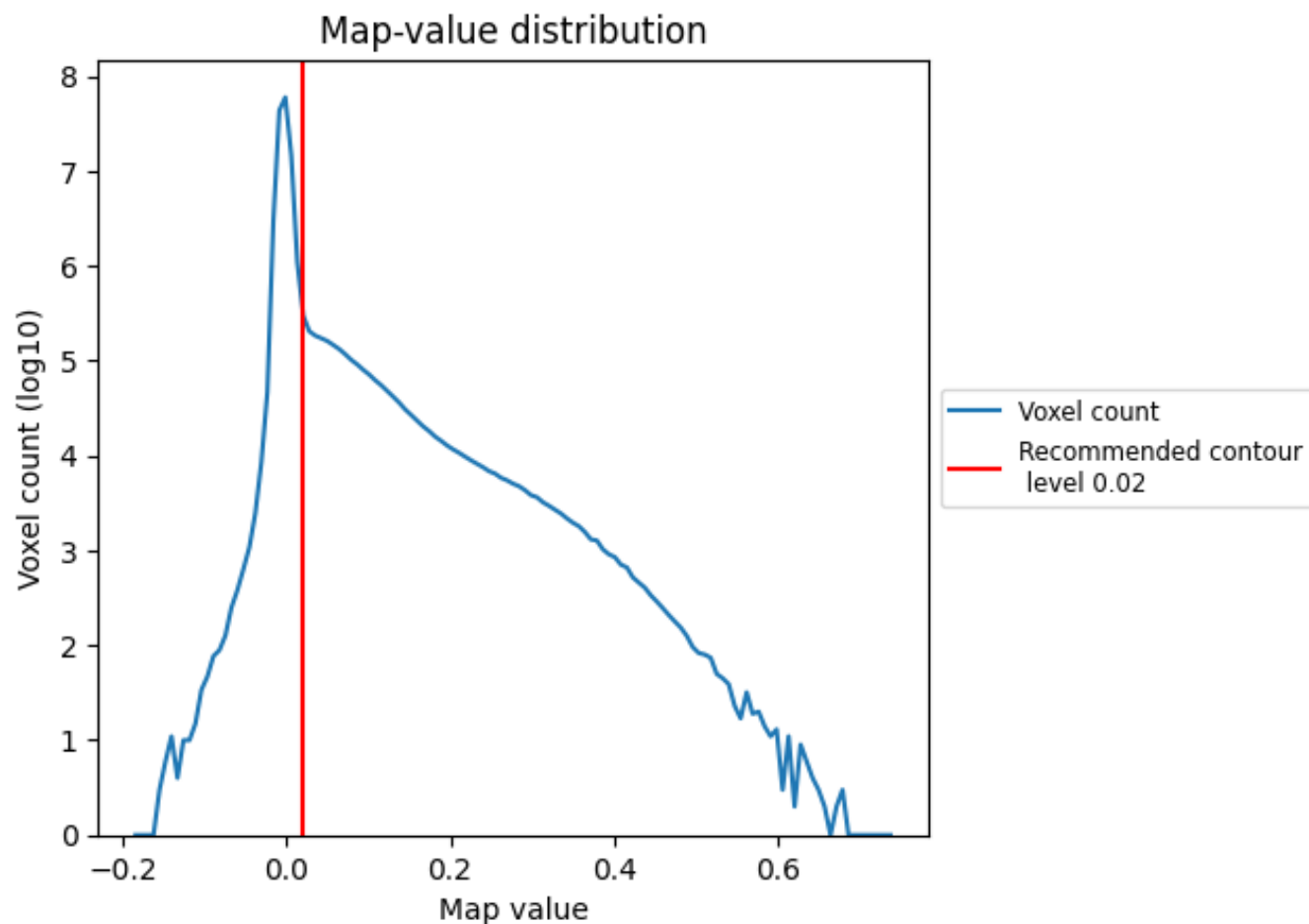
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

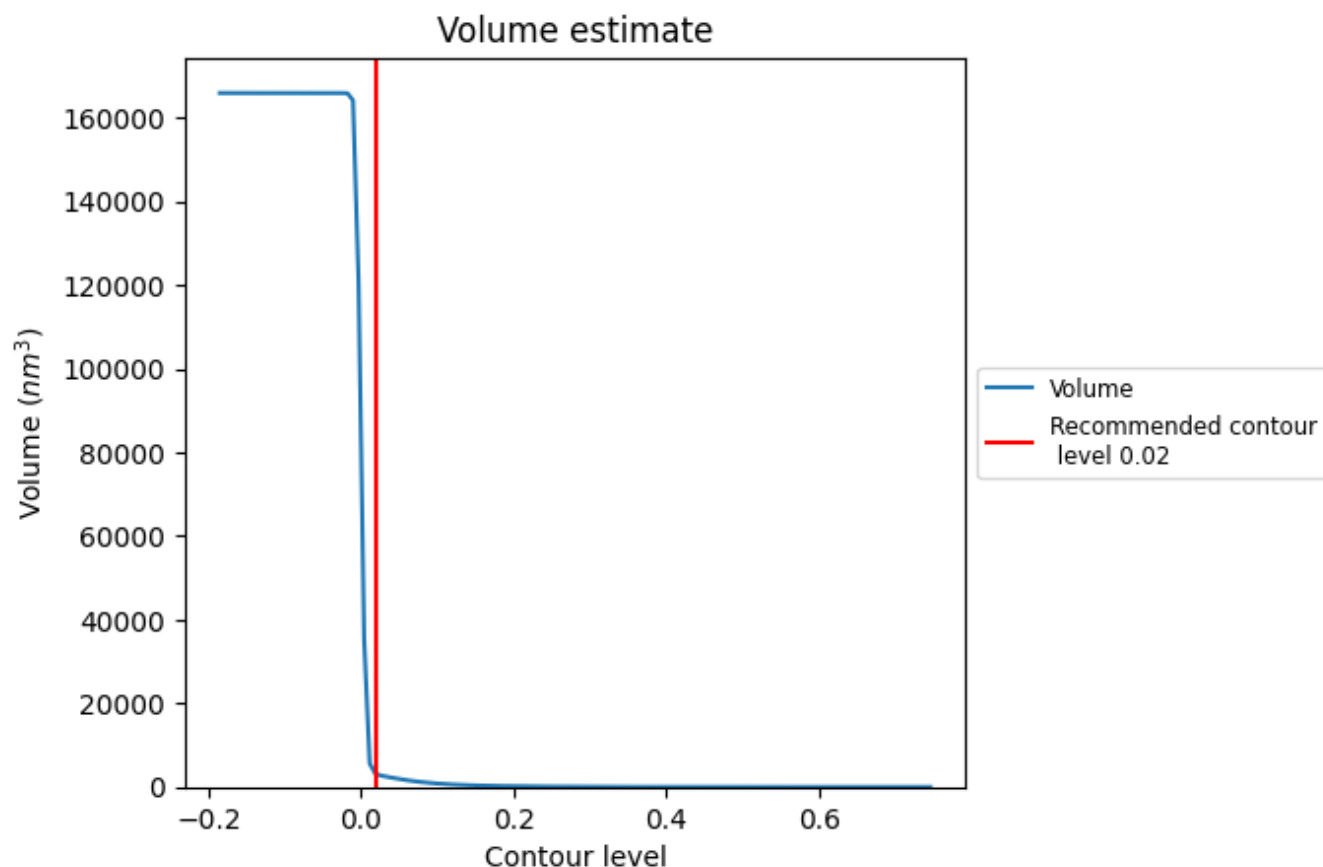
This section contains the results of statistical analysis of the map.

### 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.

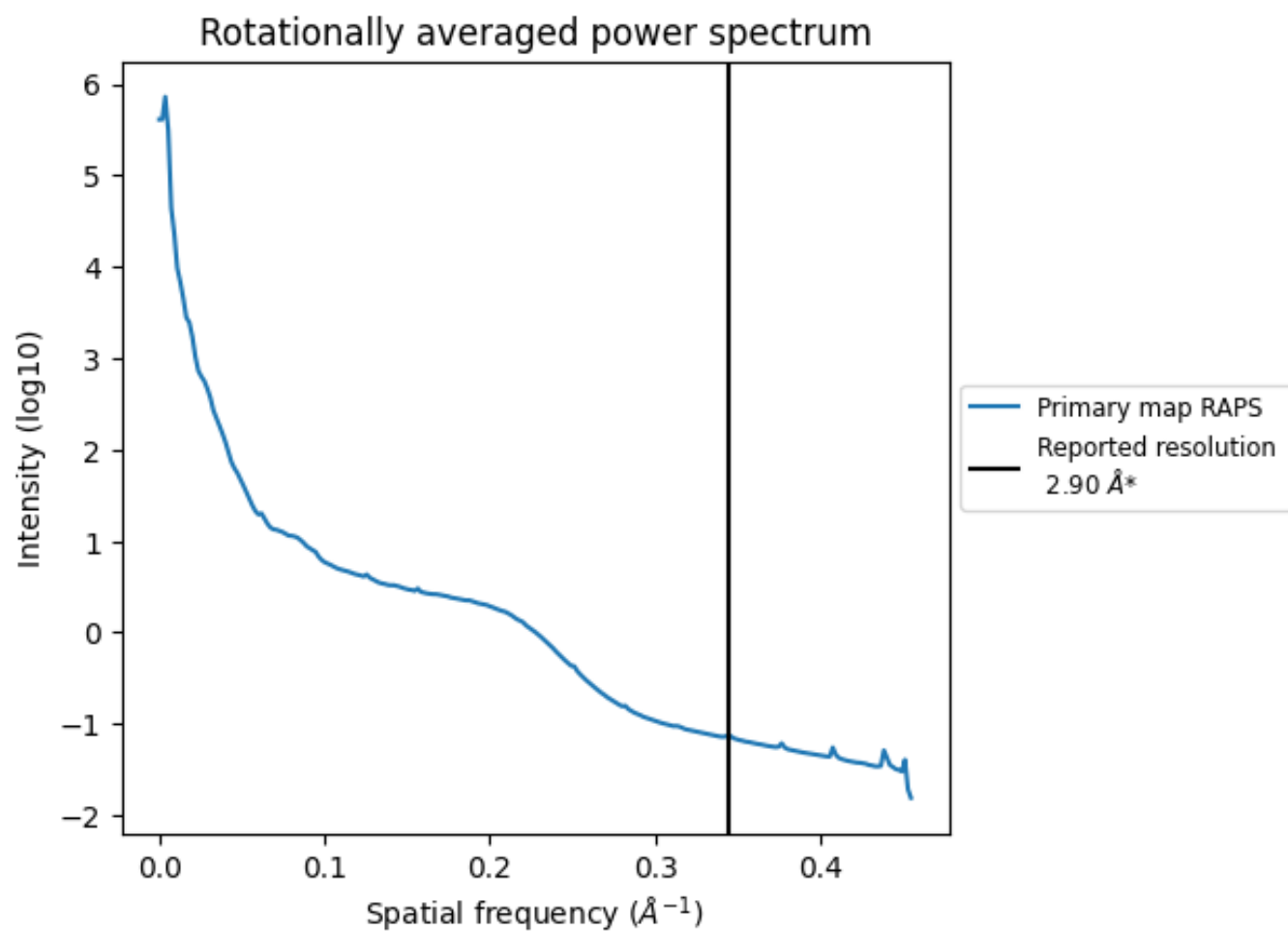
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3120 nm<sup>3</sup>; this corresponds to an approximate mass of 2818 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 0.345 Å<sup>-1</sup>

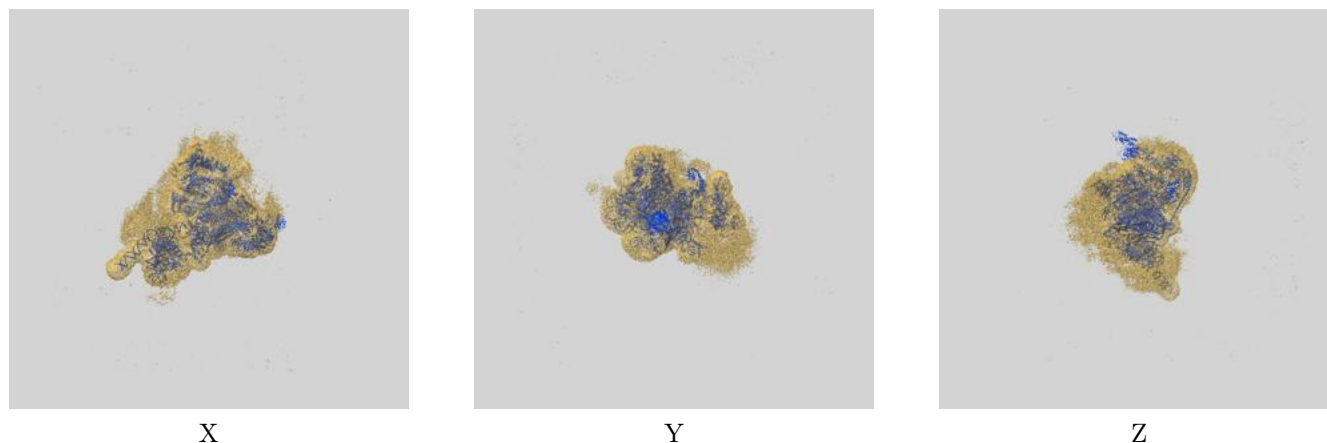
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

This section contains information regarding the fit between EMDB map EMD-48040 and PDB model 9EGY. Per-residue inclusion information can be found in section [3](#) on page [12](#).

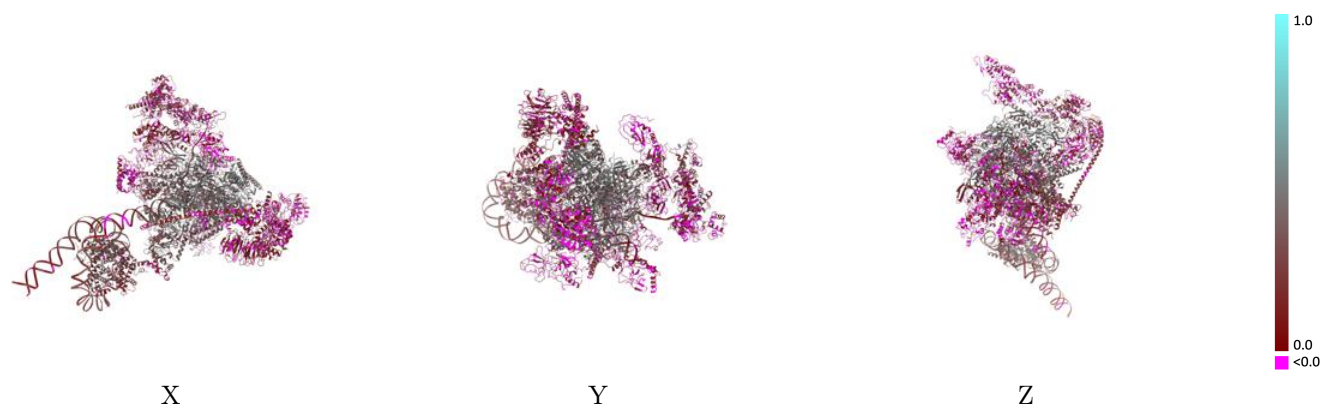
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

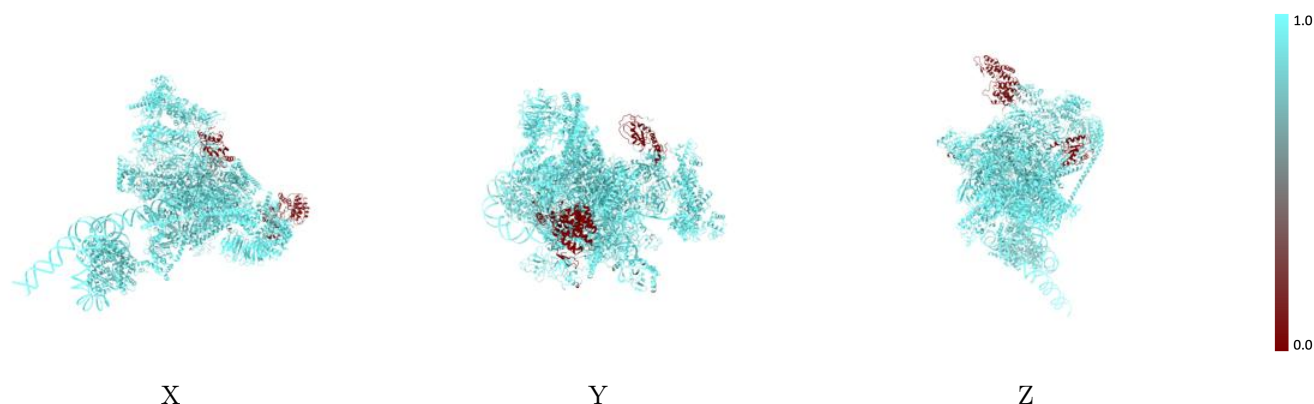


## 9.2 Q-score mapped to coordinate model [i](#)



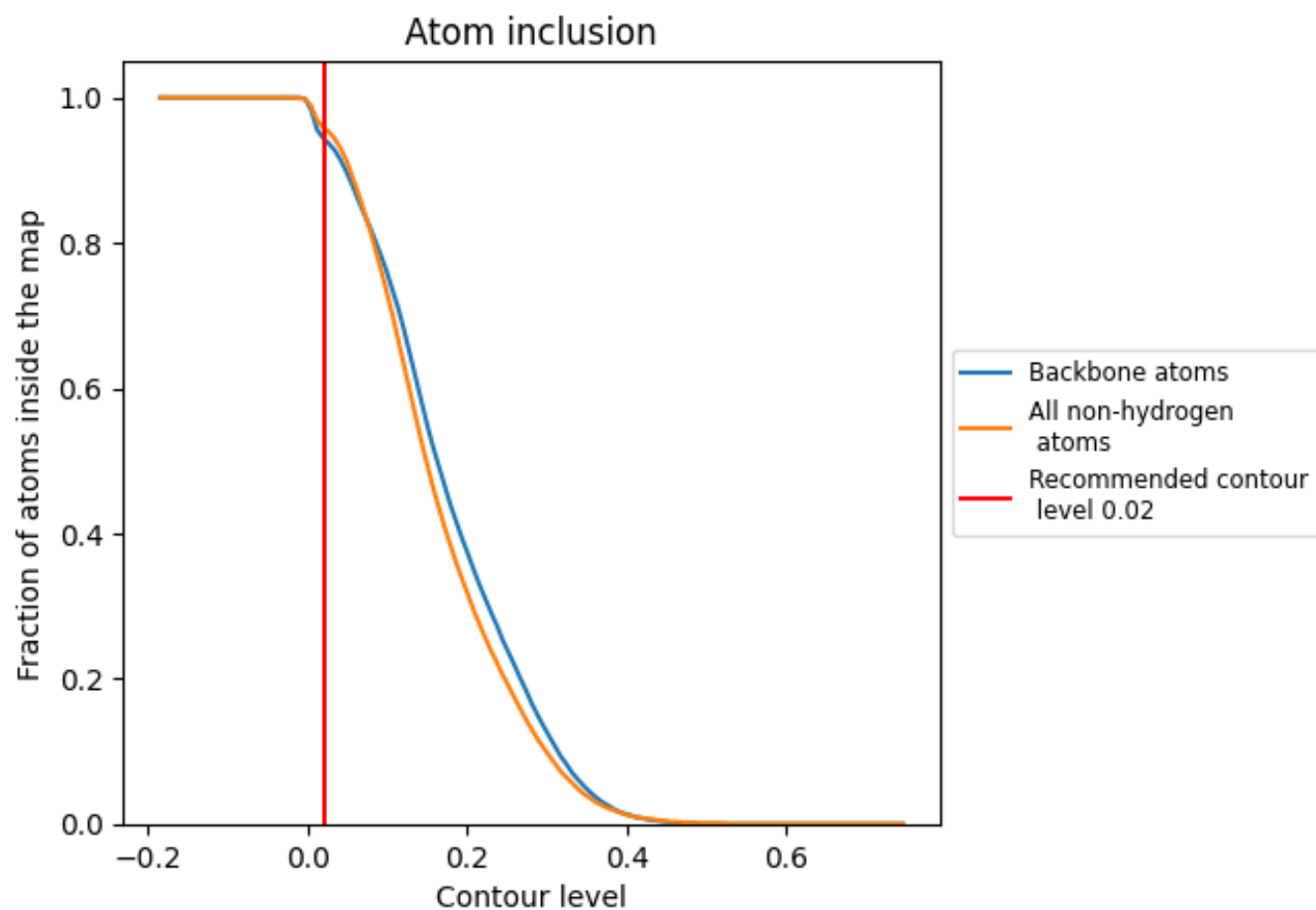
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 96% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.2560
A	 0.9920	 0.3920
B	 1.0000	 0.4070
C	 1.0000	 0.4310
D	 1.0000	 0.1860
E	 1.0000	 0.3790
F	 1.0000	 0.4340
G	 1.0000	 0.2110
H	 0.9980	 0.4220
I	 1.0000	 0.3590
J	 0.9980	 0.4150
K	 1.0000	 0.4340
L	 1.0000	 0.3690
M	 0.8460	 0.0910
N	 0.9960	 0.2020
O	 1.0000	 -0.0010
P	 1.0000	 0.1900
Q	 0.7640	 0.0890
R	 0.9040	 0.0540
S	 1.0000	 0.2010
T	 0.9950	 0.2100
U	 0.9820	 0.0890
V	 0.8080	 0.0670
W	 1.0000	 0.1380
X	 1.0000	 0.1470
Y	 1.0000	 0.0270
Z	 0.9930	 0.0810
a	 0.9930	 0.2890
b	 0.9980	 0.3080
c	 0.9970	 0.3350
d	 0.9990	 0.3120
e	 0.9950	 0.3300
f	 0.9970	 0.3340
g	 0.9950	 0.1950
h	 1.0000	 0.1990

