



wwPDB EM Validation Summary Report ⓘ

Jun 20, 2024 – 02:47 AM JST

PDB ID : 7WBV
EMDB ID : EMD-32407
Title : RNA polymerase II elongation complex bound with Elf1 and Spt4/5, stalled at SHL(-4) of the nucleosome
Authors : Osumi, K.; Kujirai, T.; Ehara, H.; Sekine, S.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2021-12-17
Resolution : 4.10 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

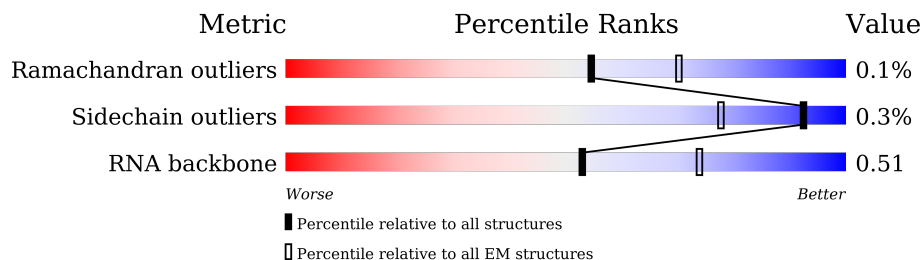
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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 ≥ 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	
2	B	1227	
3	C	304	
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	

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Mol	Chain	Length	Quality of chain
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	113	
14	N	198	
15	P	16	
16	T	198	
17	V	108	
18	W	812	
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 92340 atoms, of which 44823 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	1412	Total	C	H	N	O	S	0	0
			22279	7014	11156	1938	2101	70		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1157	Total	C	H	N	O	S	0	0
			18471	5816	9243	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	H	N	O	S	0	0
			4160	1319	2062	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	H	N	O	S	0	0
			2631	812	1317	237	263	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	213	Total	C	H	N	O	S	0	0
			3495	1094	1755	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	H	N	O	S	0	0
			1371	429	694	114	131	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2666	858	1342	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	H	N	O	S	0	0
			2104	671	1052	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	H	N	O	S	0	0
			1790	565	873	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	H	N	O	S	0	0
			1109	349	564	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	H	N	O	S	0	0
			1876	599	944	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	H	N	O	S	0	0
			722	221	363	72	61	5		

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	64	Total	C	H	N	O	S	0	0
			1005	318	500	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 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	154	Total	C	H	N	O	P	0	0
			4910	1504	1739	566	947	154		

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*GP*GP*CP*CP*GP*UP*UP*UP*UP*P*CP*GP*UP*UP*GP*U)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	16	Total	C	H	N	O	P	0	0
			504	149	169	50	120	16		

- Molecule 16 is a DNA chain called DNA (159-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
16	T	159	Total	C	H	N	O	P	0	0
			5012	1535	1771	622	926	158		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	V	102	Total	C	H	N	O	S	0	0
			1554	492	762	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 Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	W	275	Total	C	H	N	O	S	0	0
			4503	1425	2277	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 F2QUC3
W	-1	PRO	-	expression tag	UNP F2QUC3
W	0	GLY	-	expression tag	UNP F2QUC3

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	a	97	Total	C	H	N	O	S	0	0
			1632	503	835	155	137	2		
19	e	97	Total	C	H	N	O	S	0	0
			1629	501	833	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	H	N	O	S	0	0
			1315	401	677	125	111	1		
20	f	78	Total	C	H	N	O	S	0	0
			1279	391	660	120	107	1		

There are 8 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

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Chain	Residue	Modelled	Actual	Comment	Reference
b	0	MET	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
f	0	MET	-	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	H	N	O	0	0
			1645	502	849	155	139		
21	g	105	Total	C	H	N	O	0	0
			1677	511	867	158	141		

There are 8 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
c	0	MET	-	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
g	0	MET	-	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	H	N	O	S	0	0
			1518	468	772	136	140	2		
22	h	93	Total	C	H	N	O	S	0	0
			1472	456	747	130	137	2		

There are 8 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
d	-3	MET	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899
h	-3	MET	-	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

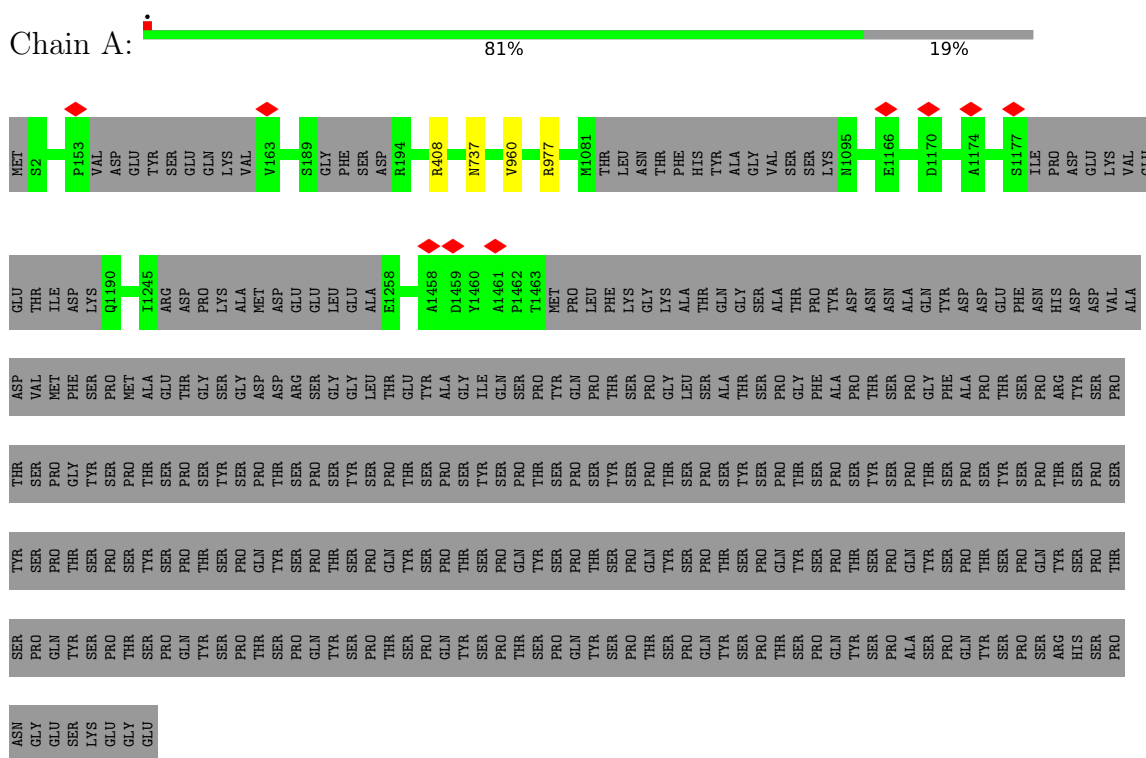
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

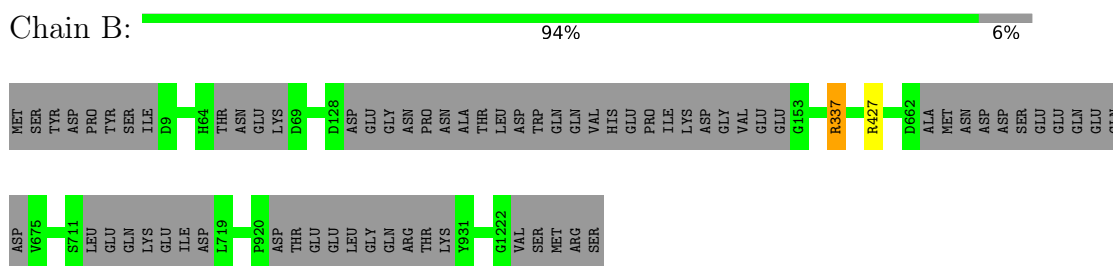
3 Residue-property plots

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.

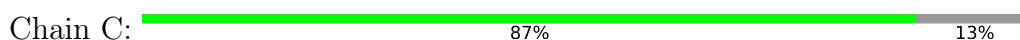
- Molecule 1: DNA-directed RNA polymerase subunit

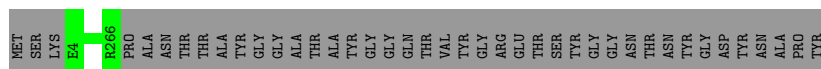


- Molecule 2: DNA-directed RNA polymerase subunit beta

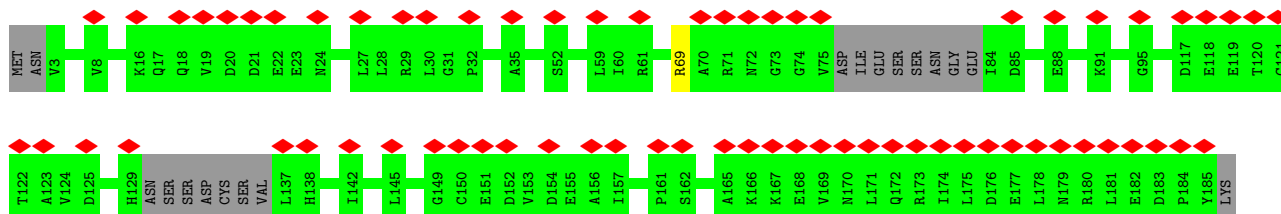
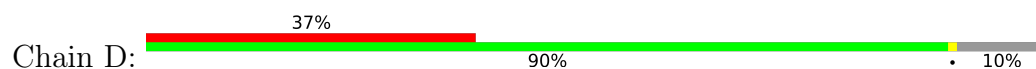


- Molecule 3: RNA polymerase II third largest subunit B44, part of central core





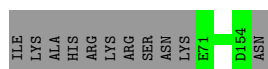
- Molecule 4: RNA polymerase II subunit B32



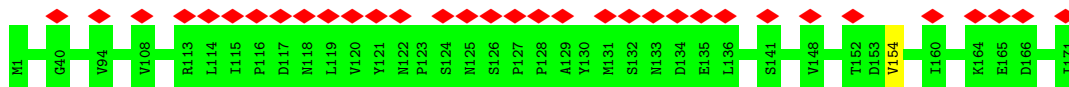
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



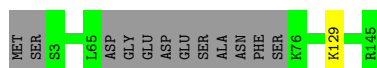
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



- Molecule 7: RNA polymerase II subunit

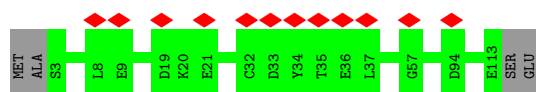


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



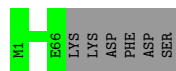
- Molecule 9: DNA-directed RNA polymerase subunit





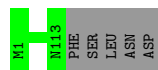
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J: 92% 8%



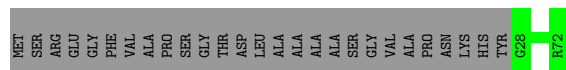
- Molecule 11: RNA polymerase II subunit B12.5

Chain K: 96% .



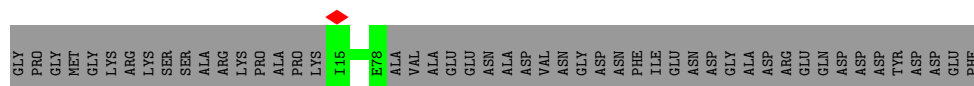
- Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L: 62% 38%



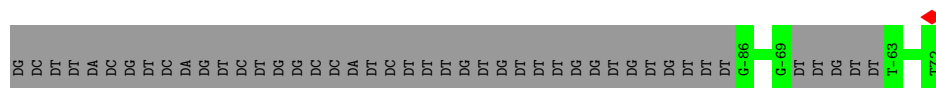
- Molecule 13: Transcription elongation factor 1 homolog

Chain M: 57% 43%



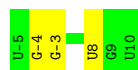
- Molecule 14: DNA (198-MER)

Chain N: 78% 22%

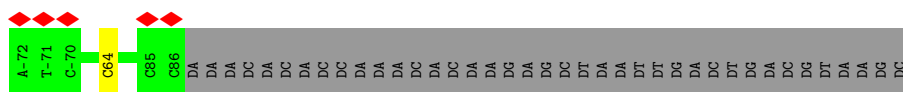


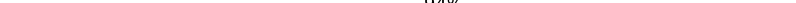
- Molecule 15: RNA (5'-R(P*UP*GP*GP*CP*CP*GP*UP*UP*UP*UP*CP*GP*UP*UP*GP*U)-3')

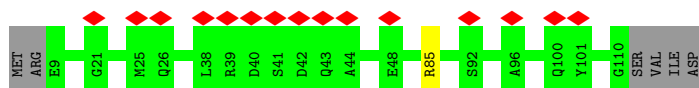
Chain P: 81% 19%



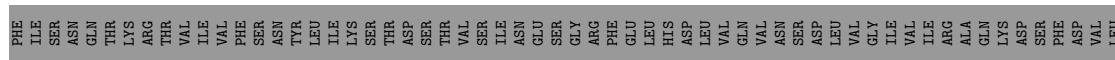
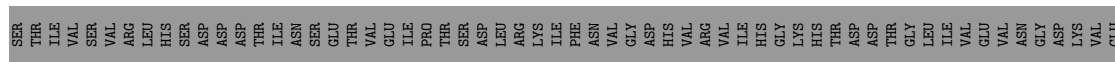
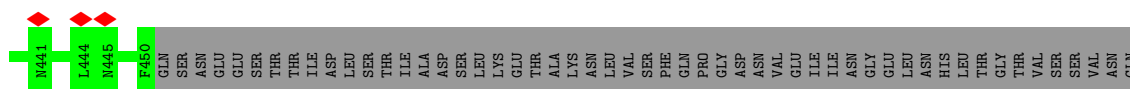
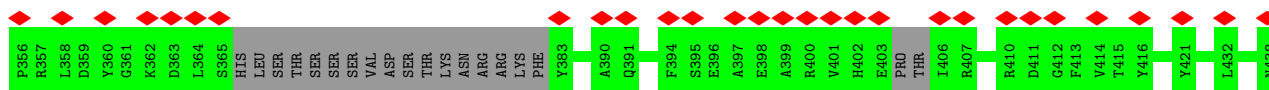
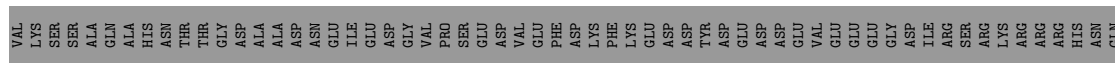
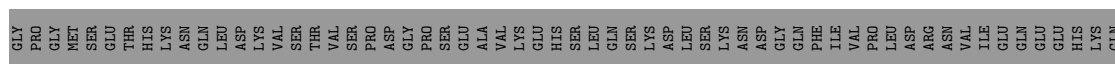
- Molecule 16: DNA (159-MER)



- Chain V:  14% 94% 6%



- Chain W: 5% 33% 66%



- 

Chain a:  70% 30%

GLY SER HIS MET MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY GLY LYS LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO SER THR GLY GLY VAL LYS LYS PRO P38 R134 ALA

- Molecule 19: Histone H3.3

Chain e:  70% 30%

GLY SER HIS MET MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY GLY LYS LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO SER THR GLY GLY VAL LYS LYS PRO H39 A135

- Molecule 20: Histone H4

Chain b:  75% 25%


GLY SER HIS MET MET SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS VAL LEU R23 R92 G102

- Molecule 20: Histone H4

Chain f:  73% 26%


GLY SER HIS MET MET SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS VAL LEU ASP R25 R92 G102

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

Chain c:  77% 23%

GLY SER HIS MET MET SER GLY ARG GLY LYS GLY GLY LYS GLY ALA ARG LYS LYS ALA LYS THR T136 K118 LYS THR GLU SER HIS HIS LYS ALA LYS LYS

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

Chain g:  79% 21%

GLY SER HIS MET MET PRO PRO ALA LYS GLN SER ALA PRO PRO ALA LYS LYS ALA ARG LYS LYS ALA LYS A14 A113 L116 P117 K118 LYS THR GLU SER ASP GLY HIS HIS LYS ALA LYS LYS LYS

- Molecule 22: Histone H2B type 1-J

Chain d:  73% 26%

GLY SER HIS MET MET PRO PRO ALA LYS GLN SER ALA PRO PRO ALA LYS LYS ALA ARG LYS LYS LYS LYS R28 K122

- Molecule 22: Histone H2B type 1-J



GLY	SER	HIS	MET	PRO	GLU	PRO	ALA	LYS	SER	ALA	PRO	ALA	PRO	LYS	LYS	GLY	SER	LYS	LYS	ALA	VAL	THR	LYS	ALA	GLN	LYS	LYS	ASP	GLY	LYS	LYS	ARG	LYS	ARG	ARG	S29	R76	A121	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00754	Depositor
Map size (Å)	356.15997, 356.15997, 356.15997	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.30	0/11329	0.50	0/15310
2	B	0.31	0/9407	0.53	0/12685
3	C	0.30	0/2139	0.50	0/2895
4	D	0.25	0/1326	0.50	0/1788
5	E	0.30	0/1772	0.52	0/2385
6	F	0.31	0/687	0.51	0/931
7	G	0.28	0/1353	0.50	0/1837
8	H	0.31	0/1069	0.50	0/1444
9	I	0.26	0/934	0.52	0/1257
10	J	0.36	0/554	0.55	0/742
11	K	0.30	0/953	0.49	0/1291
12	L	0.33	0/365	0.57	0/484
13	M	0.27	0/513	0.42	0/693
14	N	0.52	0/3551	0.93	0/5484
15	P	0.36	0/371	0.72	0/575
16	T	0.53	0/3641	0.85	1/5609 (0.0%)
17	V	0.25	0/808	0.51	0/1097
18	W	0.32	1/2267 (0.0%)	0.57	2/3048 (0.1%)
19	a	0.23	0/809	0.54	0/1085
19	e	0.25	0/807	0.55	0/1081
20	b	0.25	0/645	0.58	0/862
20	f	0.25	0/626	0.56	0/837
21	c	0.25	0/806	0.53	0/1089
21	g	0.25	0/820	0.52	0/1107
22	d	0.25	0/757	0.49	0/1015
22	h	0.24	0/736	0.45	0/990
All	All	0.34	1/49045 (0.0%)	0.60	3/67621 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	213	PRO	CG-CD	-7.90	1.24	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	213	PRO	N-CD-CG	-9.94	88.29	103.20
18	W	213	PRO	CA-N-CD	-6.34	102.63	111.50
16	T	64	DC	OP1-P-OP2	-6.29	110.16	119.60

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	1400/1743 (80%)	1305 (93%)	94 (7%)	1 (0%)	51	84
2	B	1145/1227 (93%)	1067 (93%)	77 (7%)	1 (0%)	51	84
3	C	261/304 (86%)	249 (95%)	12 (5%)	0	100	100
4	D	162/186 (87%)	155 (96%)	7 (4%)	0	100	100
5	E	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
6	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
7	G	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	25	63
8	H	129/145 (89%)	113 (88%)	16 (12%)	0	100	100
9	I	109/115 (95%)	103 (94%)	6 (6%)	0	100	100
10	J	64/72 (89%)	57 (89%)	7 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	111/118 (94%)	105 (95%)	6 (5%)	0	100	100
12	L	43/72 (60%)	38 (88%)	5 (12%)	0	100	100
13	M	62/113 (55%)	60 (97%)	2 (3%)	0	100	100
17	V	100/108 (93%)	96 (96%)	4 (4%)	0	100	100
18	W	265/812 (33%)	249 (94%)	16 (6%)	0	100	100
19	a	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
19	e	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
20	b	78/106 (74%)	75 (96%)	3 (4%)	0	100	100
20	f	76/106 (72%)	75 (99%)	1 (1%)	0	100	100
21	c	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
21	g	103/133 (77%)	99 (96%)	4 (4%)	0	100	100
22	d	93/129 (72%)	89 (96%)	4 (4%)	0	100	100
22	h	91/129 (70%)	86 (94%)	5 (6%)	0	100	100
All	All	5045/6569 (77%)	4746 (94%)	296 (6%)	3 (0%)	54	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	337	ARG
7	G	154	VAL
1	A	960	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1225/1528 (80%)	1222 (100%)	3 (0%)	93	96
2	B	1012/1077 (94%)	1010 (100%)	2 (0%)	93	96
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	143/160 (89%)	142 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	195 (100%)	1 (0%)	88	93
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%)	119 (99%)	1 (1%)	81	88
9	I	106/109 (97%)	106 (100%)	0	100	100
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%)	38 (100%)	0	100	100
13	M	61/99 (62%)	61 (100%)	0	100	100
17	V	86/92 (94%)	85 (99%)	1 (1%)	71	83
18	W	241/729 (33%)	239 (99%)	2 (1%)	81	88
19	a	83/112 (74%)	83 (100%)	0	100	100
19	e	82/112 (73%)	82 (100%)	0	100	100
20	b	65/81 (80%)	64 (98%)	1 (2%)	65	79
20	f	63/81 (78%)	62 (98%)	1 (2%)	62	78
21	c	82/102 (80%)	82 (100%)	0	100	100
21	g	83/102 (81%)	83 (100%)	0	100	100
22	d	81/107 (76%)	80 (99%)	1 (1%)	71	83
22	h	79/107 (74%)	78 (99%)	1 (1%)	69	81
All	All	4469/5705 (78%)	4454 (100%)	15 (0%)	92	95

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	129	LYS
20	f	92	ARG
17	V	85	ARG
22	h	76	ARG
20	b	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
21	g	73	ASN

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Mol	Chain	Res	Type
21	g	82	HIS
9	I	12	ASN
19	a	39	HIS
22	d	81	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	15/16 (93%)	3 (20%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	-4	G
15	P	-3	G
15	P	8	U

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

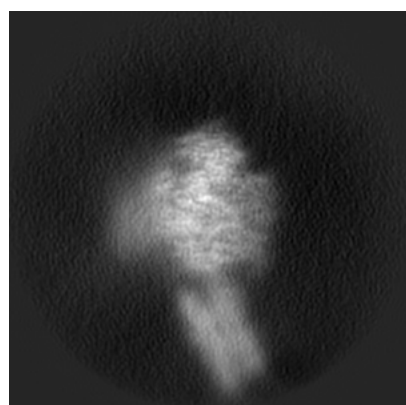
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32407. These allow visual inspection of the internal detail of the map and identification of artifacts.

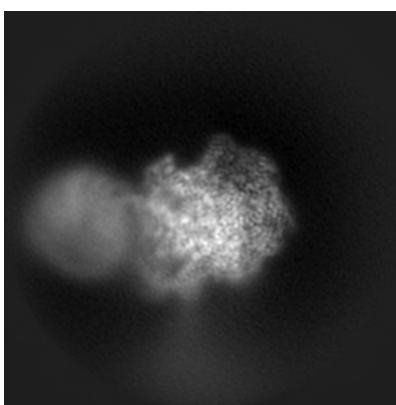
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

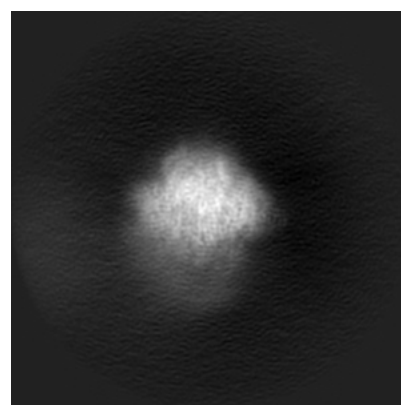
6.1.1 Primary map



X



Y

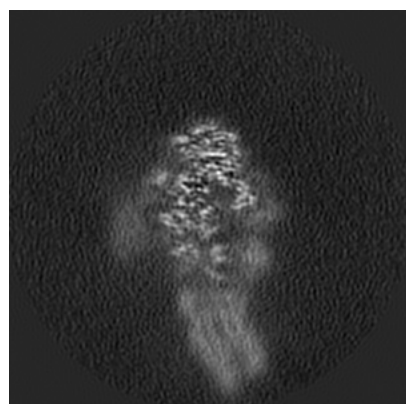


Z

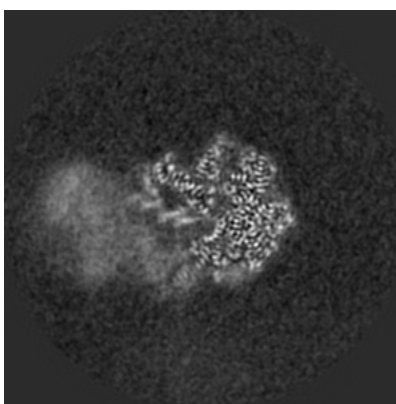
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

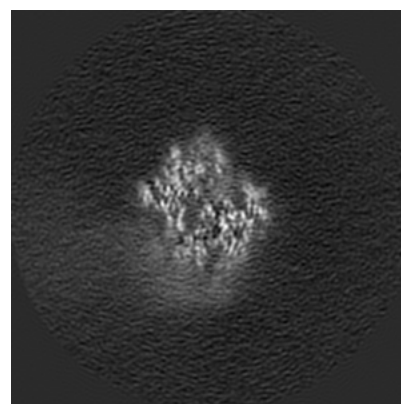
6.2.1 Primary map



X Index: 168



Y Index: 168

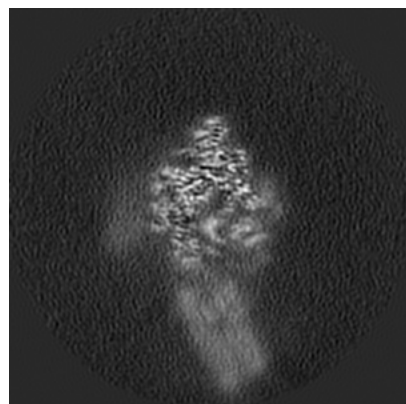


Z Index: 168

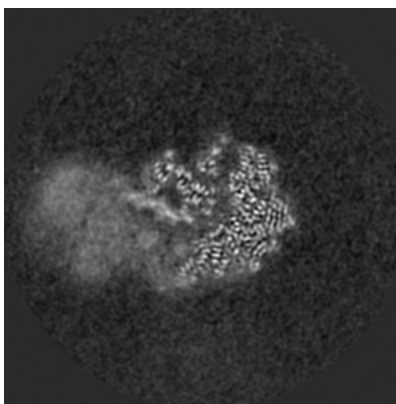
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

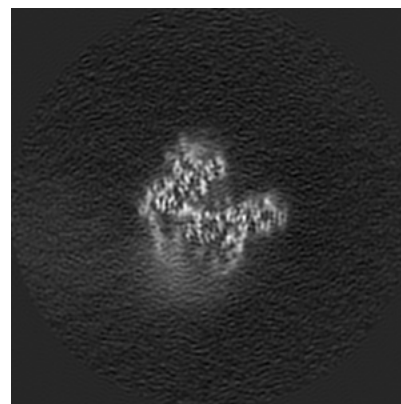
6.3.1 Primary map



X Index: 158



Y Index: 172

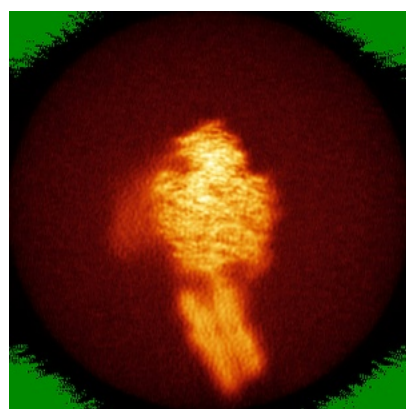


Z Index: 177

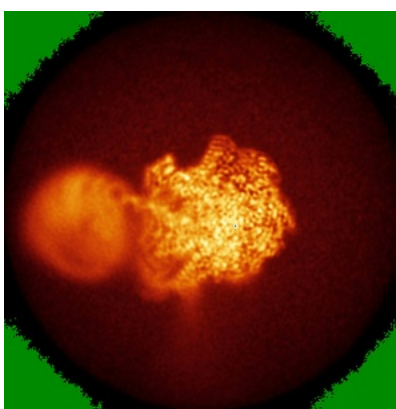
The images above show the largest variance slices of the map in three orthogonal directions.

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

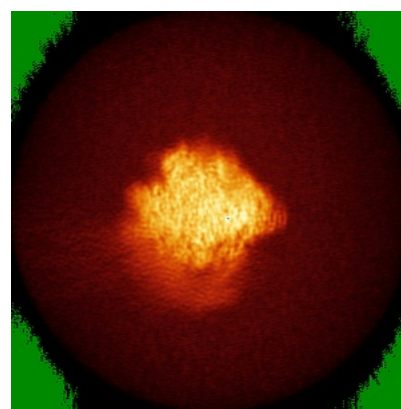
6.4.1 Primary map



X



Y

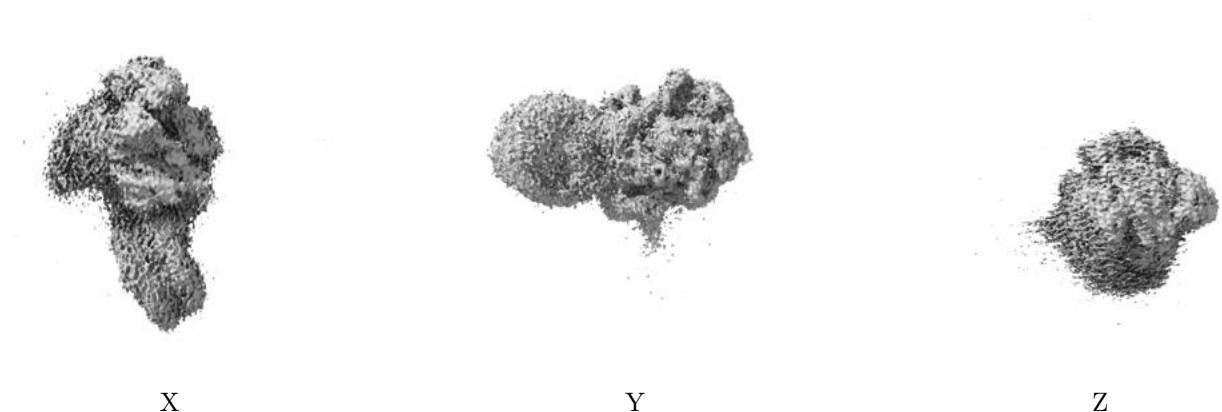


Z

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 0.00754. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

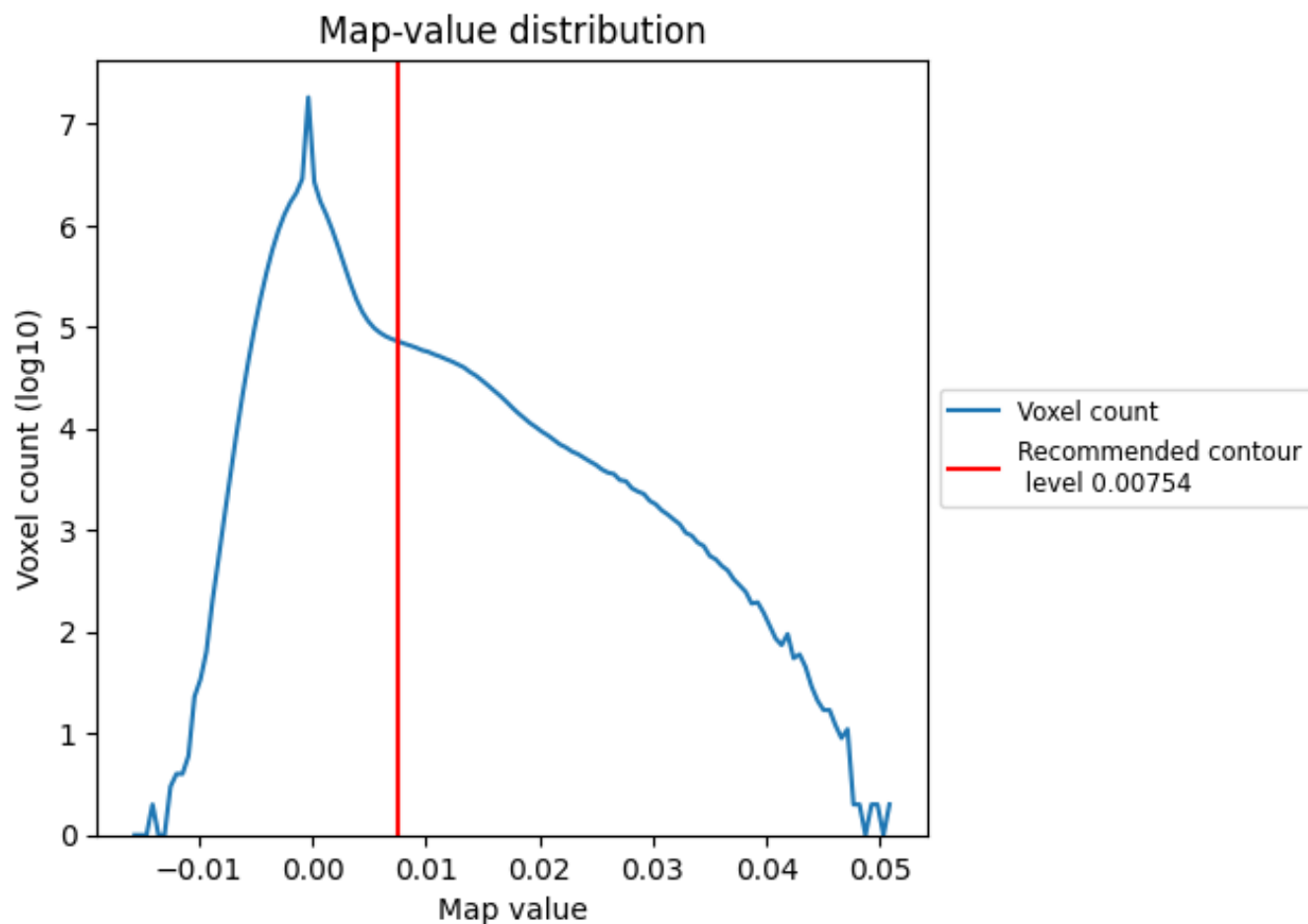
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

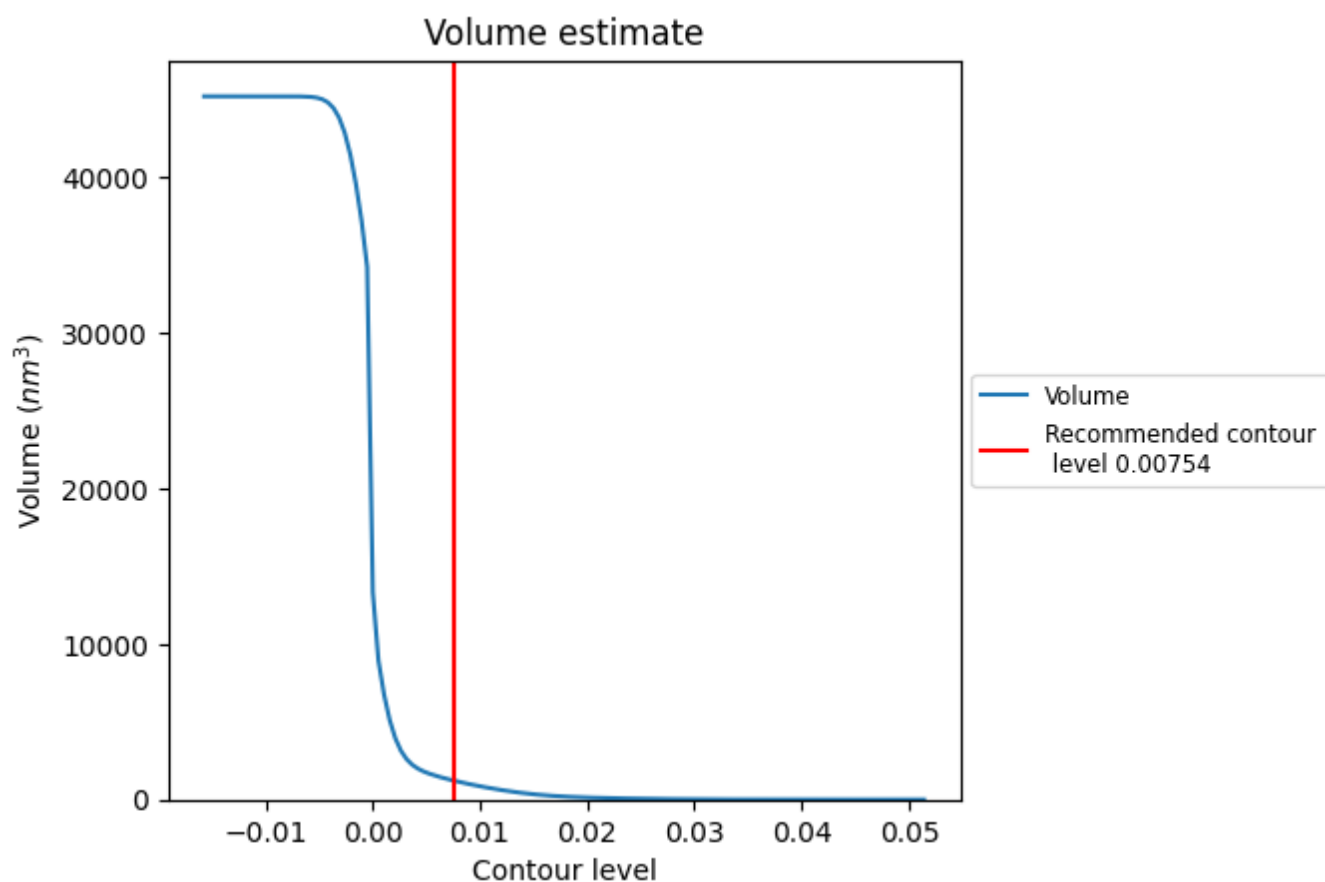
This section contains the results of statistical analysis of the map.

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.

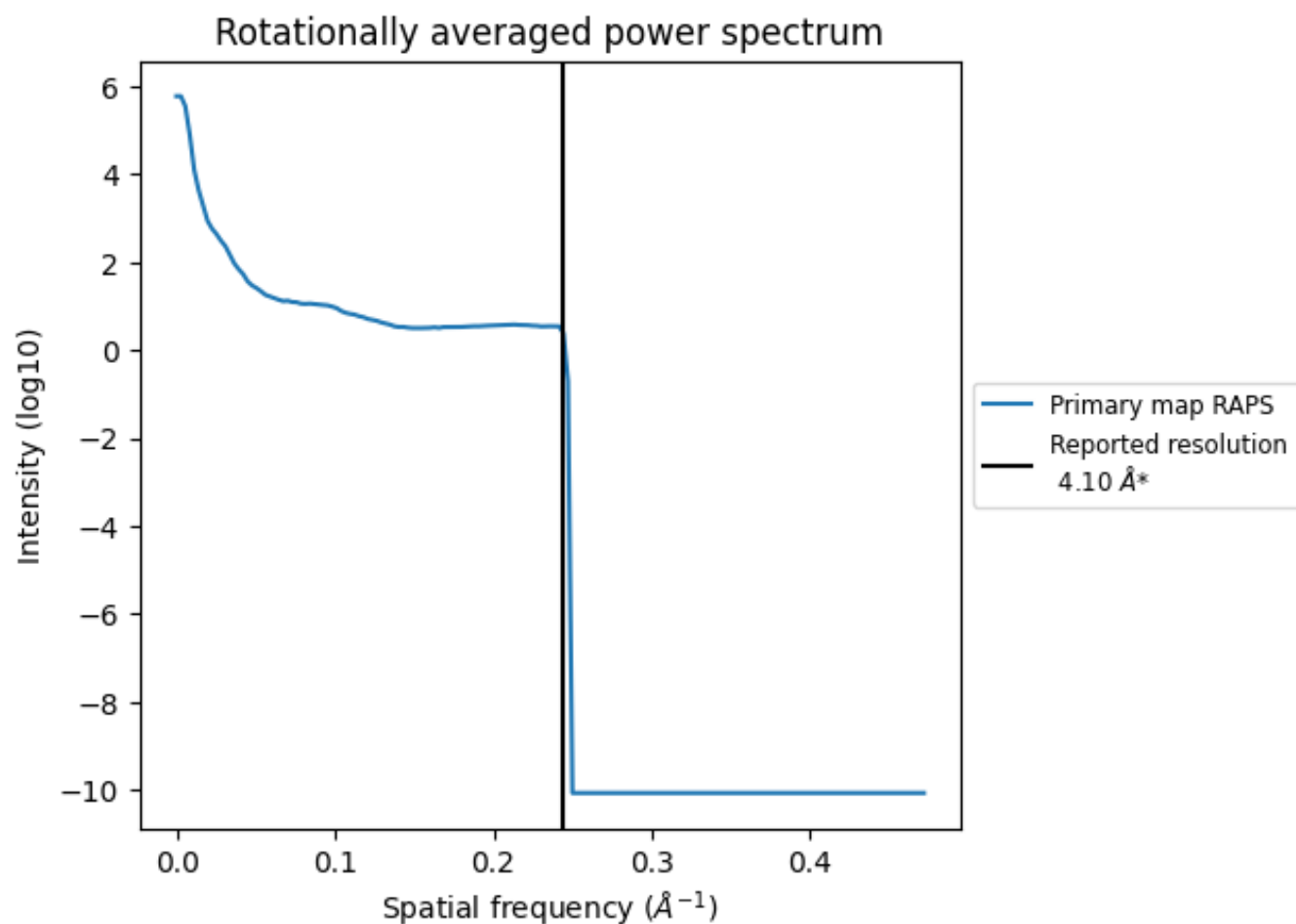
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1222 nm³; this corresponds to an approximate mass of 1104 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 ⓘ

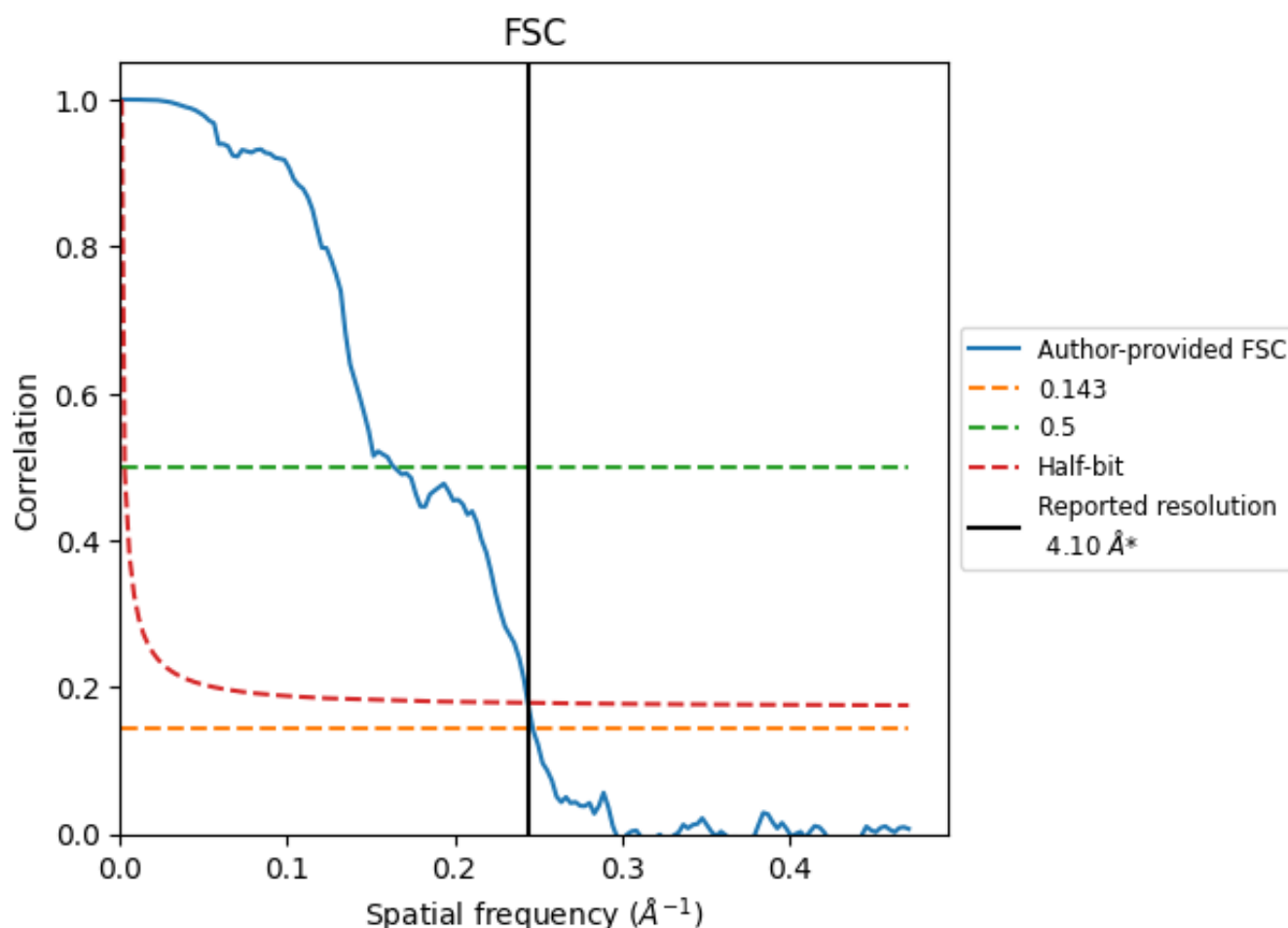


*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

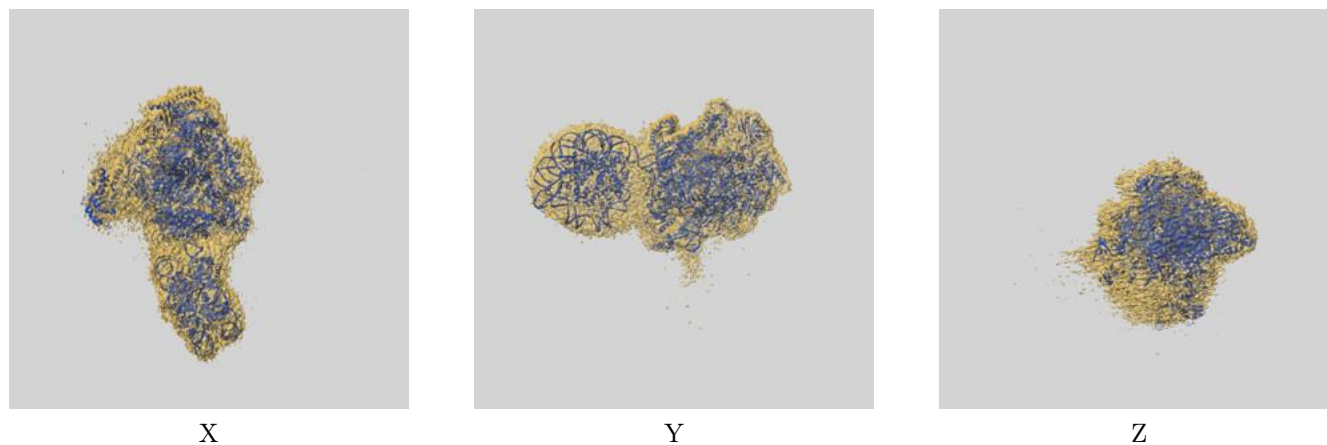
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.05	6.11	4.10
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

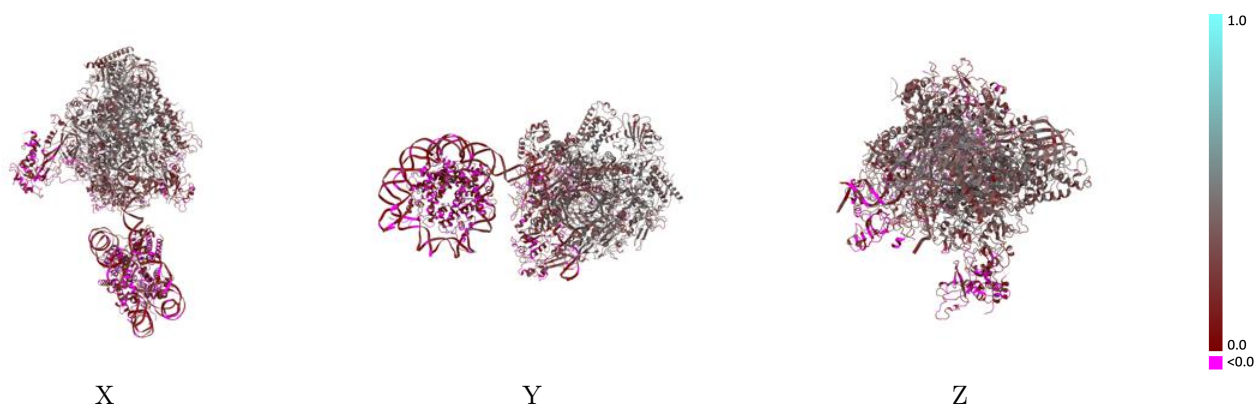
This section contains information regarding the fit between EMDB map EMD-32407 and PDB model 7WBV. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



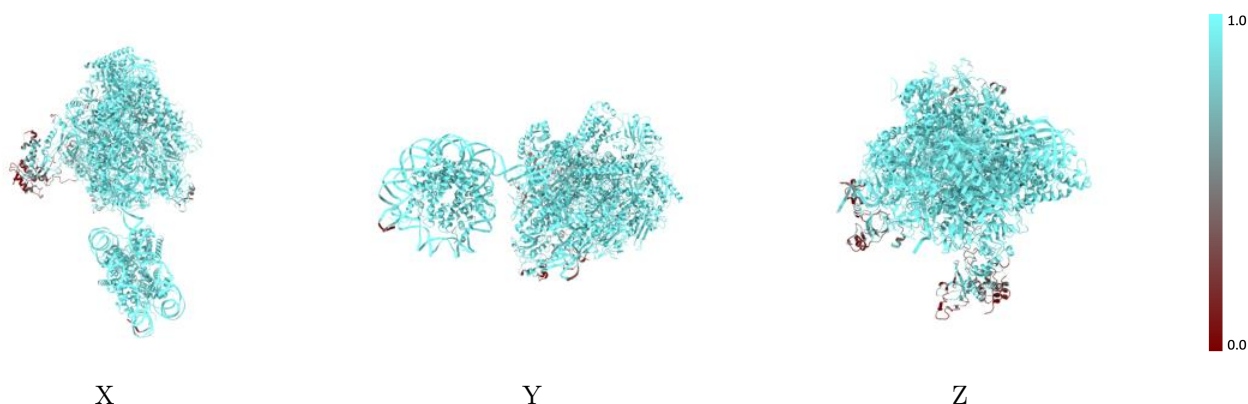
The images above show the 3D surface view of the map at the recommended contour level 0.00754 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



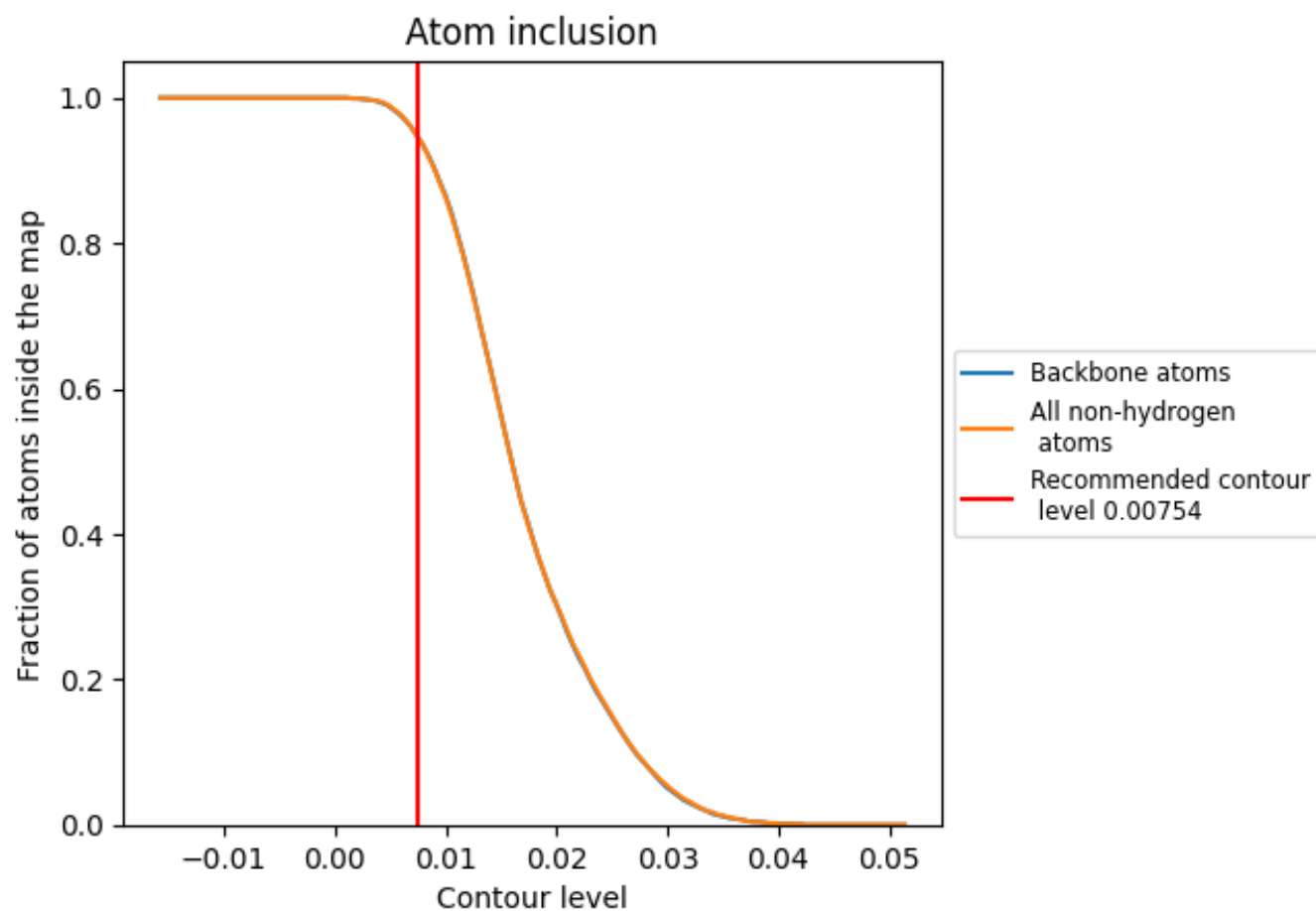
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00754).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.00754) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.2670
A	 0.9830	 0.3530
B	 0.9930	 0.3720
C	 0.9900	 0.3810
D	 0.5110	 0.1130
E	 0.9940	 0.3570
F	 0.9990	 0.3610
G	 0.7160	 0.1630
H	 0.9830	 0.3660
I	 0.8530	 0.1830
J	 0.9980	 0.3670
K	 0.9890	 0.3620
L	 1.0000	 0.3660
M	 0.9680	 0.1720
N	 0.9610	 0.1280
P	 0.9970	 0.3670
T	 0.9480	 0.1510
V	 0.7910	 0.1240
W	 0.7950	 0.1330
a	 0.9740	 0.0730
b	 0.9890	 0.1040
c	 0.9940	 0.0900
d	 0.9900	 0.1050
e	 0.9990	 0.0970
f	 1.0000	 0.0990
g	 0.9670	 0.0970
h	 0.9930	 0.1150

