



wwPDB EM Validation Summary Report ⓘ

Jul 19, 2026 – 12:24 AM JST

PDB ID : 9UXW / pdb_00009uxw
EMDB ID : EMD-64603
Title : RNA polymerase II elongation complex stalled at SHL(-0.5) in the hexasome of the overlapping dinucleosome
Authors : Chen, Z.; Ho, C.; Tanaka, H.; Kujirai, T.; Ogasawara, M.; Ehara, H.; Sekine, S.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2025-05-14
Resolution : 3.74 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.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

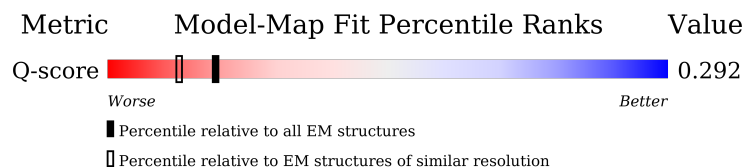
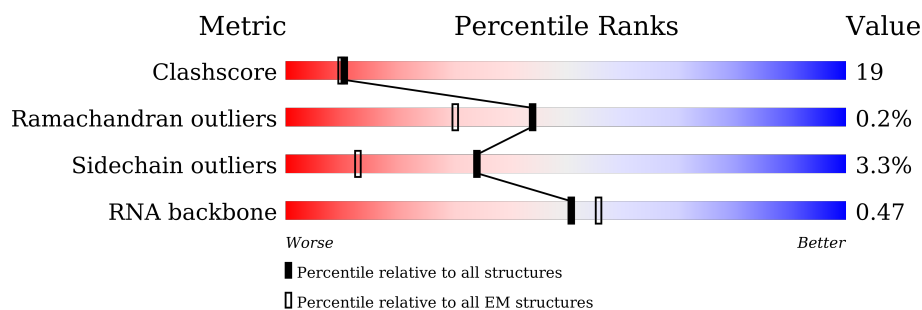
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.74 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10346 (3.24 - 4.24)

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	

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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	14	
14	T	254	
15	a	139	
15	e	139	
15	k	139	
15	m	139	
16	b	106	
16	f	106	
16	l	106	
16	n	106	
17	c	133	
17	g	133	
17	o	133	
18	d	129	
18	h	129	
18	p	129	

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Mol	Chain	Length	Quality of chain
19	N	254	17% 39% 56% 5%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51489 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	1402	Total	C	N	O	S	0	0
			11049	6966	1927	2086	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1164	Total	C	N	O	S	0	0
			9284	5848	1639	1739	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	174	Total	C	N	O	S	0	0
			1349	828	244	274	3		

- 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
			1741	1094	312	325	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
			1325	858	214	248	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
			1053	671	169	209	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	67	Total	C	N	O	S	0	0
			554	355	97	96	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*GP*UP*CP*GP*CP*UP*CP*UP*UP*C P*CP*UP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	14	Total	C	N	O	P	0	0
			286	128	41	103	14		

- Molecule 14 is a DNA chain called DNA (254-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	254	Total	C	N	O	P	0	0
			5254	2480	1021	1499	254		

- Molecule 15 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	95	Total	C	N	O	S	0	0
			779	492	150	135	2		
15	e	95	Total	C	N	O	S	0	0
			779	492	150	135	2		
15	k	73	Total	C	N	O	S	0	0
			587	373	109	103	2		
15	m	95	Total	C	N	O	S	0	0
			779	492	150	135	2		

There are 12 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
k	-3	GLY	-	expression tag	UNP P84243
k	-2	SER	-	expression tag	UNP P84243
k	-1	HIS	-	expression tag	UNP P84243
m	-3	GLY	-	expression tag	UNP P84243
m	-2	SER	-	expression tag	UNP P84243
m	-1	HIS	-	expression tag	UNP P84243

- Molecule 16 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		
16	l	71	Total	C	N	O	S	0	0
			568	357	113	97	1		
16	n	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 12 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
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
l	-3	GLY	-	expression tag	UNP P62805
l	-2	SER	-	expression tag	UNP P62805
l	-1	HIS	-	expression tag	UNP P62805
n	-3	GLY	-	expression tag	UNP P62805
n	-2	SER	-	expression tag	UNP P62805
n	-1	HIS	-	expression tag	UNP P62805

- Molecule 17 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	c	98	Total	C	N	O	0	0
			757	475	149	133		
17	g	98	Total	C	N	O	0	0
			757	475	149	133		
17	o	97	Total	C	N	O	0	0
			752	472	148	132		

There are 9 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

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

- Molecule 18 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	90	Total	C	N	O	S	0	0
			698	440	123	133	2		
18	h	89	Total	C	N	O	S	0	0
			689	435	122	130	2		
18	p	87	Total	C	N	O	S	0	0
			679	430	120	127	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-3	GLY	-	expression tag	UNP P06899
d	-2	SER	-	expression tag	UNP P06899
d	-1	HIS	-	expression tag	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899
p	-3	GLY	-	expression tag	UNP P06899
p	-2	SER	-	expression tag	UNP P06899
p	-1	HIS	-	expression tag	UNP P06899

- Molecule 19 is a DNA chain called DNA (254-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	242	Total	C	N	O	P	0	0
			4921	2342	865	1472	242		

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		AltConf
20	I	2	Total 2	Zn 2	0
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0

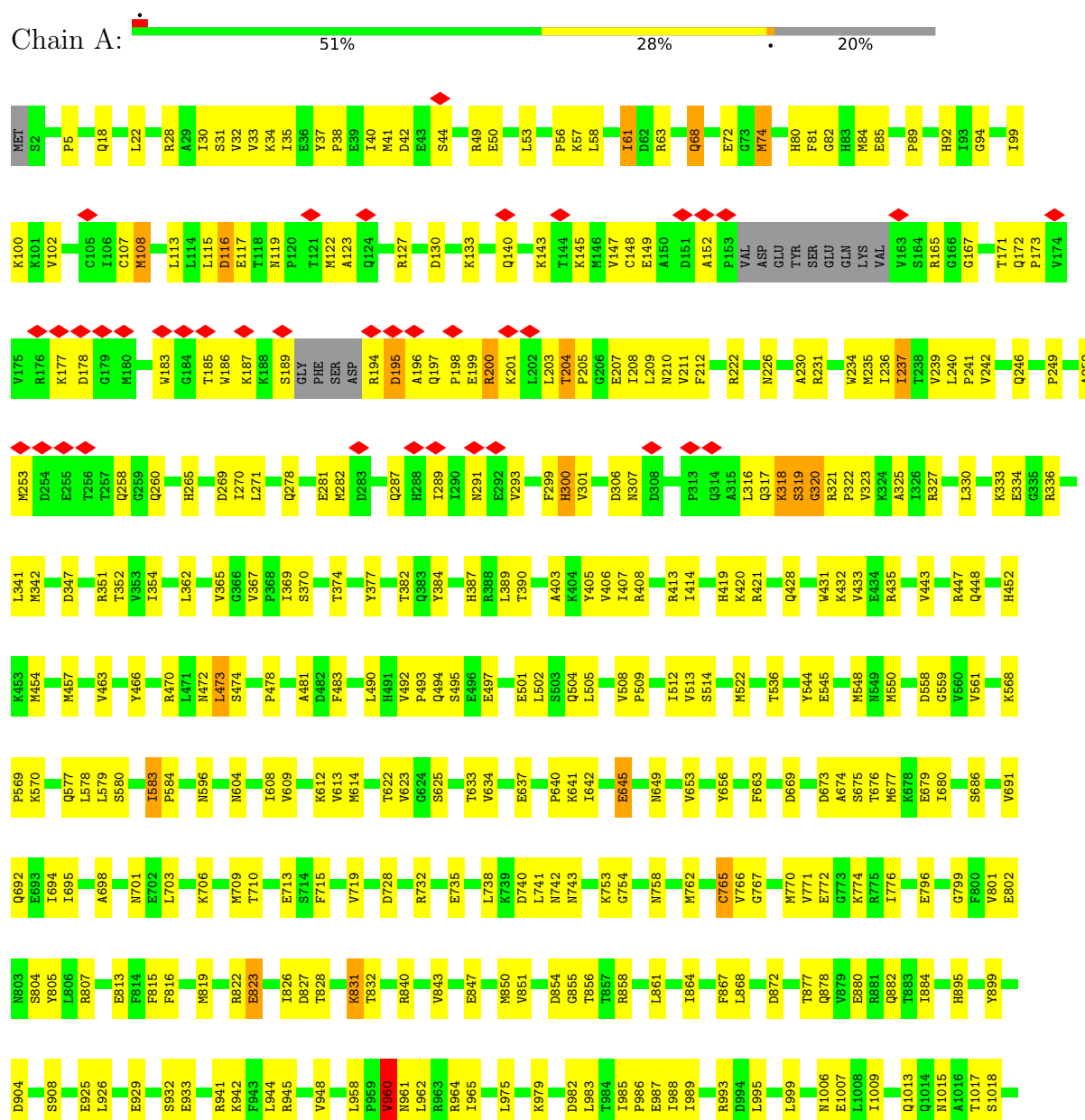
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	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.

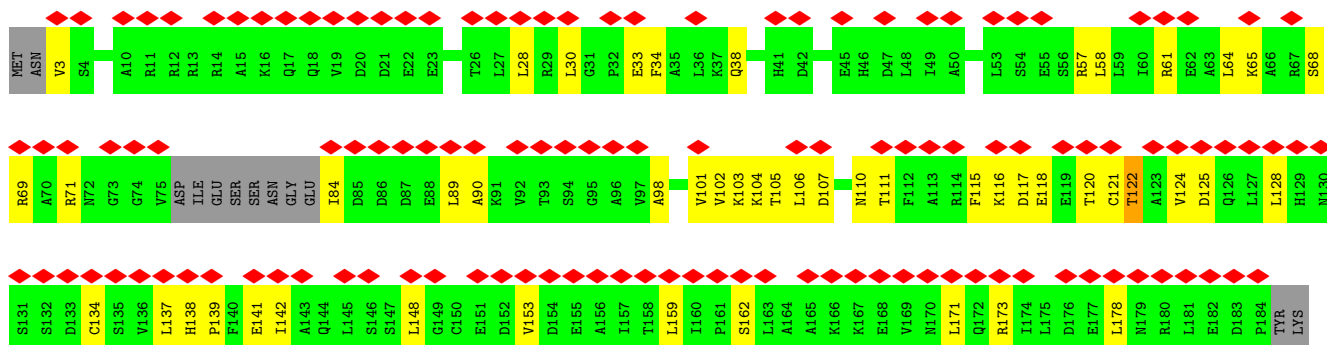
• Molecule 1: DNA-directed RNA polymerase subunit



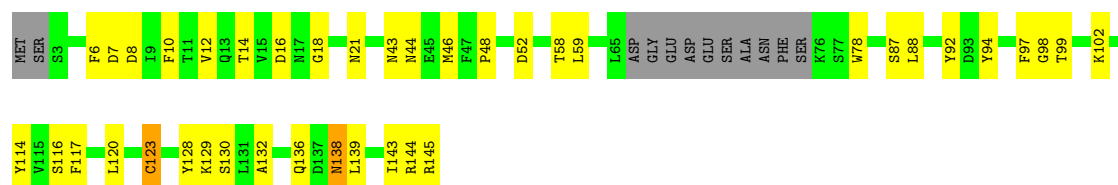


Q350	V288	M164	M89	ME1
K351	K269		T90	SER
E352		S167	ASP	TVR
L353	I272	L172	E91	PRO
	P273	S173		TVR
I357	I276	T174	T96	ILE
T358	V277	L175	M99	D9
Q359	F278	D176	F100	
E360	R279	E177	P101	T12
	A280		Q102	T13
F363		L180	E103	T14
E364	V283		A104	E15
T365	V284	K184	R105	D16
K366	P285	E185	S113	
K367		C186	P114	T19
T368	E288	F187	V115	
F369	T289	Y188	Y116	S22
	L290		L117	E27
K374			D118	
V375	T293	E200	M119	V31
N376	C294	K201	E120	
L379				
	W300	Q206	F124	L35
C381	Q301	E207		
A382	M302		I127	T44
	L303	I213	D128	S45
Q388	E304		ASP	T46
D389	M305	K218	GLU	Q47
D390	L306	R219	GLY	
R391		A220	ASN	
D392	C309	P221	ASN	Y50
H393		P222	ASN	
F394	I316	S223	ALA	L56
			THR	I57
L399	E320		LEU	L58
D400	V321	S226	ASP	D59
L401	A322	H227	TRP	Q60
A402	L323	E230	GLN	P61
	D324	Q63	GLN	A62
L409	F325		VAL	Q63
		S233	HIS	H64
L413	R329		GLU	THR
F414	G330	E236	PRO	ASN
	S331	K237	ILE	LYS
R419			LYS	D69
	I336	M245	ASP	M70
R423	R337	Q246	GLY	I71
	R338	T247	VAL	M72
Q426	E339		GLU	K73
R427	K340	R252	GLU	R74
C428	R341	R259	G153	Y75
	I342			E76
T431	Q343	T260	V156	I77
D432	Y344	I261	G159	R78
R433	A345	K262		
D434	K346			
F435	D347	L285		Y83
A436	I348	P266	P162	L84
	L340		I62	S95



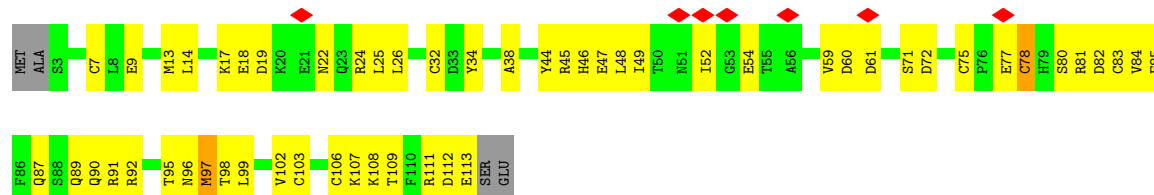


Chain H: 



- Molecule 9: DNA-directed RNA polymerase subunit

Chain I: 



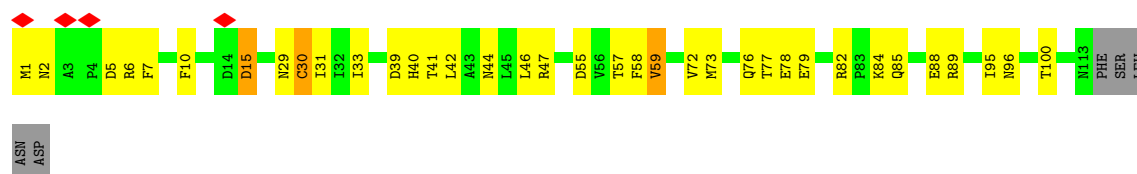
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J: 

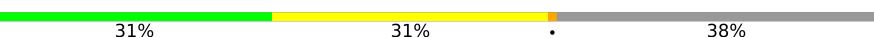


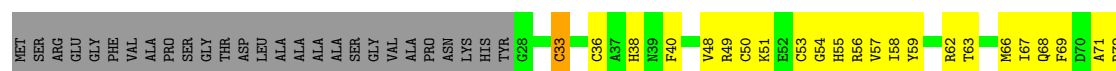
- Molecule 11: RNA polymerase II subunit B12.5

Chain K: 



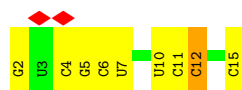
- Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L: 

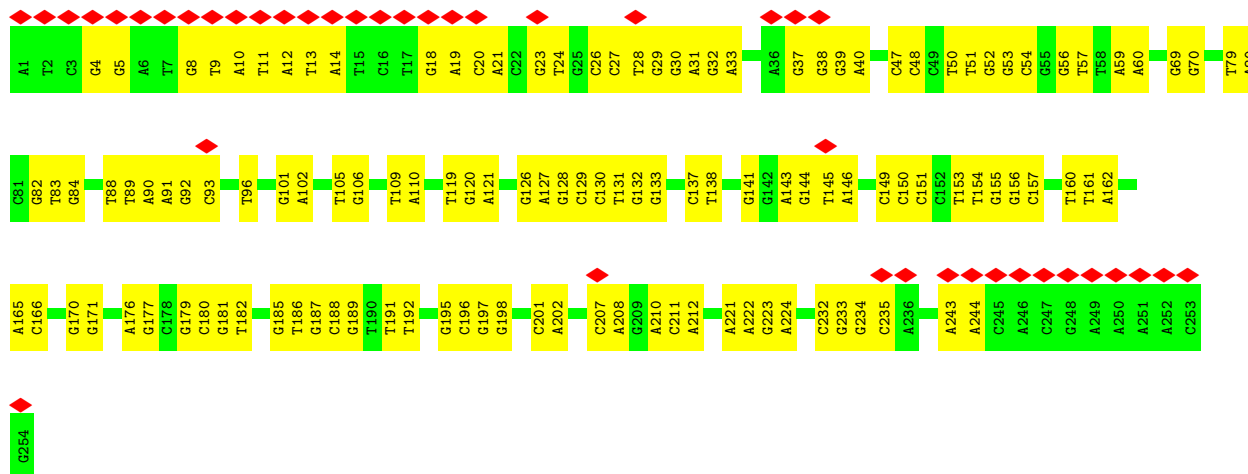


- Molecule 13: RNA (5'-R(P*GP*UP*CP*GP*CP*UP*CP*UP*UP*CP*CP*UP*CP*C)-3')

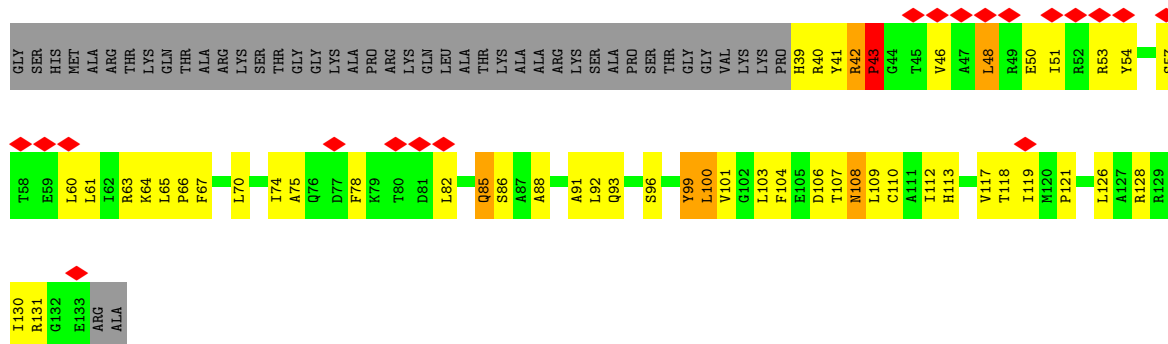
Chain P: 



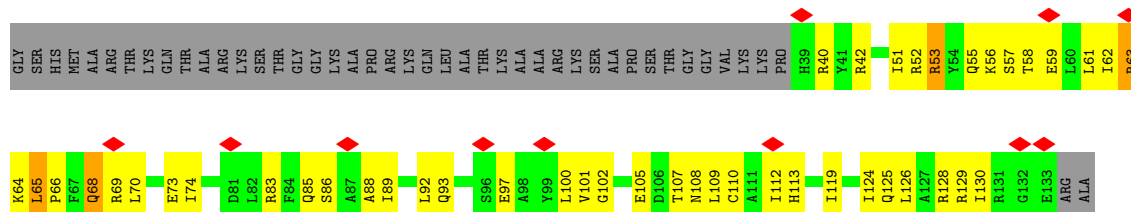
• Molecule 14: DNA (254-MER)



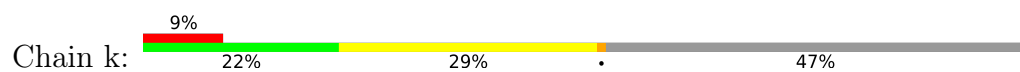
• Molecule 15: Histone H3.3



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• Molecule 15: Histone H3.3

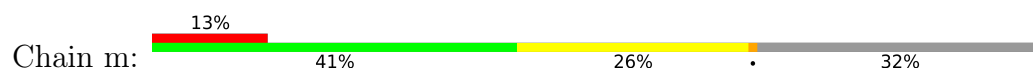


GLY SER THR GLU MET LEU ALA ARG THR LYS GLN THR ALA ARG LYS THR SER THR GLY LYS ALA PRO ARG LYS GLN LEU THR LYS ALA ARG LYS SER ALA PRO SER THR GLY VAL LYS LYS PRO HIS ARG THR ARG PRO GLY THR VAL ALA LEU ARG GLU ILE ARG TYR GLN LYS

SER THR GLU MET LEU L61 L62 L63 L64 L65 L66 L67 L68 L69 L70 L71 L72 D81 F84 A87 A88 I89 A91 A92 Q93 E94 A95 S96 E97 A98 A99 L100 L101 G102 L103 F104 E105 D106 T107 N108 L109 I112 H113 T118 T119 M120 P121 K122 D123 I124 Q125 L126 A127 R128 R129

I130 R131 G132 E133 ARG ALA

• Molecule 15: Histone H3.3



GLY SER HIS MET LEU ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY LYS ALA PRO ARG LYS GLN LEU THR LYS ALA ARG LYS SER PRO SER THR GLY VAL LYS LYS PRO H39 R40 Y41 T45 V46 A47 L48 E50 R53 Y54 Q55 K56 E59 L60

L61 L62 R63 F67 Q68 R69 L70 V71 R72 Q76 D77 F78 K79 T80 D81 L82 R83 L89 G90 A91 A92 L92 Q93 E94 A95 S96 E97 A98 Y99 L100 V101 E105 D106 T107 N108 H113 P121 I124 Q125 L126 A127 I130 R131 G132 E133 ARG ALA

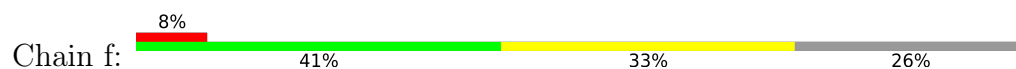
• Molecule 16: Histone H4



GLY SER HIS MET LEU SER GLY ARG GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS VAL LEU ASP N25 I26 I29 T30 K31 I34 R35 R36 L37 A38 R39 R40 G41 G42 V43 K44 R45 I46 S47 G48 L49 I50 Y51 E52 E53 E54 T55 R55 G56 V57 L58

K59 V60 F61 L62 E63 R64 V65 I66 R67 Y72 H75 V81 M84 D85 V86 V87 A89 HIS A90 L90 K91 R92 Q93 L97 Y98 G99 F100 G101 G102

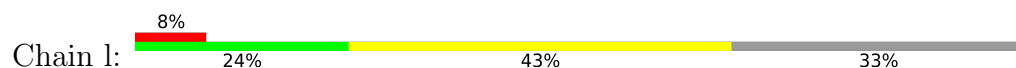
• Molecule 16: Histone H4

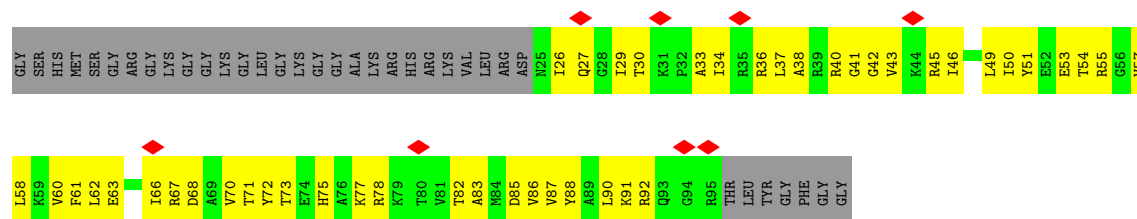


GLY SER HIS MET LEU SER GLY ARG GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS VAL LEU ASP N25 I26 Q27 G28 I29 T30 K31 I34 L37 A38 R39 R40 V43 K44 R45 I46 L49 T50 Y51 E52 G56 V57 L58 K59 V60 F61 L62

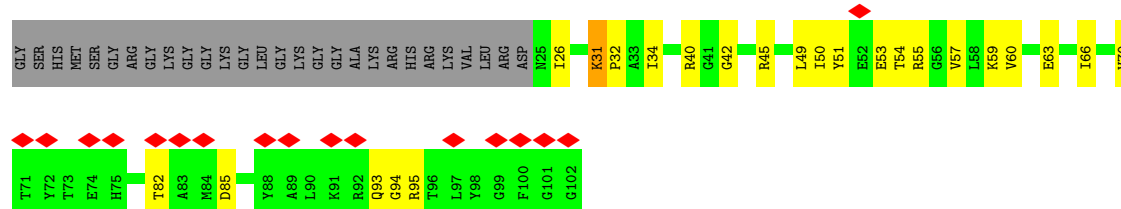
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• Molecule 16: Histone H4

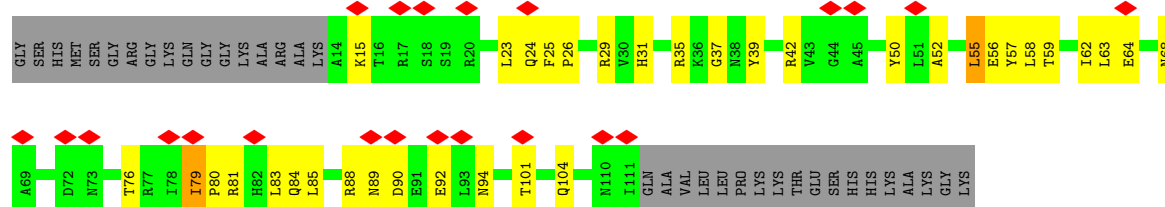




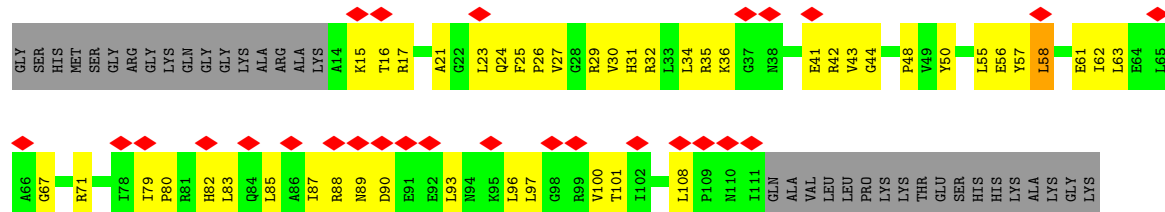
• Molecule 16: Histone H4



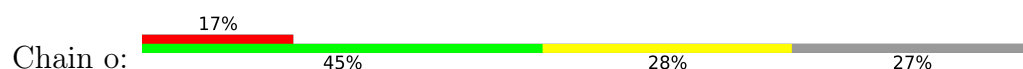
• Molecule 17: Histone H2A type 1-B/E



• Molecule 17: Histone H2A type 1-B/E

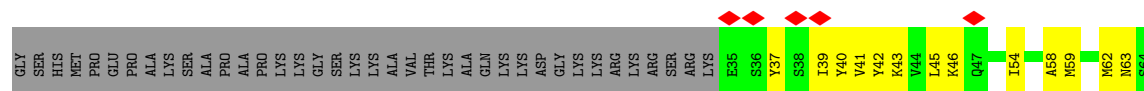
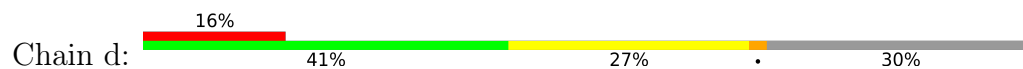


• Molecule 17: Histone H2A type 1-B/E

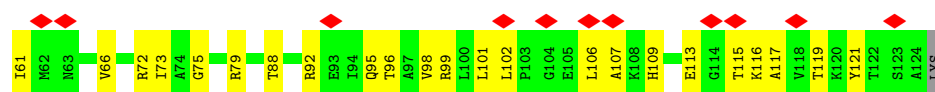




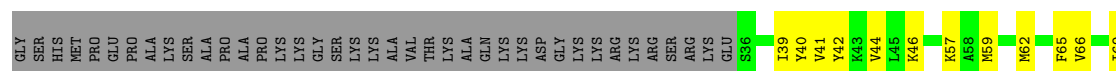
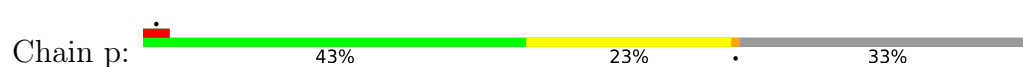
- Molecule 18: Histone H2B type 1-J



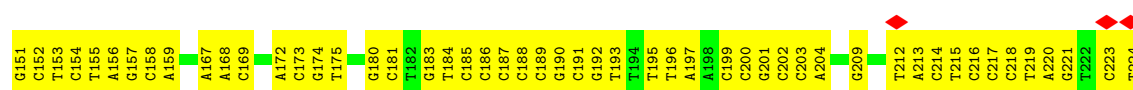
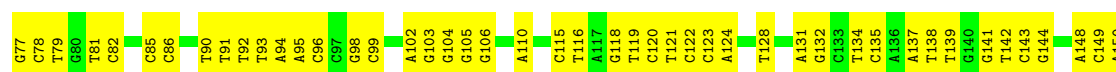
- Molecule 18: Histone H2B type 1-J



- Molecule 18: Histone H2B type 1-J



- Molecule 19: DNA (254-MER)



C225	C226	A227	G228	G229	C230	A231	C232	G233	T234	G235	T236	C237	A238	G239	A240	T241	A242	T243	A244	T245	A246	C247	A248	T249	C250	C251	G252	A253	T254
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.8	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	0.046	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00777	Depositor
Map size ($\text{\AA}$)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.41	0/11252	0.56	0/15201
2	B	0.42	0/9464	0.57	0/12763
3	C	0.39	0/2139	0.49	0/2895
4	D	0.20	0/1361	0.50	0/1837
5	E	0.38	0/1773	0.62	0/2385
6	F	0.34	0/687	0.54	0/931
7	G	0.24	0/1354	0.55	0/1837
8	H	0.35	0/1070	0.45	0/1444
9	I	0.30	0/934	0.59	0/1257
10	J	0.49	0/563	0.59	0/753
11	K	0.40	0/953	0.50	0/1291
12	L	0.30	0/365	0.54	0/484
13	P	0.75	0/315	0.84	0/486
14	T	0.63	0/5912	0.88	0/9131
15	a	0.62	0/790	0.90	0/1060
15	e	0.65	0/790	0.91	0/1060
15	k	0.54	0/594	0.89	0/797
15	m	0.64	0/790	0.98	0/1060
16	b	0.62	0/626	0.86	0/837
16	f	0.49	0/626	0.82	0/837
16	l	0.55	0/573	0.88	0/767
16	n	0.62	0/626	0.87	0/837
17	c	0.60	0/766	0.97	0/1033
17	g	0.36	0/766	0.64	0/1033
17	o	0.26	0/761	0.59	0/1026
18	d	0.47	0/709	0.69	0/955
18	h	0.35	0/700	0.61	0/943
18	p	0.29	0/690	0.59	0/930
19	N	0.63	0/5504	0.91	0/8483
All	All	0.48	0/53453	0.70	0/74353

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11049	0	11076	434	0
2	B	9284	0	9282	324	0
3	C	2098	0	2057	77	0
4	D	1349	0	1345	40	0
5	E	1741	0	1754	64	0
6	F	677	0	693	19	0
7	G	1325	0	1342	47	0
8	H	1053	0	1050	27	0
9	I	917	0	864	49	0
10	J	554	0	573	23	0
11	K	932	0	944	35	0
12	L	359	0	358	24	0
13	P	286	0	150	7	0
14	T	5254	0	2838	154	0
15	a	779	0	814	65	0
15	e	779	0	814	58	0
15	k	587	0	615	59	0
15	m	779	0	814	33	0
16	b	619	0	659	57	0
16	f	619	0	659	46	0
16	l	568	0	614	65	0
16	n	619	0	659	21	0
17	c	757	0	802	41	0
17	g	757	0	802	45	0
17	o	752	0	797	42	0
18	d	698	0	710	42	0
18	h	689	0	704	35	0
18	p	679	0	698	34	0
19	N	4921	0	2727	181	0
20	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
All	All	51489	0	47214	1837	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 1837 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:12:DA:H2''	14:T:13:DT:C7	1.34	1.55
19:N:5:DT:C2'	19:N:6:DT:H71	1.36	1.54
19:N:5:DT:H2''	19:N:6:DT:C7	1.45	1.42
19:N:8:DG:H2''	19:N:9:DT:C7	1.48	1.42
19:N:8:DG:C2'	19:N:9:DT:H72	1.49	1.40

There are no symmetry-related clashes.

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	1390/1743 (80%)	1289 (93%)	96 (7%)	5 (0%)	30	60
2	B	1154/1227 (94%)	1063 (92%)	91 (8%)	0	100	100
3	C	261/304 (86%)	249 (95%)	12 (5%)	0	100	100
4	D	170/186 (91%)	164 (96%)	6 (4%)	0	100	100
5	E	211/214 (99%)	206 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	82/155 (53%)	76 (93%)	6 (7%)	0	100	100
7	G	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
8	H	129/145 (89%)	118 (92%)	11 (8%)	0	100	100
9	I	109/115 (95%)	99 (91%)	10 (9%)	0	100	100
10	J	65/72 (90%)	63 (97%)	1 (2%)	1 (2%)	8	36
11	K	111/118 (94%)	104 (94%)	7 (6%)	0	100	100
12	L	43/72 (60%)	41 (95%)	2 (5%)	0	100	100
15	a	93/139 (67%)	85 (91%)	6 (6%)	2 (2%)	5	31
15	e	93/139 (67%)	88 (95%)	5 (5%)	0	100	100
15	k	71/139 (51%)	67 (94%)	4 (6%)	0	100	100
15	m	93/139 (67%)	87 (94%)	5 (5%)	1 (1%)	11	41
16	b	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
16	f	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
16	l	69/106 (65%)	65 (94%)	4 (6%)	0	100	100
16	n	76/106 (72%)	70 (92%)	6 (8%)	0	100	100
17	c	96/133 (72%)	92 (96%)	4 (4%)	0	100	100
17	g	96/133 (72%)	94 (98%)	1 (1%)	1 (1%)	12	43
17	o	95/133 (71%)	92 (97%)	3 (3%)	0	100	100
18	d	88/129 (68%)	85 (97%)	3 (3%)	0	100	100
18	h	87/129 (67%)	85 (98%)	2 (2%)	0	100	100
18	p	85/129 (66%)	83 (98%)	2 (2%)	0	100	100
All	All	5088/6288 (81%)	4772 (94%)	306 (6%)	10 (0%)	44	71

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1316	LEU
15	a	46	VAL
1	A	320	GLY
1	A	960	VAL
1	A	200	ARG

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	1217/1528 (80%)	1177 (97%)	40 (3%)	33	55
2	B	1018/1077 (94%)	989 (97%)	29 (3%)	38	58
3	C	236/264 (89%)	228 (97%)	8 (3%)	32	55
4	D	149/160 (93%)	148 (99%)	1 (1%)	76	77
5	E	196/197 (100%)	187 (95%)	9 (5%)	24	49
6	F	75/137 (55%)	71 (95%)	4 (5%)	20	46
7	G	148/148 (100%)	144 (97%)	4 (3%)	39	59
8	H	120/130 (92%)	115 (96%)	5 (4%)	26	51
9	I	106/109 (97%)	104 (98%)	2 (2%)	50	65
10	J	61/66 (92%)	59 (97%)	2 (3%)	33	55
11	K	104/109 (95%)	98 (94%)	6 (6%)	18	45
12	L	38/56 (68%)	37 (97%)	1 (3%)	40	60
15	a	81/112 (72%)	72 (89%)	9 (11%)	6	25
15	e	81/112 (72%)	77 (95%)	4 (5%)	22	48
15	k	61/112 (54%)	59 (97%)	2 (3%)	33	55
15	m	81/112 (72%)	75 (93%)	6 (7%)	13	39
16	b	63/81 (78%)	60 (95%)	3 (5%)	23	48
16	f	63/81 (78%)	62 (98%)	1 (2%)	55	68
16	l	59/81 (73%)	59 (100%)	0	100	100
16	n	63/81 (78%)	60 (95%)	3 (5%)	23	48
17	c	77/102 (76%)	75 (97%)	2 (3%)	40	60
17	g	77/102 (76%)	75 (97%)	2 (3%)	40	60
17	o	77/102 (76%)	77 (100%)	0	100	100
18	d	76/107 (71%)	74 (97%)	2 (3%)	40	60
18	h	75/107 (70%)	75 (100%)	0	100	100
18	p	74/107 (69%)	73 (99%)	1 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4476/5380 (83%)	4330 (97%)	146 (3%)	34 55

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	a	85	GLN
16	n	45	ARG
15	a	117	VAL
15	e	68	GLN
2	B	389	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
18	d	95	GLN
15	m	93	GLN
15	e	68	GLN
17	g	89	ASN
17	o	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	13/14 (92%)	3 (23%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	4	C
13	P	5	G
13	P	12	C

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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.

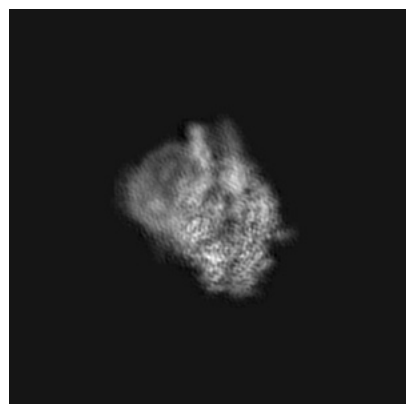
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64603. These allow visual inspection of the internal detail of the map and identification of artifacts.

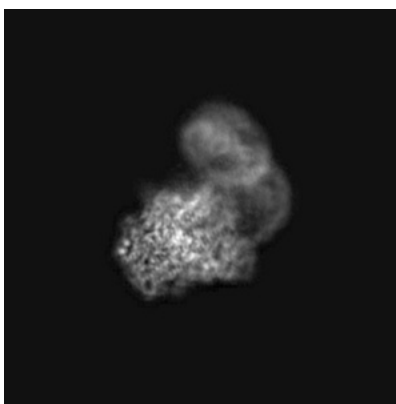
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

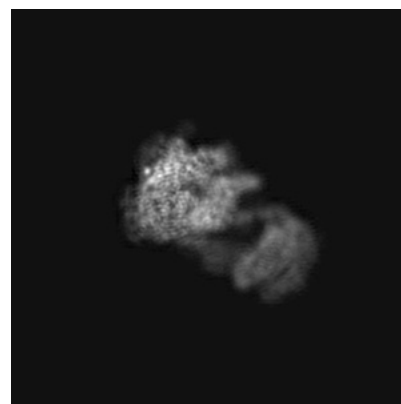
6.1.1 Primary map



X

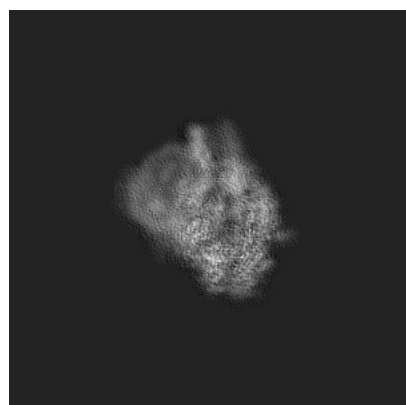


Y

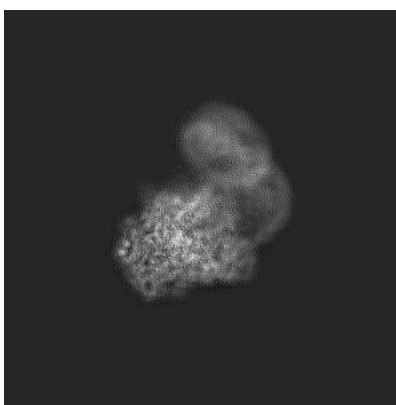


Z

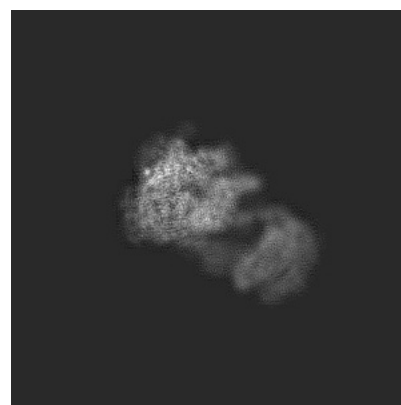
6.1.2 Raw map



X



Y

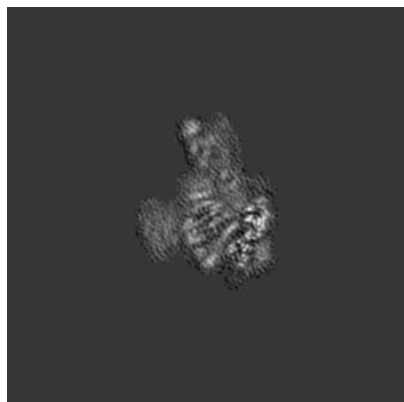


Z

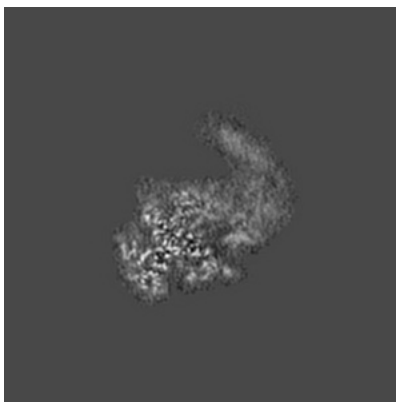
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

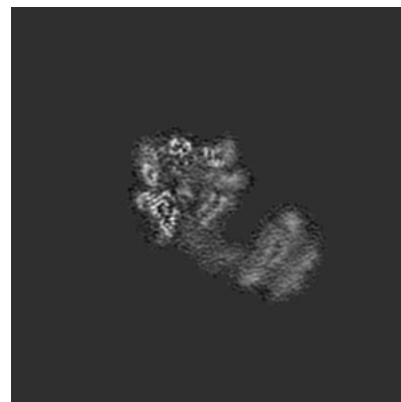
6.2.1 Primary map



X Index: 200

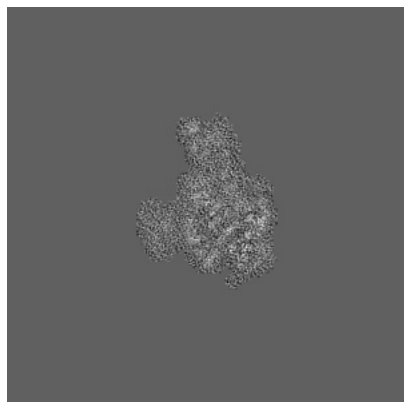


Y Index: 200

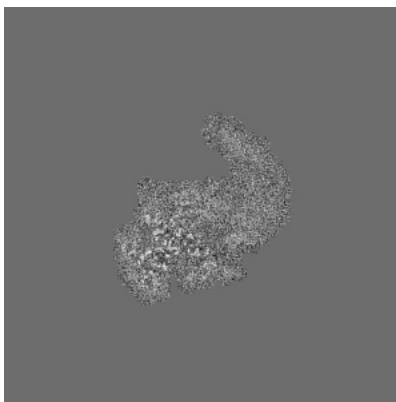


Z Index: 200

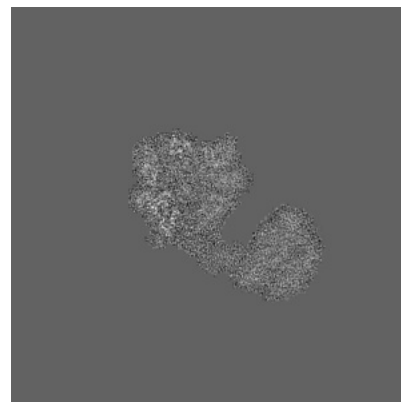
6.2.2 Raw map



X Index: 200



Y Index: 200

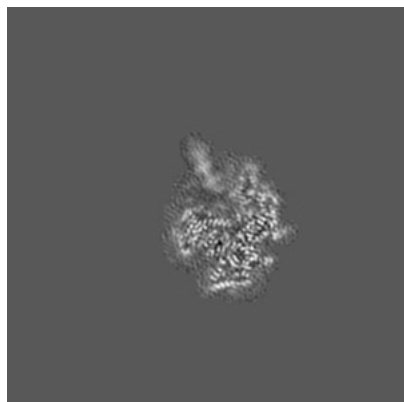


Z Index: 200

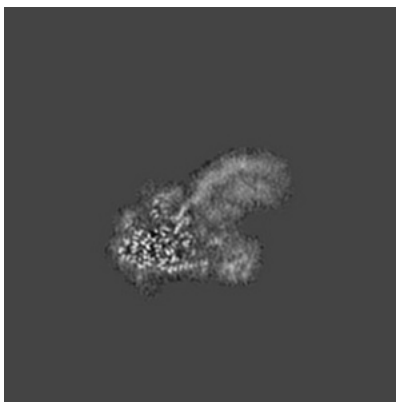
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

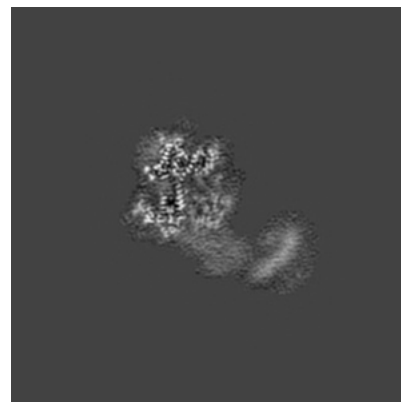
6.3.1 Primary map



X Index: 167

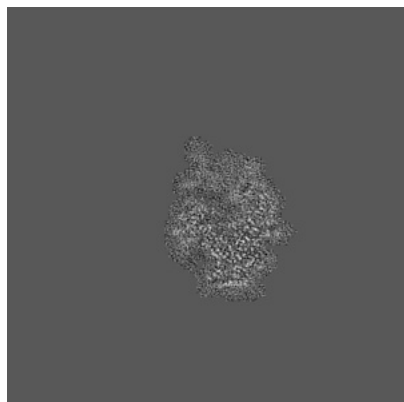


Y Index: 227

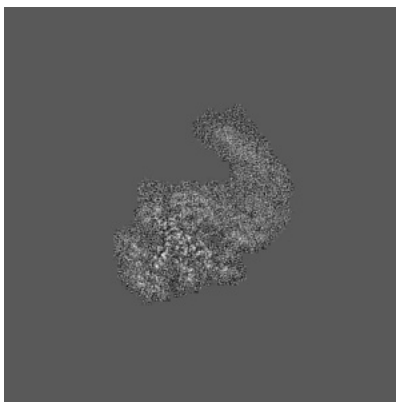


Z Index: 186

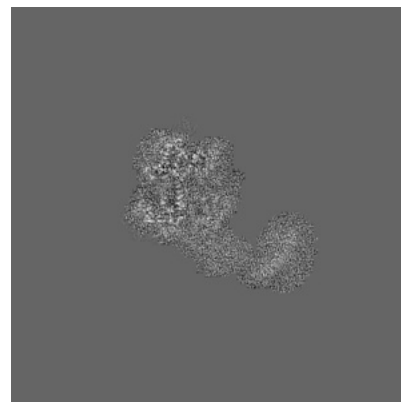
6.3.2 Raw map



X Index: 164



Y Index: 197

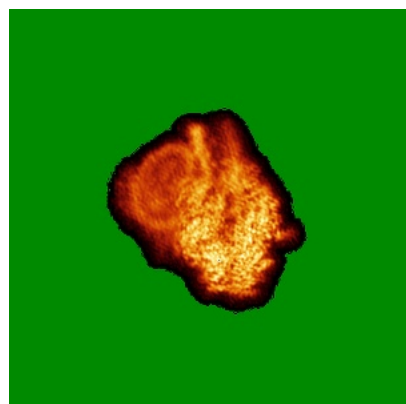


Z Index: 186

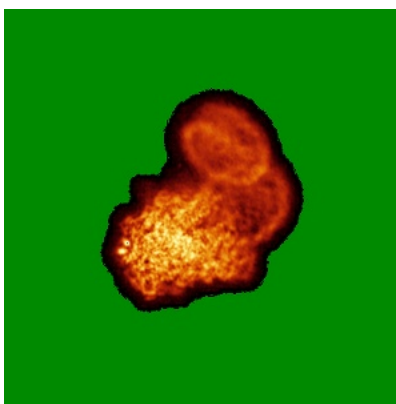
The images above show the largest variance slices of the map in three orthogonal directions.

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

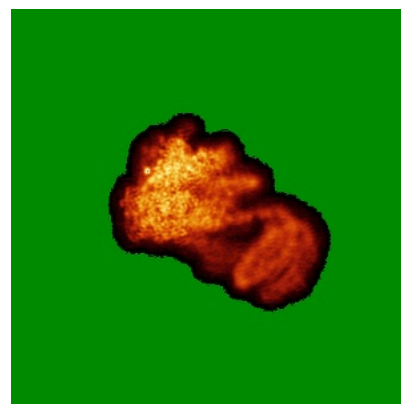
6.4.1 Primary map



X

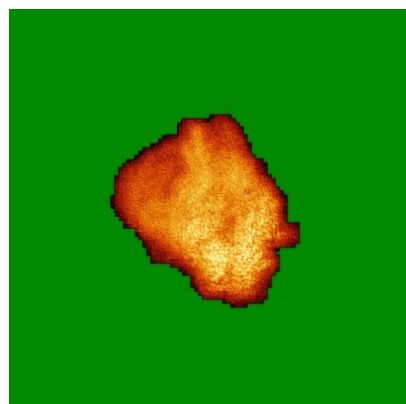


Y

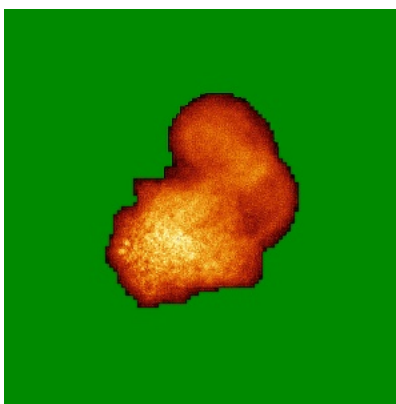


Z

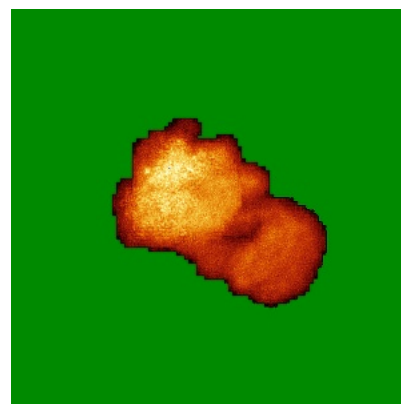
6.4.2 Raw map



X



Y

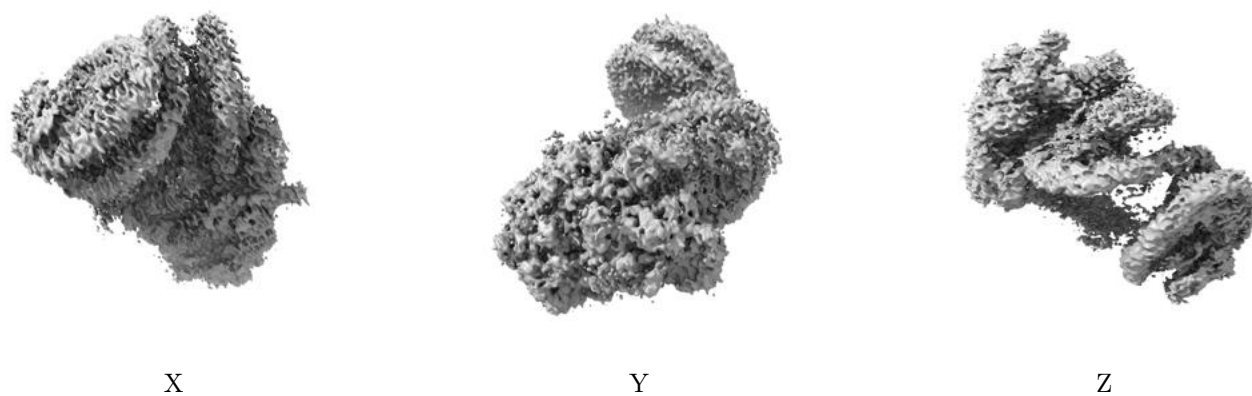


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

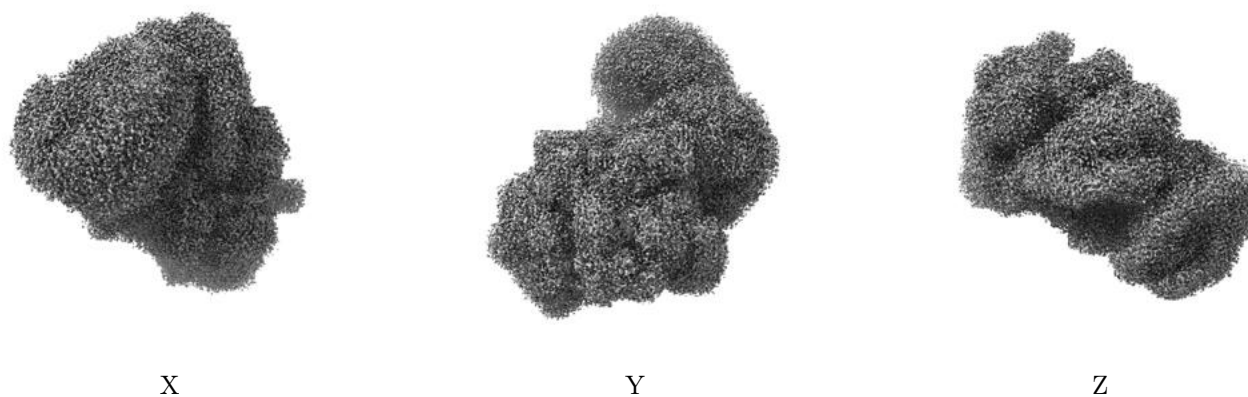
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00777. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

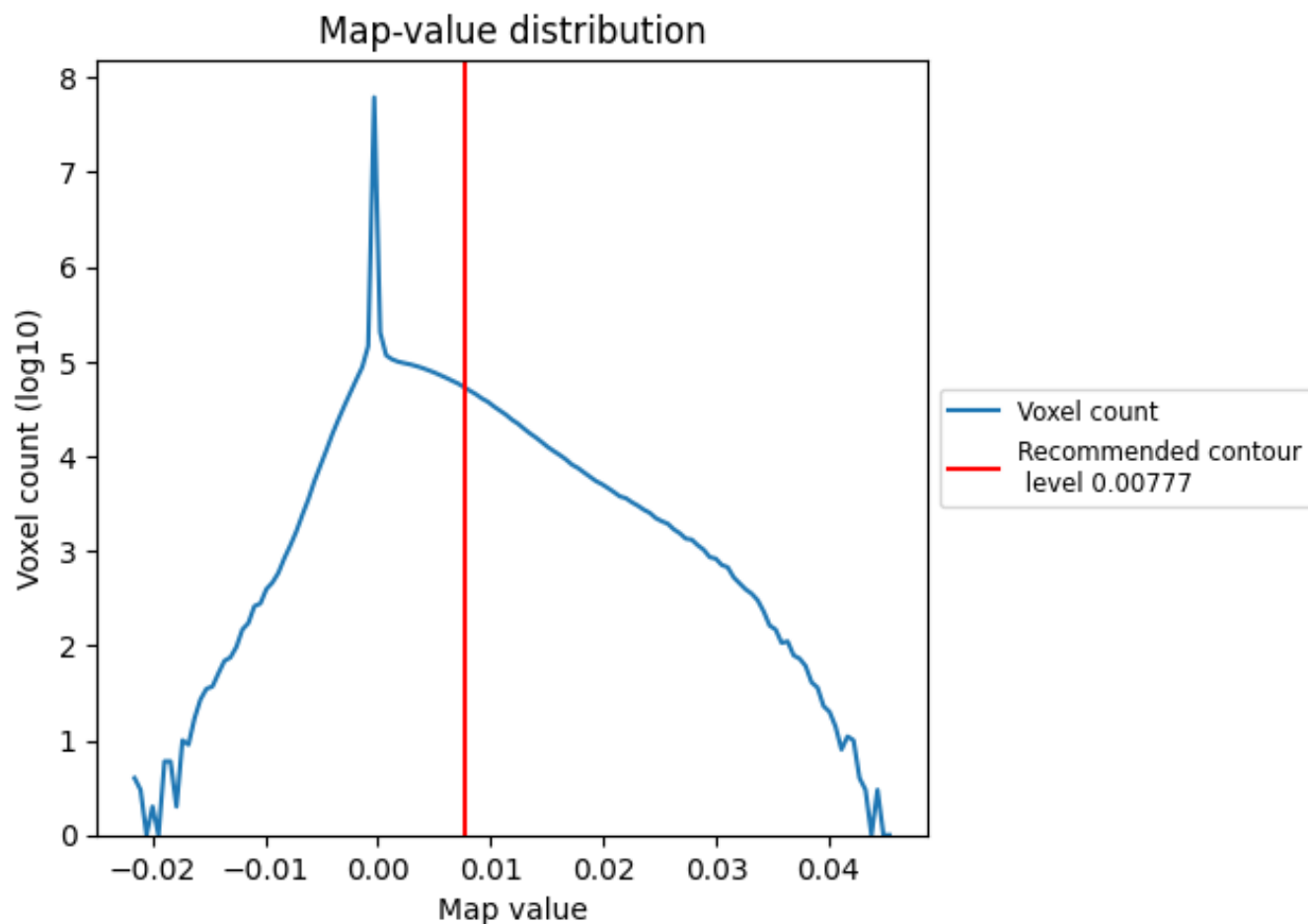
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

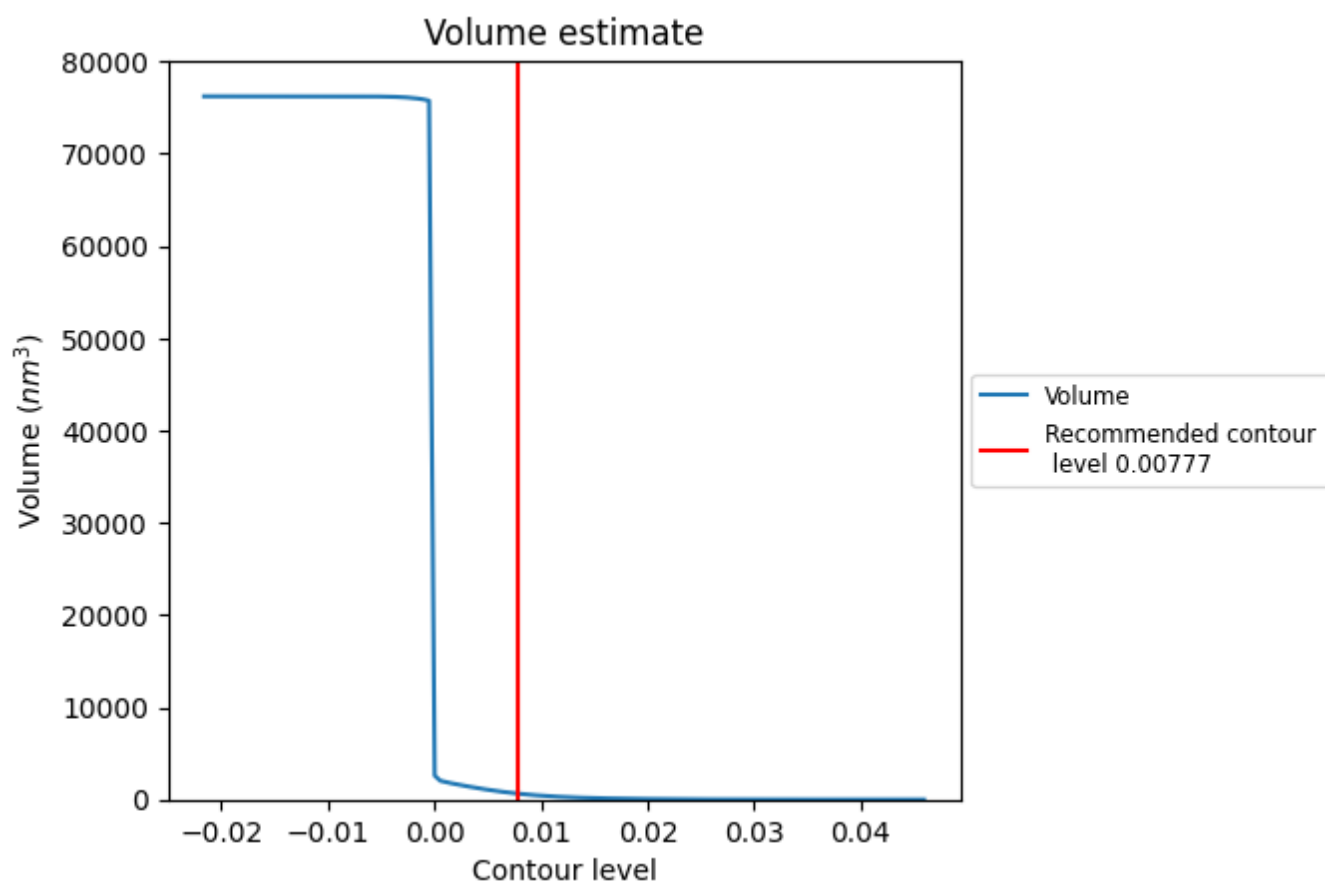
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

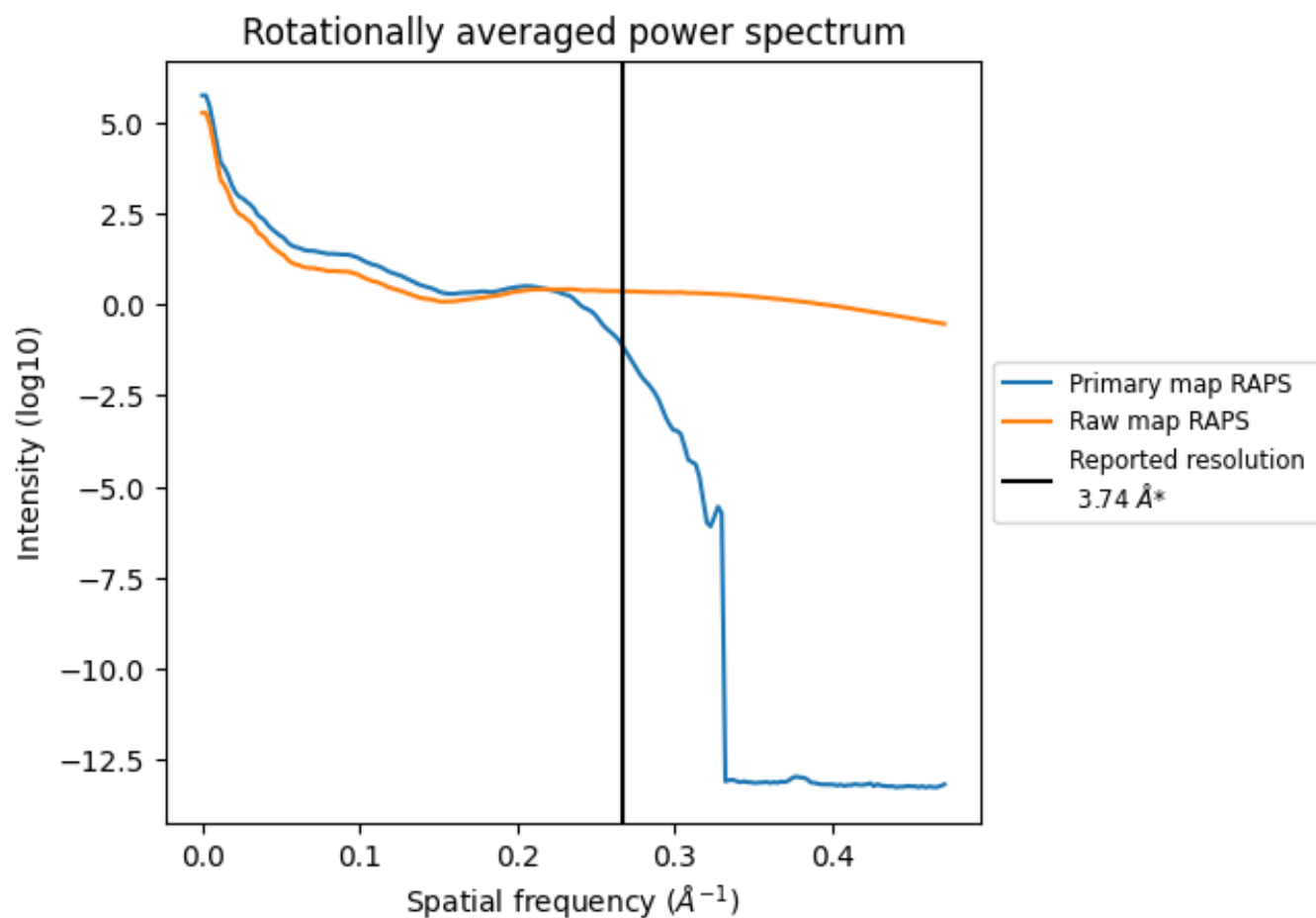
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 654 nm³; this corresponds to an approximate mass of 591 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 ⓘ

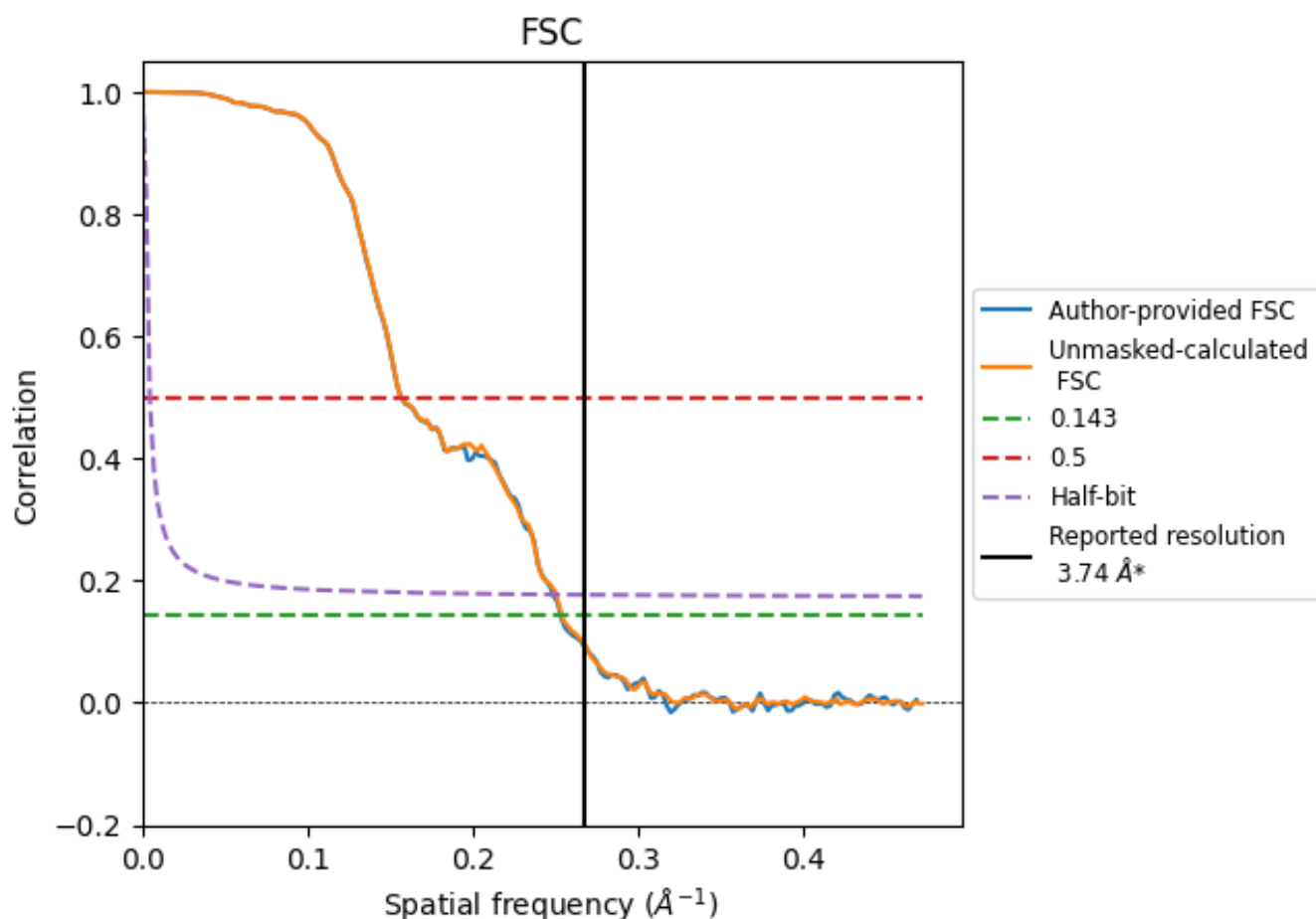


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 $0.267 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

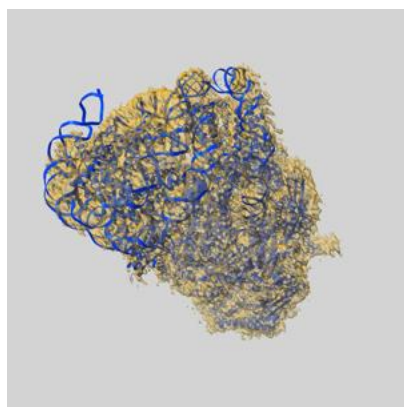
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	3.95	6.38	4.02
Unmasked-calculated*	3.94	6.37	4.00

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

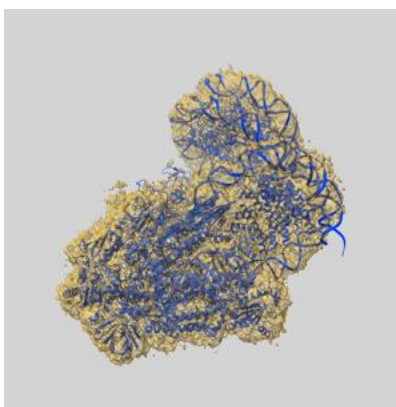
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64603 and PDB model 9UXW. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

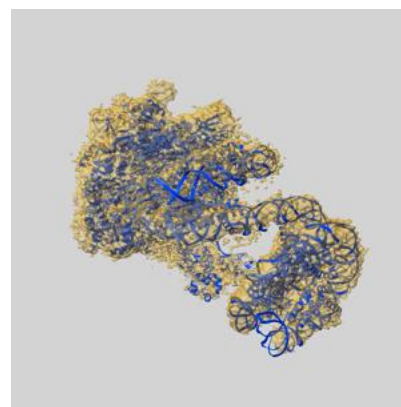
9.1 Map-model overlay [i](#)



X



Y



Z

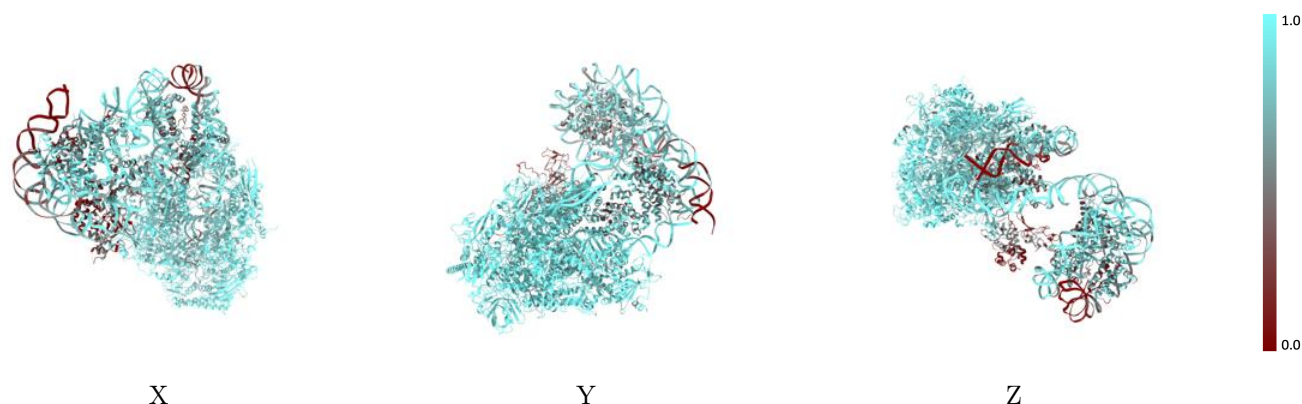
The images above show the 3D surface view of the map at the recommended contour level 0.00777 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



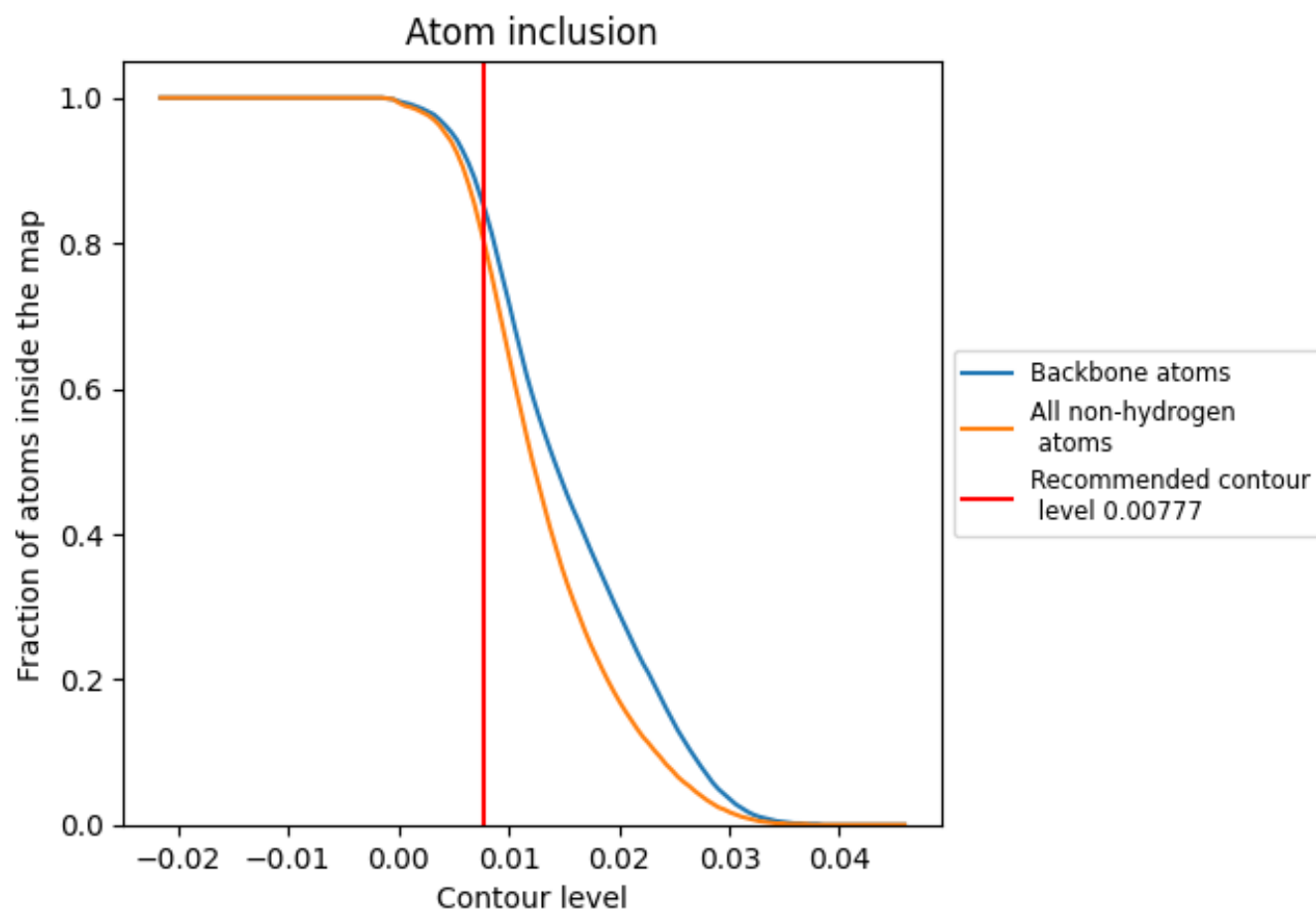
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00777).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.00777) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.2920
A	 0.9050	 0.3960
B	 0.9150	 0.4240
C	 0.9580	 0.4490
D	 0.2640	 0.1120
E	 0.9470	 0.4070
F	 0.9680	 0.4320
G	 0.4770	 0.1940
H	 0.9830	 0.4450
I	 0.8770	 0.2630
J	 0.9670	 0.4430
K	 0.9390	 0.4310
L	 0.9400	 0.3880
N	 0.6890	 0.1100
P	 0.7940	 0.2530
T	 0.6980	 0.1160
a	 0.6370	 0.1420
b	 0.7330	 0.1620
c	 0.6460	 0.1520
d	 0.6660	 0.1500
e	 0.7550	 0.1650
f	 0.7330	 0.1490
g	 0.6310	 0.1540
h	 0.6840	 0.1450
k	 0.6910	 0.2480
l	 0.6830	 0.2160
m	 0.6410	 0.2010
n	 0.6170	 0.2150
o	 0.6710	 0.1480
p	 0.7820	 0.1750

