



# wwPDB EM Validation Summary Report ⓘ

May 2, 2026 – 07:38 am BST

PDB ID : 9G0A / pdb\_00009g0a  
EMDB ID : EMD-50927  
Title : Influenza A/H7N9 polymerase post-cleavage cap-snatching complex  
Authors : Rotsch, A.H.; Li, D.; Dienemann, C.; Cusack, S.; Cramer, P.  
Deposited on : 2024-07-07  
Resolution : 3.10 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](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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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) : 2.49

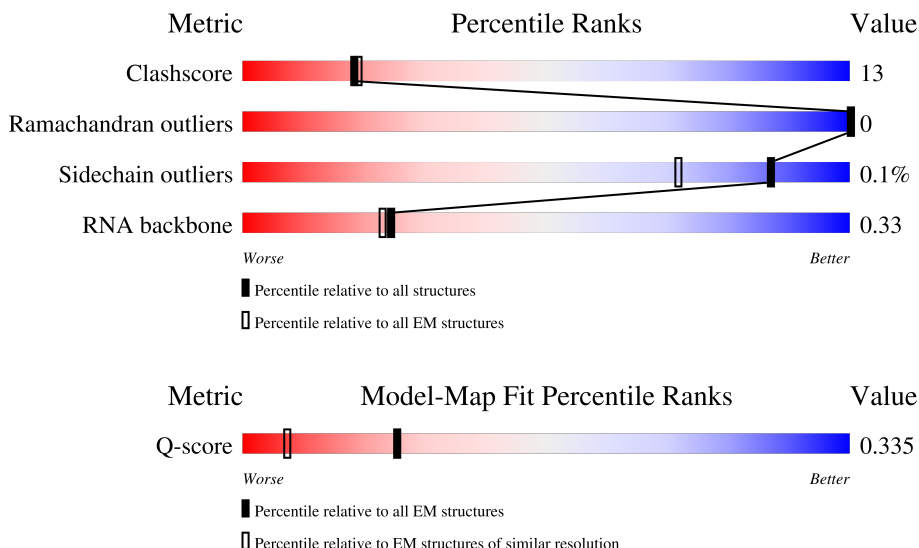
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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)	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	14724 ( 2.60 - 3.60 )

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	Z	1087	
2	Y	117	
3	A	1641	

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Mol	Chain	Length	Quality of chain
4	P	35	
5	a	717	
6	b	757	
7	c	759	
8	r	13	
9	v	14	
10	X	14	
11	B	1174	
12	C	275	
13	E	210	
14	F	127	
15	H	150	
16	I	125	
17	J	67	
18	K	117	
19	L	58	
20	N	43	
21	T	43	
22	D	184	
23	G	172	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SEP	A	3004	-	-	X	-

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55859 atoms, of which 29 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 Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	472	Total	C	N	O	S	0	0
			3787	2405	669	696	17		

- Molecule 2 is a protein called Transcription elongation factor SPT4.

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

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	1440	Total	C	N	O	P	S	0	0
			11410	7170	2036	2132	2	70		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	527	THR	-	insertion	UNP I3LJR4
A	1300	GLY	-	insertion	UNP I3LJR4

- Molecule 4 is a RNA chain called 5' cap(1) RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	23	Total	C	N	O	P	0	0
			499	223	101	152	23		

- Molecule 5 is a protein called Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	717	Total	C	N	O	S	0	0
			5807	3672	987	1107	41		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	0	GLY	-	expression tag	UNP M9TI86
a	119	ASP	GLU	engineered mutation	UNP M9TI86

- Molecule 6 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	736	Total	C	N	O	S	0	0
			5865	3688	1026	1105	46		

- Molecule 7 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	734	Total	C	N	O	S	0	0
			5816	3655	1046	1075	40		

- Molecule 8 is a RNA chain called 3' vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	r	8	Total	C	N	O	P	0	0
			163	73	22	60	8		

- Molecule 9 is a RNA chain called 5' vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	v	14	Total	C	N	O	P	0	0
			306	137	62	93	14		

- Molecule 10 is a protein called likely linker between KOWx4 and KOW5 domains of SPT5.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	14	Total	C	N	O	0	0
			77	48	14	15		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	1131	Total	C	N	O	S	0	0
			9053	5727	1592	1670	64		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	261	Total	C	N	O	S	0	0
			2096	1314	360	416	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	82	Total	C	N	O	S	0	0
			658	418	113	122	5		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 19 is a protein called RNA polymerase II, I and III subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 20 is a DNA chain called nontemplate DNA (43-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	26	Total	C	N	O	P	0	0
			537	257	97	157	26		

- Molecule 21 is a DNA chain called template DNA (43-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	35	Total	C	N	O	P	0	0
			713	343	128	208	34		

- Molecule 22 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	126	Total	C	N	O	S	0	0
			1030	642	175	209	4		

- Molecule 23 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

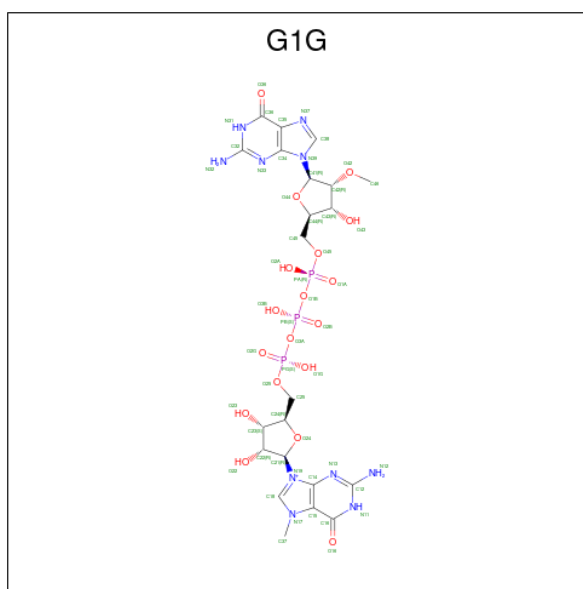
- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	Mg	0
			1	1	
25	a	1	Total	Mg	0
			1	1	

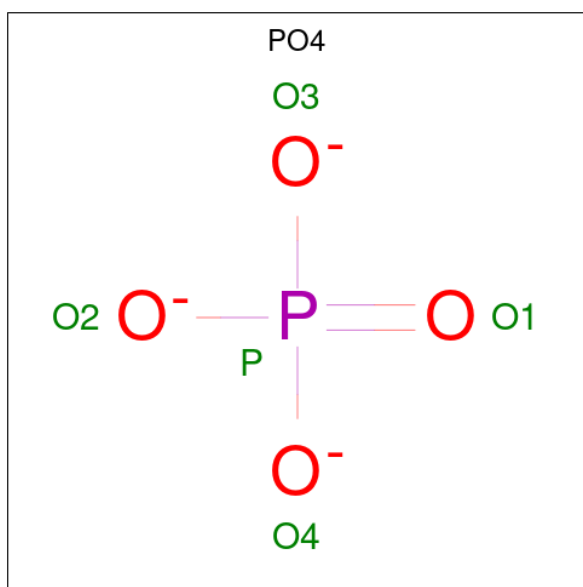
- Molecule 26 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-(2'-O-METHYL)-GUANOSINE (CCD ID: G1G) (formula: C<sub>22</sub>H<sub>32</sub>N<sub>10</sub>O<sub>18</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
26	P	1	Total	C	H	N	O	P	0
			82	22	29	10	18	3	

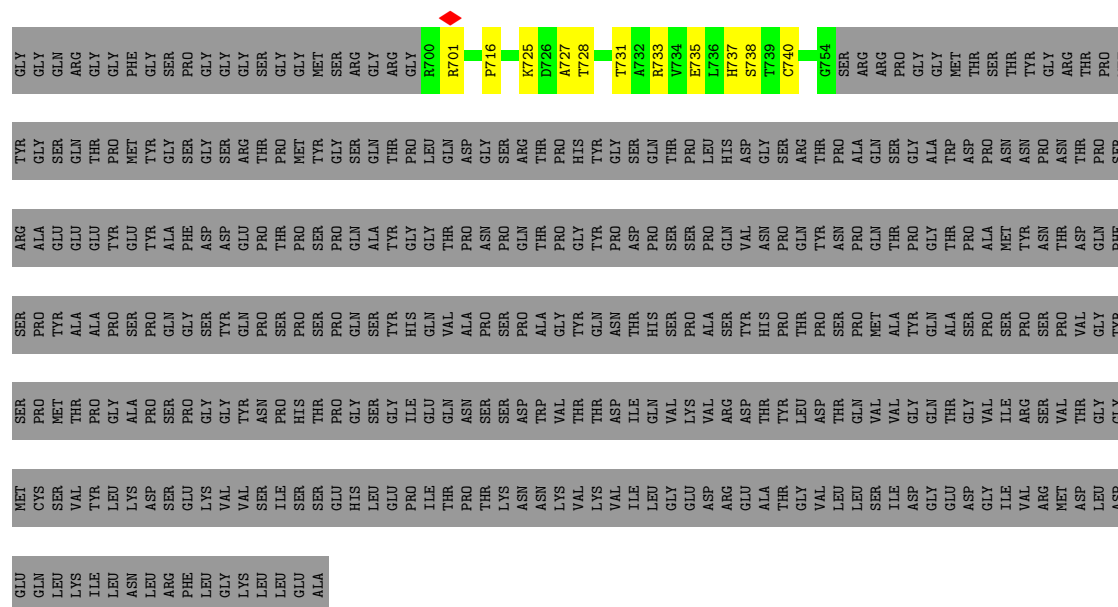
- Molecule 27 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



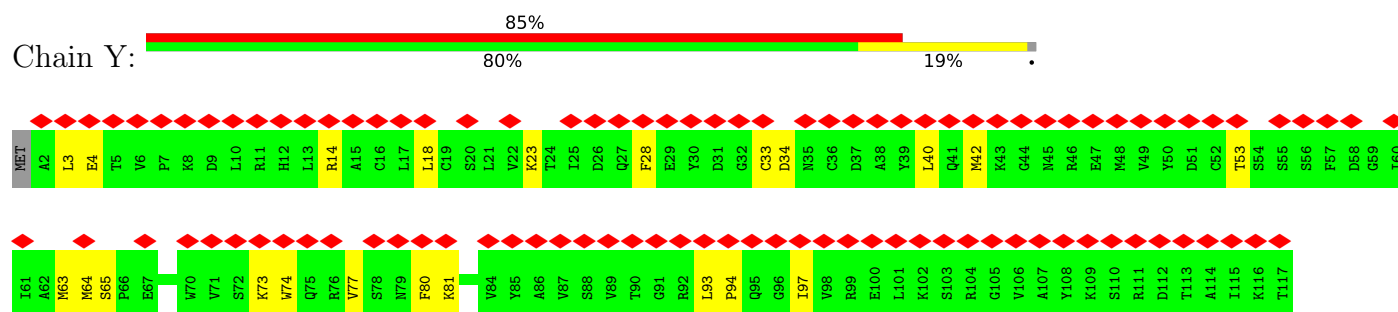


Mol	Chain	Residues	Atoms			AltConf
27	a	1	Total	O	P	0
			5	4	1	
27	a	1	Total	O	P	0
			5	4	1	
27	c	1	Total	O	P	0
			5	4	1	

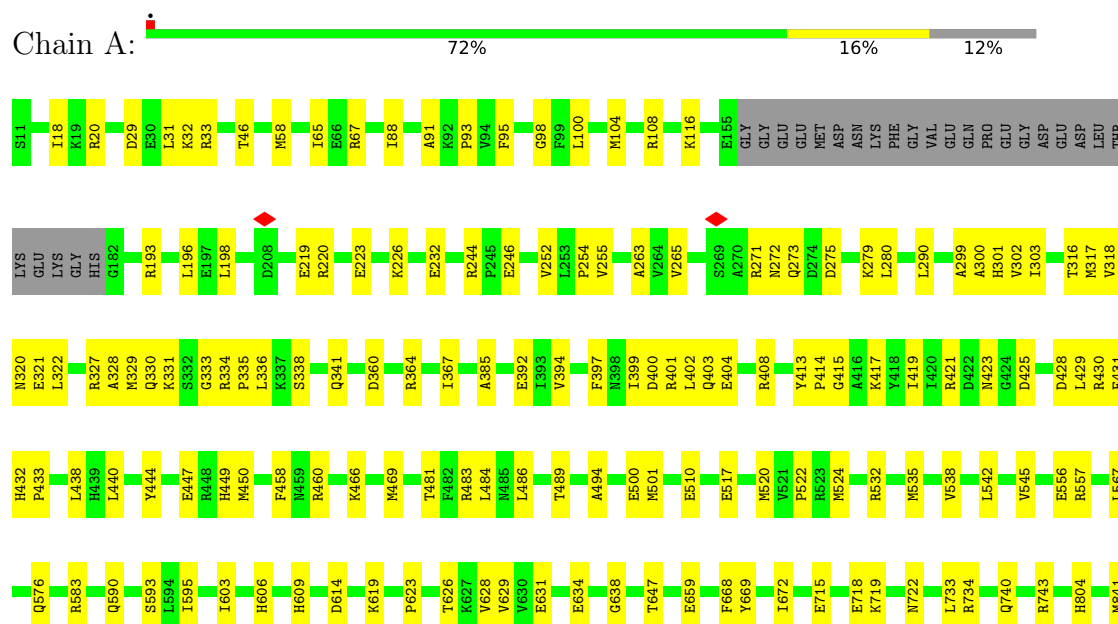




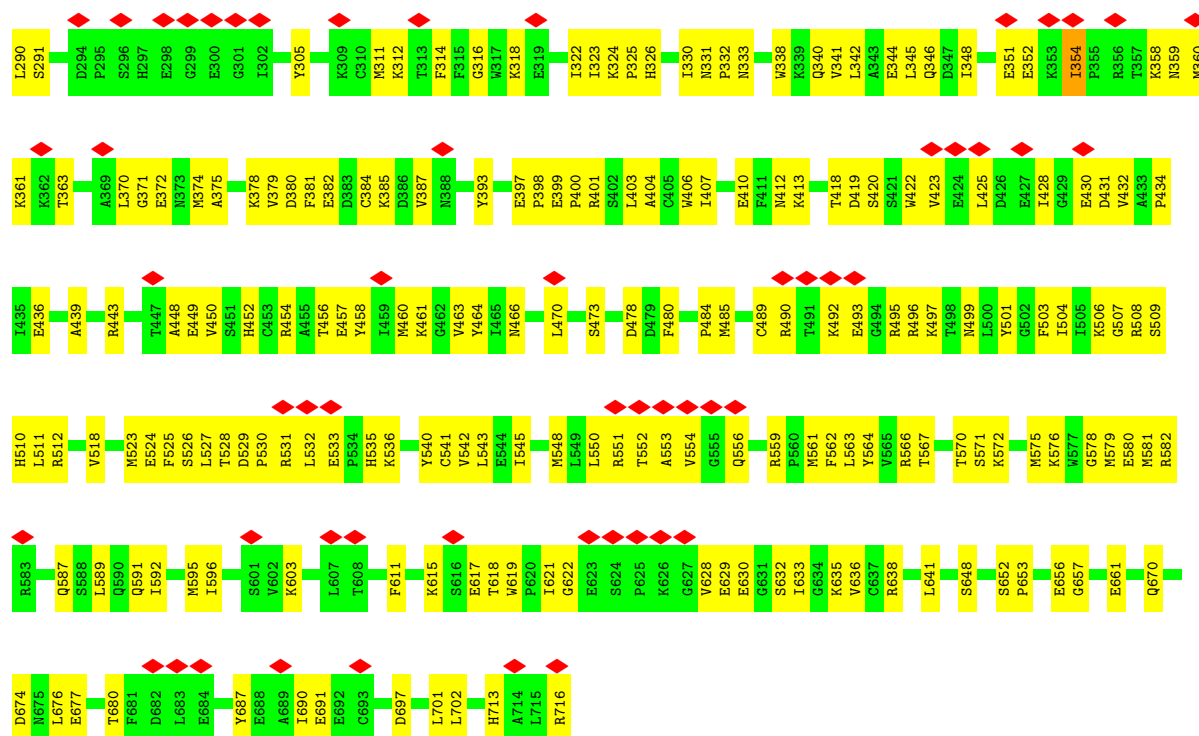
### • Molecule 2: Transcription elongation factor SPT4



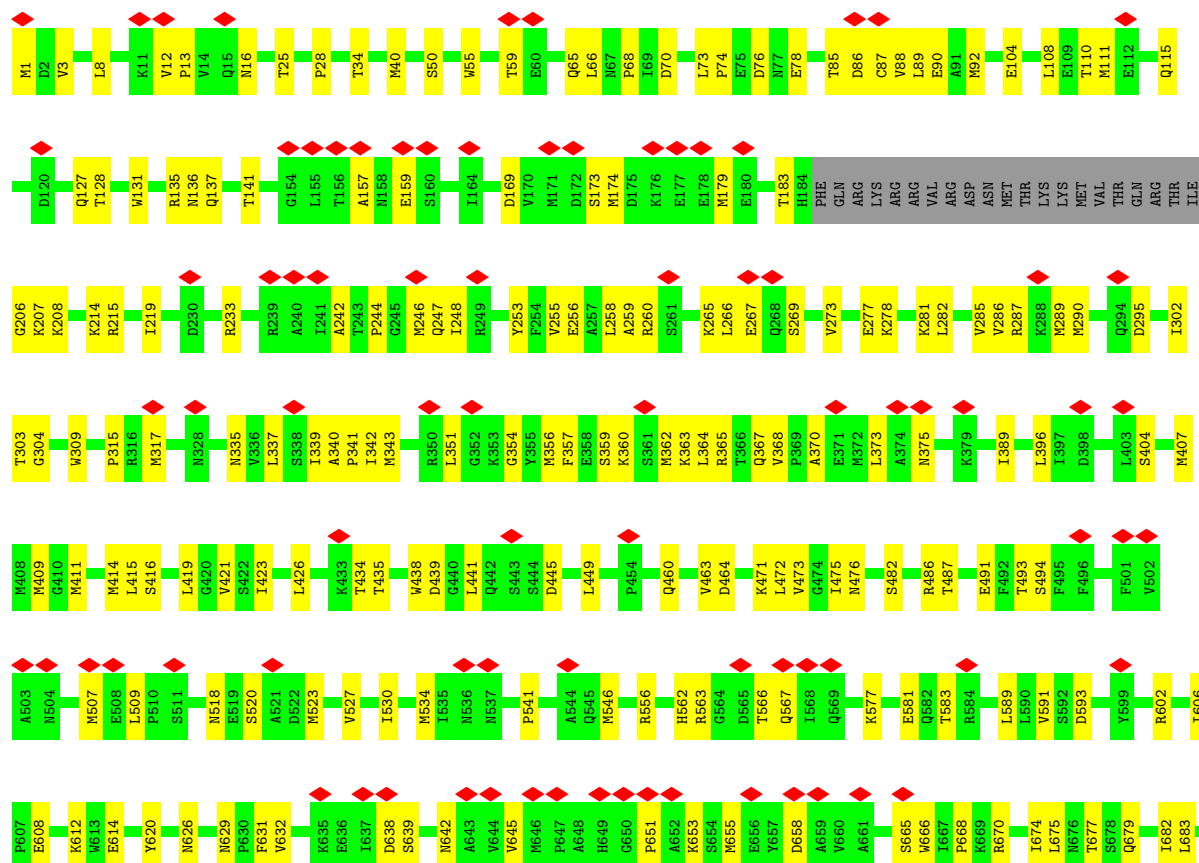
### • Molecule 3: DNA-directed RNA polymerase subunit





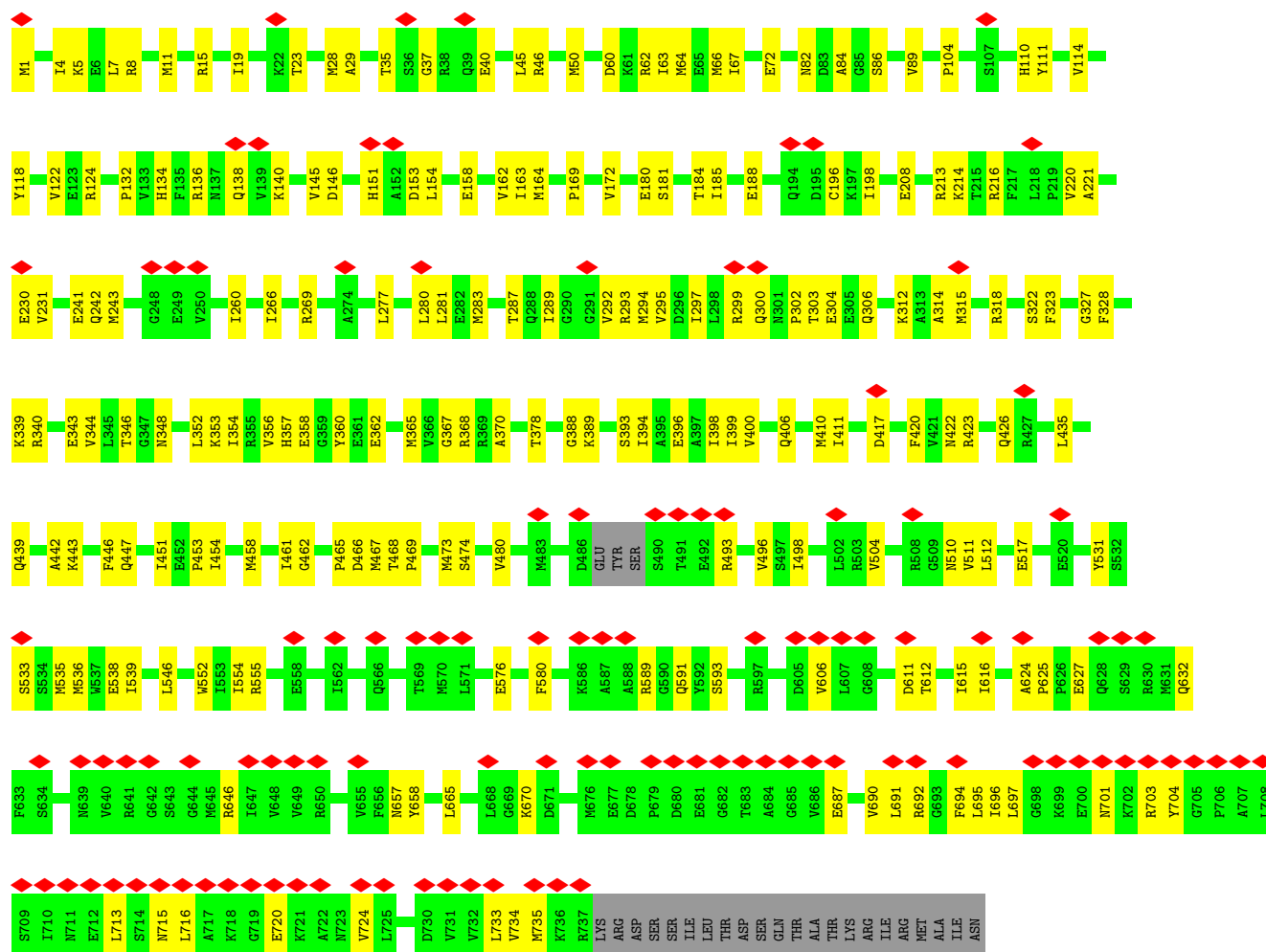


• Molecule 6: RNA-directed RNA polymerase catalytic subunit

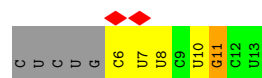
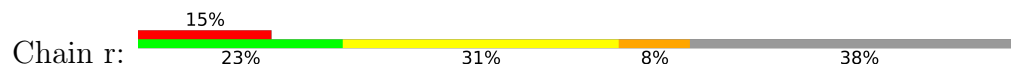




• Molecule 7: Polymerase basic protein 2



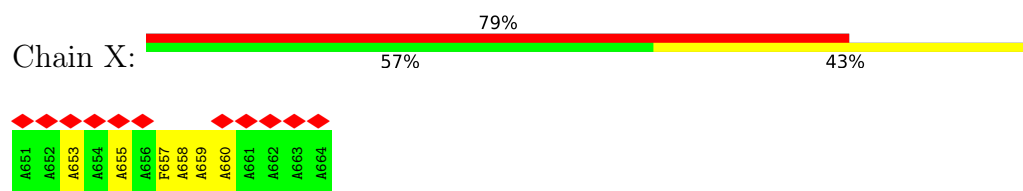
• Molecule 8: 3' vRNA



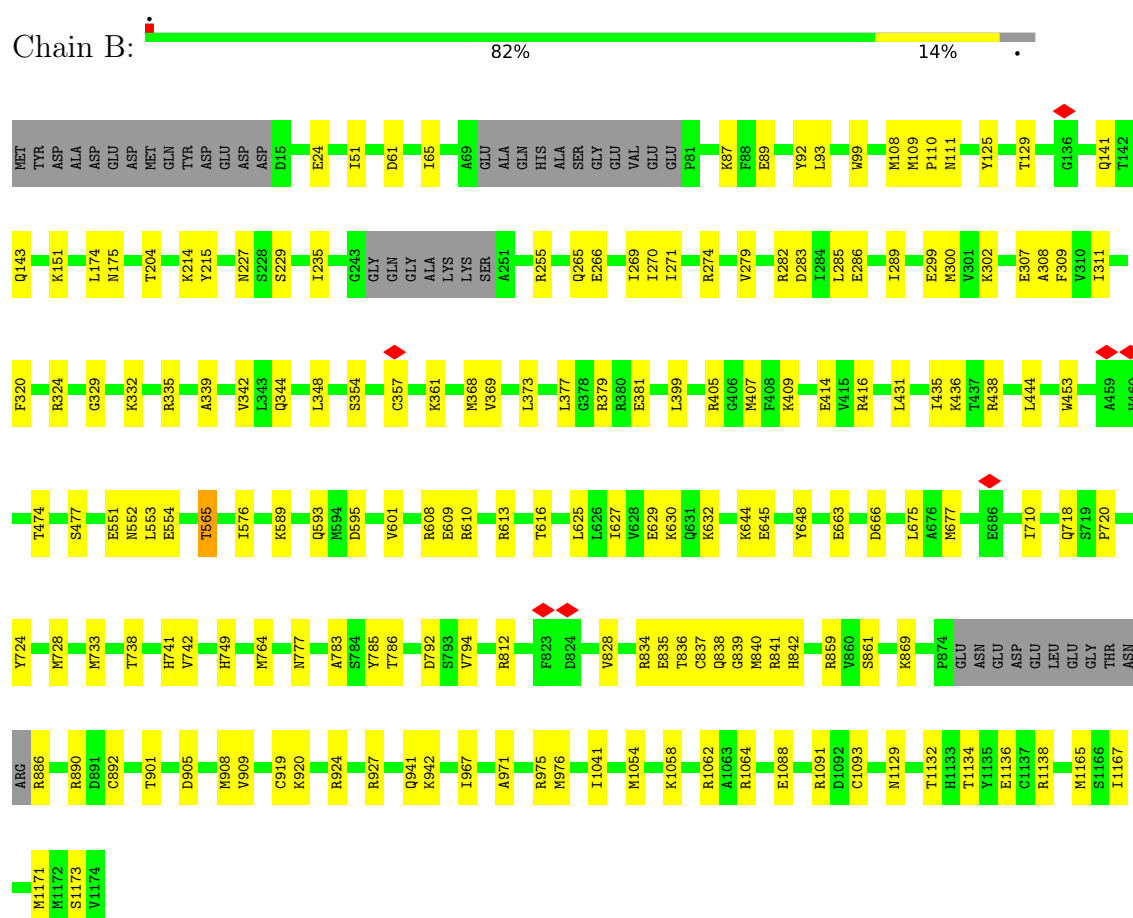
• Molecule 9: 5' vRNA



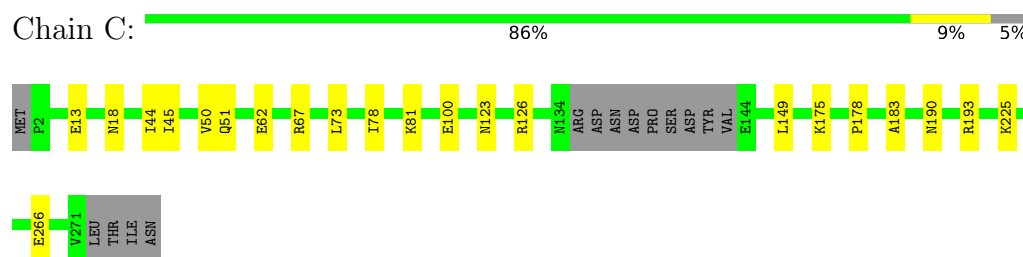
- Molecule 10: likely linker between KOWx4 and KOW5 domains of SPT5



- Molecule 11: DNA-directed RNA polymerase subunit beta



- Molecule 12: DNA-directed RNA polymerase II subunit RPB3

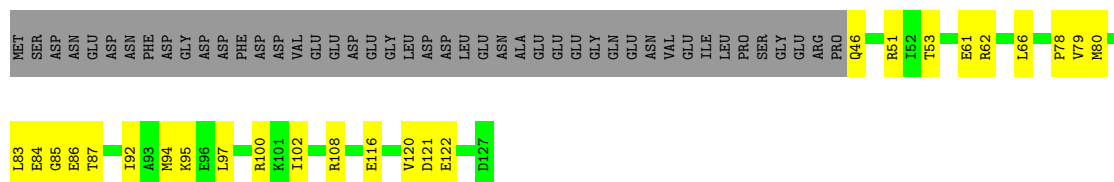


- Molecule 13: DNA-directed RNA polymerase II subunit E

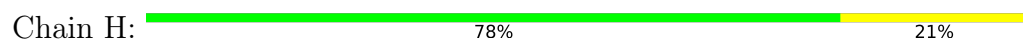




- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2



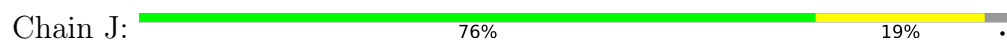
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC3



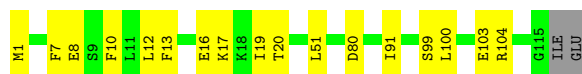
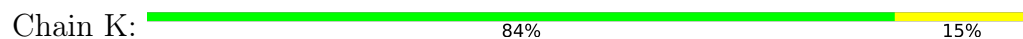
- Molecule 16: DNA-directed RNA polymerase II subunit RPB9



- Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 18: DNA-directed RNA polymerase II subunit RPB11-a



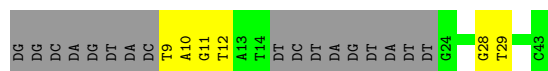
- Molecule 19: RNA polymerase II, I and III subunit K



- Molecule 20: nontemplate DNA (43-mer)

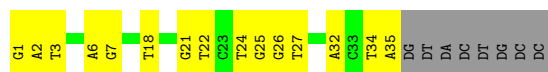


Chain N:  47% 14% 40%



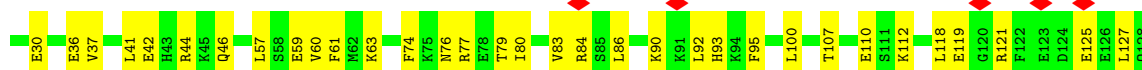
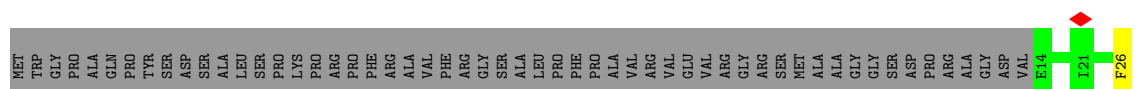
- Molecule 21: template DNA (43-mer)

Chain T:  47% 35% 19%



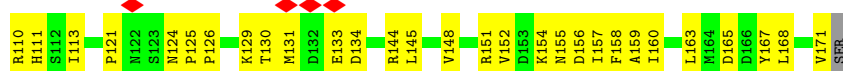
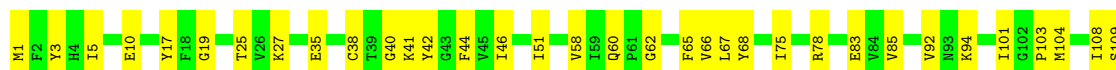
- Molecule 22: RNA polymerase II subunit D

Chain D:  48% 20% 32%



- Molecule 23: DNA-directed RNA polymerase subunit

Chain G:  63% 37%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63230	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 ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.018	Depositor
Minimum map value	-0.756	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	470.39996, 470.39996, 470.39996	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SEP, G1G, PO4

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	Z	0.40	0/3853	0.73	0/5187
2	Y	0.13	0/927	0.34	0/1250
3	A	0.36	0/11599	0.70	0/15658
4	P	0.56	0/558	0.87	0/864
5	a	0.43	0/5931	0.70	0/7998
6	b	0.31	0/5980	0.58	0/8063
7	c	0.29	0/5912	0.56	0/7972
8	r	0.30	0/179	0.63	0/275
9	v	0.40	0/344	0.81	1/535 (0.2%)
10	X	1.00	0/77	1.14	0/104
11	B	0.35	0/9234	0.69	0/12463
12	C	0.32	0/2139	0.65	0/2906
13	E	0.36	0/1752	0.72	0/2366
14	F	0.32	0/668	0.69	0/901
15	H	0.35	0/1207	0.69	0/1628
16	I	0.44	0/973	0.97	1/1316 (0.1%)
17	J	0.36	0/516	0.72	0/696
18	K	0.33	0/939	0.64	0/1271
19	L	0.51	0/395	0.91	0/524
20	N	0.37	0/601	0.67	0/924
21	T	0.39	0/799	0.68	0/1231
22	D	0.52	0/1043	0.95	0/1400
23	G	0.52	0/1382	1.02	0/1874
All	All	0.37	0/57008	0.69	2/77406 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	v	2	G	O3'-P-O5'	-5.71	95.43	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	58	ILE	CA-CB-CG1	5.19	119.22	110.40

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	Z	3787	0	3830	140	0
2	Y	911	0	908	16	0
3	A	11410	0	11503	222	0
4	P	499	0	255	34	0
5	a	5807	0	5726	400	0
6	b	5865	0	5853	209	0
7	c	5816	0	5946	201	0
8	r	163	0	85	9	0
9	v	306	0	153	8	0
10	X	77	0	73	16	0
11	B	9053	0	9087	133	0
12	C	2096	0	2040	20	0
13	E	1721	0	1737	16	0
14	F	658	0	684	22	0
15	H	1186	0	1147	18	0
16	I	950	0	879	31	0
17	J	507	0	523	10	0
18	K	920	0	942	14	0
19	L	389	0	394	24	0
20	N	537	0	297	6	0
21	T	713	0	398	20	0
22	D	1030	0	1016	35	0
23	G	1351	0	1358	77	0
24	A	2	0	0	0	0
24	B	1	0	0	0	0
24	C	1	0	0	0	0
24	I	2	0	0	0	0
24	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	L	1	0	0	0	0
25	A	1	0	0	0	0
25	a	1	0	0	0	0
26	P	53	29	28	2	0
27	a	10	0	0	1	0
27	c	5	0	0	0	0
All	All	55830	29	54862	1447	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 13.

The worst 5 of 1447 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)
5:a:189:ASP:HB3	11:B:835:GLU:HB2	1.37	1.05
5:a:122:VAL:HA	5:a:148:PHE:O	1.71	0.90
1:Z:737:HIS:CE1	19:L:53:VAL:HG23	2.09	0.87
23:G:163:LEU:HA	23:G:168:LEU:HD23	1.55	0.86
1:Z:588:ASP:HB3	1:Z:594:ILE:HD11	1.57	0.86

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	Z	460/1087 (42%)	446 (97%)	14 (3%)	0	100	100
2	Y	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
3	A	1426/1641 (87%)	1369 (96%)	57 (4%)	0	100	100
5	a	715/717 (100%)	662 (93%)	53 (7%)	0	100	100
6	b	732/757 (97%)	716 (98%)	16 (2%)	0	100	100

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	c	730/759 (96%)	714 (98%)	16 (2%)	0	100	100
10	X	12/14 (86%)	8 (67%)	4 (33%)	0	100	100
11	B	1123/1174 (96%)	1088 (97%)	35 (3%)	0	100	100
12	C	257/275 (94%)	252 (98%)	5 (2%)	0	100	100
13	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
14	F	80/127 (63%)	76 (95%)	4 (5%)	0	100	100
15	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
16	I	115/125 (92%)	110 (96%)	5 (4%)	0	100	100
17	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
18	K	113/117 (97%)	113 (100%)	0	0	100	100
19	L	44/58 (76%)	37 (84%)	7 (16%)	0	100	100
22	D	124/184 (67%)	118 (95%)	6 (5%)	0	100	100
23	G	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
All	All	6629/7751 (86%)	6388 (96%)	241 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Z	417/940 (44%)	415 (100%)	2 (0%)	81	85
2	Y	102/103 (99%)	102 (100%)	0	100	100
3	A	1268/1425 (89%)	1268 (100%)	0	100	100
5	a	644/645 (100%)	643 (100%)	1 (0%)	87	89
6	b	647/668 (97%)	646 (100%)	1 (0%)	87	89
7	c	643/666 (96%)	643 (100%)	0	100	100
10	X	1/1 (100%)	1 (100%)	0	100	100
11	B	992/1027 (97%)	991 (100%)	1 (0%)	88	90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	C	238/252 (94%)	238 (100%)	0	100	100
13	E	191/192 (100%)	191 (100%)	0	100	100
14	F	71/111 (64%)	71 (100%)	0	100	100
15	H	129/131 (98%)	129 (100%)	0	100	100
16	I	105/112 (94%)	105 (100%)	0	100	100
17	J	53/56 (95%)	53 (100%)	0	100	100
18	K	104/106 (98%)	104 (100%)	0	100	100
19	L	43/55 (78%)	43 (100%)	0	100	100
22	D	116/160 (72%)	116 (100%)	0	100	100
23	G	152/153 (99%)	152 (100%)	0	100	100
All	All	5916/6803 (87%)	5911 (100%)	5 (0%)	87	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	184	CYS
1	Z	285	ILE
5	a	354	ILE
6	b	744	MET
11	B	565	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
6	b	367	GLN
7	c	447	GLN
23	G	60	GLN
13	E	95	GLN
6	b	425	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	P	20/35 (57%)	8 (40%)	0
8	r	7/13 (53%)	1 (14%)	0
9	v	13/14 (92%)	6 (46%)	0

*Continued on next page...*

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	40/62 (64%)	15 (37%)	0

5 of 15 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	P	5	C
4	P	6	G
4	P	7	A
4	P	13	A
4	P	14	C

There are no RNA pucker outliers to report.

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

2 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	$\# Z  > 2$
3	SEP	A	3004	3	8,9,10	0.65	0	8,12,14	0.62	0
3	SEP	A	3018	3	8,9,10	0.64	0	8,12,14	0.65	0

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
3	SEP	A	3004	3	-	1/5/8/10	-
3	SEP	A	3018	3	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3004	SEP	N-CA-CB-OG
3	A	3018	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3004	SEP	5	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
27	PO4	a	1002	-	4,4,4	0.93	0	6,6,6	0.42	0
26	G1G	P	101	4	52,58,58	1.78	11 (21%)	74,91,91	2.36	21 (28%)
27	PO4	a	1003	-	4,4,4	0.92	0	6,6,6	0.43	0
27	PO4	c	801	-	4,4,4	0.93	0	6,6,6	0.41	0

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
26	G1G	P	101	4	-	6/32/66/66	0/6/6/6

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	101	G1G	C15-C16	-4.60	1.31	1.43
26	P	101	G1G	C15-N17	-3.98	1.31	1.38
26	P	101	G1G	C35-C36	-3.73	1.30	1.44
26	P	101	G1G	C14-N19	-3.54	1.31	1.37
26	P	101	G1G	C35-N37	-3.51	1.32	1.39

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	101	G1G	C12-N13-C14	7.74	120.01	112.71
26	P	101	G1G	O24-C21-C22	-7.26	96.31	106.93
26	P	101	G1G	C15-C16-N11	4.89	119.60	110.99
26	P	101	G1G	N13-C14-N19	4.38	130.85	125.61
26	P	101	G1G	C24-O24-C21	-4.19	105.86	109.85

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	P	101	G1G	C45-O45-PA-O1A
26	P	101	G1G	C45-O45-PA-O1B
26	P	101	G1G	PG-O3A-PB-O2B
26	P	101	G1G	C45-O45-PA-O2A
26	P	101	G1G	O44-C44-C45-O45

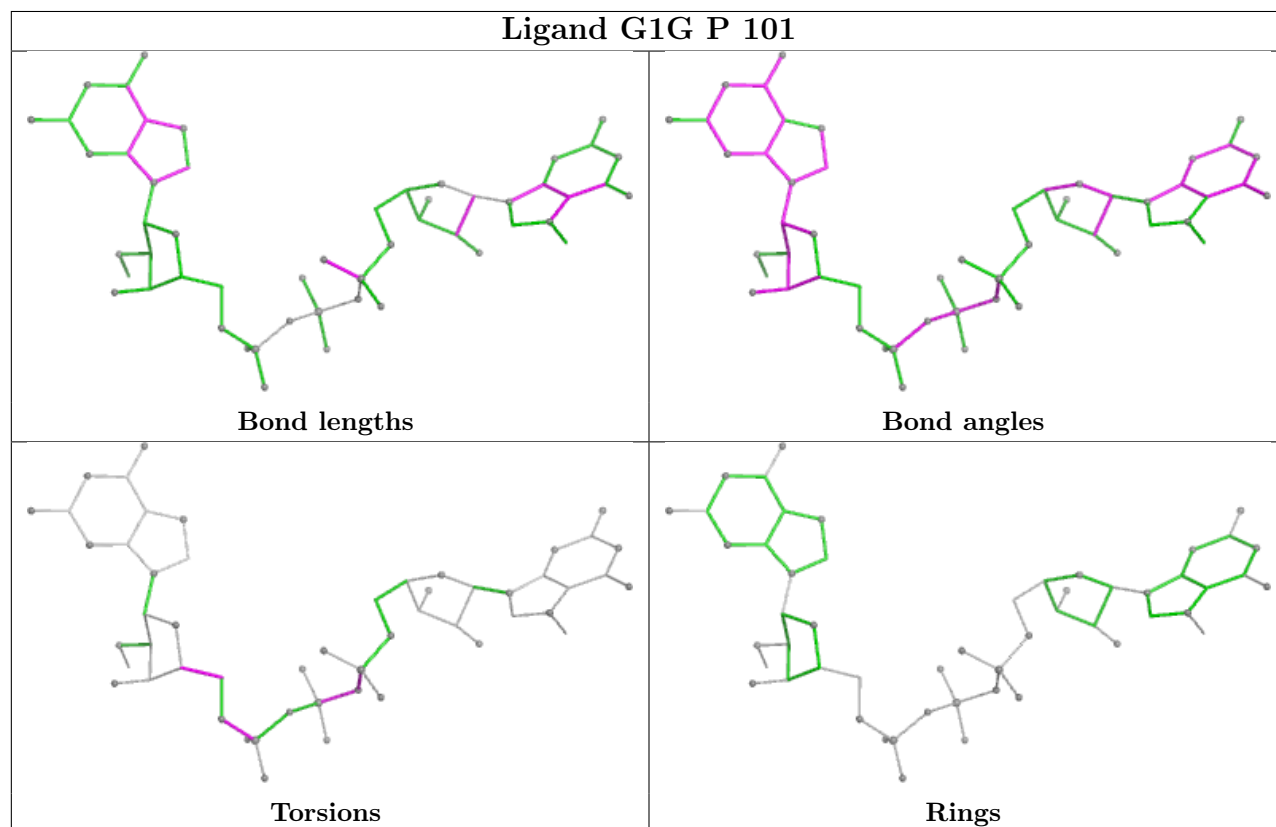
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	101	G1G	2	0
27	a	1003	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

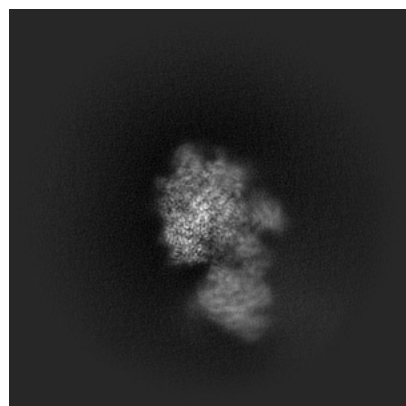
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50927. These allow visual inspection of the internal detail of the map and identification of artifacts.

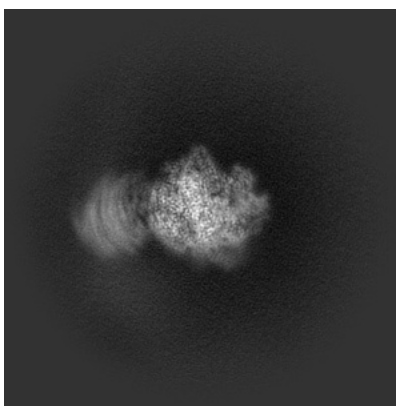
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

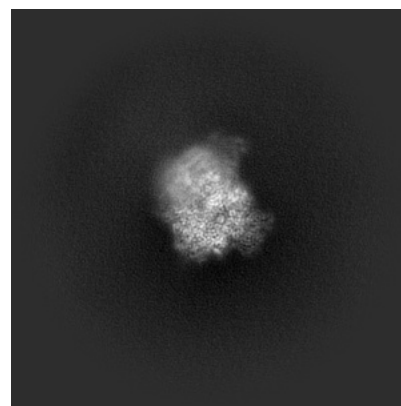
#### 6.1.1 Primary map



X

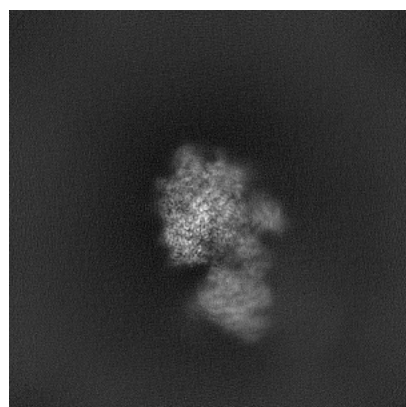


Y

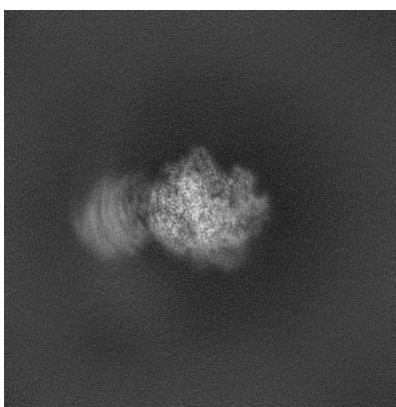


Z

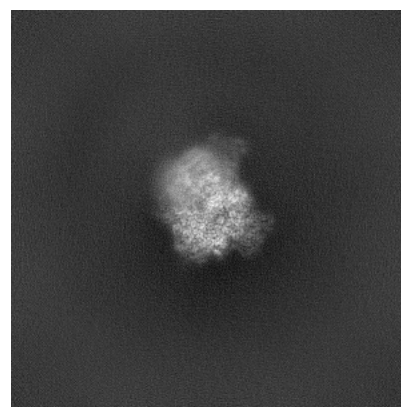
#### 6.1.2 Raw map



X



Y

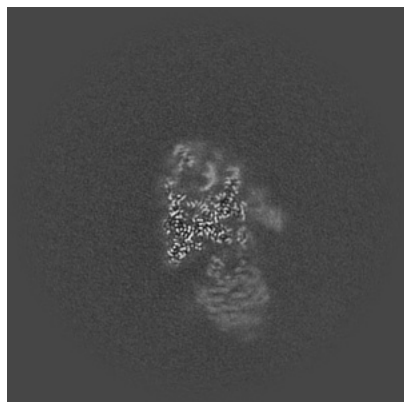


Z

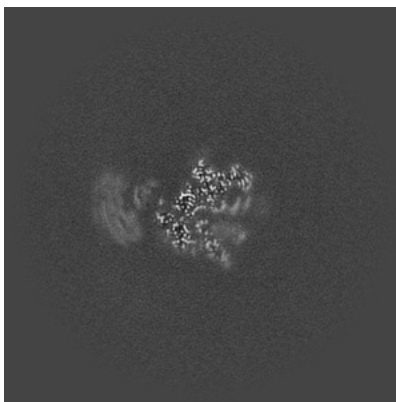
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

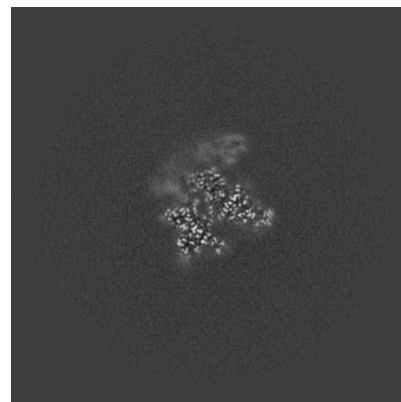
### 6.2.1 Primary map



X Index: 224



Y Index: 224

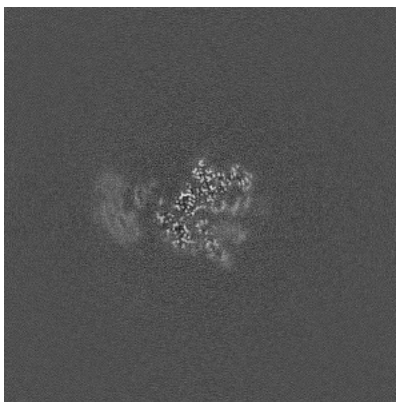


Z Index: 224

### 6.2.2 Raw map



X Index: 224



Y Index: 224

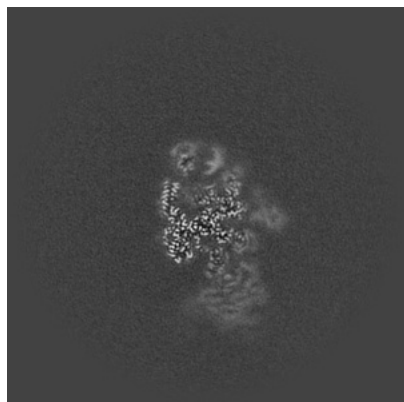


Z Index: 224

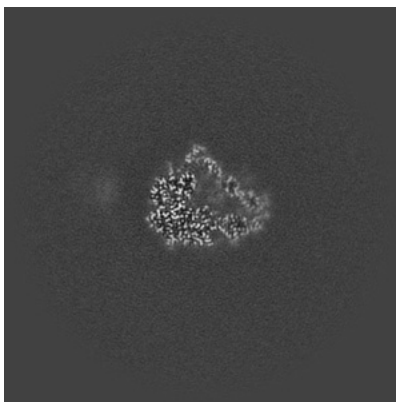
The images above show central slices of the map in three orthogonal directions.

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

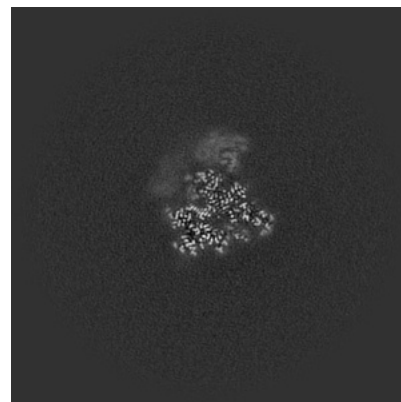
### 6.3.1 Primary map



X Index: 230

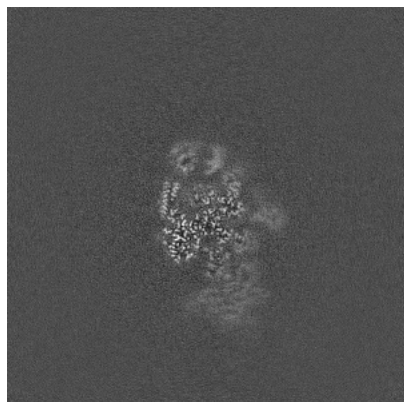


Y Index: 203

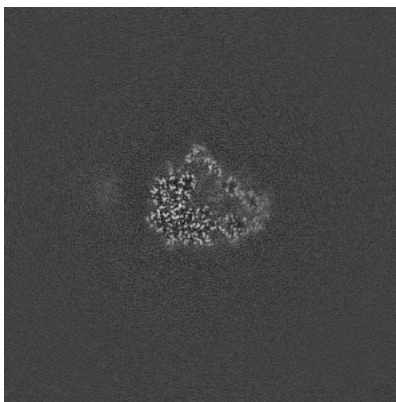


Z Index: 216

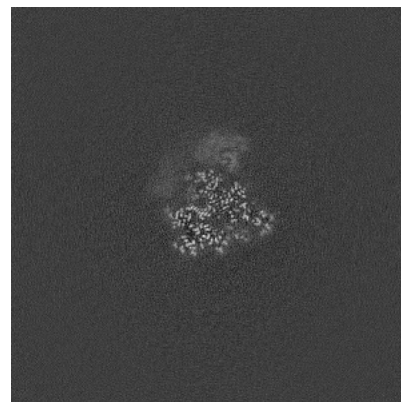
### 6.3.2 Raw map



X Index: 231



Y Index: 203



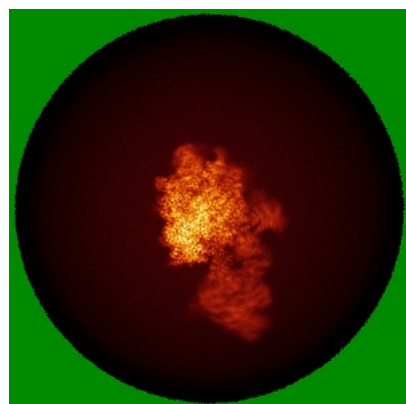
Z Index: 216

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

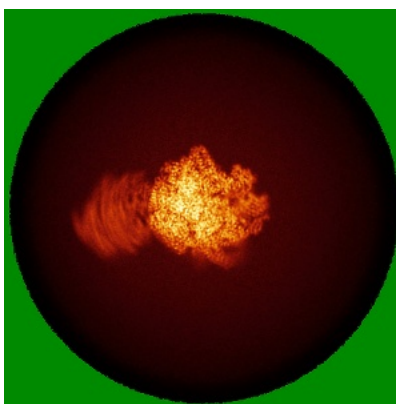


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

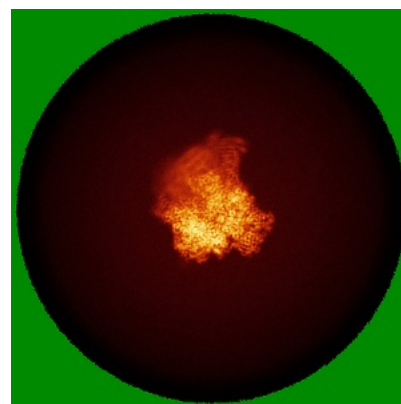
### 6.4.1 Primary map



X

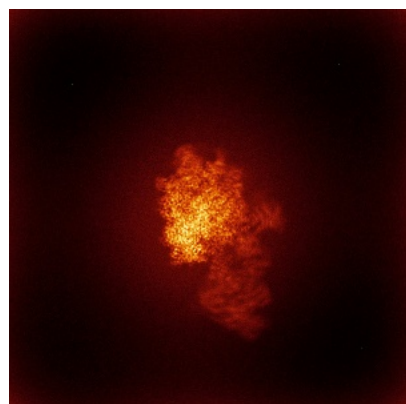


Y

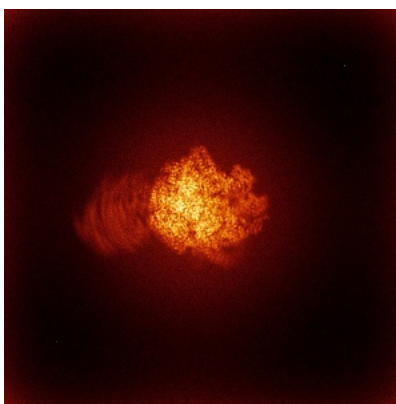


Z

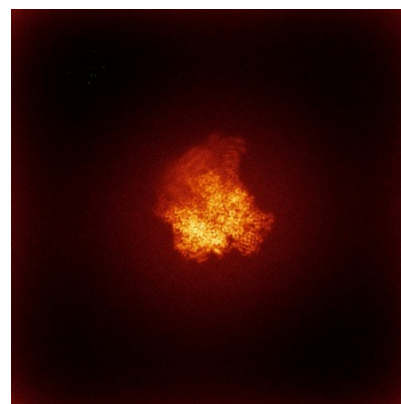
### 6.4.2 Raw map



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



X



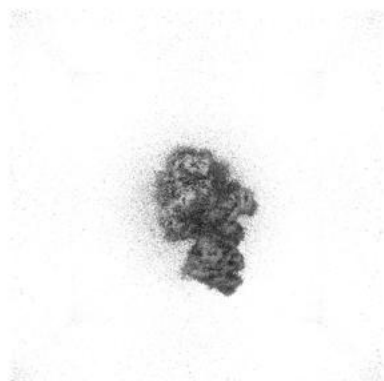
Y



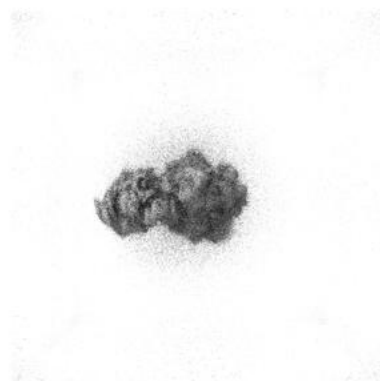
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

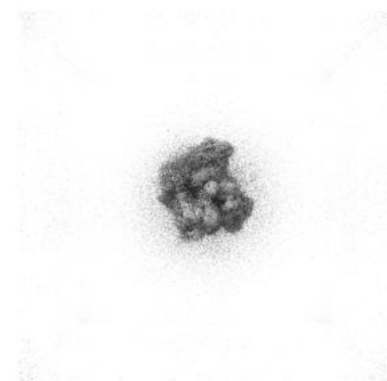
### 6.5.2 Raw map



X



Y



Z

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



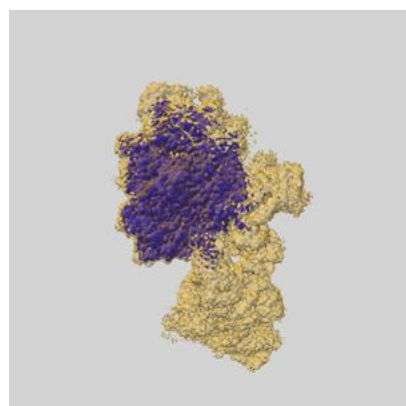
## 6.6 Mask visualisation [i](#)

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

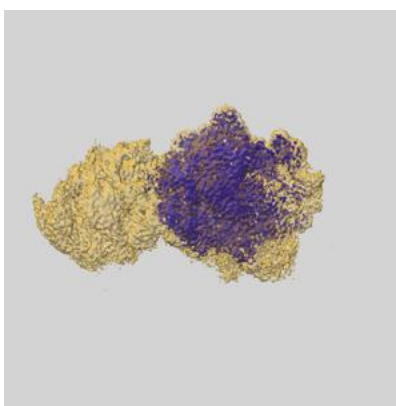
A mask typically either:

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

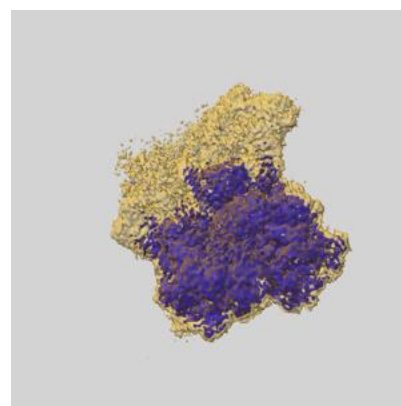
### 6.6.1 emd\_50927\_msk\_1.map [i](#)



X



Y

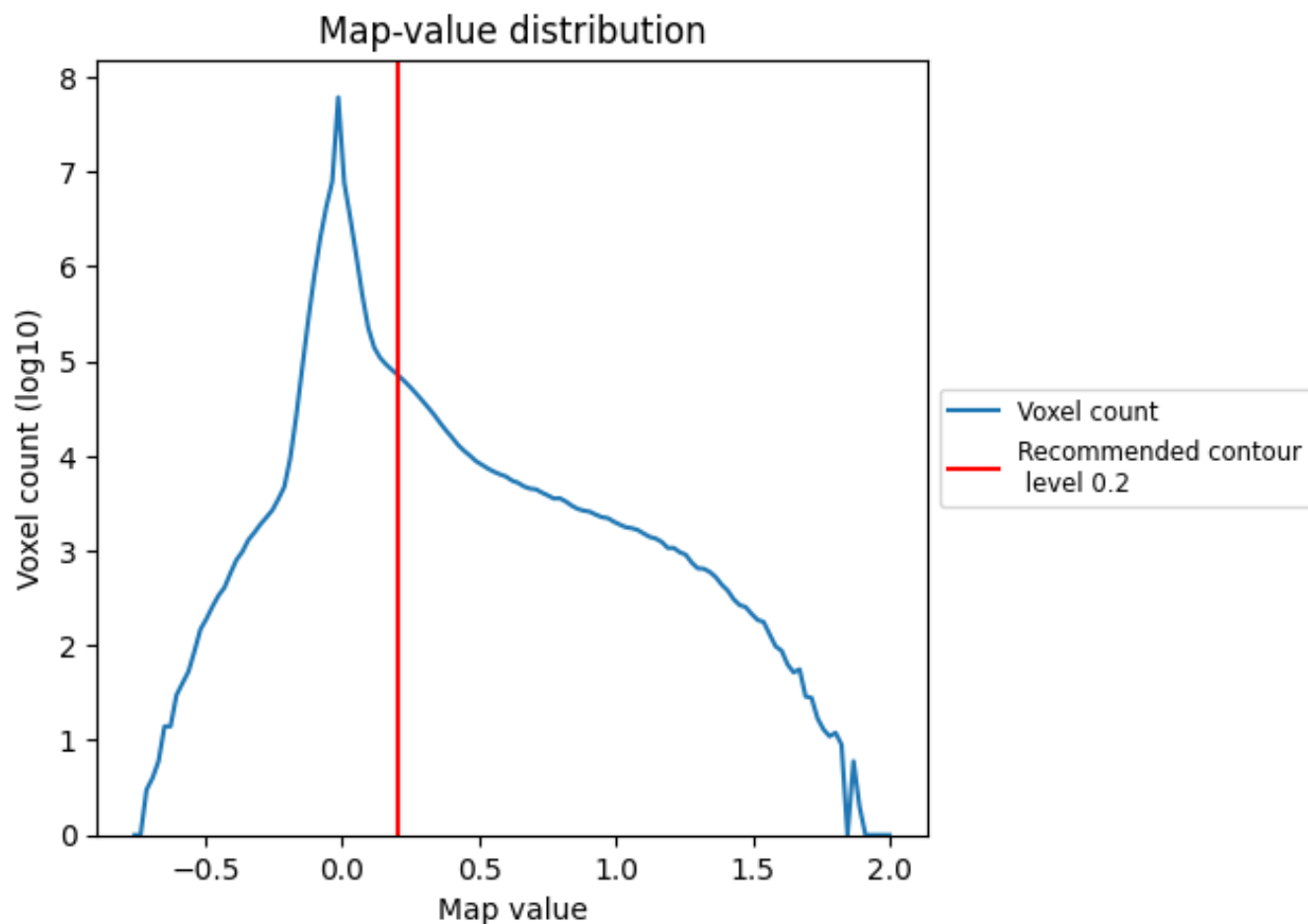


Z

## 7 Map analysis [i](#)

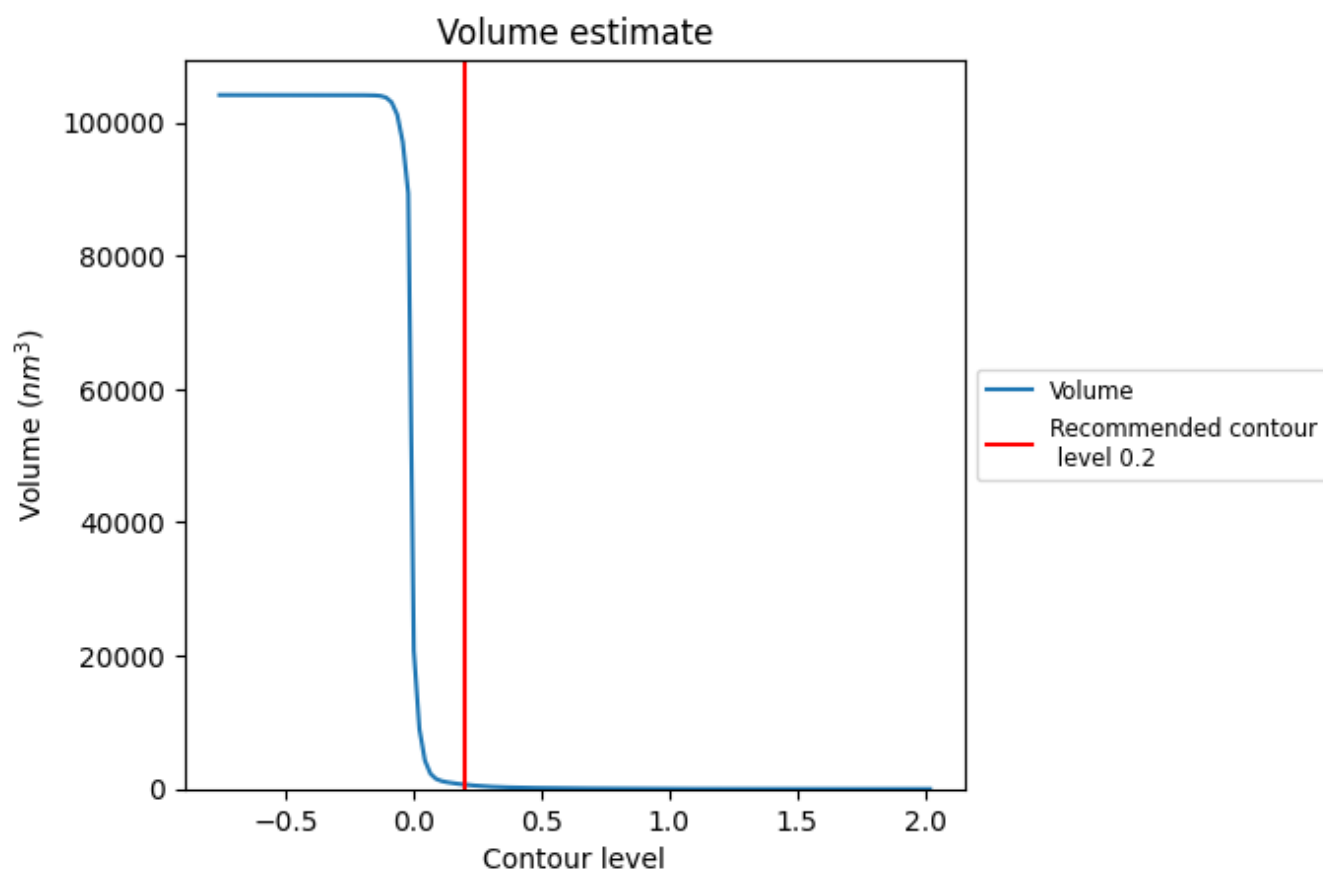
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

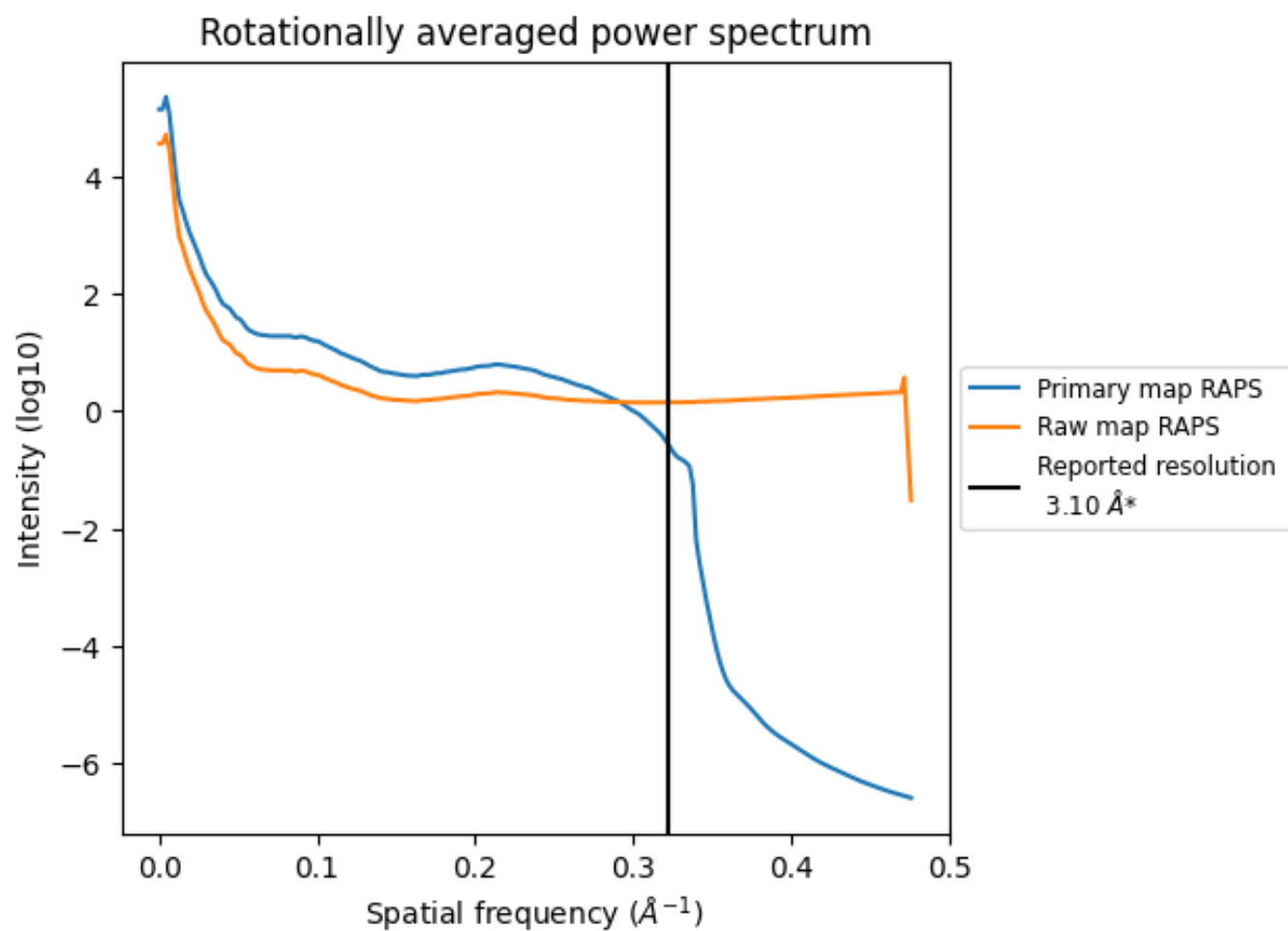
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 656  $\text{nm}^3$ ; this corresponds to an approximate mass of 592 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 ⓘ

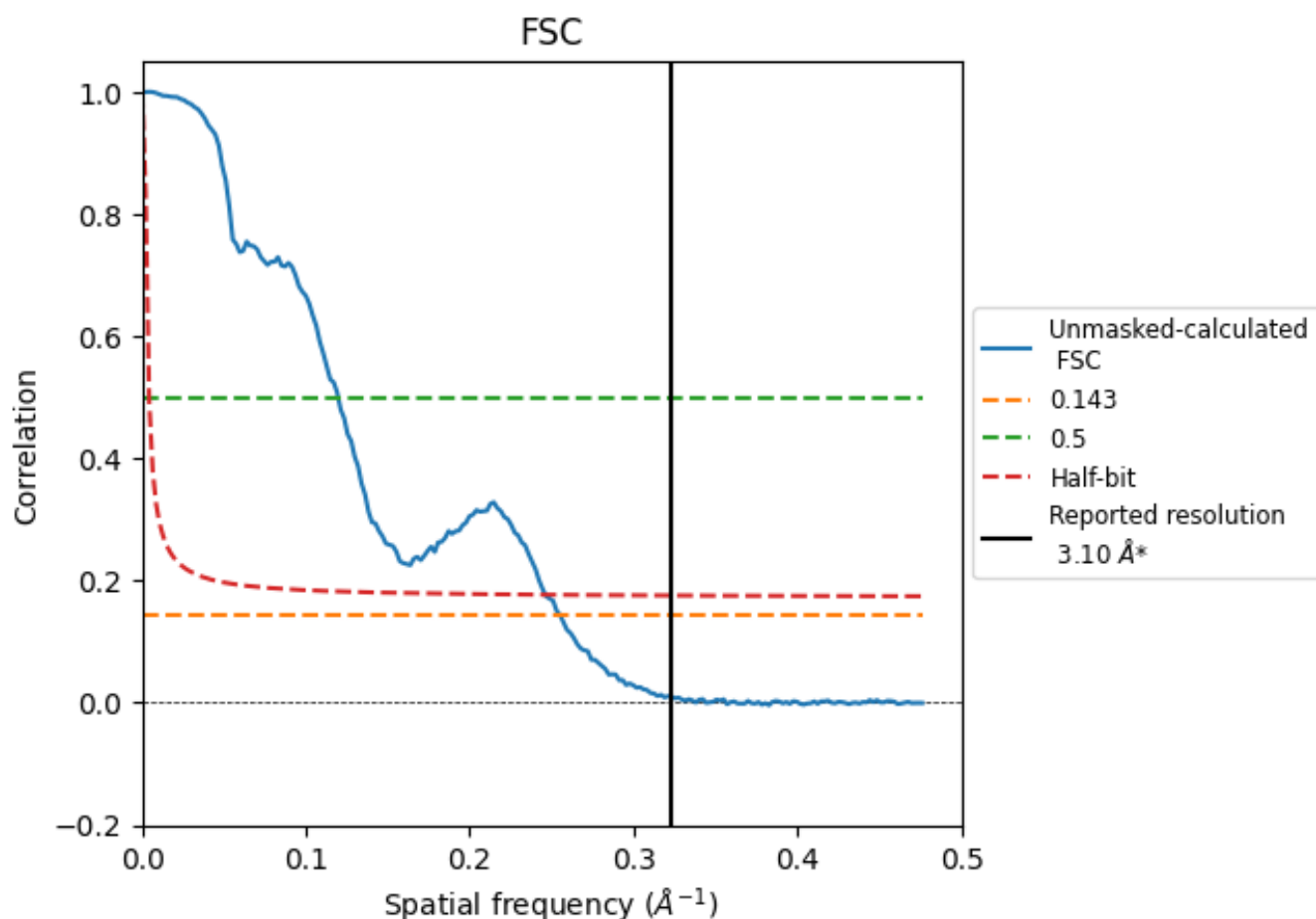


\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

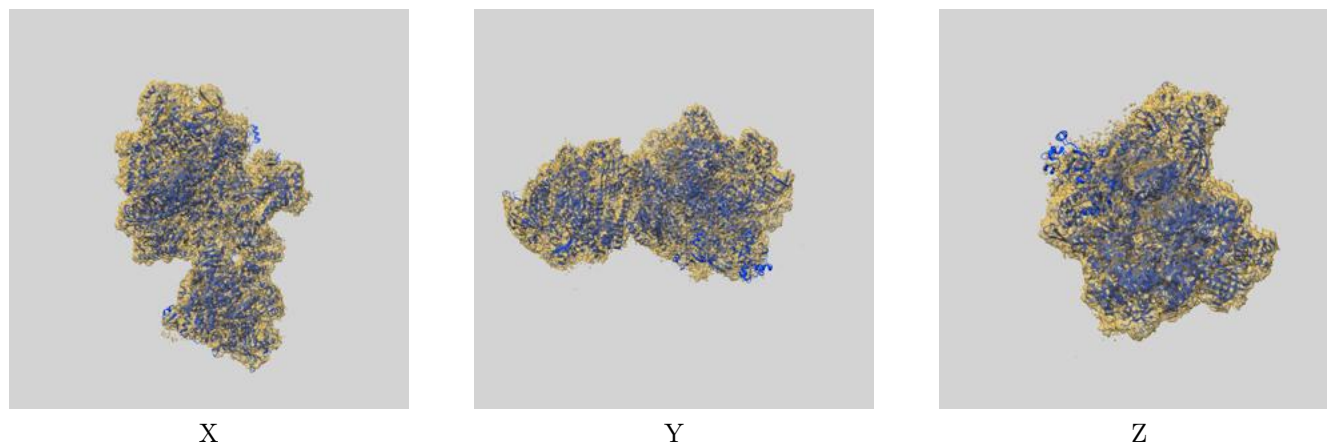
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	8.36	4.06

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.1 by more than 10 %

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

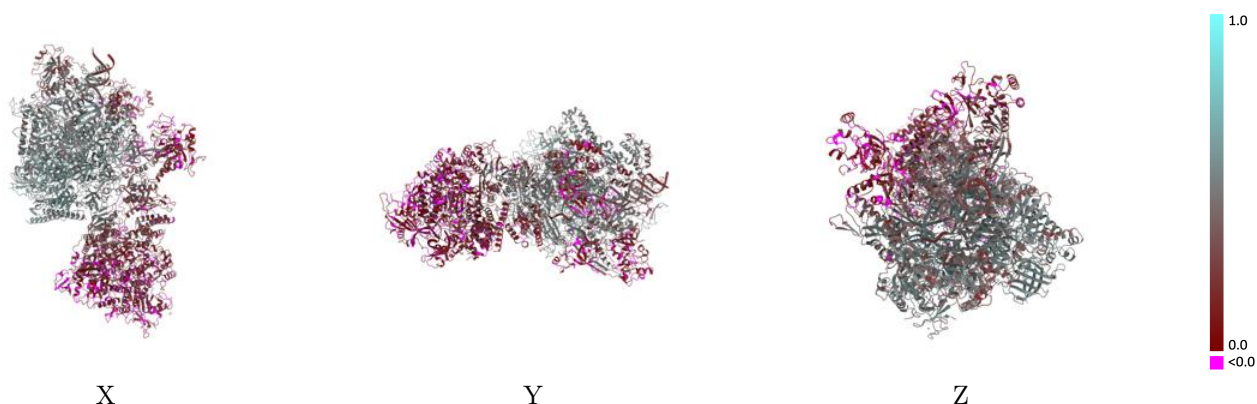
This section contains information regarding the fit between EMDB map EMD-50927 and PDB model 9G0A. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

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



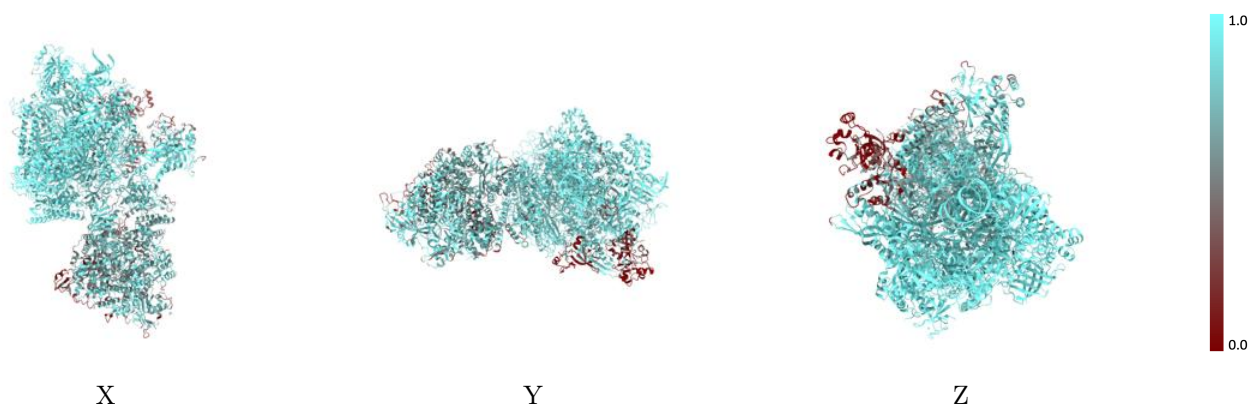
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

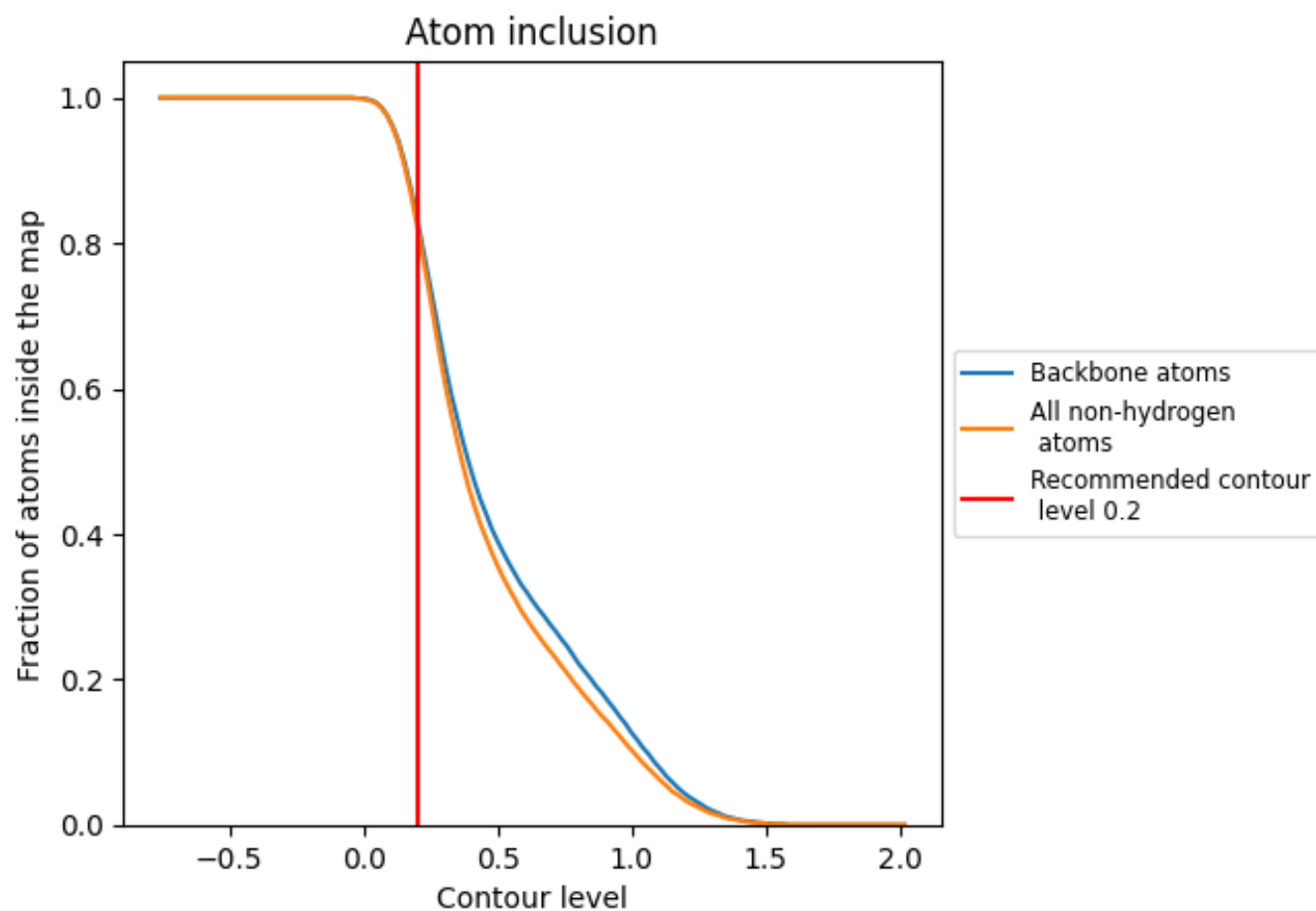
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.2).



















































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8250	 0.3350
A	 0.9440	 0.4780
B	 0.9550	 0.4950
C	 0.9620	 0.5290
D	 0.7920	 0.1650
E	 0.9600	 0.4730
F	 0.9330	 0.4970
G	 0.9080	 0.2710
H	 0.9550	 0.5180
I	 0.9510	 0.4190
J	 0.9780	 0.5440
K	 0.9620	 0.5380
L	 0.9440	 0.4490
N	 0.9720	 0.2780
P	 0.9440	 0.3640
T	 0.9660	 0.3680
X	 0.2210	 0.0560
Y	 0.1370	 0.0860
Z	 0.4990	 0.1660
a	 0.7370	 0.1270
b	 0.7230	 0.1320
c	 0.6850	 0.1980
r	 0.6500	 0.1020
v	 0.9740	 0.0940

