



## wwPDB EM Validation Summary Report ⓘ

Jun 8, 2025 – 01:23 AM JST

PDB ID : 9K3V / pdb\_00009k3v  
EMDB ID : EMD-62030  
Title : Human RNA Polymerase III de novo transcribing complex 4 (TC4)  
Authors : Wang, Q.; Ren, Y.; Jin, Q.; Chen, X.; Xu, Y.  
Deposited on : 2024-10-20  
Resolution : 3.50 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.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

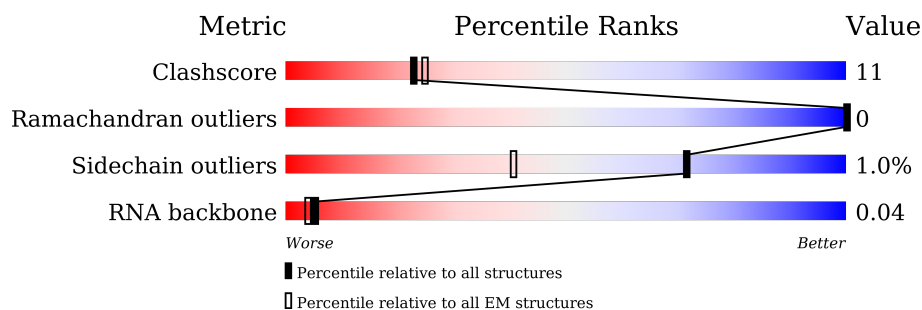
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	368	
2	3	411	
3	4	1469	
4	A	1390	
5	B	1133	
6	C	346	
7	D	148	

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Mol	Chain	Length	Quality of chain
8	E	210	
9	F	127	
10	G	204	
11	H	150	
12	I	108	
13	J	67	
14	K	133	
15	L	58	
16	M	708	
17	N	398	
18	O	534	
19	P	316	
20	Q	223	
21	U	339	
22	V	419	
23	W	2624	
24	X	96	
25	Y	96	
26	Z	3	

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
29	SF4	P	401	-	-	X	-
31	GTP	Z	102	-	-	X	-

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 56769 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 snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	145	Total	C	N	O	S	0	0
			1226	799	211	208	8		

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	374	Total	C	N	O	S	0	0
			3038	1925	521	571	21		

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	247	Total	C	N	O	S	0	0
			2066	1295	378	388	5		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1378	Total	C	N	O	S	0	0
			10814	6850	1886	2005	73		

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1097	Total	C	N	O	S	0	0
			8680	5499	1516	1597	68		

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	343	Total	C	N	O	S	0	0
			2736	1723	488	514	11		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	122	Total	C	N	O	S	0	0
			985	614	172	196	3		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	166	Total	C	N	O	S	0	0
			1337	876	211	245	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	54	Total	C	N	O	S	0	0
			426	267	79	74	6		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	303	Total	C	N	O	S	0	0
			2403	1516	411	460	16		

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	178	Total	C	N	O	S	1	0
			1411	915	246	243	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 23 is a protein called Transcription factor TFIIB component B'' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (96-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	76	Total	C	N	O	P	0	0
			1558	747	273	462	76		

- Molecule 25 is a DNA chain called DNA (96-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	77	Total	C	N	O	P	0	0
			1580	755	292	456	77		

- Molecule 26 is a RNA chain called RNA (5'-R(P\*UP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	3	Total	C	N	O	P	0	0
			63	28	10	22	3		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

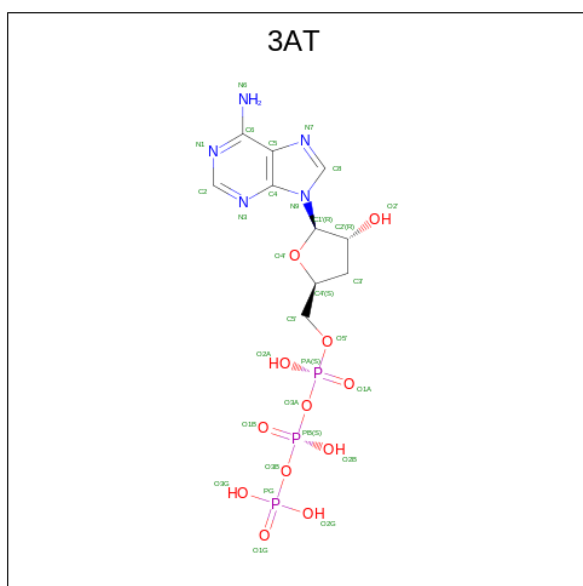
Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Zn	0
			2	2	
27	B	1	Total	Zn	0
			1	1	
27	I	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
27	J	1	Total	Zn	0
			1	1	
27	L	1	Total	Zn	0
			1	1	
27	V	1	Total	Zn	0
			1	1	

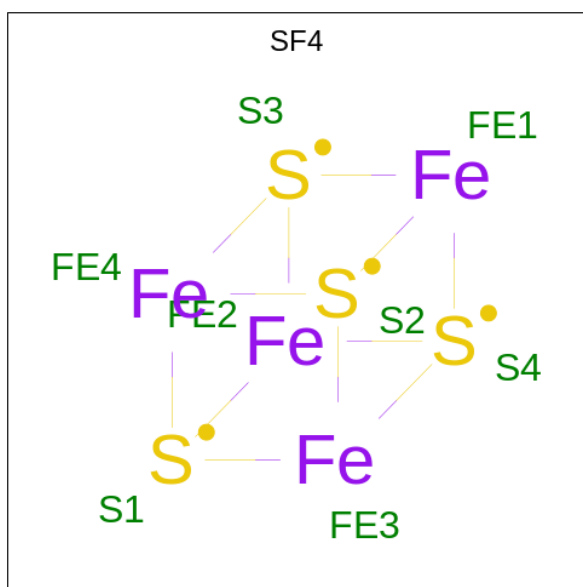
- Molecule 28 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $Fe_4S_4$ ).



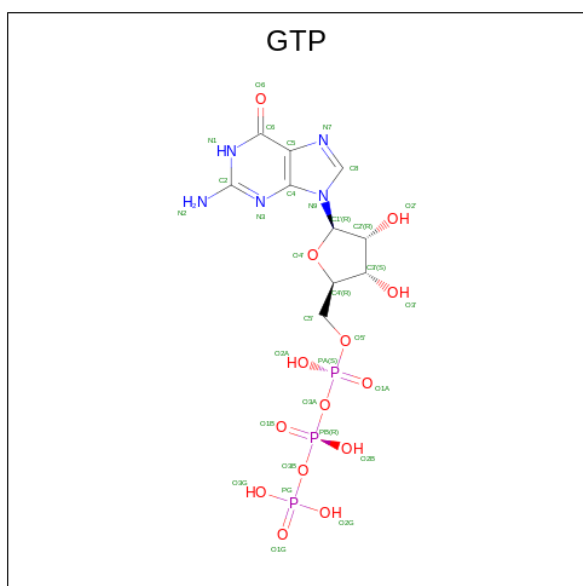


Mol	Chain	Residues	Atoms			AltConf
29	P	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

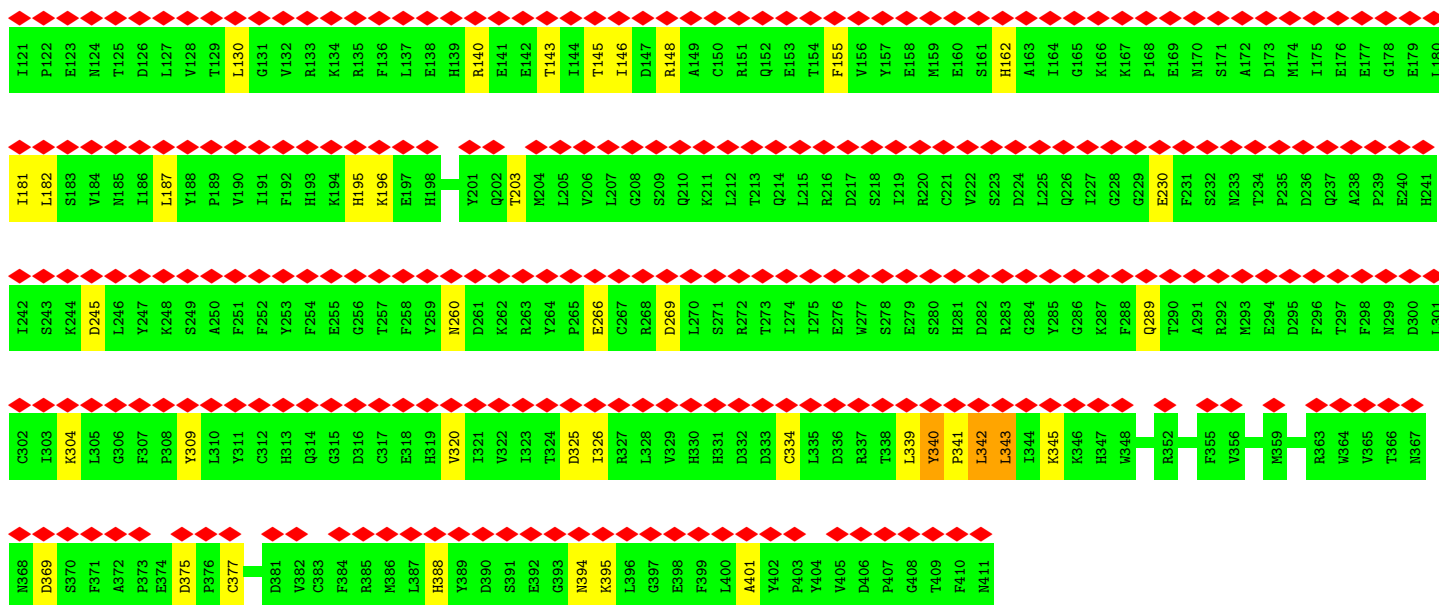
Mol	Chain	Residues	Atoms		AltConf
30	Z	1	Total	Mg	0
			1	1	

- Molecule 31 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

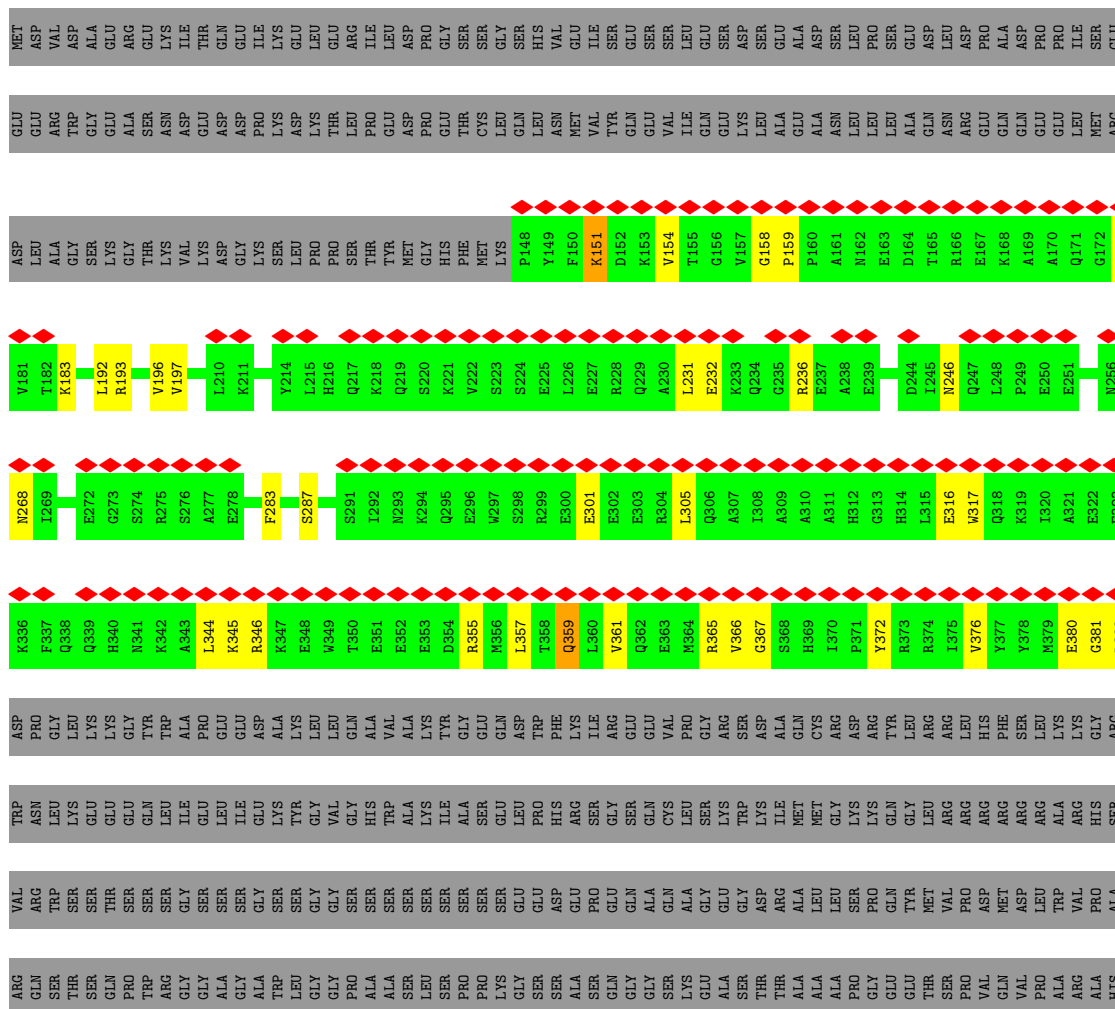


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
31	Z	1	32	10	5	14	3	0

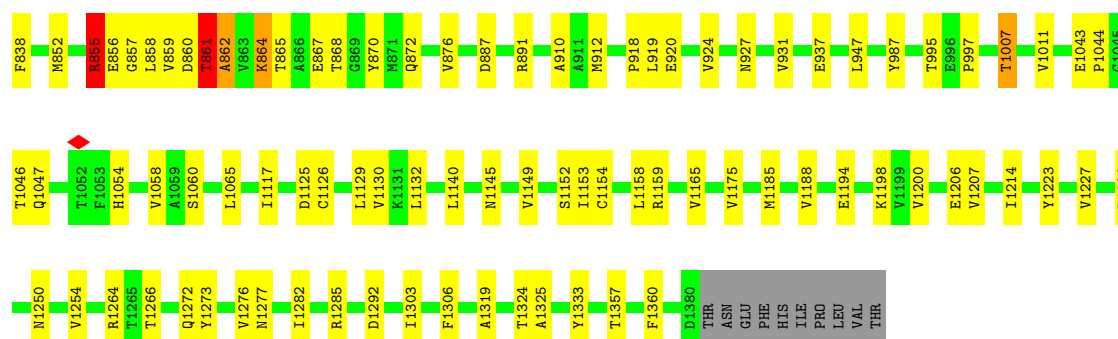




• Molecule 3: snRNA-activating protein complex subunit 4

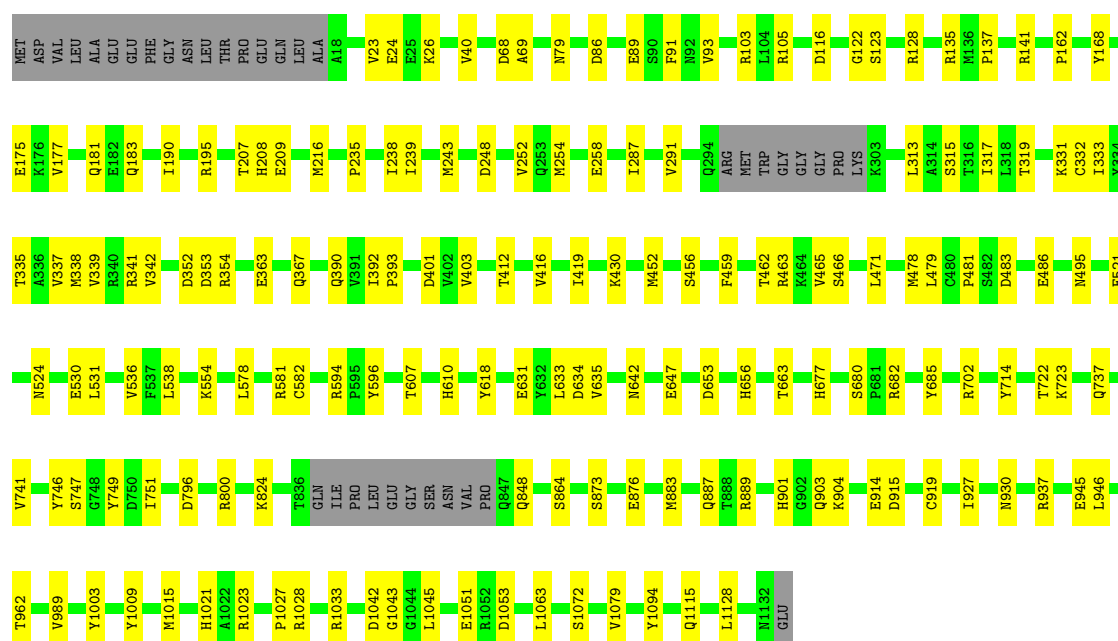






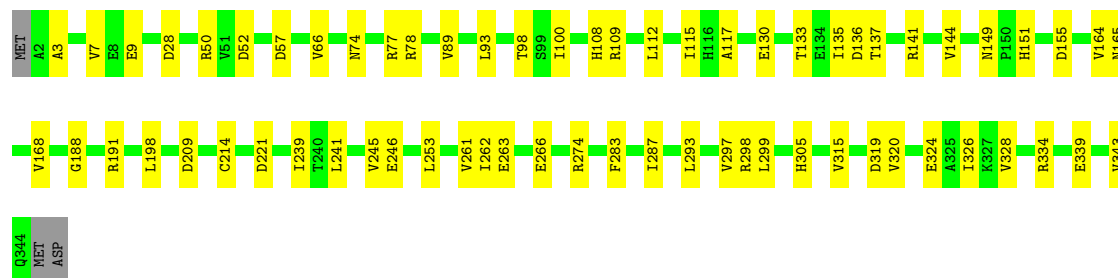
• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

Chain B: 82% 14%



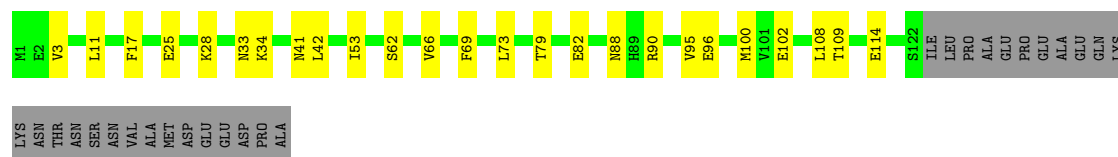
• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 80% 19%



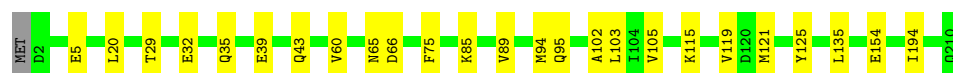
• Molecule 7: DNA-directed RNA polymerase III subunit RPC9

Chain D: 66% 17% 18%



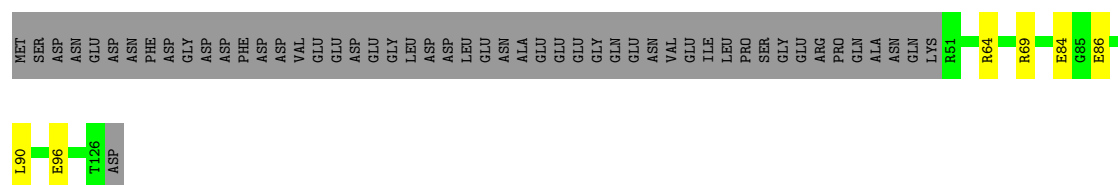
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 88% 12%



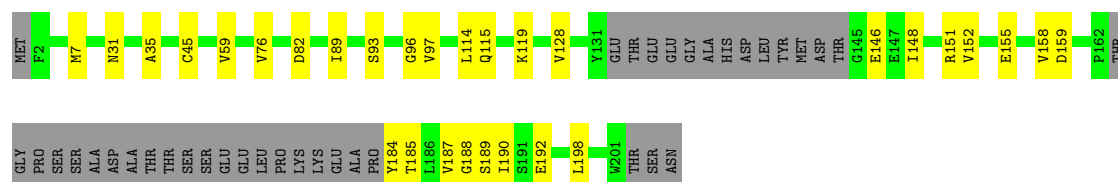
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 55% 5% 40%



- Molecule 10: DNA-directed RNA polymerase III subunit RPC8

Chain G: 67% 15% 19%



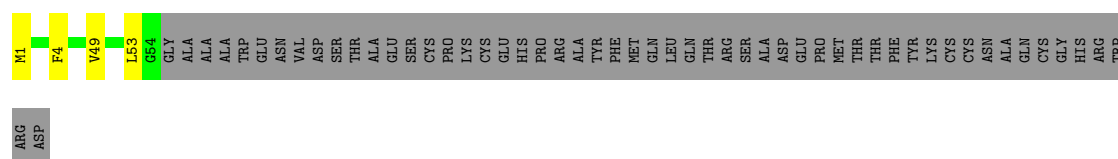
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 78% 21%



- Molecule 12: DNA-directed RNA polymerase III subunit RPC10

Chain I: 46% 50%



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

M1	I2	I3	P4		G10	G11	V14		E28	Y29	T30	E31	G32	D33	A34	L35	D36	L40		R46		L49		L65	G1U	LYS
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- Chain K: 

MET	GLU	GLU	ASP	GLN	GLU	LEU	LEU	GLU	ARG	LYS	ILE	GLY	GLY	LEU	LYS	THR	SER	MET	ALA	GLU	GLY	GLU	ARG	K24	E28	A33	L55	I59	M60	K61	N62	P63	E64	R87	M104	L111	A126	SER	ARG	ASN	GLU	SER	THR	PRO
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- Chain L:  72% 7% 21%

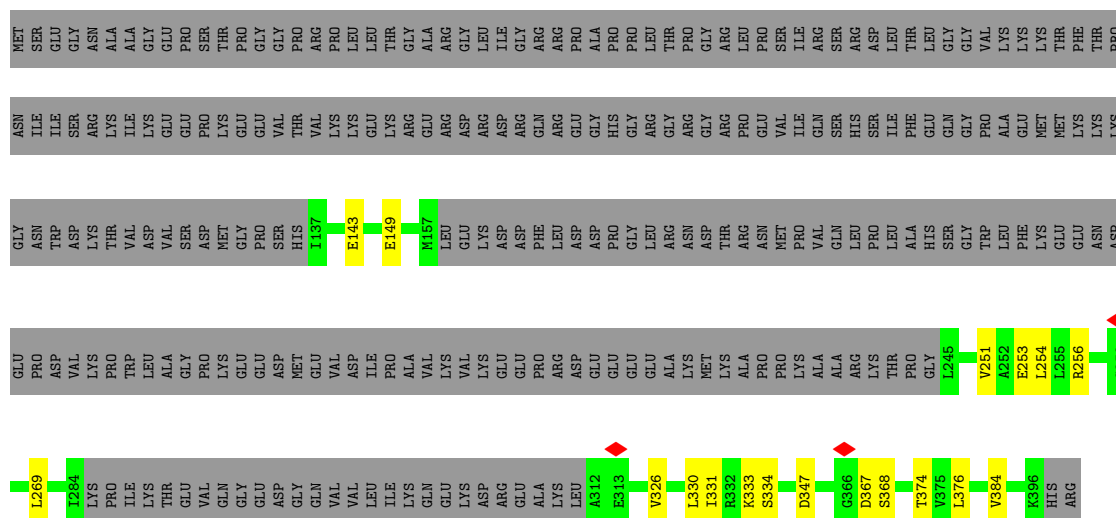
MET  
 ASP  
 THR  
 GLN  
 LYS  
 ASP  
 VAL  
 GLN  
 PRO  
 PRO  
 LYS  
 GLN  
 Q13  
 N26  
 C36  
 R42  
 R58

- Chain M: 

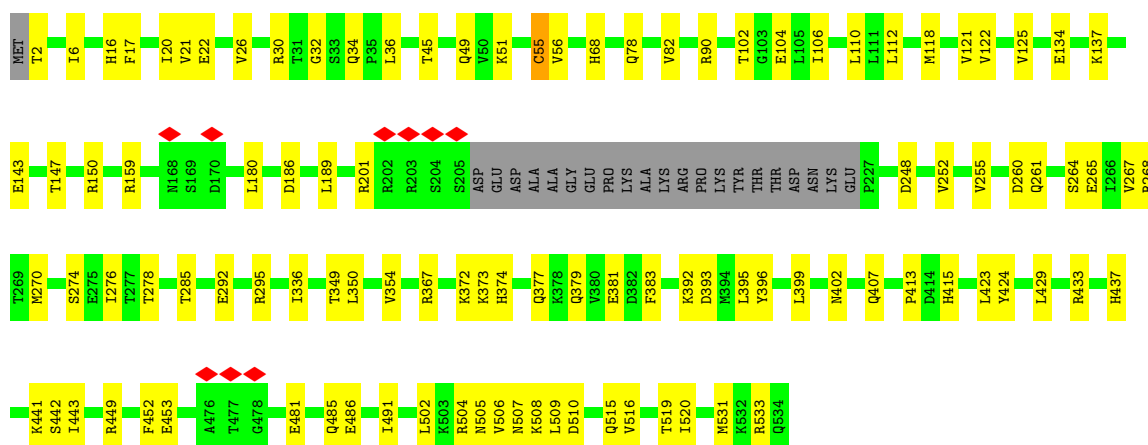
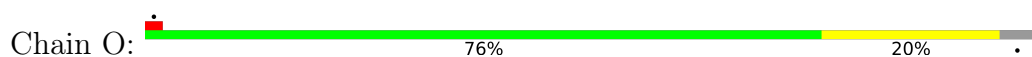
GLU	VAL	ASP	LYS	VAL	LEU	LYS	LYS	PRO	ALA	GLU	LYS	G343	H200	MET
VAL	ASP	ASP	LYS	VAL	LEU	GLY	GLY	GLN	PHE	GLY	PRO	G343	H200	ALA
LYS	LYS	LYS	THR	GLU	VAL	GLY	GLY	THR	VAL	GLY	ASP	A346	D215	ASN
VAL	VAL	VAL	ALA	ALA	THR	ASP	GLU	ALA	ALA	GLU	GLN	E347	S216	GLU
LEU	LEU	LEU	ALA	THR	THR	ASP	ASP	ALA	THR	ASP	SER	V348	S218	GLU
LYS	LYS	LYS	SER	PHE	THR	GLY	GLU	GLU	PHE	GLY	GLY	R351	E221	V9
ASP	ASP	ASP	GLN	GLN	GLN	GLN	GLU	GLU	GLN	GLN	PRO	G352	V10	Q11
CYS	CYS	CYS	ASP	ARG	GLN	GLY	GLU	GLU	ARG	GLY	ALA	R353	L225	
VAL	VAL	VAL	GLN	PHE	VAL	VAL	ALA	ALA	PHE	VAL	VAL	D354	N235	L17
SER	TYR	TYR	VAL	VAL	GLU	GLU	GLU	GLU	VAL	CYS	VAL	F355	L246	A18
GLY	GLY	GLY	THR	THR	GLU	GLU	GLU	GLU	LEU	GLY	GLY	V356	L249	S36
GLY	GLY	GLY	ALA	ALA	PRO	PRO	PRO	PRO	ASP	ASP	GLY	F360	M250	N37
MET	MET	TRP	LEU	SER	SER	ASP	GLN	GLN	SER	GLN	ARG	S363	L249	
TRP	TRP	TRP	TRP	GLU	LEU	THR	THR	THR	LEU	THR	ILE	V367	M250	K50
TYR	TYR	SER	SER	GLY	LEU	SER	SER	SER	LEU	GLN	GLN	V367	Q254	Q53
LEU	LYS	LYS	GLY	ARG	LYS	PRO	PRO	PRO	VAL	VAL	VAL	V370	GLU	V56
GLY	GLY	GLY	ASP	LEU	SER	SER	SER	GLY	LEU	GLY	LYS	E370	GLU	
THR	THR	THR	MET	PHE	LEU	GLY	GLY	GLY	ALA	ALA	ALA	V371	GLU	
VAL	VAL	VAL	SER	ASN	LEU	LEU	LEU	THR	ASN	THR	LYS	V374	LYS	I77
GLN	GLN	GLN	ASP	LEU	LEU	HIS	HIS	LYS	LEU	ALA	ALA	V374	ASP	V81
SER	SER	SER	HIS	HIS	SER	SER	SER	ALA	GLY	GLY	ALA	D381	LYS	
HIS	HIS	HIS	ARG	LEU	LEU	LYS	LYS	GLN	LEU	GLN	GLN	D381	PRO	
ARG	ARG	ARG	ALA	ALA	LEU	GLY	GLY	GLN	ALA	ASN	ASN	E387	VAL	Y92
GLN	GLN	GLN	SER	SER	SER	ASN	ASN	HIS	LEU	ALA	HIS	E387	ALA	
VAL	VAL	VAL	GLN	LEU	LEU	LEU	LEU	ALA	PRO	GLY	ALA	P264	S265	S104
LEU	LEU	LEU	VAL	PRO	GLY	PRO	PRO	ALA	GLY	GLY	ALA	S265	S265	Q134
LEU	LEU	GLY	GLY	PRO	GLY	PRO	PRO	LEU	GLY	PRO	LEU	I394	N266	
ILE	ILE	ILE	ILE	HIS	HIS	LEU	LEU	LEU	LEU	LEU	GLU	N395	V267	L135
PHE	PHE	PHE	THR	THR	THR	GLY	GLY	ARG	THR	GLY	ARG	K396	L268	R136
SER	SER	SER	THR	LEU	LEU	ARG	ARG	GLU	PHE	GLU	GLU	E399	L268	
LYS	LYS	LYS	LEU	PHE	LEU	ALA	ALA	LEU	LEU	LEU	LEU	E399	L276	A158
ASN	ASN	ASN	ASN	SER	SER	ALA	ALA	GLN	SER	GLN	GLN	F400	L276	G159
TYR	TYR	TYR	TYR	GLY	GLY	GLY	GLY	ARG	GLY	ARG	ARG	I401	Q281	D160
ARG	ARG	ARG	ARG	ILE	ILE	THR	THR	ARG	THR	THR	THR	I401	Q281	
VAL	VAL	VAL	SER	SER	SER	ASP	ASP	LYS	ASP	LYS	LYS	D405	V289	S161
ARG	ARG	ARG	ASP	ARG	ARG	PHE	PHE	GLU	ASP	GLU	GLU	G406	K290	S162
ASN	ASN	ASN	MET	MET	MET	ASN	ASN	GLN	LEU	GLN	GLN	G406	V291	Q163
MET	MET	MET	LEU	LEU	LEU	GLY	GLY	LEU	GLY	ARG	ARG	I409	M298	D164
ILE	ILE	ILE	GLN	GLN	GLN	GLY	GLY	VAL	GLY	VAL	VAL	I409	M298	
GLN	GLN	GLN	ASP	ASP	THR	HIS	HIS							

- Chain N:  32% 5% 63%

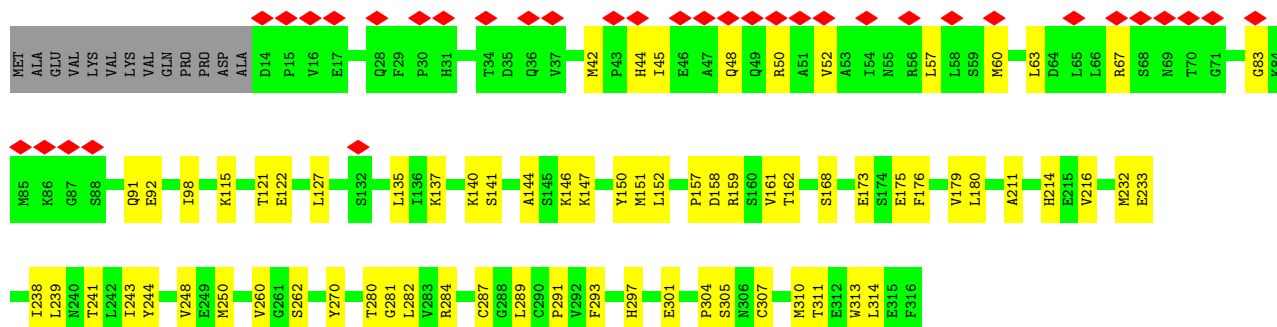
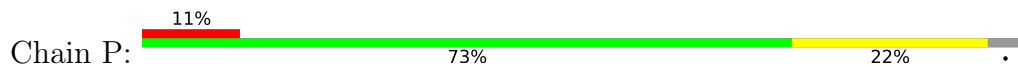




• Molecule 18: DNA-directed RNA polymerase III subunit RPC3



• Molecule 19: DNA-directed RNA polymerase III subunit RPC6



• Molecule 20: DNA-directed RNA polymerase III subunit RPC7



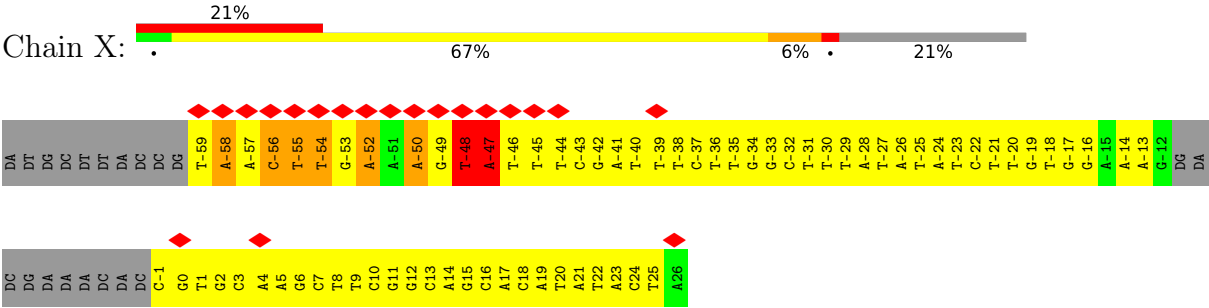




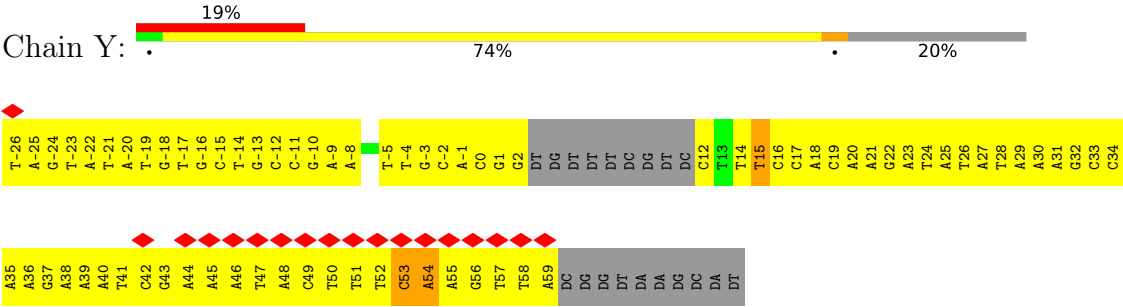


PRO	GLN	PRO	GLN	PRO	GLN	ASP	GLU	MET	LEU	VAL	SER	LEU	ARG	LYS	ASP	LYS	GLU	GLU	ILE	THR	ASP	ALA	ALA	PRO	LYS	SER	GLN	GLN	MET	ASP	SER	ARG	THR	SER	SER	SER	SER	SER	GLN	GLU	GLU	LYS	ALA	SER	LEU	SER	ARG	GLY	PRO	ARG	PRO	LEU	GLY	PHE	VAL	THR	THR	GLN	ILE	LEU	LEU	CYS	LYS	ILE	ASN	SER	LEU	GLU	ALA	SER	ASP
GLU	PRO	MET	GLN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

• Molecule 24: DNA (96-MER)



• Molecule 25: DNA (96-MER)



• Molecule 26: RNA (5'-R(P\*UP\*GP\*C)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	235000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.505	Depositor
Minimum map value	-4.247	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.143	Depositor
Map size (Å)	429.07724, 429.07724, 429.07724	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332538, 1.332538, 1.332538	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, MG, GTP, 3AT

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	1	0.21	0/1257	0.48	1/1692 (0.1%)
2	3	0.14	0/3113	0.33	0/4206
3	4	0.12	0/2107	0.27	0/2828
4	A	0.21	2/11008 (0.0%)	0.28	2/14842 (0.0%)
5	B	0.11	0/8845	0.24	0/11930
6	C	0.11	0/2790	0.24	0/3782
7	D	0.12	0/997	0.24	0/1343
8	E	0.12	0/1745	0.23	0/2358
9	F	0.13	0/620	0.24	0/839
10	G	0.12	0/1374	0.26	0/1868
11	H	0.12	0/1207	0.24	0/1628
12	I	0.13	0/434	0.22	0/584
13	J	0.13	0/521	0.25	0/703
14	K	0.13	0/837	0.25	0/1129
15	L	0.15	0/394	0.26	0/524
16	M	0.11	0/3455	0.23	0/4673
17	N	0.11	0/1137	0.24	0/1530
18	O	0.11	0/4141	0.24	0/5592
19	P	0.11	0/2446	0.22	0/3301
20	Q	0.13	0/777	0.23	0/1050
21	U	0.22	0/1439	0.52	1/1938 (0.1%)
22	V	0.12	0/2904	0.25	0/3941
23	W	0.14	0/967	0.27	0/1293
24	X	0.38	2/1744 (0.1%)	0.89	12/2688 (0.4%)
25	Y	0.30	2/1773 (0.1%)	0.57	5/2731 (0.2%)
26	Z	0.57	0/69	1.00	1/105 (1.0%)
All	All	0.17	6/58101 (0.0%)	0.33	22/79098 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
5	B	0	1
24	X	0	2
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	X	-56	DC	O3'-P	9.26	1.75	1.61
25	Y	15	DT	C4'-O4'	7.87	1.61	1.45
4	A	861	THR	CA-C	-6.88	1.44	1.52
4	A	861	THR	N-CA	-6.72	1.38	1.46
24	X	-58	DA	O3'-P	-6.17	1.51	1.61

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	54	DA	O3'-P-O5'	-17.63	77.56	104.00
24	X	-54	DT	O3'-P-O5'	-16.51	79.23	104.00
24	X	-55	DT	O3'-P-O5'	16.07	128.11	104.00
24	X	-47	DA	C5'-C4'-O4'	16.04	133.45	109.40
24	X	-50	DA	C2'-C3'-O3'	-13.84	90.74	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	855	ARG	Sidechain
5	B	682	ARG	Sidechain
24	X	-47	DA	Sidechain
24	X	-48	DT	Sidechain

## 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	1	1226	0	1224	24	0
2	3	3038	0	2911	62	0
3	4	2066	0	2049	33	0
4	A	10814	0	11058	238	0
5	B	8680	0	8805	122	0
6	C	2736	0	2712	44	0
7	D	985	0	1006	16	0
8	E	1715	0	1733	18	0
9	F	610	0	642	6	0
10	G	1337	0	1306	22	0
11	H	1186	0	1147	21	0
12	I	426	0	429	6	0
13	J	512	0	525	8	0
14	K	822	0	810	8	0
15	L	388	0	393	3	0
16	M	3382	0	3376	58	0
17	N	1128	0	1181	16	0
18	O	4075	0	4149	162	0
19	P	2403	0	2408	95	0
20	Q	754	0	759	38	0
21	U	1411	0	1499	42	0
22	V	2853	0	2890	47	0
23	W	943	0	924	26	0
24	X	1558	0	865	213	0
25	Y	1580	0	870	192	0
26	Z	63	0	32	28	0
27	A	2	0	0	0	0
27	B	1	0	0	0	0
27	I	1	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
27	V	1	0	0	0	0
28	B	30	0	12	4	0
29	P	8	0	0	2	0
30	Z	1	0	0	0	0
31	Z	32	0	11	21	0
All	All	56769	0	55726	1230	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 11.

The worst 5 of 1230 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)
24:X:-49:DG:H22	25:Y:49:DC:N4	1.15	1.41
24:X:-49:DG:N2	25:Y:49:DC:H42	1.09	1.41
2:3:181:ILE:HD11	2:3:340:TYR:OH	1.12	1.29
26:Z:2:U:C5'	31:Z:102:GTP:O2'	1.81	1.27
2:3:181:ILE:CD1	2:3:340:TYR:OH	1.84	1.24

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	1	141/368 (38%)	128 (91%)	13 (9%)	0	100	100
2	3	368/411 (90%)	354 (96%)	14 (4%)	0	100	100
3	4	245/1469 (17%)	237 (97%)	8 (3%)	0	100	100
4	A	1376/1390 (99%)	1337 (97%)	39 (3%)	0	100	100
5	B	1091/1133 (96%)	1066 (98%)	25 (2%)	0	100	100
6	C	341/346 (99%)	337 (99%)	4 (1%)	0	100	100
7	D	120/148 (81%)	118 (98%)	2 (2%)	0	100	100
8	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
9	F	74/127 (58%)	70 (95%)	4 (5%)	0	100	100
10	G	160/204 (78%)	149 (93%)	11 (7%)	0	100	100
11	H	146/150 (97%)	146 (100%)	0	0	100	100
12	I	52/108 (48%)	52 (100%)	0	0	100	100
13	J	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
14	K	101/133 (76%)	98 (97%)	3 (3%)	0	100	100
15	L	44/58 (76%)	41 (93%)	3 (7%)	0	100	100
16	M	418/708 (59%)	402 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	N	140/398 (35%)	140 (100%)	0	0	100	100
18	O	508/534 (95%)	496 (98%)	12 (2%)	0	100	100
19	P	301/316 (95%)	292 (97%)	9 (3%)	0	100	100
20	Q	85/223 (38%)	83 (98%)	2 (2%)	0	100	100
21	U	177/339 (52%)	174 (98%)	3 (2%)	0	100	100
22	V	358/419 (85%)	347 (97%)	11 (3%)	0	100	100
23	W	109/2624 (4%)	102 (94%)	7 (6%)	0	100	100
All	All	6625/11883 (56%)	6432 (97%)	193 (3%)	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	1	129/334 (39%)	118 (92%)	11 (8%)	8	32
2	3	330/356 (93%)	317 (96%)	13 (4%)	27	56
3	4	221/1213 (18%)	217 (98%)	4 (2%)	54	74
4	A	1200/1212 (99%)	1191 (99%)	9 (1%)	79	88
5	B	959/988 (97%)	958 (100%)	1 (0%)	92	97
6	C	299/302 (99%)	299 (100%)	0	100	100
7	D	114/136 (84%)	114 (100%)	0	100	100
8	E	191/192 (100%)	191 (100%)	0	100	100
9	F	66/111 (60%)	66 (100%)	0	100	100
10	G	149/181 (82%)	148 (99%)	1 (1%)	81	89
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	48/93 (52%)	48 (100%)	0	100	100
13	J	53/56 (95%)	53 (100%)	0	100	100
14	K	92/119 (77%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	L	43/55 (78%)	43 (100%)	0	100	100
16	M	377/622 (61%)	377 (100%)	0	100	100
17	N	131/347 (38%)	131 (100%)	0	100	100
18	O	458/476 (96%)	457 (100%)	1 (0%)	92	97
19	P	269/280 (96%)	269 (100%)	0	100	100
20	Q	84/195 (43%)	84 (100%)	0	100	100
21	U	154/293 (53%)	148 (96%)	6 (4%)	27	56
22	V	325/365 (89%)	316 (97%)	9 (3%)	38	65
23	W	102/2381 (4%)	98 (96%)	4 (4%)	27	56
All	All	5923/10438 (57%)	5864 (99%)	59 (1%)	71	84

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	428	MET
23	W	289	THR
4	A	861	THR
22	V	384	ILE
22	V	128	GLN

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

Mol	Chain	Res	Type
5	B	552	HIS
11	H	131	ASN
23	W	383	GLN
21	U	166	GLN
5	B	785	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	Z	2/3 (66%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	Z	4	C

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\# Z  > 2$
28	3AT	B	1202	-	25,32,32	0.98	1 (4%)	28,50,50	1.62	5 (17%)
29	SF4	P	401	19	0,12,12	-	-	-	-	-
31	GTP	Z	102	-	26,34,34	1.43	4 (15%)	32,54,54	2.65	8 (25%)

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
29	SF4	P	401	19	-	-	0/6/5/5
28	3AT	B	1202	-	-	6/18/34/34	0/3/3/3
31	GTP	Z	102	-	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	102	GTP	C3'-C4'	3.71	1.62	1.53
31	Z	102	GTP	C5-C6	-2.81	1.41	1.47
31	Z	102	GTP	O4'-C1'	2.70	1.44	1.41
31	Z	102	GTP	C8-N7	-2.66	1.30	1.35
28	B	1202	3AT	C5-C4	2.51	1.47	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Z	102	GTP	O4'-C4'-C5'	7.64	134.50	109.37
31	Z	102	GTP	PA-O3A-PB	-7.58	106.81	132.83
31	Z	102	GTP	PB-O3B-PG	-7.53	106.97	132.83
28	B	1202	3AT	PA-O3A-PB	-3.62	120.40	132.83
28	B	1202	3AT	PB-O3B-PG	-3.61	120.42	132.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	B	1202	3AT	C5'-O5'-PA-O3A
28	B	1202	3AT	O4'-C4'-C5'-O5'
28	B	1202	3AT	C3'-C4'-C5'-O5'
31	Z	102	GTP	O4'-C4'-C5'-O5'
31	Z	102	GTP	C3'-C4'-C5'-O5'

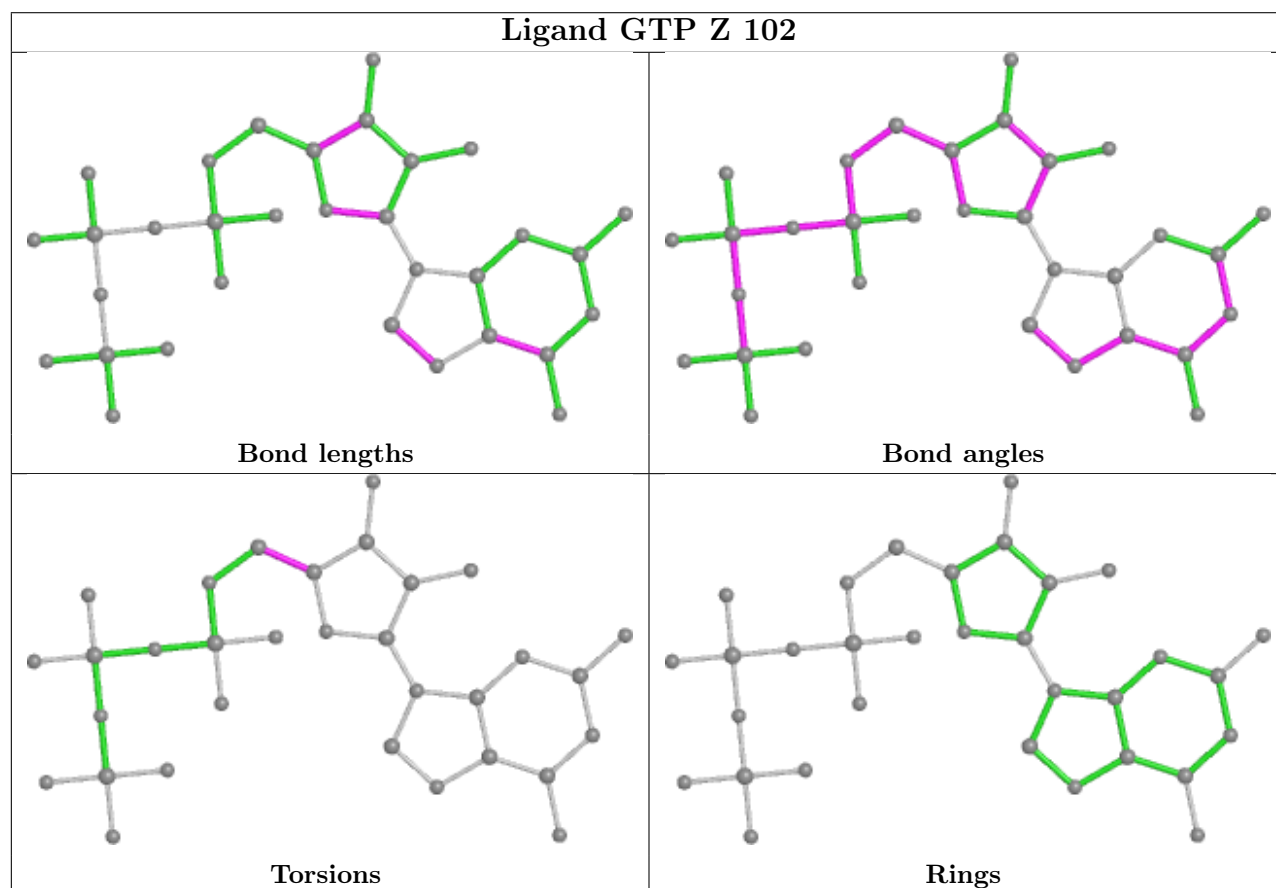
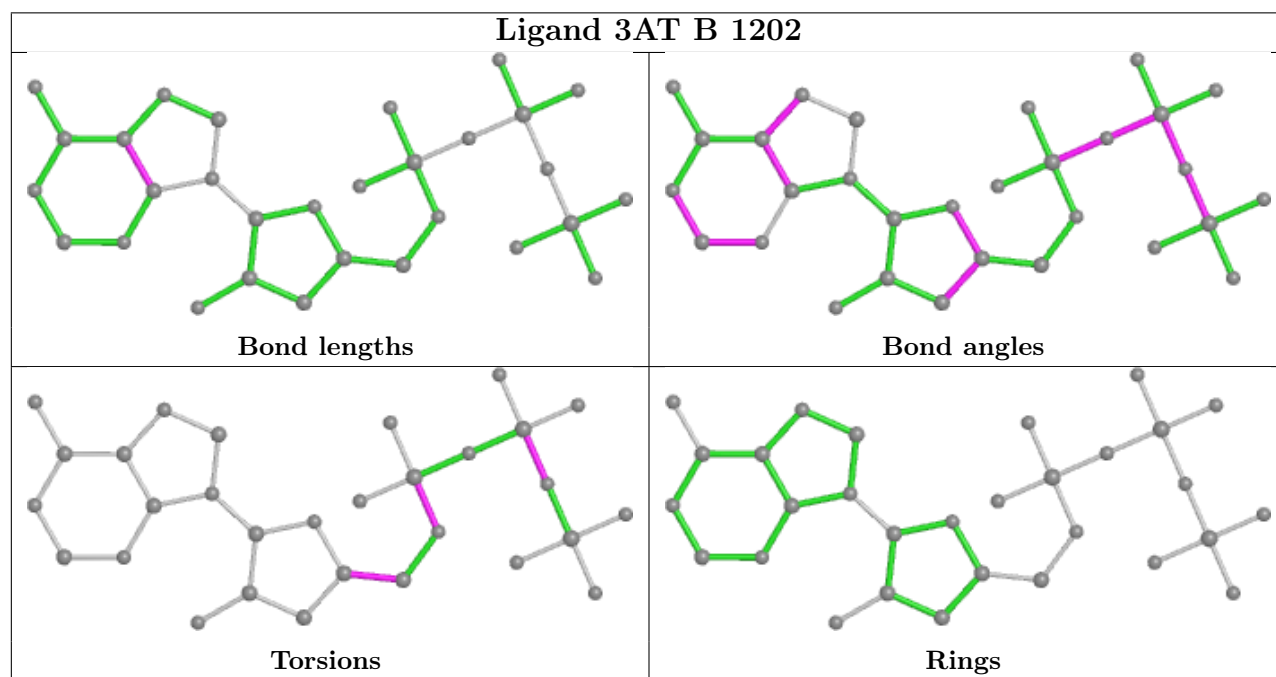
There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	1202	3AT	4	0
29	P	401	SF4	2	0
31	Z	102	GTP	21	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.



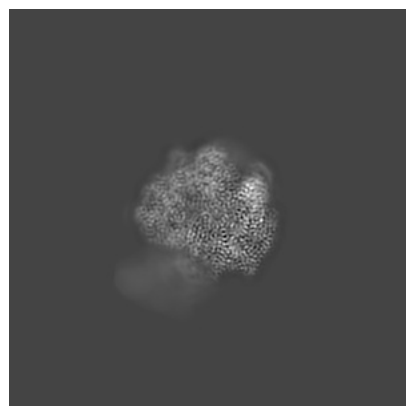
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62030. These allow visual inspection of the internal detail of the map and identification of artifacts.

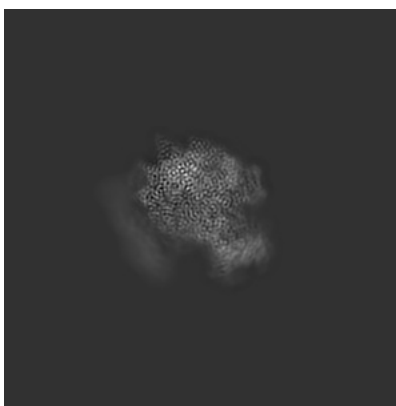
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

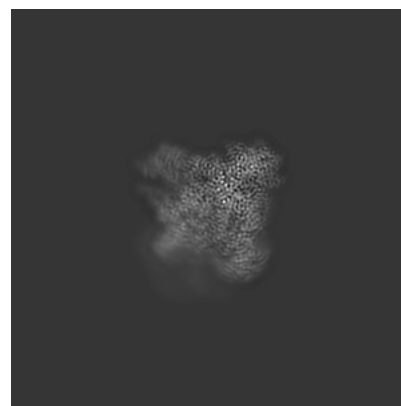
#### 6.1.1 Primary map



X

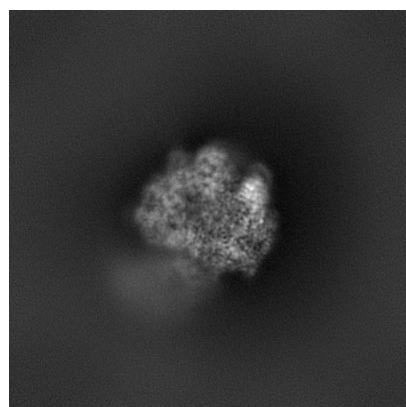


Y

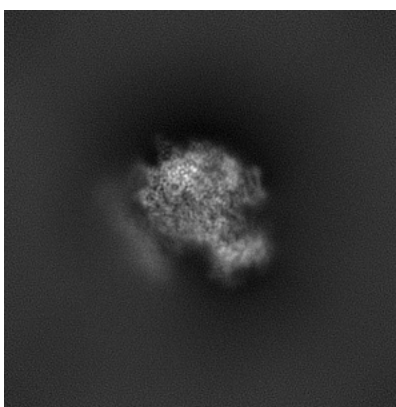


Z

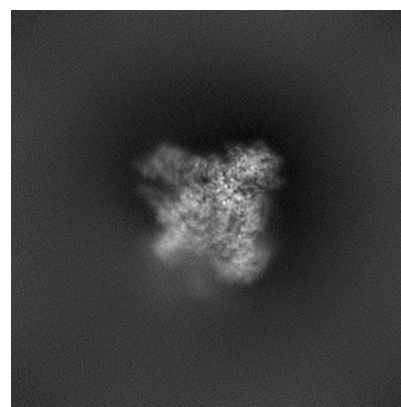
#### 6.1.2 Raw map



X



Y

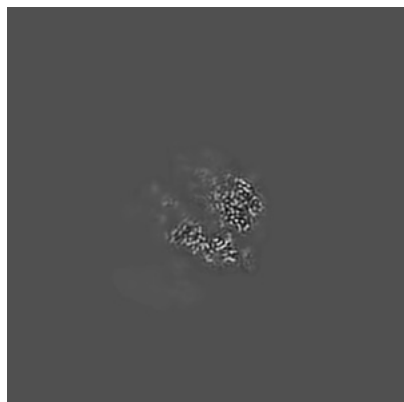


Z

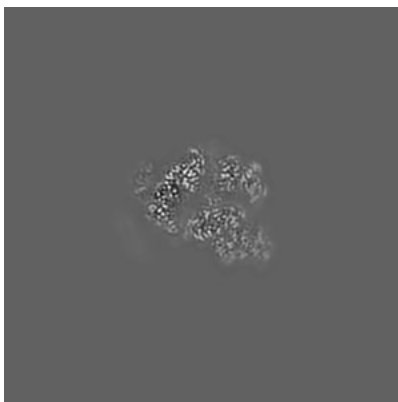
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

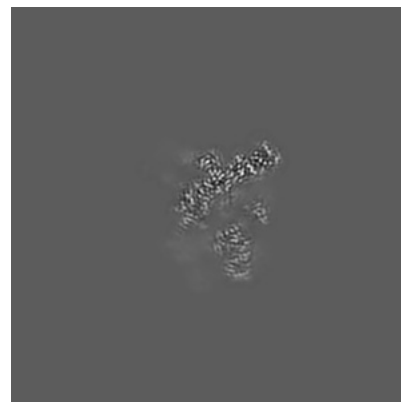
### 6.2.1 Primary map



X Index: 161



Y Index: 161

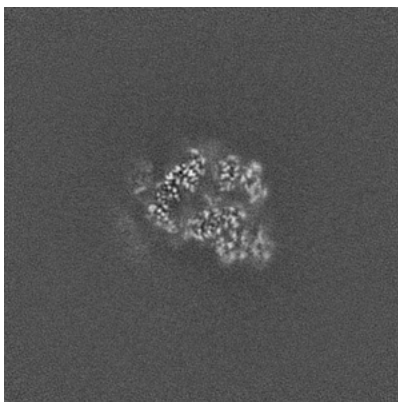


Z Index: 161

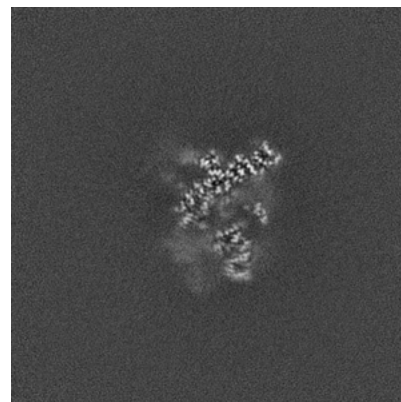
### 6.2.2 Raw map



X Index: 161



Y Index: 161

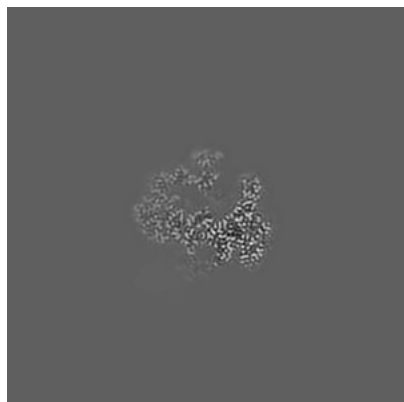


Z Index: 161

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

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

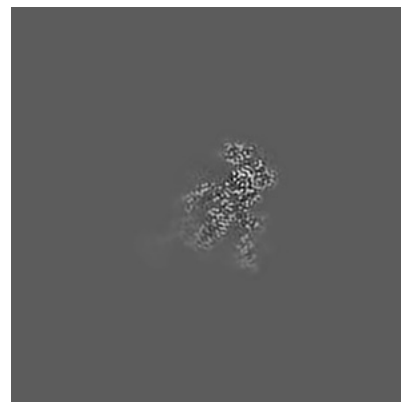
### 6.3.1 Primary map



X Index: 189

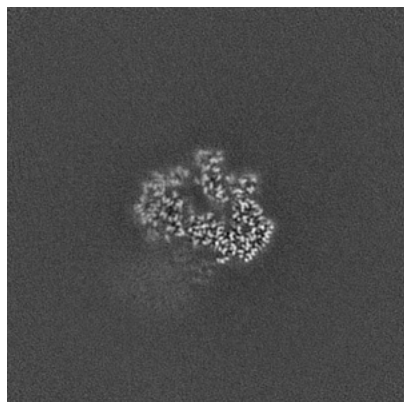


Y Index: 190

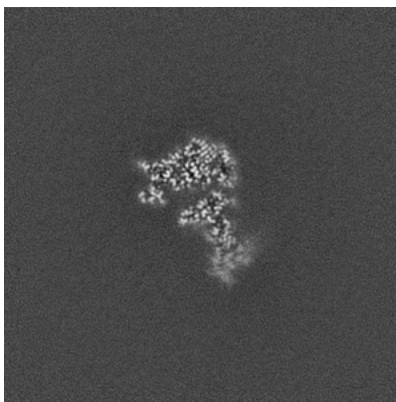


Z Index: 136

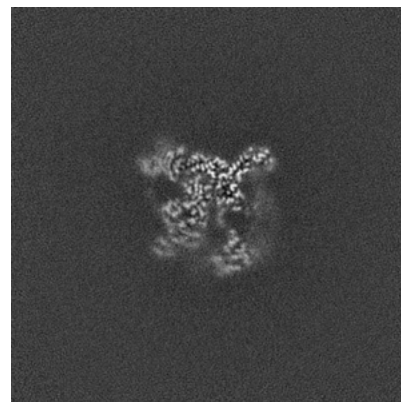
### 6.3.2 Raw map



X Index: 183



Y Index: 196

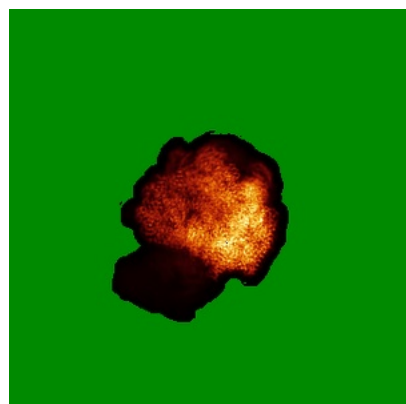


Z Index: 173

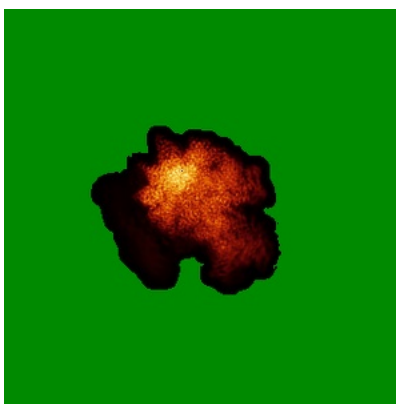
The images above show the largest variance slices of the map in three orthogonal directions.

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

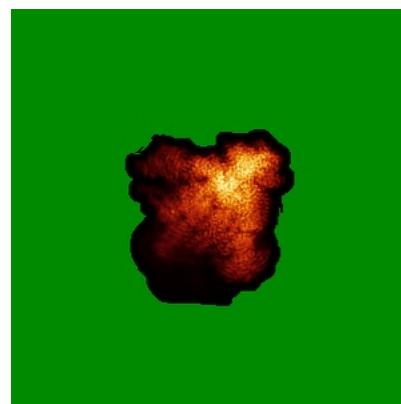
### 6.4.1 Primary map



X

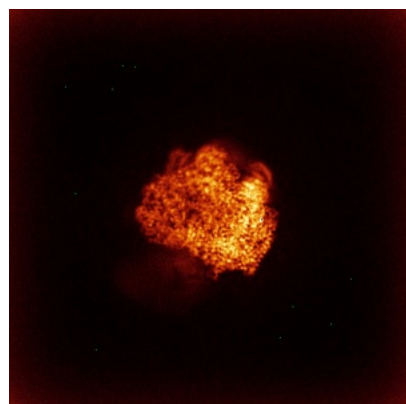


Y

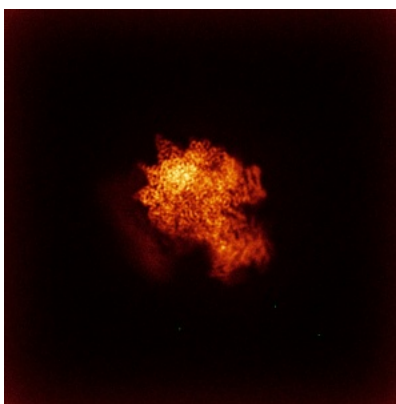


Z

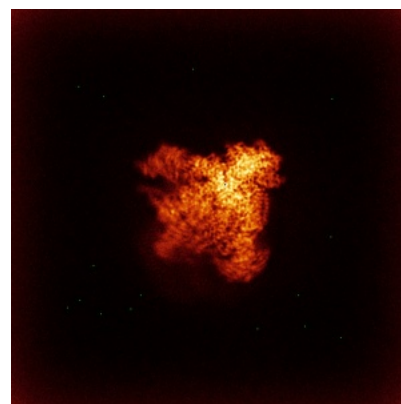
### 6.4.2 Raw map



X



Y

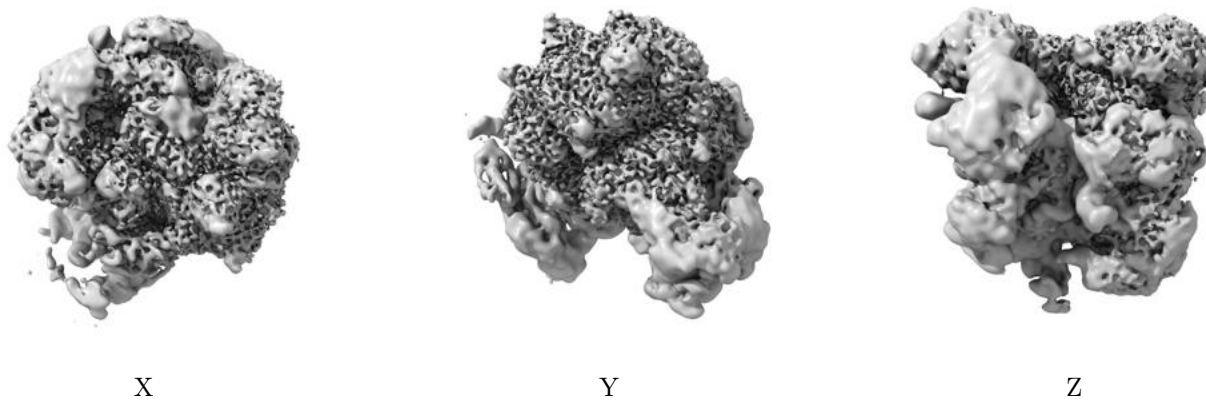


Z

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.

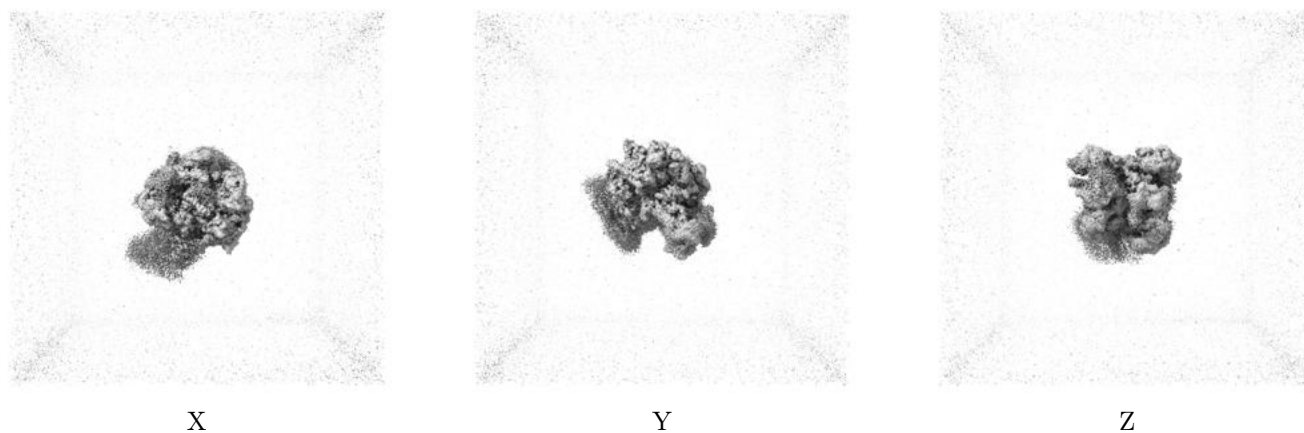
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.143. 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.

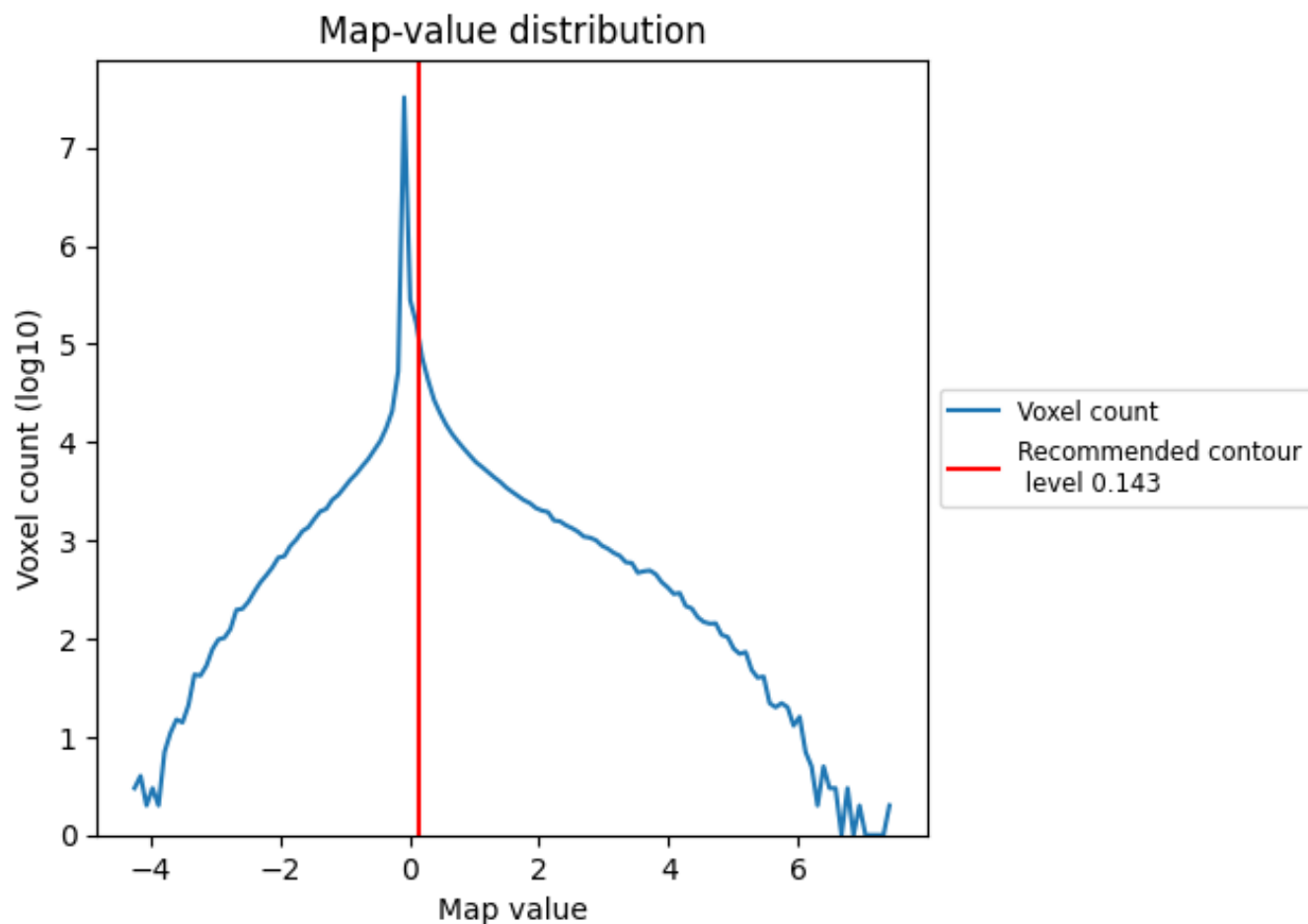
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

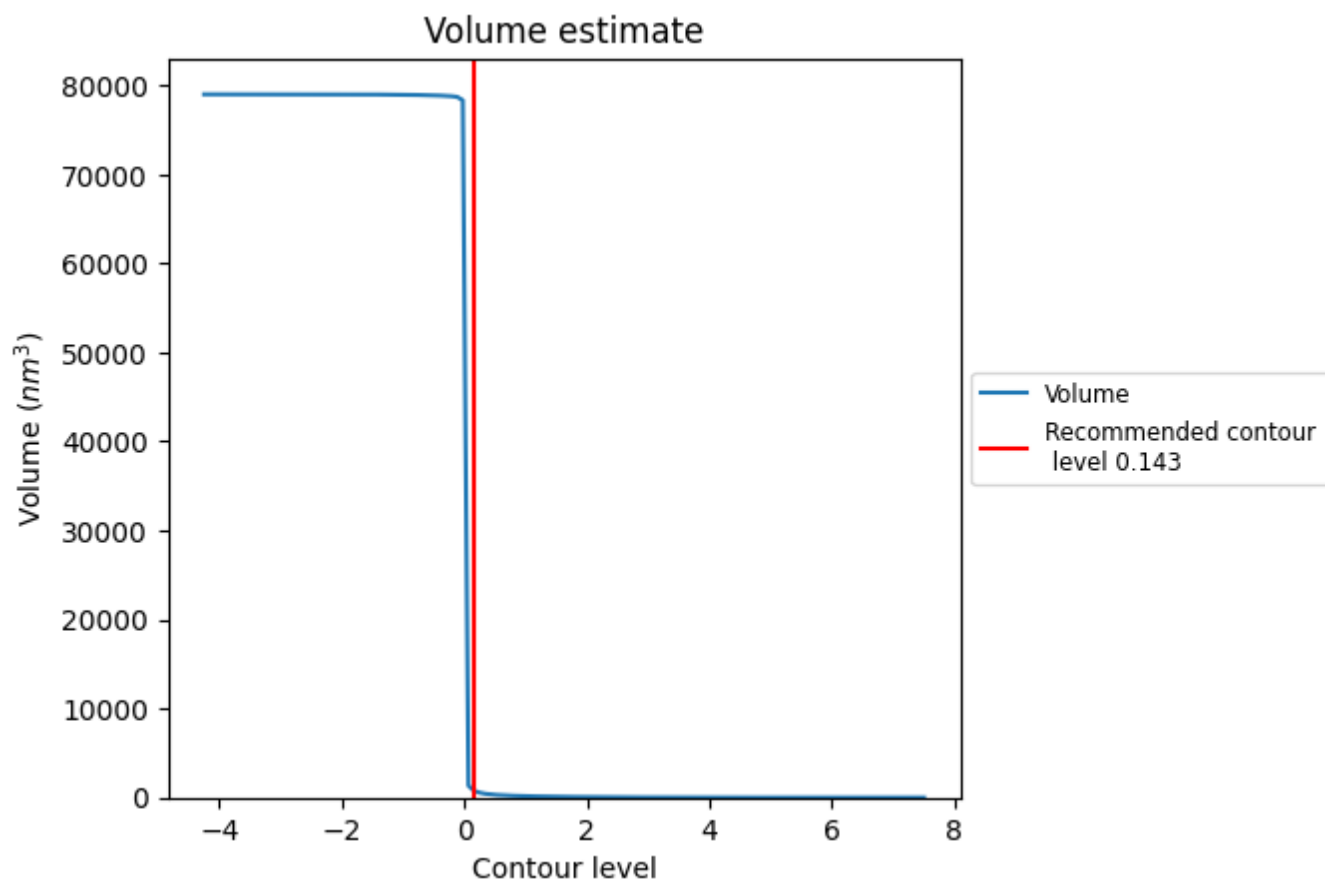
This section contains the results of statistical analysis of the map.

### 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.

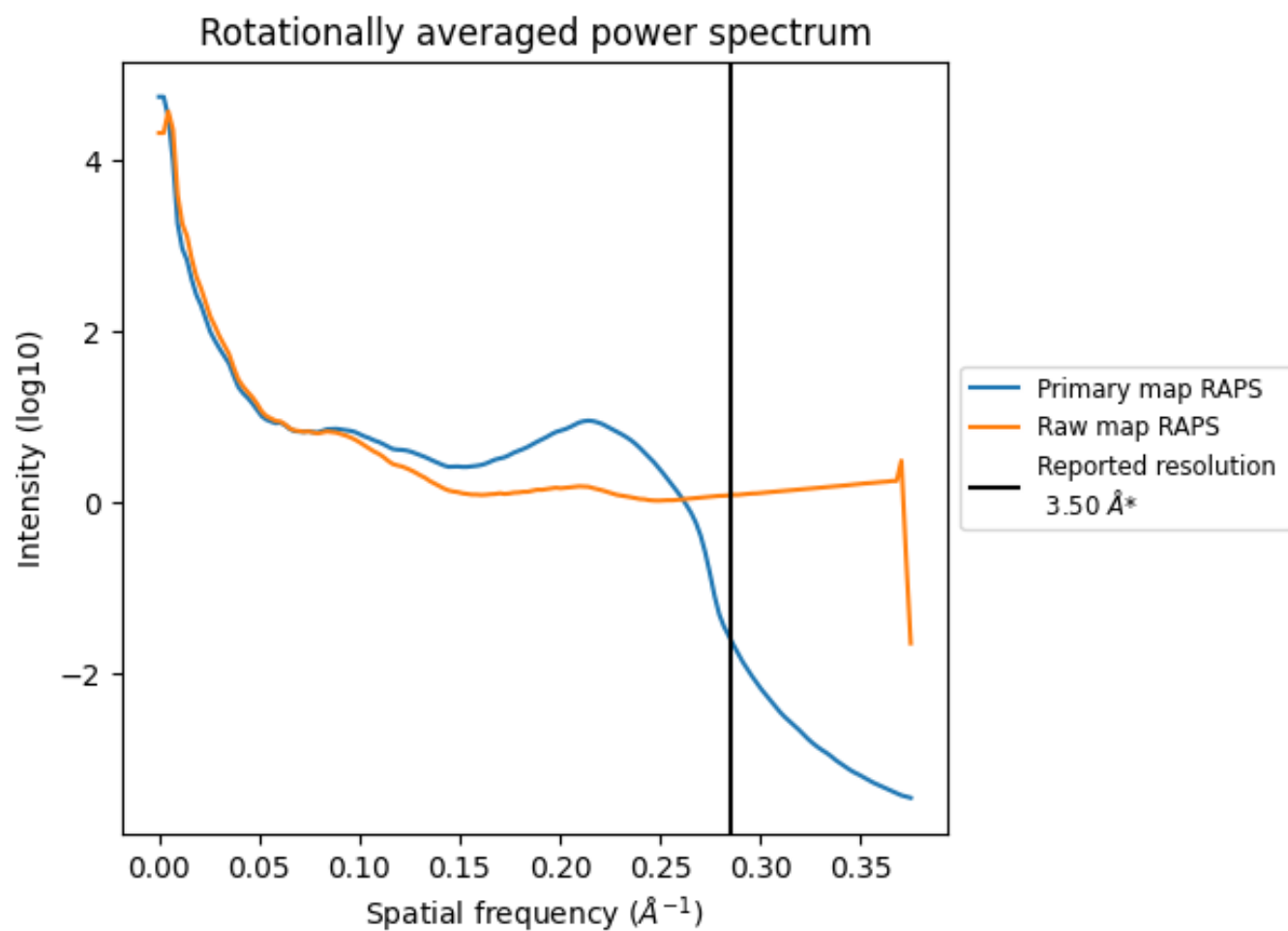
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 867  $\text{nm}^3$ ; this corresponds to an approximate mass of 783 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 ⓘ



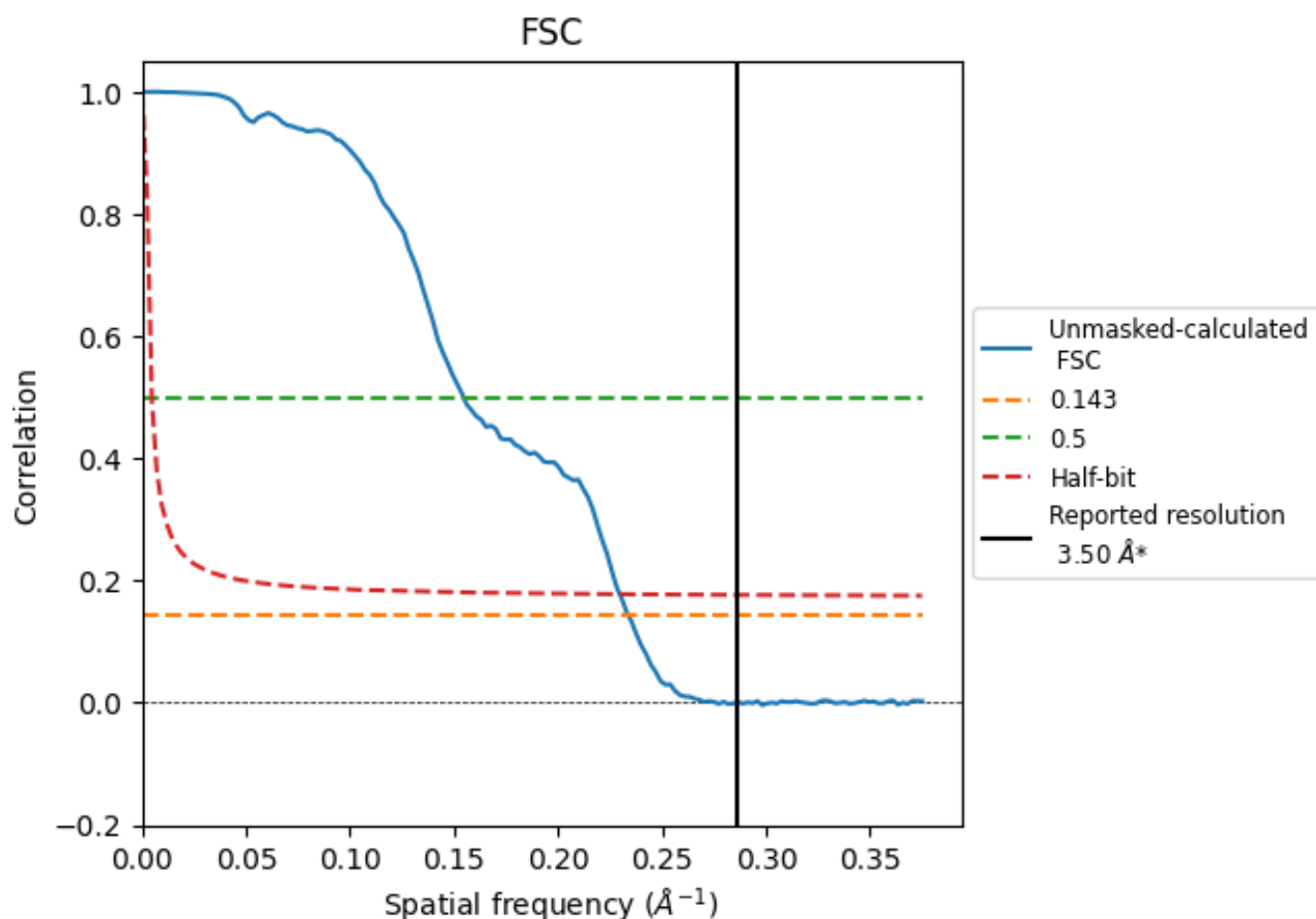
\*Reported resolution corresponds to spatial frequency of  $0.286 \text{ \AA}^{-1}$



## 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 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

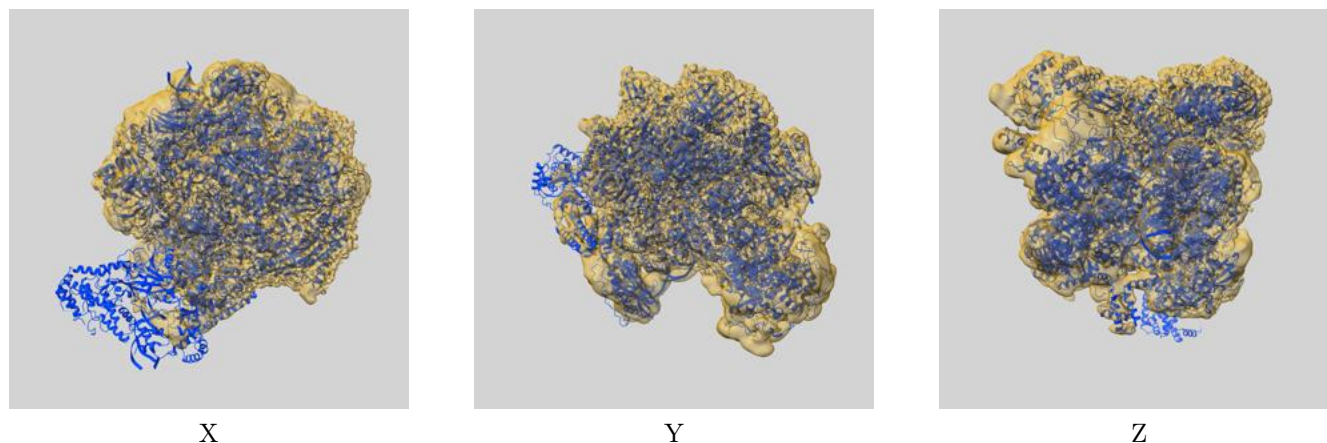
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	6.47	4.35

\*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 4.28 differs from the reported value 3.5 by more than 10 %

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

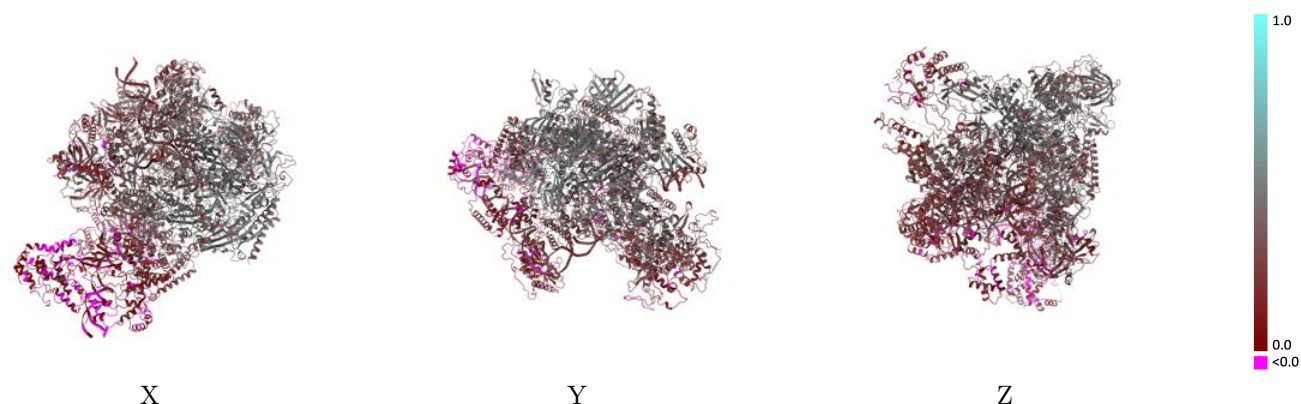
This section contains information regarding the fit between EMDB map EMD-62030 and PDB model 9K3V. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

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



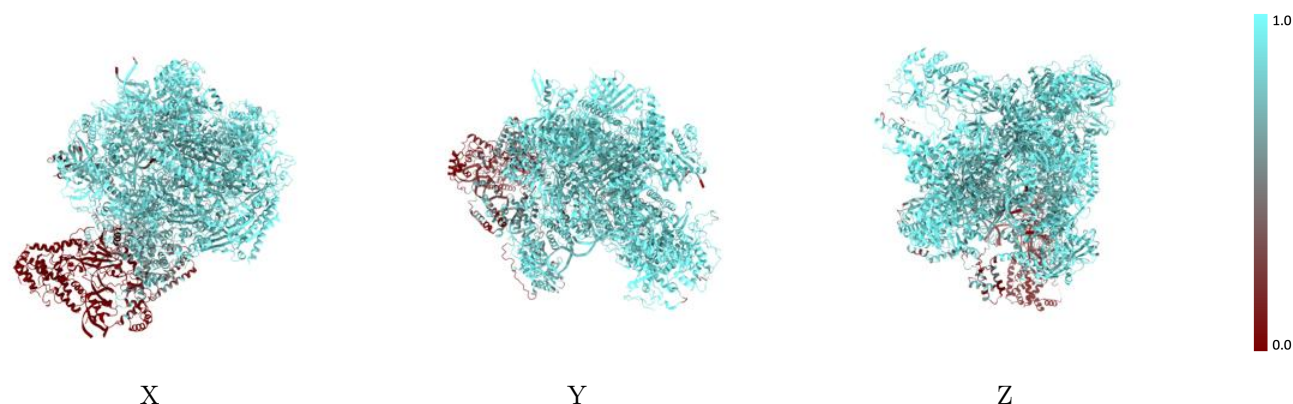
The images above show the 3D surface view of the map at the recommended contour level 0.143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



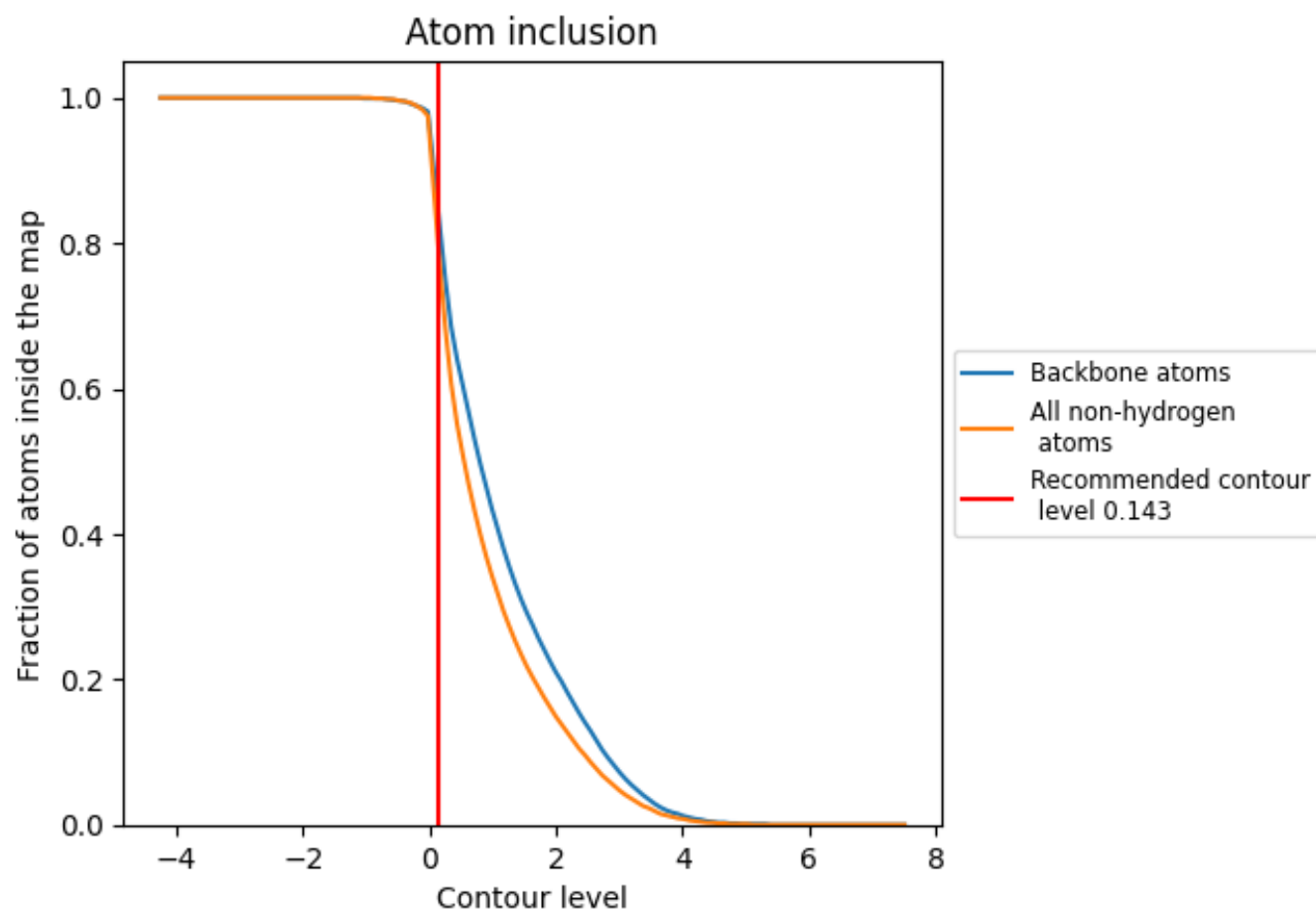
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.143).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.2960
1	 0.0000	 0.0370
3	 0.0520	 0.0420
4	 0.2230	 0.0680
A	 0.9190	 0.3960
B	 0.9150	 0.4150
C	 0.9320	 0.4460
D	 0.9560	 0.2300
E	 0.9500	 0.3520
F	 0.9360	 0.4430
G	 0.9390	 0.3150
H	 0.9270	 0.4290
I	 0.9450	 0.3450
J	 0.9200	 0.4250
K	 0.9180	 0.4290
L	 0.9460	 0.3930
M	 0.7730	 0.2580
N	 0.9060	 0.2350
O	 0.9380	 0.2960
P	 0.8340	 0.1930
Q	 0.9520	 0.2890
U	 0.8730	 0.1280
V	 0.7560	 0.2110
W	 0.7450	 0.1060
X	 0.6580	 0.1440
Y	 0.7120	 0.1830
Z	 0.7190	 0.2930

