



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 10:22 PM 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

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
Mogul : 1.8.5 (274361), 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) : 2.50

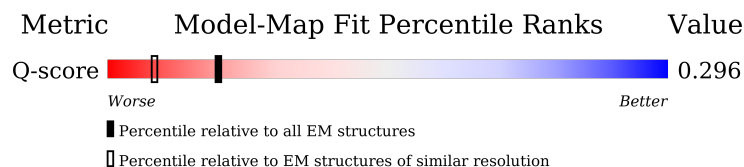
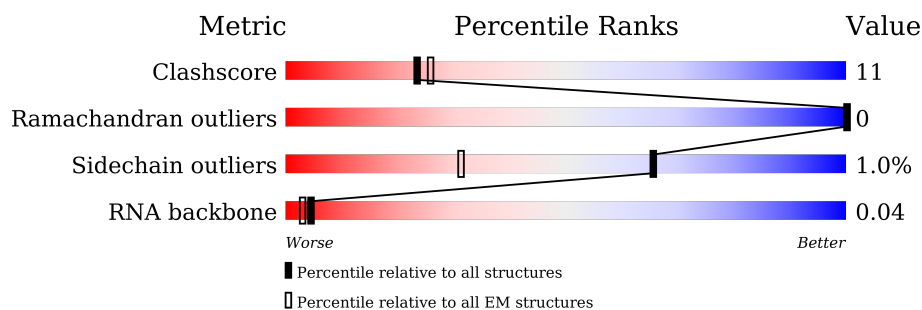
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



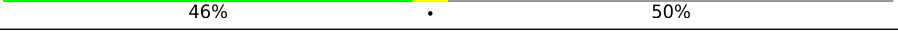
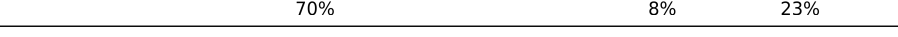
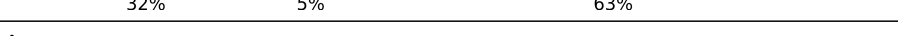
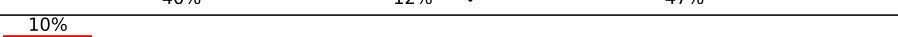
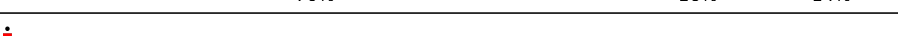
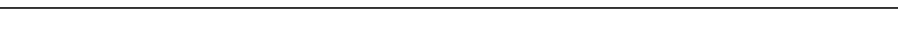
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	1	368	
2	3	411	
3	4	1469	

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Mol	Chain	Length	Quality of chain
4	A	1390	
5	B	1133	
6	C	346	
7	D	148	
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).

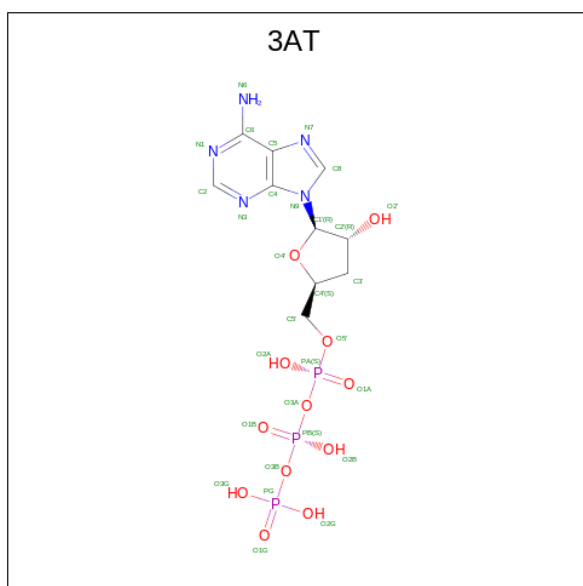
Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Zn	0
			2	2	
27	B	1	Total	Zn	0
			1	1	
27	I	1	Total	Zn	0
			1	1	

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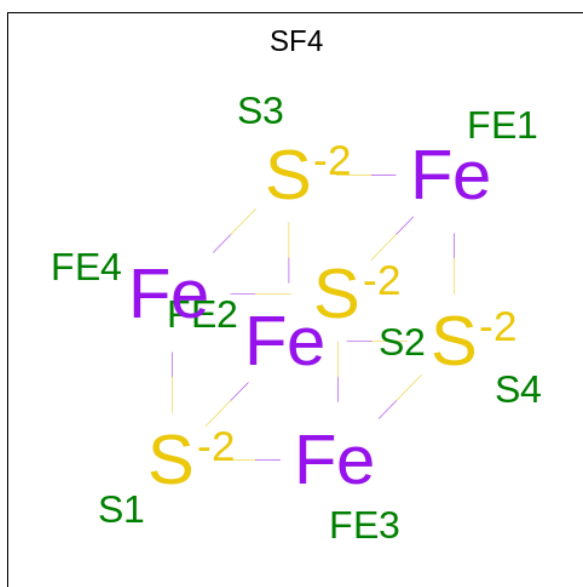
Mol	Chain	Residues	Atoms		AltConf
27	J	1	Total	Zn	0
			1	1	
27	L	1	Total	Zn	0
			1	1	
27	V	1	Total	Zn	0
			1	1	

- 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).

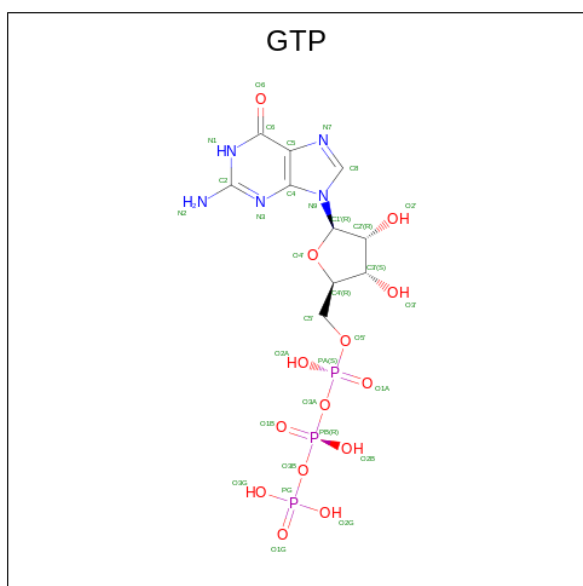


Mol	Chain	Residues	Atoms			AltConf
29	P	1	Total	Fe	S	0
			8	4	4	

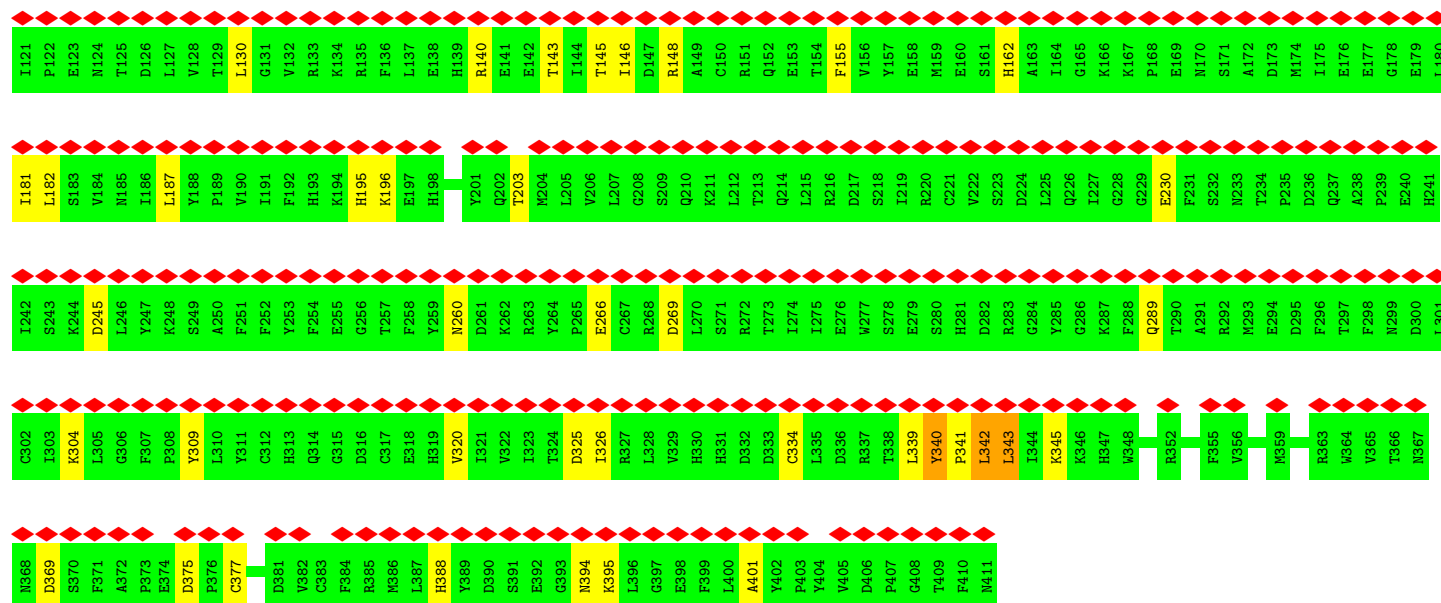
- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

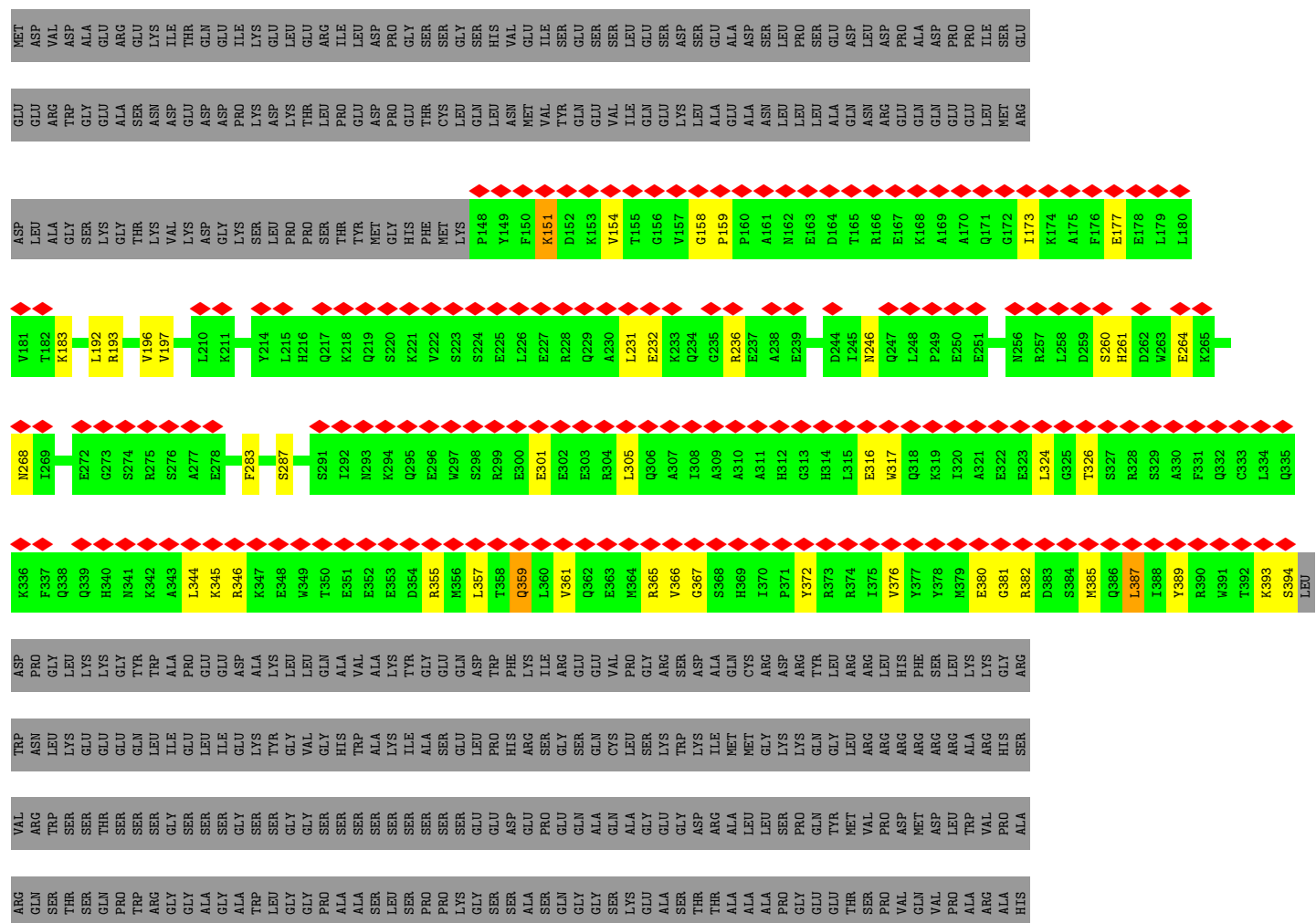
- Molecule 31 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

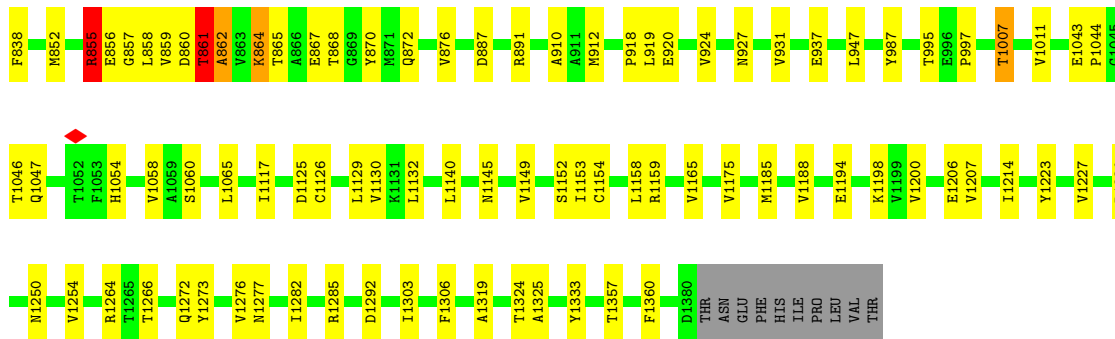


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
31	Z	1	32	10	5	14	3	0



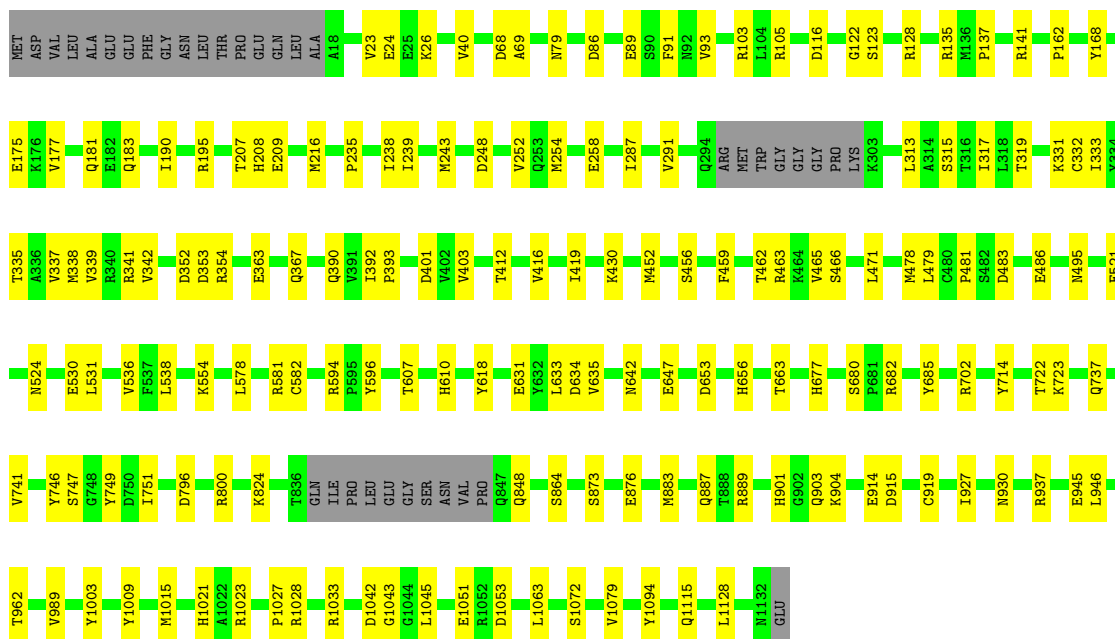
• Molecule 3: snRNA-activating protein complex subunit 4





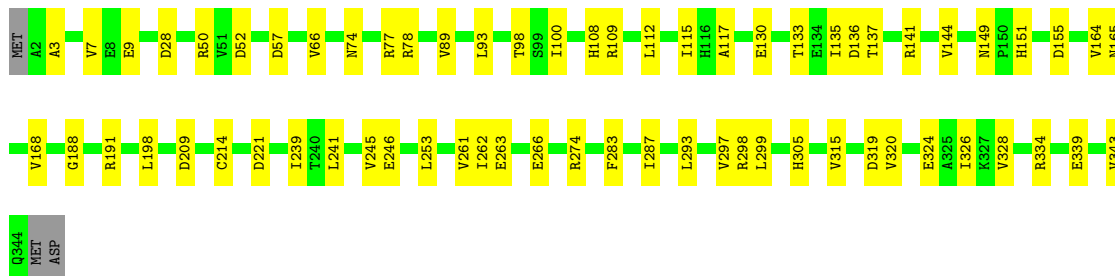
• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

Chain B: 82% 14%



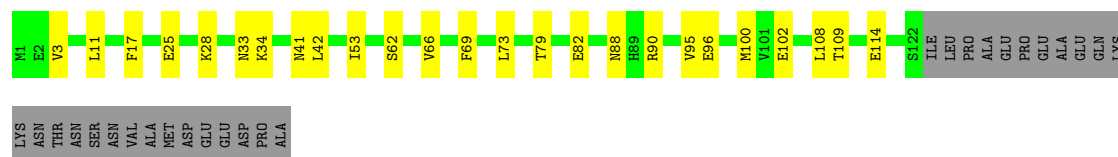
• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 80% 19%



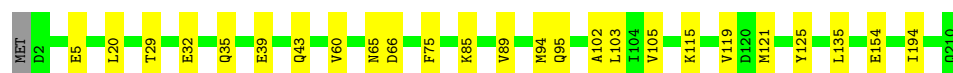
• Molecule 7: DNA-directed RNA polymerase III subunit RPC9

Chain D: 66% 17% 18%



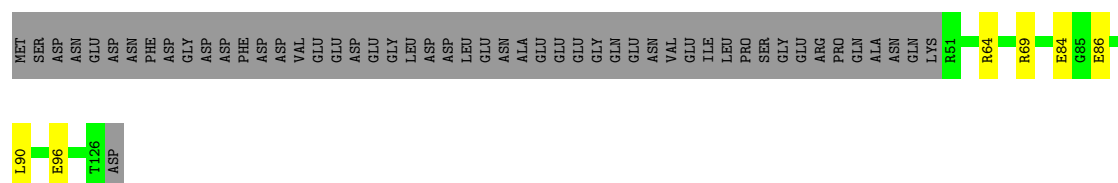
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 88% 12%



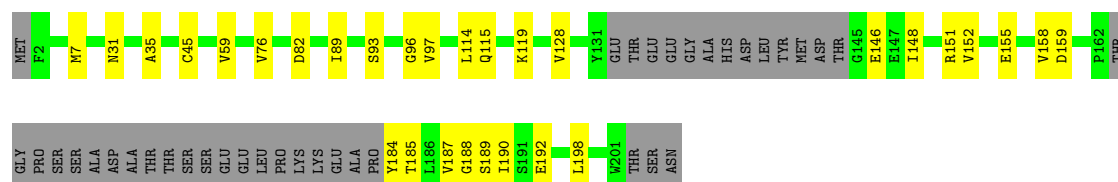
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 55% 5% 40%



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

Chain G: 67% 15% 19%



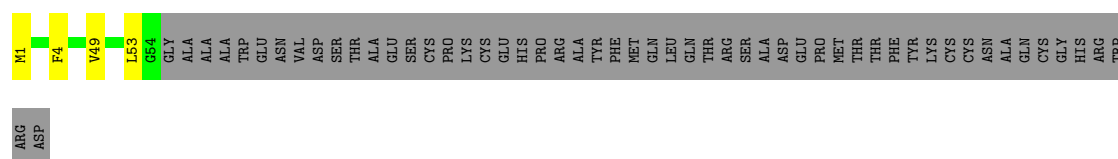
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

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

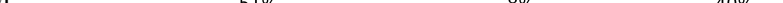
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- Chain K: 70% 8% 23%

MET	GLU	GLU	ASP	GLU	GLU	LEU	GLU	ARG	ARG	LYS	SER	GLY	LEU	LYS	THR	SER	MET	ALA	GLU	GLY	ARG	K24	E28	A33	I55	I59	M60	K61	M62	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: 

MET				D6	V9	V10	Q11	L17	A18	S36	M37	K50	Q53	V56	L77	V81	Y92	S104	Q134	L135	R136	A158	G159	D160	S161	S162	O163	D164	E165	A166	E167	D168	D169	V170	K171	Q172	I173	T174	V175	R176	F177	R186	V190
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E347	0.000000	Red	LVS
V348	0.000000	Red	GLU
R351	0.000000	Green	THR
G352	0.000000	Green	MET
R353	0.000000	Green	PRO
D354	0.000000	Red	LVS
F355	0.000000	Green	GLU
V356	0.000000	Green	THR
F360	0.000000	Green	MET
S363	0.000000	Red	PRO
V367	0.000000	Green	LVS
E370	0.000000	Green	GLU
V371	0.000000	Green	THR
V374	0.000000	Green	MET
D381	0.000000	Red	PRO
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E399	0.000000	Green	LVS
F400	0.000000	Green	GLU
I401	0.000000	Green	THR
D405	0.000000	Red	LVS
G406	0.000000	Red	VAL
I409	0.000000	Red	VAL
H412	0.000000	Green	LVS
V416	0.000000	Green	GLU
Q419	0.000000	Green	THR
K429	0.000000	Green	MET
K432	0.000000	Red	PRO
V433	0.000000	Green	LVS
L436	0.000000	Red	VAL

LYS PRO PRO ASP ALA GLN SER GLY PRO PRO ALA ALA LEU VAL CYS GLY ASP GLN ARG ARG ILE GLN VAL ALA ALA LYS THR THR LYS ALA LEU LEU GLU GLU LEU GLN ARG ARG LYS LYS GLN LEU VAL VAL PRO PRO PRO GLY VAL VAL ILE LYS VAL PRO PRO VAL VAL

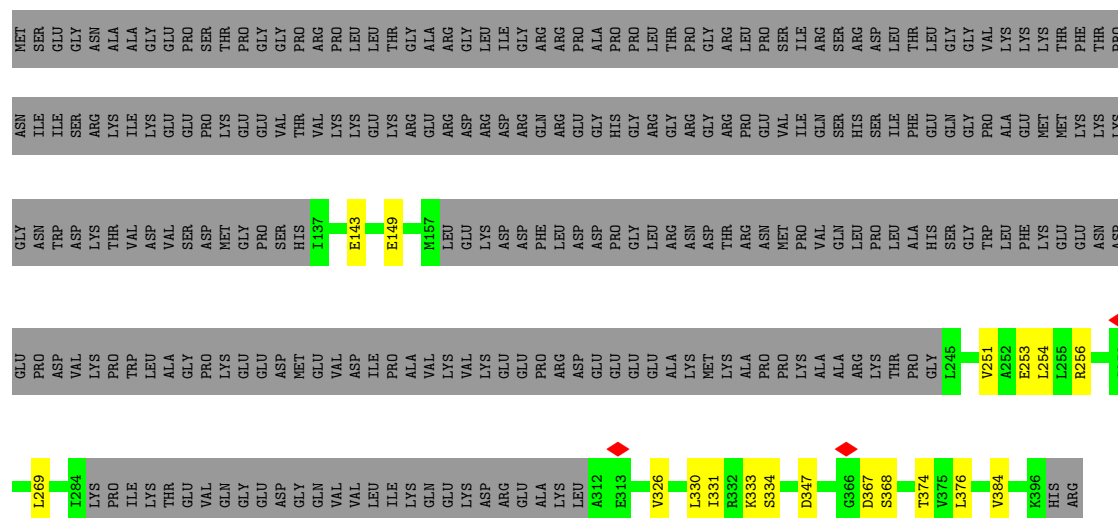
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ALA PHE VAL GLU ALA THR PHE GLN ARG GLN PHE VAL LEU THR LEU LEU LEU LEU LEU LYS ARG LEU LEU ALA SER LEU SER PRO PRO GLY HIS THR THR PHE SER SER GLY ILE SER ASP ARG MET LEU GLN ASP THR VAL LEU LEU ALA ALA GLY CYS LYS GLN ILE LEU VAL VAL PRO PHE

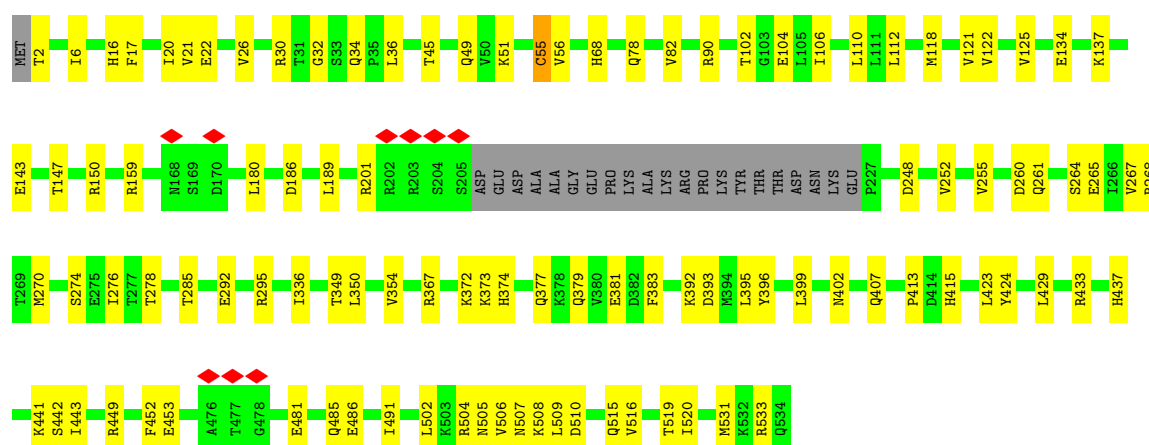
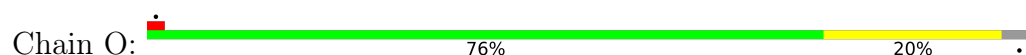
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GLU VAL ASP LYS VAL LEU LYS ASP CYS CYS VAL SER TYR GLY GLY MET TRP TYR LEU LYS GLY THR VAL GLN SER

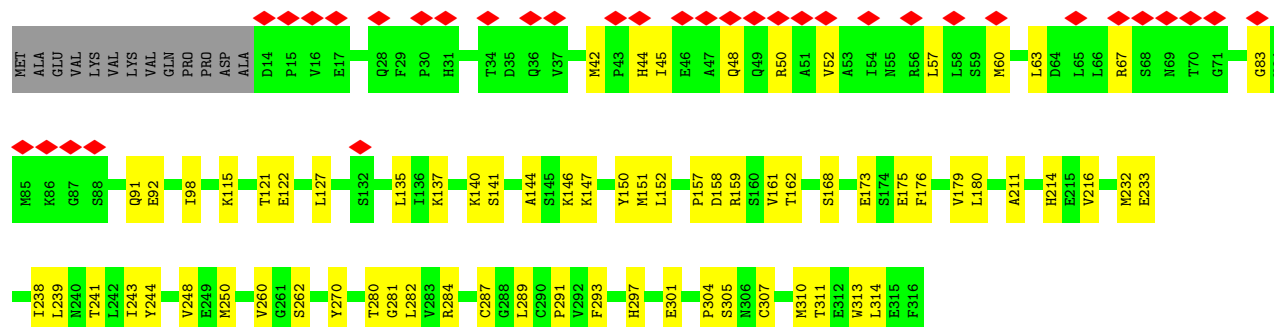
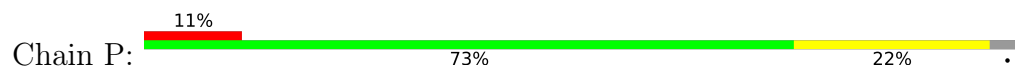
- Chain N: 32% 5% 63%



• 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









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 [i](#)

5.1 Standard geometry [i](#)

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

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%)	10	34
2	3	330/356 (93%)	317 (96%)	13 (4%)	28	54
3	4	221/1213 (18%)	217 (98%)	4 (2%)	51	69
4	A	1200/1212 (99%)	1191 (99%)	9 (1%)	73	77
5	B	959/988 (97%)	958 (100%)	1 (0%)	88	87
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%)	76	78
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%)	87	85
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%)	28	54
22	V	325/365 (89%)	316 (97%)	9 (3%)	38	61
23	W	102/2381 (4%)	98 (96%)	4 (4%)	28	54
All	All	5923/10438 (57%)	5864 (99%)	59 (1%)	65	75

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	-	27,32,32	1.36	4 (14%)	38,50,50	2.16	11 (28%)
31	GTP	Z	102	-	30,34,34	1.07	1 (3%)	46,54,54	2.58	13 (28%)
29	SF4	P	401	19	0,12,12	-	-	-		

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
28	3AT	B	1202	-	-	8/22/34/34	0/3/3/3
31	GTP	Z	102	-	-	2/22/38/38	0/3/3/3
29	SF4	P	401	19	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	1202	3AT	C5-C4	4.58	1.47	1.39
31	Z	102	GTP	C3'-C4'	3.71	1.62	1.53
28	B	1202	3AT	C5-C6	2.72	1.48	1.41
28	B	1202	3AT	C8-N7	2.40	1.36	1.31
28	B	1202	3AT	C5-N7	-2.07	1.35	1.39

The worst 5 of 24 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	C5-C4-N3	-6.20	118.66	126.75
31	Z	102	GTP	C5-C4-N3	-5.43	119.66	128.46

There are no chirality outliers.

5 of 10 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'

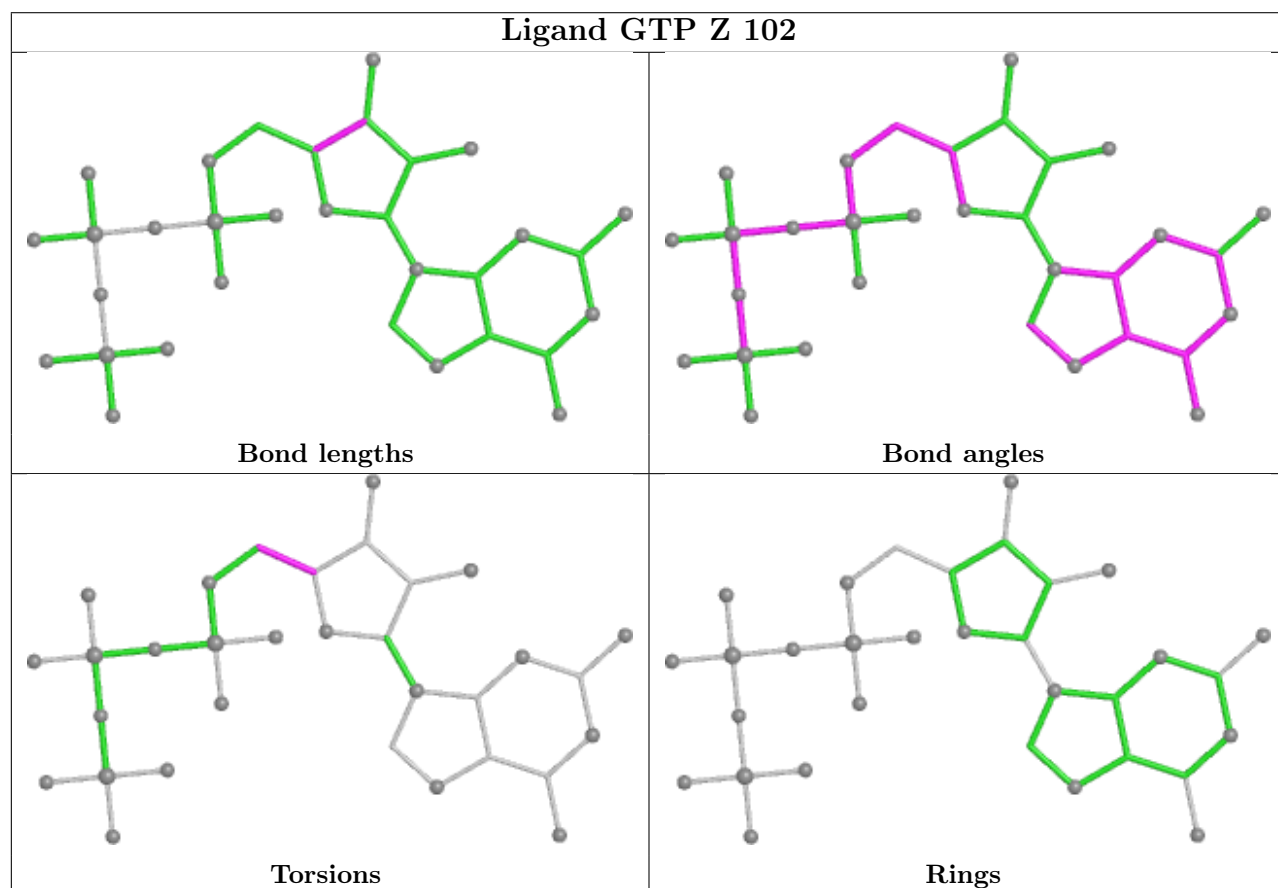
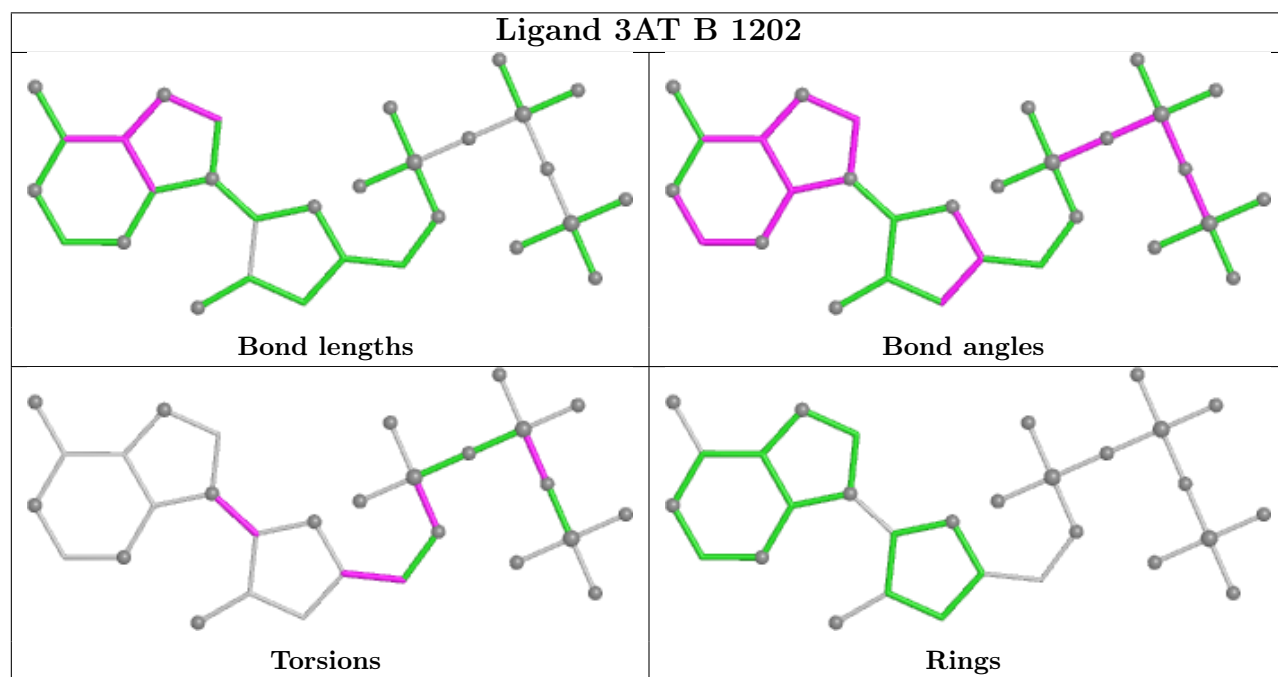
There are no ring outliers.

3 monomers are involved in 27 short contacts:

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

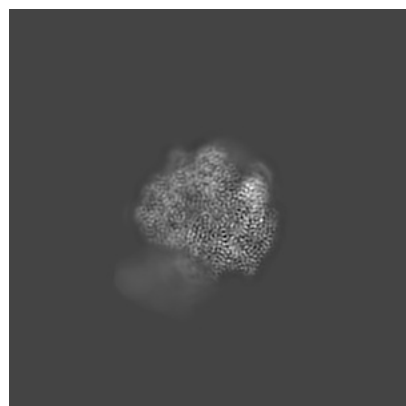
6 Map visualisation [i](#)

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.

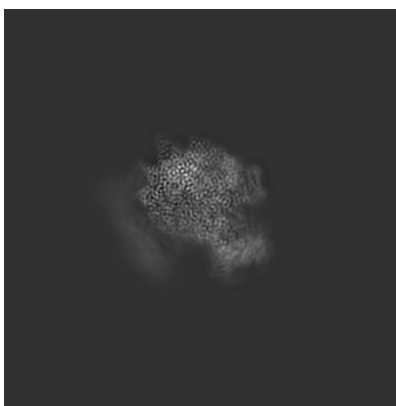
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

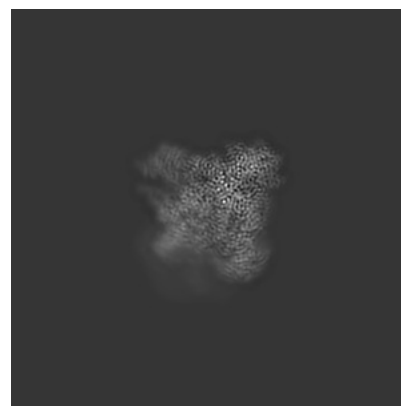
6.1.1 Primary map



X

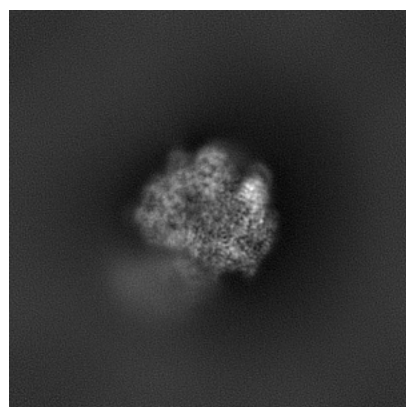


Y

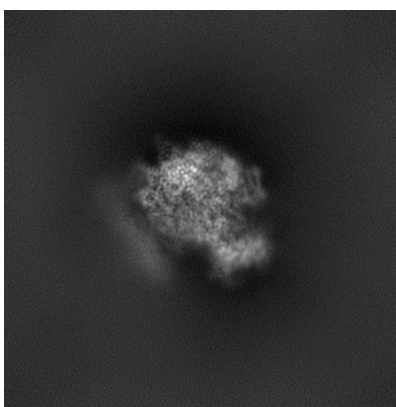


Z

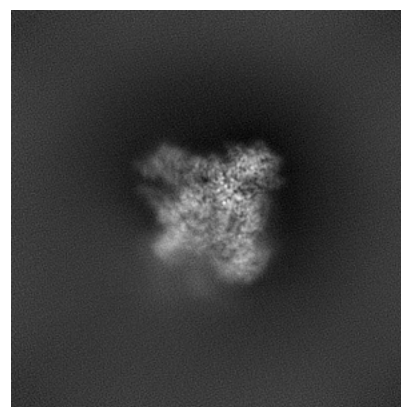
6.1.2 Raw map



X



Y

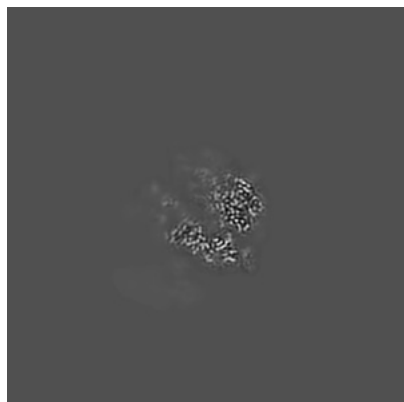


Z

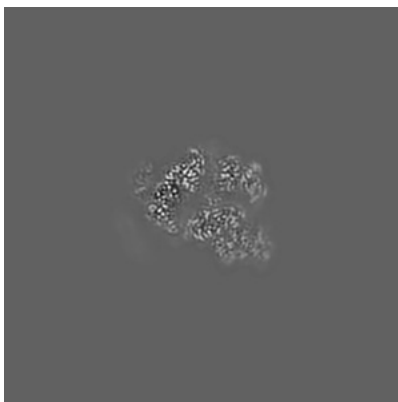
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

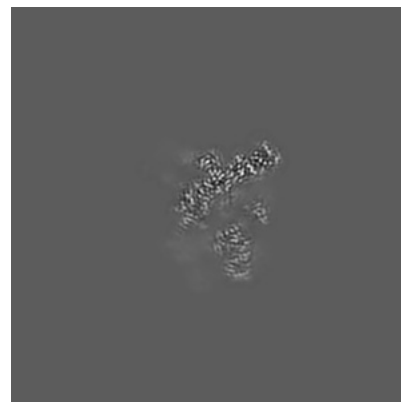
6.2.1 Primary map



X Index: 161



Y Index: 161

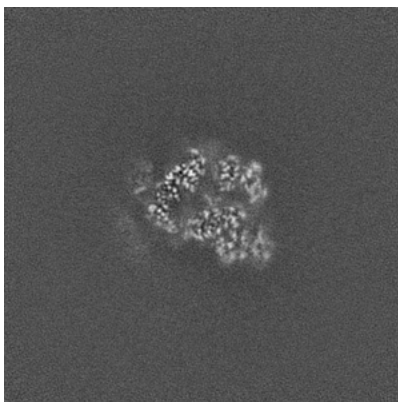


Z Index: 161

6.2.2 Raw map



X Index: 161



Y Index: 161

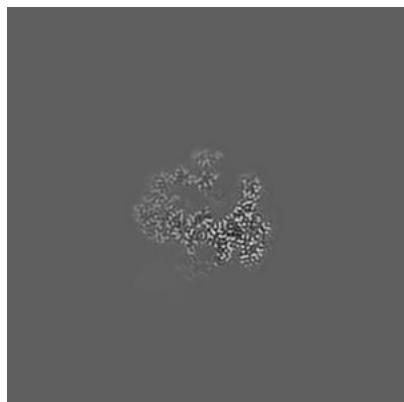


Z Index: 161

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

6.3 Largest variance slices [i](#)

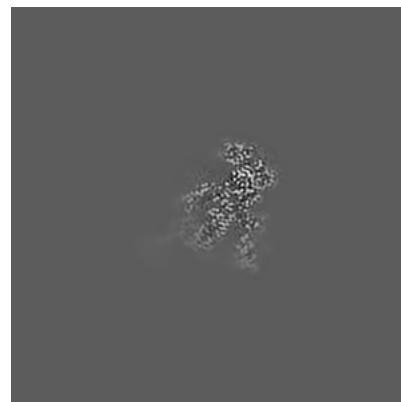
6.3.1 Primary map



X Index: 189

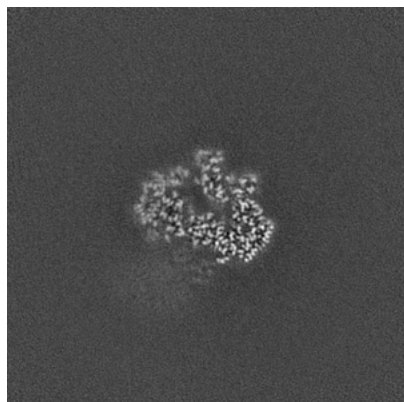


Y Index: 190

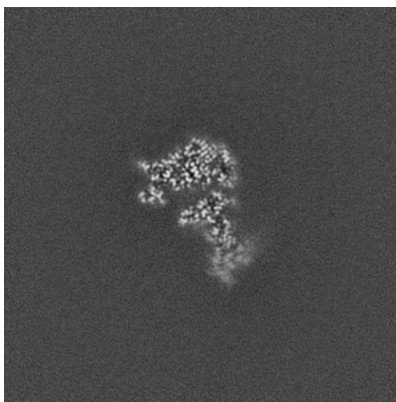


Z Index: 136

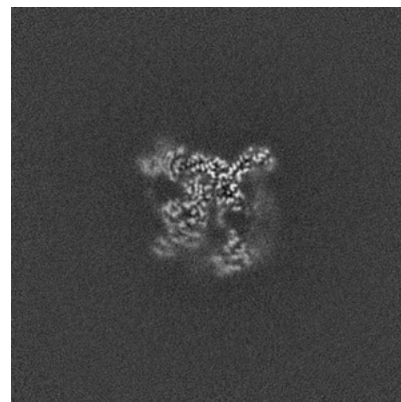
6.3.2 Raw map



X Index: 183



Y Index: 196

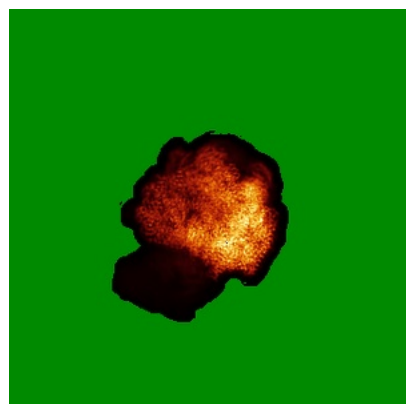


Z Index: 173

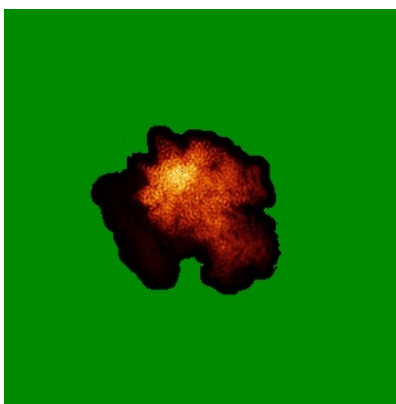
The images above show the largest variance slices of the map in three orthogonal directions.

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

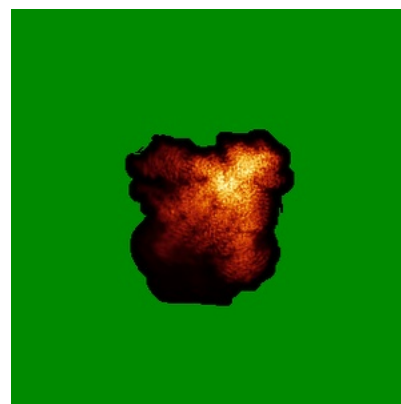
6.4.1 Primary map



X

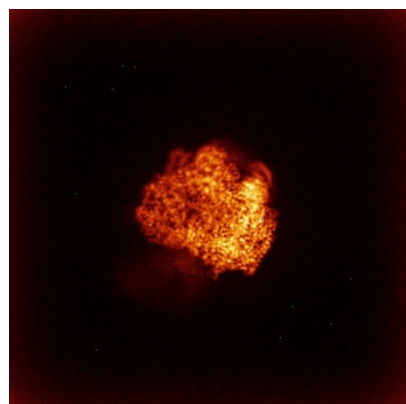


Y

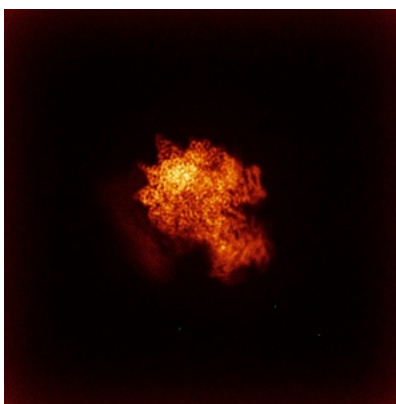


Z

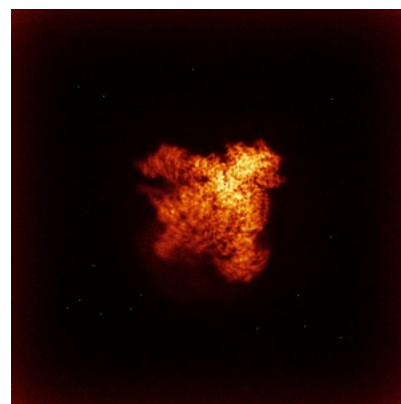
6.4.2 Raw map



X



Y

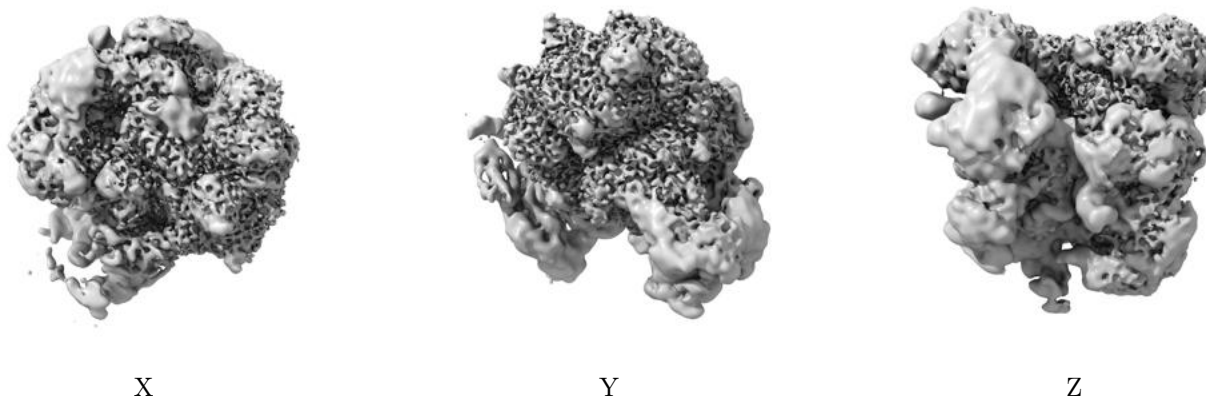


Z

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.

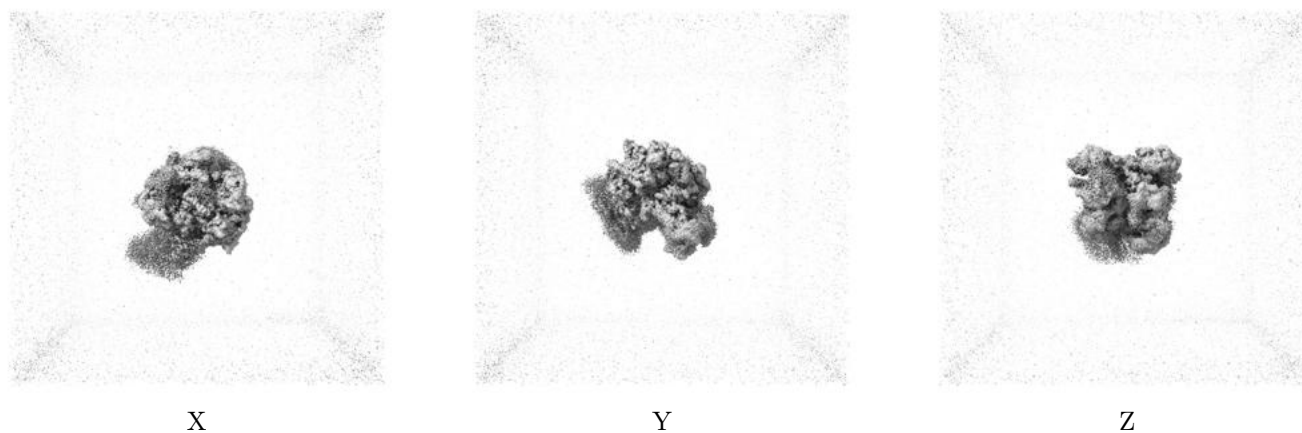
6.5 Orthogonal surface views [i](#)

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.

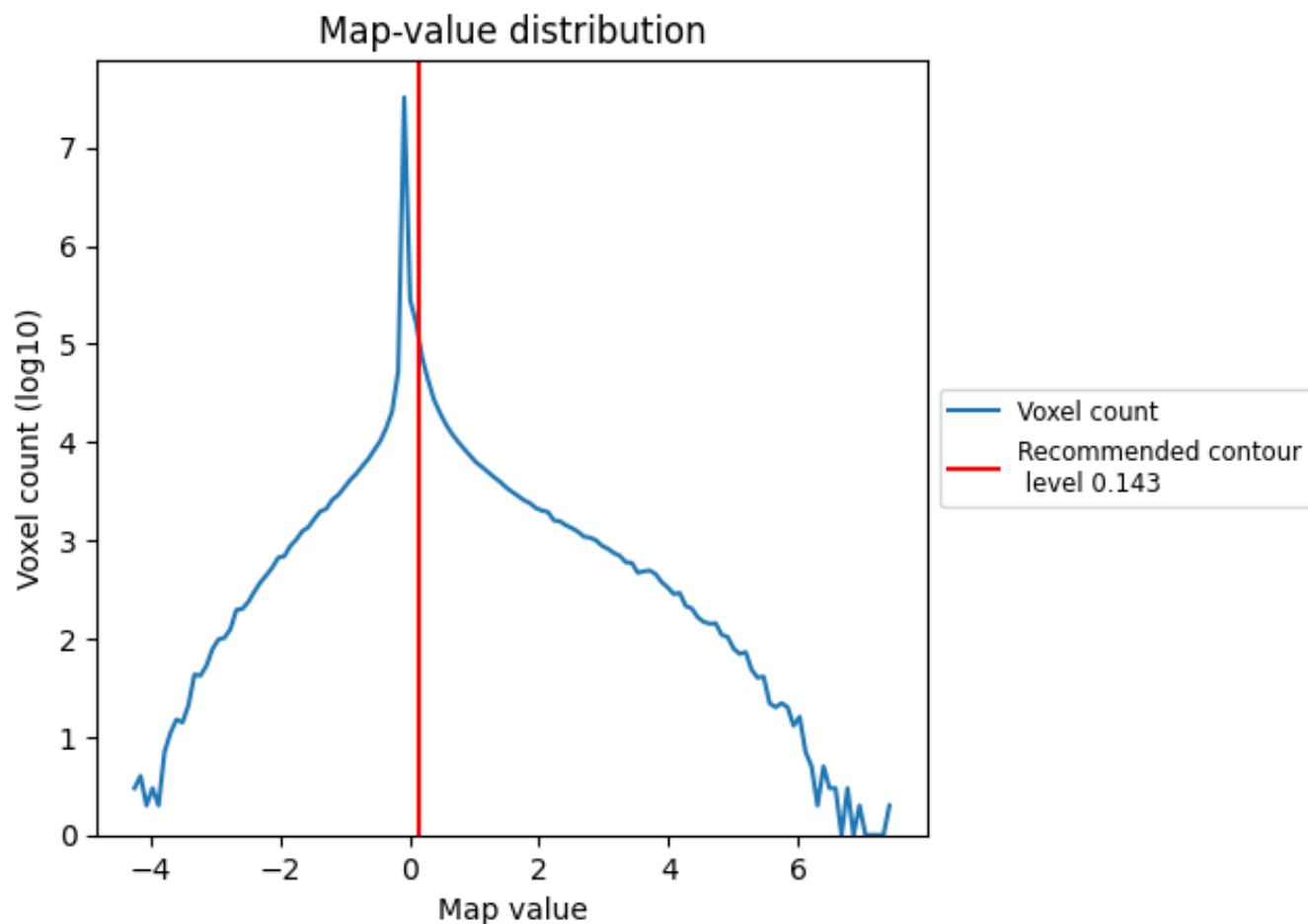
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

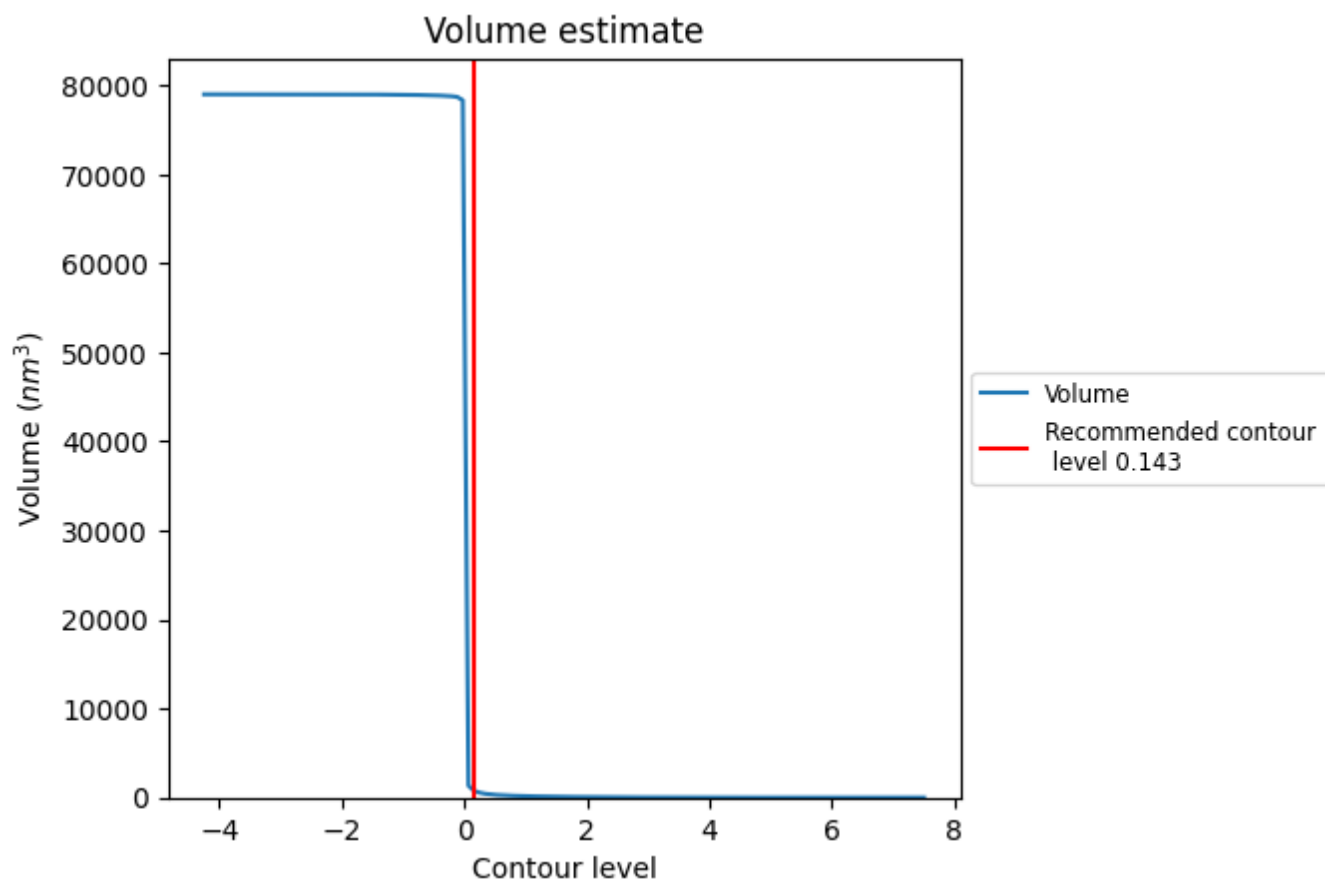
This section contains the results of statistical analysis of the map.

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.

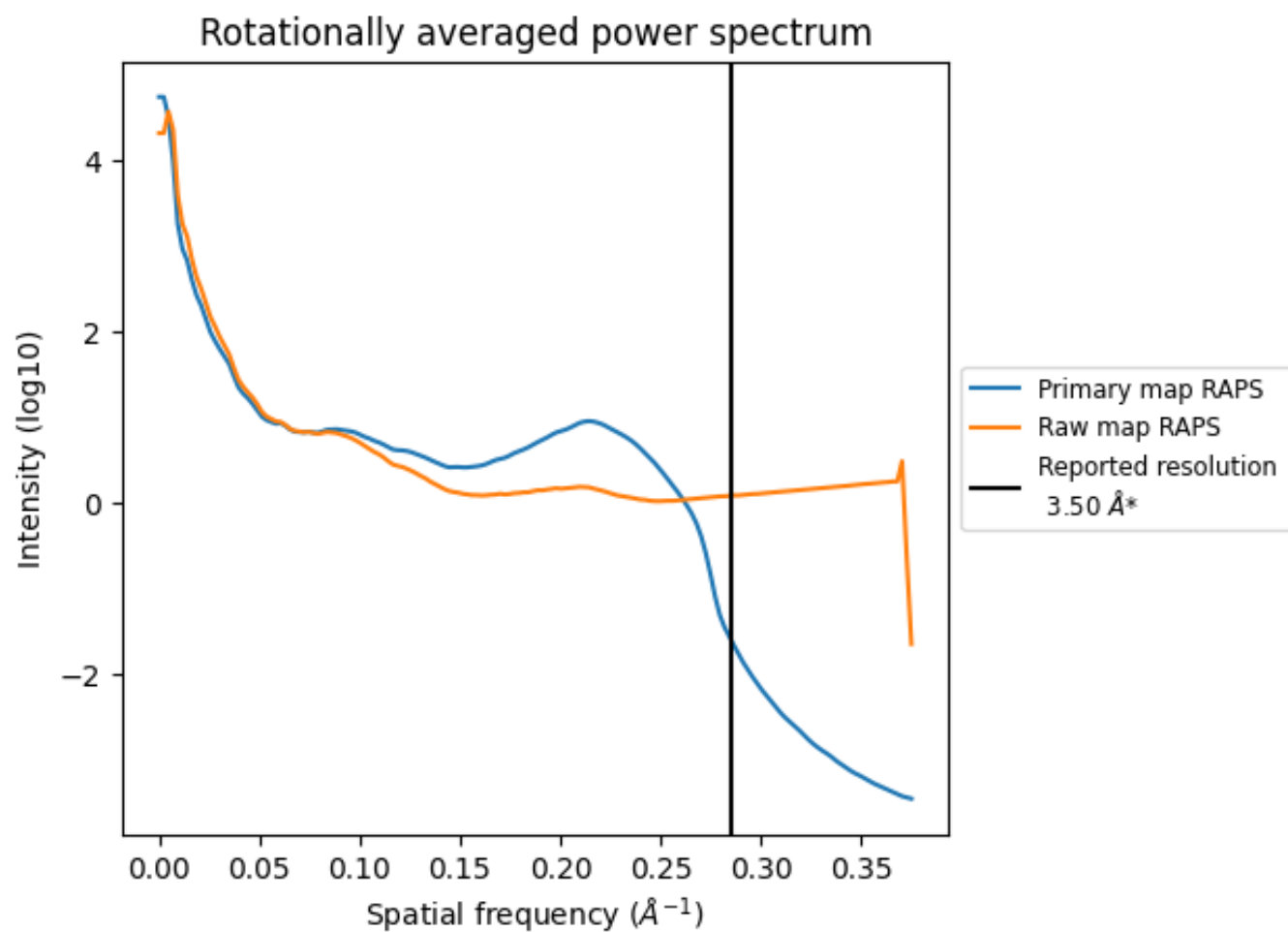
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 867 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 ⓘ

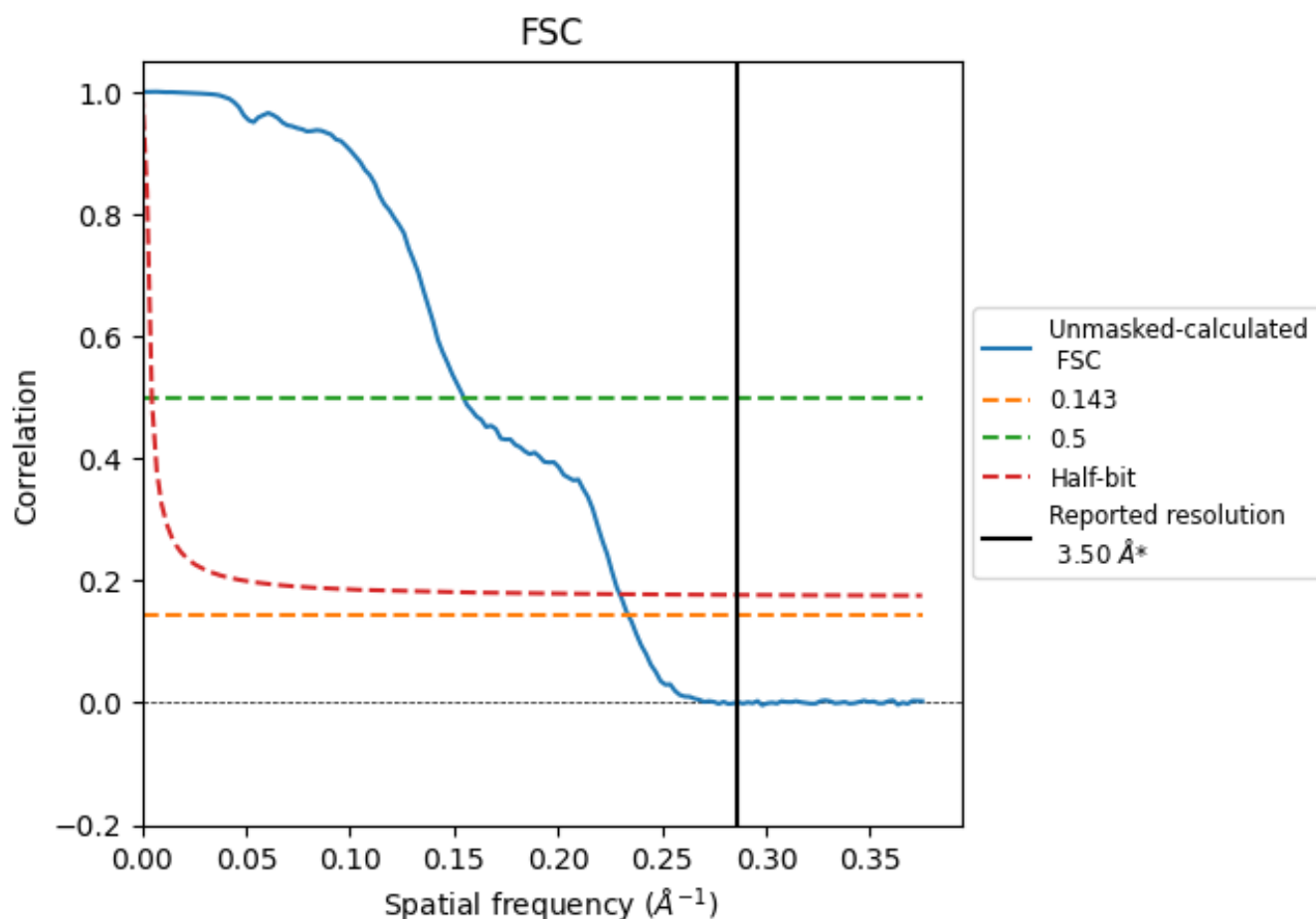


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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⁻¹

8.2 Resolution estimates [i](#)

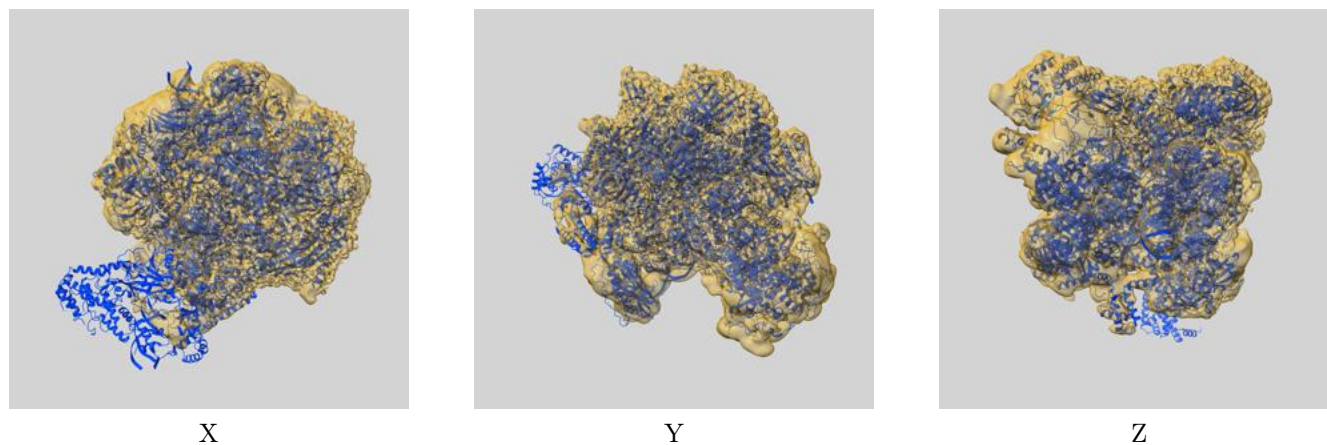
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	6.47	4.35

*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](#)

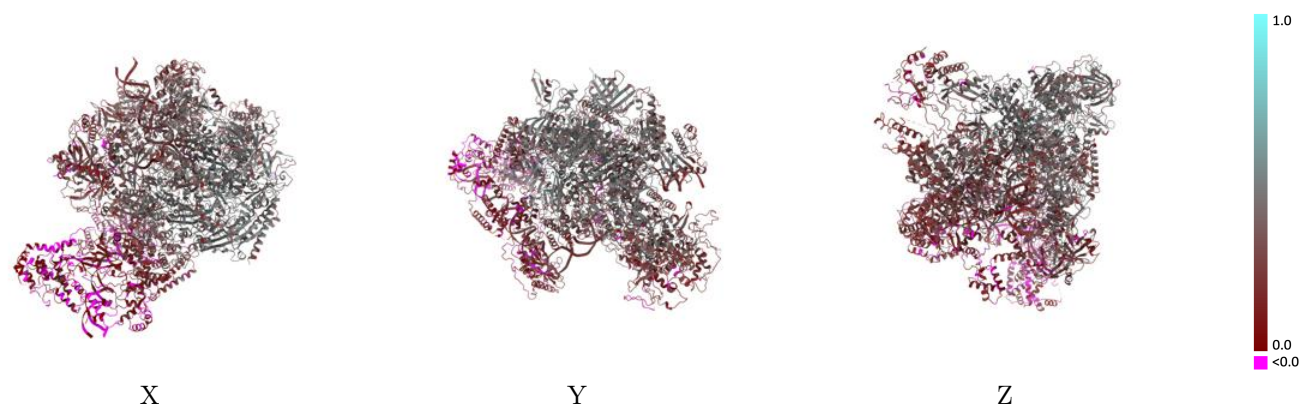
This section contains information regarding the fit between EMDB map EMD-62030 and PDB model 9K3V. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



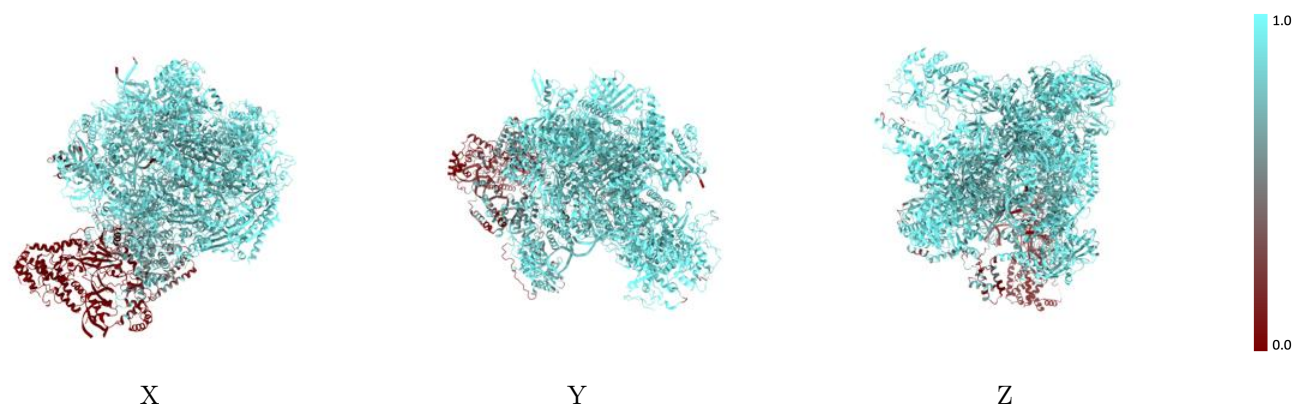
The images above show the 3D surface view of the map at the recommended contour level 0.143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



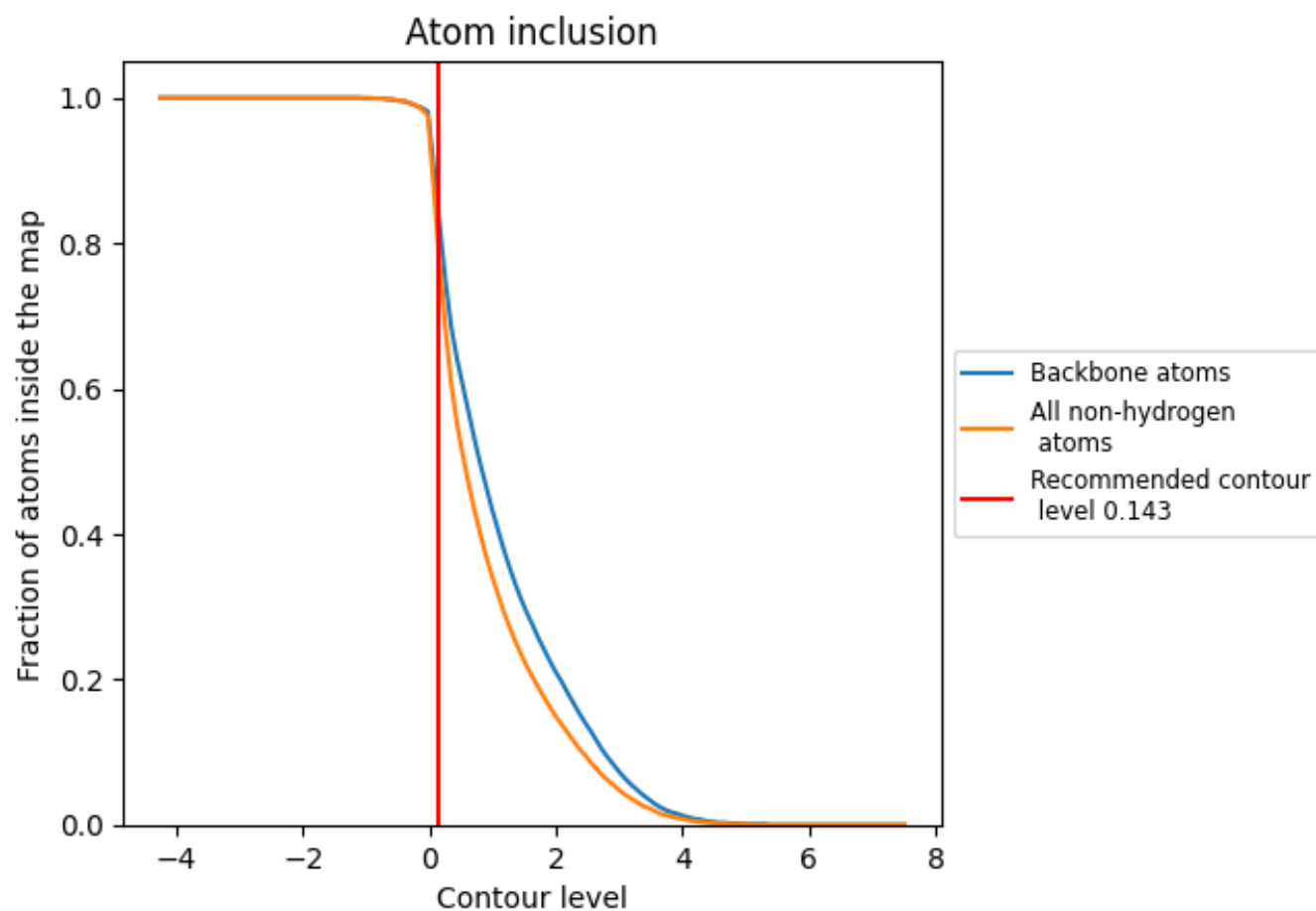
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

