



wwPDB EM Validation Summary Report ⓘ

Apr 10, 2025 – 12:33 PM JST

PDB ID : 9K2G / pdb_00009k2g
EMDB ID : EMD-61994
Title : Human RNA Polymerase III de novo transcribing complex 13 (TC13)
Authors : Wang, Q.; Ren, Y.; Jin, Q.; Chen, X.; Xu, Y.
Deposited on : 2024-10-17
Resolution : 3.00 Å(reported)

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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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
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) : 2.42

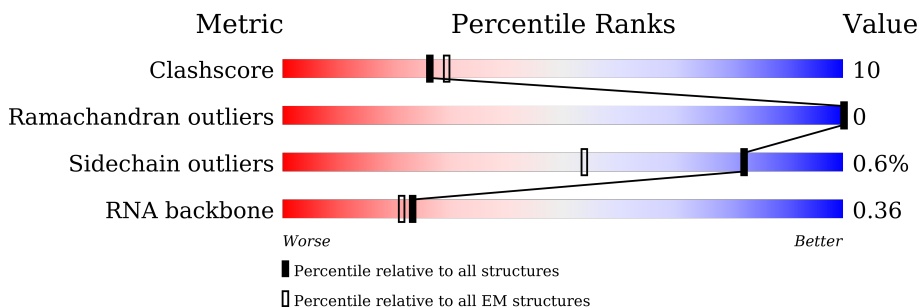
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1390	 79% 20% .
2	B	1133	 77% 20% ..
3	C	346	 81% 18% .
4	D	148	 63% 20% 18%
5	E	210	 80% 19%
6	F	127	 49% 11% 40%
7	G	204	 55% 26% 19%

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	108	
10	J	67	
11	K	133	
12	L	58	
13	M	708	
14	N	398	
15	O	534	
16	P	316	
17	Q	223	
18	V	419	
19	X	104	
20	Y	104	
21	Z	10	

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
24	3AT	B	1202	-	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 44605 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase III subunit RPC1.

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

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1105	Total	C	N	O	S	0	0
			8741	5538	1529	1605	69		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

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

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

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

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

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

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

- Molecule 18 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	34	Total	C	N	O	S	0	0
			246	144	41	56	5		

- Molecule 19 is a DNA chain called DNA (104-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	51	Total	C	N	O	P	0	0
			1051	499	206	295	51		

- Molecule 20 is a DNA chain called DNA (104-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	51	Total	C	N	O	P	0	0
			1040	499	173	317	51		

- Molecule 21 is a RNA chain called RNA (5'-R(P*CP*UP*CP*GP*CP*UP*UP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	10	Total	C	N	O	P	0	0
			209	93	33	73	10		

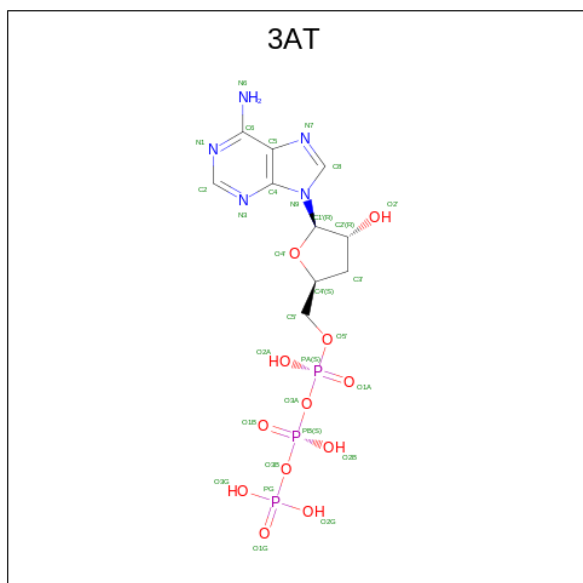
- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

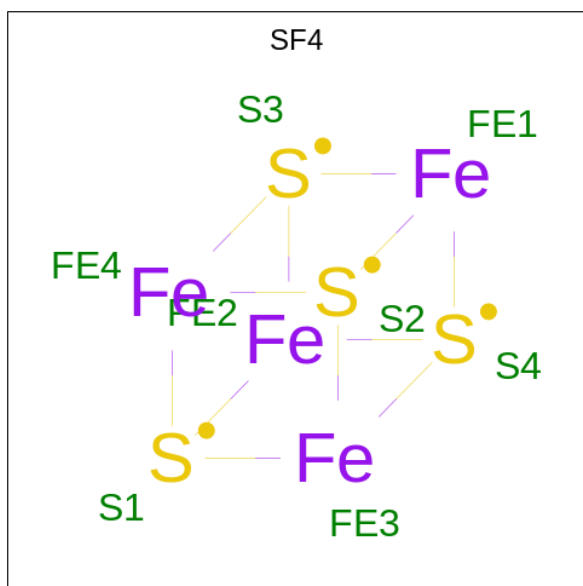
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Mg	0
			1	1	

- Molecule 24 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃).



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

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

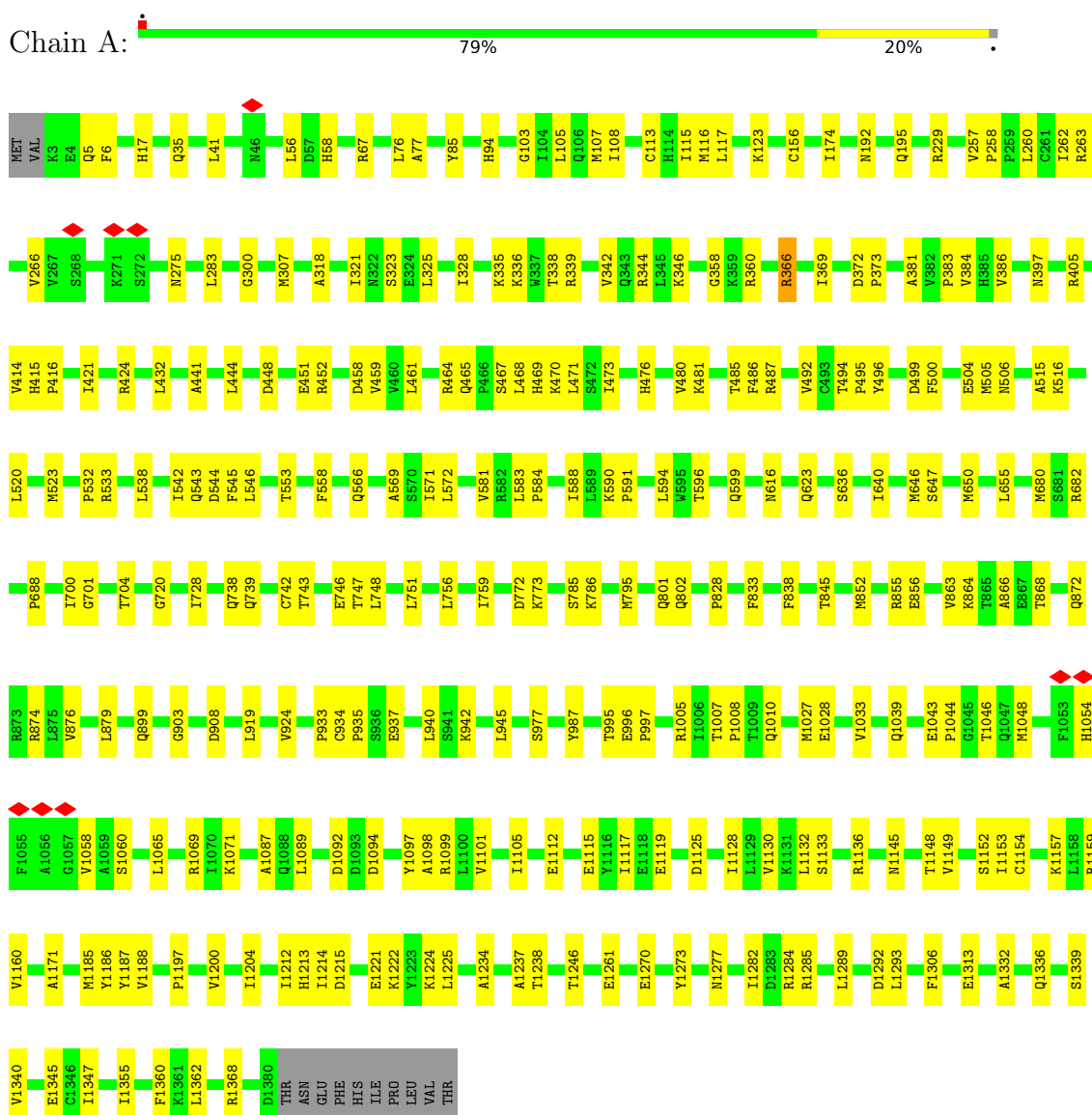


Mol	Chain	Residues	Atoms			AltConf
25	P	1	Total	Fe	S	0
			8	4	4	


3 Residue-property plots

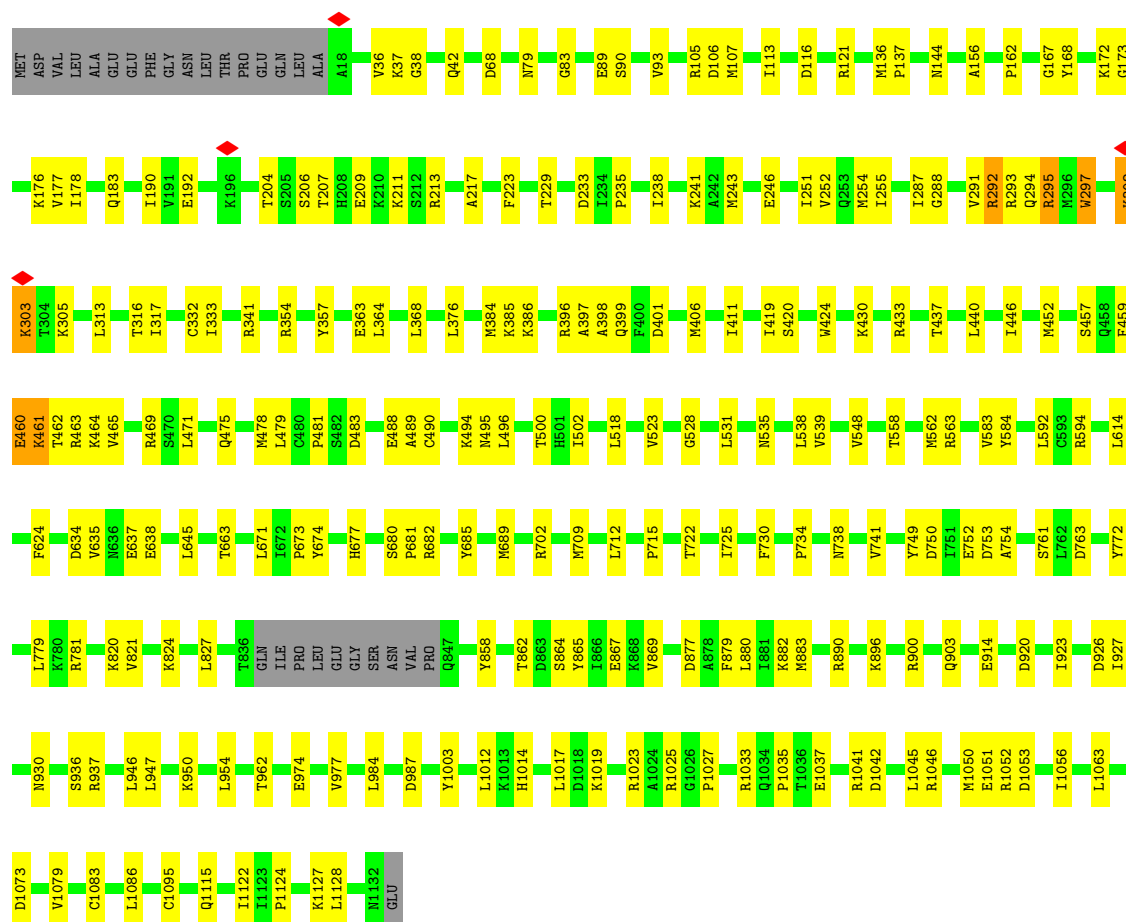
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase III subunit RPC1




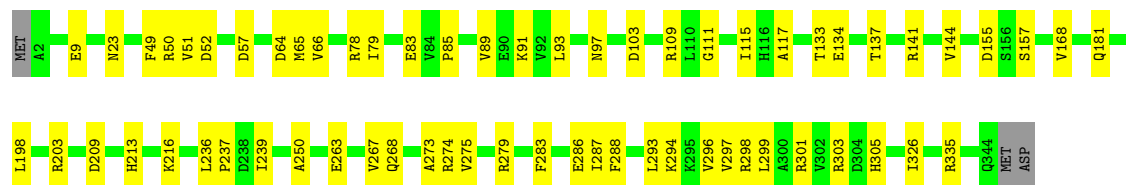
- Molecule 2: DNA-directed RNA polymerase III subunit RPC2

Chain B:  77% 20% ..



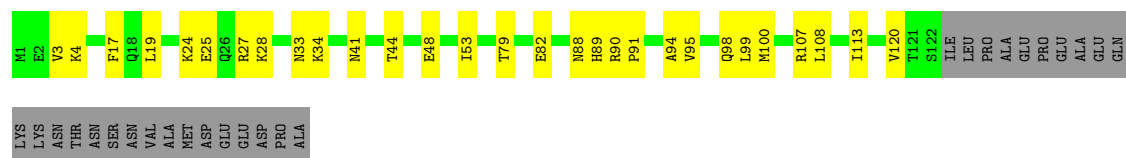
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:  81% 18% .

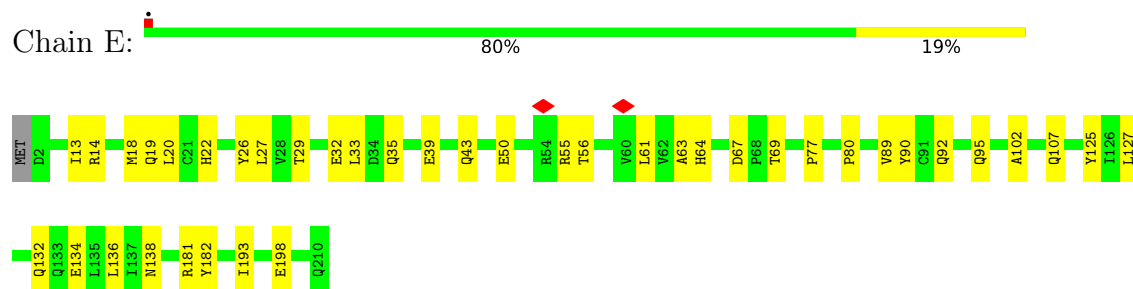


- Molecule 4: DNA-directed RNA polymerase III subunit RPC9

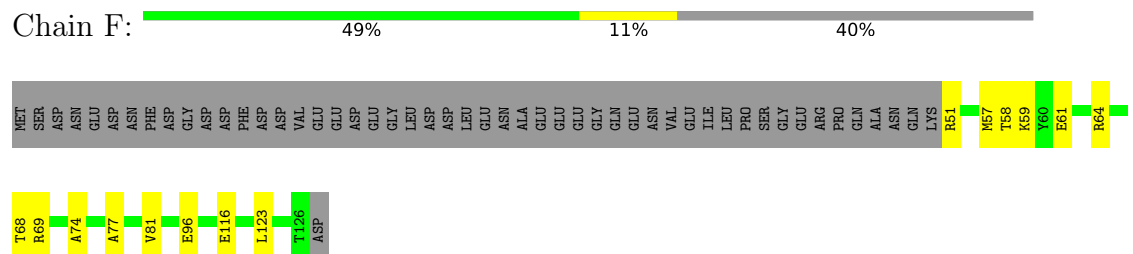
Chain D:  63% 20% 18%



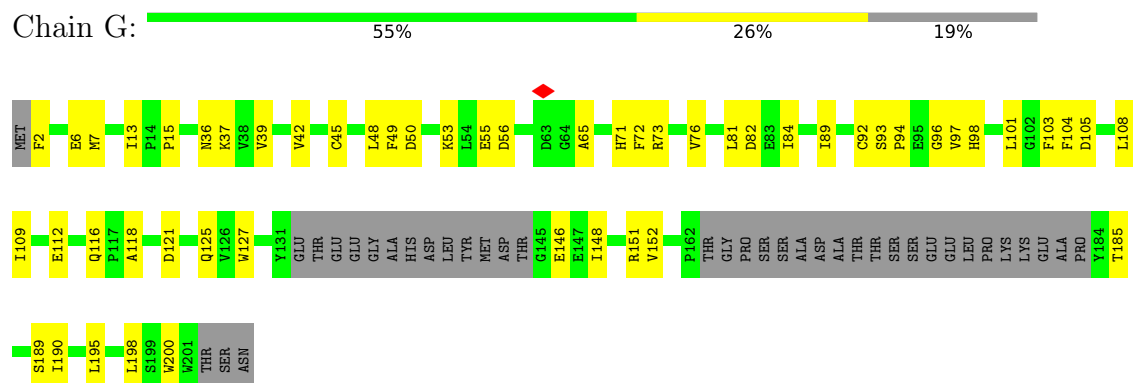
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



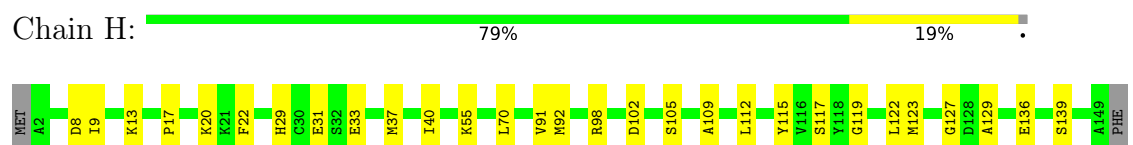
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



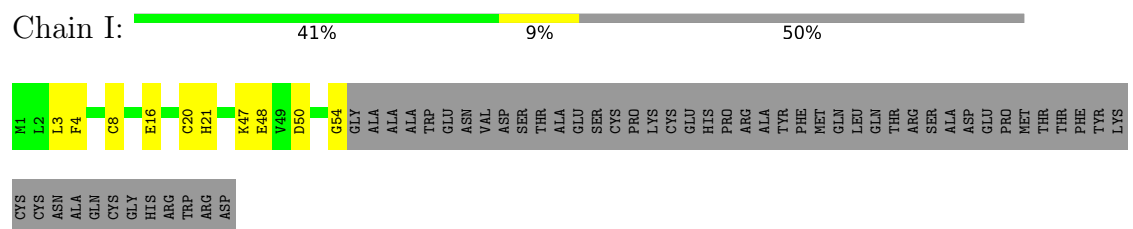
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



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



- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



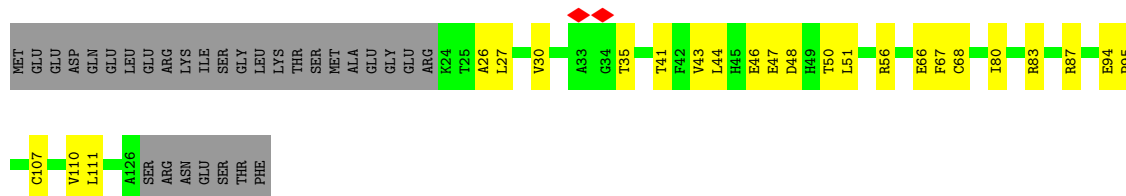
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  70% 27% .



- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:  59% 18% 23%



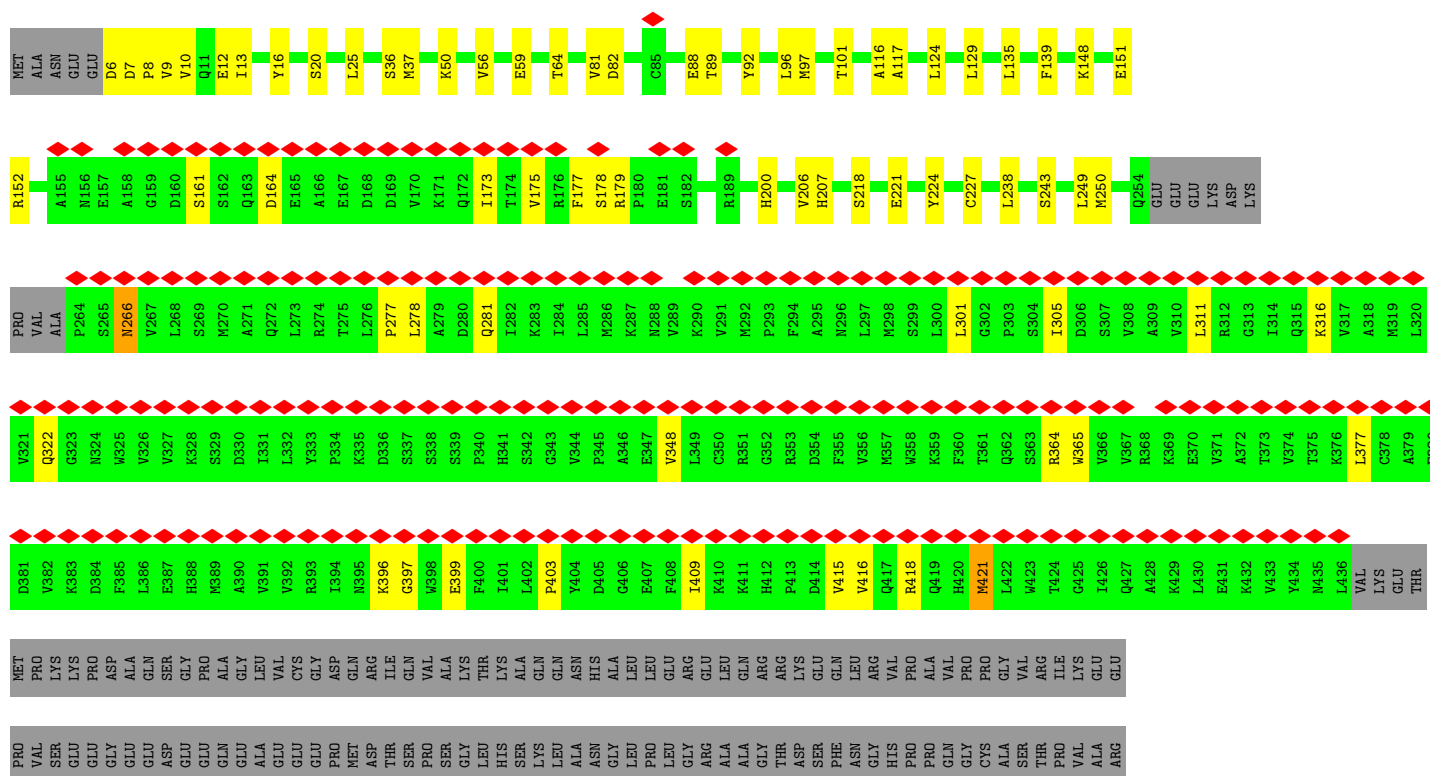
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

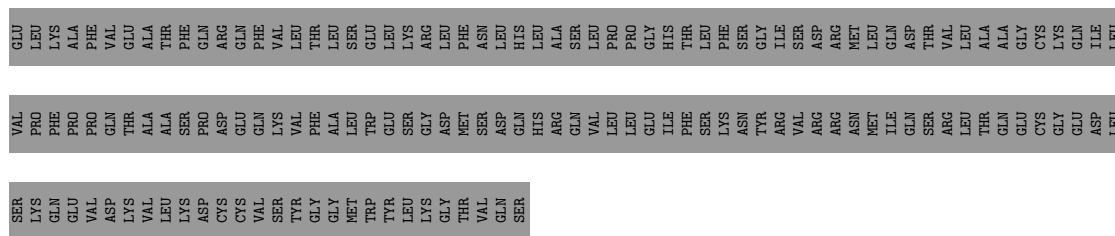
Chain L:  50% 29% 21%



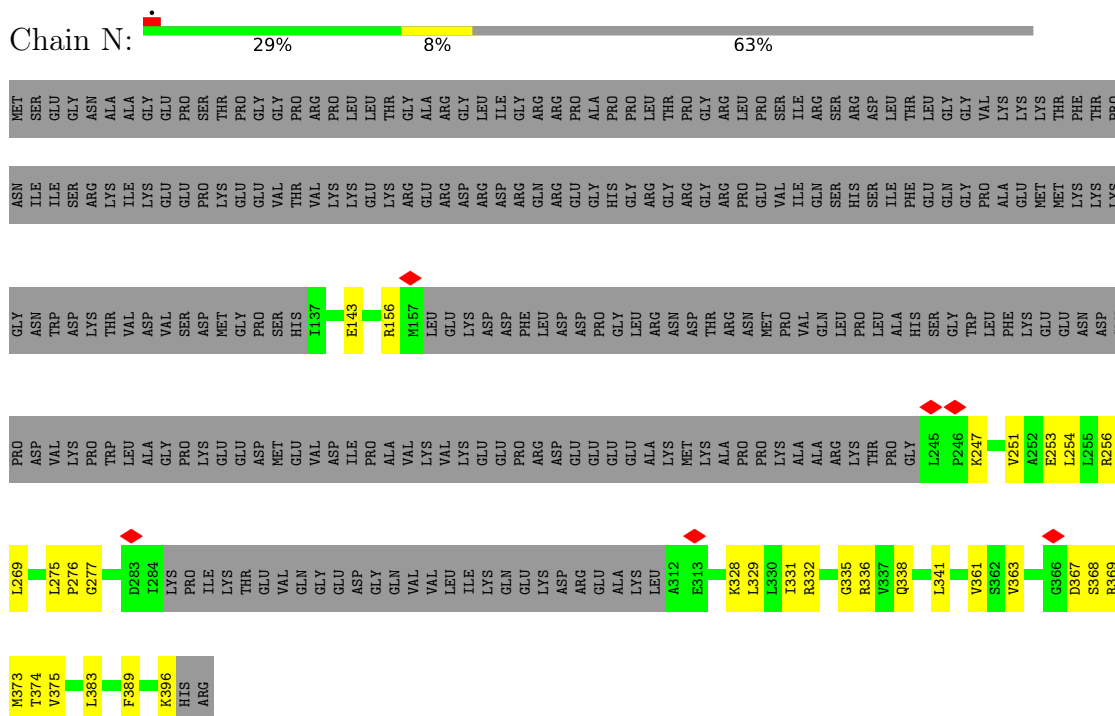
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

Chain M:  28% 49% 10% 40%

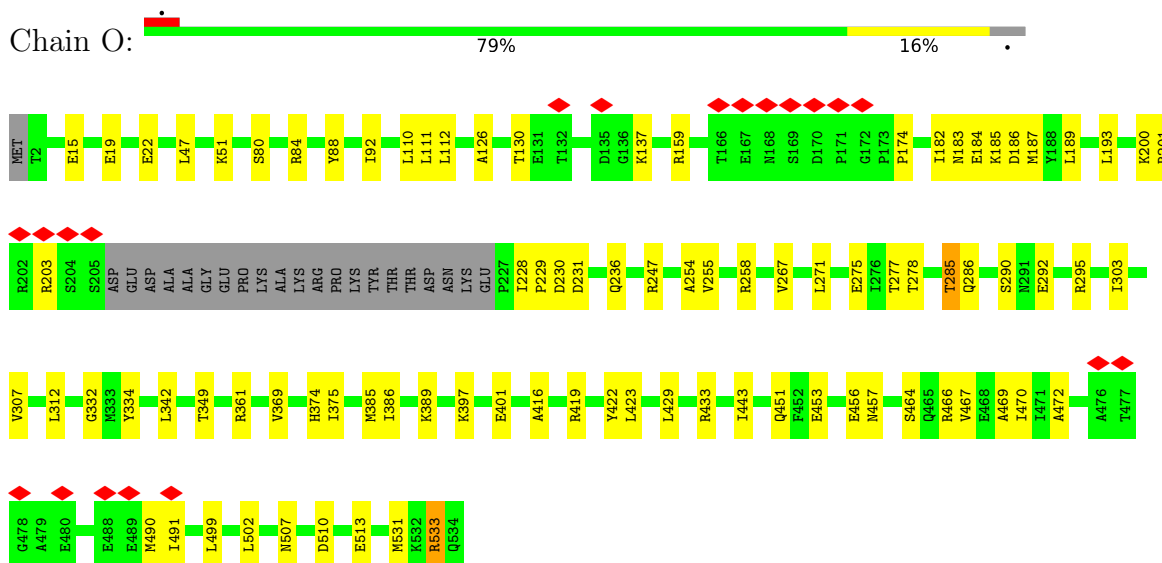




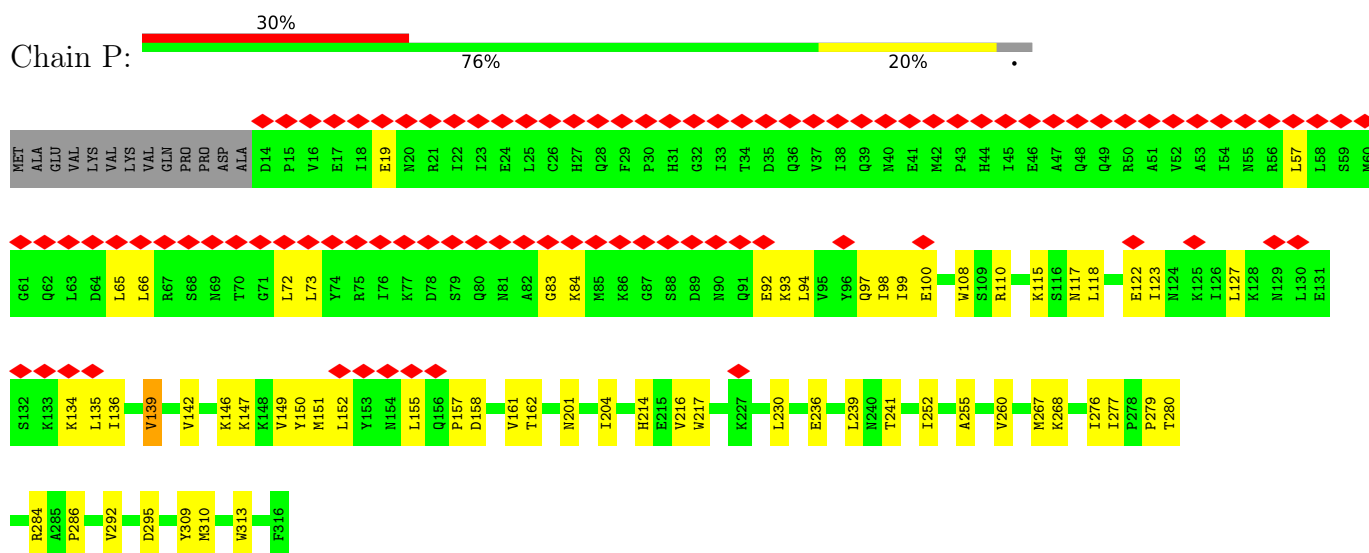
- Molecule 14: DNA-directed RNA polymerase III subunit RPC4



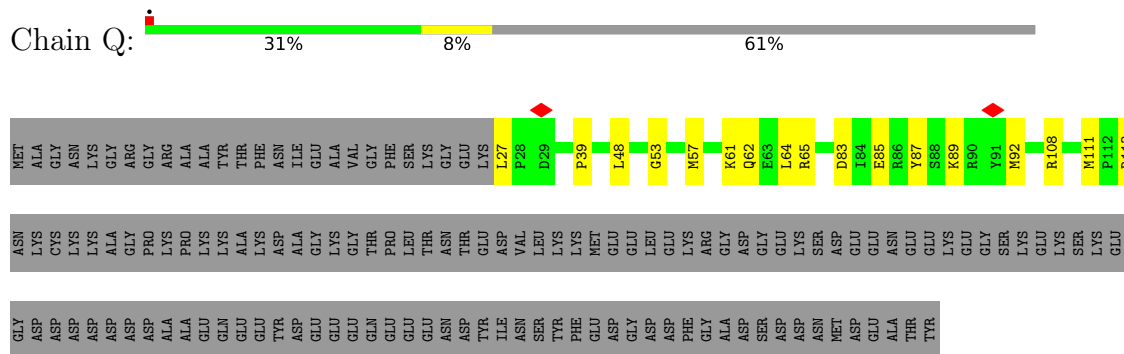
- Molecule 15: DNA-directed RNA polymerase III subunit RPC3



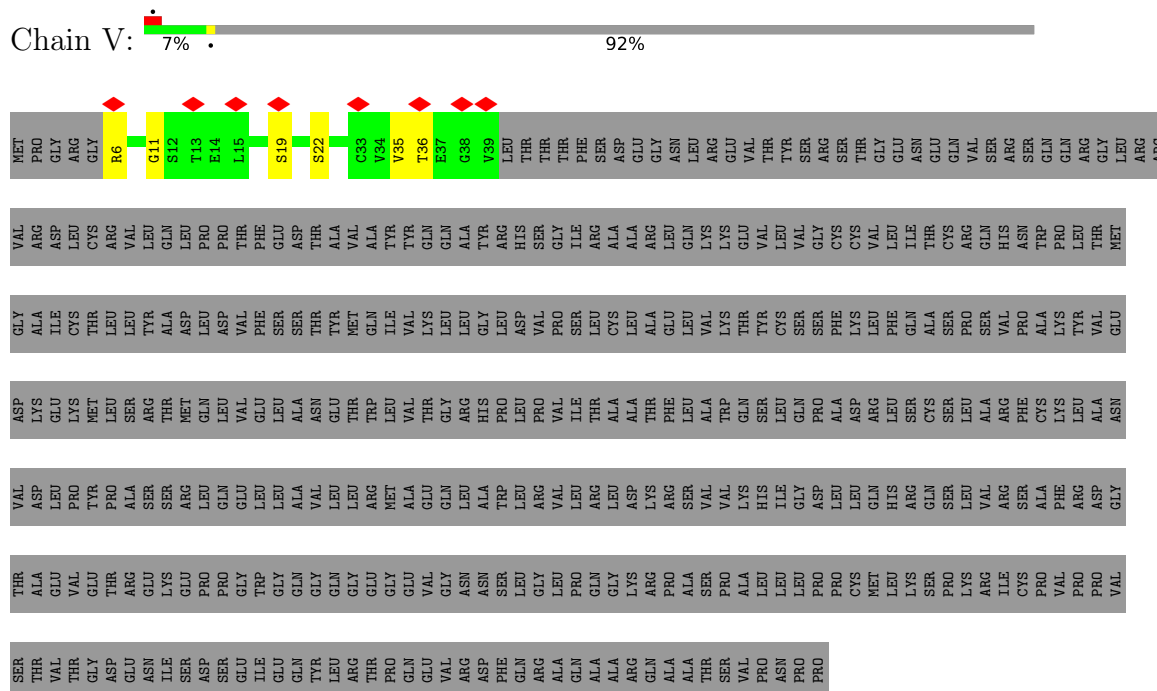
- Molecule 16: DNA-directed RNA polymerase III subunit RPC6



• Molecule 17: DNA-directed RNA polymerase III subunit RPC7



• Molecule 18: Transcription factor IIIB 50 kDa subunit





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	351000	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	7.893	Depositor
Minimum map value	-4.903	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.218	Depositor
Map size (Å)	429.22598, 429.22598, 429.22598	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.333, 1.333, 1.333	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: MG, 3AT, SF4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.26	0/11008	0.47	0/14842
2	B	0.27	0/8910	0.48	0/12018
3	C	0.25	0/2790	0.50	0/3782
4	D	0.24	0/997	0.45	0/1343
5	E	0.25	0/1745	0.48	0/2358
6	F	0.24	0/620	0.50	0/839
7	G	0.27	0/1374	0.48	0/1868
8	H	0.26	0/1207	0.50	0/1628
9	I	0.27	0/434	0.52	0/584
10	J	0.26	0/521	0.46	0/703
11	K	0.26	0/837	0.49	0/1129
12	L	0.27	0/394	0.61	0/524
13	M	0.26	0/3455	0.46	0/4673
14	N	0.25	0/1137	0.51	0/1530
15	O	0.25	0/4141	0.48	0/5592
16	P	0.26	0/2446	0.44	0/3301
17	Q	0.26	0/777	0.50	0/1050
18	V	0.28	0/248	0.48	0/336
19	X	1.51	23/1183 (1.9%)	1.26	16/1823 (0.9%)
20	Y	1.48	23/1161 (2.0%)	1.65	32/1790 (1.8%)
21	Z	0.76	1/231 (0.4%)	0.97	0/357
All	All	0.43	47/45616 (0.1%)	0.59	48/62070 (0.1%)

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	X	2	DG	O3'-P	-16.03	1.42	1.61
19	X	22	DT	O3'-P	-15.98	1.42	1.61
20	Y	2	DG	C2'-C1'	-15.65	1.36	1.52
20	Y	-3	DG	O3'-P	-15.32	1.42	1.61
19	X	-13	DA	C4'-O4'	-15.19	1.29	1.45

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	-2	DC	O5'-P-OP2	-21.00	85.50	110.70
20	Y	7	DT	P-O3'-C3'	-17.16	99.11	119.70
20	Y	0	DC	OP1-P-O3'	13.95	135.89	105.20
20	Y	0	DC	P-O3'-C3'	-12.20	105.06	119.70
20	Y	-20	DA	C3'-C2'-C1'	-11.43	88.78	102.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10814	0	11057	215	0
2	B	8741	0	8865	214	0
3	C	2736	0	2712	43	0
4	D	985	0	1006	22	0
5	E	1715	0	1733	22	0
6	F	610	0	642	12	0
7	G	1337	0	1306	41	0
8	H	1186	0	1147	18	0
9	I	426	0	428	11	0
10	J	512	0	525	15	0
11	K	822	0	810	19	0
12	L	388	0	393	11	0
13	M	3382	0	3376	54	0
14	N	1128	0	1181	23	0
15	O	4075	0	4149	54	0
16	P	2403	0	2405	43	0
17	Q	754	0	759	16	0
18	V	246	0	221	9	0
19	X	1051	0	570	109	0
20	Y	1040	0	582	96	0
21	Z	209	0	107	21	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
23	A	1	0	0	0	0
24	B	30	0	12	13	0
25	P	8	0	0	0	0
All	All	44605	0	43986	872	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 10.

The worst 5 of 872 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)
20:Y:2:DG:C8	20:Y:3:DT:H72	1.60	1.34
2:B:295:ARG:CG	19:X:9:DT:H72	1.69	1.20
19:X:3:DC:H6	19:X:3:DC:H5"	1.01	1.14
2:B:295:ARG:HG3	19:X:9:DT:C7	1.78	1.13
2:B:295:ARG:HG3	19:X:9:DT:H72	1.09	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1376/1390 (99%)	1335 (97%)	41 (3%)	0	100	100
2	B	1101/1133 (97%)	1050 (95%)	51 (5%)	0	100	100
3	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
4	D	120/148 (81%)	114 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	74/127 (58%)	73 (99%)	1 (1%)	0	100	100
7	G	160/204 (78%)	142 (89%)	18 (11%)	0	100	100
8	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
9	I	52/108 (48%)	50 (96%)	2 (4%)	0	100	100
10	J	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
11	K	101/133 (76%)	96 (95%)	5 (5%)	0	100	100
12	L	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
13	M	418/708 (59%)	399 (96%)	19 (4%)	0	100	100
14	N	140/398 (35%)	136 (97%)	4 (3%)	0	100	100
15	O	508/534 (95%)	493 (97%)	15 (3%)	0	100	100
16	P	301/316 (95%)	292 (97%)	9 (3%)	0	100	100
17	Q	85/223 (38%)	83 (98%)	2 (2%)	0	100	100
18	V	32/419 (8%)	29 (91%)	3 (9%)	0	100	100
All	All	5269/6672 (79%)	5075 (96%)	194 (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	A	1200/1212 (99%)	1198 (100%)	2 (0%)	92	97
2	B	964/988 (98%)	953 (99%)	11 (1%)	70	87
3	C	299/302 (99%)	299 (100%)	0	100	100
4	D	114/136 (84%)	114 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	66/111 (60%)	66 (100%)	0	100	100
7	G	149/181 (82%)	149 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	48/93 (52%)	48 (100%)	0	100	100
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	92/119 (77%)	92 (100%)	0	100	100
12	L	43/55 (78%)	41 (95%)	2 (5%)	22	56
13	M	377/622 (61%)	375 (100%)	2 (0%)	86	94
14	N	131/347 (38%)	130 (99%)	1 (1%)	79	90
15	O	458/476 (96%)	456 (100%)	2 (0%)	89	95
16	P	269/280 (96%)	263 (98%)	6 (2%)	47	76
17	Q	84/195 (43%)	84 (100%)	0	100	100
18	V	31/365 (8%)	31 (100%)	0	100	100
All	All	4698/5861 (80%)	4672 (99%)	26 (1%)	82	93

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	29	LYS
14	N	156	ARG
16	P	135	LEU
13	M	421	MET
15	O	285	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	125	GLN
8	H	29	HIS
16	P	117	ASN
14	N	282	GLN
14	N	381	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	Z	9/10 (90%)	7 (77%)	0

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	Z	5	U
21	Z	7	G
21	Z	8	C
21	Z	10	U
21	Z	11	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 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	$\# Z > 2$
24	3AT	B	1202	-	25,32,32	1.00	1 (4%)	28,50,50	1.63	5 (17%)
25	SF4	P	401	16	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
24	3AT	B	1202	-	-	6/18/34/34	0/3/3/3
25	SF4	P	401	16	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1202	3AT	C5-C4	2.52	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1202	3AT	PA-O3A-PB	-3.63	120.36	132.83
24	B	1202	3AT	PB-O3B-PG	-3.59	120.50	132.83
24	B	1202	3AT	N3-C2-N1	-3.14	123.77	128.68
24	B	1202	3AT	C4-C5-N7	-2.64	106.65	109.40
24	B	1202	3AT	O4'-C4'-C3'	2.17	107.86	105.07

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

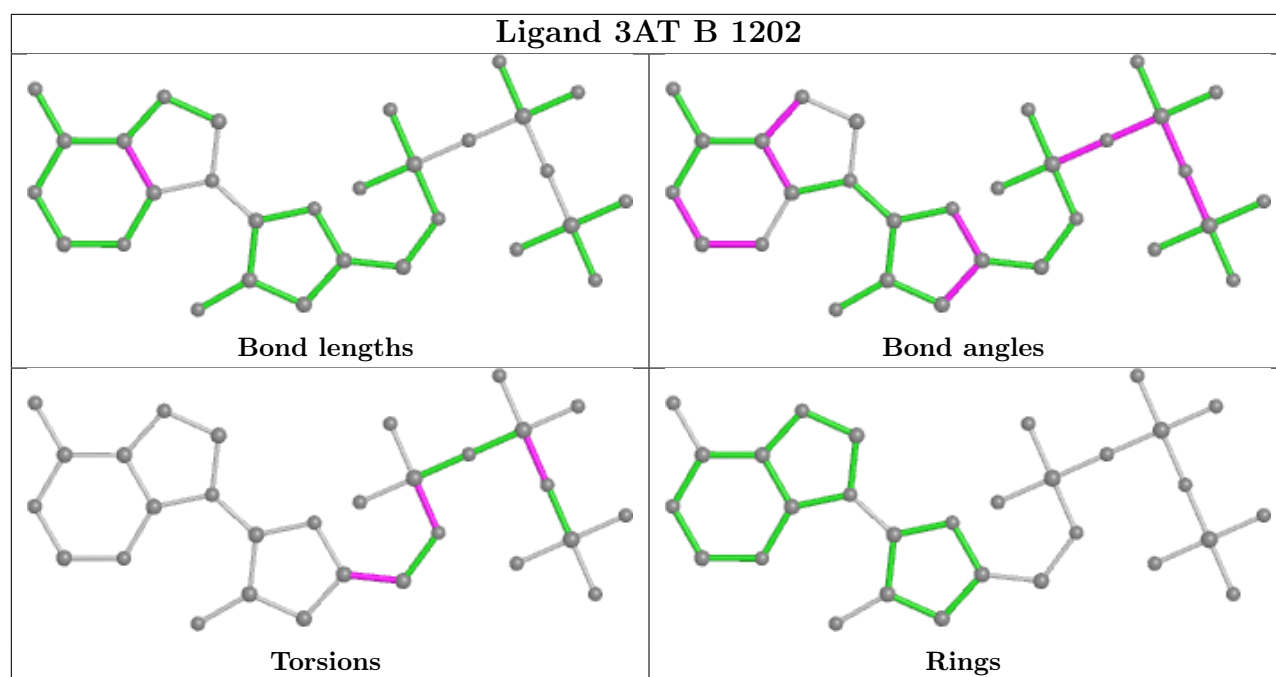
Mol	Chain	Res	Type	Atoms
24	B	1202	3AT	C5'-O5'-PA-O3A
24	B	1202	3AT	O4'-C4'-C5'-O5'
24	B	1202	3AT	C3'-C4'-C5'-O5'
24	B	1202	3AT	C5'-O5'-PA-O2A
24	B	1202	3AT	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	1202	3AT	13	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.

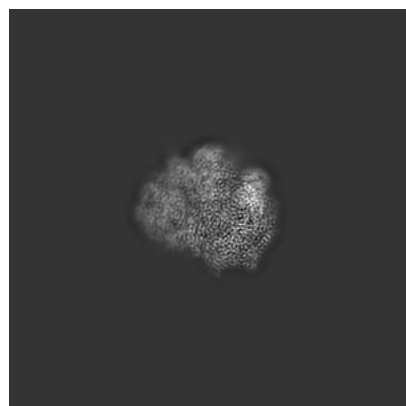
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61994. These allow visual inspection of the internal detail of the map and identification of artifacts.

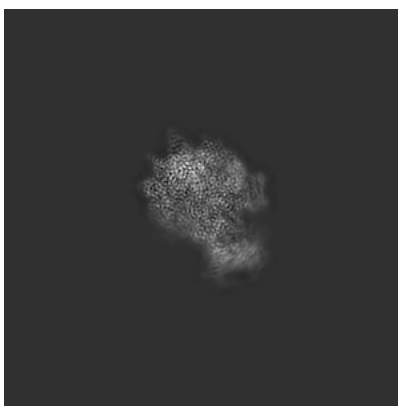
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

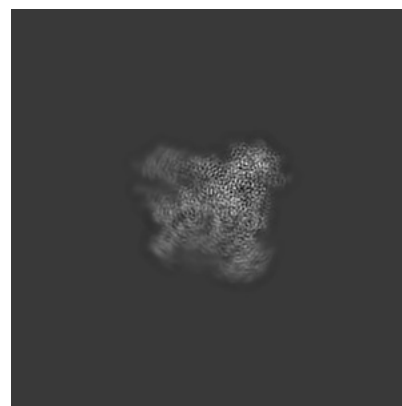
6.1.1 Primary map



X

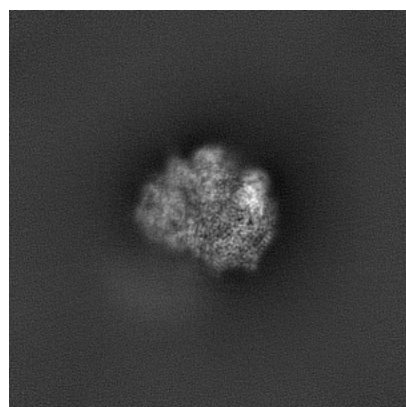


Y

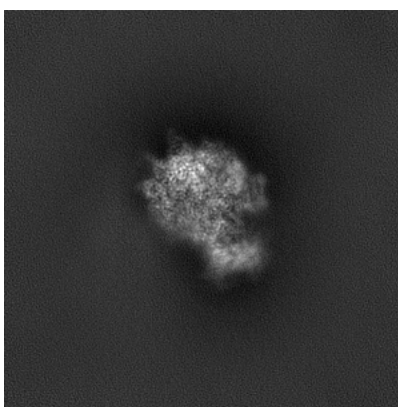


Z

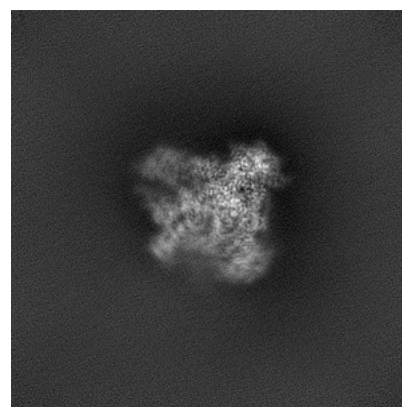
6.1.2 Raw map



X



Y

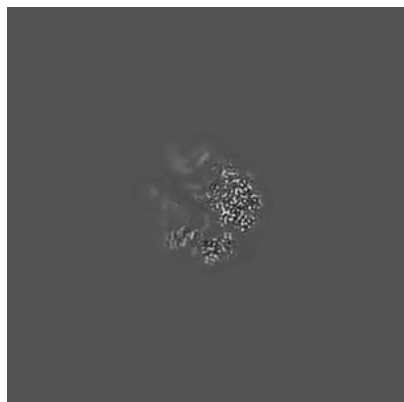


Z

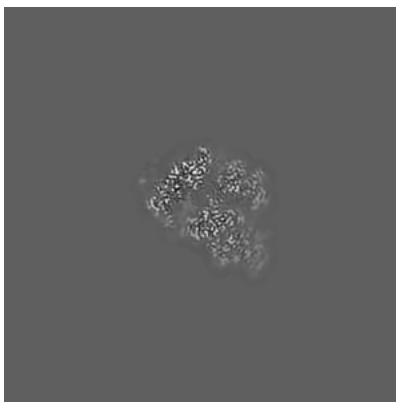
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

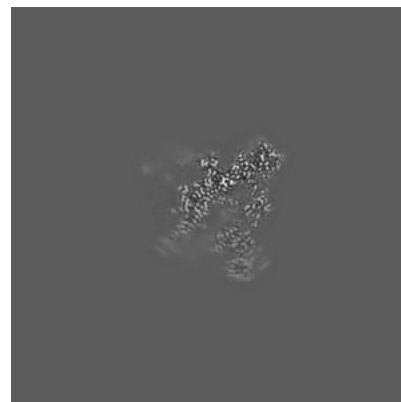
6.2.1 Primary map



X Index: 161

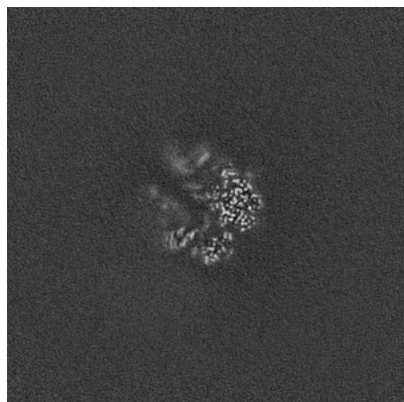


Y Index: 161

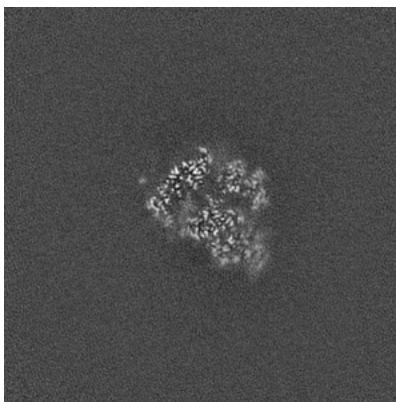


Z Index: 161

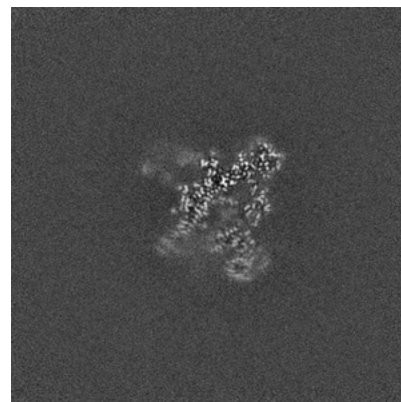
6.2.2 Raw map



X Index: 161



Y Index: 161

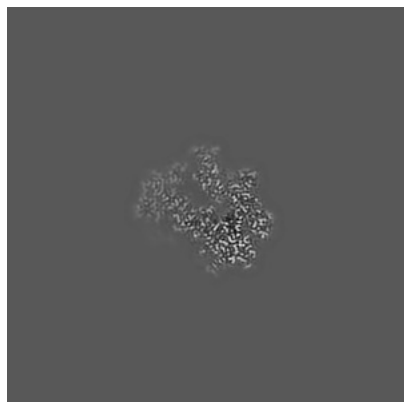


Z Index: 161

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

6.3 Largest variance slices [i](#)

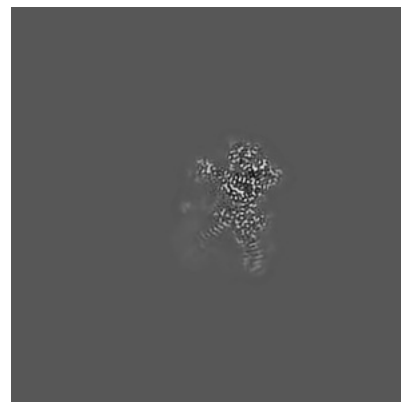
6.3.1 Primary map



X Index: 181

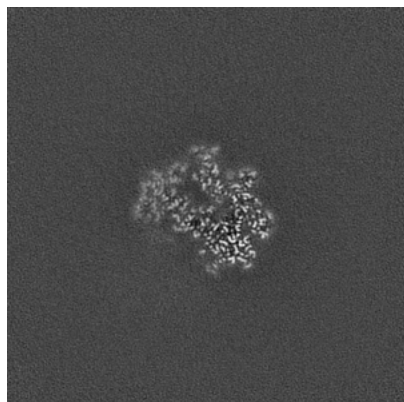


Y Index: 190

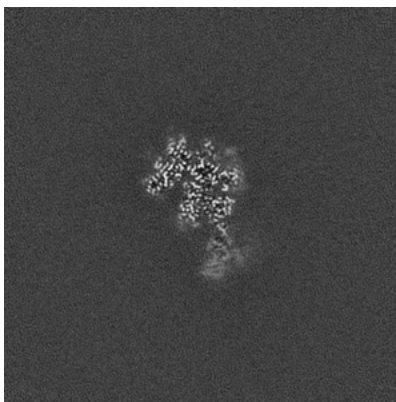


Z Index: 144

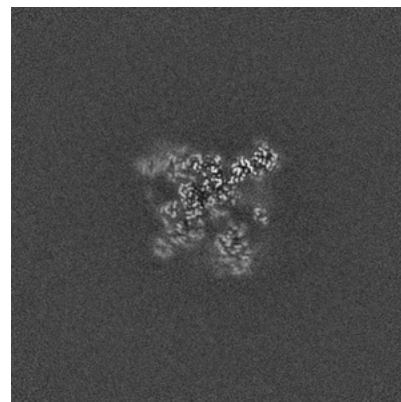
6.3.2 Raw map



X Index: 181



Y Index: 190

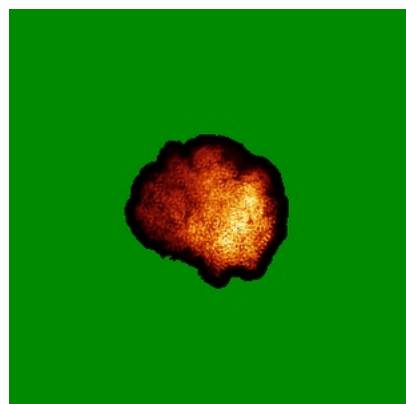


Z Index: 168

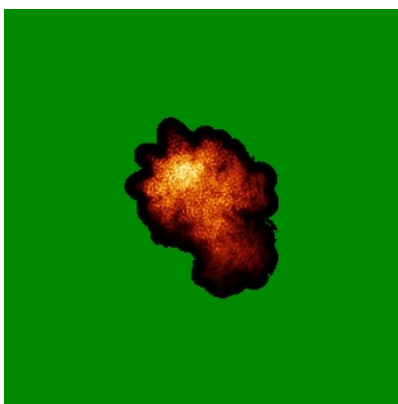
The images above show the largest variance slices of the map in three orthogonal directions.

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

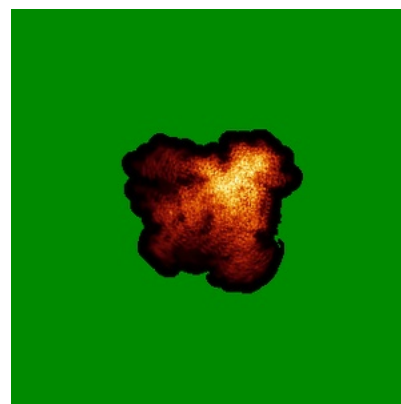
6.4.1 Primary map



X

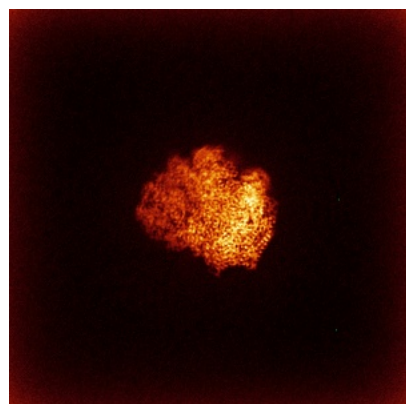


Y

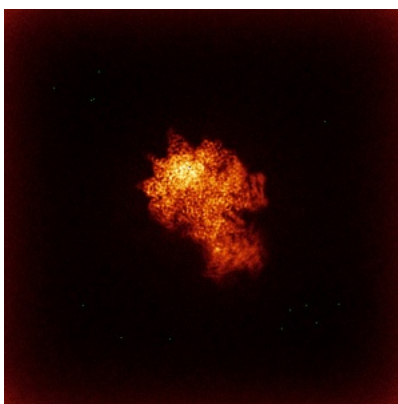


Z

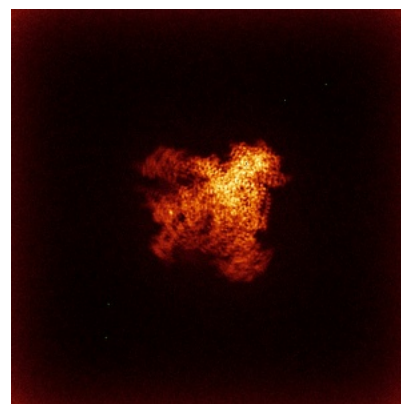
6.4.2 Raw map



X



Y

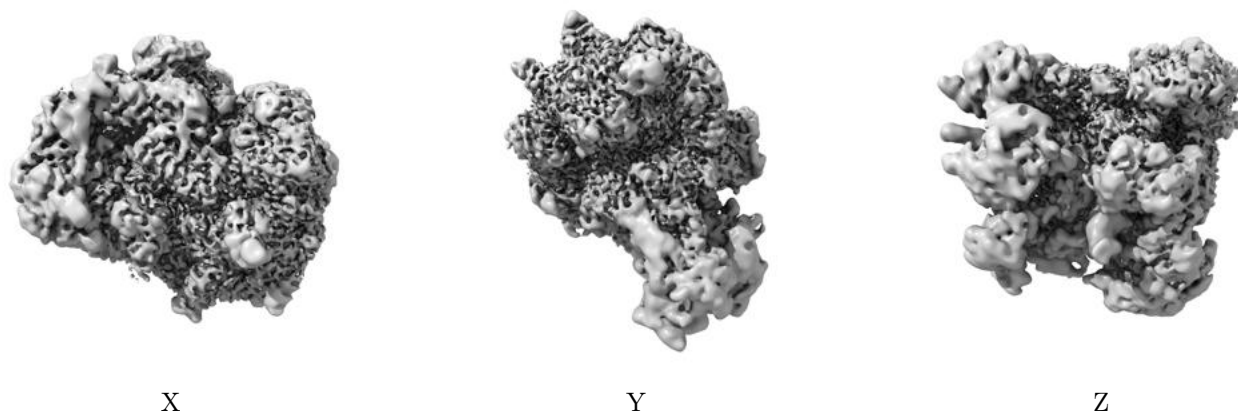


Z

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.

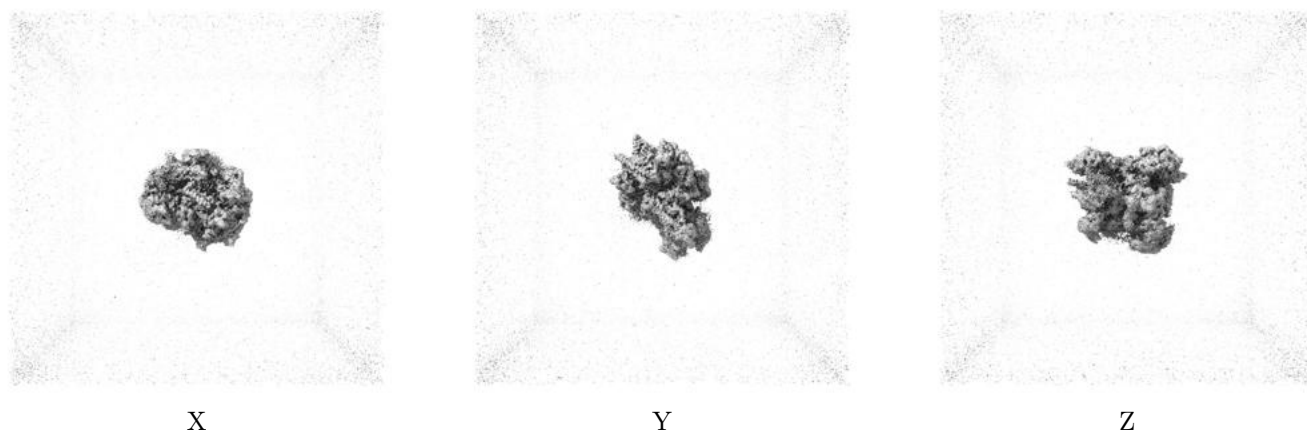
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.218. 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.

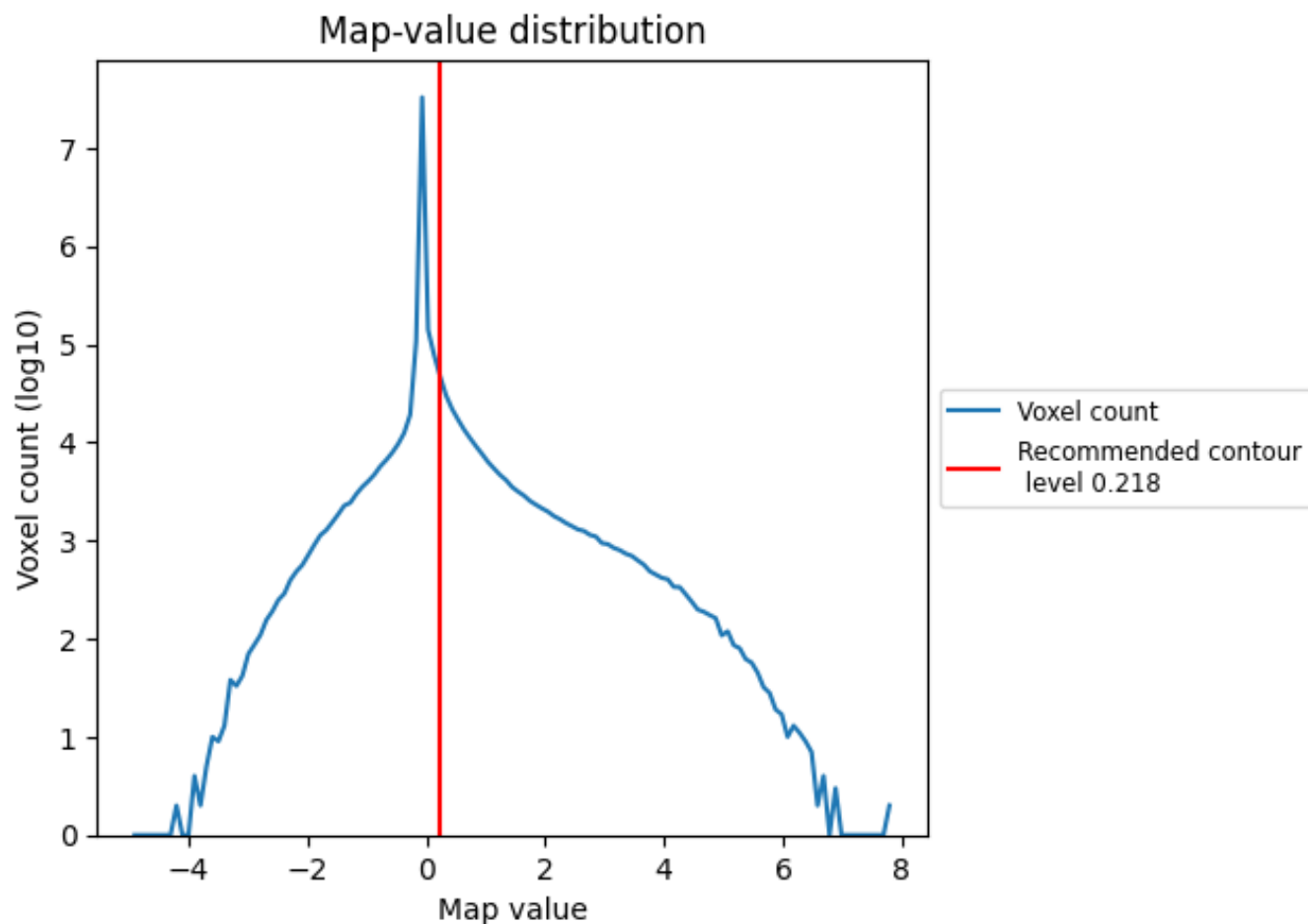
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

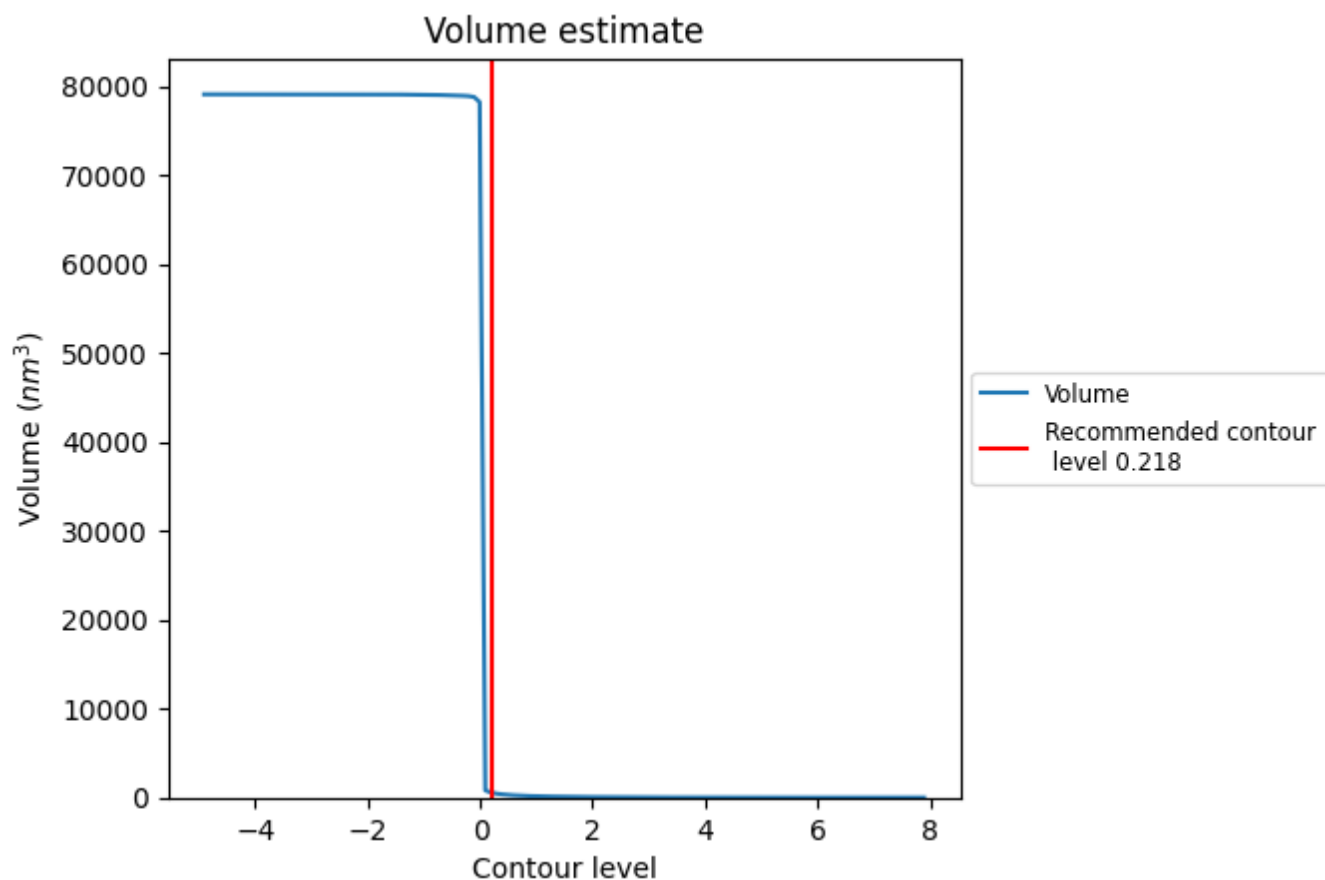
This section contains the results of statistical analysis of the map.

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.

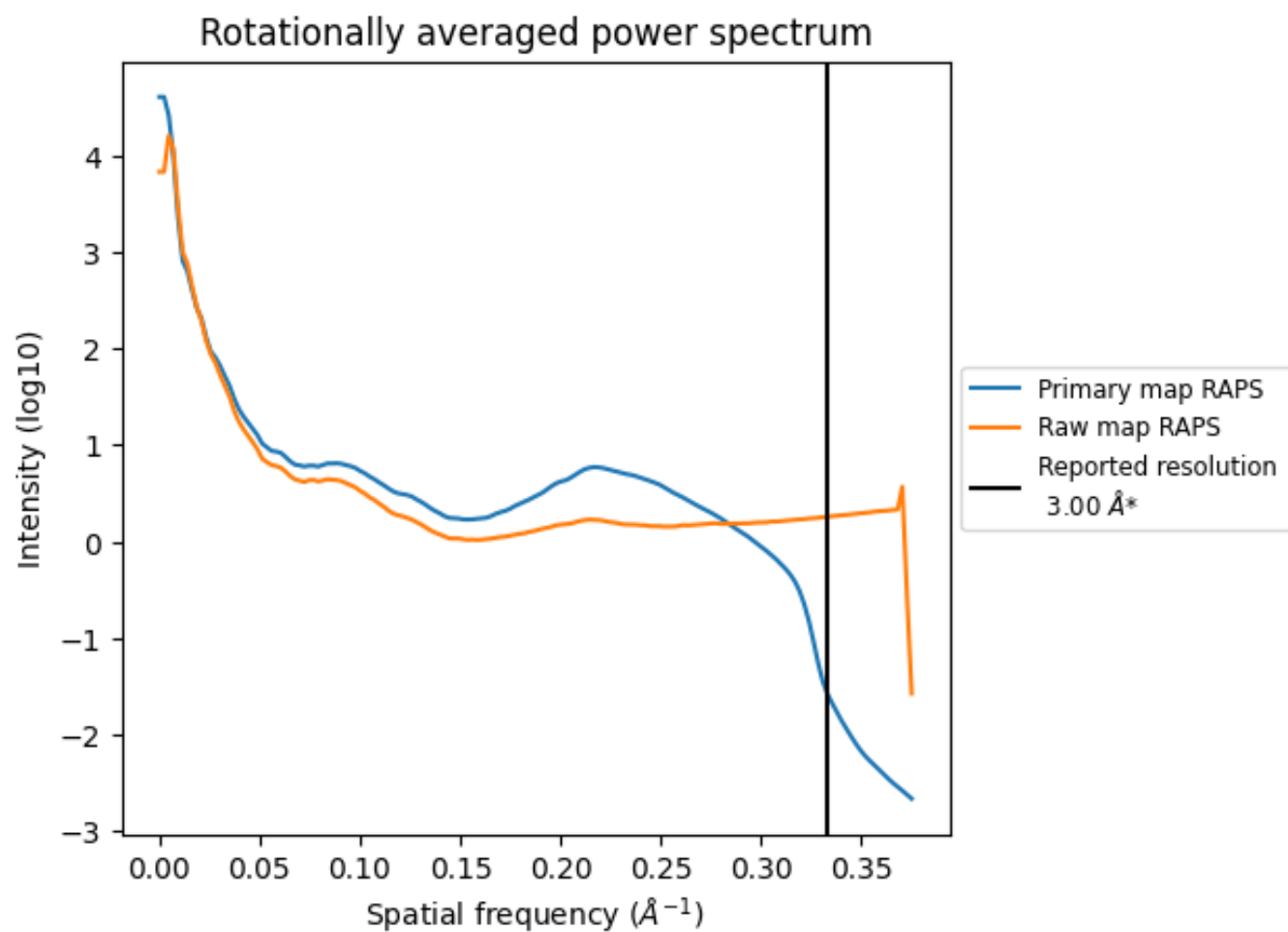
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 548 nm^3 ; this corresponds to an approximate mass of 495 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 ⓘ

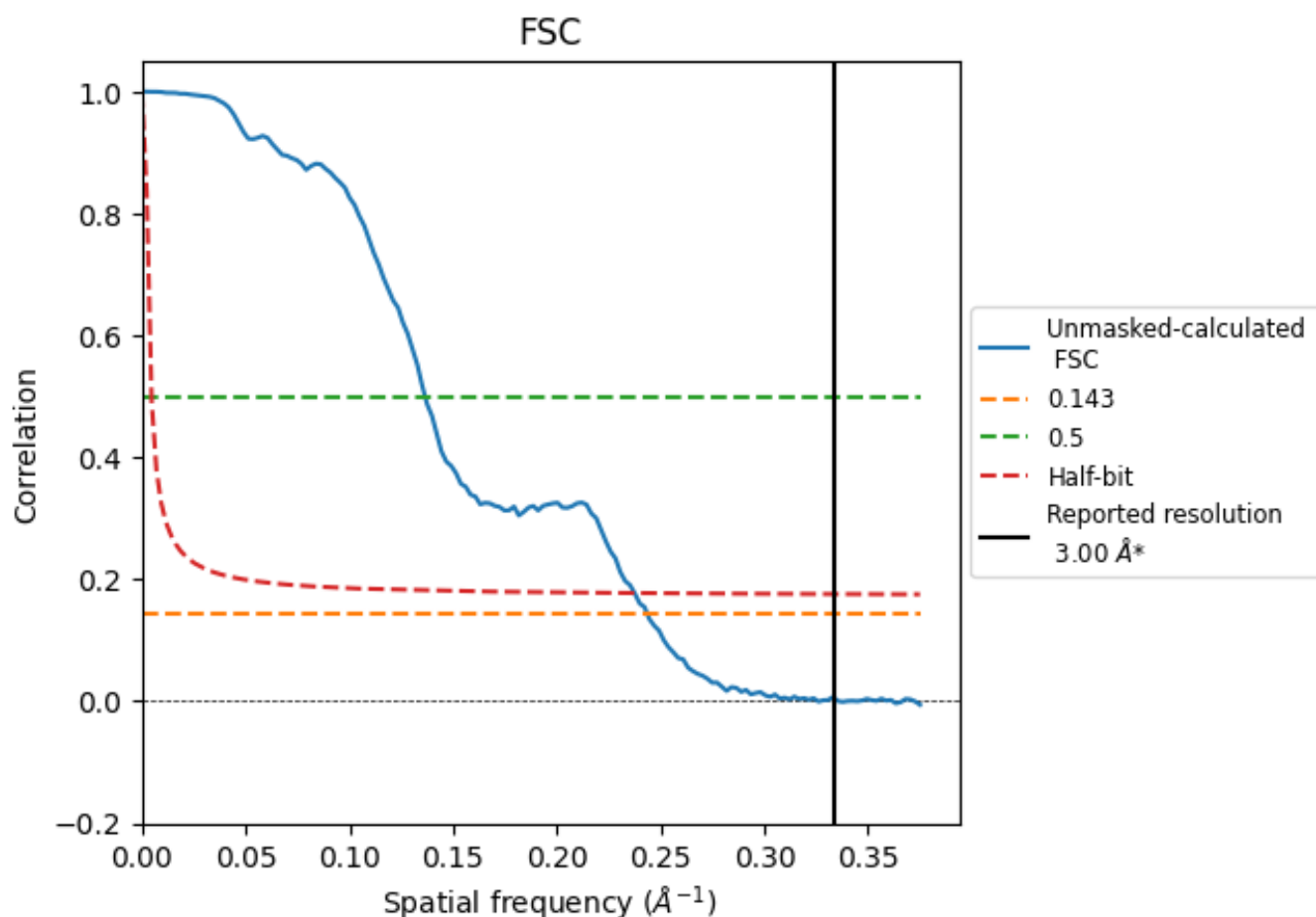


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

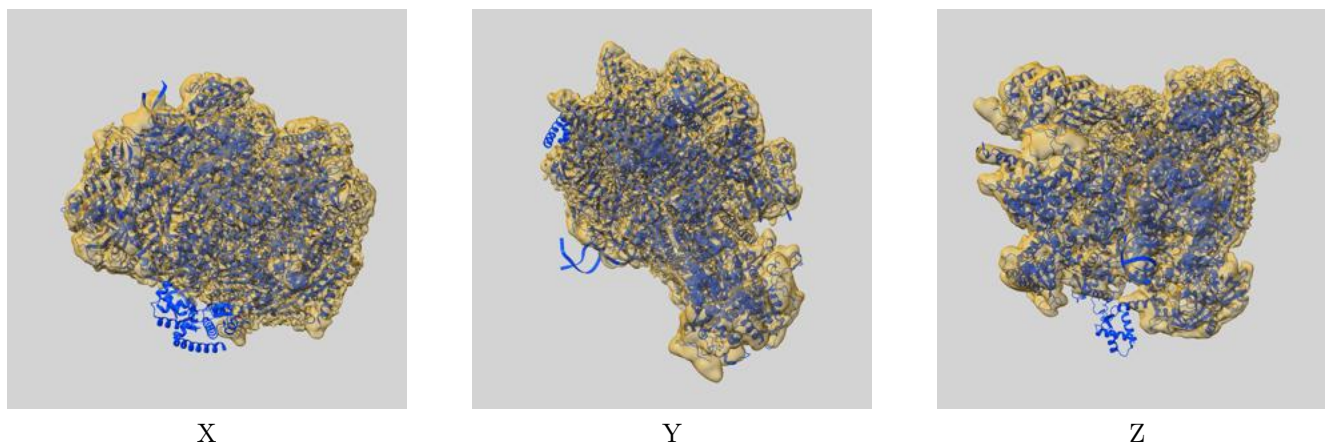
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.11	7.33	4.21

*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 4.11 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

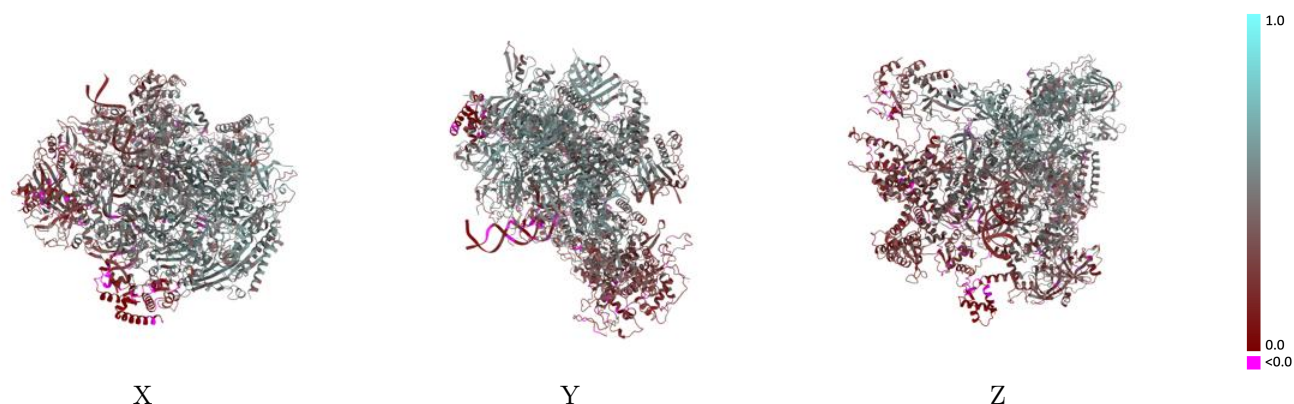
This section contains information regarding the fit between EMDB map EMD-61994 and PDB model 9K2G. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



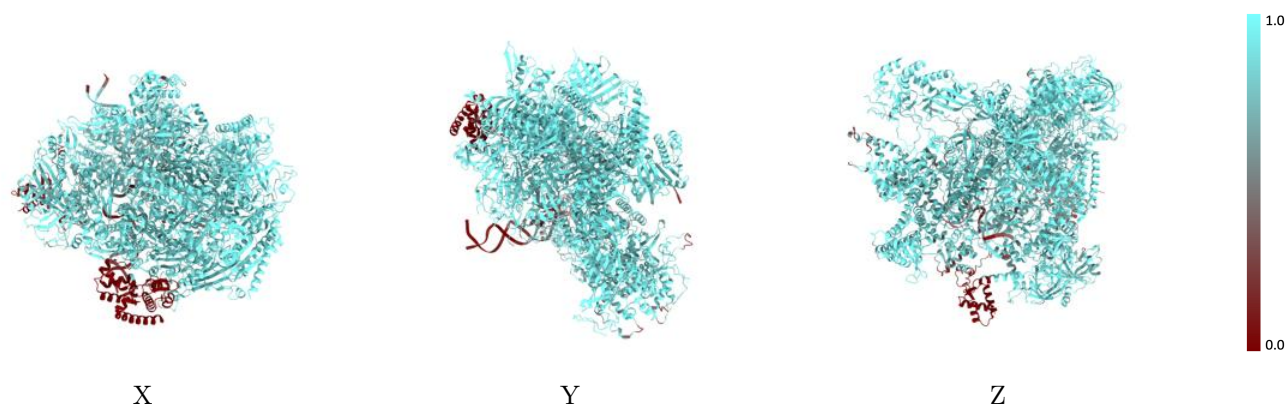
The images above show the 3D surface view of the map at the recommended contour level 0.218 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



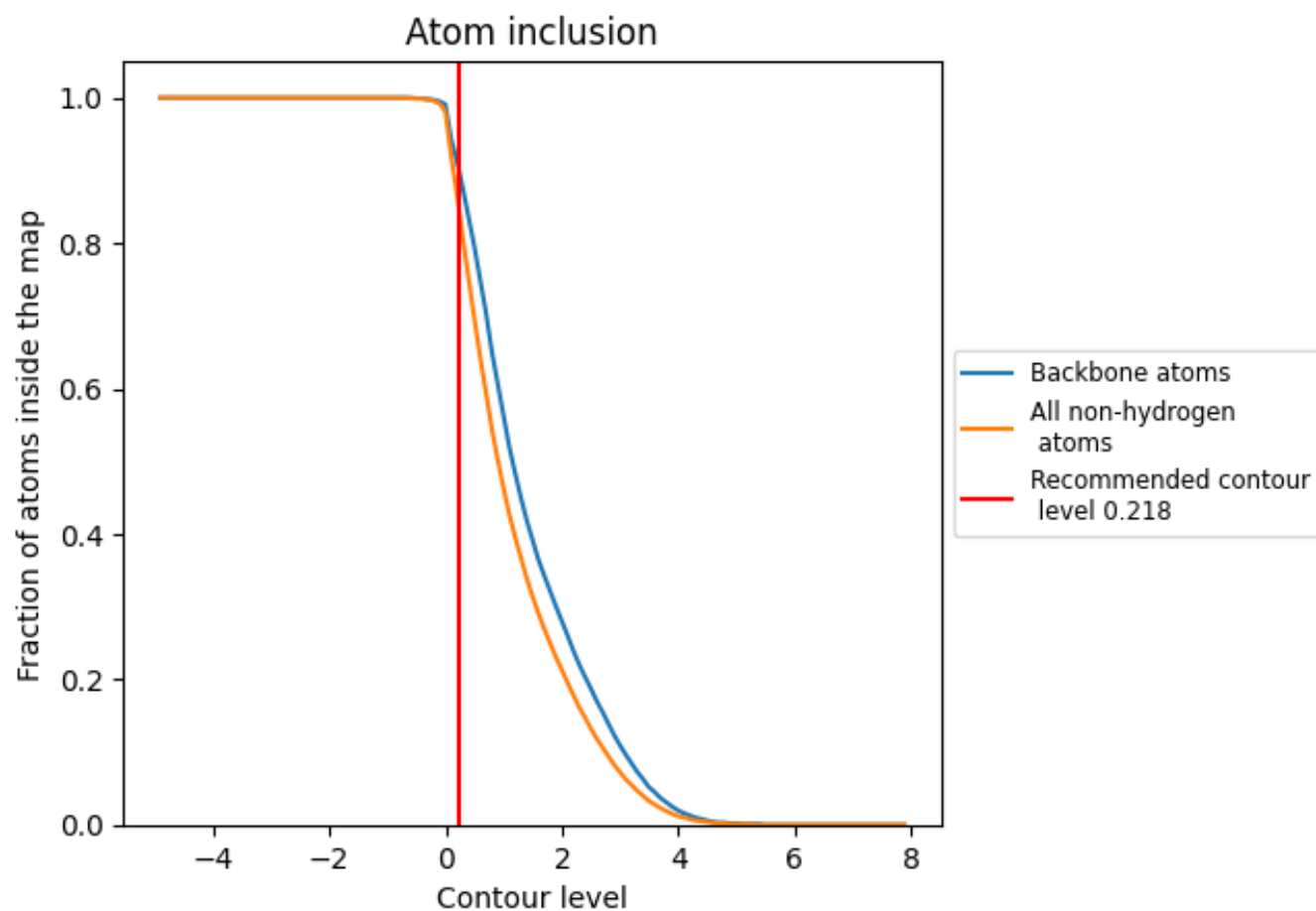
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.218).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.3770
A	 0.9340	 0.4680
B	 0.9320	 0.4630
C	 0.9510	 0.4960
D	 0.9290	 0.2870
E	 0.9460	 0.4000
F	 0.9650	 0.5280
G	 0.9320	 0.3540
H	 0.9600	 0.4890
I	 0.9110	 0.3240
J	 0.9500	 0.4970
K	 0.9490	 0.4970
L	 0.9440	 0.4220
M	 0.4950	 0.1970
N	 0.8550	 0.2670
O	 0.8540	 0.2560
P	 0.6120	 0.1550
Q	 0.8500	 0.2110
V	 0.5350	 0.0300
X	 0.5080	 0.1360
Y	 0.6260	 0.2290
Z	 0.9090	 0.4090

