



# wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 06:17 am BST

PDB ID : 7Z1L  
EMDB ID : EMD-14447  
Title : Structure of yeast RNA Polymerase III Pre-Termination Complex (PTC)  
Authors : Girbig, M.; Mueller, C.W.  
Deposited on : 2022-02-24  
Resolution : 2.80 Å(reported)  
Based on initial model : 6TUT

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.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

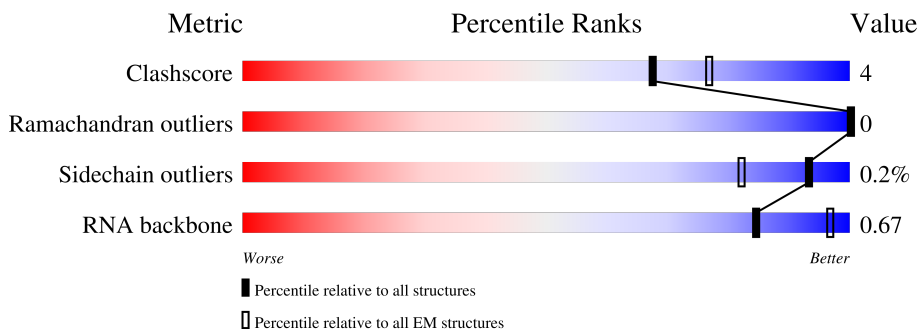
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	1460	
2	B	1149	
3	C	335	
4	D	161	
5	E	215	
6	F	155	
7	G	212	

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	R	24	
19	S	44	
20	T	44	

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 42330 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	1436	Total	C	N	O	S	0	0
			11228	7080	1981	2106	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1101	Total	C	N	O	S	0	0
			8693	5503	1499	1631	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	334	Total	C	N	O	S	0	0
			2647	1676	453	510	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	145	Total	C	N	O	S	0	0
			1185	755	200	224	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	199	Total	C	N	O	S	0	0
			1594	1038	258	291	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	135	Total	C	N	O	S	0	0
			1084	683	183	214	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	110	Total	C	N	O	S	0	0
			873	546	145	171	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	102	Total	C	N	O	S	0	0
			801	501	131	164	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	196	Total	C	N	O	S	0	0
			1594	1012	272	309	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	153	Total	C	N	O	S	0	0
			1196	754	220	219	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	570	Total	C	N	O	S	0	0
			4577	2908	787	863	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	140	Total	C	N	O	S	0	0
			1159	756	179	220	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	123	Total	C	N	O	S	0	0
			981	633	163	182	3		

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	9	Total	C	N	O	P	0	0
			195	87	39	60	9		

- Molecule 19 is a DNA chain called NT-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	25	Total	C	N	O	P	0	0
			507	246	78	158	25		

- Molecule 20 is a DNA chain called T-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	29	Total	C	N	O	P	0	0
			597	284	109	175	29		

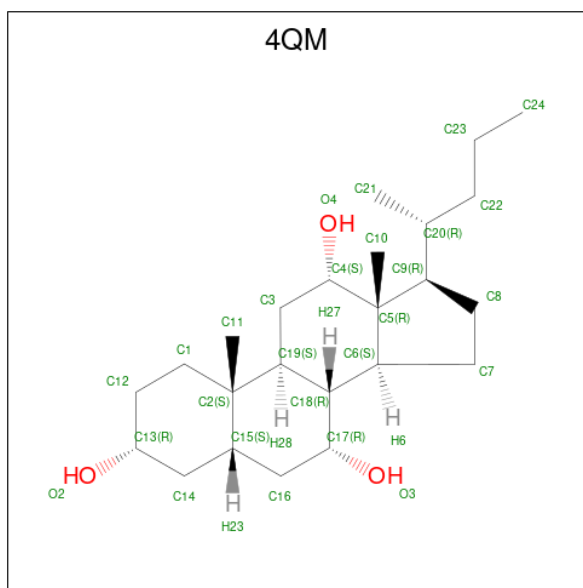
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 23 is (3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-10,13-dimethyl-17-[(2R)-pentan-2-yl]-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol (three-letter code: 4QM) (formula: C<sub>24</sub>H<sub>42</sub>O<sub>3</sub>).

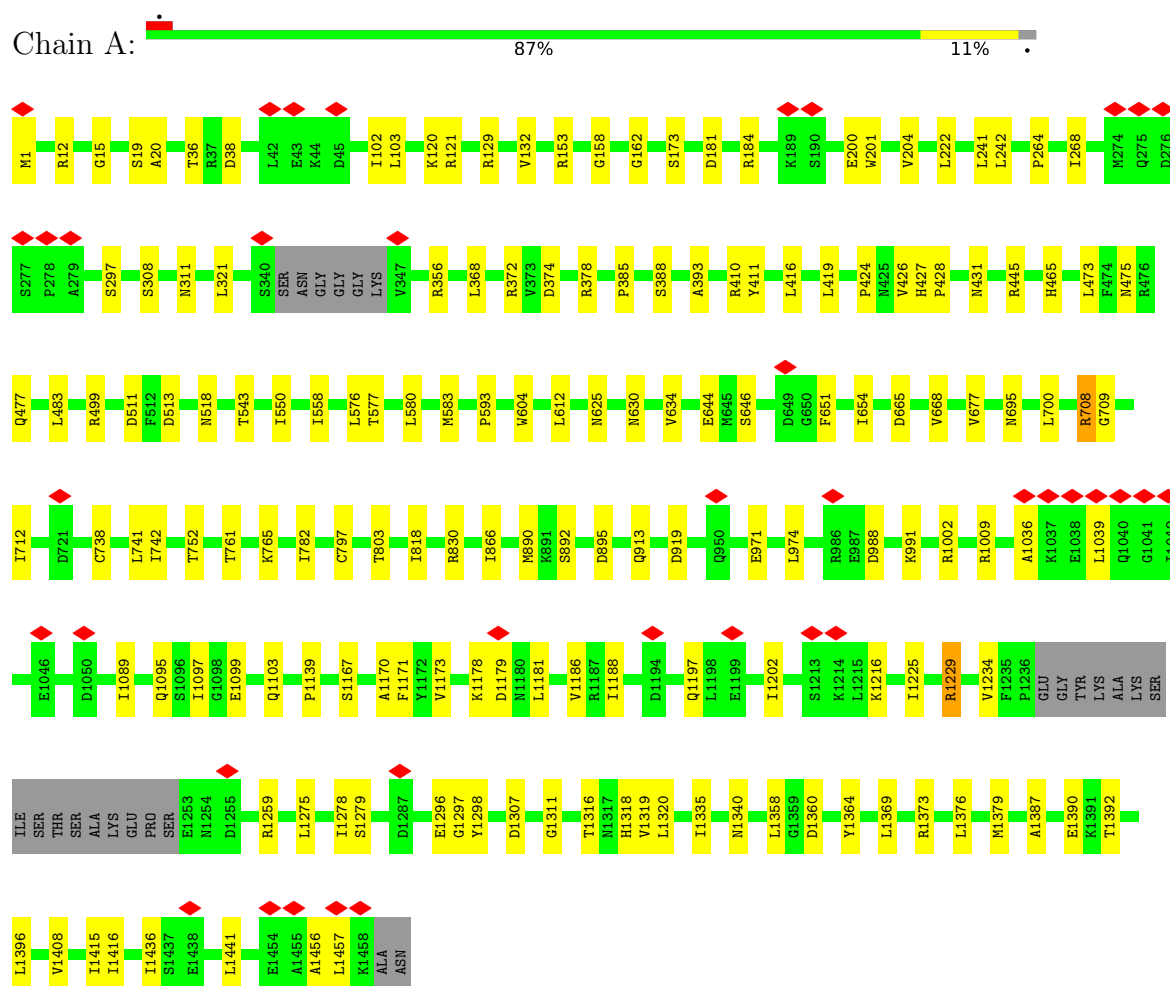


Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			27	24	3	
23	C	1	Total	C	O	0
			27	24	3	

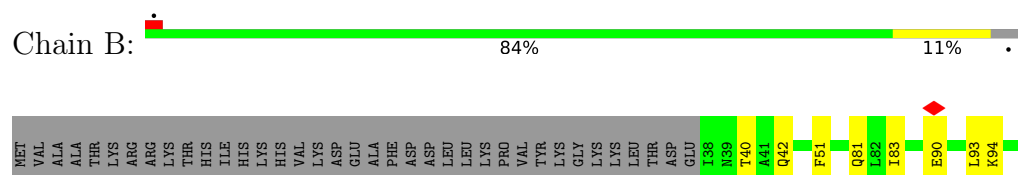
### 3 Residue-property plots

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.

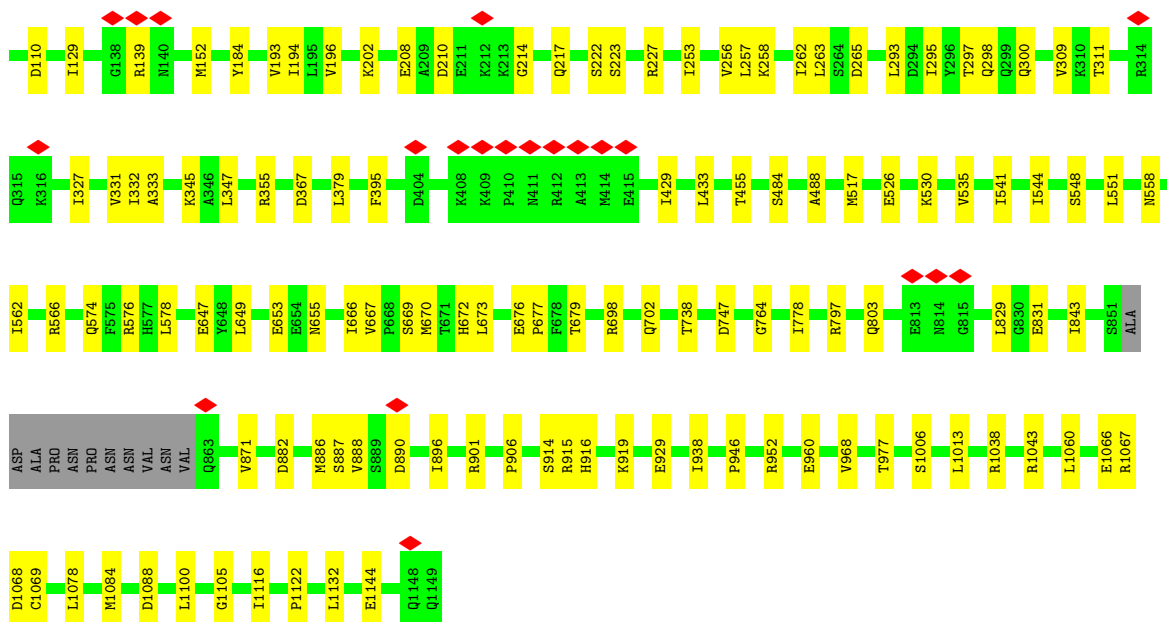
#### • Molecule 1: DNA-directed RNA polymerase III subunit RPC1



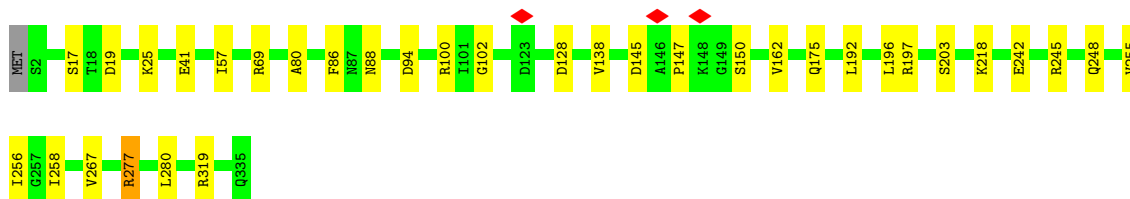
#### • Molecule 2: DNA-directed RNA polymerase III subunit RPC2



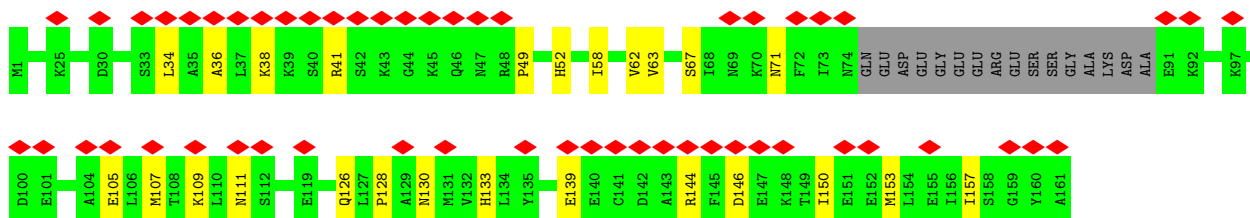
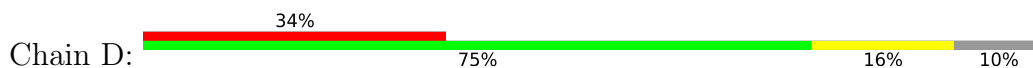




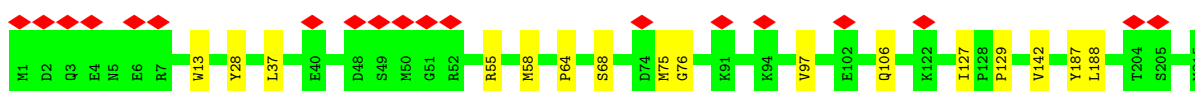
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



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



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




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

Chain F: 

MET SER ASP TTR GLU GLU ALA PHE ASP GLY ASN GLU ASN PHE ASP ASP VAL HIS PHE SER ASP GLU THR TTR GLU LYS PRO GLN PHE LYS ASP GLY THR THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY GLY ASN GLY PRO ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS E71 R79 A80 T81 M85 D116 R119 R136 E150 L151 I152 V153 ASP LEU


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

Chain G: 

M1 D9 L10 I13 I26 N32 N36 V42 I46 V54 V76 F77 E83 I84 V85 T86 G87 W88 I89 S90 K91 K96 I104 F105 D106 D107 M114 G118 C119 Y120 Y121 E124 E125 S126 S127 A127 W128 I129 W130 P131 M132 D133 E134 E135 T136 K137


L138 Y139 F140 V142 N143 E144 K145 I146 R147 E151 E167 L168 E169 E170 R171 A172 Q173 L174 E175 ASN GLU ILE GLY LYS ASN GLU THR PRO GLN ASN E189 K190 G198 G204 L207 V208 S209 W210 W211 E212

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

Chain H: 

MET S2 N3 F10 A28 T31 T32 Q33 D34 C35 C36 P48 V57 L65 GLU ASP THR PRO ALA ASN ASP SER SER ALA T76 D91 E106 D110 E126 R130 I144 R145 R146

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

Chain I: 

M1 C5 P6 S7 H10 G17 D18 S19 G20 T23 L24 S28 C29 F33 P34 L46 F47 R48 K49 E50 V51 D52 D53 V54 L55 G56 G57 G58 G59 D60 N61 V62 D63 Q64 T65 K66 T67 Q68 C69 P70 M71 Y72 D73 T74 C75 G76 G77 E78 S79 A80 Y81 F82 F83

R88 D91 E92 P93 H94 T95 T96 F97 Y98 K99 C100 V101 M102 C103 G104 H105 R106 W107 K108 E109 M110

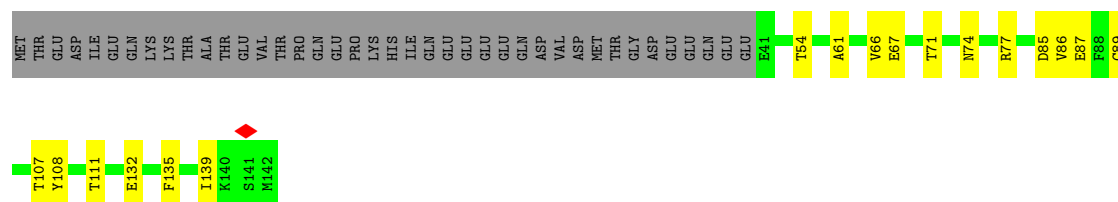
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 

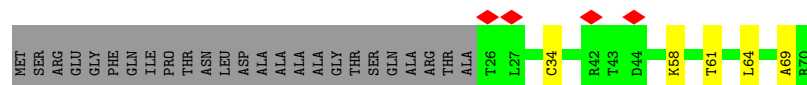
M1 C10 G11 R43 Y44 R48 T52 K68 R69 ASP

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

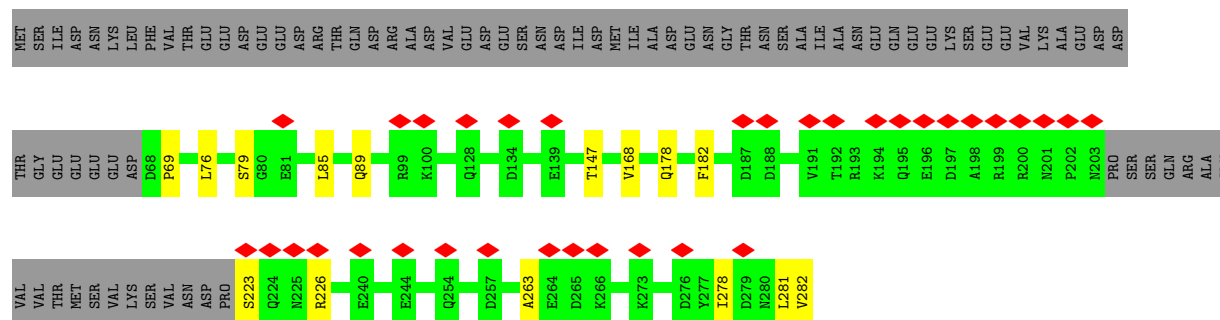
Chain K: 



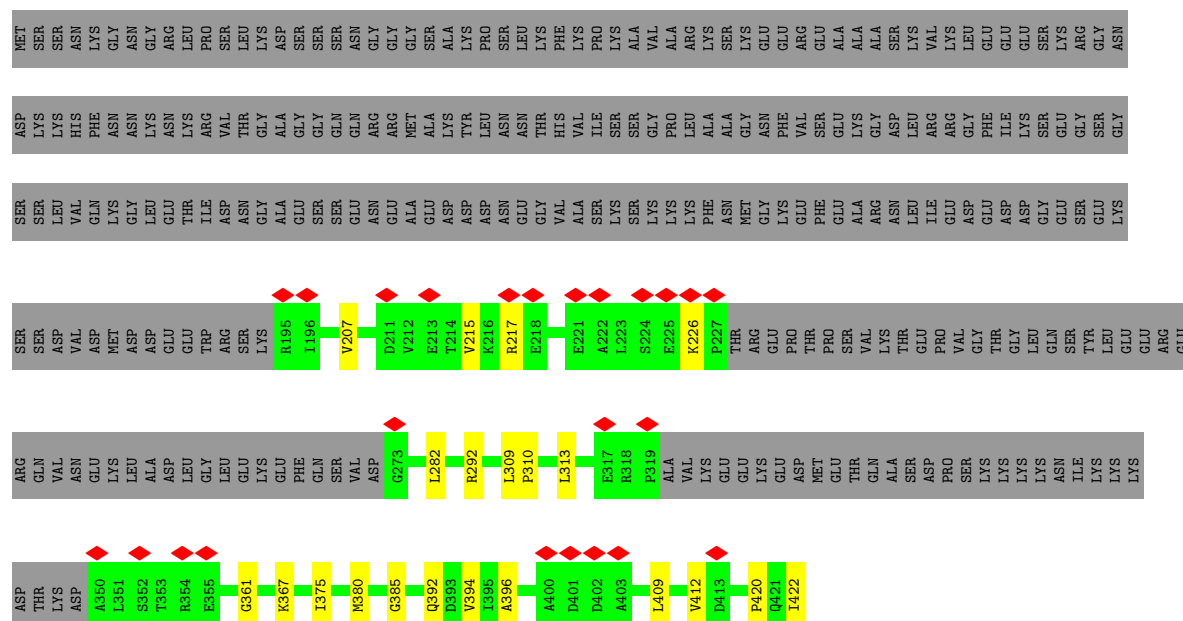
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



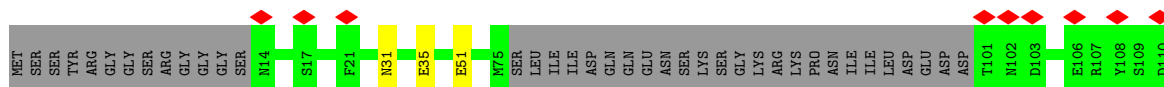
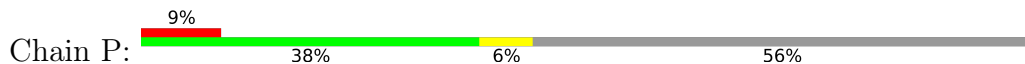
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

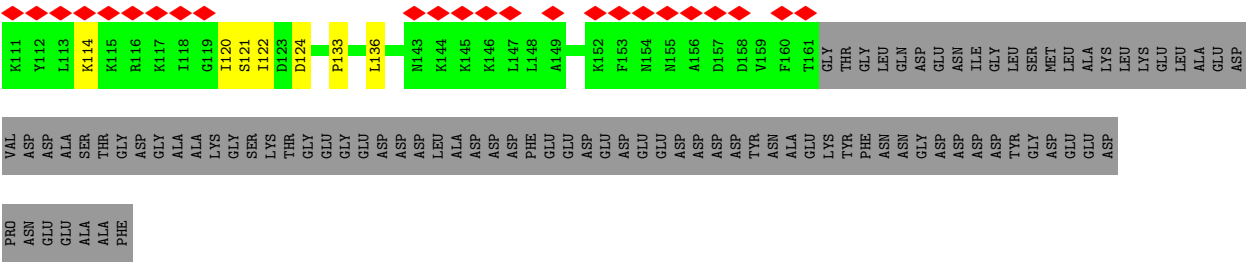


- Molecule 14: DNA-directed RNA polymerase III subunit RPC4

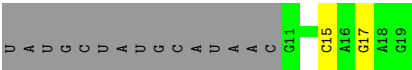


Chain O:  7% 78% 9% 13%

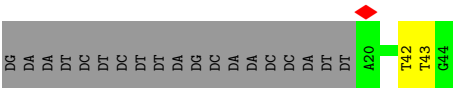




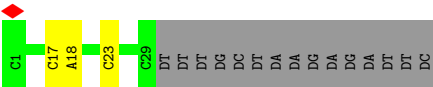
● Molecule 18: RNA



● Molecule 19: NT-DNA



● Molecule 20: T-DNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47279	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 ( $e^-/\text{\AA}^2$ )	40.9	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	Not provided	
Image detector	GATAN K2 IS (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	364.35, 364.35, 364.35	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 4QM, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/11429	0.52	0/15440
2	B	0.27	0/8845	0.51	0/11929
3	C	0.26	0/2703	0.50	0/3666
4	D	0.26	0/1203	0.47	0/1610
5	E	0.27	0/1795	0.53	0/2416
6	F	0.26	0/683	0.52	0/923
7	G	0.26	0/1634	0.51	0/2217
8	H	0.27	0/1102	0.57	0/1492
9	I	0.26	0/894	0.51	0/1208
10	J	0.26	0/577	0.54	0/772
11	K	0.26	0/812	0.52	0/1096
12	L	0.25	0/360	0.65	0/478
13	M	0.25	0/1628	0.49	0/2204
14	N	0.24	0/1210	0.53	0/1625
15	O	0.25	0/4646	0.49	0/6267
16	P	0.27	0/1190	0.48	1/1616 (0.1%)
17	Q	0.27	0/1004	0.48	0/1354
18	R	0.18	0/218	0.71	0/338
19	S	0.53	0/564	1.06	0/868
20	T	0.49	0/669	0.89	0/1031
All	All	0.27	0/43166	0.53	1/58550 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	251	ASP	CB-CG-OD1	5.45	123.21	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11228	0	11362	104	0
2	B	8693	0	8820	87	0
3	C	2647	0	2616	25	0
4	D	1185	0	1206	18	0
5	E	1759	0	1788	9	0
6	F	671	0	692	4	0
7	G	1594	0	1580	18	0
8	H	1084	0	1057	9	0
9	I	873	0	818	10	0
10	J	569	0	584	7	0
11	K	801	0	795	11	0
12	L	358	0	381	5	0
13	M	1594	0	1552	10	0
14	N	1196	0	1257	17	0
15	O	4577	0	4754	36	0
16	P	1159	0	1109	11	0
17	Q	981	0	979	6	0
18	R	195	0	99	0	0
19	S	507	0	289	1	0
20	T	597	0	328	3	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	A	1	0	0	0	0
23	A	27	0	0	0	0
23	C	27	0	0	0	0
All	All	42330	0	42066	330	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 4.

The worst 5 of 330 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:217:ARG:HH12	14:N:282:LEU:HD13	1.50	0.76
1:A:36:THR:HG22	1:A:38:ASP:H	1.58	0.69
15:O:603:LEU:HD21	15:O:630:VAL:HG11	1.74	0.69
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.75	0.68
1:A:162:GLY:HA3	1:A:181:ASP:O	1.93	0.68

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	1428/1460 (98%)	1391 (97%)	37 (3%)	0	100	100
2	B	1097/1149 (96%)	1068 (97%)	29 (3%)	0	100	100
3	C	332/335 (99%)	323 (97%)	9 (3%)	0	100	100
4	D	141/161 (88%)	136 (96%)	5 (4%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
7	G	195/212 (92%)	186 (95%)	9 (5%)	0	100	100
8	H	131/146 (90%)	129 (98%)	2 (2%)	0	100	100
9	I	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
10	J	65/70 (93%)	64 (98%)	1 (2%)	0	100	100
11	K	100/142 (70%)	98 (98%)	2 (2%)	0	100	100
12	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
13	M	192/282 (68%)	186 (97%)	6 (3%)	0	100	100
14	N	147/422 (35%)	143 (97%)	4 (3%)	0	100	100
15	O	566/654 (86%)	557 (98%)	9 (2%)	0	100	100
16	P	136/317 (43%)	133 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	119/251 (47%)	112 (94%)	7 (6%)	0	100	100
All	All	5094/6151 (83%)	4953 (97%)	141 (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	A	1239/1257 (99%)	1235 (100%)	4 (0%)	92	98
2	B	964/1006 (96%)	964 (100%)	0	100	100
3	C	295/296 (100%)	294 (100%)	1 (0%)	92	98
4	D	133/145 (92%)	133 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	73/137 (53%)	72 (99%)	1 (1%)	67	90
7	G	173/190 (91%)	173 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	98/98 (100%)	97 (99%)	1 (1%)	76	93
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	92/130 (71%)	92 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	171/249 (69%)	171 (100%)	0	100	100
14	N	131/360 (36%)	131 (100%)	0	100	100
15	O	524/593 (88%)	524 (100%)	0	100	100
16	P	130/285 (46%)	130 (100%)	0	100	100
17	Q	109/212 (51%)	108 (99%)	1 (1%)	78	94
All	All	4552/5405 (84%)	4544 (100%)	8 (0%)	93	98

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	114	LYS
9	I	49	LYS
3	C	277	ARG
1	A	1340	ASN
6	F	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	702	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	8/24 (33%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	15	C
18	R	17	G

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 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
23	4QM	A	2003	-	30,30,30	1.87	11 (36%)	47,48,48	3.38	26 (55%)
23	4QM	C	401	-	30,30,30	1.87	11 (36%)	47,48,48	3.43	26 (55%)

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
23	4QM	A	2003	-	-	1/7/72/72	0/4/4/4
23	4QM	C	401	-	-	1/7/72/72	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	2003	4QM	C16-C17	3.80	1.59	1.52
23	C	401	4QM	C16-C17	3.79	1.59	1.52
23	C	401	4QM	C16-C15	3.71	1.59	1.53
23	A	2003	4QM	C16-C15	3.69	1.59	1.53
23	A	2003	4QM	C7-C6	-3.25	1.47	1.54

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	401	4QM	C10-C5-C4	8.00	117.21	109.07
23	A	2003	4QM	C10-C5-C4	7.74	116.95	109.07
23	C	401	4QM	C10-C5-C6	-6.61	100.87	111.21
23	A	2003	4QM	C10-C5-C6	-6.31	101.34	111.21
23	C	401	4QM	C2-C19-C18	5.99	118.25	111.82

There are no chirality outliers.

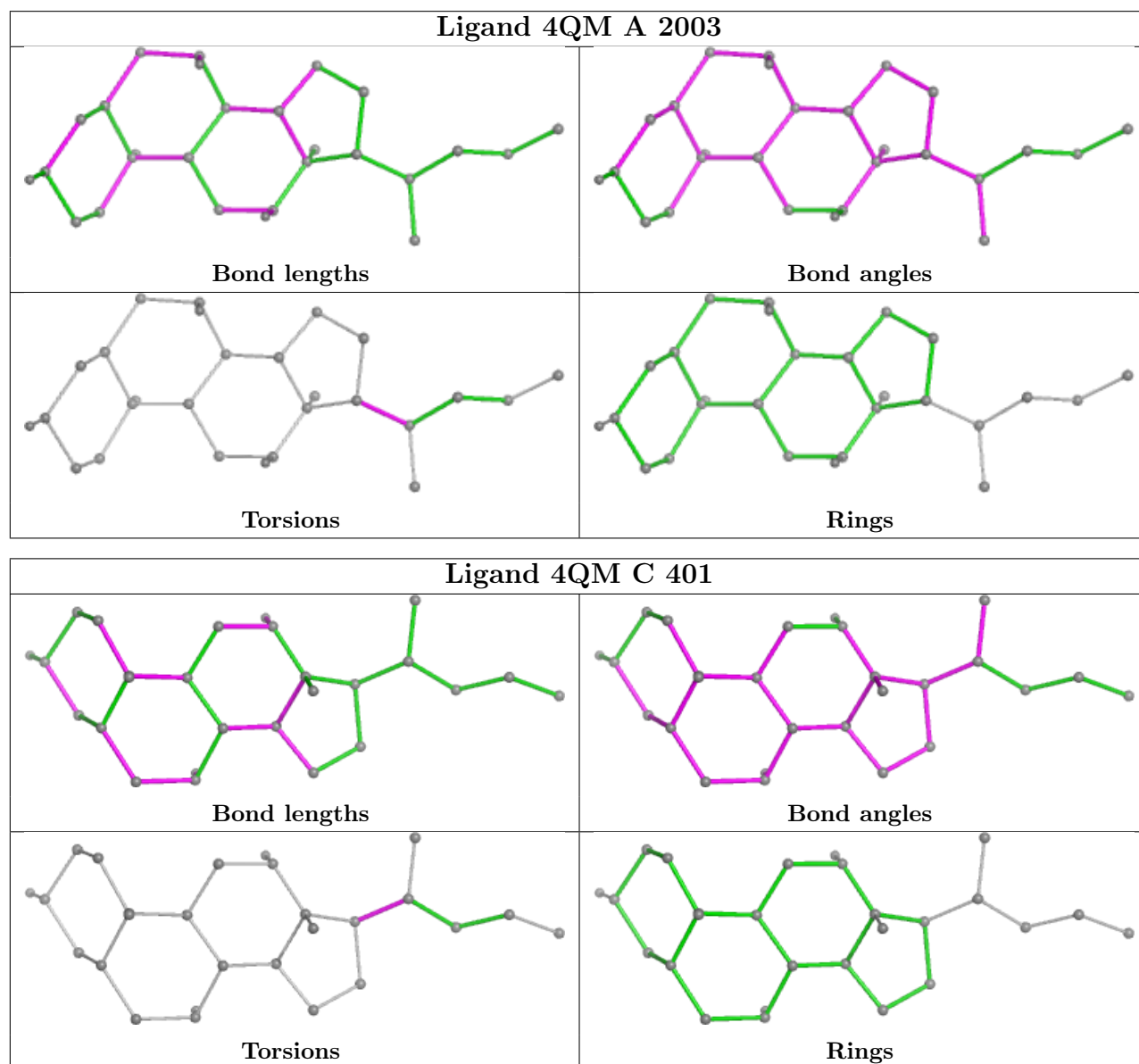
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	C	401	4QM	C22-C20-C9-C5
23	A	2003	4QM	C22-C20-C9-C5

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
10	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1456:ALA	C	1457:LEU	N	3.23
1	J	67:GLU	C	68:LYS	N	3.12

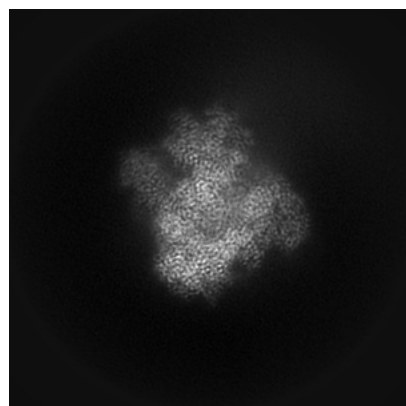
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14447. These allow visual inspection of the internal detail of the map and identification of artifacts.

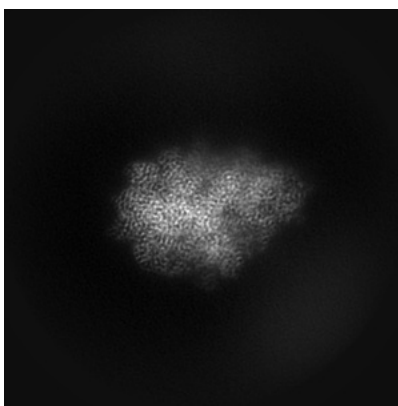
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

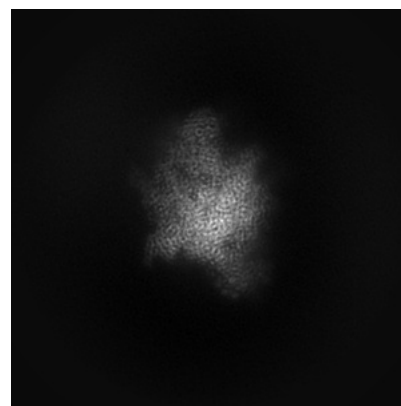
#### 6.1.1 Primary map



X

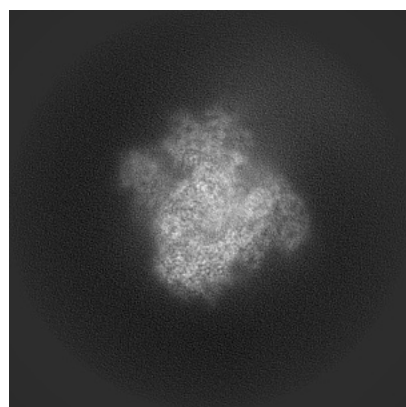


Y

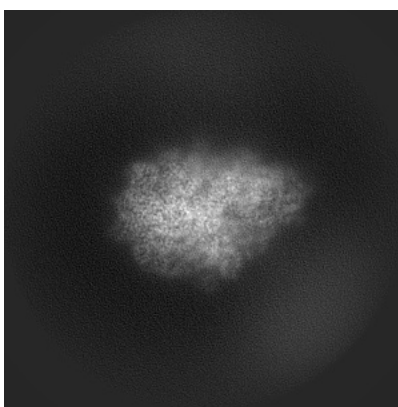


Z

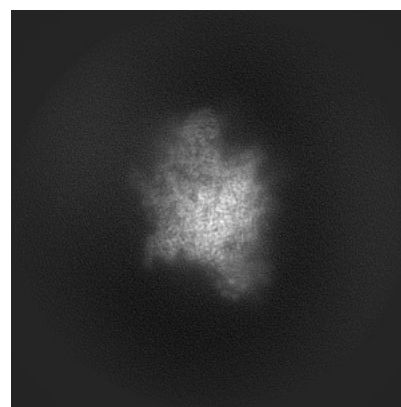
#### 6.1.2 Raw map



X



Y

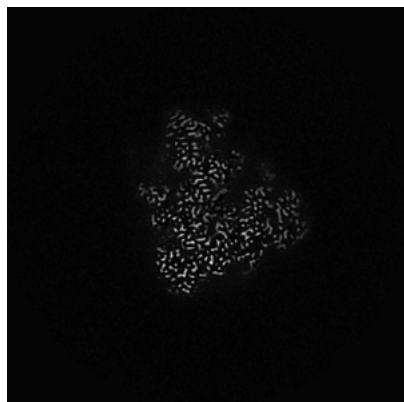


Z

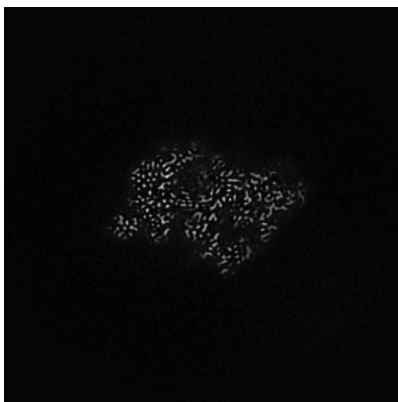
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

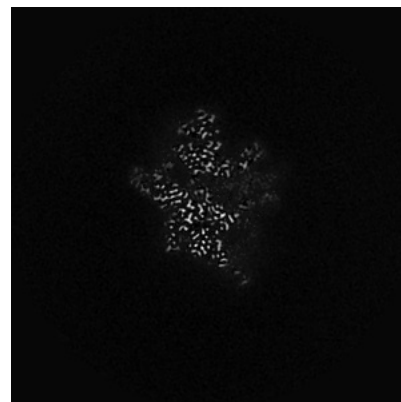
### 6.2.1 Primary map



X Index: 175

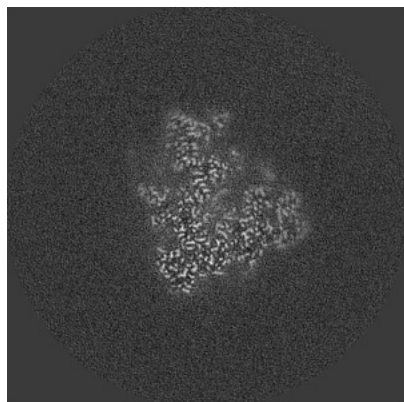


Y Index: 175

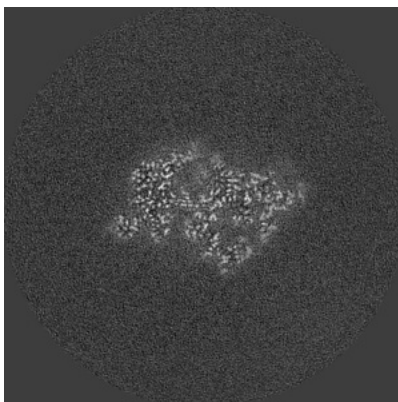


Z Index: 175

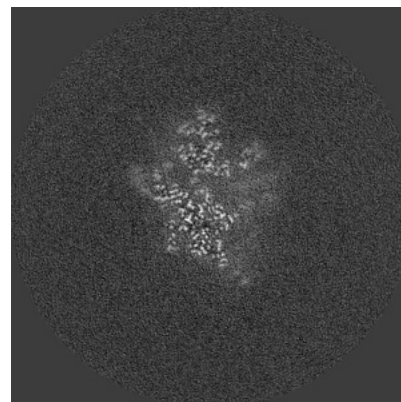
### 6.2.2 Raw map



X Index: 175



Y Index: 175



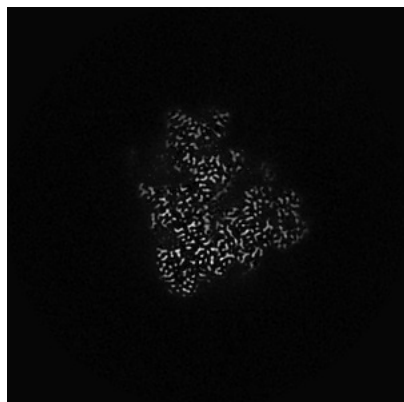
Z Index: 175

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

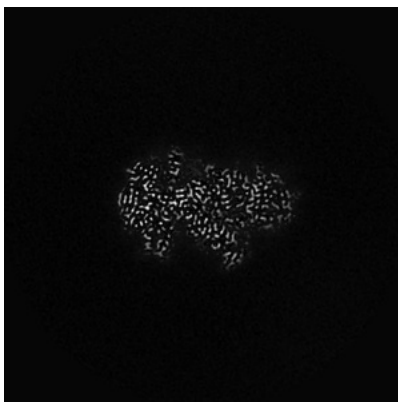


## 6.3 Largest variance slices [i](#)

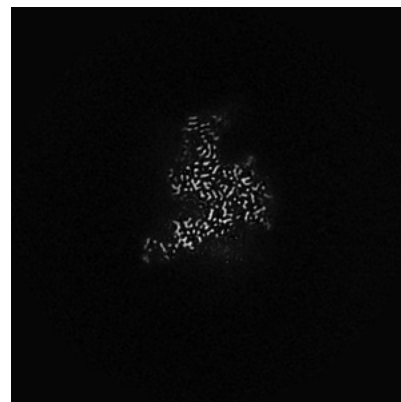
### 6.3.1 Primary map



X Index: 176

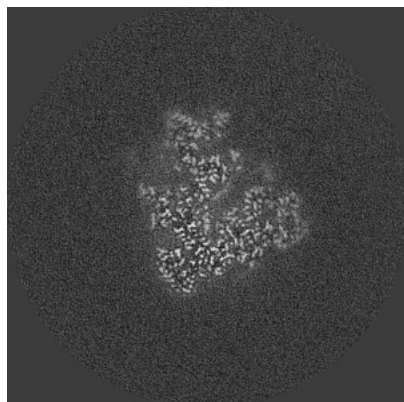


Y Index: 164

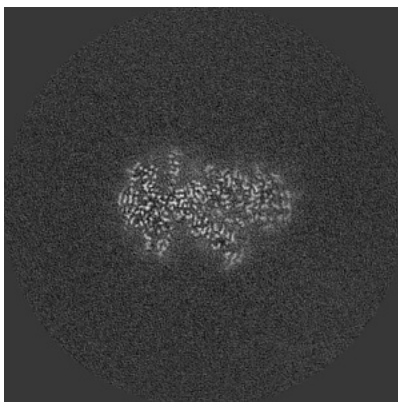


Z Index: 146

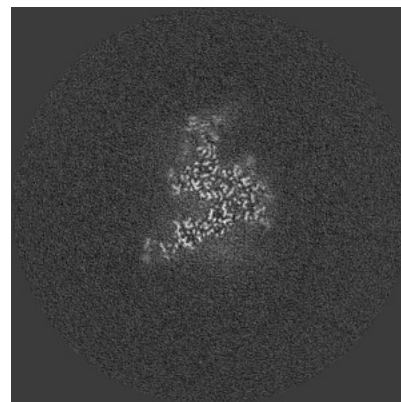
### 6.3.2 Raw map



X Index: 176



Y Index: 164

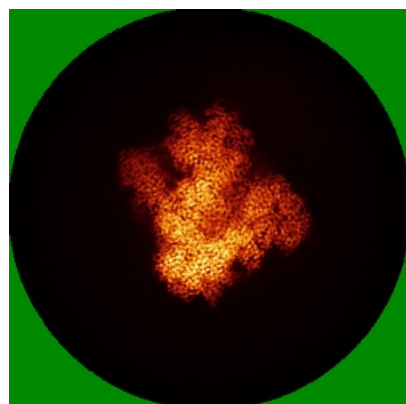


Z Index: 146

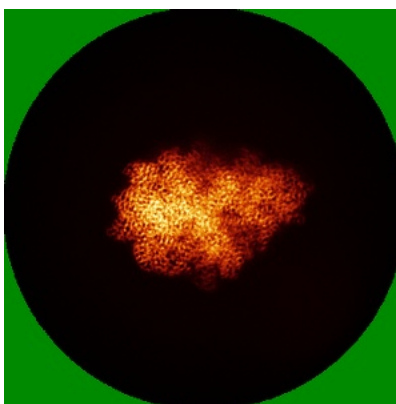
The images above show the largest variance slices of the map in three orthogonal directions.

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

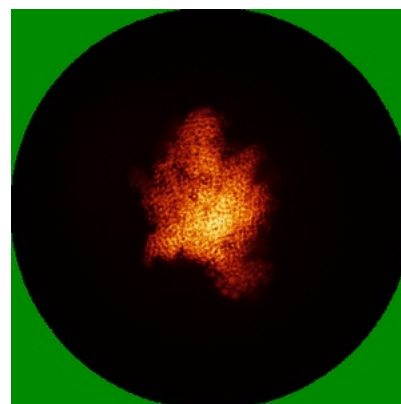
### 6.4.1 Primary map



X

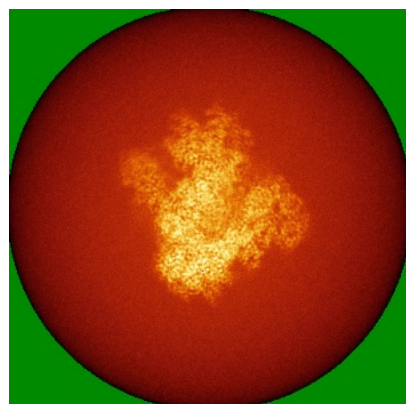


Y

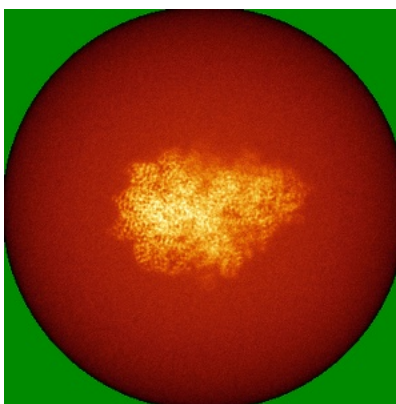


Z

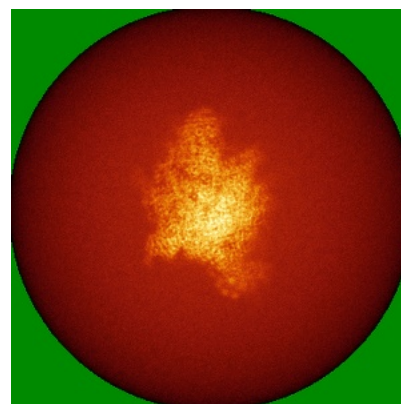
### 6.4.2 Raw map



X



Y

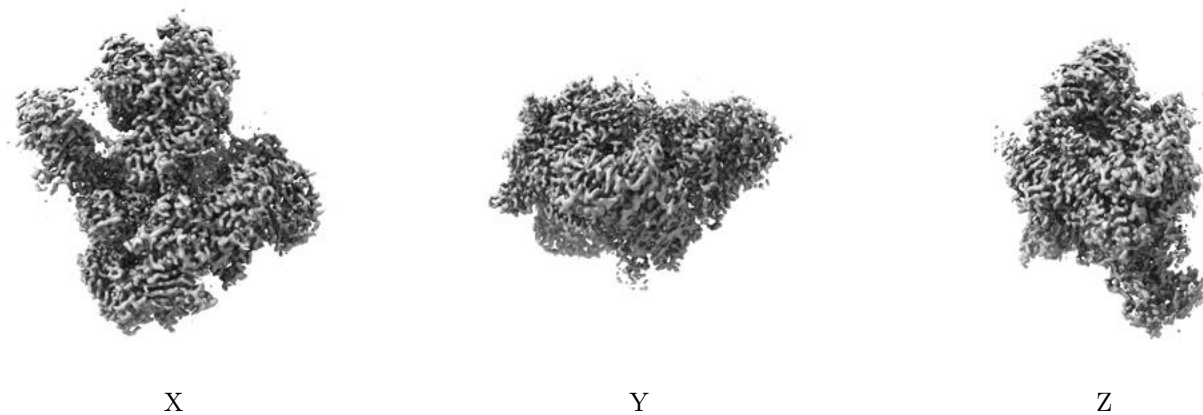


Z

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.

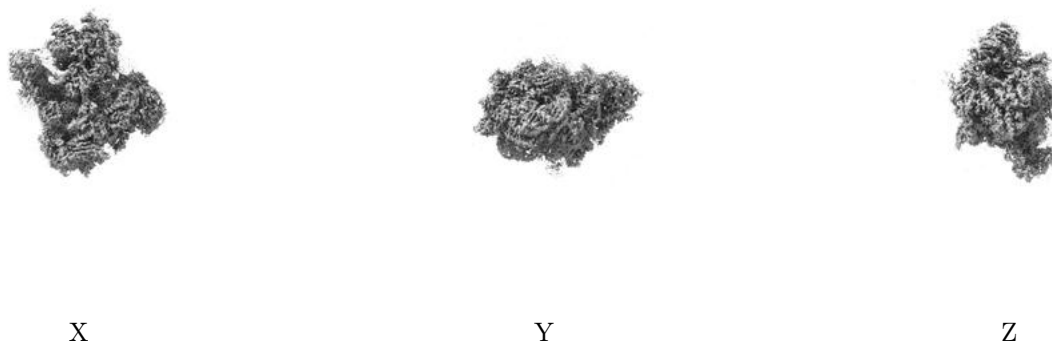
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

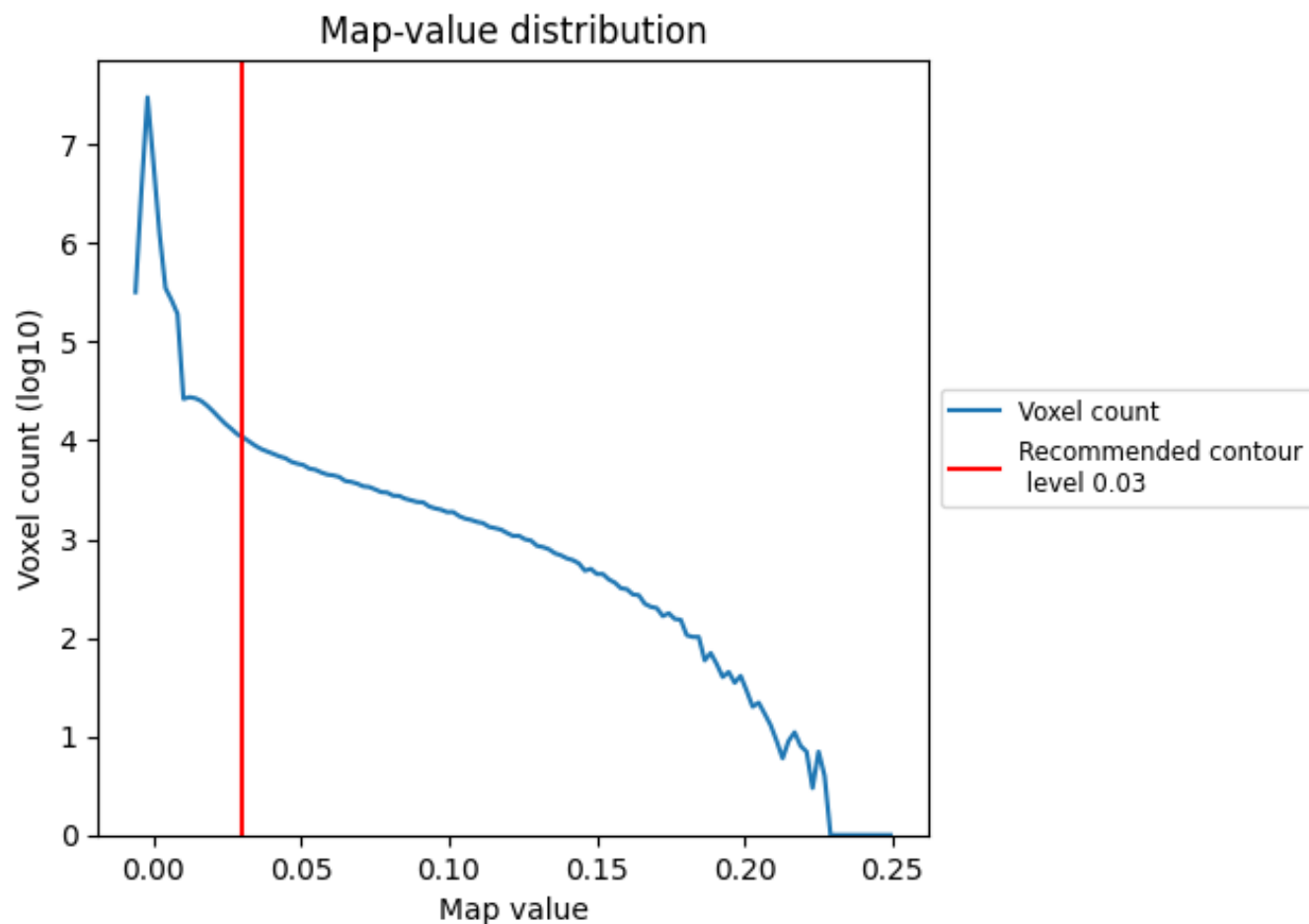
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

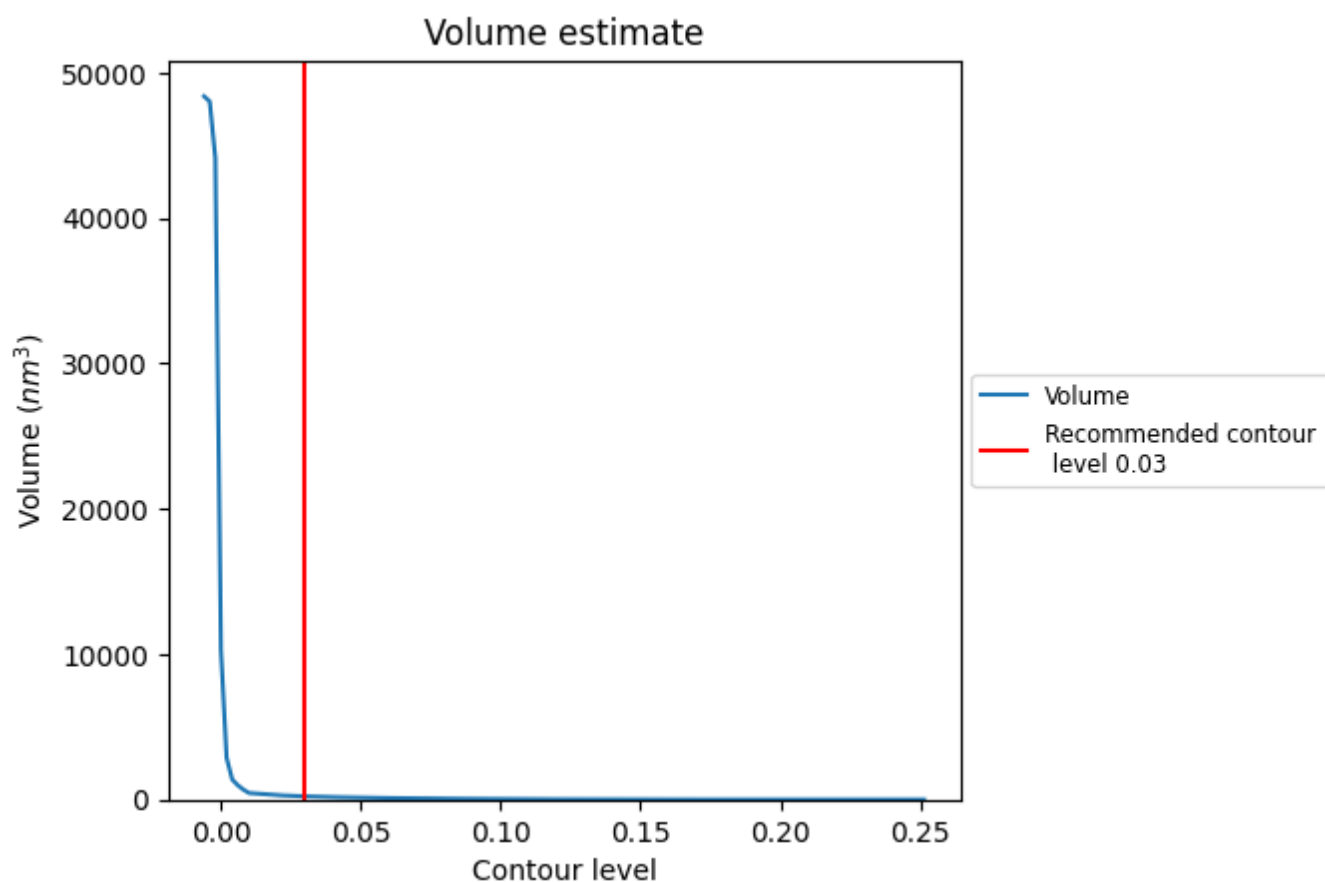
This section contains the results of statistical analysis of the map.

### 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.

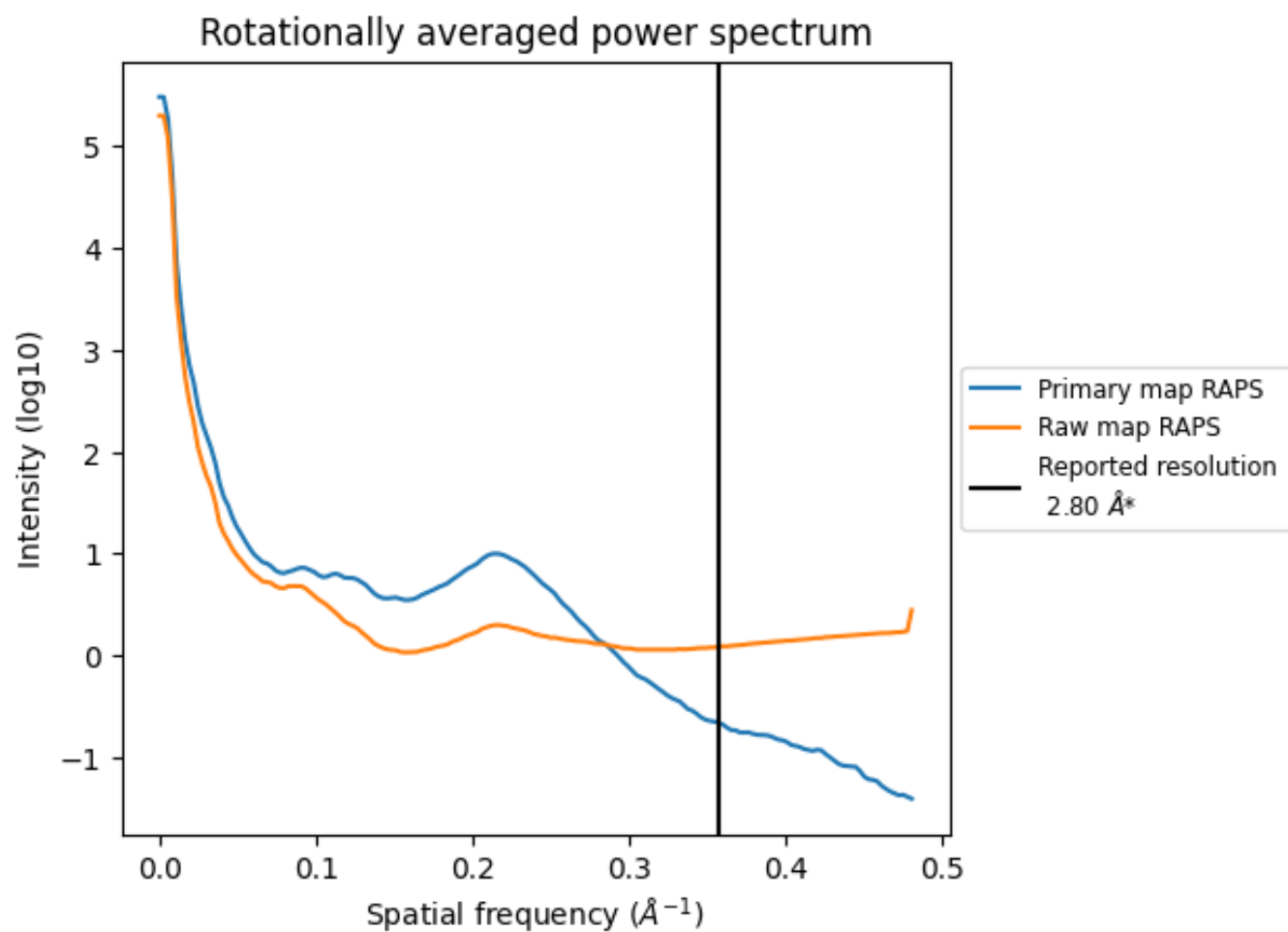
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm<sup>3</sup>; this corresponds to an approximate mass of 200 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 ⓘ

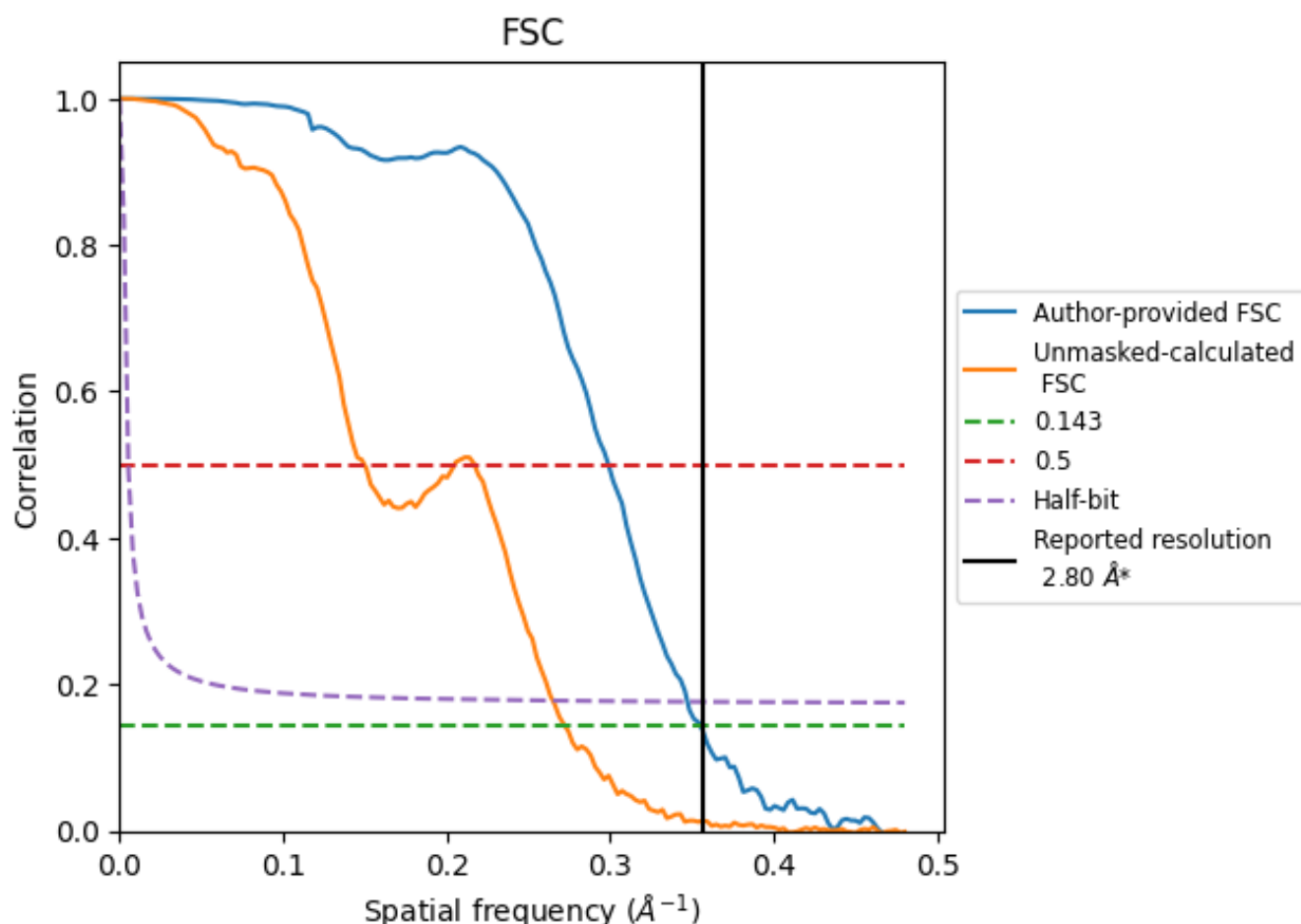


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.34	2.88
Unmasked-calculated*	3.67	6.68	3.77

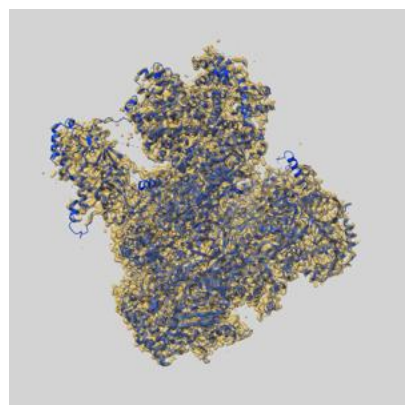
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.8 by more than 10 %



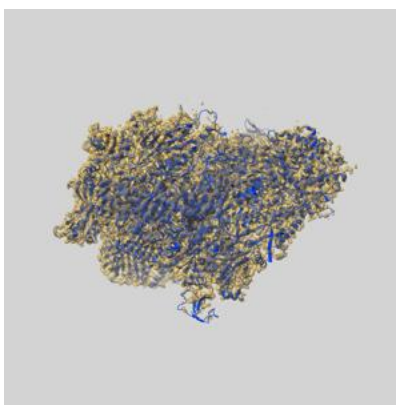
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14447 and PDB model 7Z1L. Per-residue inclusion information can be found in section [3](#) on page [8](#).

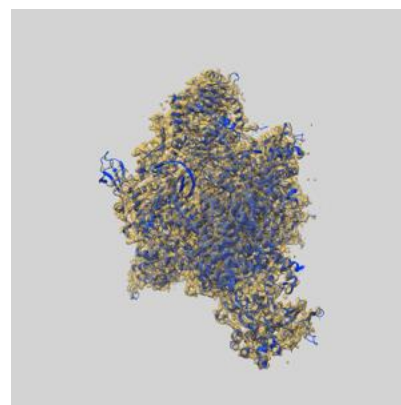
### 9.1 Map-model overlay [i](#)



X



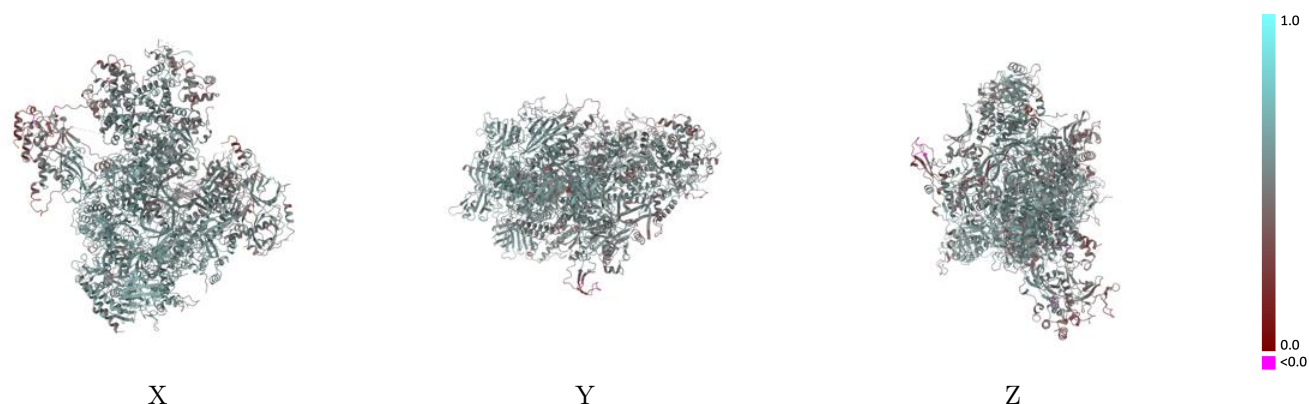
Y



Z

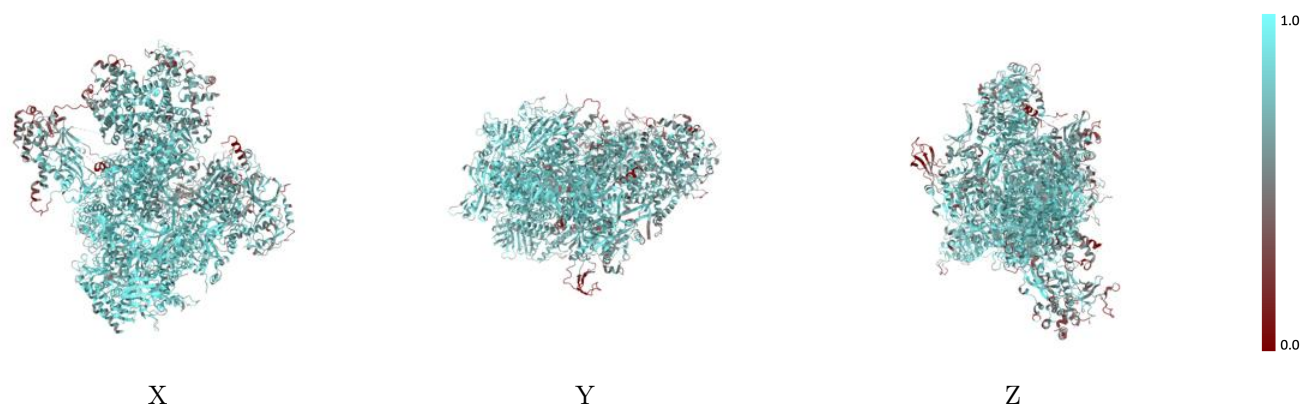
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



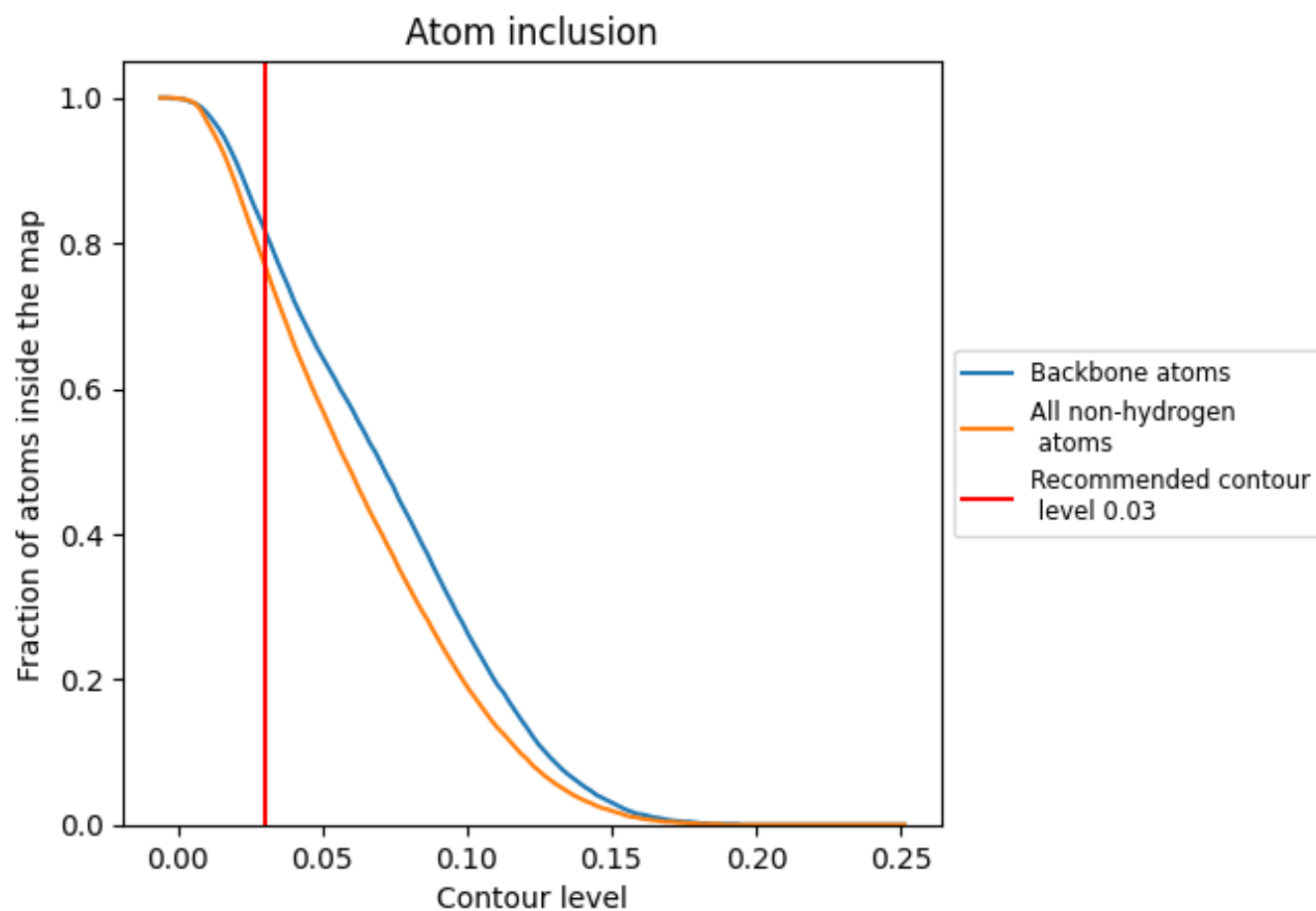
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.5380
A	 0.8310	 0.5620
B	 0.8460	 0.5700
C	 0.8380	 0.5740
D	 0.5110	 0.4110
E	 0.7460	 0.5220
F	 0.8500	 0.5670
G	 0.6420	 0.4760
H	 0.8110	 0.5680
I	 0.4480	 0.4170
J	 0.8710	 0.5860
K	 0.8320	 0.5640
L	 0.7720	 0.5520
M	 0.6420	 0.4860
N	 0.6450	 0.4910
O	 0.7170	 0.5130
P	 0.6180	 0.4720
Q	 0.5990	 0.4790
R	 0.8620	 0.5490
S	 0.8440	 0.5490
T	 0.8410	 0.5540

