



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 11:04 AM EST

PDB ID : 7MEI  
EMDB ID : EMD-23789  
Title : Composite structure of EC+EC  
Authors : Yang, C.; Murakami, K.  
Deposited on : 2021-04-06  
Resolution : 3.54 Å(reported)  
Based on initial models : 5C4J, 3PO2, 5FMF

This is a Full wwPDB EM Validation 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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

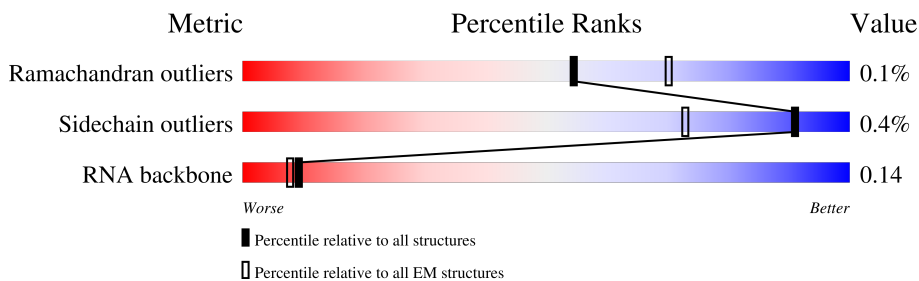
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.54 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)
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	N	74	
2	O	74	
3	A	1733	
3	a	1733	
4	B	1224	
4	b	1224	
5	C	318	
5	c	318	

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Mol	Chain	Length	Quality of chain
6	D	221	33% 76% 24%
6	d	221	75% 24%
7	E	215	100%
7	e	215	99% 24%
8	F	155	56% 44%
8	f	155	56% 44%
9	G	171	39% 99% 24%
9	g	171	99% 24%
10	H	146	90% 8%
10	h	146	91% 8%
11	I	122	93% 7%
11	i	122	93% 7%
12	J	70	94% 6%
12	j	70	94% 6%
13	K	120	7% 96% 24%
13	k	120	7% 96% 24%
14	L	70	63% 37%
14	l	70	61% 37%
15	r	16	38% 62%
16	R	15	20% 40% 60%
17	Q	735	29% 71%
18	M	400	34% 66%

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 69281 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 DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	N	74	1519	727	290	428	74	0	0

- Molecule 2 is a DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	O	74	1524	730	263	457	74	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	a	1425	11189	7046	1955	2126	62	0	0
3	A	1425	11167	7036	1948	2121	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	b	1160	9197	5805	1614	1723	55	0	0
4	B	1166	9227	5823	1619	1729	56	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	265	2086	1312	347	414	13	0	0
5	C	265	2086	1312	347	414	13	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	168	Total	C	N	O	S	0	0
			1331	822	237	270	2		
6	D	168	Total	C	N	O	S	0	0
			1331	822	237	270	2		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		
7	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	87	Total	C	N	O	S	0	0
			705	451	119	132	3		
8	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		
9	G	171	Total	C	N	O	S	0	0
			1335	858	221	248	8		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	h	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		
10	H	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	114	Total	C	N	O	S	0	0
			927	571	168	178	10		
11	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	j	66	Total	C	N	O	S	0	0
			540	345	94	95	6		
12	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	k	115	Total	C	N	O	S	0	0
			924	593	157	172	2		
13	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 14 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	44	Total	C	N	O	S	0	0
			352	217	70	61	4		
14	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 15 is a RNA chain called RNA (5'-R(P\*AP\*AP\*CP\*UP\*AP\*GP\*UP\*UP\*AP\*A P\*GP\*AP\*GP\*GP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	16	Total	C	N	O	P	0	0
			333	150	55	112	16		

- Molecule 16 is a RNA chain called RNA (5'-R(P\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*U P\*CP\*CP\*CP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	15	Total	C	N	O	P	0	0
			312	141	56	100	15		

- Molecule 17 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	214	1619	1017	297	299	6	0	0

- Molecule 18 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	M	135	1106	694	197	210	5	0	0

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	a	2	Total 2	Zn 2	0
19	b	1	Total 1	Zn 1	0
19	c	1	Total 1	Zn 1	0
19	i	2	Total 2	Zn 2	0
19	j	1	Total 1	Zn 1	0
19	l	1	Total 1	Zn 1	0
19	A	2	Total 2	Zn 2	0
19	B	1	Total 1	Zn 1	0
19	C	1	Total 1	Zn 1	0
19	I	2	Total 2	Zn 2	0
19	J	1	Total 1	Zn 1	0
19	L	1	Total 1	Zn 1	0

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

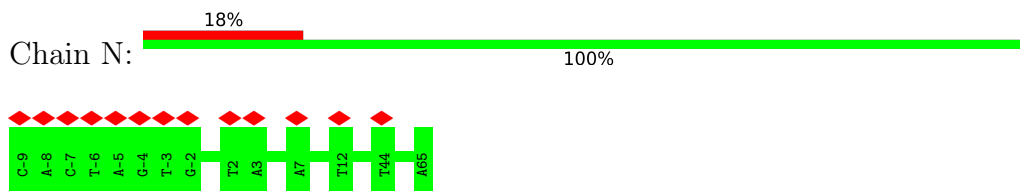
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
20	a	2	Total 2	Mg 2	0
20	A	1	Total 1	Mg 1	0
20	R	1	Total 1	Mg 1	0



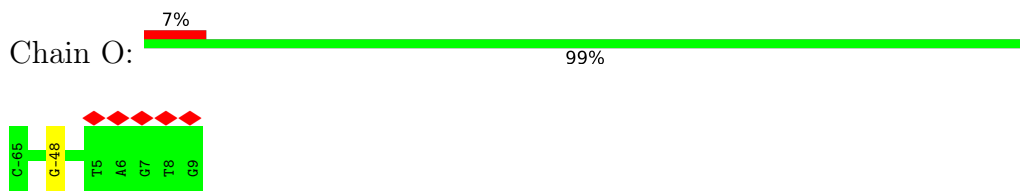
### 3 Residue-property plots [i](#)

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.

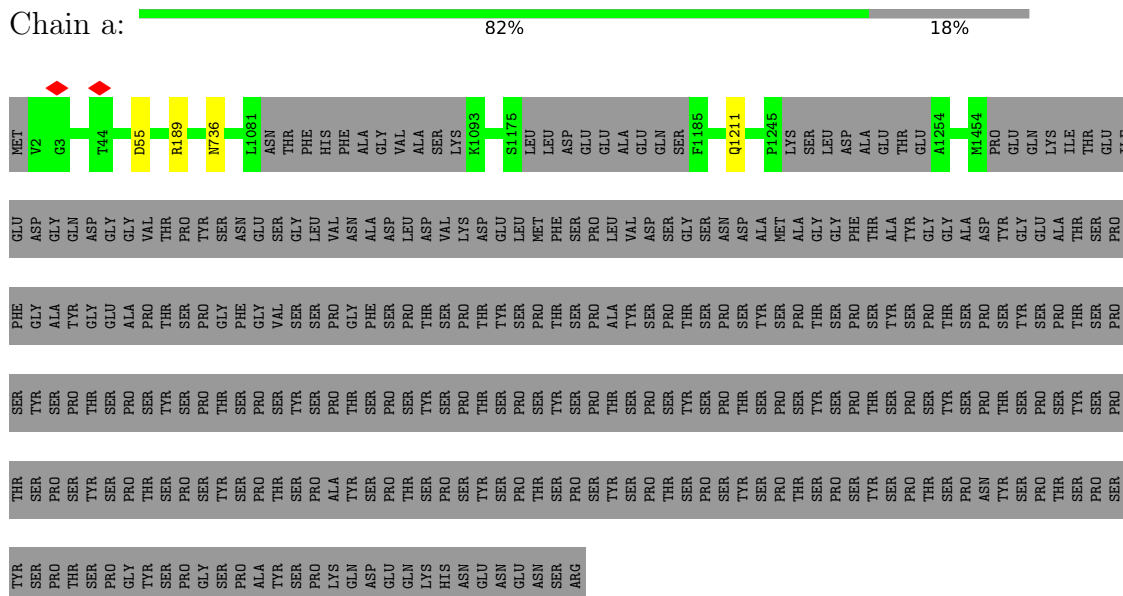
- Molecule 1: DNA (74-MER)



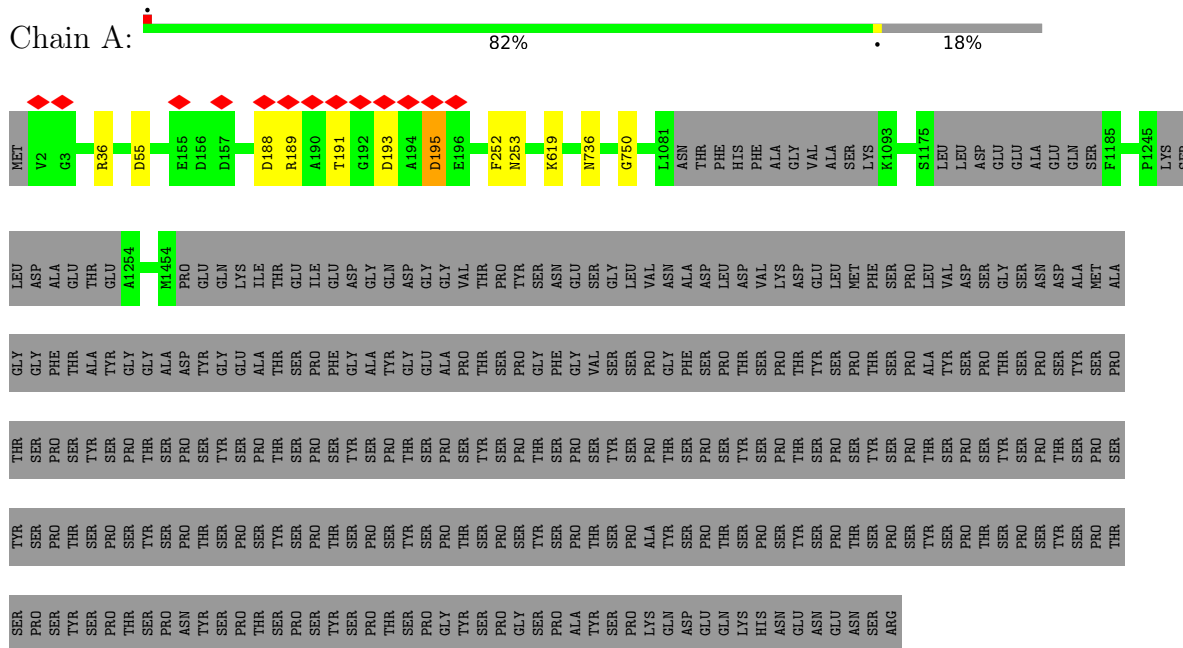
- Molecule 2: DNA (74-MER)



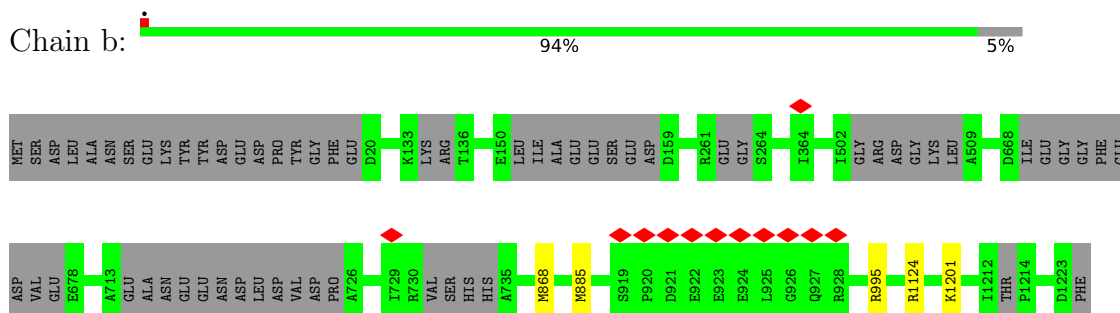
- Molecule 3: DNA-directed RNA polymerase subunit



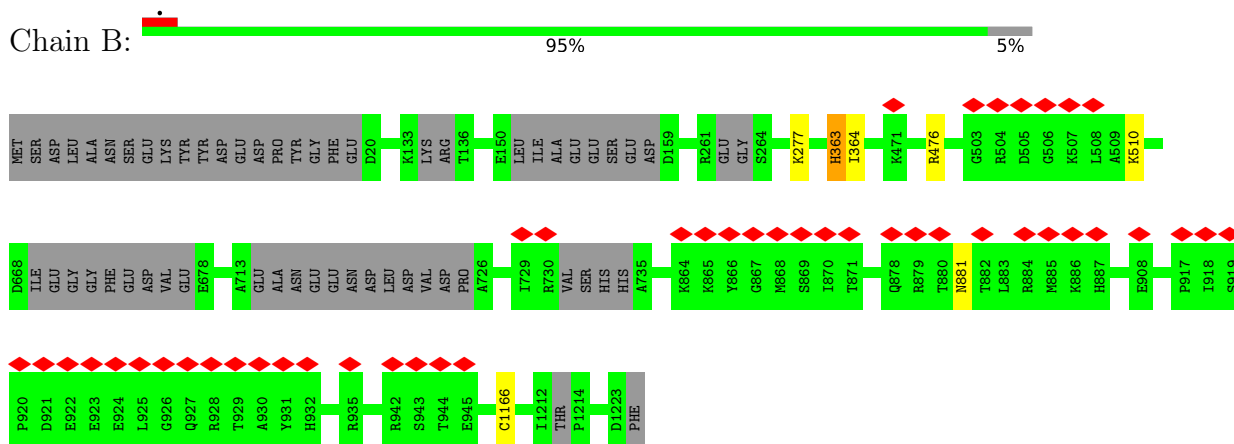
- Molecule 3: DNA-directed RNA polymerase subunit



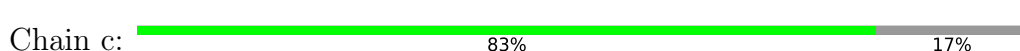
• Molecule 4: DNA-directed RNA polymerase subunit beta

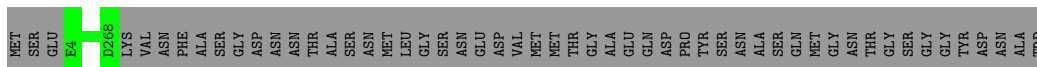


• Molecule 4: DNA-directed RNA polymerase subunit beta

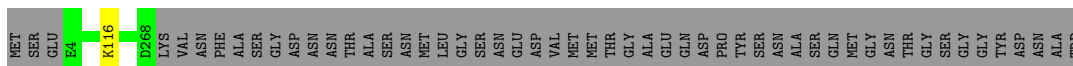
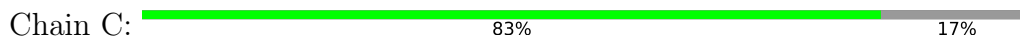


• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

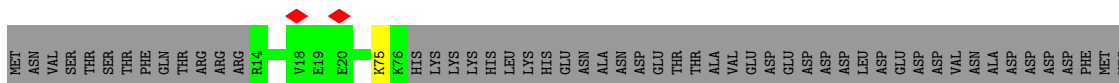




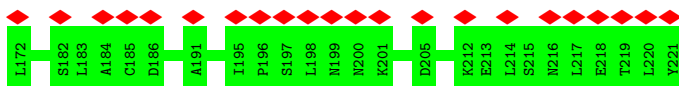
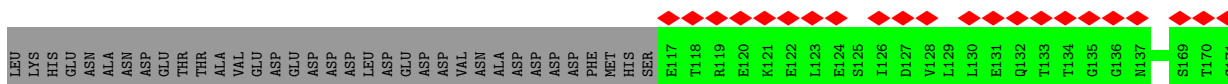
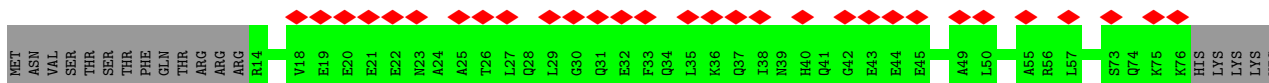
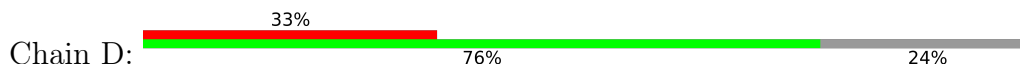
- Molecule 5: DNA-directed RNA polymerase II subunit RPB3



- Molecule 6: DNA-directed RNA polymerase II subunit RPB4



- Molecule 6: DNA-directed RNA polymerase II subunit RPB4



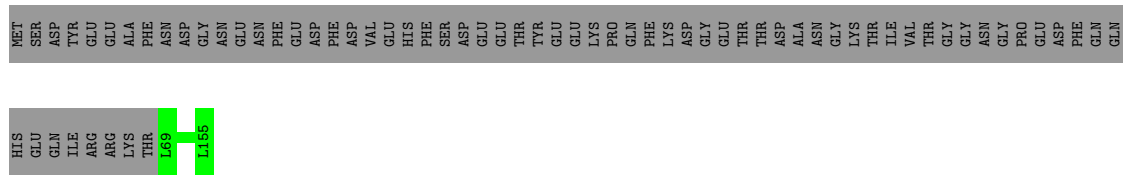
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



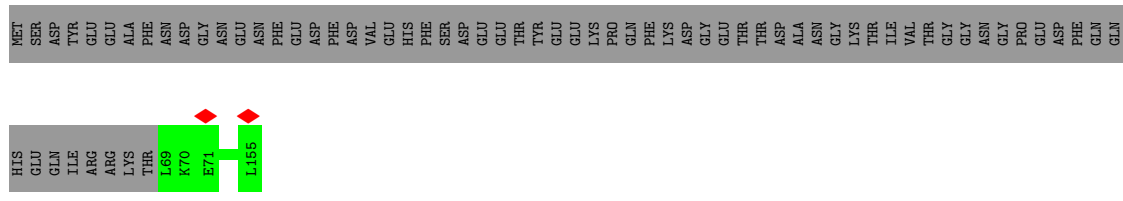
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



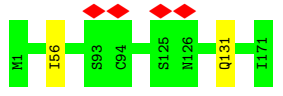
• Molecule 8: DNA-directed RNA polymerases I,II,and III subunit RPABC2



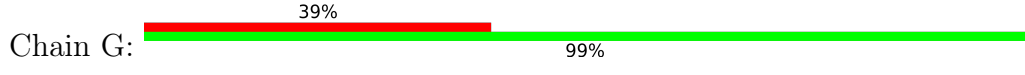
• Molecule 8: DNA-directed RNA polymerases I,II,and III subunit RPABC2



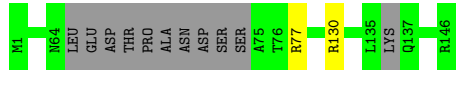
• Molecule 9: DNA-directed RNA polymerase II subunit RPB7



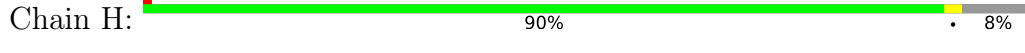
• Molecule 9: DNA-directed RNA polymerase II subunit RPB7

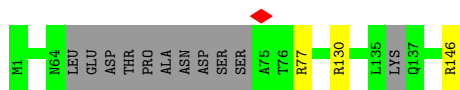


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3





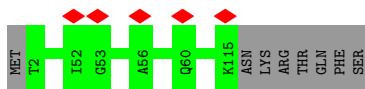
- Molecule 11: DNA-directed RNA polymerase II subunit RPB9

Chain i: 93% 7%



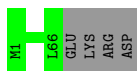
- Molecule 11: DNA-directed RNA polymerase II subunit RPB9

Chain I: 93% 7%



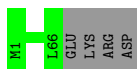
- Molecule 12: DNA-directed RNA polymerases II subunit RPABC5

Chain j: 94% 6%



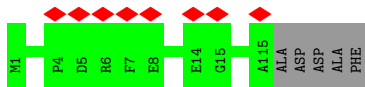
- Molecule 12: DNA-directed RNA polymerases II subunit RPABC5

Chain J: 94% 6%



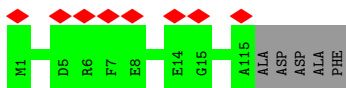
- Molecule 13: DNA-directed RNA polymerase II subunit RPB11

Chain k: 7% 96% .



- Molecule 13: DNA-directed RNA polymerase II subunit RPB11

Chain K: 7% 96% .



- Molecule 14: DNA-directed RNA polymerases II subunit RPABC4





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57690	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0088	Depositor
Map size ( $\text{\AA}$ )	367.2, 367.2, 367.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	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, 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	N	0.59	0/1709	0.92	0/2633
2	O	0.69	0/1706	0.99	1/2635 (0.0%)
3	A	0.32	0/11368	0.49	0/15383
3	a	0.34	0/11390	0.50	0/15408
4	B	0.34	0/9402	0.52	1/12680 (0.0%)
4	b	0.36	0/9371	0.52	1/12636 (0.0%)
5	C	0.32	0/2124	0.50	0/2879
5	c	0.34	0/2124	0.47	0/2879
6	D	0.24	0/1339	0.44	0/1793
6	d	0.26	0/1339	0.50	0/1793
7	E	0.32	0/1788	0.45	0/2406
7	e	0.34	0/1788	0.46	0/2406
8	F	0.35	0/717	0.51	0/967
8	f	0.37	0/717	0.54	0/967
9	G	0.29	0/1363	0.49	0/1840
9	g	0.31	0/1367	0.54	0/1844
10	H	0.33	0/1097	0.52	0/1484
10	h	0.34	0/1097	0.50	0/1484
11	I	0.30	0/945	0.45	0/1273
11	i	0.31	0/945	0.48	0/1273
12	J	0.40	0/549	0.51	0/738
12	j	0.41	0/549	0.47	0/738
13	K	0.32	0/942	0.48	0/1272
13	k	0.33	0/942	0.48	0/1272
14	L	0.28	0/354	0.57	0/468
14	l	0.31	0/354	0.48	0/468
15	r	0.80	0/370	0.88	1/572 (0.2%)
16	R	0.57	0/347	0.85	1/536 (0.2%)
17	Q	0.27	0/1648	0.45	1/2226 (0.0%)
18	M	0.25	0/1124	0.47	0/1517
All	All	0.36	0/70875	0.54	6/96470 (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
3	A	0	3
3	a	0	1
4	B	0	3
4	b	0	1
7	e	0	1
9	G	0	1
9	g	0	2
All	All	0	12

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1166	CYS	CB-CA-C	-6.85	96.70	110.40
15	r	40	U	N1-C1'-C2'	-6.56	104.79	112.00
2	O	-48	DG	O4'-C4'-C3'	-5.96	102.12	104.50
16	R	12	A	O5'-P-OP1	-5.83	100.45	105.70
17	Q	421	PRO	N-CA-CB	5.72	110.17	103.30
4	b	885	MET	CA-CB-CG	5.07	121.91	113.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	252	PHE	Peptide
3	A	55	ASP	Peptide
3	A	750	GLY	Peptide
4	B	363	HIS	Peptide
4	B	510	LYS	Peptide
4	B	881	ASN	Peptide
9	G	154	VAL	Peptide
3	a	55	ASP	Peptide
4	b	868	MET	Peptide
7	e	171	LYS	Peptide
9	g	131	GLN	Peptide
9	g	56	ILE	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	
3	A	1417/1733 (82%)	1266 (89%)	148 (10%)	3 (0%)	47	80
3	a	1417/1733 (82%)	1235 (87%)	182 (13%)	0	100	100
4	B	1150/1224 (94%)	1000 (87%)	148 (13%)	2 (0%)	47	80
4	b	1142/1224 (93%)	984 (86%)	158 (14%)	0	100	100
5	C	263/318 (83%)	231 (88%)	32 (12%)	0	100	100
5	c	263/318 (83%)	225 (86%)	38 (14%)	0	100	100
6	D	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
6	d	164/221 (74%)	156 (95%)	8 (5%)	0	100	100
7	E	212/215 (99%)	196 (92%)	16 (8%)	0	100	100
7	e	212/215 (99%)	193 (91%)	18 (8%)	1 (0%)	29	68
8	F	85/155 (55%)	77 (91%)	8 (9%)	0	100	100
8	f	85/155 (55%)	77 (91%)	8 (9%)	0	100	100
9	G	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
9	g	169/171 (99%)	152 (90%)	17 (10%)	0	100	100
10	H	129/146 (88%)	110 (85%)	19 (15%)	0	100	100
10	h	129/146 (88%)	111 (86%)	18 (14%)	0	100	100
11	I	112/122 (92%)	102 (91%)	10 (9%)	0	100	100
11	i	112/122 (92%)	104 (93%)	8 (7%)	0	100	100
12	J	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
12	j	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
13	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	k	113/120 (94%)	106 (94%)	7 (6%)	0	100	100
14	L	42/70 (60%)	30 (71%)	12 (29%)	0	100	100
14	l	42/70 (60%)	30 (71%)	12 (29%)	0	100	100
17	Q	208/735 (28%)	202 (97%)	6 (3%)	0	100	100
18	M	131/400 (33%)	123 (94%)	8 (6%)	0	100	100
All	All	8171/10265 (80%)	7240 (89%)	925 (11%)	6 (0%)	54	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	188	ASP
4	B	364	ILE
3	A	195	ASP
3	A	253	ASN
4	B	363	HIS
7	e	172	GLU

### 5.3.2 Protein sidechains [i](#)

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	
3	A	1235/1520 (81%)	1228 (99%)	7 (1%)	86	94
3	a	1240/1520 (82%)	1237 (100%)	3 (0%)	93	98
4	B	1000/1061 (94%)	998 (100%)	2 (0%)	93	98
4	b	999/1061 (94%)	996 (100%)	3 (0%)	92	98
5	C	233/274 (85%)	232 (100%)	1 (0%)	91	97
5	c	233/274 (85%)	233 (100%)	0	100	100
6	D	146/200 (73%)	146 (100%)	0	100	100
6	d	146/200 (73%)	144 (99%)	2 (1%)	67	85
7	E	196/197 (100%)	196 (100%)	0	100	100
7	e	196/197 (100%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	77/137 (56%)	77 (100%)	0	100	100
8	f	77/137 (56%)	77 (100%)	0	100	100
9	G	151/152 (99%)	151 (100%)	0	100	100
9	g	152/152 (100%)	152 (100%)	0	100	100
10	H	118/128 (92%)	115 (98%)	3 (2%)	47	76
10	h	118/128 (92%)	116 (98%)	2 (2%)	60	83
11	I	108/116 (93%)	108 (100%)	0	100	100
11	i	108/116 (93%)	108 (100%)	0	100	100
12	J	61/65 (94%)	61 (100%)	0	100	100
12	j	61/65 (94%)	61 (100%)	0	100	100
13	K	99/102 (97%)	99 (100%)	0	100	100
13	k	99/102 (97%)	99 (100%)	0	100	100
14	L	39/57 (68%)	39 (100%)	0	100	100
14	l	39/57 (68%)	38 (97%)	1 (3%)	46	75
17	Q	147/641 (23%)	145 (99%)	2 (1%)	67	85
18	M	125/363 (34%)	125 (100%)	0	100	100
All	All	7203/9022 (80%)	7177 (100%)	26 (0%)	91	97

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	a	189	ARG
3	a	736	ASN
3	a	1211	GLN
4	b	995	ARG
4	b	1124	ARG
4	b	1201	LYS
6	d	75	LYS
6	d	121	LYS
10	h	77	ARG
10	h	130	ARG
14	l	49	LYS
3	A	36	ARG
3	A	189	ARG
3	A	191	THR
3	A	193	ASP

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Mol	Chain	Res	Type
3	A	195	ASP
3	A	619	LYS
3	A	736	ASN
4	B	277	LYS
4	B	476	ARG
5	C	116	LYS
10	H	77	ARG
10	H	130	ARG
10	H	146	ARG
17	Q	330	ARG
17	Q	333	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	a	209	ASN
3	a	659	HIS
3	a	768	GLN
3	a	881	GLN
3	a	965	GLN
3	a	1171	GLN
3	a	1432	GLN
4	b	47	GLN
4	b	357	GLN
4	b	395	GLN
4	b	776	GLN
4	b	794	ASN
4	b	821	GLN
4	b	834	ASN
4	b	1076	HIS
5	c	65	HIS
12	j	53	HIS
3	A	68	GLN
3	A	71	GLN
3	A	451	HIS
3	A	768	GLN
3	A	802	ASN
3	A	851	HIS
3	A	1128	GLN
3	A	1171	GLN
3	A	1390	ASN
4	B	110	HIS

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Mol	Chain	Res	Type
4	B	538	ASN
4	B	834	ASN
4	B	881	ASN
5	C	102	GLN
6	D	39	ASN
6	D	41	GLN
6	D	74	GLN
6	D	150	ASN
8	F	100	GLN
11	I	87	GLN
11	I	89	GLN
13	K	40	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	r	15/16 (93%)	9 (60%)	0
16	R	14/15 (93%)	8 (57%)	0
All	All	29/31 (93%)	17 (58%)	0

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	r	35	C
15	r	36	U
15	r	38	G
15	r	41	C
15	r	42	U
15	r	43	A
15	r	45	U
15	r	47	U
15	r	48	C
16	R	5	C
16	R	8	A
16	R	9	C
16	R	10	A
16	R	11	A
16	R	13	U
16	R	15	C
16	R	18	A

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 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 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.



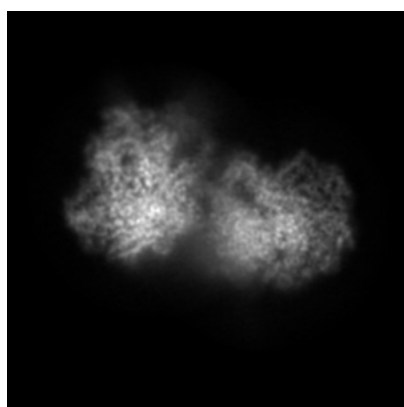
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23789. These allow visual inspection of the internal detail of the map and identification of artifacts.

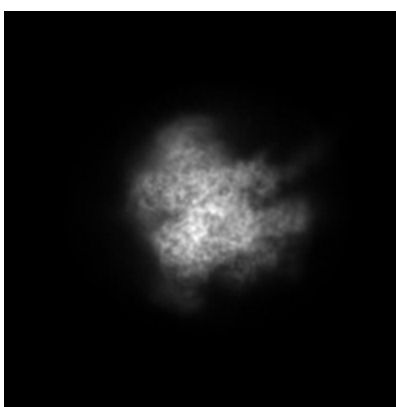
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

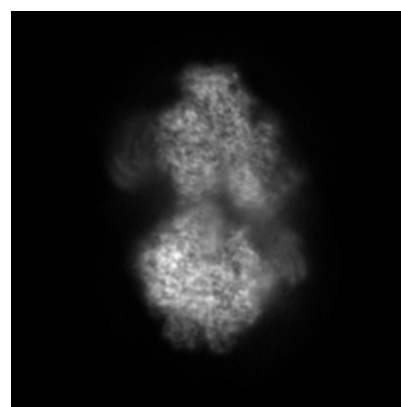
#### 6.1.1 Primary map



X



Y

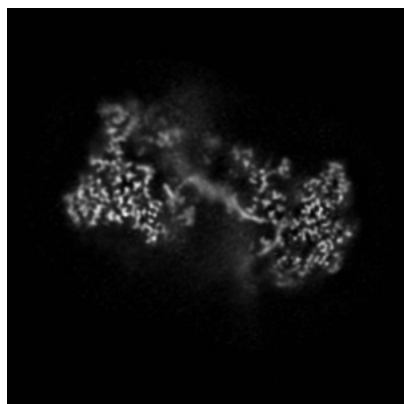


Z

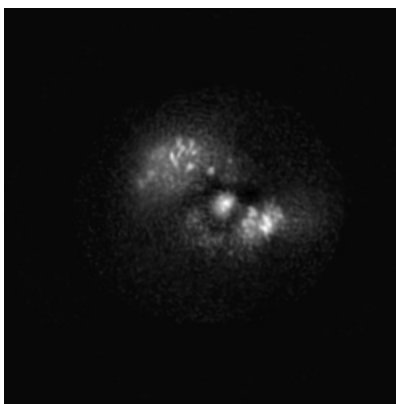
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

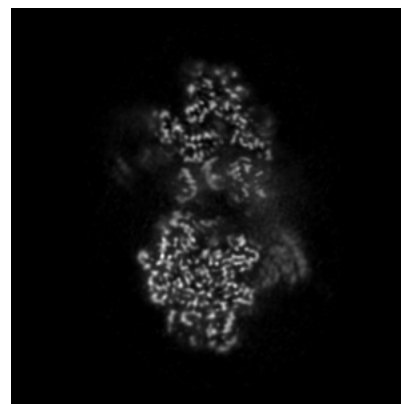
#### 6.2.1 Primary map



X Index: 170



Y Index: 170

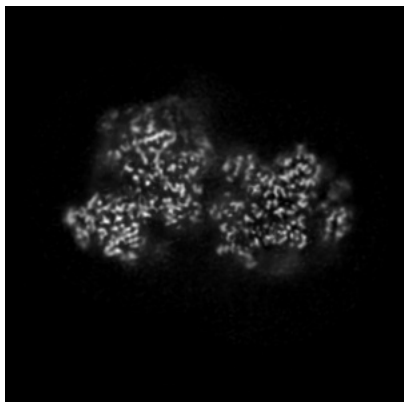


Z Index: 170

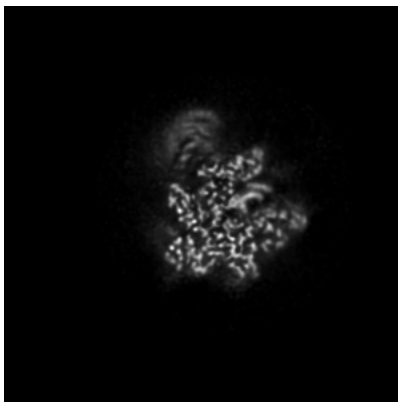
The images above show central slices of the map in three orthogonal directions.

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

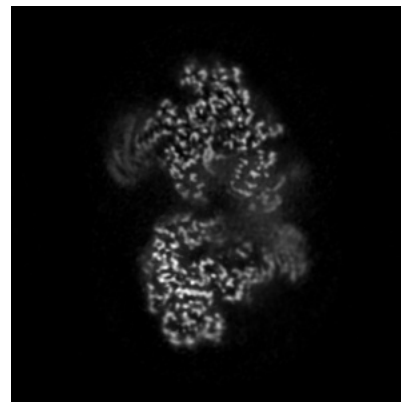
### 6.3.1 Primary map



X Index: 150



Y Index: 119

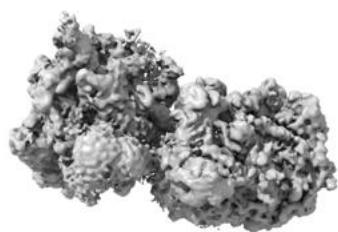


Z Index: 159

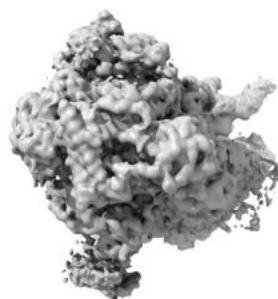
The images above show the largest variance slices of the map in three orthogonal directions.

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

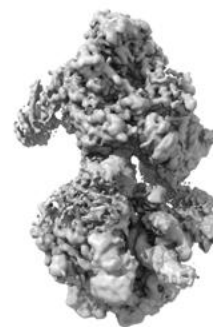
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

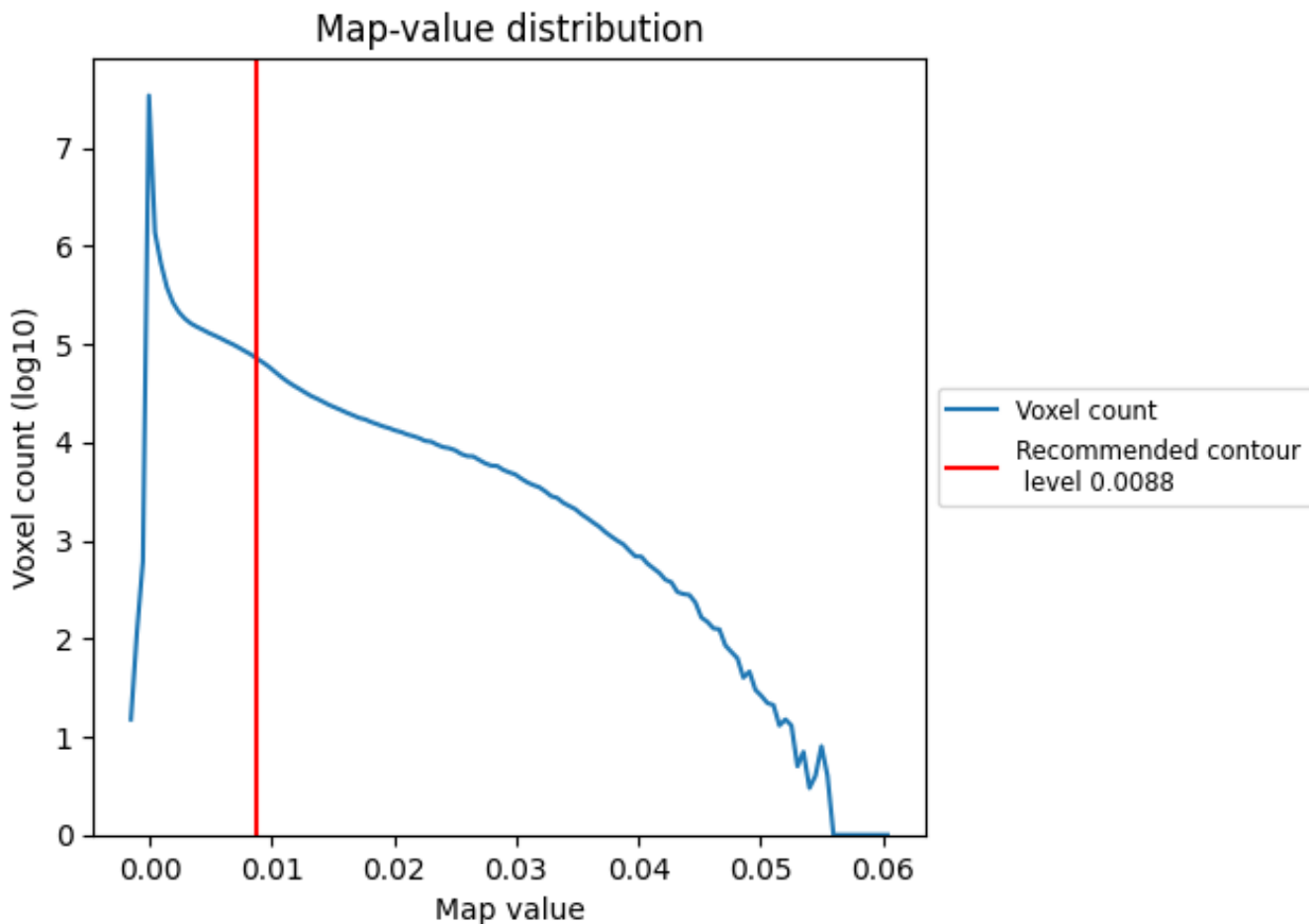
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

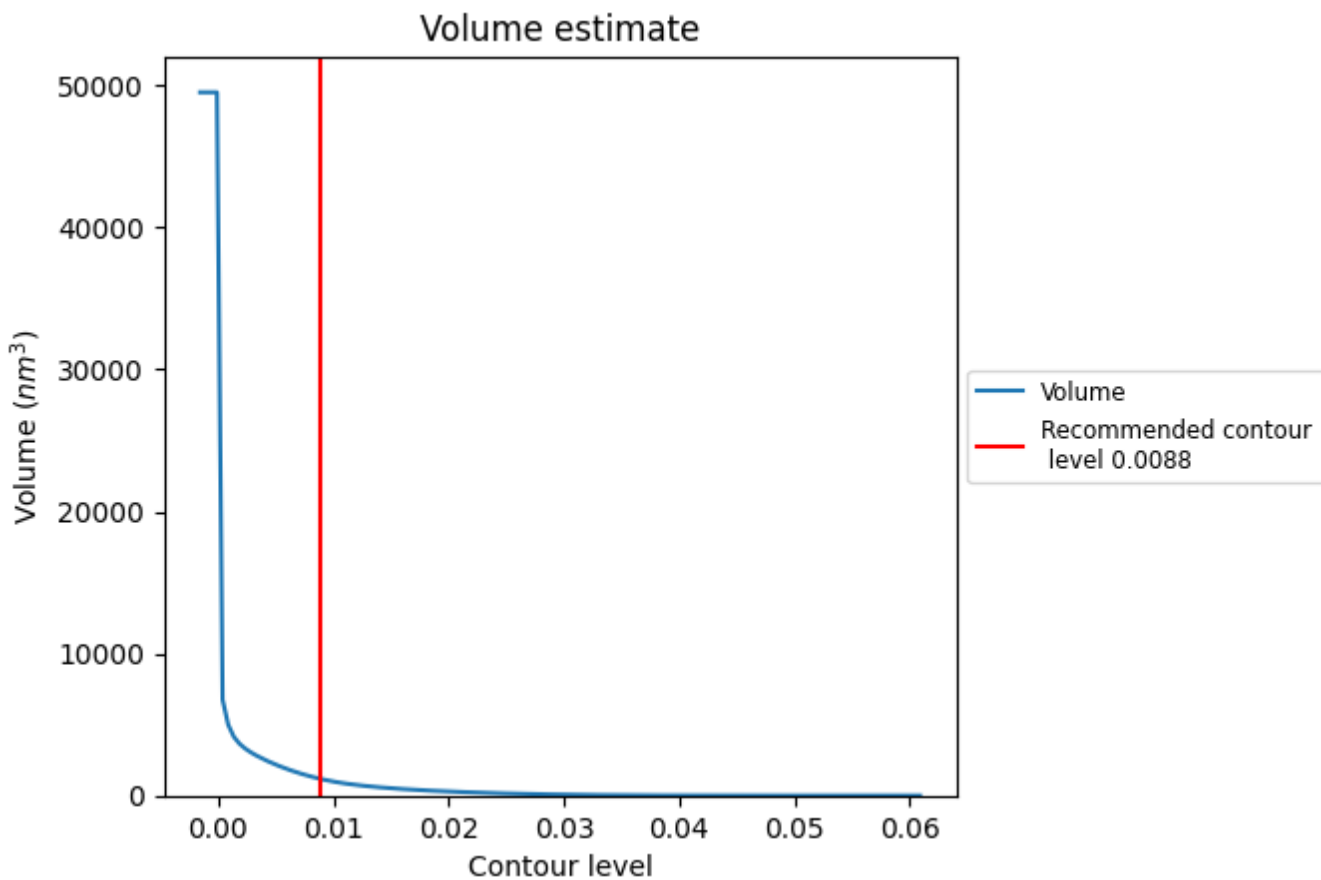
This section contains the results of statistical analysis of the map.

### 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.

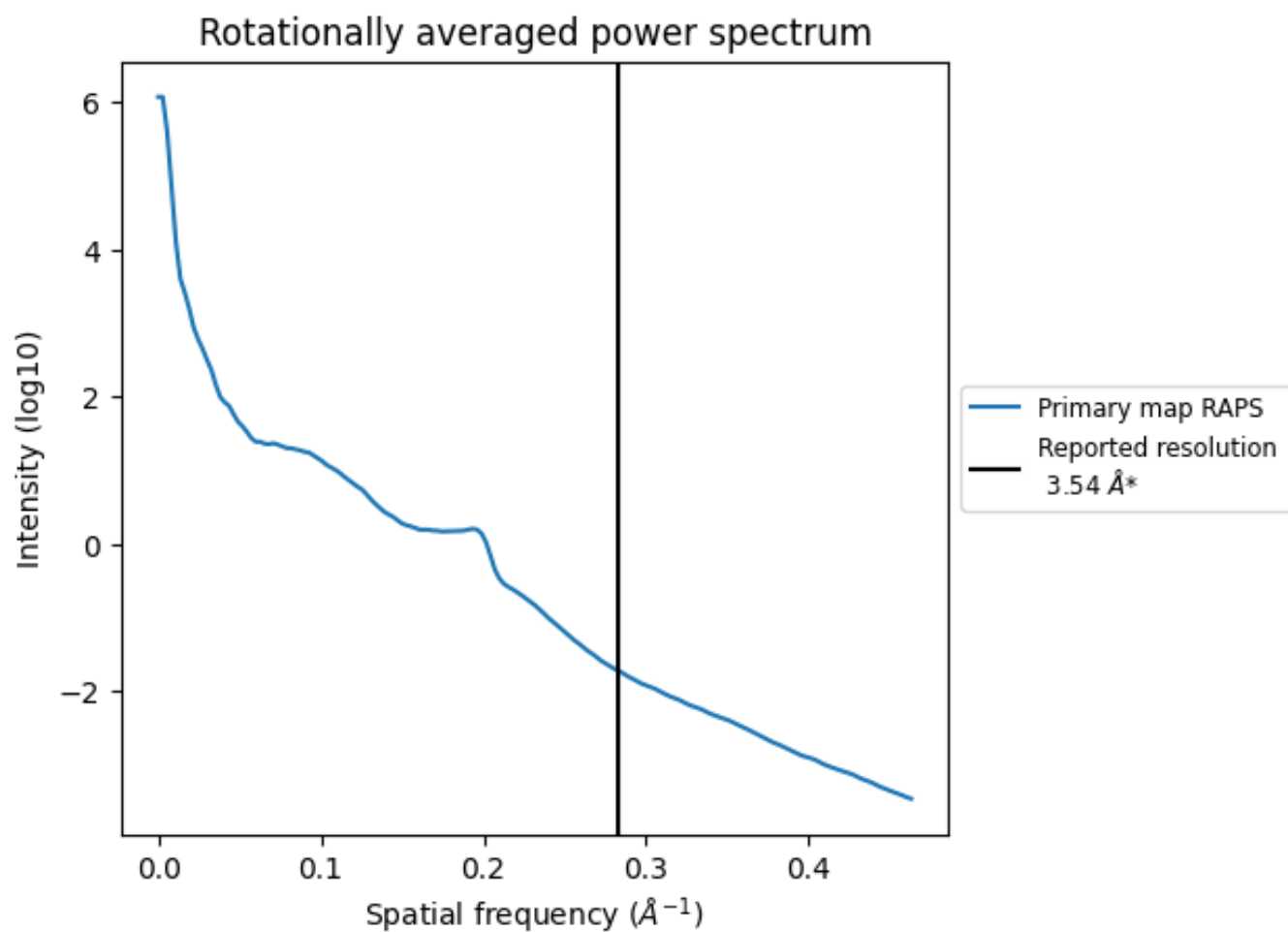
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1192  $\text{nm}^3$ ; this corresponds to an approximate mass of 1077 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 i



\*Reported resolution corresponds to spatial frequency of 0.282 Å<sup>-1</sup>

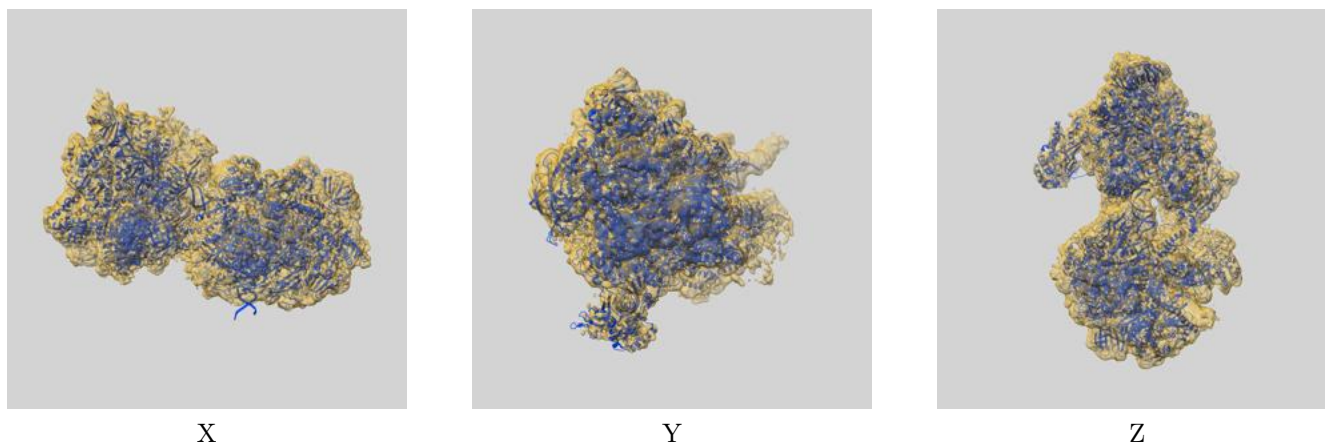
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

This section contains information regarding the fit between EMDB map EMD-23789 and PDB model 7MEI. Per-residue inclusion information can be found in section 3 on page 9.

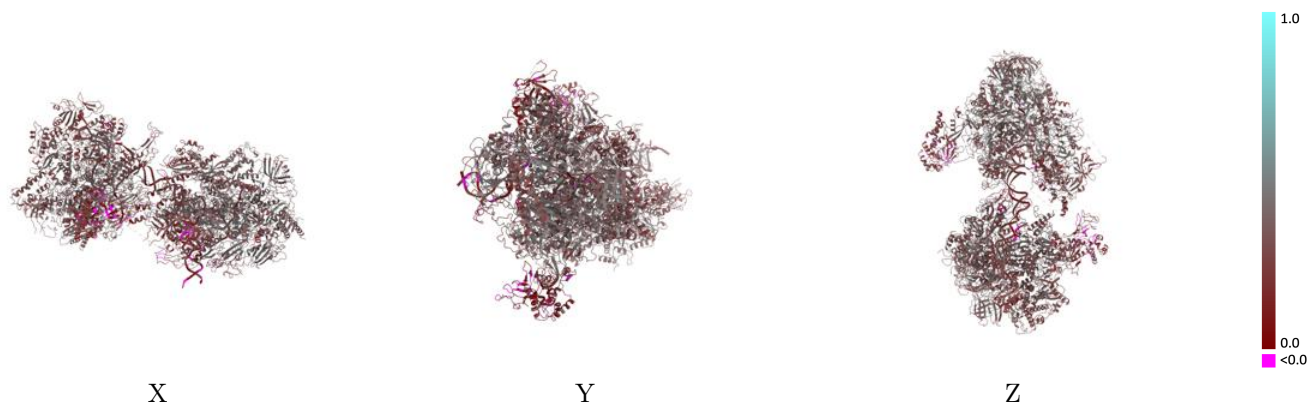
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0088 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.

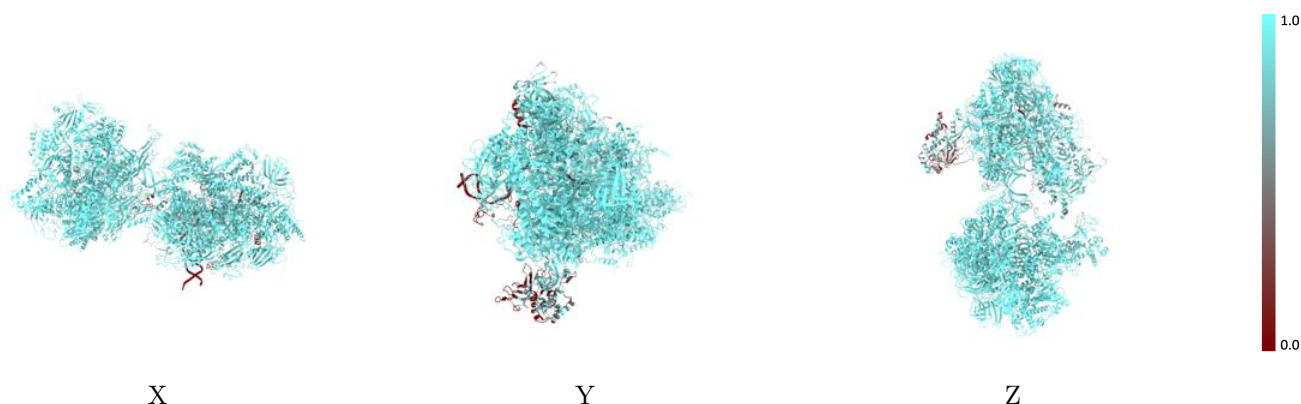


## 9.2 Q-score mapped to coordinate model [i](#)



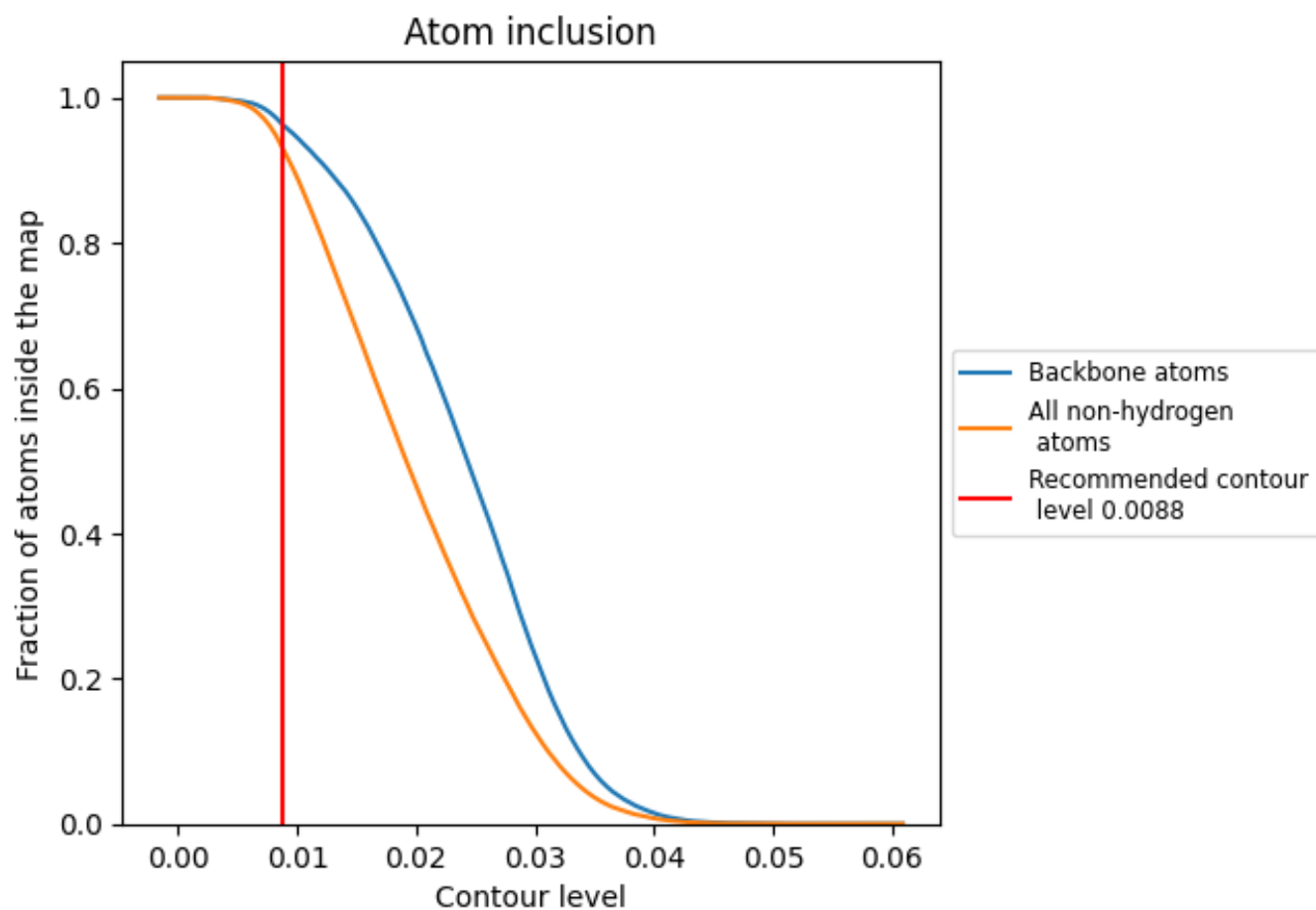
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0088).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.0088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9303	 0.3350
A	 0.9471	 0.3680
B	 0.9211	 0.3680
C	 0.9607	 0.3920
D	 0.4652	 0.1990
E	 0.9602	 0.3480
F	 0.9549	 0.3820
G	 0.5368	 0.2010
H	 0.9677	 0.3690
I	 0.9325	 0.3360
J	 0.9829	 0.3960
K	 0.8880	 0.3340
L	 0.9559	 0.3390
M	 0.8413	 0.2300
N	 0.7735	 0.1950
O	 0.8924	 0.2700
Q	 0.8352	 0.2660
R	 0.7859	 0.2650
a	 0.9861	 0.3450
b	 0.9742	 0.3520
c	 0.9913	 0.3650
d	 0.9297	 0.1650
e	 0.9941	 0.3490
f	 0.9854	 0.3520
g	 0.9500	 0.2100
h	 0.9848	 0.3470
i	 0.9690	 0.3160
j	 0.9962	 0.3620
k	 0.9177	 0.3320
l	 0.9794	 0.3520
r	 0.9369	 0.2630

