



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:52 AM UTC

PDB ID : 6CNB / pdb_00006cnb
EMDB ID : EMD-7530
Title : Yeast RNA polymerase III initial transcribing complex
Authors : Han, Y.; He, Y.
Deposited on : 2018-03-08
Resolution : 4.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

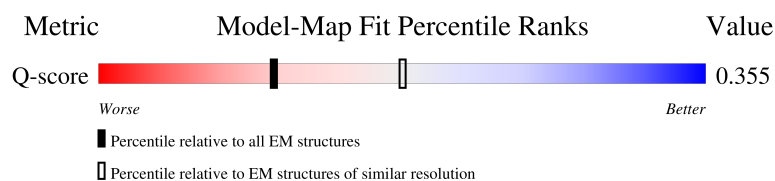
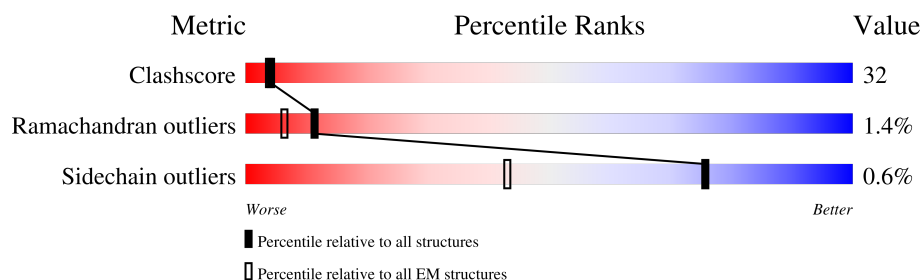
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



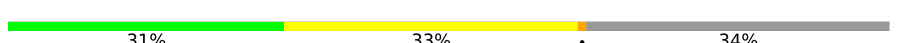
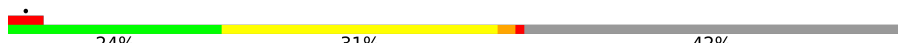
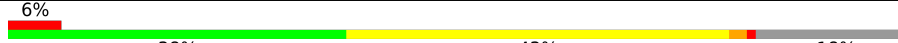
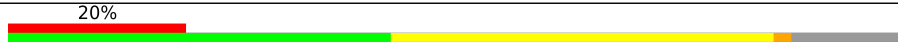
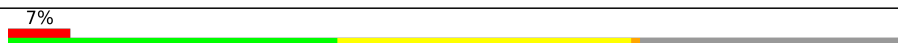
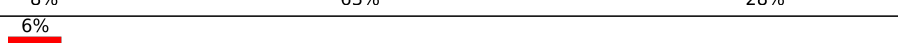
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	1460	
2	B	1149	
3	C	335	
4	D	161	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	212	
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	736	
19	S	594	
20	X	71	
21	Y	71	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 47837 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	1428	Total	C	N	O	S	0	0
			11159	7029	1972	2099	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	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	184	Total	C	N	O	S	0	0
			1484	972	239	267	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	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	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	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	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	277	Total	C	N	O	S	0	0
			2242	1438	368	425	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	54	Total	C	N	O	0	0
			368	238	64	66		

- Molecule 18 is a protein called Transcription factor IIIB 70 kDa subunit,TATA-box-binding protein,Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	522	Total	C	N	O	S	0	0
			4131	2621	733	757	20		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	383	ALA	-	linker	UNP P29056
R	384	MET	-	linker	UNP P29056
R	385	PRO	-	linker	UNP P29056
R	386	TRP	-	linker	UNP P29056
R	567	GLY	-	linker	UNP P13393
R	568	SER	-	linker	UNP P13393
R	569	GLY	-	linker	UNP P13393
R	570	SER	-	linker	UNP P13393
R	571	GLY	-	linker	UNP P13393

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Chain	Residue	Modelled	Actual	Comment	Reference
R	572	SER	-	linker	UNP P13393
R	573	GLY	-	linker	UNP P13393
R	574	SER	-	linker	UNP P13393
R	575	GLY	-	linker	UNP P13393
R	576	SER	-	linker	UNP P13393
R	577	GLY	-	linker	UNP P13393
R	578	SER	CYS	engineered mutation	UNP P29056

- Molecule 19 is a protein called Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B".

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	217	Total	C	N	O	S	0	0
			1649	1035	286	321	7		

- Molecule 20 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	51	Total	C	N	O	P	0	0
			1036	501	177	308	50		

- Molecule 21 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	61	Total	C	N	O	P	0	0
			1254	603	228	363	60		

- 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	

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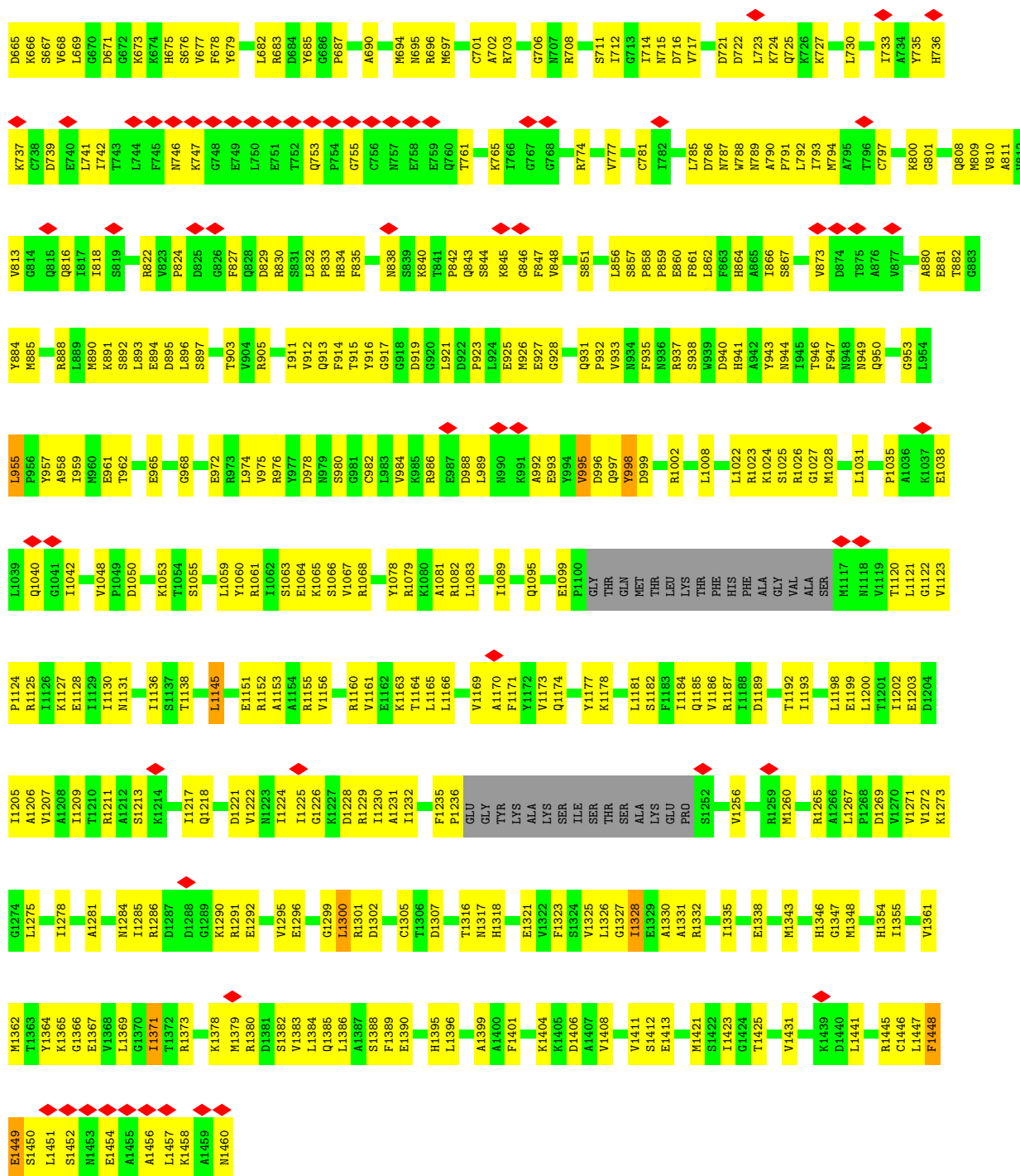
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	R	1	1	1	0

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.

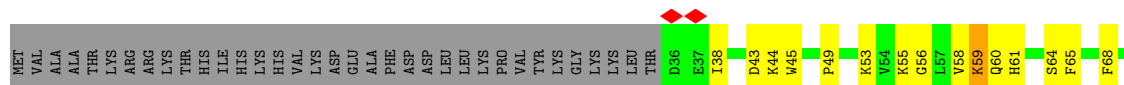
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1





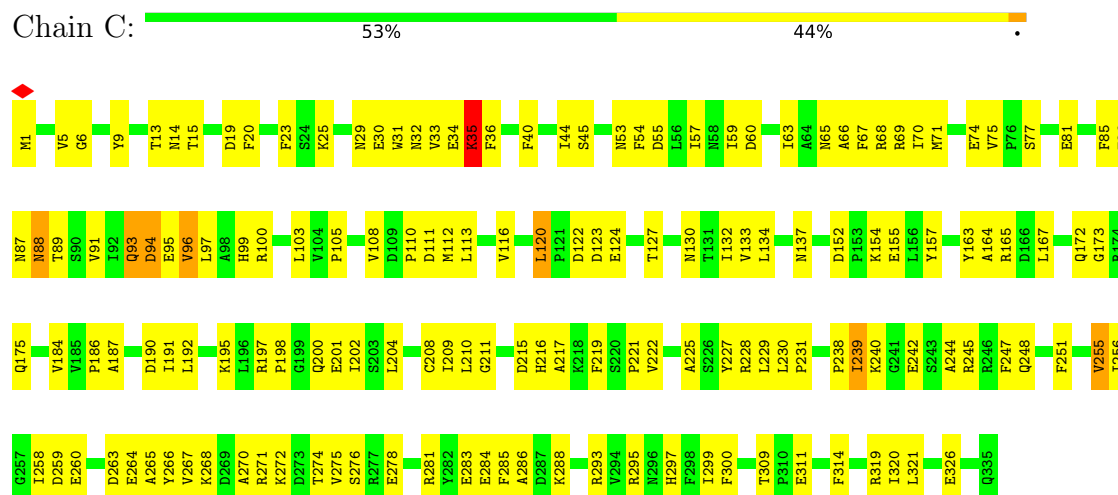
● Molecule 2: DNA-directed RNA polymerase III subunit RPC2

Chain B:

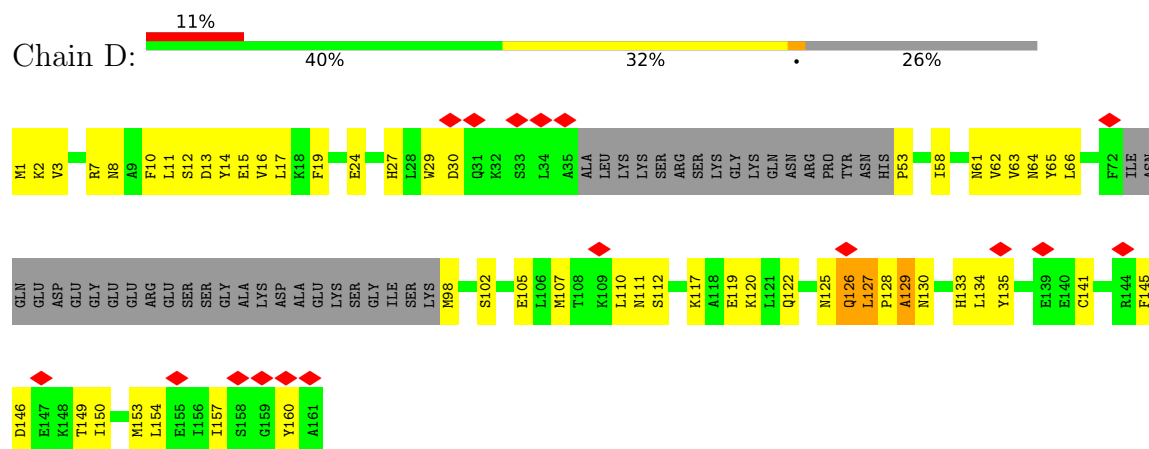




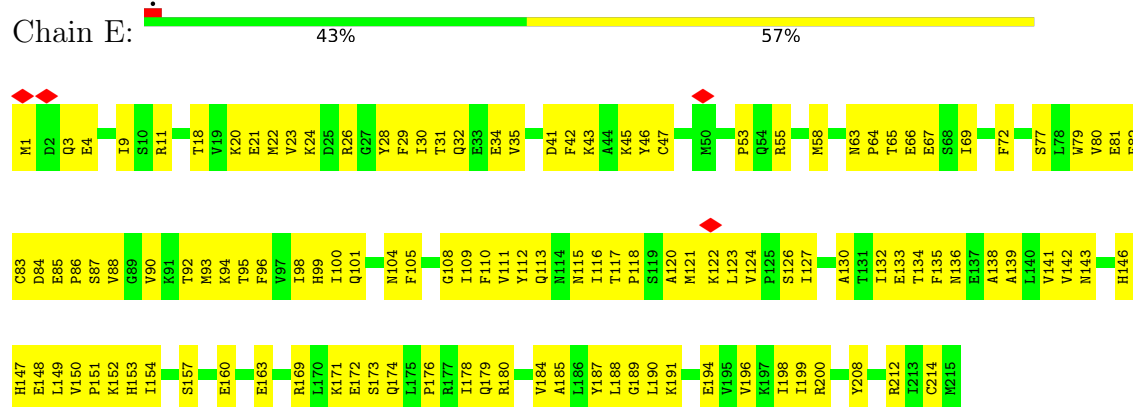
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



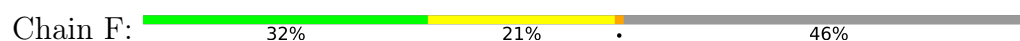
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

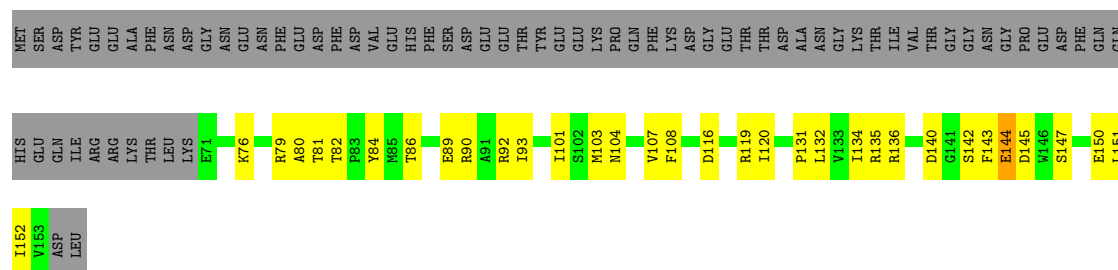


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

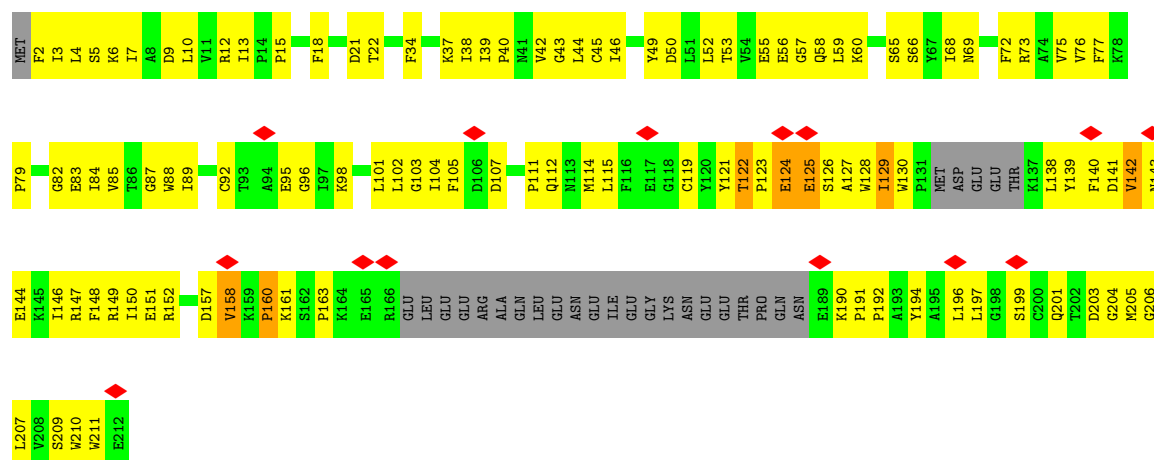


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

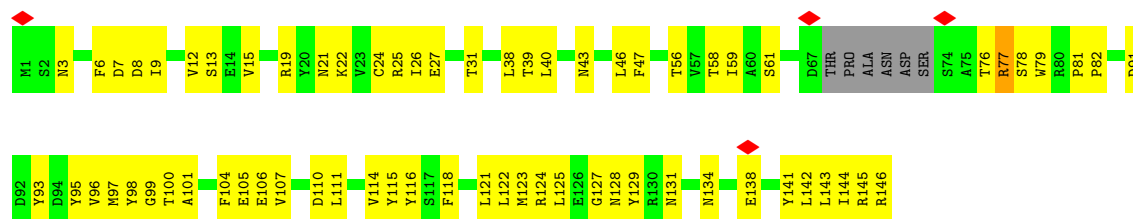




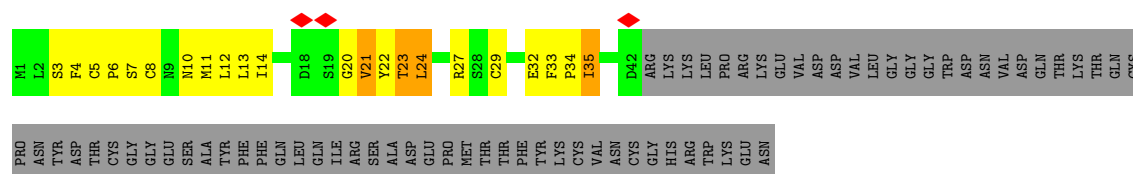
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8



• 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

M1	I2		V5	R6	C7	F8	S9	C10	D16	K17		Y21		E32	L36		L39		R43	Y44	C45		R48	M49		T52	H53	V54	D55	L56	I57		F60	L61		E67	LVS	ASP	ARP
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- Chain K:  45% 25% . 29%

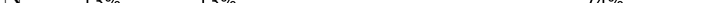
[illegible]

- Chain L: 31% 33% . 34%

NET	SER	ARG	GLY	GLY	PRO	THR	ASP	LEU	ALA	ALA	ALA	ALA	GLY	THR	GLN	ARG	THR	A25	T26	L27	K28	Y29	L30	C31		C34		K37	L40	S41		D44		C48	C51	G52	H53		L56	L57	K58	A59	R60	T61	K62	R63	L64		F67		F70
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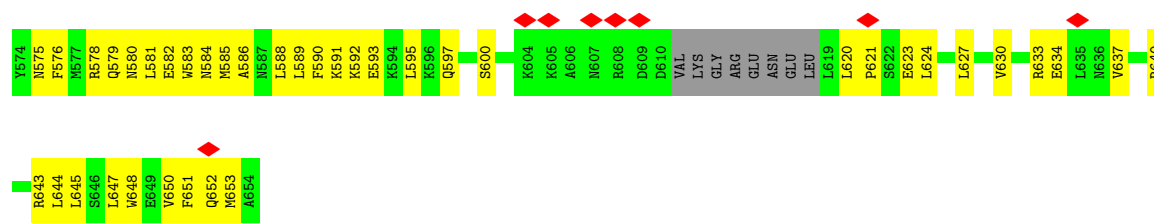
- Chain M: 24% 31% .. 42%

K261 E262	ASP	E196	P124 L125	MET		
	ALA	ASP			GLY	SER
	GLU	ARG			GLU	ILE
	ASP	ARG			GLU	ASP
	LYS	ASN			GLU	ASN
	THR	PRO			GLU	LEU
	LEU	ASN			ASP	PHE
	VAL	PRO			VAL	THR
	ALA	SER			VAL	THR
	LEU	SER			E72	GLU
GLU	GLN	E73	GLU	GLU		
LYS	ARG	F74	GLU	GLU		
GLN	ALA	F75	GLU	GLU		
GLU	GLN	F76	GLU	ASP		
ASP	VAL	L76	ARG	ASP		
TYR	VAL	K77	THR	THR		
ILE	THR	L78	THR	THR		
ASP	MET	S79	GLN	GLN		
ASN	SER	C80	ASP	ASP		
LEU	VAL	E81	ARG	ARG		
LEU	LYS	E82	ALA	ALA		
VAL	SER	F83	VAL	VAL		
VAL	VAL	S84	GLU	GLU		
ASN	ASN	L85	ASP	ASP		
ASP	ASP	H86	GLU	GLU		
PRO	PRO	V151	GLY	SER		
SER	SER	G152	THR	THR		
GLN	GLN	F153	ASN	ASN		
N225 R226	N225	E154	Y90	ILE		
	R226	E155	N92	ILE		
	L227	Y159	R93	MET		
	S230	A160	P94	ILE		
	L231	P95	R95	ALA		
	H234	V163	L96	ASP		
	A237	K164	ASN	GLU		
	A241	V168	ASN	GLY		
	N242	V169	THR	THR		
	L243	L170	ASN	ASN		
E244	V171	P101	SER			
L245	P172	E102	SER			
L246	E103	ALA	ALA			
W247	H104	ILE	ILE			
A248	P105	F106	ALA			
E249	R175	ASN	ASN			
G250	Q176	THR	GLY			
T251	L179	GLN	GLN			
F252	L179	GLU	GLU			
Q254	P181	LYS	LYS			
F255	F182	P114	SER			
K256	F183	K115	GLU			
D257	K184	S116	VAL			
T258	Y185	H117	LYS			
L259	F186	L118	ALA			
V260	D187	W119	GLU			
	M190	E120	ASP			
	K194	I121	ASP			
		D122				
		L123				

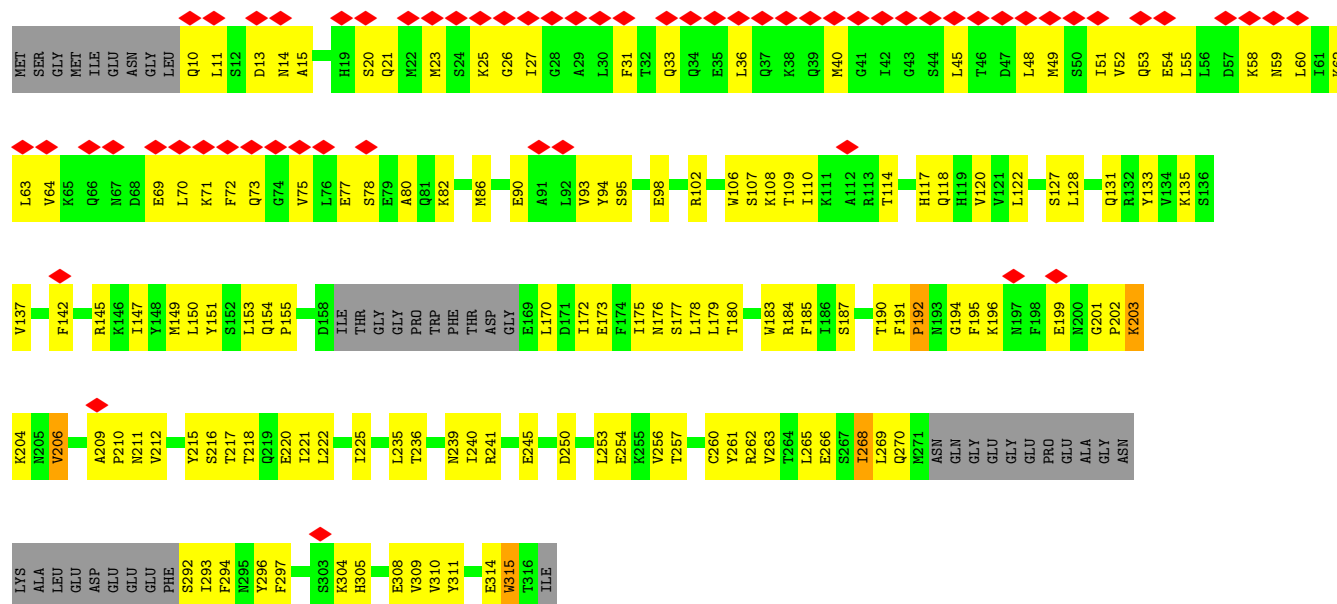
- Chain N:  13% 13% 74%

[illegible]

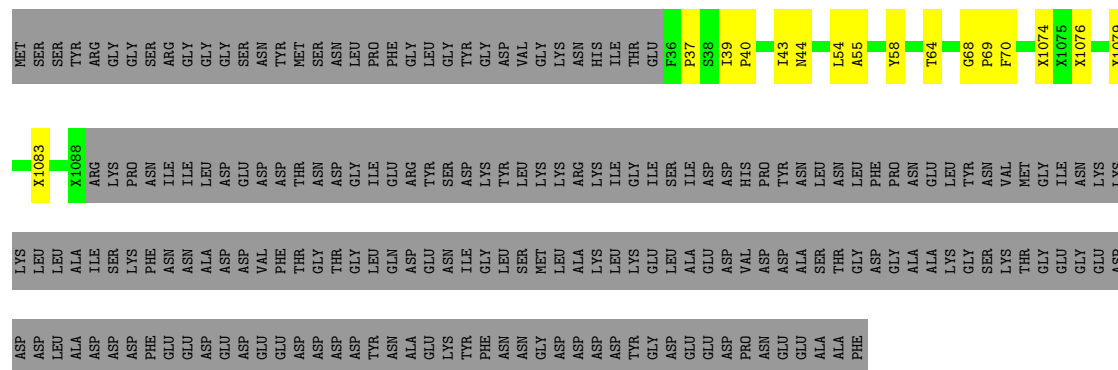




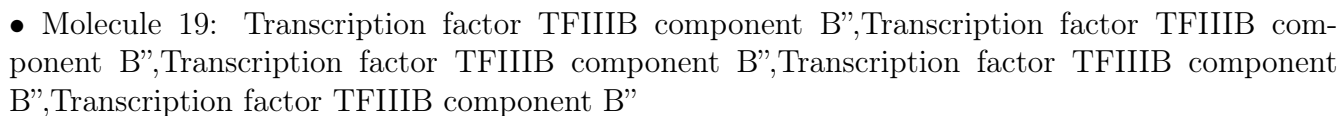
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

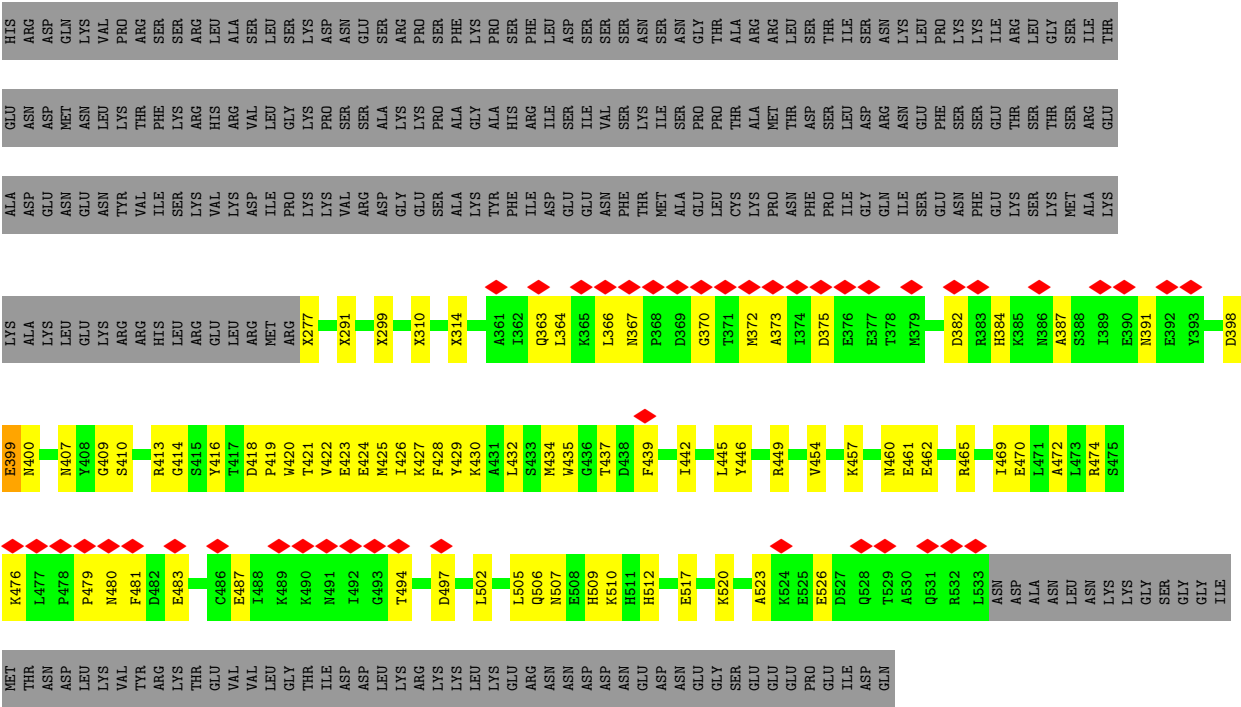


• Molecule 17: DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7

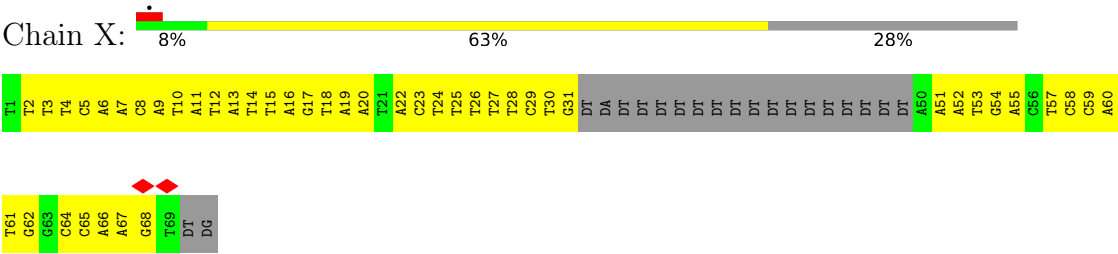


• Molecule 18: Transcription factor IIIB 70 kDa subunit, TATA-box-binding protein, Transcription factor IIIB 70 kDa subunit

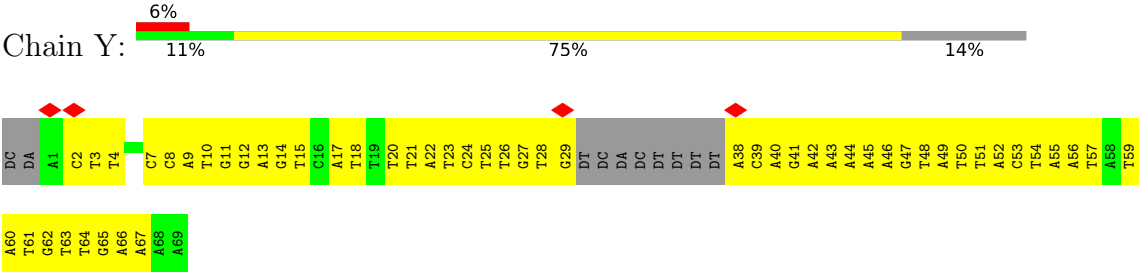




• Molecule 20: DNA (71-MER)



• Molecule 21: DNA (71-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0334	Depositor
Map size (Å)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18, 1.18, 1.18	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: 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	0.40	0/11358	0.79	16/15345 (0.1%)
2	B	0.41	1/8943 (0.0%)	0.79	15/12068 (0.1%)
3	C	0.40	0/2711	0.78	7/3676 (0.2%)
4	D	0.21	0/991	0.66	1/1328 (0.1%)
5	E	0.32	0/1795	0.65	0/2416
6	F	0.40	0/683	0.76	0/923
7	G	0.28	0/1523	0.70	2/2066 (0.1%)
8	H	0.34	0/1138	0.65	0/1540
9	I	0.34	0/328	0.77	0/445
10	J	0.45	0/558	0.75	0/750
11	K	0.42	0/803	0.79	1/1083 (0.1%)
12	L	0.33	0/365	0.81	1/485 (0.2%)
13	M	0.32	1/1369 (0.1%)	0.82	5/1851 (0.3%)
14	N	0.24	0/855	0.73	2/1149 (0.2%)
15	O	0.32	0/4394	0.76	5/5928 (0.1%)
16	P	0.25	0/2282	0.69	6/3075 (0.2%)
17	Q	0.26	0/281	0.55	0/381
18	R	0.27	1/4200 (0.0%)	0.63	3/5659 (0.1%)
19	S	0.18	0/1464	0.60	3/1971 (0.2%)
20	X	0.28	0/1158	0.51	0/1782
21	Y	0.28	0/1407	0.50	0/2169
All	All	0.35	3/48606 (0.0%)	0.73	67/66090 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	151	GLN	CA-C	7.22	1.62	1.52
2	B	517	MET	CA-CB	-5.59	1.45	1.53
13	M	103	GLU	CA-C	5.00	1.59	1.52

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	184	LYS	N-CA-C	-10.46	100.52	113.18
3	C	96	VAL	N-CA-C	9.77	120.39	110.23
2	B	335	LEU	N-CA-C	-9.44	100.71	112.88
2	B	428	ASN	N-CA-C	-9.26	101.09	112.38
15	O	556	ASP	N-CA-C	-9.14	100.25	111.40

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	11159	0	11285	815	0
2	B	8788	0	8901	659	0
3	C	2655	0	2628	170	0
4	D	977	0	983	87	0
5	E	1759	0	1788	109	0
6	F	671	0	692	35	0
7	G	1484	0	1485	130	0
8	H	1120	0	1089	68	0
9	I	321	0	303	43	0
10	J	549	0	559	37	0
11	K	792	0	790	38	0
12	L	363	0	386	35	0
13	M	1338	0	1307	148	0
14	N	845	0	891	68	0
15	O	4329	0	4497	364	0
16	P	2242	0	2265	146	0
17	Q	368	0	307	14	0
18	R	4131	0	4230	261	0
19	S	1649	0	1456	72	0
20	X	1036	0	584	76	0
21	Y	1254	0	695	94	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	1	0	0	0	0
22	R	1	0	0	0	0
All	All	47837	0	47121	3055	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 32.

The worst 5 of 3055 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:X:4:DT:H2''	20:X:5:DC:C5'	1.26	1.57
2:B:587:PHE:CZ	2:B:607:ARG:HD3	1.32	1.56
20:X:4:DT:C2'	20:X:5:DC:H5'	1.35	1.54
1:A:200:GLU:HB3	15:O:516:LEU:CD2	1.48	1.43
1:A:235:LYS:HD3	15:O:44:PRO:CG	1.49	1.40

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	1422/1460 (97%)	1142 (80%)	260 (18%)	20 (1%)	9	39
2	B	1112/1149 (97%)	907 (82%)	185 (17%)	20 (2%)	6	35
3	C	333/335 (99%)	272 (82%)	58 (17%)	3 (1%)	14	49
4	D	113/161 (70%)	85 (75%)	26 (23%)	2 (2%)	6	35
5	E	213/215 (99%)	177 (83%)	35 (16%)	1 (0%)	24	61
6	F	81/155 (52%)	71 (88%)	9 (11%)	1 (1%)	10	42
7	G	178/212 (84%)	146 (82%)	27 (15%)	5 (3%)	4	27
8	H	136/146 (93%)	114 (84%)	21 (15%)	1 (1%)	18	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	40/110 (36%)	29 (72%)	8 (20%)	3 (8%)	1	12
10	J	65/70 (93%)	51 (78%)	14 (22%)	0	100	100
11	K	99/142 (70%)	79 (80%)	20 (20%)	0	100	100
12	L	44/70 (63%)	36 (82%)	8 (18%)	0	100	100
13	M	160/282 (57%)	128 (80%)	27 (17%)	5 (3%)	3	25
14	N	106/422 (25%)	80 (76%)	26 (24%)	0	100	100
15	O	533/654 (82%)	405 (76%)	116 (22%)	12 (2%)	5	31
16	P	271/317 (86%)	223 (82%)	45 (17%)	3 (1%)	11	44
17	Q	33/251 (13%)	27 (82%)	6 (18%)	0	100	100
18	R	514/736 (70%)	436 (85%)	75 (15%)	3 (1%)	21	58
19	S	172/594 (29%)	157 (91%)	15 (9%)	0	100	100
All	All	5625/7481 (75%)	4565 (81%)	981 (17%)	79 (1%)	11	39

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	A	236	SER
1	A	587	ILE
1	A	599	LYS
1	A	601	TYR

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	1232/1257 (98%)	1226 (100%)	6 (0%)	81	82
2	B	975/1006 (97%)	968 (99%)	7 (1%)	76	79
3	C	296/296 (100%)	293 (99%)	3 (1%)	68	76
4	D	110/145 (76%)	110 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	164/190 (86%)	161 (98%)	3 (2%)	51	67
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	38/98 (39%)	37 (97%)	1 (3%)	40	61
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	39 (98%)	1 (2%)	42	62
13	M	142/249 (57%)	141 (99%)	1 (1%)	76	79
14	N	92/360 (26%)	92 (100%)	0	100	100
15	O	495/593 (84%)	489 (99%)	6 (1%)	63	73
16	P	255/285 (90%)	255 (100%)	0	100	100
17	Q	31/195 (16%)	31 (100%)	0	100	100
18	R	450/623 (72%)	448 (100%)	2 (0%)	84	83
19	S	157/494 (32%)	157 (100%)	0	100	100
All	All	5023/6505 (77%)	4993 (99%)	30 (1%)	76	80

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	120	LEU
15	O	557	ARG
7	G	124	GLU
18	R	515	LEU
15	O	187	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	200	GLN
13	M	89	GLN
18	R	278	ASN
3	C	330	ASN
5	E	153	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 7 ligands modelled in this entry, 7 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	S	1
17	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	319:UNK	C	360:THR	N	37.31

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	70:PHE	C	1070:UNK	N	13.25

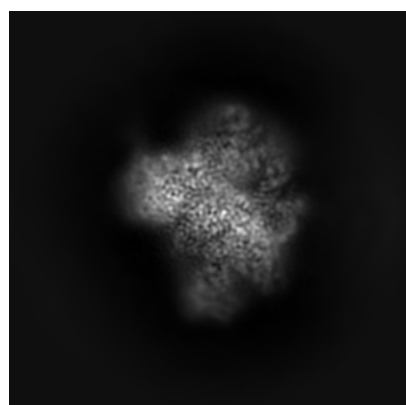
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7530. These allow visual inspection of the internal detail of the map and identification of artifacts.

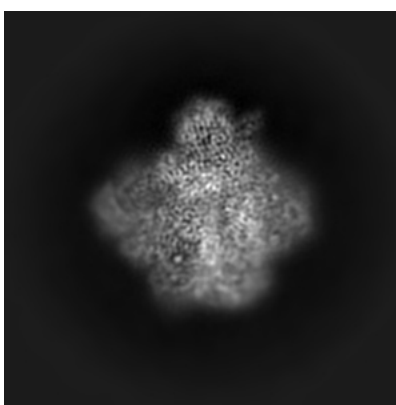
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

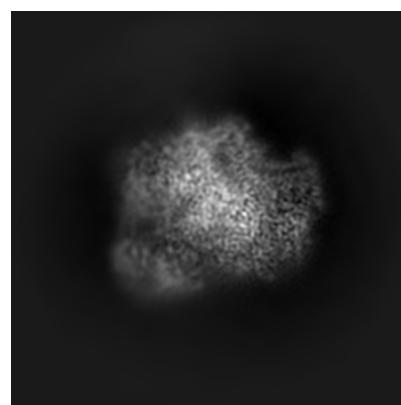
6.1.1 Primary map



X



Y

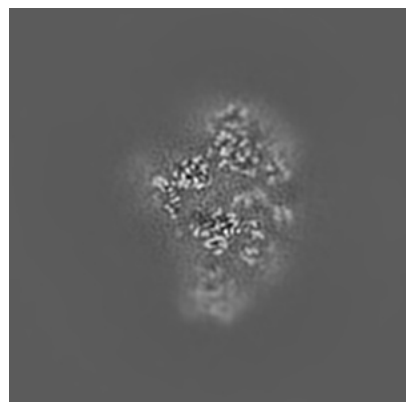


Z

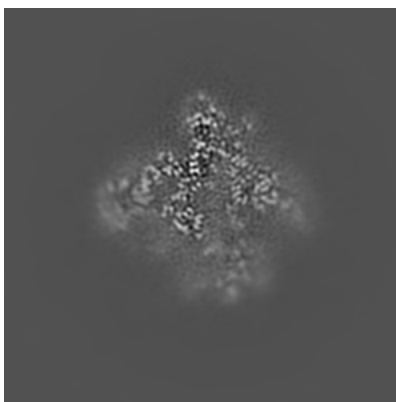
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

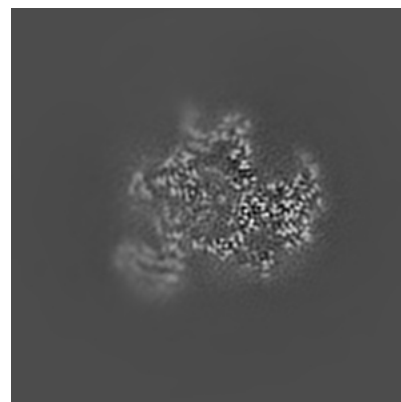
6.2.1 Primary map



X Index: 144



Y Index: 144

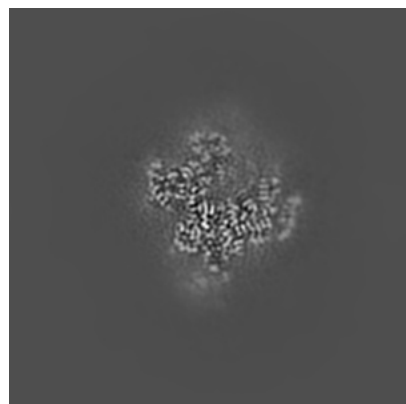


Z Index: 144

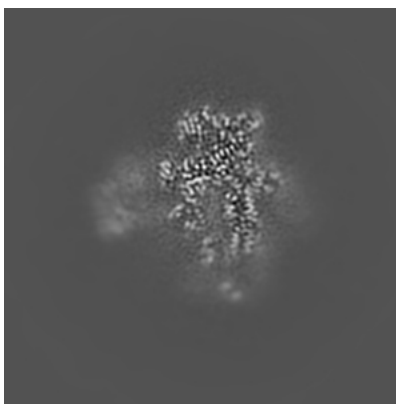
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

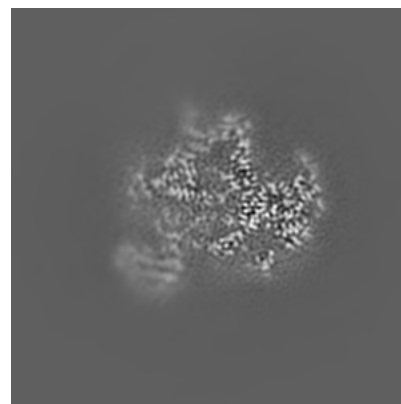
6.3.1 Primary map



X Index: 168



Y Index: 134

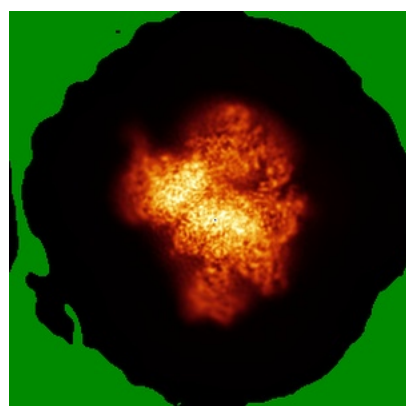


Z Index: 143

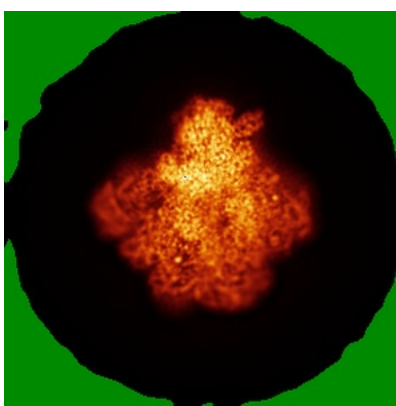
The images above show the largest variance slices of the map in three orthogonal directions.

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

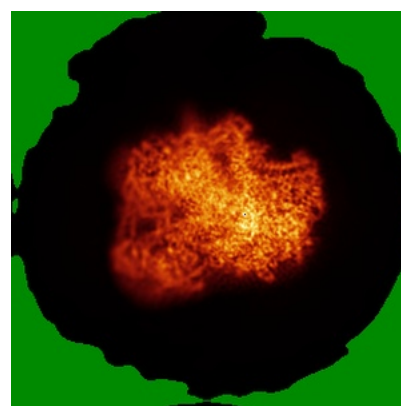
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

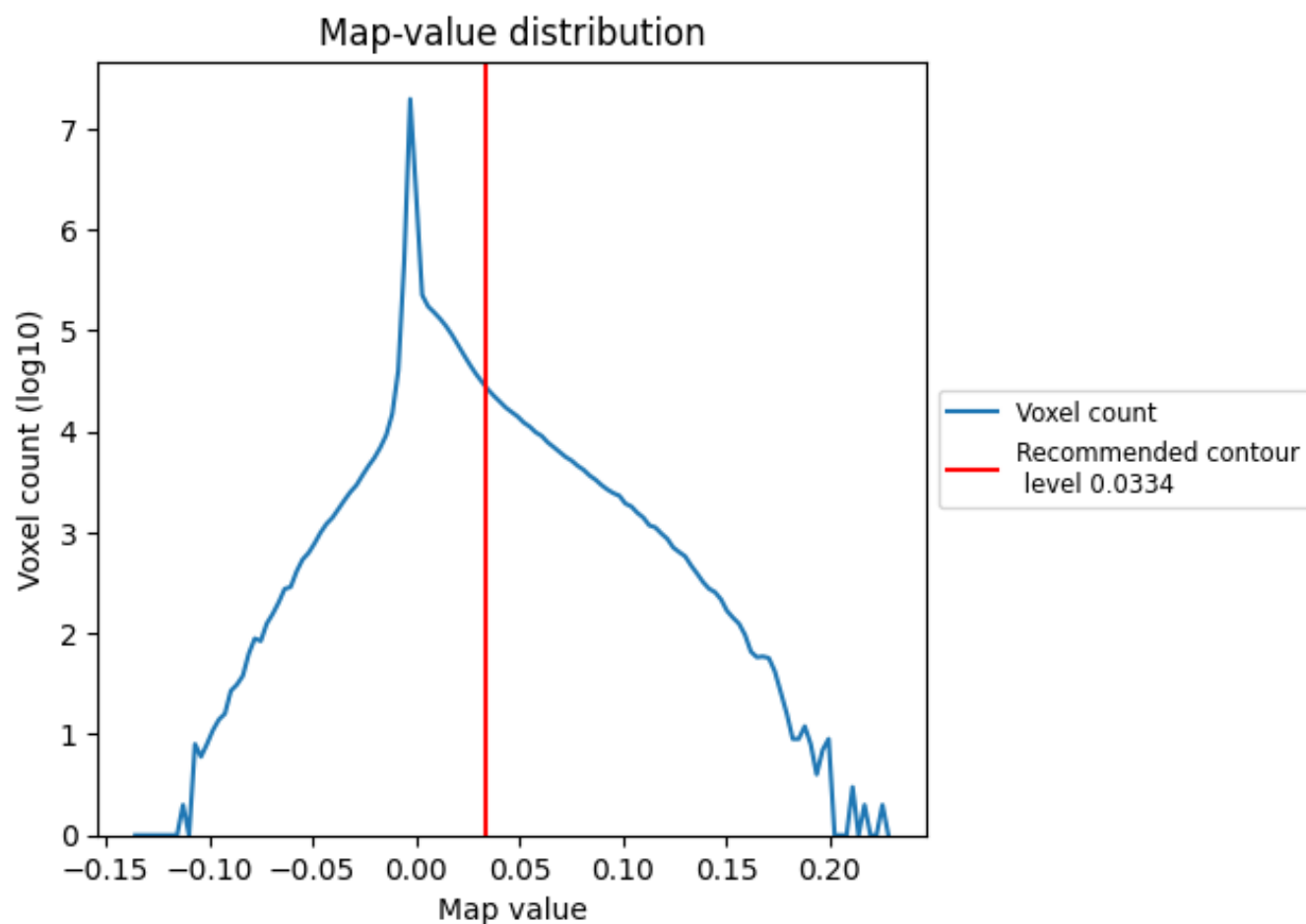
6.6 Mask visualisation

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

7 Map analysis [i](#)

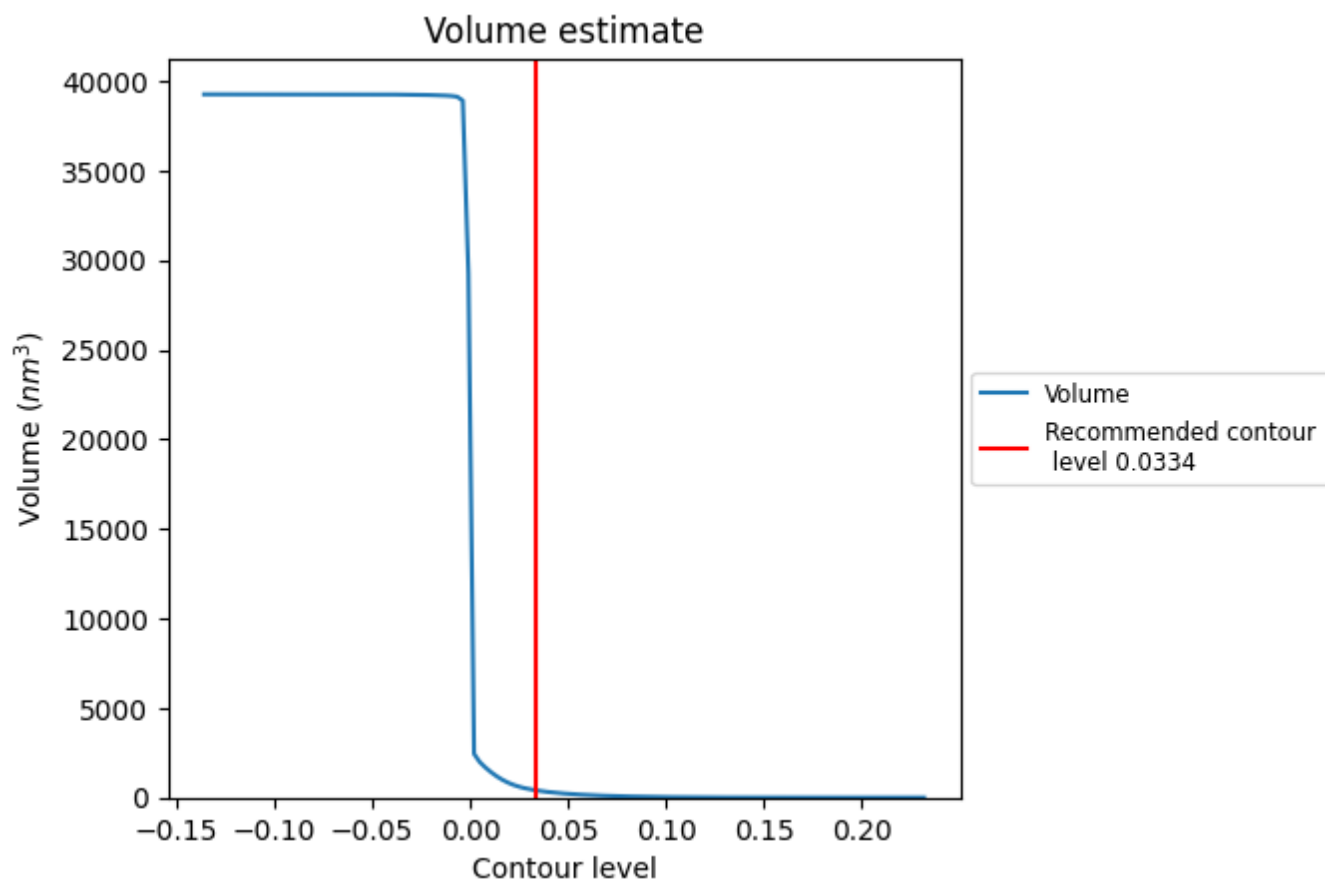
This section contains the results of statistical analysis of the map.

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.

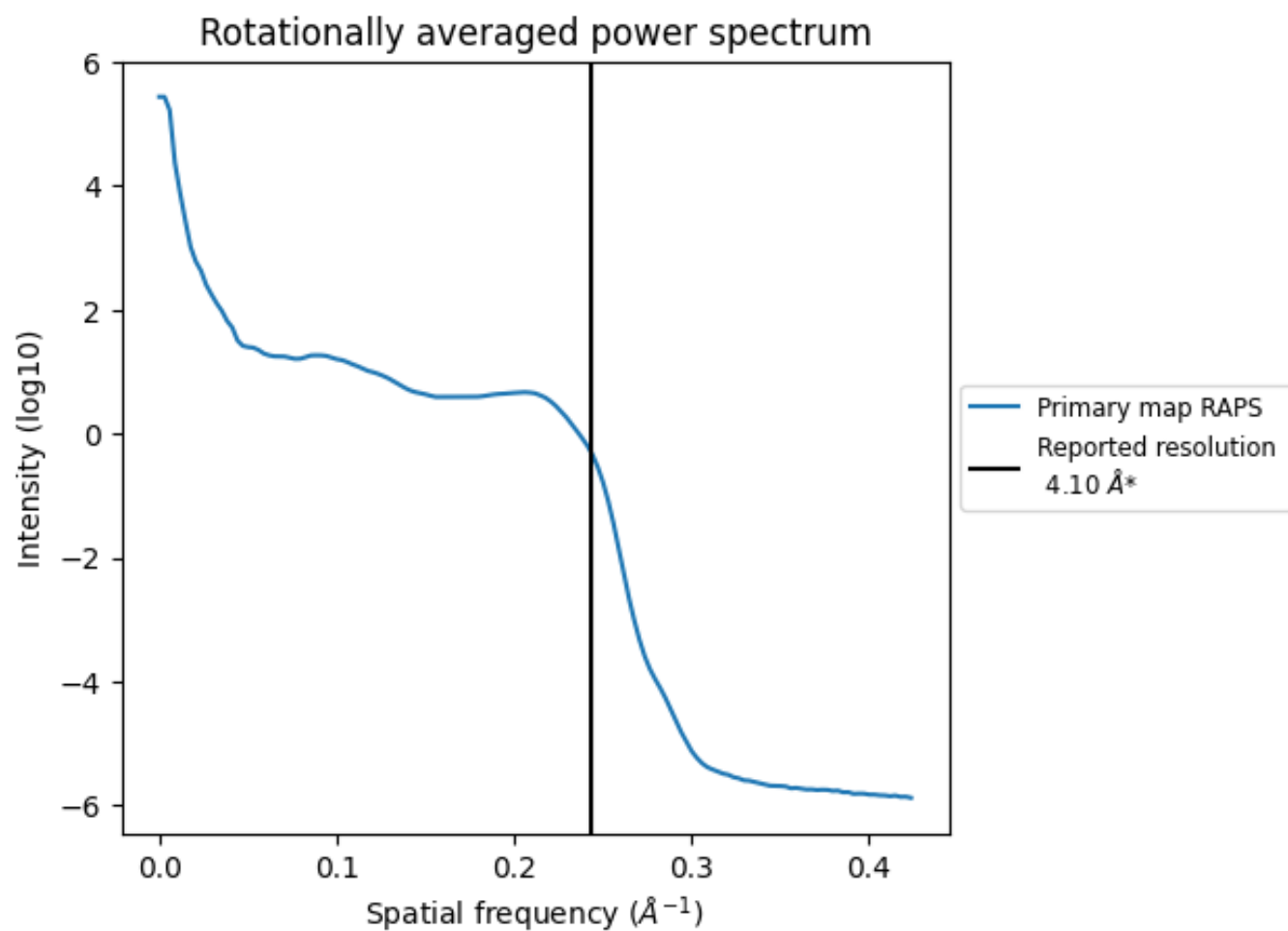
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 406 nm³; this corresponds to an approximate mass of 366 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 ⓘ

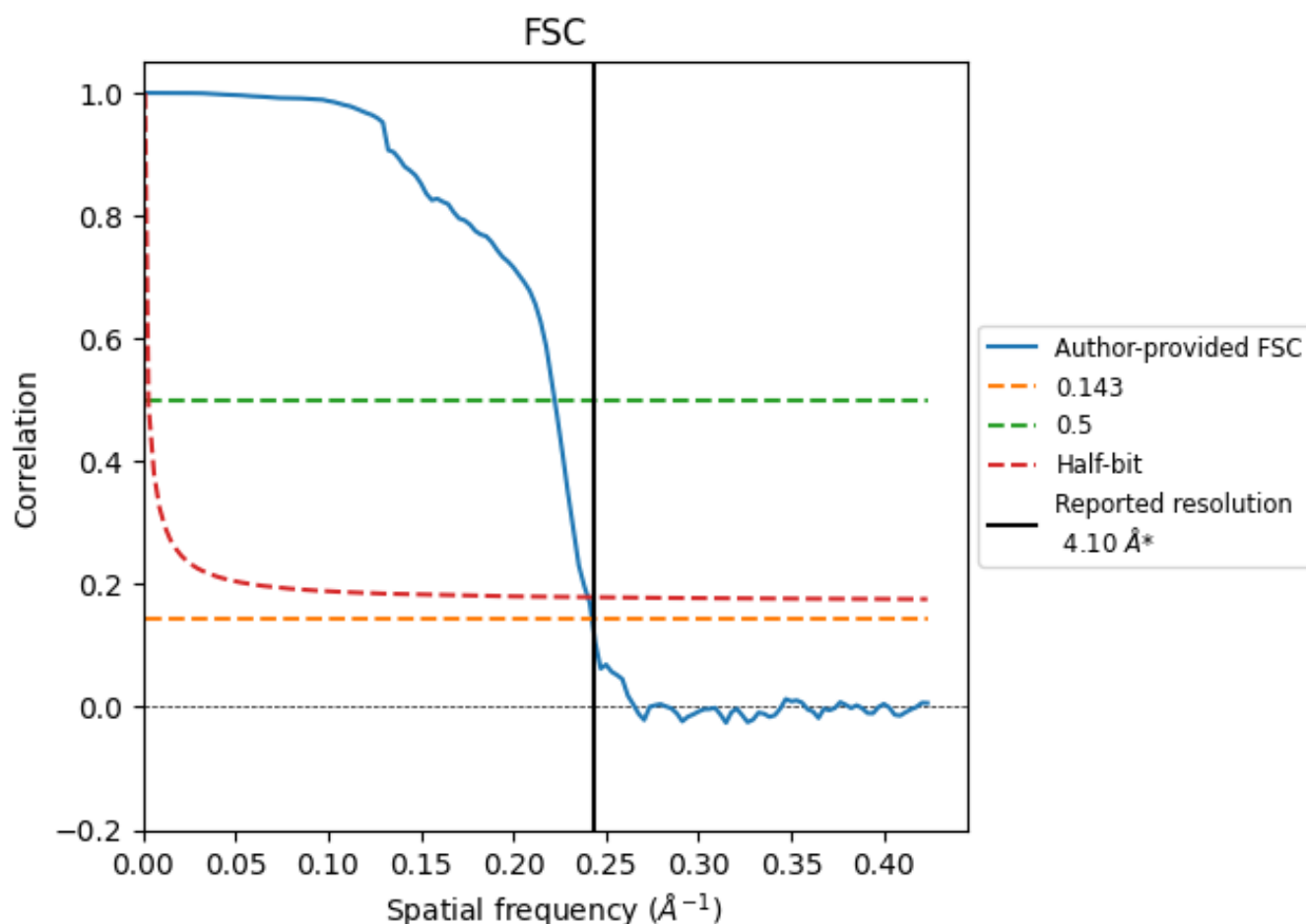


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	4.50	4.16
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

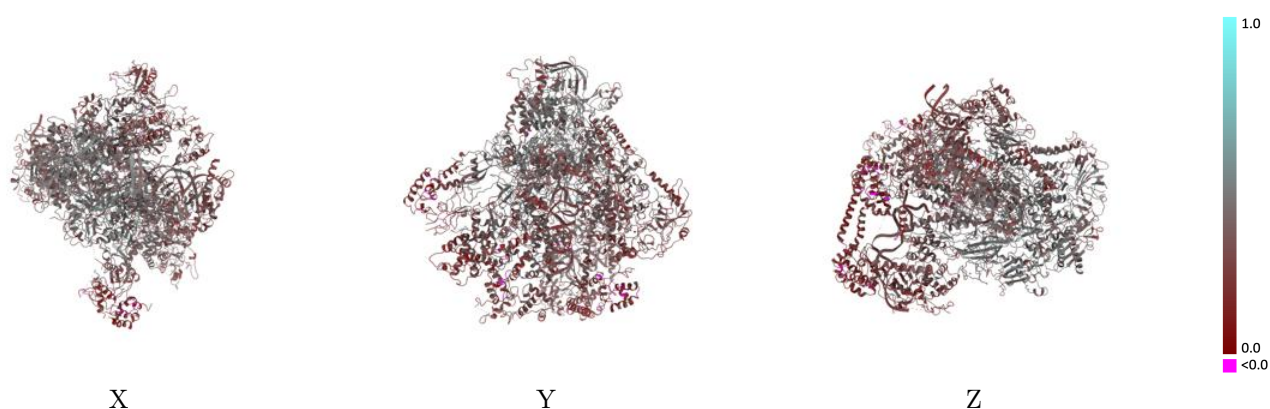
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7530 and PDB model 6CNB. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

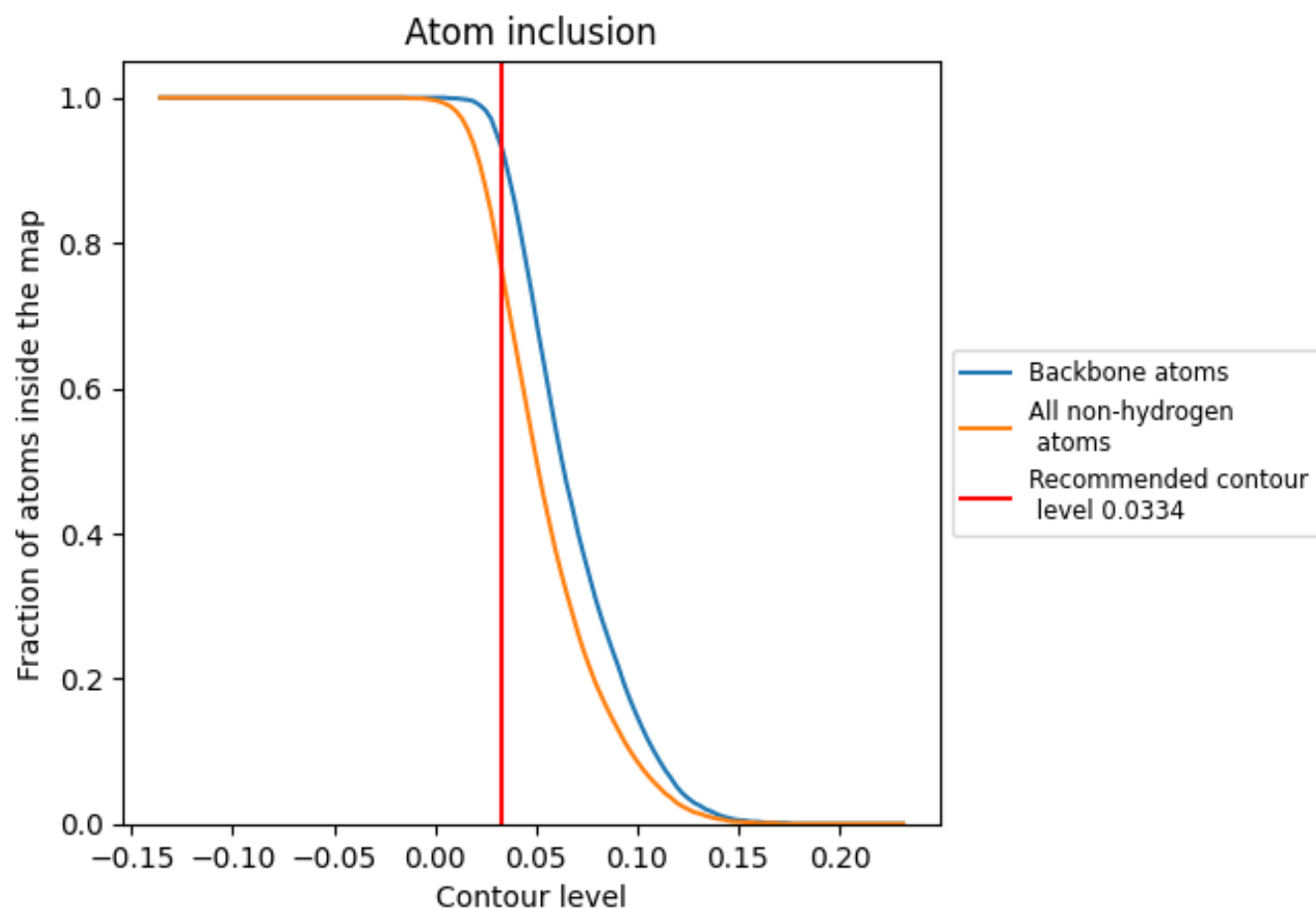


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% 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 (0.0334) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.3550
A	 0.7800	 0.3950
B	 0.7980	 0.4100
C	 0.8810	 0.4270
D	 0.6120	 0.2080
E	 0.7900	 0.3510
F	 0.8790	 0.4450
G	 0.7440	 0.2830
H	 0.8350	 0.4160
I	 0.7350	 0.3120
J	 0.8950	 0.4390
K	 0.8610	 0.4380
L	 0.8210	 0.4270
M	 0.6700	 0.2820
N	 0.7000	 0.2880
O	 0.7070	 0.3040
P	 0.6070	 0.2680
Q	 0.8660	 0.3680
R	 0.6680	 0.2830
S	 0.5590	 0.2440
X	 0.8890	 0.3240
Y	 0.8460	 0.3270

