



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:39 AM UTC

PDB ID : 5W64 / pdb_00005w64
EMDB ID : EMD-8774
Title : RNA Polymerase I Initial Transcribing Complex State 1
Authors : Han, Y.; He, Y.
Deposited on : 2017-06-16
Resolution : 4.20 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:

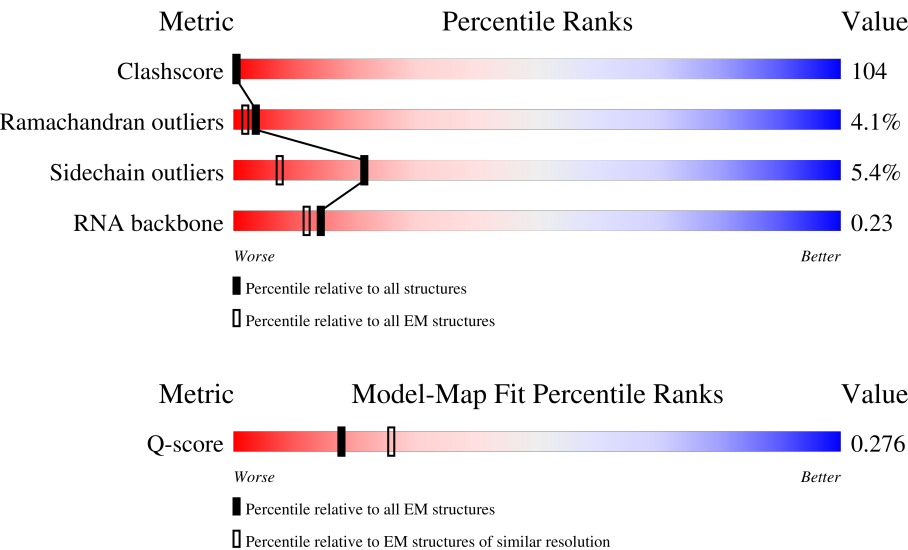
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



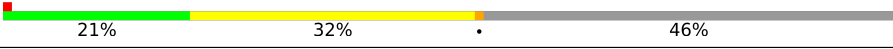
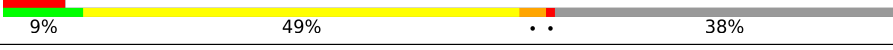
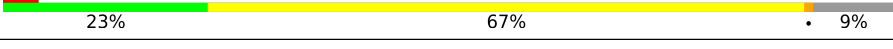
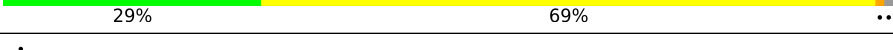
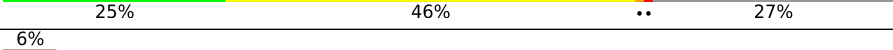
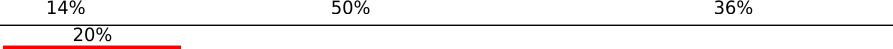
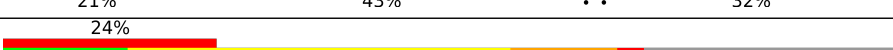
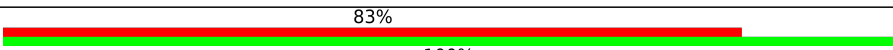
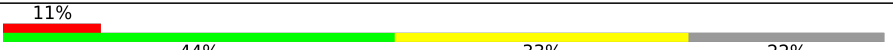
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	1664	30%55%12%
2	B	1203	32%64%
3	C	335	33%56%9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	894	
16	P	514	
17	Q	507	
18	R	6	
19	S	54	
20	T	54	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 46512 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1461	Total	C	N	O	S	0	0
			11542	7292	2004	2184	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1178	Total	C	N	O	S	0	0
			9351	5911	1639	1750	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	306	Total	C	N	O	S	0	0
			2432	1544	417	463	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	59	Total	C	N	O	0	0
			467	293	80	94		

- 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
			1760	1116	310	322	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
			670	428	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	201	Total	C	N	O	S	0	0
			1592	1022	275	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1071	676	181	210	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	65	Total	C	N	O	S	0	0
			479	300	79	96	4		

- 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	103	Total	C	N	O	S	0	0
			811	506	132	168	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
			359	221	71	63	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	106	Total	C	N	O	0	0
			841	534	139	168		

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	158	Total	C	N	O	S	0	0
			1254	799	205	246	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	640	Total	C	N	O	S	0	0
			5063	3218	872	964	9		

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	3	UNK	ALA	SEE REMARK 999	UNP P32786
O	4	UNK	GLU	SEE REMARK 999	UNP P32786
O	5	UNK	ASP	SEE REMARK 999	UNP P32786
O	6	UNK	ALA	SEE REMARK 999	UNP P32786
O	7	UNK	LEU	SEE REMARK 999	UNP P32786
O	8	UNK	ASP	SEE REMARK 999	UNP P32786
O	9	UNK	LEU	SEE REMARK 999	UNP P32786
O	10	UNK	HIS	SEE REMARK 999	UNP P32786
O	11	UNK	ILE	SEE REMARK 999	UNP P32786
O	12	UNK	VAL	SEE REMARK 999	UNP P32786
O	13	UNK	VAL	SEE REMARK 999	UNP P32786
O	14	UNK	LYS	SEE REMARK 999	UNP P32786
O	15	UNK	SER	SEE REMARK 999	UNP P32786
O	16	UNK	LEU	SEE REMARK 999	UNP P32786
O	17	UNK	LEU	SEE REMARK 999	UNP P32786
O	18	UNK	CYS	SEE REMARK 999	UNP P32786
O	19	UNK	ASP	SEE REMARK 999	UNP P32786
O	20	UNK	THR	SEE REMARK 999	UNP P32786
O	21	UNK	ALA	SEE REMARK 999	UNP P32786
O	22	UNK	ILE	SEE REMARK 999	UNP P32786
O	23	UNK	ARG	SEE REMARK 999	UNP P32786
O	24	UNK	TYR	SEE REMARK 999	UNP P32786
O	25	UNK	ILE	SEE REMARK 999	UNP P32786
O	26	UNK	SER	SEE REMARK 999	UNP P32786
O	27	UNK	ASP	SEE REMARK 999	UNP P32786
O	28	UNK	ASP	SEE REMARK 999	UNP P32786
O	41	UNK	TYR	SEE REMARK 999	UNP P32786
O	42	UNK	ILE	SEE REMARK 999	UNP P32786
O	43	UNK	PRO	SEE REMARK 999	UNP P32786
O	44	UNK	SER	SEE REMARK 999	UNP P32786

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	45	UNK	ASP	SEE REMARK 999	UNP P32786
O	46	UNK	LEU	SEE REMARK 999	UNP P32786
O	47	UNK	LEU	SEE REMARK 999	UNP P32786
O	48	UNK	ARG	SEE REMARK 999	UNP P32786
O	49	UNK	ASN	SEE REMARK 999	UNP P32786
O	50	UNK	LEU	SEE REMARK 999	UNP P32786
O	51	UNK	ASP	SEE REMARK 999	UNP P32786
O	52	UNK	ASP	SEE REMARK 999	UNP P32786
O	53	UNK	THR	SEE REMARK 999	UNP P32786
O	54	UNK	LEU	SEE REMARK 999	UNP P32786
O	55	UNK	GLN	SEE REMARK 999	UNP P32786
O	56	UNK	GLU	SEE REMARK 999	UNP P32786
O	57	UNK	SER	SEE REMARK 999	UNP P32786
O	58	UNK	THR	SEE REMARK 999	UNP P32786
O	59	UNK	ASN	SEE REMARK 999	UNP P32786
O	60	UNK	SER	SEE REMARK 999	UNP P32786
O	61	UNK	SER	SEE REMARK 999	UNP P32786
O	62	UNK	ARG	SEE REMARK 999	UNP P32786
O	63	UNK	PRO	SEE REMARK 999	UNP P32786
O	64	UNK	MET	SEE REMARK 999	UNP P32786
O	65	UNK	GLN	SEE REMARK 999	UNP P32786
O	66	UNK	ASP	SEE REMARK 999	UNP P32786
O	67	UNK	ALA	SEE REMARK 999	UNP P32786

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	387	Total	C	N	O	S	0	0
			3238	2105	540	576	17		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	349	Total	C	N	O	S	0	0
			2923	1881	513	518	11		

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	6	Total	C	N	O	P	0	0
			127	58	25	39	5		

- Molecule 19 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	42	Total	C	N	O	P	0	0
			875	417	168	249	41		

- Molecule 20 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	54	Total	C	N	O	P	0	0
			1082	522	177	330	53		

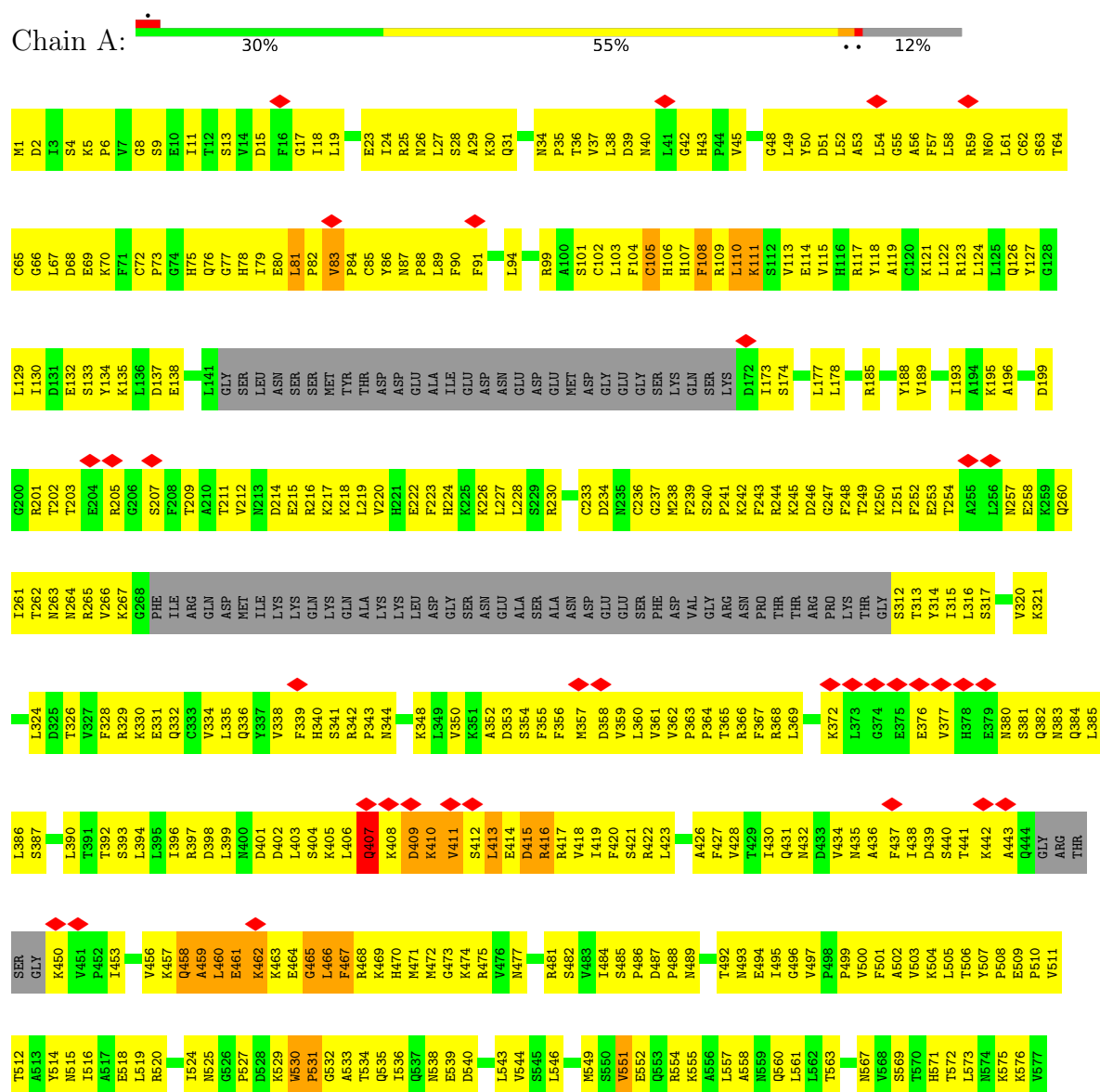
- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

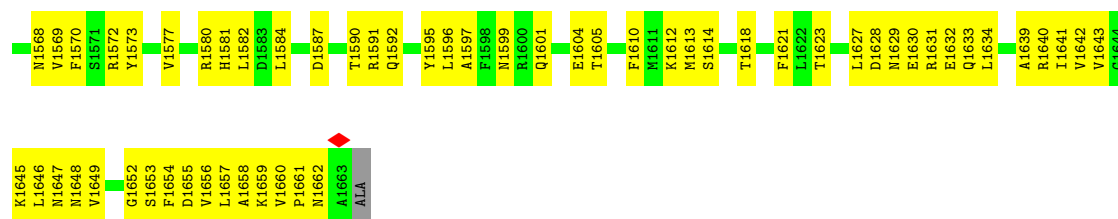
3 Residue-property plots

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 I subunit RPA190

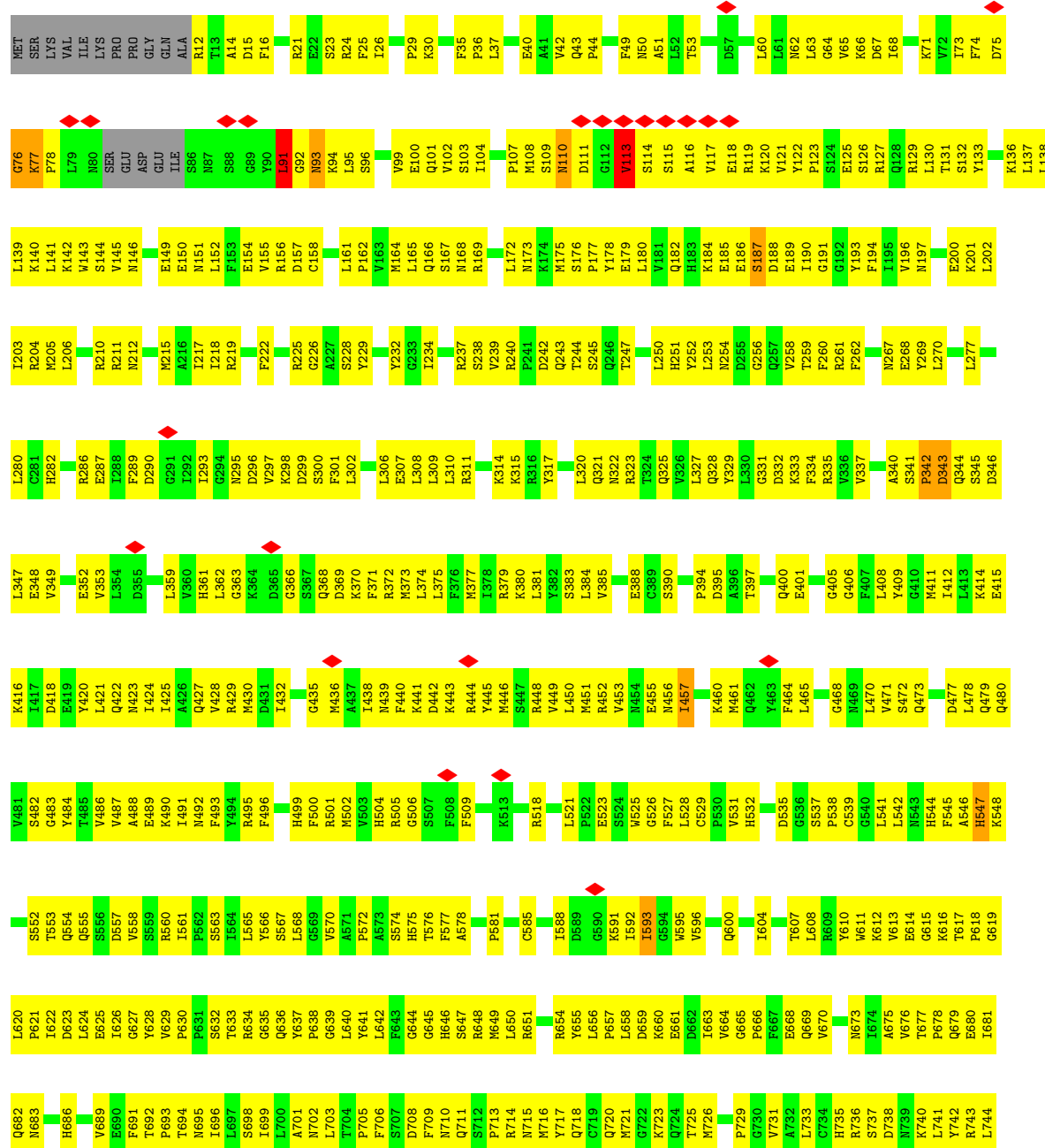


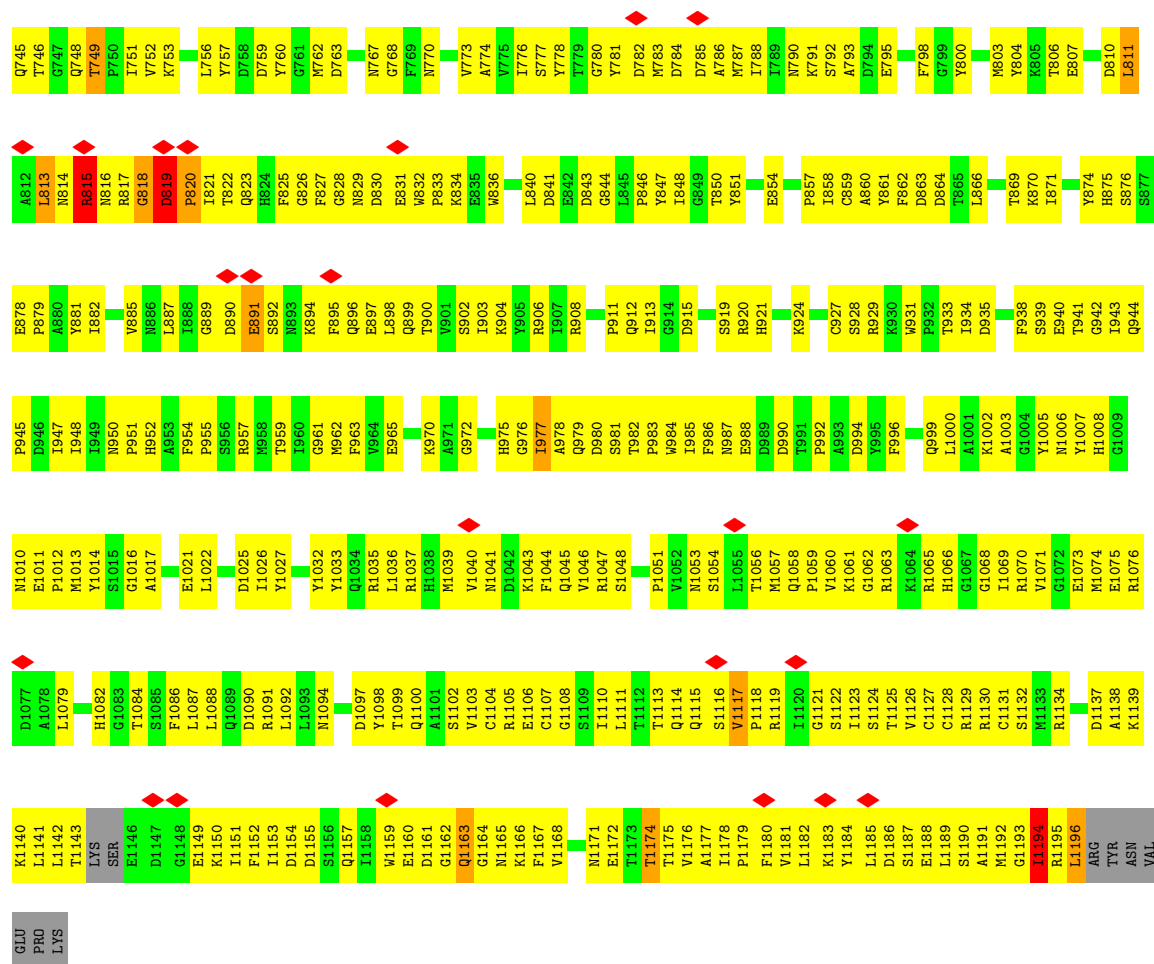
R1494	LYS	ASP	Y1306	W1243	K1173	K1107	S1037	K934	V861	S784	I719	A645
S1495	SER	GLU	D1307	V1246	M1174	H1108	I1038	G935	T862	Q785	F720	E646
S1496	ILE	GLU	V1308	S1247	M1175	S1109	R1039	S936	N863	Y786	K721	A647
I1497	VAL	GLN	S1309	S1248	L1176	LYS	R1039	N937	L864	G787	P722	L648
I1498	GLU	SER	K1310	D1248	L1178	GLU	A1041	V938	D865	A788	W723	N649
R1499	ALA	HIS	E1311	E1249	I1179	P1112	P1042	N939	K866	S789	P724	
Q1500	ASN	LYS	E1312	Q1250	H1180	H1113	G1043	V940	D867	K790	L725	D654
I1501	ASN	LYS	L1313	F1254	P1181	H1113	L1045	M944	D872	G792	W726	
P1502	N1438	THR	Q1314	C1255	E1182	X1115	L1045	C945	G793	I793	T727	Y657
H1503	N1439	LYS	N1315	K1256	G1183	Q1116	F1048	P873	R873	K794	G728	L658
N1504	K1440	GLN	V1316	S1257	G1186	Q1116	A1041	L947	E874	W794	K729	T659
D1505	T1441	ALA	I1317	K1258	G1187	V1118	Y1050	L946	H795	Q730	N590	
R1506	V1442	VAL	S1318	I1258	I1187	S1117	Y1050	G948	R878	S796	I731	P600
C1507	Q1443	SER	N1319	S1259	I1188	K1119	G1051		L879	S796	I732	
V1508	Q1443	TYR	Q1320	K1260	I1188	Y1120	G1052	A951	D872	G792	W726	
H1509	R1444	ASP	F1321	V1261	Q1191	D1121	D1053	E881	E874	I799	G728	
	Q1447	GLU	I1322	L1262	Q1191	F1122	A1054	I882		W794	K729	
		PRO	H1323	L1263	E1195	V1123	D1056	R955		H795	Q730	
		ASP	L1324	S1264	P1196	L1124	I1057	R956		S796	I731	
		GLU	L1325	E1265			D1056	R955		L797	I732	
		ASP	E1326	V1266			I1057	R956		K798	W726	
		GLU	A1327	D1267			T1058	V957		I799	G728	
		ILE	A1328	K1268			E1060	P958		V800	L736	
		GLU	E1332	V1270			S1061	V959		A806	W743	
		MET		I1271			H1062	M960		A807	M744	
		THR		V1272			L1133	V961		K808	P745	
		ARG	Q1336	I1272			G1134	G963		V809	G746	
		GLU	K1337	T1273			S1135	R964		F817	I747	
		ALA	ARG	E1274			V1136	K964		T818	N748	
		GLU	THR	T1275			S1137	P967		N819	L749	
		LYS	THR	T1276			E1138	S968		I820	S751	
		SER	GLY	GLY			N1139	P969		L821	K752	
		SER	GLY	THR			K1143	K970		T822	N753	
		ASP	ASN	THR			L1144	K970		A825	K756	
		GLU	ILE	ASN			F1147	Y872		F826	I755	
		GLU	GLY	THR			L1148	E973		T827	N757	
		GLY	VAL	ALA			D1149			C828		
		ILE	ALA	GLY			K1150			G829		
		ASP	VAL	GLY			L1085			M830		
		SER	ASN	ASN			L1085			D831		
		ASP	ARG	A1286			L1085			D832		
		LYS	LEU	A1287			H1088			D832		
		GLU	GLN	R1288			L1089			D833		
		SER	THR	S1289			F1154			D833		
		ASP	THR	Y1290			D1090			R834		
		ASP	ASP	V1291			V1091			L835		
		SER	VAL	I1292			K1156					
		ASP	ALA	H1293			E1092					
		SER	ASN	K1293			S1093					
		GLU	SER	M1294			A1094					
		ASP	SER	R1295			L1095					
		GLU	SER	F1296			K1096					
		ASP	SER	D1297			V1097					
		VAL	SER	D1298			S1098					
		ASP	ASN	N1299			T1101					
		LYS	LYS	P1236			L1102					
		ASP	ARG	N1300			K1165					
		GLU	ASN	Q1237			F1166					
		GLU	GLU	Y1302			R1167					
		ILE	GLU	S1303			A1168					
		ASN	ASP	E1304			L1169					
		ASN	ASN	E1305			K1106					



• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

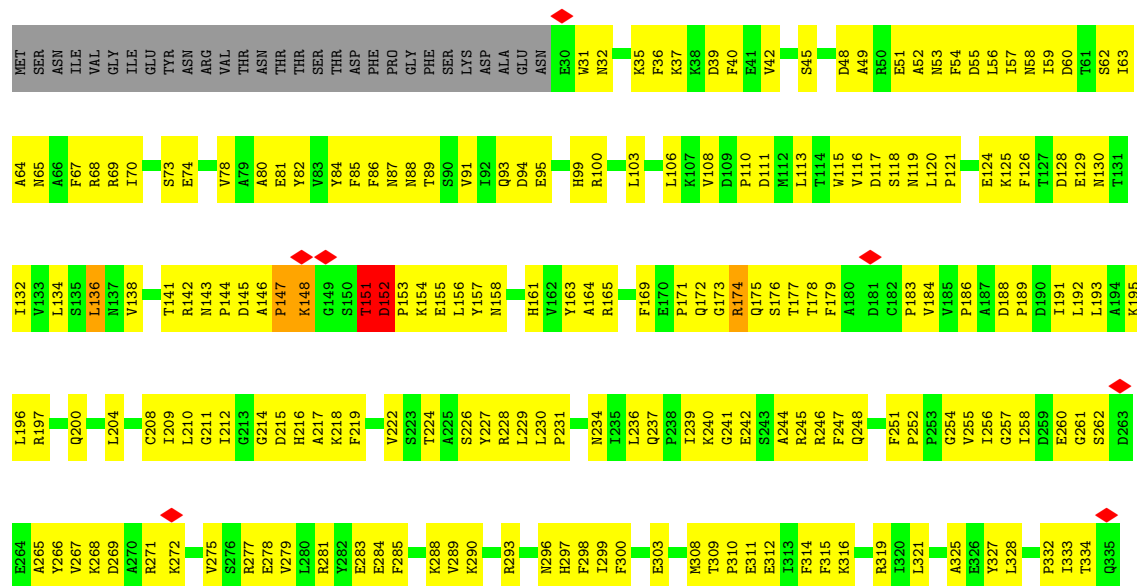
Chain B: 32% 64%



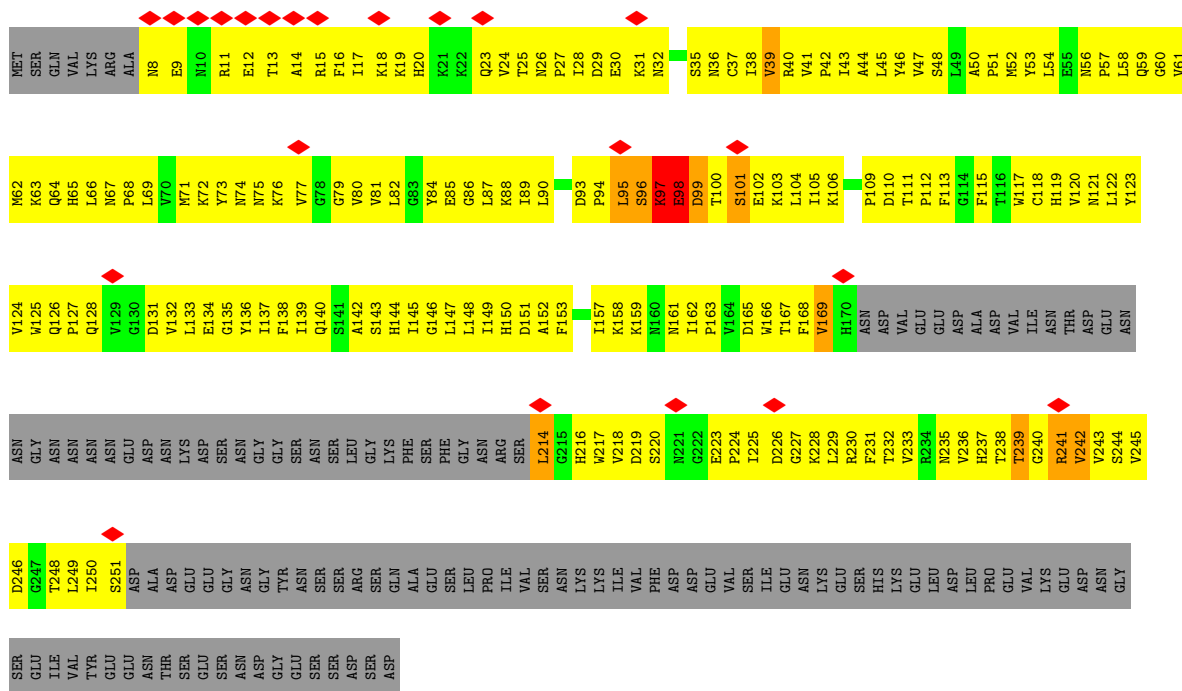


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

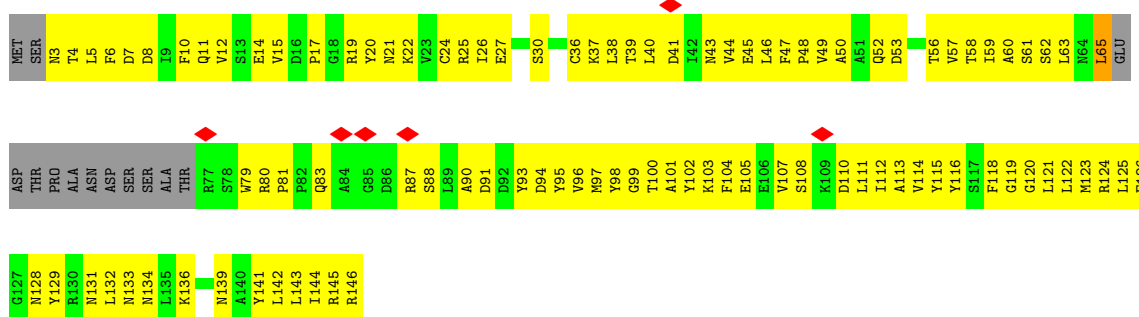
Chain C: 33% 56% 9%



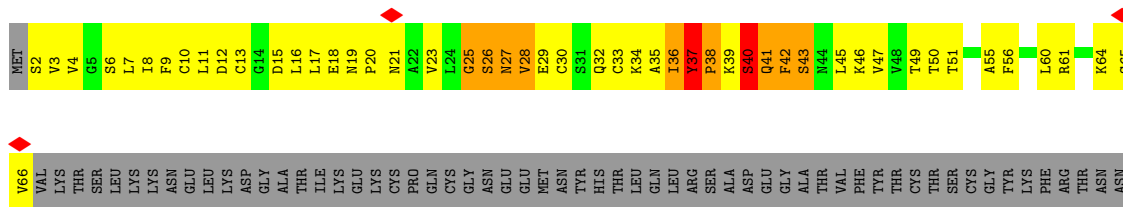




- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



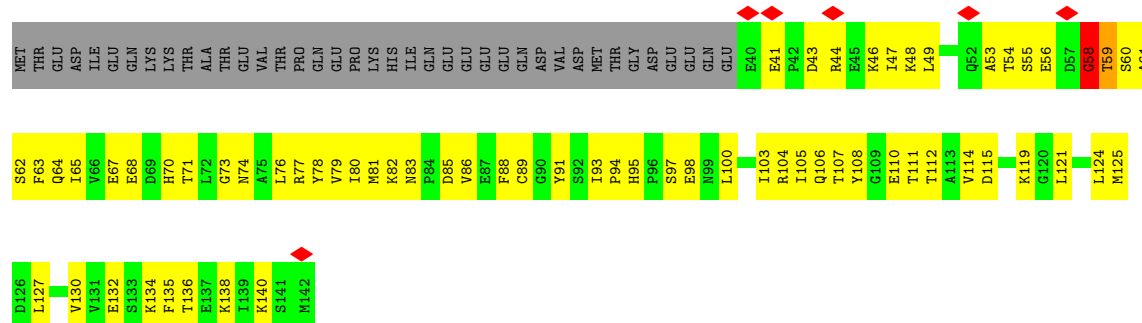
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5





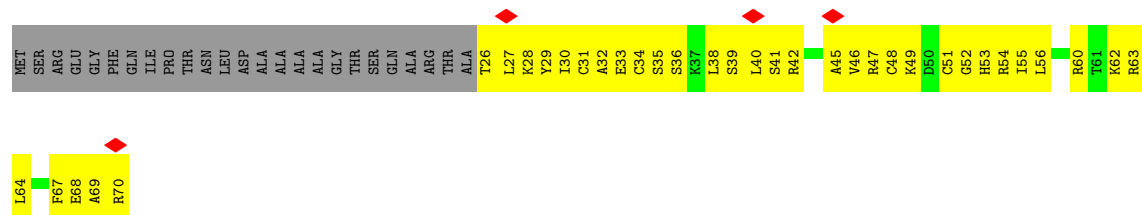
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 25% 46% 27%



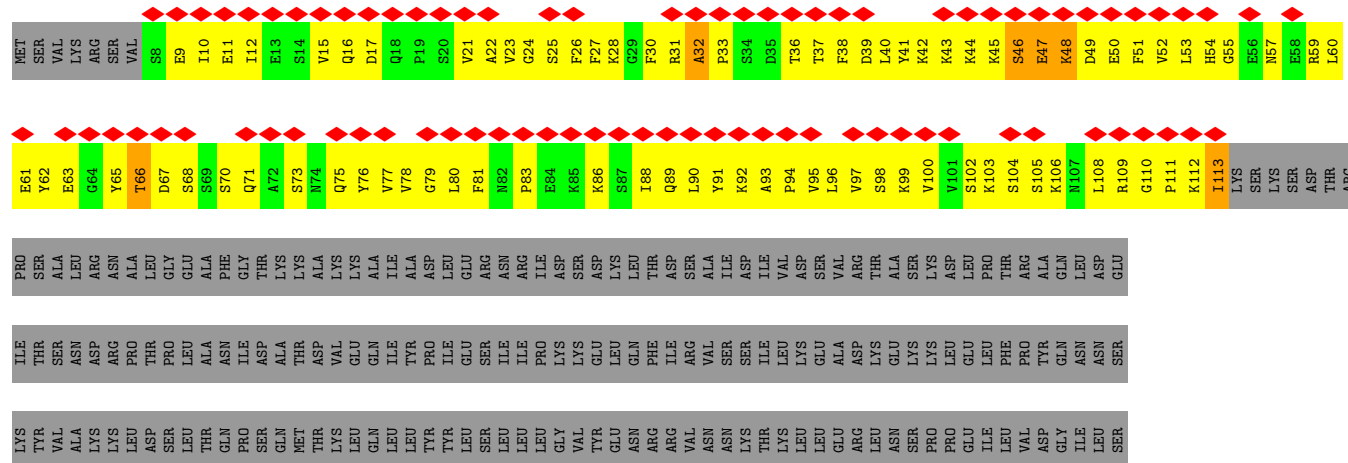
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 6% 14% 50% 36%



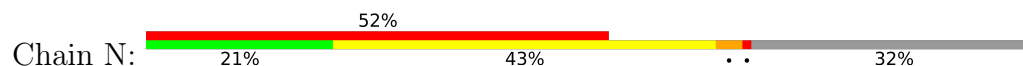
• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain M: 5% 20% 19% 74%



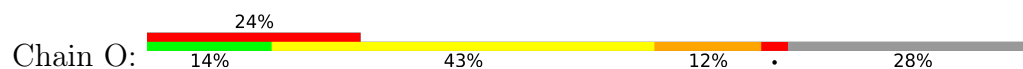
ARG	PHE	THR	LYS	THR	ILE	LYS	PRO	GLY	GLN	PHE	GLY	ASP	LYS	ASP	LYS	VAL
VAL	SER	LEU	PHE	VAL	ARG	VAL	LEU	GLY	ALA	VAL	GLY	THR	ALA	VAL	THR	ARG

● Molecule 14: DNA-directed RNA polymerase I subunit RPA34



MET	SER	LEU	LEU	SER	LYS	ASP	TYR	VAL	VAL	ASP	ASP	SER	SER	ASP	ASP	ASP
M61	V62	D63	I64	S65	K66	L67	K68	S69	P71	V72	D73	F74	E75	S76	S77	T78
T79	M80	T81	I82	D83	K84	H85	D86	K87	K88	I89	M90	D91	D92	T93	D94	I95
E96	S97	S98	L99	T100	Q101	D102	N103	L104	S105	N106	M107	T108	L109	L110	V111	P112
E114	S115	K116	E117	S118	L119	K120										
I121	A122	S123	T124	A125	K126	D127	N128	A129	P130	L131	Q132	F133	D134	K135	V136	F137
S138	F139	E141	T142	K143	K144	I145	P146	A147	I148	D149	Y150	V153	R154	V155	P156	R157
K158	D159	V160	V163	L166	K167	L168	E169	H170	F171	A172	Y175	D176	E177	E178	D179	F180
HIS	VAL	ALA	GLU													
GLU	VAL	LYS	GLU	ASN	LYS	PRO	LYS	ARG	GLY	HIS	HIS	ASP	GLU	GLU	GLY	ASP

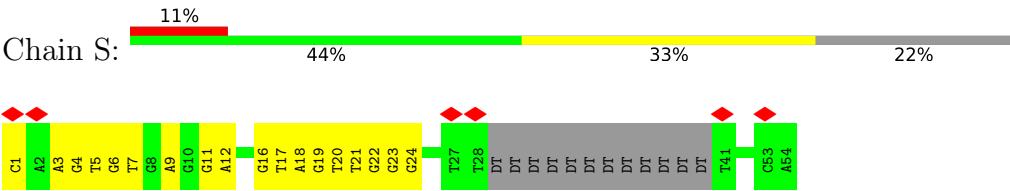
● Molecule 15: RNA polymerase I-specific transcription initiation factor RRN6



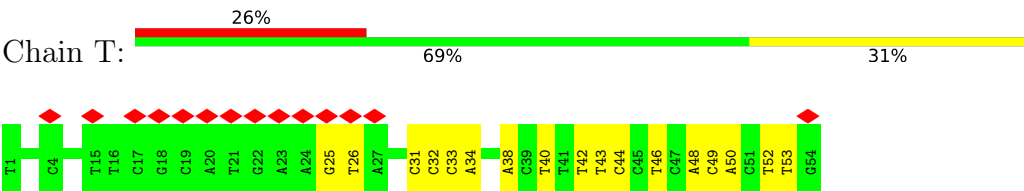
MET	SER	GLY	GLY	ILE	PRO	SER	SER	ASP	VAL	LEU	GLY	SER	SER	GLN	LEU	GLN
X13	X14	X15	X16	X17	X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28	X29
X30	X31	X32	X33	X34	X35	X36	X37	X38	X39	X40	X41	X42	X43	X44	X45	X46
X47	X48	X49	X50	X51	X52	X53	X54	X55	X56	X57	X58	X59	X60	X61	X62	X63
X64	X65	X66	X67	F172	F173	D175	V178	A179	M180	R181	D183	Q185	Y186	I187		
Q188	T189	A190	S191	D192	L193	R194	N195	Y196	R197	D198	G199	T200	E201	I202	V203	P204
G205	A206	S207	G208	K209	T210	G211	S212	V213	L214	N215	I216	A217	V218	L219	T220	X221
Q222	N223	T224	H225	L227	N228	R229	H230	N231	N232	T233	T234	S235	I236	E237	L238	H239
S240	I242	K243	S184	Q185	Y186	I187										
P248	G249	A250	S251	S253	I254	G255	R256	R257	S258	N259	L260	G261	G262	I263	T264	T265
E266	F269	Q270	I271	F272	R273	I274	E275	S276	V277	H278	S279	R280	S281	C282	D283	V284
M285	V286	S287	S288	S289	E290	P291	L292	Y293	F294	V295	E296	I297	D298	L299	M300	P301
Q301	K302	V303	D304	I245	K246	F307	N308									
P309	W310	D311	L312	Q313	Q314	F315	A316	I317	I318	D319	I320	K321	G322	N323	W324	S325
I326	G327	R328	W389	Q390	P391	E392	V393	V394	Q395	A396	K397	A398	W399	S400	N401	I402
I403	R404	D405	K406	R407	I408	D409	D410	K411	N412	G413	I414	L415	L416	T417	S418	R419
E420	I421	I422	I423	V424	G425	A426	S427	E428								



• Molecule 19: non-template strand DNA



• Molecule 20: template strand DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28297	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	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.199	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	249.59999, 249.59999, 249.59999	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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

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	0.39	1/11752 (0.0%)	0.78	20/15870 (0.1%)
2	B	0.44	1/9556 (0.0%)	0.79	12/12916 (0.1%)
3	C	0.37	0/2484	0.73	3/3366 (0.1%)
4	D	0.34	0/473	0.71	2/641 (0.3%)
5	E	0.32	0/1796	0.68	0/2416
6	F	0.35	0/682	0.62	0/922
7	G	0.28	0/1630	0.68	2/2216 (0.1%)
8	H	0.33	0/1089	0.67	0/1474
9	I	0.35	0/485	1.13	4/657 (0.6%)
10	J	0.43	0/578	0.82	1/775 (0.1%)
11	K	0.37	0/822	0.73	4/1108 (0.4%)
12	L	0.35	0/361	0.72	0/478
13	M	0.25	0/857	0.69	1/1151 (0.1%)
14	N	0.23	0/1279	0.91	5/1724 (0.3%)
15	O	0.67	8/4902 (0.2%)	1.45	84/6641 (1.3%)
16	P	0.64	6/3316 (0.2%)	1.77	132/4477 (2.9%)
17	Q	0.75	1/2990 (0.0%)	1.52	42/4030 (1.0%)
18	R	0.31	0/142	0.86	0/220
19	S	0.49	0/984	0.84	0/1519
20	T	0.49	0/1206	0.82	2/1855 (0.1%)
All	All	0.48	17/47384 (0.0%)	1.02	314/64456 (0.5%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	PRO	N-CD	-10.66	1.32	1.47
15	O	573	GLU	CA-C	8.89	1.64	1.52
15	O	297	ILE	CA-C	8.64	1.63	1.53
1	A	460	LEU	CA-C	8.09	1.63	1.52
16	P	262	LEU	CA-C	7.85	1.62	1.52

The worst 5 of 314 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	617	HIS	N-CA-C	-22.89	85.95	113.19
16	P	356	VAL	N-CA-C	-20.80	92.41	112.17
15	O	705	HIS	N-CA-C	-19.32	90.99	113.21
17	Q	152	ILE	N-CA-C	-18.82	95.13	113.20
2	B	77	LYS	CA-C-N	-17.61	100.39	120.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11542	0	11623	1803	0
2	B	9351	0	9239	1339	0
3	C	2432	0	2418	359	0
4	D	467	0	468	79	0
5	E	1760	0	1788	296	0
6	F	670	0	690	72	0
7	G	1592	0	1600	375	0
8	H	1071	0	1045	184	0
9	I	479	0	478	240	0
10	J	569	0	585	93	0
11	K	811	0	801	118	0
12	L	359	0	381	68	0
13	M	841	0	837	200	0
14	N	1254	0	1264	251	0
15	O	5063	0	4796	2326	0
16	P	3238	0	3256	1758	0
17	Q	2923	0	2967	1058	0
18	R	127	0	67	0	0
19	S	875	0	477	31	0
20	T	1082	0	615	43	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	J	1	0	0	0	0
21	L	1	0	0	0	0
All	All	46512	0	45395	9219	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 104.

The worst 5 of 9219 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)
15:O:421:ILE:HD11	17:Q:138:PHE:CD2	1.21	1.72
15:O:589:ILE:HG22	16:P:320:PHE:CD2	1.25	1.70
16:P:123:MET:HB2	16:P:125:PHE:CE1	1.19	1.70
16:P:171:HIS:CE1	16:P:243:PHE:CE1	1.81	1.67
15:O:421:ILE:CD1	17:Q:138:PHE:CD2	1.75	1.67

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	1445/1664 (87%)	1333 (92%)	87 (6%)	25 (2%)	7	35
2	B	1172/1203 (97%)	1088 (93%)	65 (6%)	19 (2%)	7	37
3	C	304/335 (91%)	283 (93%)	17 (6%)	4 (1%)	9	41
4	D	55/137 (40%)	51 (93%)	4 (7%)	0	100	100
5	E	213/215 (99%)	204 (96%)	8 (4%)	1 (0%)	24	62
6	F	81/155 (52%)	73 (90%)	7 (9%)	1 (1%)	10	42
7	G	197/326 (60%)	181 (92%)	12 (6%)	4 (2%)	6	32
8	H	129/146 (88%)	122 (95%)	7 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	63/125 (50%)	51 (81%)	7 (11%)	5 (8%)	1	10
10	J	67/70 (96%)	59 (88%)	7 (10%)	1 (2%)	8	38
11	K	101/142 (71%)	95 (94%)	4 (4%)	2 (2%)	6	32
12	L	43/70 (61%)	37 (86%)	5 (12%)	1 (2%)	5	29
13	M	104/415 (25%)	98 (94%)	4 (4%)	2 (2%)	6	32
14	N	156/233 (67%)	127 (81%)	23 (15%)	6 (4%)	2	20
15	O	581/894 (65%)	407 (70%)	119 (20%)	55 (10%)	0	8
16	P	378/514 (74%)	275 (73%)	52 (14%)	51 (14%)	0	3
17	Q	343/507 (68%)	248 (72%)	50 (15%)	45 (13%)	0	3
All	All	5432/7151 (76%)	4732 (87%)	478 (9%)	222 (4%)	4	18

5 of 222 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	TRP
1	A	531	PRO
1	A	721	LYS
1	A	791	TYR
1	A	912	VAL

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	1292/1465 (88%)	1262 (98%)	30 (2%)	44	64
2	B	1030/1053 (98%)	1007 (98%)	23 (2%)	45	64
3	C	270/296 (91%)	265 (98%)	5 (2%)	50	66
4	D	56/116 (48%)	56 (100%)	0	100	100
5	E	197/197 (100%)	196 (100%)	1 (0%)	81	81
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	179/291 (62%)	169 (94%)	10 (6%)	19	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	117/128 (91%)	116 (99%)	1 (1%)	70	75
9	I	57/110 (52%)	51 (90%)	6 (10%)	6	23
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	93/130 (72%)	93 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	96/371 (26%)	91 (95%)	5 (5%)	21	44
14	N	146/220 (66%)	142 (97%)	4 (3%)	39	60
15	O	545/779 (70%)	486 (89%)	59 (11%)	6	22
16	P	362/476 (76%)	299 (83%)	63 (17%)	2	12
17	Q	331/474 (70%)	273 (82%)	58 (18%)	2	11
All	All	4948/6365 (78%)	4683 (95%)	265 (5%)	21	43

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	208	TYR
17	Q	277	ILE
17	Q	392	LEU
15	O	260	LEU
15	O	234	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	36	ASN
15	O	239	HIS
17	Q	212	HIS
7	G	65	HIS
14	N	51	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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
15	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	67:UNK	C	172:PHE	N	32.54

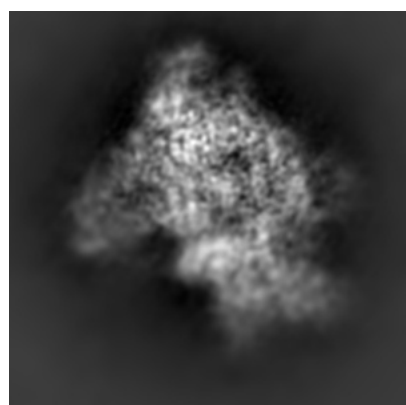
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8774. These allow visual inspection of the internal detail of the map and identification of artifacts.

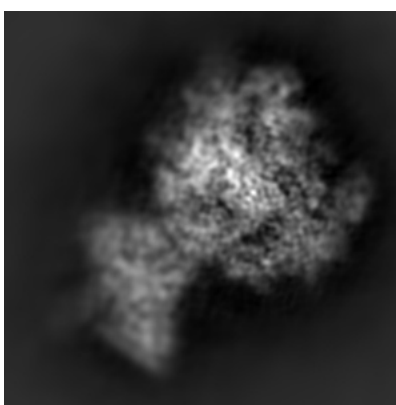
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

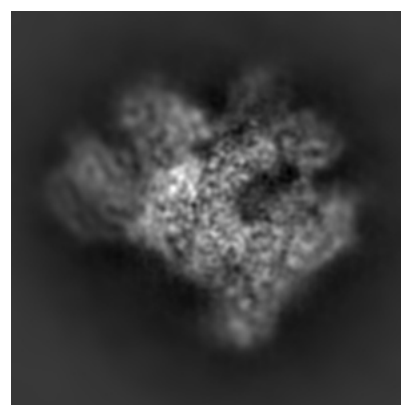
6.1.1 Primary map



X



Y

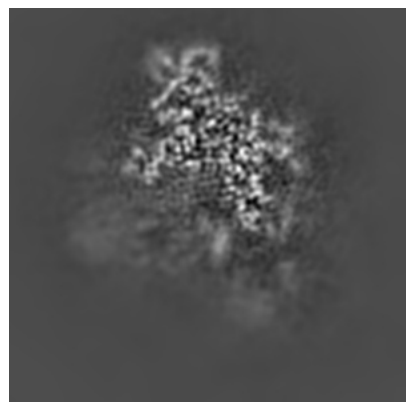


Z

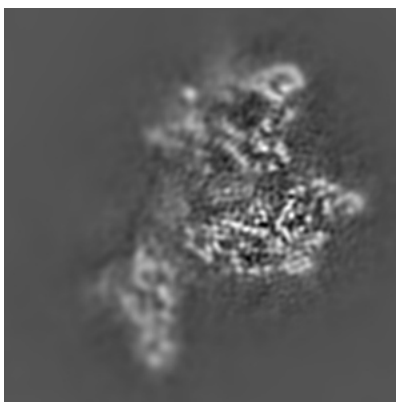
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

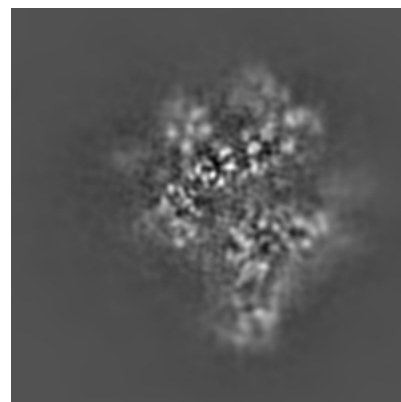
6.2.1 Primary map



X Index: 96



Y Index: 96

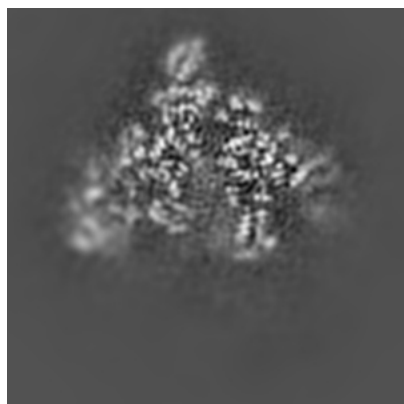


Z Index: 96

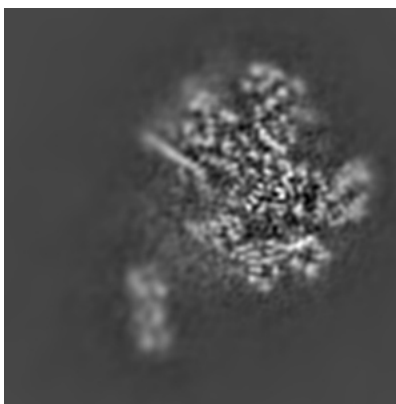
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

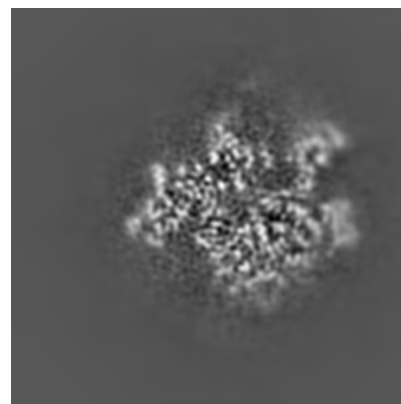
6.3.1 Primary map



X Index: 108



Y Index: 86

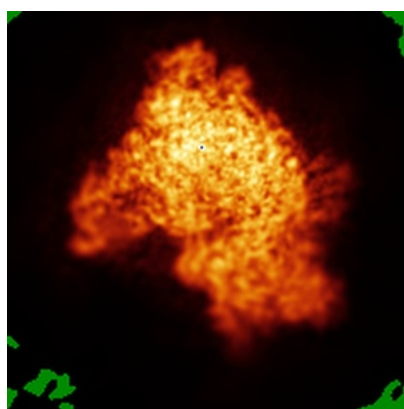


Z Index: 126

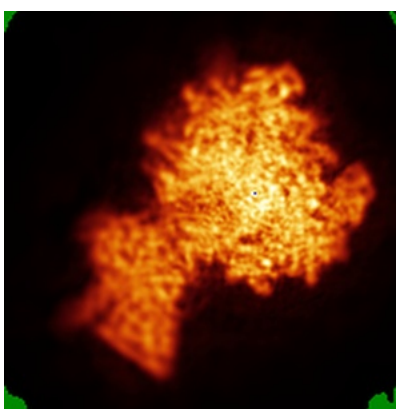
The images above show the largest variance slices of the map in three orthogonal directions.

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

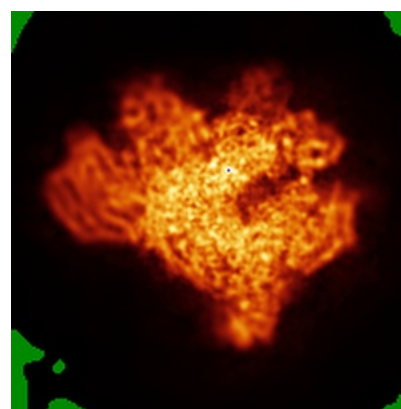
6.4.1 Primary map



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.

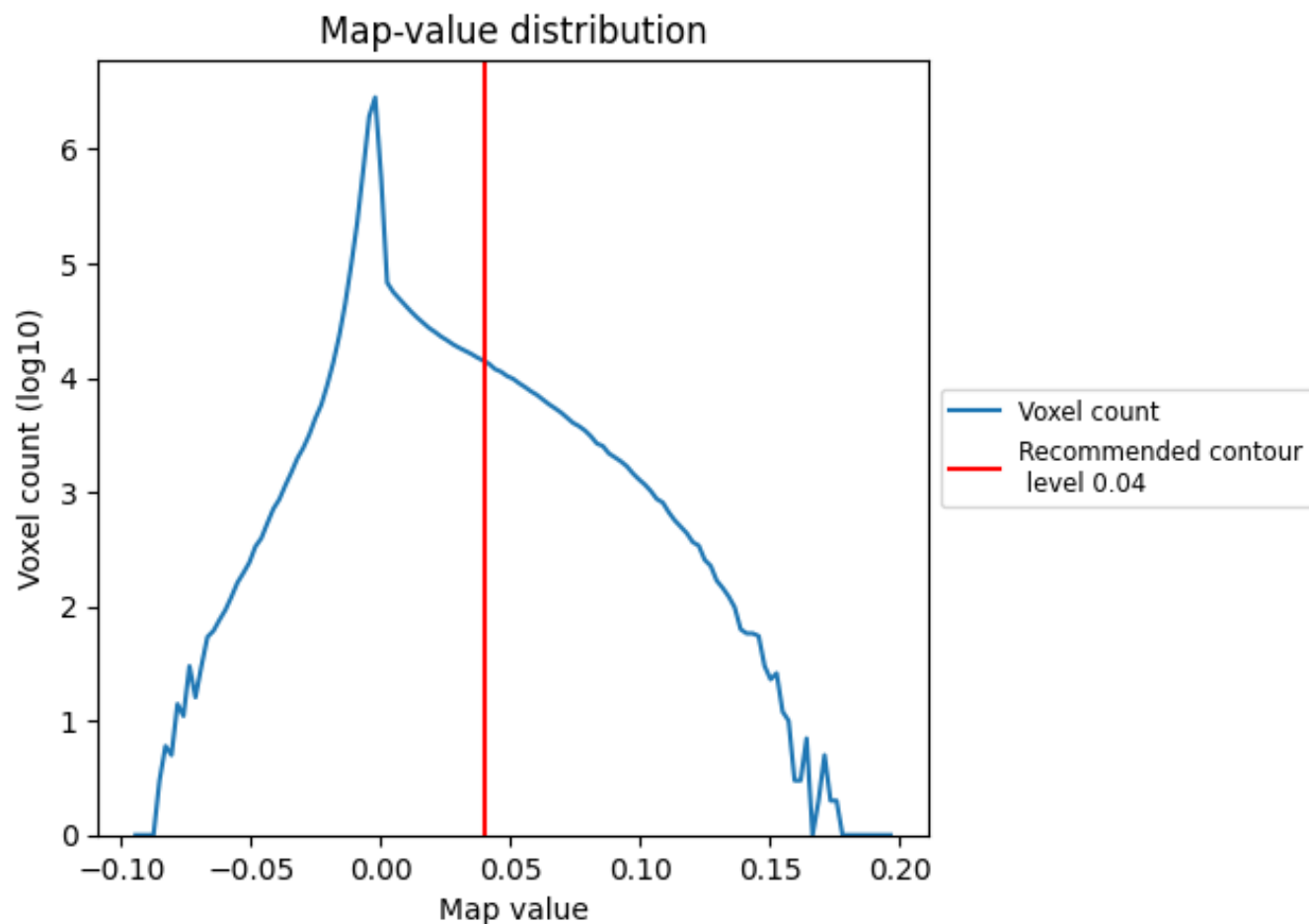
6.6 Mask visualisation

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

7 Map analysis [i](#)

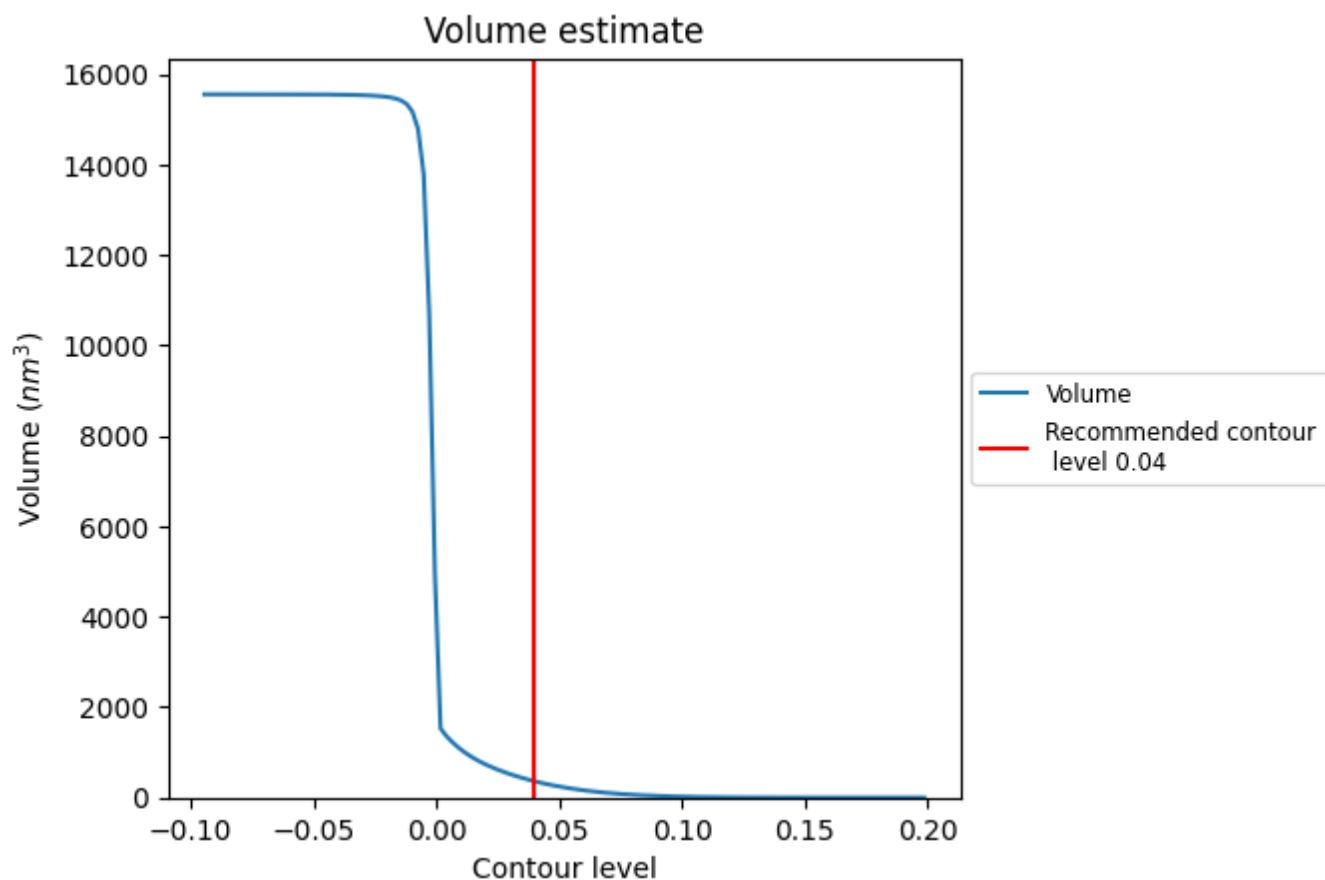
This section contains the results of statistical analysis of the map.

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.

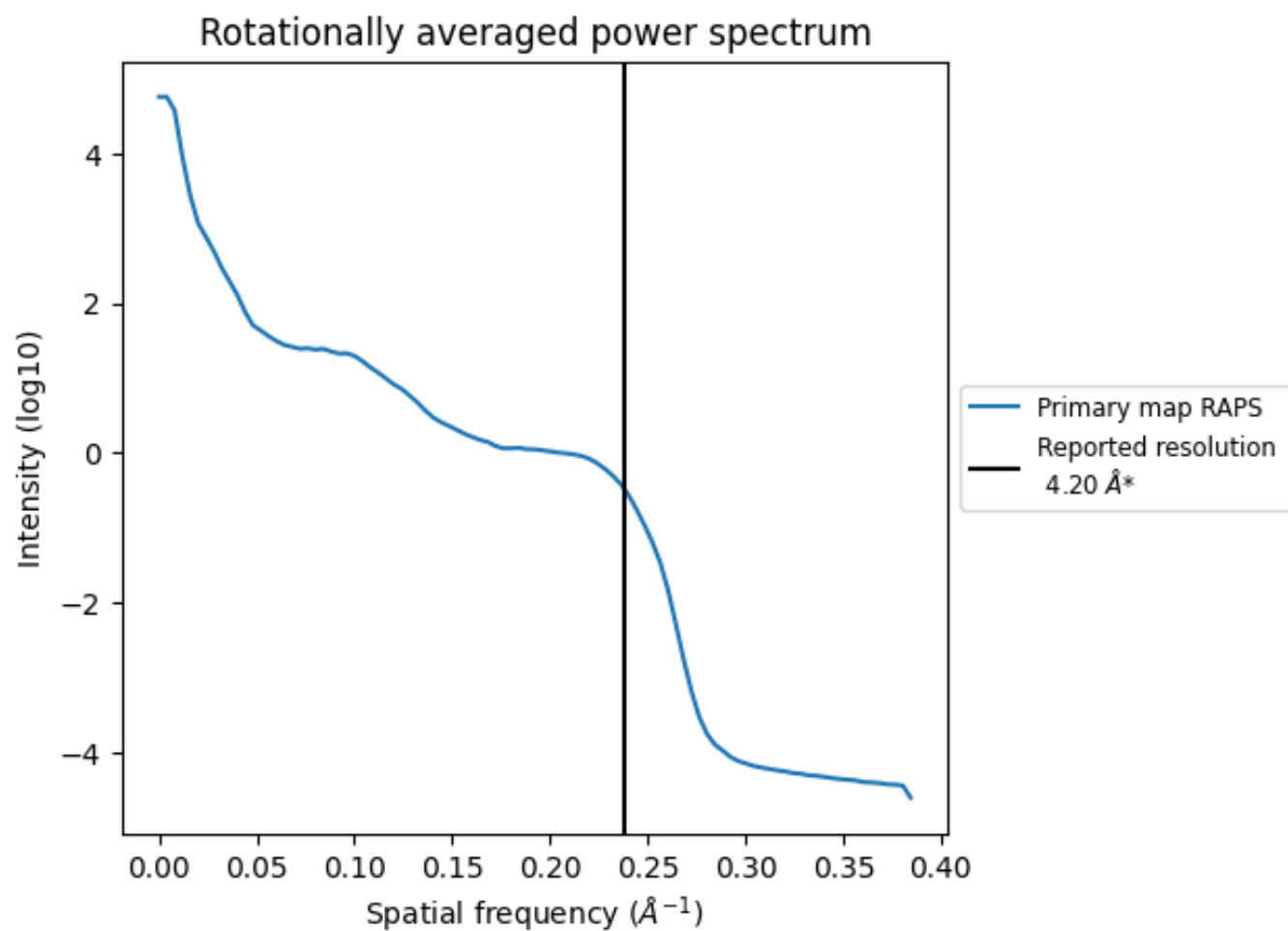
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 361 nm³; this corresponds to an approximate mass of 326 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 ⓘ

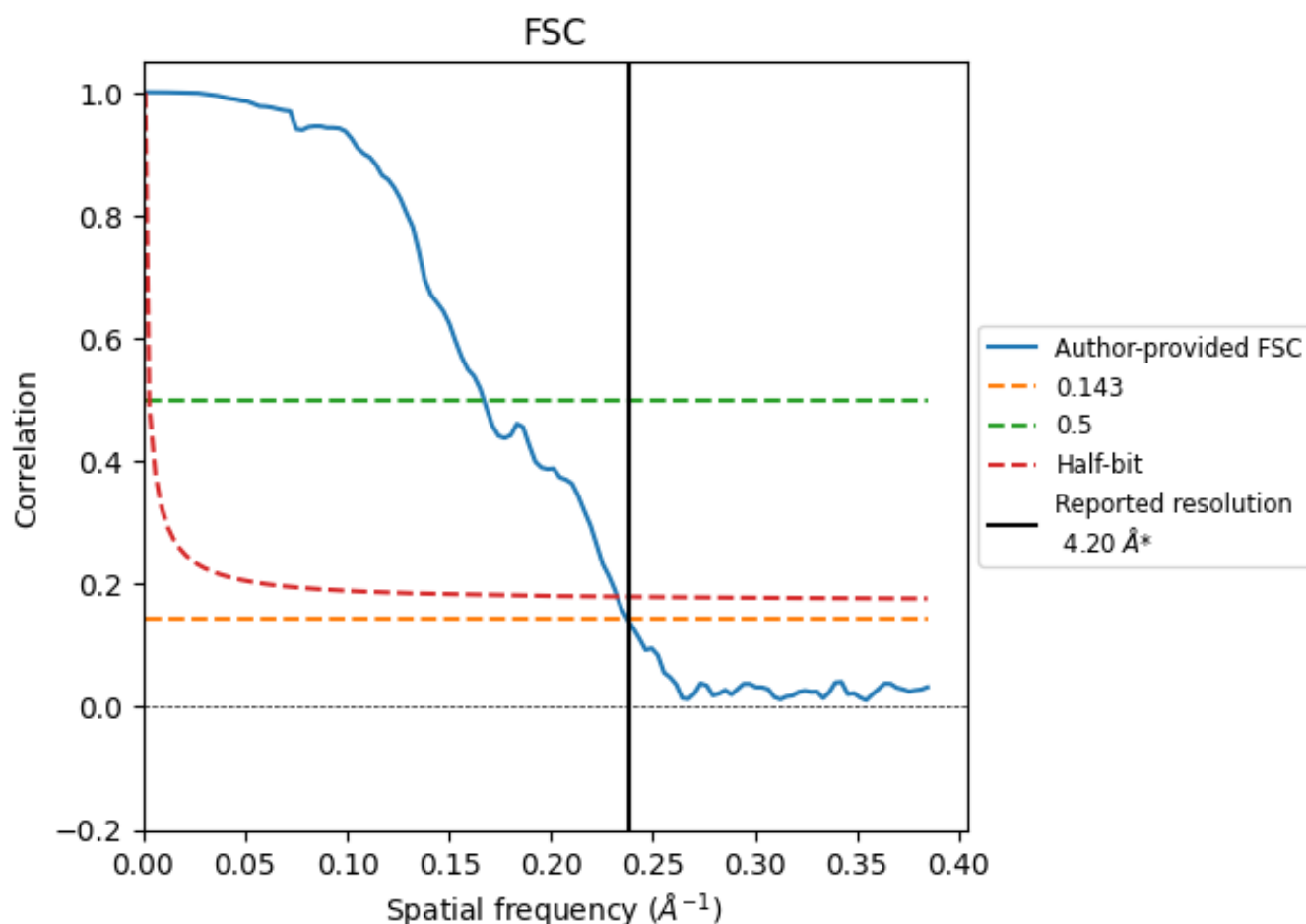


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

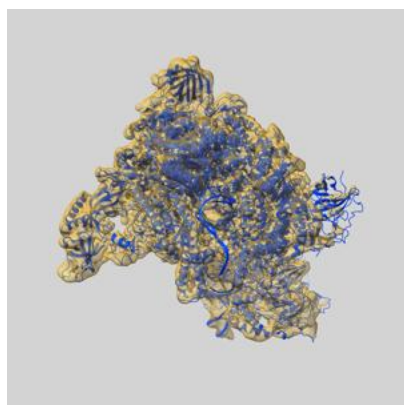
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.21	5.99	4.30
Unmasked-calculated*	-	-	-

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

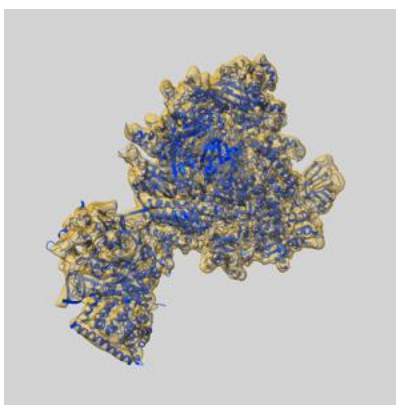
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8774 and PDB model 5W64. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

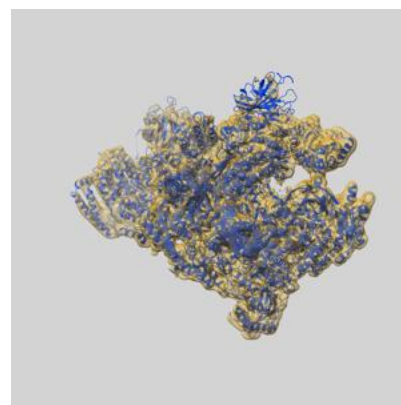
9.1 Map-model overlay [i](#)



X



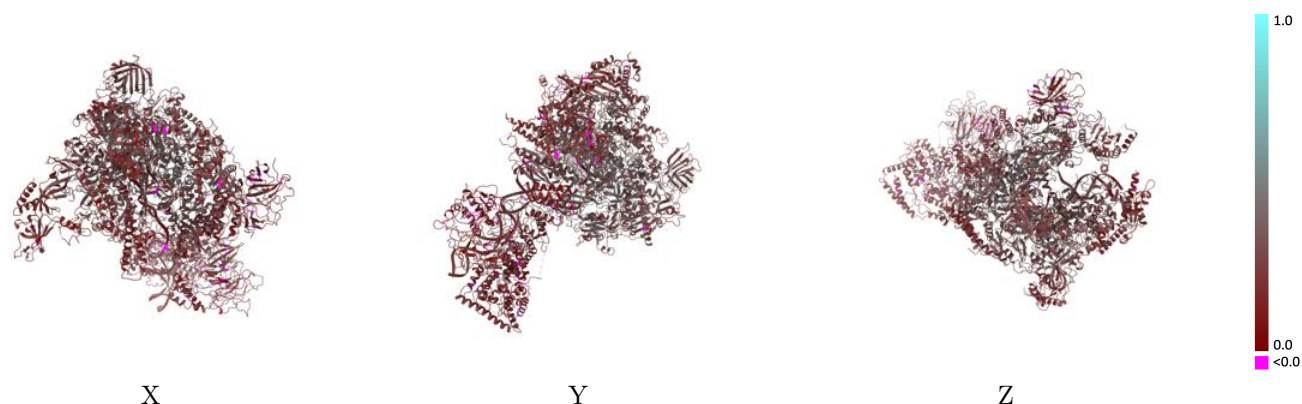
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)

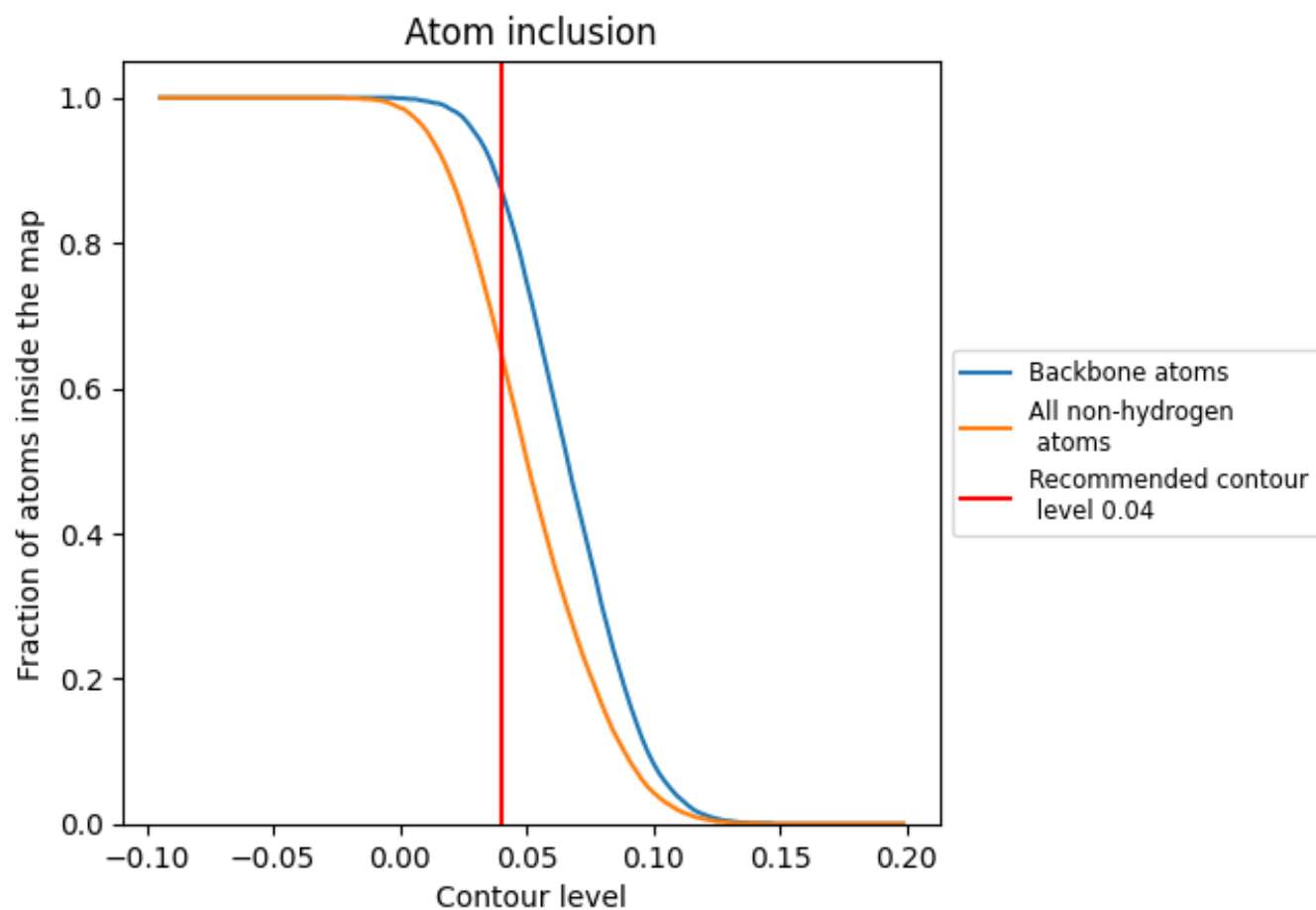


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 65% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6510	 0.2760
A	 0.7100	 0.3130
B	 0.7290	 0.3540
C	 0.7650	 0.3280
D	 0.6980	 0.2400
E	 0.7300	 0.2700
F	 0.7180	 0.3260
G	 0.6780	 0.2280
H	 0.7490	 0.2920
I	 0.7280	 0.2820
J	 0.7790	 0.3560
K	 0.7130	 0.3020
L	 0.7150	 0.3360
M	 0.2110	 0.2090
N	 0.2010	 0.2190
O	 0.5110	 0.1810
P	 0.5830	 0.1710
Q	 0.5410	 0.1820
R	 0.1730	 0.1870
S	 0.7190	 0.2590
T	 0.6200	 0.2230

