



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 12:10 PM UTC

PDB ID : 9G2C / pdb_00009g2c
EMDB ID : EMD-50972
Title : Yeast RNA polymerase I elongation complex stalled by an apurinic site, open state
Authors : Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on : 2024-07-10
Resolution : 3.50 Å(reported)
Based on initial model : 6hko

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:

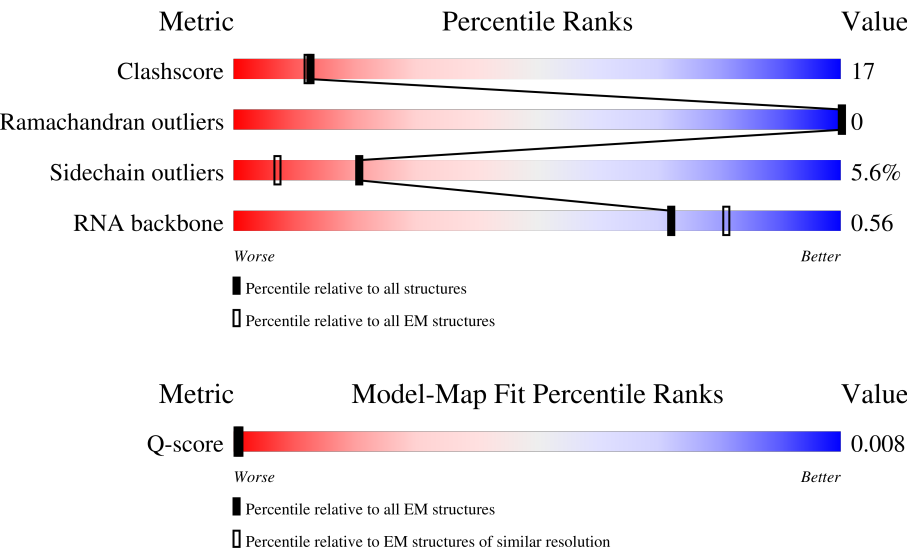
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.50 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	13950 (3.00 - 4.00)

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	60% 46% 23% • 30%
2	B	1203	82% 55% 36% • 6%
3	C	335	82% 59% 29% • 9%

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Mol	Chain	Length	Quality of chain
4	E	215	
5	F	155	
6	G	326	
7	H	146	
8	I	125	
9	J	70	
10	K	142	
11	L	70	
12	M	415	
13	N	233	
14	R	12	
15	S	38	
16	T	38	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 29270 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	1172	Total	C	N	O	S	0	0
			9243	5827	1599	1768	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1127	Total	C	N	O	S	0	0
			8963	5676	1577	1660	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2415	1535	414	458	8		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	181	Total	C	N	O	S	0	0
			1488	943	263	274	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	103	Total	C	N	O	S	0	0
			839	530	148	158	3		

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	60	Total	C	N	O	S	0	0
			472	305	75	89	3		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 8 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	57	Total	C	N	O	S	0	0
			423	267	70	82	4		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	68	Total	C	N	O	S	0	0
			561	357	100	99	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	97	Total	C	N	O	S	0	0
			758	476	123	155	4		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	71	Total	C	N	O	0	0
			571	359	99	113		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	86	Total	C	N	O	S	0	0
			679	437	116	124	2		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	9	Total	C	N	O	P	0	0
			197	88	40	60	9		

- Molecule 15 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	27	Total	C	N	O	P	0	0
			546	262	89	168	27		

- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	35	Total	C	N	O	P	0	0
			707	337	127	208	35		

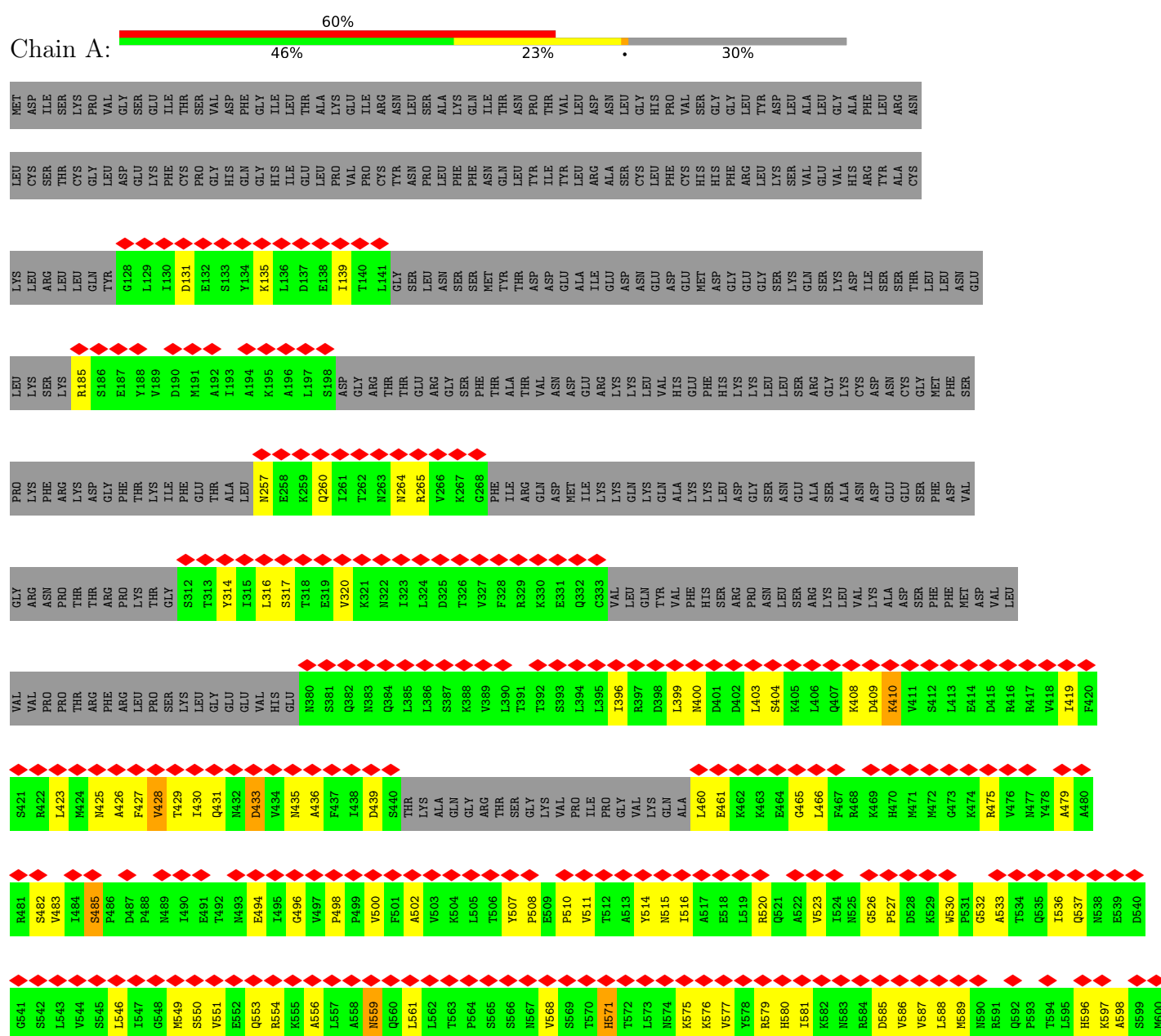
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	B	1	Total	Zn	0
			1	1	
17	I	1	Total	Zn	0
			1	1	
17	J	1	Total	Zn	0
			1	1	
17	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.

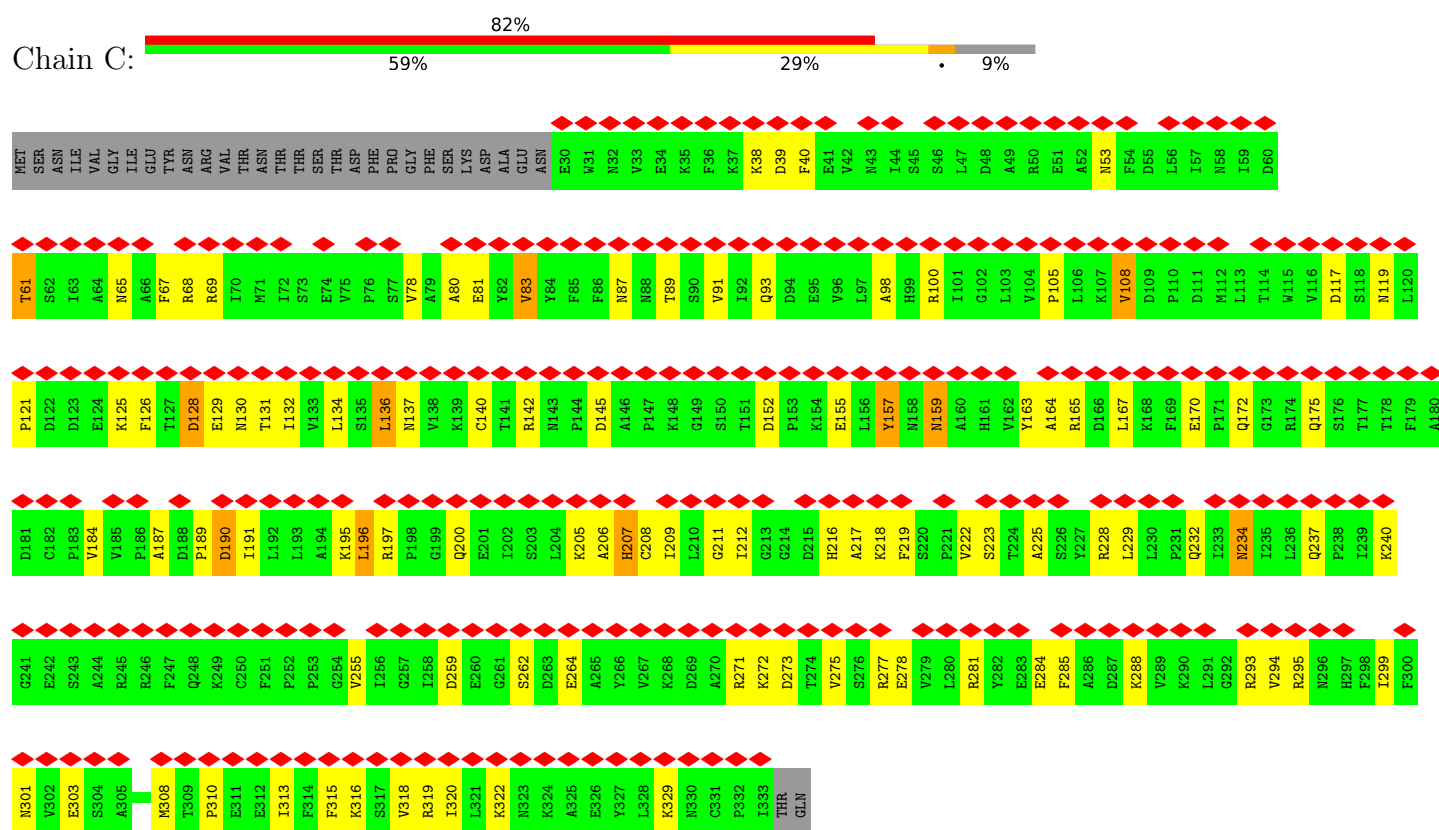
• Molecule 1: DNA-directed RNA polymerase I subunit RPA190



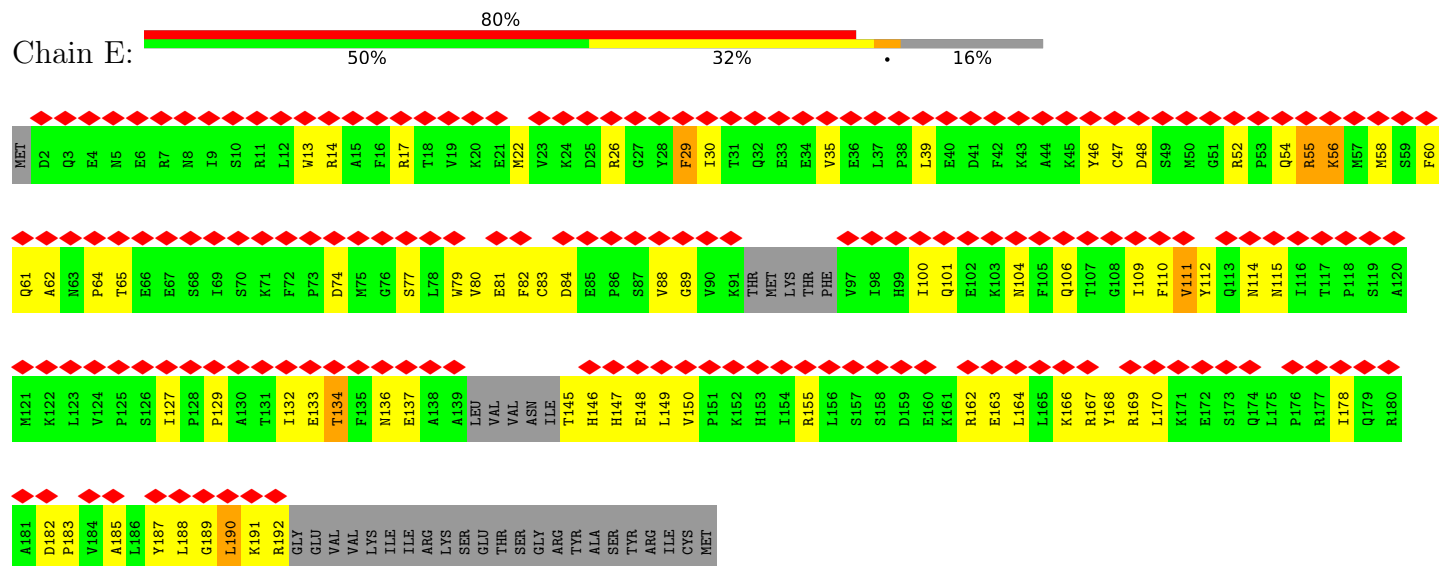
A1328	D1268	ALA	L1027	T965	G1033	H1088	L1148	V1270	K1269	I1329	A1328	G663	M601
I1329	K1269	GLY	E1028	I966	E1029	L1089	D1149	I1271	I1270	V1330	H603	G664	G602
K1331	I1271	ALA	H1031	S968	H1030	V1091	K1150	I1272	M1151	E1331	K604	V666	K604
I1333	T1273	ALA	S1093	P969	S1093	E1092	S1152	T1274	S1152	E1332	V605	R667	V605
K1334	E1274	LEU	D1035	K970	S1033	A1094	K1153	T1275	K1153	I1333	R606	G668	R606
K1335	T1275	PHE	N1036	P971	Y1034	L1095	LEU	T1276	S1152	I1334	V607	L669	V607
Q1336	T1276	LYS	N1036	Y972	D1035	L1096	PHE	T1277	S1152	K1334	L608	I670	L608
K1337	G1277	SER	N1036	E973	N1036	K1096	LYS	T1278	S1152	Q1336	P609	Q671	P609
R1338	THR	ASP	I1038	T974	I1038	Y1097	SER	T1279	S1152	K1337	N610	D672	N610
THR	ASN	P1220	S1098	D975	S1098	K1099	ASP	T1280	S1152	R1338	E611	H673	E611
THR	THR	R1221	K1099	A976	K1099	K1099	GLI160	P1221	S1152	THR	K612	I674	K612
PRO	ALA	L1222	K1100	M977	K1100	T1101	V1161	R1222	S1152	PRO	T613	S675	T613
ASP	GLY	R1223	L1102	A978	L1102	T1101	M1162	E1223	S1152	ASP	L614	A678	L614
ILE	GLY	E1224	K1103	G979	K1103	K1103	E1163	I1225	S1152	ILE	R615	G677	R615
GLY	ASN	K1165	T1044	G980	K1104	K1104	K1164	V1226	S1152	GLY	L616	V678	L616
VAL	ALA	K1165	L1045	Y981	R1105	R1105	K1165	M1227	S1152	VAL	L617	W679	L617
ALA	ALA	F1166	V1046	K983	K1106	K1106	F1166	M1227	S1152	ALA	H617	L680	H617
VAL	ALA	R1167	Q1047	K984	K1107	K1107	R1167	M1228	S1152	VAL	Y618	T681	Y618
PRO	ARG	A1168	Q1047	K985	K1107	K1107	A1168	T1229	S1152	PRO	A619	S682	A619
ARG	LEU	L1169	F1048	P986	H1108	H1108	L1169	A1229	S1152	ARG	N620	S682	N620
LEU	GLN	M1170	Y1050	S924	S1109	S1109	M1170	S1230	S1152	LEU	T621	G683	T621
THR	THR	Q1171	G1051	M925	K1110	K1110	Q1171	A1231	S1152	THR	G622	D684	G622
ASP	ASP	L1172	G1052	Q926	K1111	K1111	L1172	I1231	S1152	ASP	A623	S685	A623
VAL	VAL	K1173	D1053	A927	P1112	P1112	K1173	A1232	S1152	VAL	Y624	F686	Y624
ALA	ALA	Y1174	D1053	N928	P1112	P1112	Y1174	I1233	S1152	ALA	N625	F687	N625
ASN	ASN	M1175	A1054	P992	H1113	H1113	M1175	K1234	S1152	ASN	A626	T688	A626
LEU	LEU	R1176	I1055	Q931	Y1114	Y1114	R1176	T1235	S1152	LEU	ASP	PHE	ASP
GLU	GLU	S1177	I1056	G932	K1115	K1115	S1177	P1236	S1152	GLU	ASP	GLY	ASP
ASP	ASP	L1178	I1057	A933	Q1116	Q1116	L1178	Q1237	S1152	ASP	ASP	GLY	ASP
ASP	ASP	T1179	T1058	K934	Y996	Y996	T1179	M1238	S1152	ASP	ASP	GLY	ASP
ASP	ASP	V1118	T1058	G935	P997	P997	V1118	T1239	S1152	ASP	ASP	GLY	ASP
GLU	GLU	K1119	E1059	S936	H998	H998	K1119	E1240	S1152	GLU	E632	Q693	E632
GLN	GLN	P1181	E1060	N937	N937	N937	P1181	I1241	S1152	GLN	M633	Q694	M633
LEU	LEU	G1182	S1061	V938	N938	N938	G1182	I1242	S1152	LEU	N634	Q695	N634
GLU	GLU	E1183	H1062	N939	N939	N939	E1183	I1243	S1152	GLU	M635	Q697	M635
GLU	GLU	A1184	T1064	Q942	Q942	Q942	A1184	Q1250	S1152	GLU	H636	F637	H636
GLU	GLU	V1185	Q1065	Q943	Q943	Q943	V1185	Q1251	S1152	GLU	F638	Q699	F638
GLN	GLN	G1186	Q1065	Q944	Q944	Q944	G1186	I1252	S1152	GLN	Q639	Q701	Q639
GLN	GLN	I1187	F1068	C945	C945	C945	I1187	S1247	S1152	GLN	N640	P702	N640
GLN	GLN	I1188	C1069	L946	L946	L946	I1188	D1248	S1152	GLN	E641	P703	E641
GLN	GLN	Y1189	L1070	L947	L947	L947	Y1189	E1249	S1152	GLN	N642	D704	N642
GLN	GLN	S1190	D1071	Q948	Q948	Q948	S1190	Q1250	S1152	GLN	A643	G705	A643
GLN	GLN	Q1191	N1072	Q950	Q950	Q950	Q1191	I1251	S1152	GLN	R644	H706	R644
GLN	GLN	S1192	Y1073	A951	A951	A951	S1192	D1252	S1152	GLN	E646	T707	E646
GLN	GLN	V1193	Y1074	L952	L952	L952	V1193	T1253	S1152	GLN	A647	T708	A647
GLN	GLN	G1194	A1075	E953	E953	E953	G1194	F1254	S1152	GLN	N648	R709	N648
GLN	GLN	P1196	L1076	G954	G954	G954	P1196	C1255	S1152	GLN	L650	S710	L650
GLN	GLN	S1197	L1077	R955	R955	R955	S1197	C1256	S1152	GLN	A651	I712	A651
GLN	GLN	T1198	K1078	R956	R956	R956	T1198	S1257	S1152	GLN	T653	T713	T653
GLN	GLN	Q1199	K1079	V957	V957	V957	Q1199	I1258	S1152	GLN	D654	L715	D654
GLN	GLN	Y1199	S1137	V957	V957	V957	Y1199	S1259	S1152	GLN	S655	P716	S655
GLN	GLN	M1200	E1138	P958	P958	P958	M1200	K1260	S1152	GLN	Q656	T718	Q656
GLN	GLN	T1201	N1081	V959	V959	V959	T1201	V1261	S1152	GLN	Y657	F720	Y657
GLN	GLN	L1202	P1082	N960	N960	N960	L1202	I1262	S1152	GLN	L658	T721	L658
GLN	GLN	M1203	S1083	V961	V961	V961	M1203	L1263	S1152	GLN	P660		
GLN	GLN	T1204	A1084	S962	S962	S962	T1204	S1264	S1152	GLN			
GLN	GLN	PHE	L1085	G963	G963	G963	PHE	V1266	S1152	GLN			
GLN	GLN	HIS	I1086	K964	K964	K964	HIS		S1152	GLN			
GLN	GLN	PHE	E1087				PHE		S1152	GLN			
GLN	GLN	S1146					S1146		S1152	GLN			
GLN	GLN	F1147					F1147		S1152	GLN			

ILE	PHE	ILE	ASP	D1155	S1156	Q1157	I1158	TRP	GLU	GLN	ASP	GLY	PHE	V1168	G1169	G1170	N1171	E1172	T1173	T1174	T1175	V1176	A1177	I1178	P1179	F1180	V1181	L1182	K1183	Y1184	L1185	D1186	S1187	E1188	L1189	S1190	A1191	M1192	G1193	I1194	R1195	L1196	R1197	Y1198	M1199	V1200	E1201	P1202	K1203											
R1091	L1092	L1093	N1094	SER	ASP	ASP	THR	THR	GLN	ALA	SER	V1103	C1104	E1106	C1107	G1108	S1109	ILE	THR	T1113	Q1114	Q1115	S1116	V1117	R1119	I1120	G1121	S1122	I1123	S1124	L1125	V1126	C1127	C1128	R1129	R1130	R1131	SER	MET	ARG	PHE	GLU	ASP	ALA	LYS	LYS	LEU	LEU	THR	LYS	GLU	GLY	GLU	LYS						
V1031	Y1032	Y1033	Q1034	R1035	L1036	L1037	H1038	M1039	VAL	ASN	ASN	K1043	F1044	Q1045	V1046	R1047	S1048	T1049	G1050	P1051	V1052	ASN	SER	SER	T1056	M1057	Q1058	P1059	V1060	K1061	G1062	K1063	K1064	R1065	H1066	G1067	G1068	I1069	R1070	V1071	G1072	ARG	E1073	M1074	E1075	R1076	D1077	L1078	L1079	L1080	G1081	H1082	G1083	T1084	S1085	F1086	L1087	L1088	Q1089	D1090
A968	Q969	K970	A971	G972	A973	L974	H975	G976	I977	A978	Q979	D980	S981	T982	P983	W984	I985	E988	D989	D990		A993	D994	Y995	P996	G997	E998	Q999	L1000	A1001	K1002	A1003	G1004	Y1005	N1006		G1009	M1010	E1011	P1012	M1013	Y1014	S1015	G1016	P1017	A1017	T1018	G1019	F954	P955	S956	R957	N958		G961	N962	E965	S966	G1029	V1030
R906	I907	R908	R909	T910	P911	Q912	I913	G914	D915	R916	F917	S918	S919	R920	H921	G922	Q923	R924	G925	Y926	C927	S928	R929	R930	W931	P932	T933	I934	D935	N936	P937	F938	S939	E940	T941	G942	I943	Q944	P945	D946	I947	I948	I949	N950	P951	H952	A953	F954	P955	S956	R957	N958		G961	N962	E965	S966	L967		
P846	Y847	I848	G849	T850	H851	H852	E853	E854	G855	D856	P857	I858	C859	A860	H861	F862	D863	H864	T865	L866	H867	K868	T869	K870	L871	K872	H873	H874	H875	S876	S877	E878	P879	A880	Y881	I882	E883	E884	H885	L887	I888	G889	D890	E891	S892	N893	K894	F895	Q896	E897	L898	Q899	T900	Y901	S902	T903	K904	Y905		
A786	M787	I788	I789	N790	S791	H792	A793	D794	E795	R796	F798	G799	Y800	G801	T802	M803	Y804	K805	T806	E807	K808	H809	D810	L811	A812	L813	R814	R815	N816	R817	G818	D819	P820	I821	T822	Q823	H824	F825	G826	F827	G828	N829	D830	E831	W832	P833	K834	E835	W836	L837	E838	K839	L840	D841	E842	D843	G844	L845		
T725	M726	G727	T728	E729	G730	V731	A732	L733	C734	H735	R736	D738	N739	K740	L741	Y742	R743	L744	Q745	T746	G747	Q748	T749	P750	I751	V752	K753	A754	N755	L756	Y757	D758	D759		M762	D763	T764	F765	P766	N767	G768	F769	N770	A771	V772	V773	A774	V775	I776	S777	Y778	T779	Y781	D782	M783	D784	D785			
I603	I604	A605	D606	T607	L608	R609	Y610	W611	K612	V613	G615	K616	T617	P618	G619	L620	P621	I622	D623	L624	E625	G626	Y628	V629	P630	P631	S632	T633	R634	G635	Q636	Y637	P638	G639	L640	Y641	L642	F643	G644	G645	H646	S647	R648	M649	L650	R651	P652	G653	R654	Y655	L656	P657	L658	E659	K660	E661	D662			
N543	H544	F545	H547	K548	C549	I551	S552	T553	Q554	Q555	S556	D557	V558	S559	R560	I561	S562	S563	I564	L565	Y566	S567	L568	G569	V570	A571	P572	A573	S574	H575	T576	F577	A578	A579	G580	P581	S582	L583	C584	C585	V586	Q587	I588	D589	G590	K591	I592	I593	Q594	W595	V596	S597	H598	E599	Q600	G601	K602			
S482	G483	Y484	T485	V486	V487	A488	E489	K490	I491	M492	Y493	R495	F496	I497	S498	H499	F500	R501	M502	V503	H504	R505	G506	S507	F508	F509	A510	Q511	L512	K513	T514	T515	T516	V517	R518	K519	L520	L521	P522	E523	S524	W525	G526	F527	L528	C529	H532	T533	P534	D535	G536	S537	P538	C539	G540	L541	L542			
Q422	N423	I424	I425	A426	Q427	V428	R429	M430	D431	I432	N433	R434	G435	M436	A437	I438	N439	F440	K441	D442	K443	R444	Y445	G446	S447	R448	V449	L450	M451	R452	V453	N454	E455	N456	I457	G458	S459	K460	M461	Q462	Y463	F464	L465	S466	T467	G468	N469	L470	V471	S472	Q473	G475	L476	D477	L478	Q479	Q480	V481		

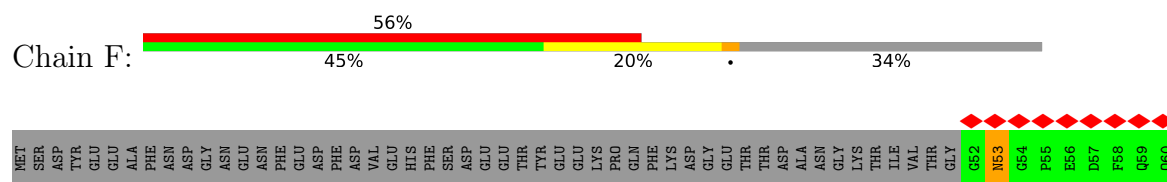
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

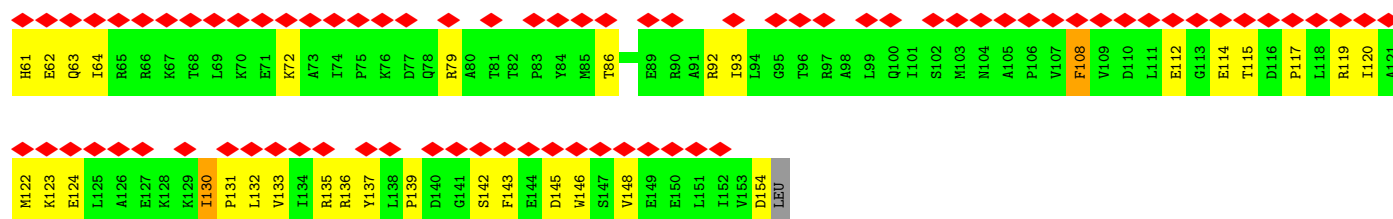


- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

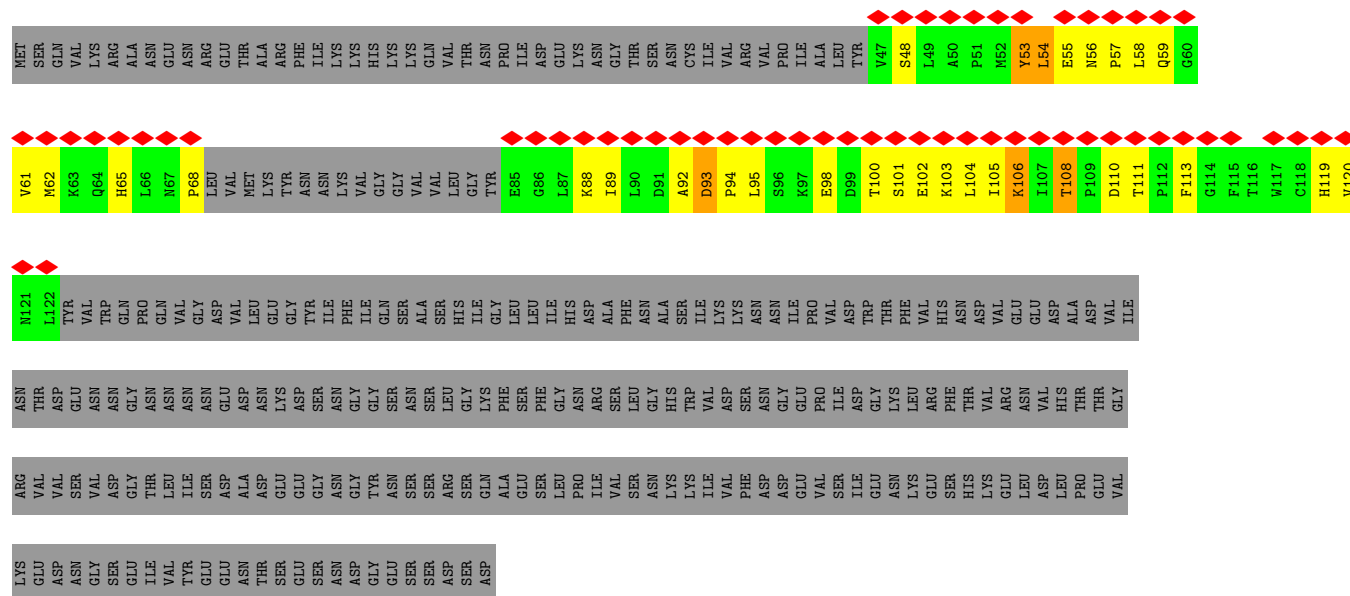


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

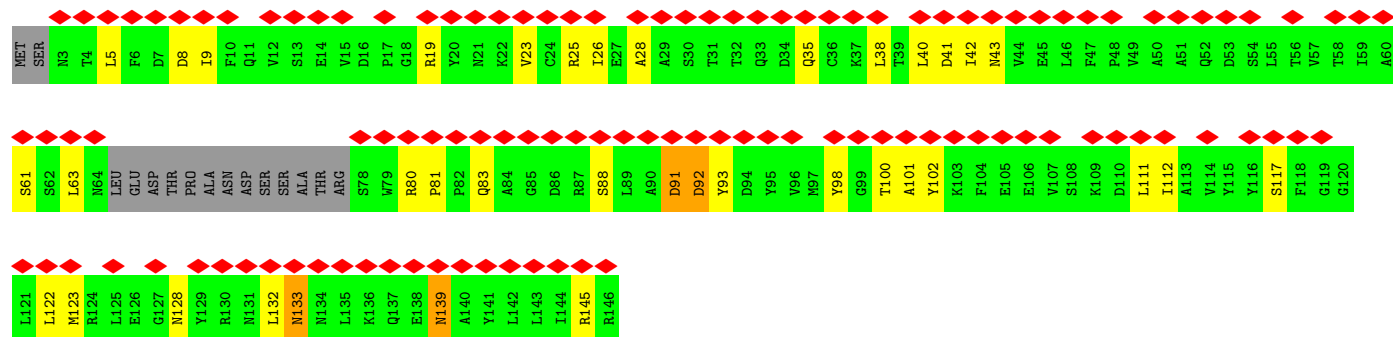
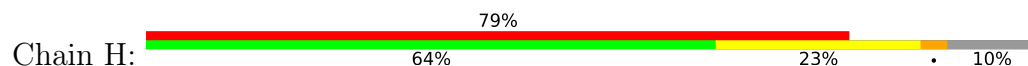




• Molecule 6: DNA-directed RNA polymerase I subunit RPA43

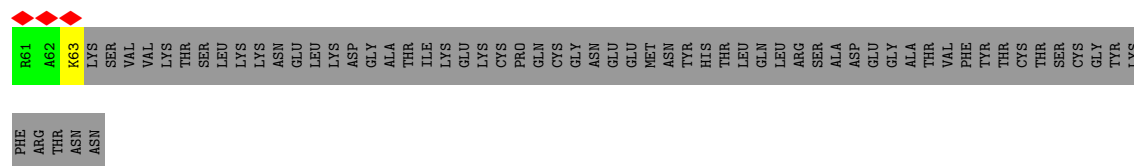


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

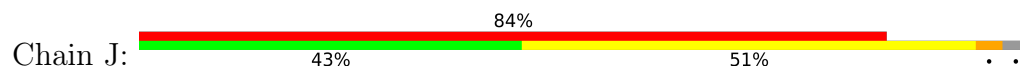


• Molecule 8: DNA-directed RNA polymerase I subunit RPA12

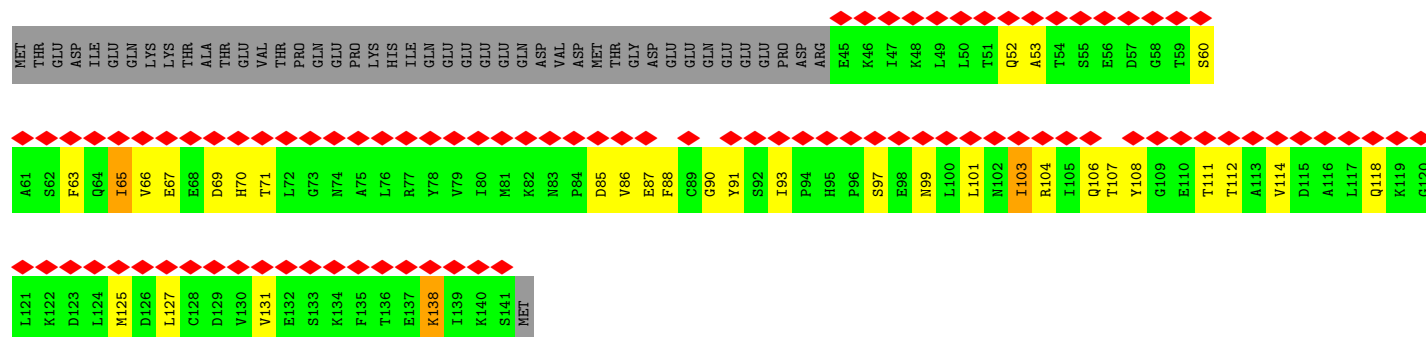




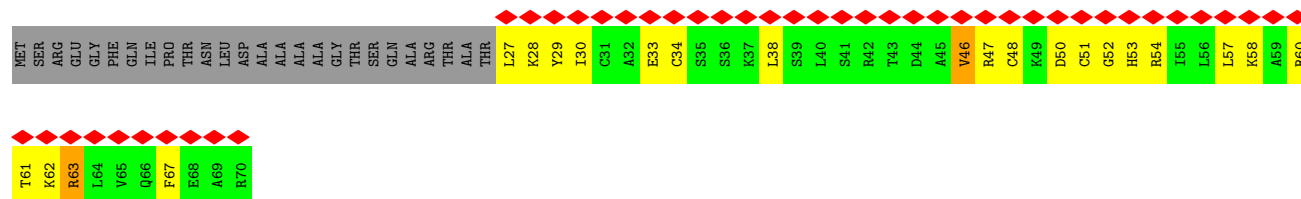
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5



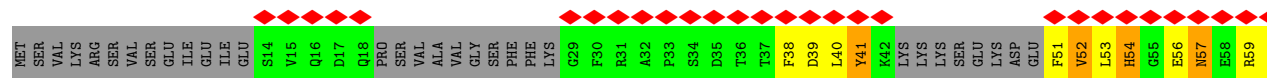
- Molecule 10: DNA-directed RNA polymerases I and III subunit RPAC2

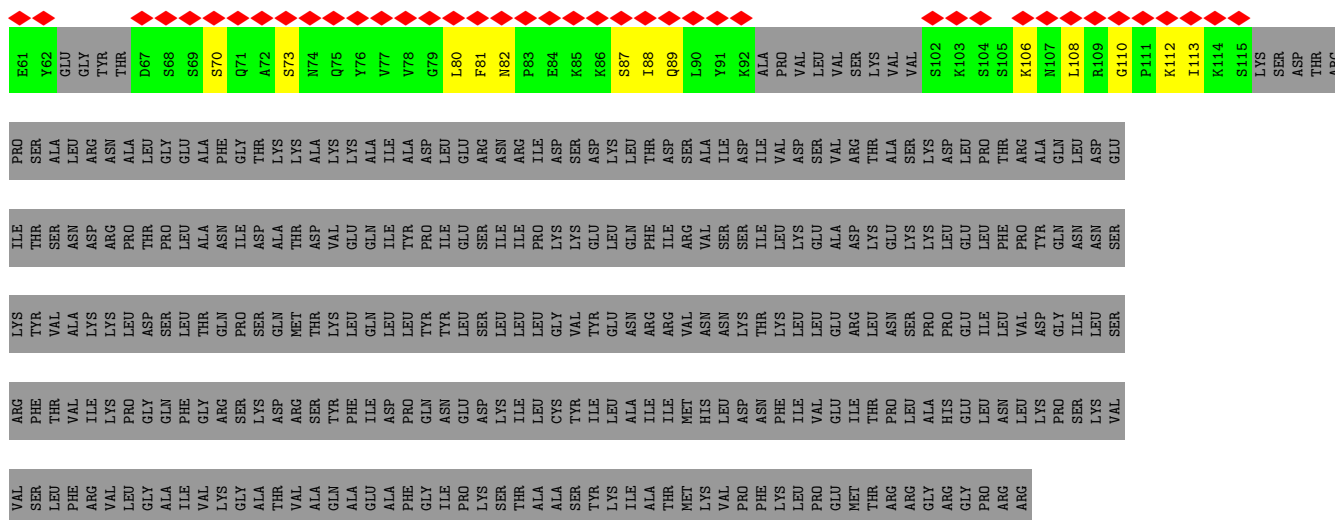


- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

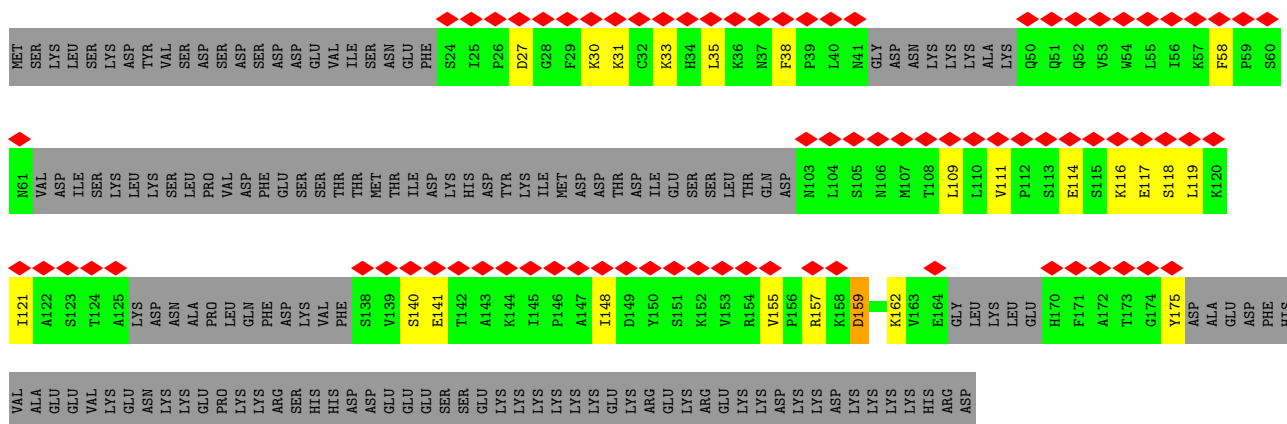


- Molecule 12: DNA-directed RNA polymerase I subunit RPA49

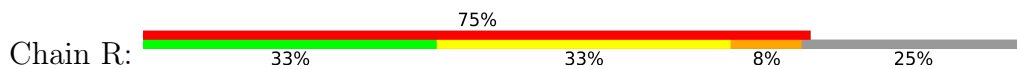




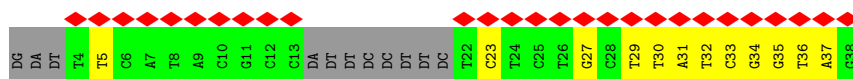
- Molecule 13: DNA-directed RNA polymerase I subunit RPA34



- Molecule 14: RNA



- Molecule 15: Non-template DNA



- Molecule 16: Template DNA



C1	T2	A3	C4	C5	G6	A7	T8	A9	A10	G11	C12	A13	G14	A15	T16	N17	C18	T19	C20	T21	C22	G23	A24	T25	T26	G27	C28	G29	T30	A31	T32	G33	A34	A35	DA	DT	DC
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117941	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	301.536, 301.536, 301.536	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR, 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	0.16	0/9393	0.31	0/12678
2	B	0.19	0/9158	0.30	0/12370
3	C	0.18	0/2467	0.27	0/3344
4	E	0.15	0/1519	0.34	0/2044
5	F	0.15	0/854	0.31	0/1151
6	G	0.14	0/483	0.35	0/656
7	H	0.16	0/1070	0.24	0/1449
8	I	0.14	0/428	0.35	0/578
9	J	0.22	0/570	0.30	0/765
10	K	0.17	0/768	0.25	0/1037
11	L	0.16	0/354	0.31	0/468
12	M	0.11	0/578	0.29	0/768
13	N	0.13	0/691	0.32	0/928
14	R	0.10	0/221	0.21	0/343
15	S	0.17	0/607	0.37	0/931
16	T	0.18	0/779	0.36	0/1197
All	All	0.17	0/29940	0.30	0/40707

There are no bond length outliers.

There are no bond angle outliers.

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	9243	0	9314	312	0
2	B	8963	0	8881	354	0
3	C	2415	0	2403	88	0
4	E	1488	0	1490	64	0
5	F	839	0	852	27	0
6	G	472	0	474	23	0
7	H	1052	0	1021	29	0
8	I	423	0	425	20	0
9	J	561	0	573	46	0
10	K	758	0	756	28	0
11	L	352	0	374	22	0
12	M	571	0	557	23	0
13	N	679	0	699	19	0
14	R	197	0	99	7	0
15	S	546	0	309	11	0
16	T	707	0	392	12	0
17	B	1	0	0	0	0
17	I	1	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
All	All	29270	0	28619	957	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 17.

The worst 5 of 957 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)
9:J:43:ARG:HD2	9:J:45:CYS:SG	1.92	1.09
2:B:1104:CYS:SG	2:B:1107:CYS:HB2	2.07	0.93
8:I:30:CYS:SG	8:I:33:CYS:HB2	2.17	0.85
1:A:1325:LEU:HD13	1:A:1492:ILE:HG23	1.56	0.85
9:J:57:ILE:O	9:J:61:LEU:HB2	1.81	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1146/1664 (69%)	1044 (91%)	102 (9%)	0	100	100
2	B	1109/1203 (92%)	1013 (91%)	96 (9%)	0	100	100
3	C	302/335 (90%)	291 (96%)	11 (4%)	0	100	100
4	E	175/215 (81%)	146 (83%)	29 (17%)	0	100	100
5	F	101/155 (65%)	91 (90%)	10 (10%)	0	100	100
6	G	56/326 (17%)	43 (77%)	13 (23%)	0	100	100
7	H	127/146 (87%)	120 (94%)	7 (6%)	0	100	100
8	I	53/125 (42%)	34 (64%)	19 (36%)	0	100	100
9	J	66/70 (94%)	58 (88%)	8 (12%)	0	100	100
10	K	95/142 (67%)	92 (97%)	3 (3%)	0	100	100
11	L	42/70 (60%)	36 (86%)	6 (14%)	0	100	100
12	M	61/415 (15%)	50 (82%)	11 (18%)	0	100	100
13	N	76/233 (33%)	59 (78%)	17 (22%)	0	100	100
All	All	3409/5099 (67%)	3077 (90%)	332 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1033/1465 (70%)	991 (96%)	42 (4%)	27	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	985/1053 (94%)	927 (94%)	58 (6%)	18	44
3	C	268/296 (90%)	252 (94%)	16 (6%)	17	44
4	E	166/197 (84%)	154 (93%)	12 (7%)	13	38
5	F	91/137 (66%)	86 (94%)	5 (6%)	19	46
6	G	55/291 (19%)	48 (87%)	7 (13%)	4	21
7	H	115/128 (90%)	110 (96%)	5 (4%)	26	51
8	I	50/110 (46%)	42 (84%)	8 (16%)	2	14
9	J	63/65 (97%)	59 (94%)	4 (6%)	16	42
10	K	87/130 (67%)	83 (95%)	4 (5%)	24	50
11	L	39/57 (68%)	36 (92%)	3 (8%)	12	37
12	M	65/371 (18%)	61 (94%)	4 (6%)	16	43
13	N	79/220 (36%)	73 (92%)	6 (8%)	12	37
All	All	3096/4520 (68%)	2922 (94%)	174 (6%)	21	46

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	234	ASN
7	H	133	ASN
4	E	55	ARG
5	F	108	PHE
8	I	48	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	101	GLN
5	F	63	GLN
11	L	66	GLN
1	A	1461	ASN
1	A	1447	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	8/12 (66%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	R	5	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	3DR	T	17	16	8,11,12	1.49	1 (12%)	7,14,17	1.58	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	3DR	T	17	16	-	0/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	17	3DR	C2'-C1'	2.58	1.58	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	17	3DR	O4'-C4'-C3'	3.69	109.15	103.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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.

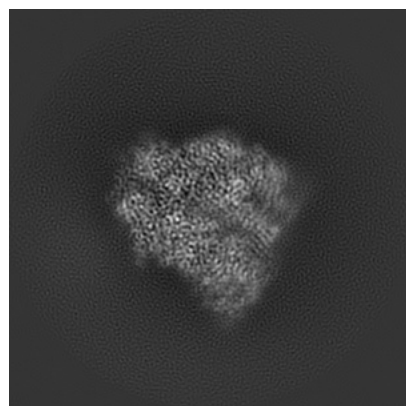
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50972. These allow visual inspection of the internal detail of the map and identification of artifacts.

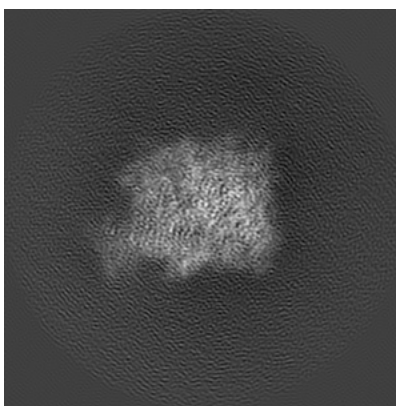
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

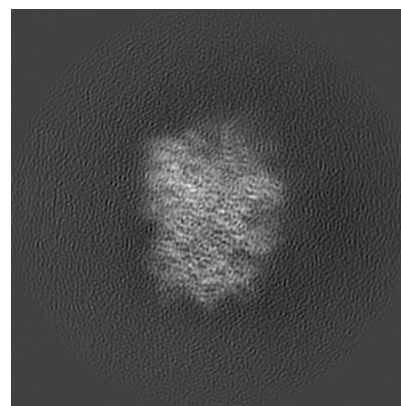
6.1.1 Primary map



X

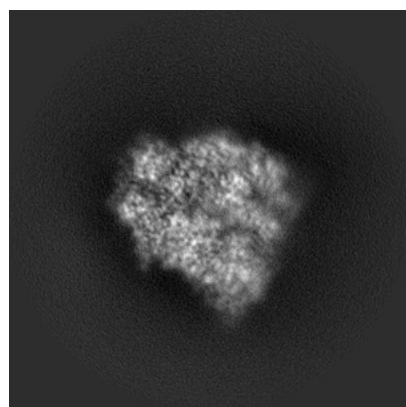


Y

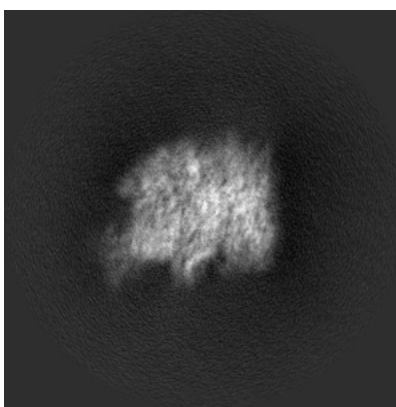


Z

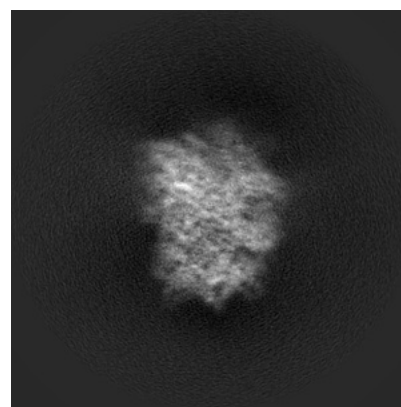
6.1.2 Raw map



X



Y

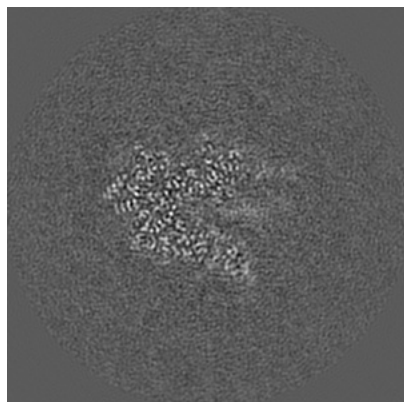


Z

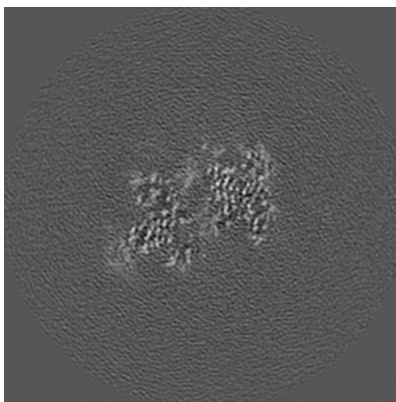
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

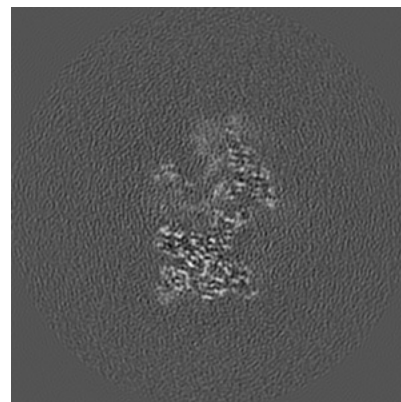
6.2.1 Primary map



X Index: 144

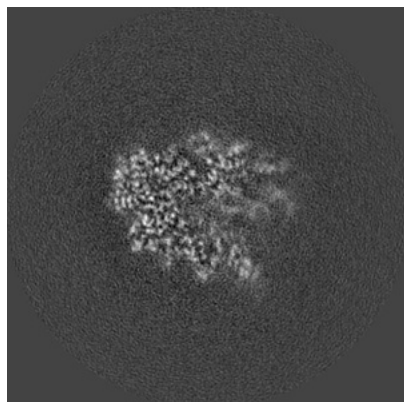


Y Index: 144

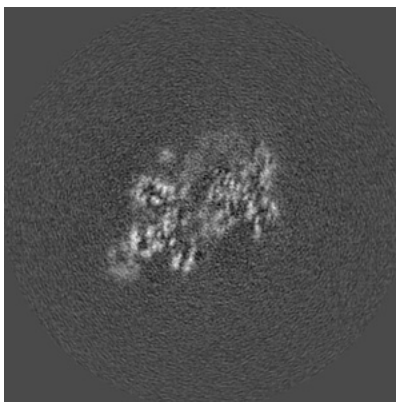


Z Index: 144

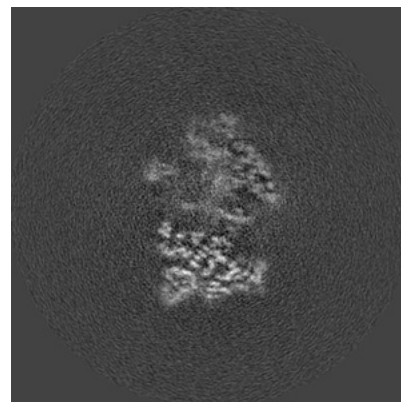
6.2.2 Raw map



X Index: 144



Y Index: 144

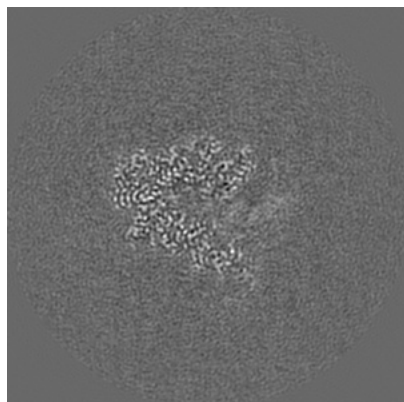


Z Index: 144

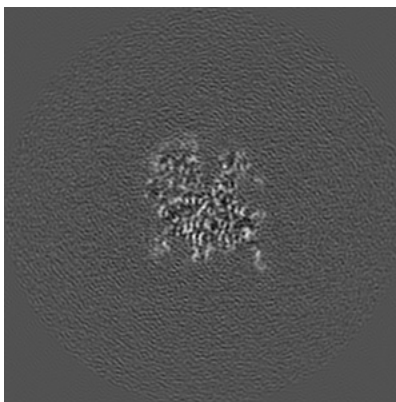
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

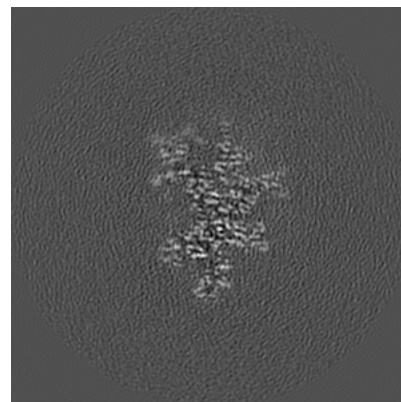
6.3.1 Primary map



X Index: 139

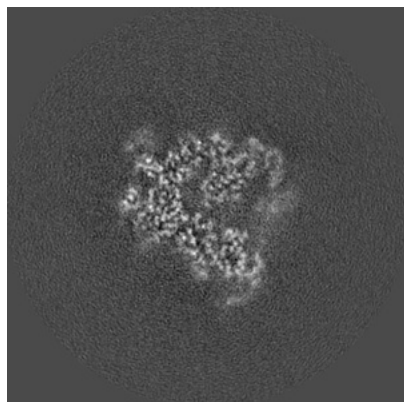


Y Index: 120

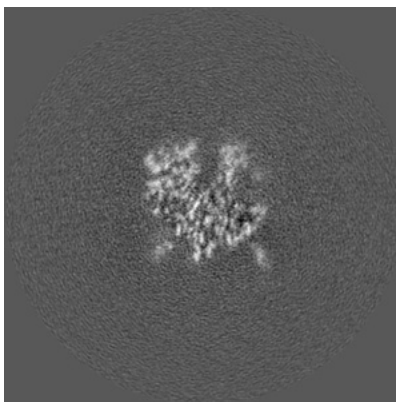


Z Index: 162

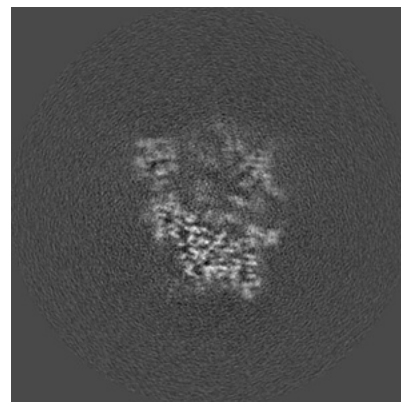
6.3.2 Raw map



X Index: 131



Y Index: 119

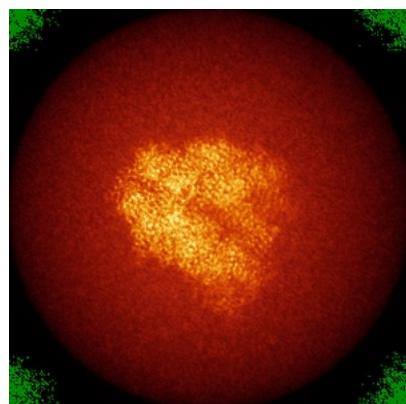


Z Index: 135

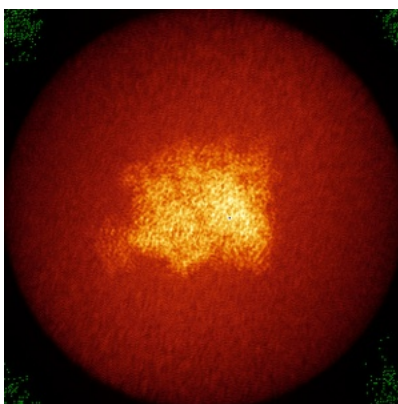
The images above show the largest variance slices of the map in three orthogonal directions.

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

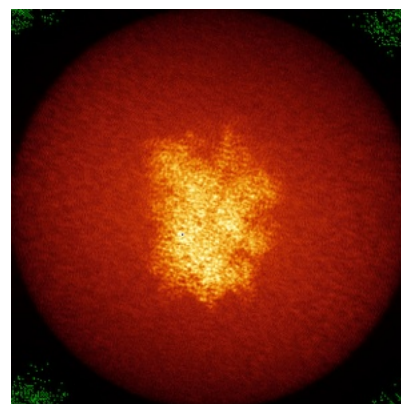
6.4.1 Primary map



X

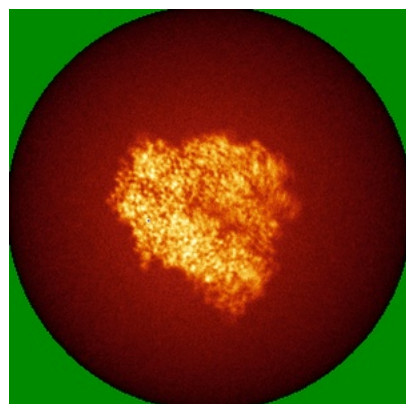


Y

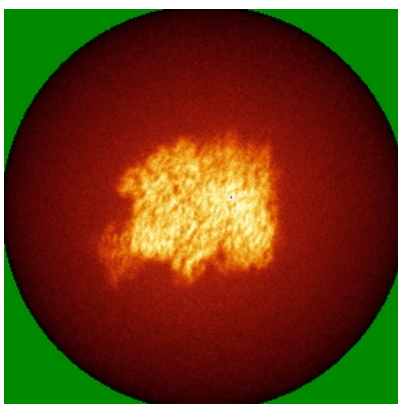


Z

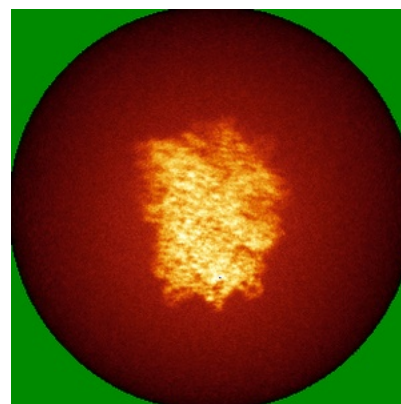
6.4.2 Raw map



X



Y

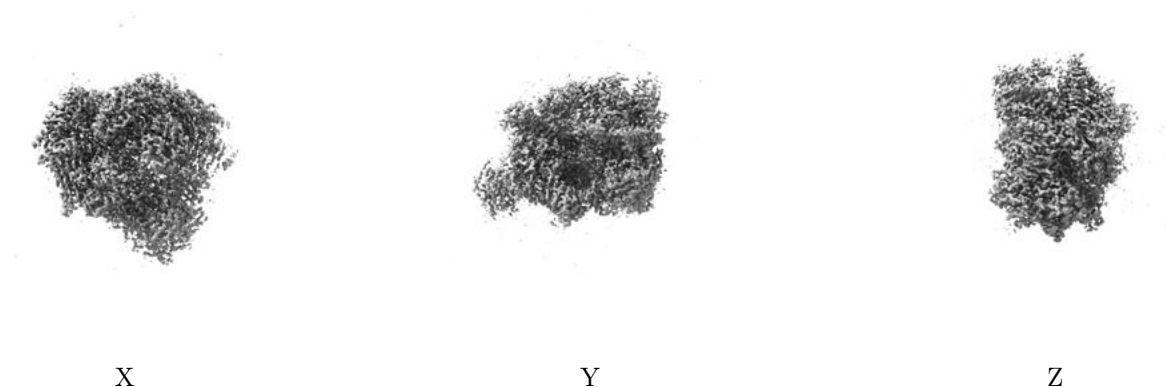


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

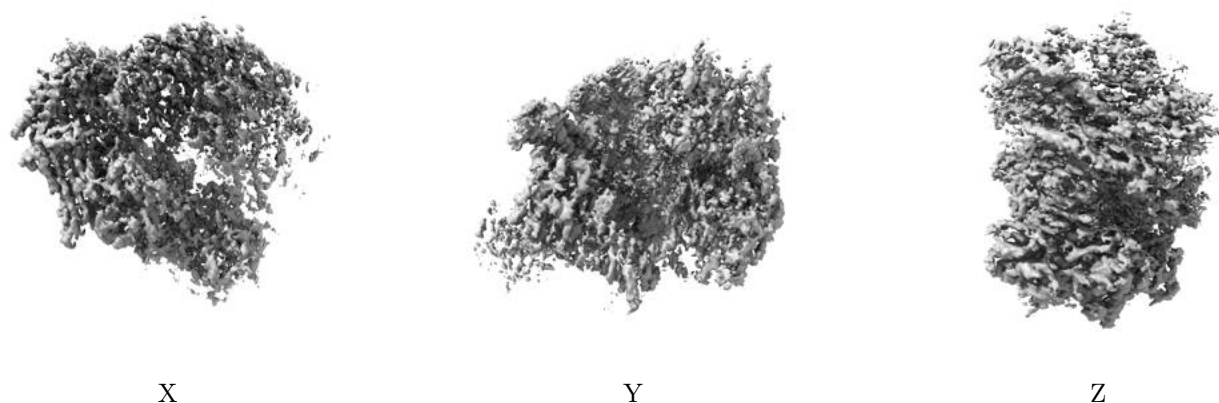
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

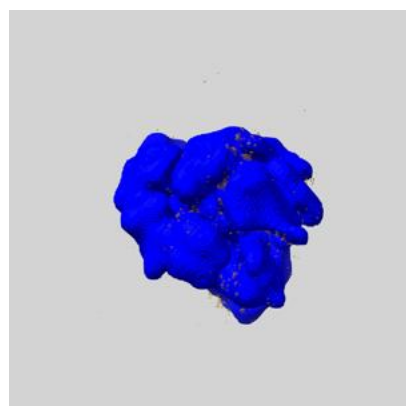
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

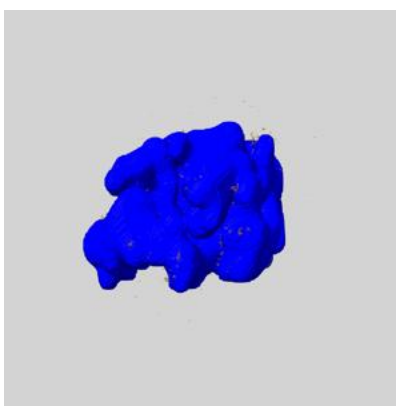
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

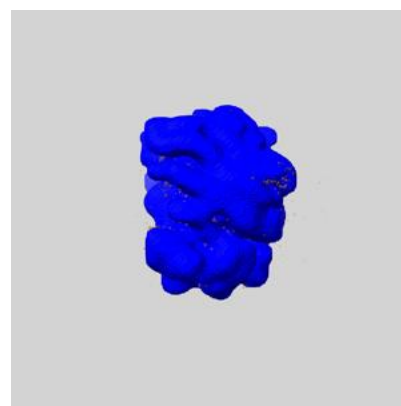
6.6.1 emd_50972_msk_1.map [i](#)



X



Y

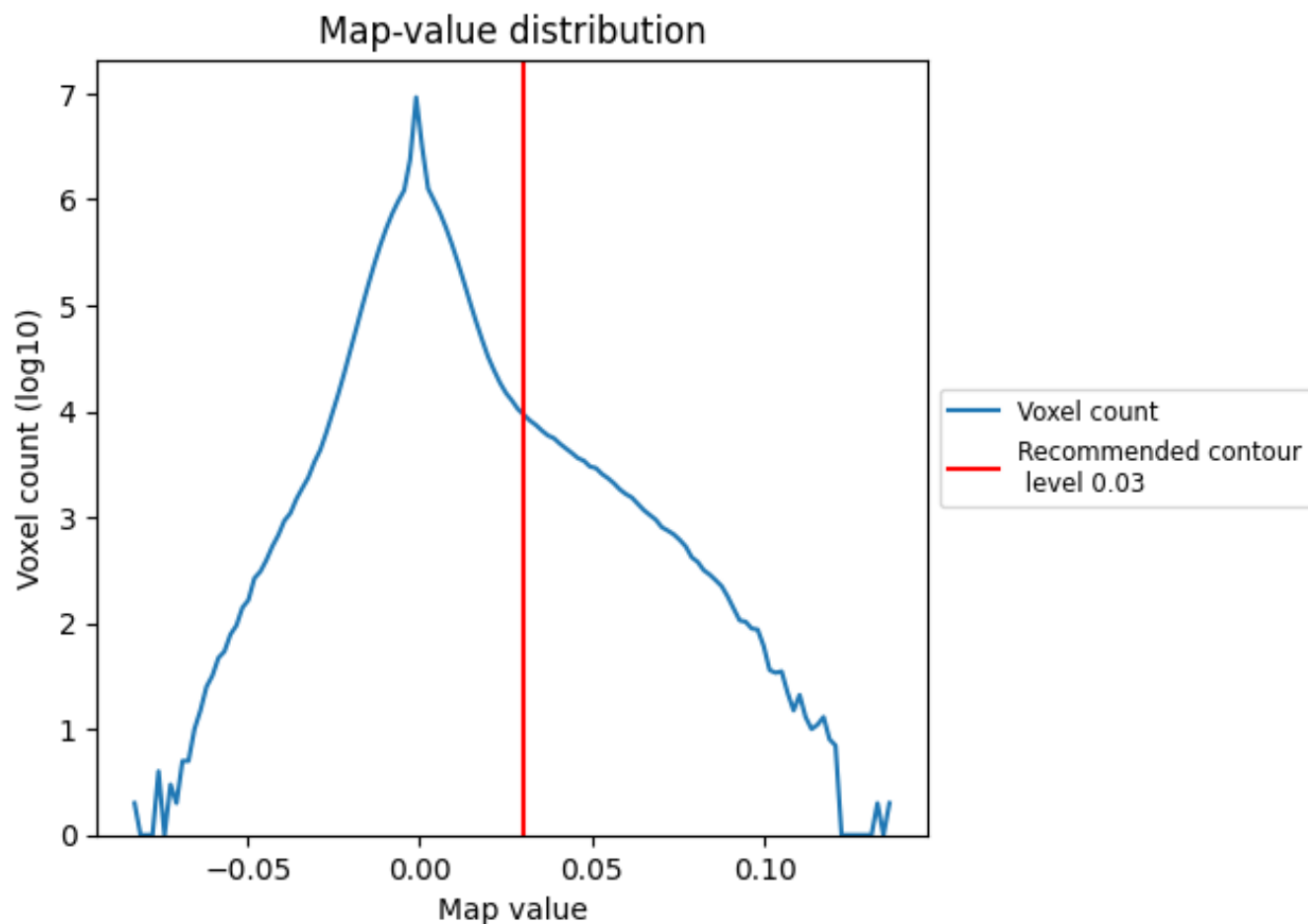


Z

7 Map analysis [i](#)

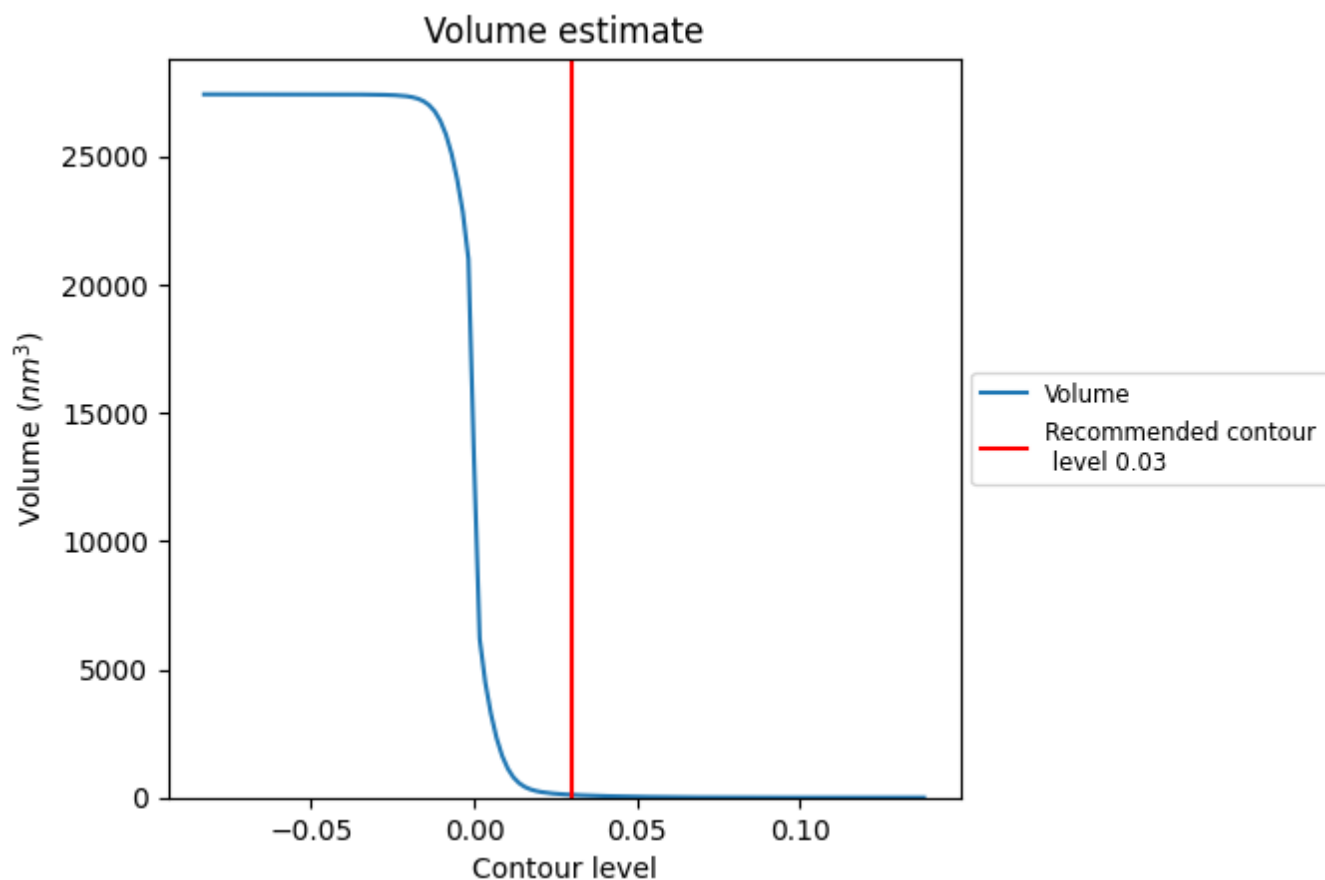
This section contains the results of statistical analysis of the map.

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.

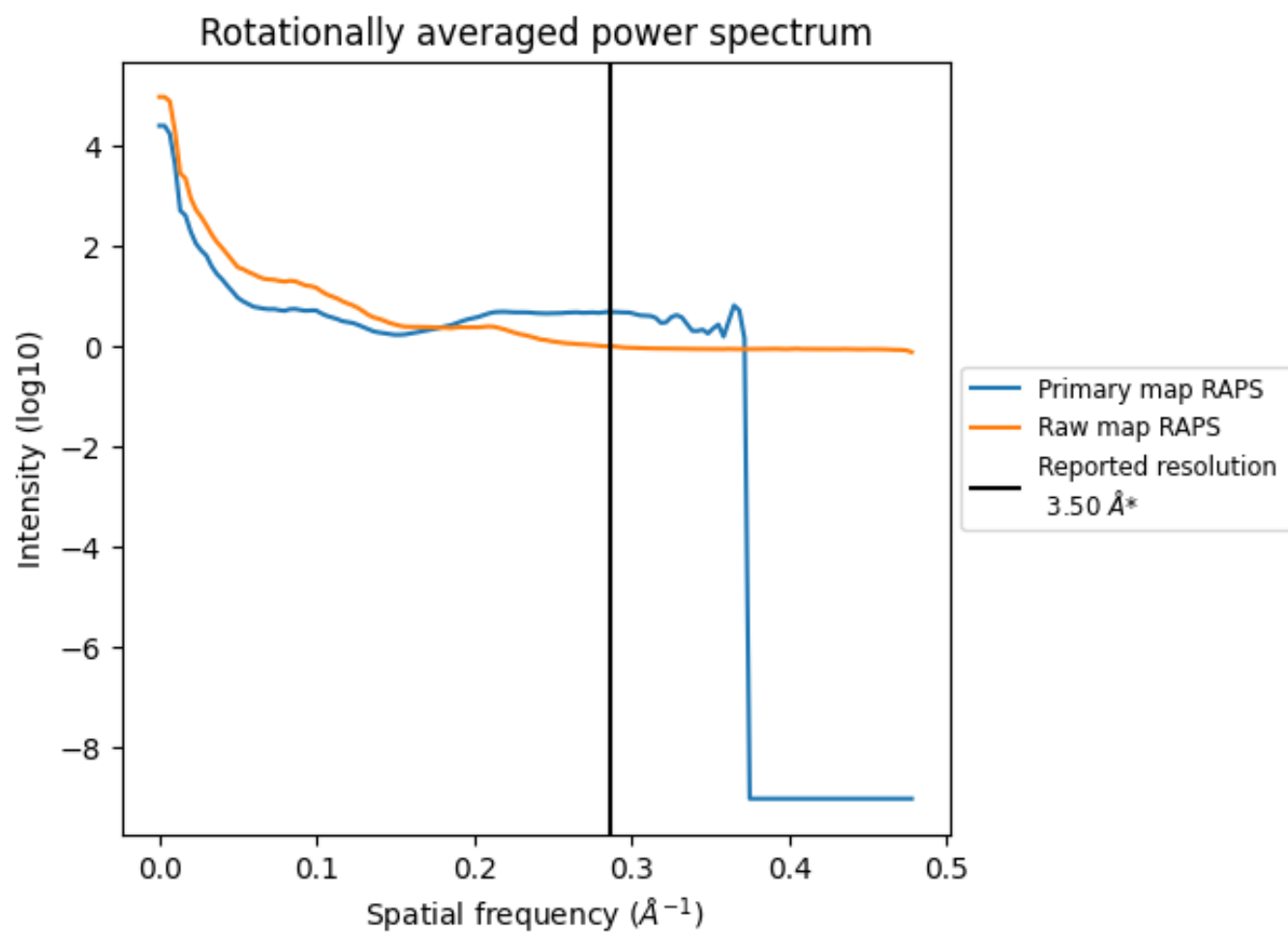
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 97 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 ⓘ

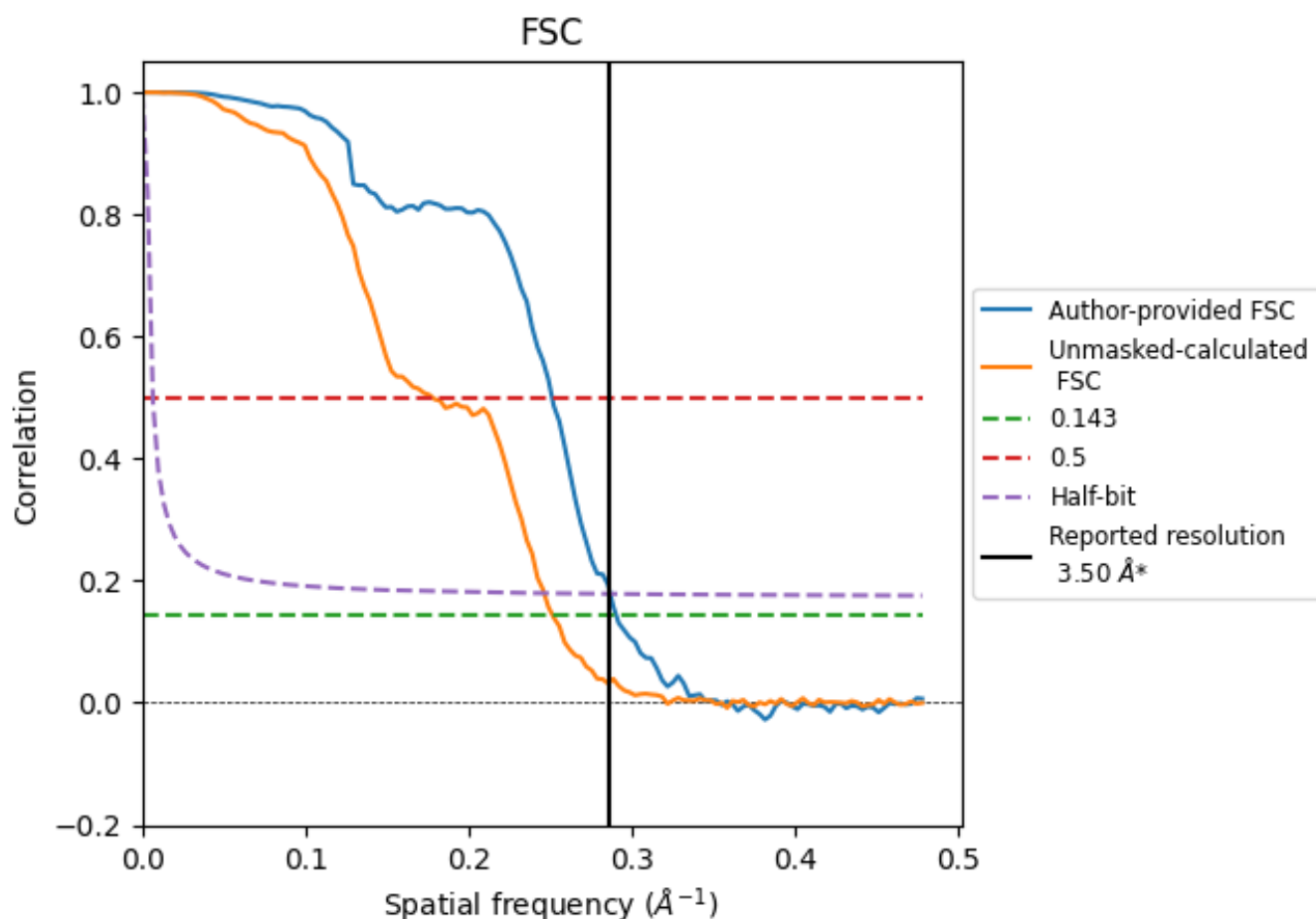


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

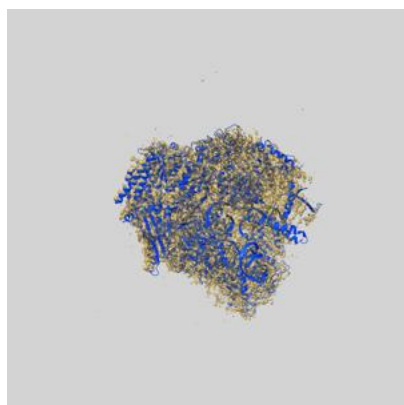
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.98	3.49
Unmasked-calculated*	3.98	5.62	4.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.5 by more than 10 %

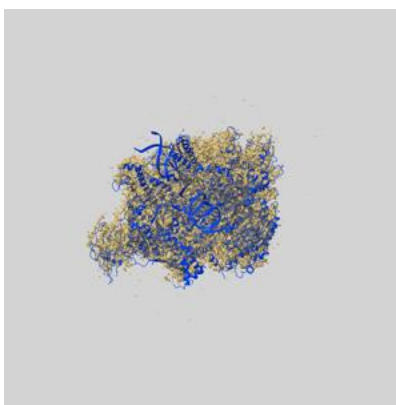
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50972 and PDB model 9G2C. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

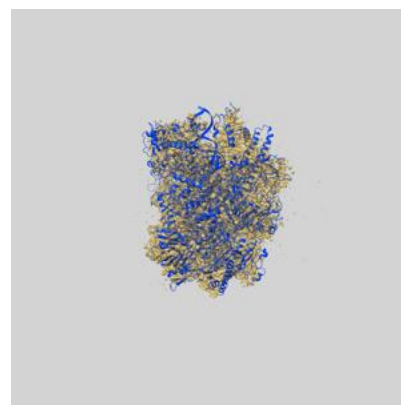
9.1 Map-model overlay [i](#)



X



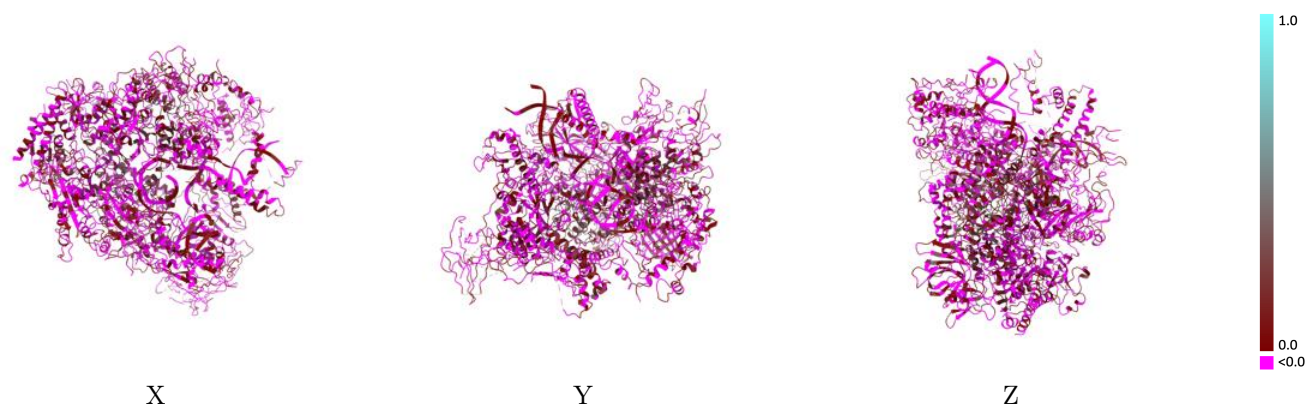
Y



Z

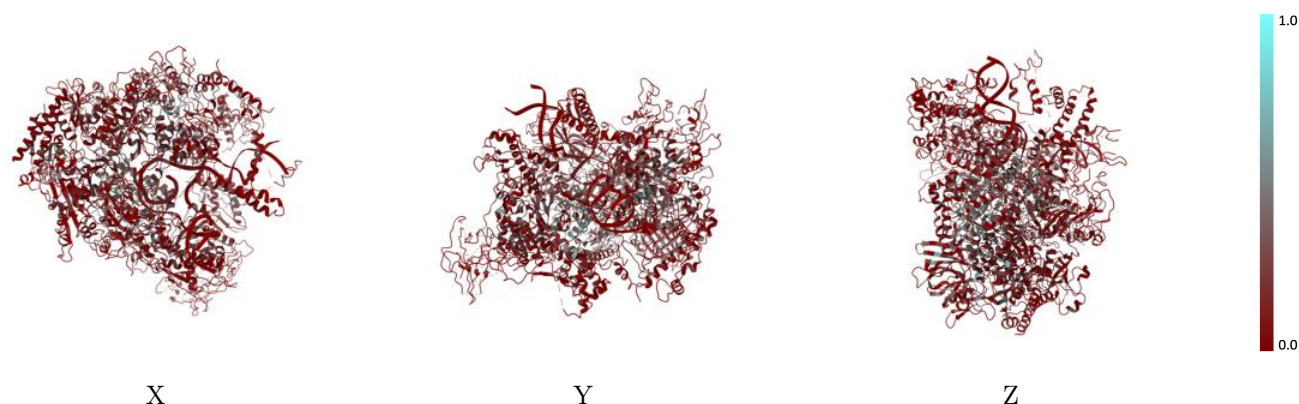
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



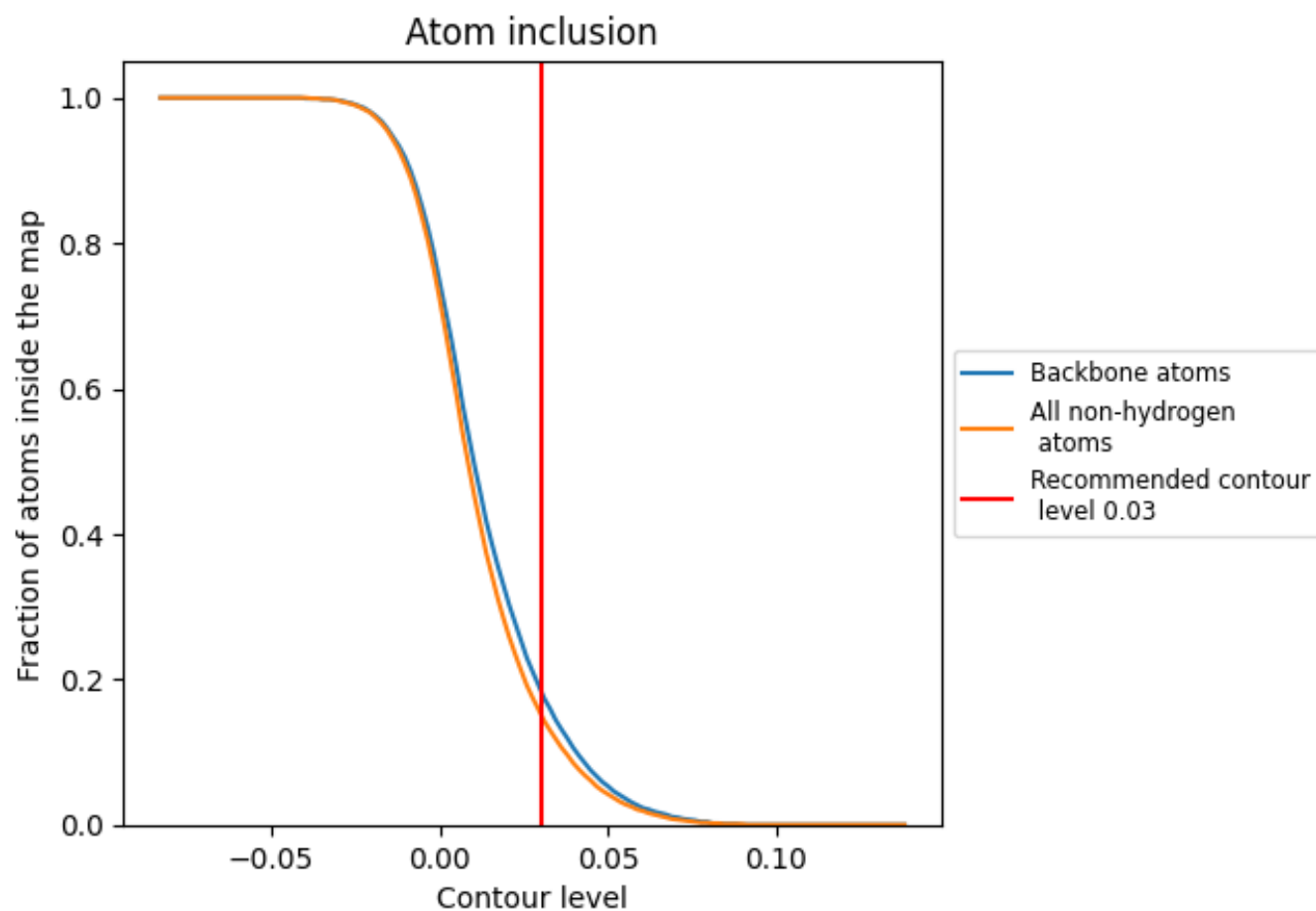
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion ⓘ



At the recommended contour level, 19% of all backbone atoms, 15% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1530	 0.0080
A	 0.1840	 0.0300
B	 0.1700	 -0.0090
C	 0.1460	 0.0110
E	 0.0930	 -0.0340
F	 0.2100	 0.0900
G	 0.1130	 0.0330
H	 0.1530	 0.0080
I	 0.0740	 0.0280
J	 0.1530	 -0.0810
K	 0.0870	 -0.0290
L	 0.0760	 0.0240
M	 0.0530	 -0.0300
N	 0.0830	 0.0190
R	 0.1320	 -0.0100
S	 0.0130	 0.0120
T	 0.0450	 0.0090

