



wwPDB EM Validation Summary Report ⓘ

Jun 8, 2025 – 04:19 pm BST

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

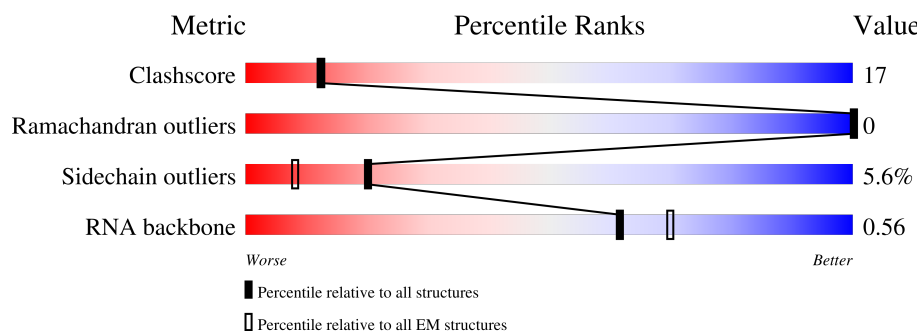
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	<div> <div>60%</div> <div>46% 23% . 30%</div> </div>
2	B	1203	<div> <div>82%</div> <div>55% 36% . 6%</div> </div>
3	C	335	<div> <div>82%</div> <div>59% 29% . 9%</div> </div>
4	E	215	<div> <div>80%</div> <div>50% 32% . 16%</div> </div>
5	F	155	<div> <div>56%</div> <div>45% 20% . 34%</div> </div>
6	G	326	<div> <div>18%</div> <div>9% 8% . 82%</div> </div>
7	H	146	<div> <div>79%</div> <div>64% 23% . 10%</div> </div>

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Mol	Chain	Length	Quality of chain
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		

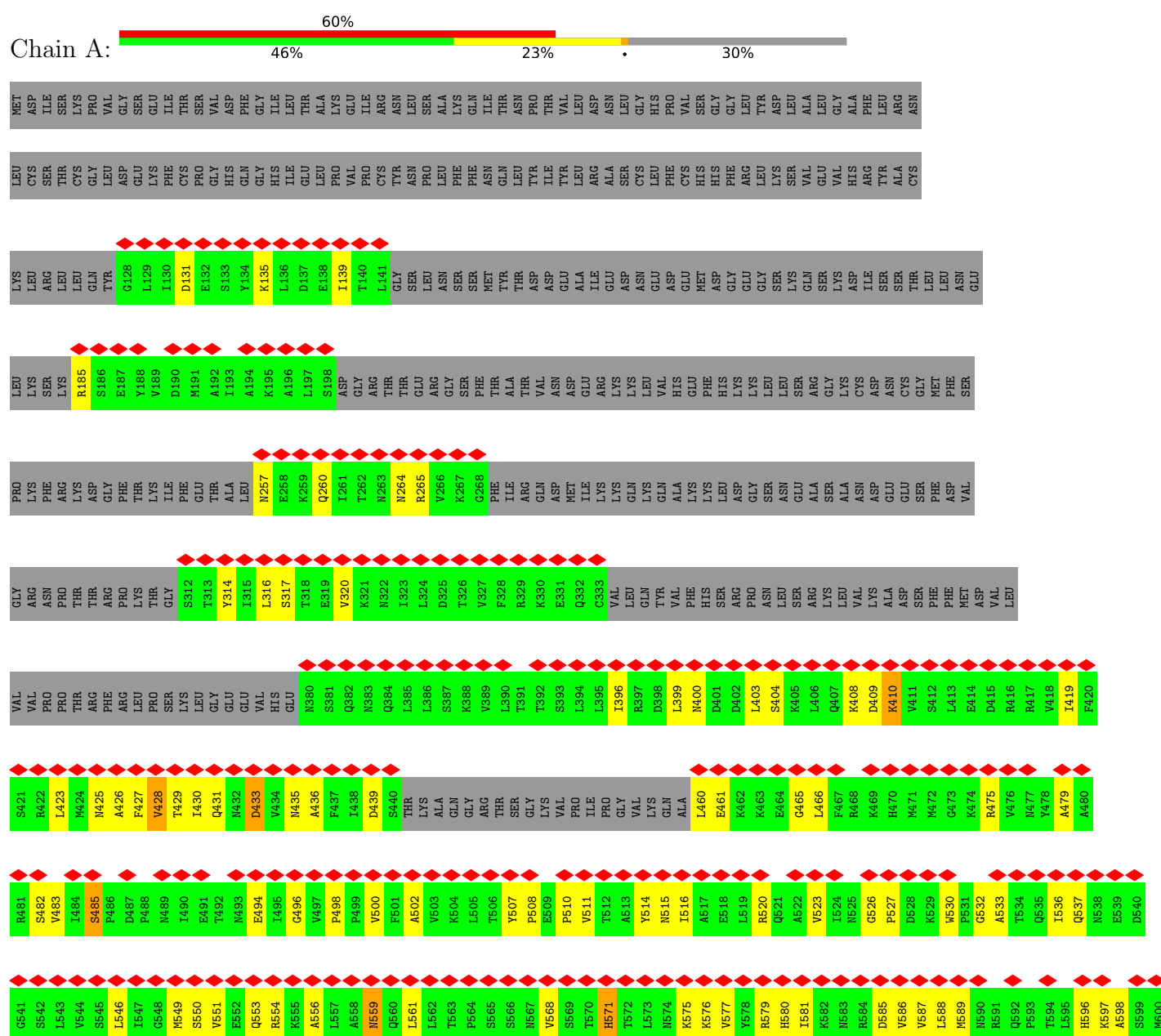
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	

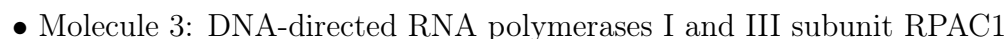
3 Residue-property plots

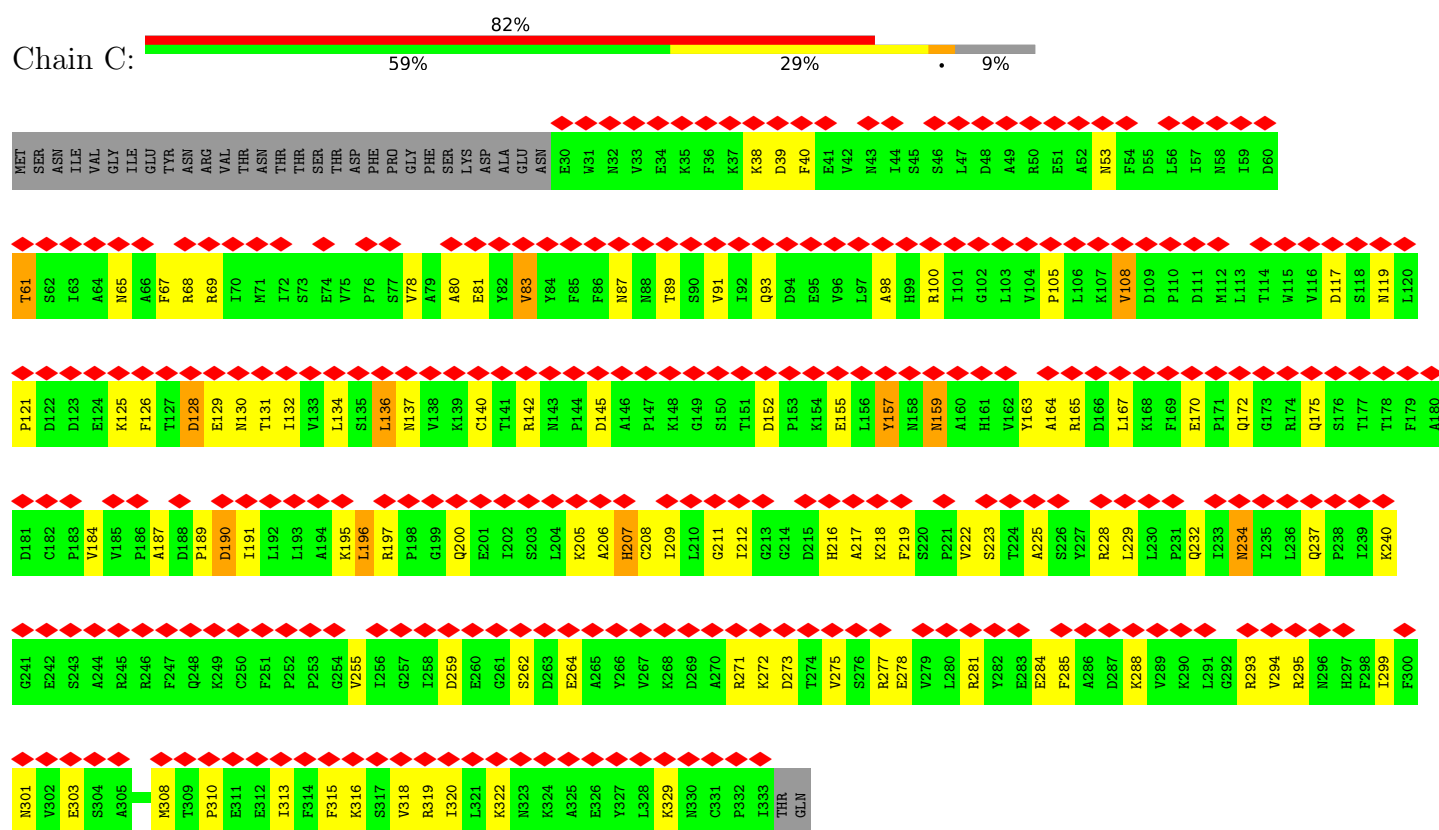
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

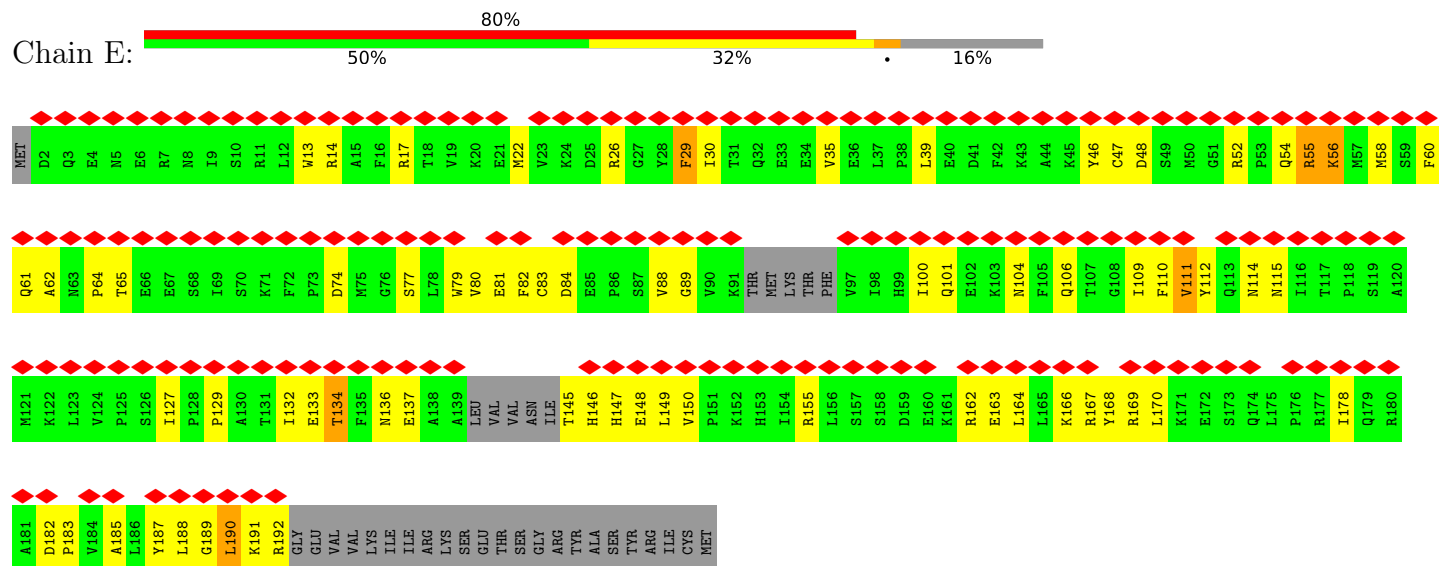


A1328	D1268	ALA	L1027	T965	G1033	H1088	L1148	V1270	K1269	I1329	A1328
I1329	K1269	GLY	E1028	I966	E1029	L1089	D1149	I1271	I1271	I1330	I1329
V1330	V1270	GLY	G1030	P967	G1031	D1090	K1150	I1272	K1150	V1331	V1330
K1331	I1271	ALA	H1031	S968	H1032	V1091	M1151	I1273	M1151	K1332	K1331
I1332	I1272	ALA	S1033	P969	S1034	E1092	S1152	I1274	S1152	E1333	I1332
E1333	I1273	ALA	Y1034	K970	Y1035	A1094	K1153	I1275	K970	I1334	E1333
K1334	I1274	ALA	D1035	P971	D1036	L1095	LEU	I1276	P971	K1335	K1334
K1335	I1275	ALA	N1036	Y972	N1037	L1096	PHE	I1277	Y972	Q1336	K1335
Q1336	I1276	ALA	I1038	E973	I1039	K1096	LYS	I1278	E973	Q1337	Q1336
Q1337	I1277	ALA	I1039	T974	I1040	Y1097	SER	I1279	T974	K1338	Q1337
R1338	I1278	ALA	A1041	D975	A1042	K1098	ASP	I1280	D975	R1339	R1338
THR	THR	THR	G1043	A976	G1044	K1099	G1160	I1281	A976	THR	THR
THR	ASN	THR	T1044	M977	T1045	K1100	V1161	I1282	M977	THR	THR
THR	PRO	THR	L1046	A978	L1047	T1101	M1162	I1283	A978	PRO	THR
THR	ALA	THR	L1048	G979	L1049	L1102	E1163	I1284	G979	ALA	THR
THR	GLY	THR	Y1050	G980	Y1051	K1103	E1164	I1285	G980	GLY	THR
THR	ILE	THR	M1049	Y981	M1050	K1104	K1165	I1286	Y981	ILE	THR
THR	GLY	THR	G982	K983	G983	L1105	F1166	I1287	K983	GLY	THR
THR	ASN	THR	C922	P984	C923	K1106	R1167	I1288	P984	ASN	THR
THR	VAL	THR	S924	G985	S925	K1107	A1168	I1289	G985	VAL	THR
THR	ALA	THR	M925	P986	M926	H1108	L1169	I1290	P986	ALA	THR
THR	ASP	THR	A927	K987	A928	S1109	M1170	I1291	K987	ASP	THR
THR	ASN	THR	N928	S988	N929	K1110	Q1171	I1292	S988	ASN	THR
THR	GLU	THR	S931	I990	S932	P1112	L1172	I1293	I990	GLU	THR
THR	LEU	THR	G932	K991	G933	H1113	K1173	I1294	K991	LEU	THR
THR	GLU	THR	A933	P992	A934	Y1114	Y1174	I1295	P992	GLU	THR
THR	ASP	THR	K934	Q993	K935	K1115	M1175	I1296	Q993	ASP	THR
THR	ASN	THR	G935	E994	G936	T1116	R1176	I1297	E994	ASN	THR
THR	GLN	THR	S936	Y995	S937	Q1116	S1177	I1298	Y995	GLN	THR
THR	ARG	THR	N937	K996	N938	V1117	L1178	I1299	K996	ARG	THR
THR	LEU	THR	V938	H998	V939	V1118	I1179	I1300	H998	LEU	THR
THR	GLU	THR	N939	A1001	N940	K1119	M1180	I1301	A1001	GLU	THR
THR	ASP	THR	Q942	G1002	Q943	Y1120	P1181	I1302	G1002	ASP	THR
THR	ASN	THR	I943	I1003	I944	D1121	G1182	I1303	I1003	ASN	THR
THR	GLN	THR	C945	E1004	C946	Y1122	E1183	I1304	E1004	GLN	THR
THR	PRO	THR	N945	I1007	N946	L1124	V1185	I1305	I1007	PRO	THR
THR	LEU	THR	L946	D1008	L947	A1125	G1186	I1306	D1008	LEU	THR
THR	GLU	THR	C947	T1009	C948	K1126	I1187	I1307	T1009	GLU	THR
THR	ASP	THR	I947	A1010	I948	Y1127	I1188	I1308	A1010	ASP	THR
THR	ASN	THR	Q949	T1011	Q950	N1128	A1189	I1309	T1011	ASN	THR
THR	GLN	THR	Q951	L1012	Q952	P1129	S1190	I1310	L1012	GLN	THR
THR	LEU	THR	A951	R1013	A952	A1130	Q1191	I1311	R1013	LEU	THR
THR	GLU	THR	N953	T1014	N954	K1131	S1192	I1312	T1014	GLU	THR
THR	ASP	THR	G954	S1015	G955	Y1132	G1194	I1313	S1015	ASP	THR
THR	ASN	THR	R955	R1016	R956	L1133	E1195	I1314	R1016	ASN	THR
THR	PRO	THR	N957	G1017	N958	G1134	P1196	I1315	G1017	PRO	THR
THR	LEU	THR	V957	Y1018	V958	V1135	S1197	I1316	Y1018	LEU	THR
THR	GLU	THR	P957	L1019	P958	S1137	T1198	I1317	L1019	GLU	THR
THR	ASP	THR	C957	Q1020	C958	E1138	Q1199	I1318	Q1020	ASP	THR
THR	ASN	THR	N959	R1021	N960	N1139	M1200	I1319	R1021	ASN	THR
THR	GLN	THR	V959	C1022	V960	F1140	T1201	I1320	C1022	GLN	THR
THR	LEU	THR	N961	L1023	N962	F1141	L1202	I1321	L1023	LEU	THR
THR	GLU	THR	G963	L1024	G964	D1142	M1203	I1322	L1024	GLU	THR
THR	ASP	THR	K964	K1025	K965	K1143	T1204	I1323	K1025	ASP	THR
THR	ASN	THR	Q1026	Q1026	Q1027	L1144	PHE	I1324	Q1026	ASN	THR
THR	PRO	THR	E1087	E1088	E1089	L1145	HIS	I1325	E1088	PRO	THR
THR	LEU	THR	F1147	F1148	F1149	S1146	PHE	I1326	F1147	LEU	THR
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THR	ASN	THR								ASN	THR
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THR	LEU	THR								LEU	THR
THR	GLU	THR								GLU	THR
THR	ASP	THR								ASP	THR
THR	ASN	THR								ASN	THR
THR	VAL	THR								VAL	THR
THR	ALA	THR								ALA	THR
THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
THR	LEU	THR								LEU	THR
THR	GLN	THR								GLN	THR
THR	THR	THR								THR	THR
THR	ASP	THR								ASP	THR
THR	ASN	THR								ASN	THR
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THR	ALA	THR								ALA	THR
THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
THR	LEU	THR								LEU	THR
THR	GLN	THR								GLN	THR
THR	THR	THR								THR	THR
THR	ASP	THR								ASP	THR
THR	ASN	THR								ASN	THR
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THR	ALA	THR								ALA	THR
THR	ASN	THR								ASN	THR
THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
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THR	GLU	THR								GLU	THR
THR	ASP	THR								ASP	THR
THR	ASN	THR								ASN	THR
THR	VAL	THR								VAL	THR
THR	ALA	THR								ALA	THR
THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
THR	LEU	THR								LEU	THR
THR	GLN	THR								GLN	THR
THR	THR	THR								THR	THR
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THR	ASN	THR								ASN	THR
THR	VAL	THR								VAL	THR
THR	ALA	THR								ALA	THR
THR	ASN	THR								ASN	THR
THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
THR	LEU	THR								LEU	THR
THR	GLU	THR								GLU	THR
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THR	LEU	THR								LEU	THR
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THR	ASN	THR								ASN	THR
THR	VAL	THR								VAL	THR
THR	ALA	THR								ALA	THR
THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
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THR	GLU	THR								GLU	THR
THR	ASP	THR								ASP	THR
THR	ASN	THR								ASN	THR
THR	VAL	THR								VAL	THR
THR	ALA	THR								ALA	THR
THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
THR	LEU	THR								LEU	THR
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THR	ALA	THR								ALA	THR
THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
THR	LEU	THR								LEU	THR
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THR	ASN	THR								ASN	THR
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THR	PRO	THR								PRO	THR
THR	ARG	THR								ARG	THR
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THR	ARG	THR		</							

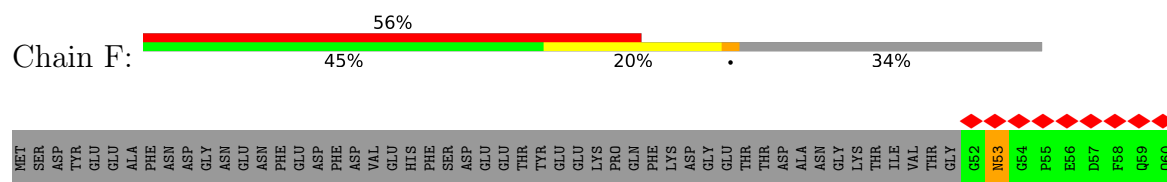


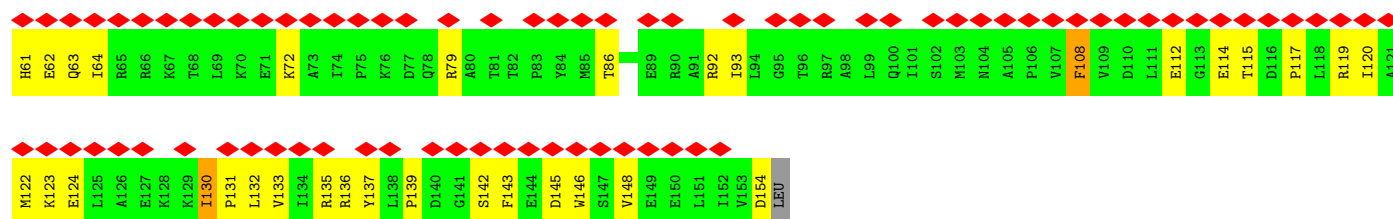


- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

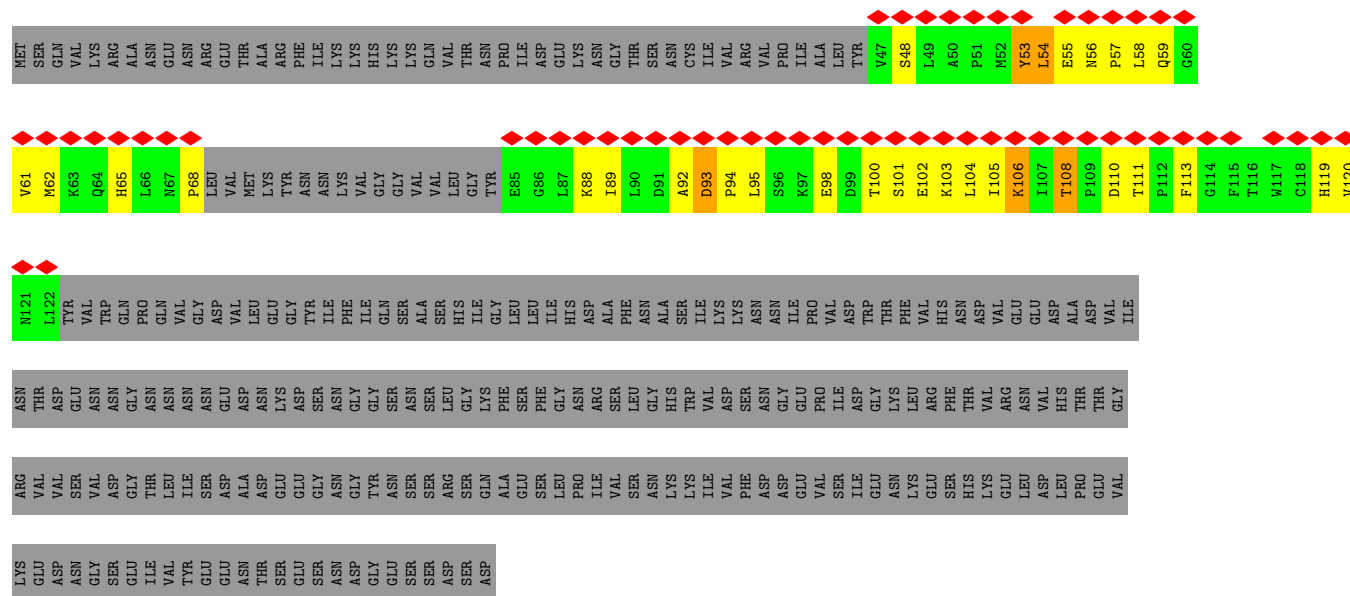


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

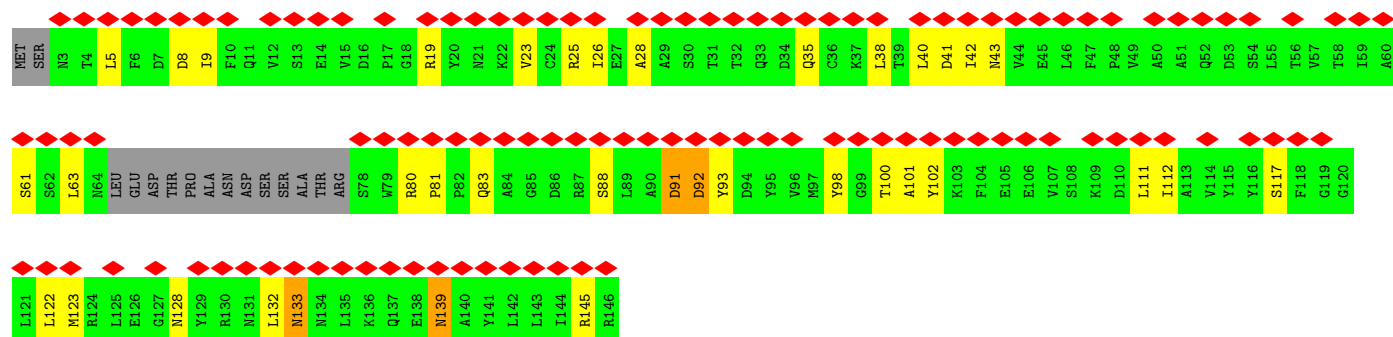
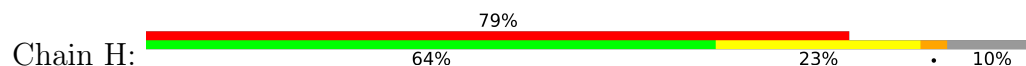




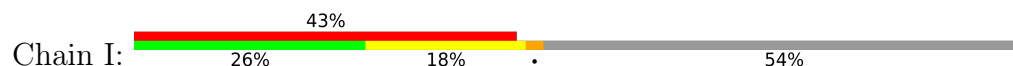
• Molecule 6: DNA-directed RNA polymerase I subunit RPA43

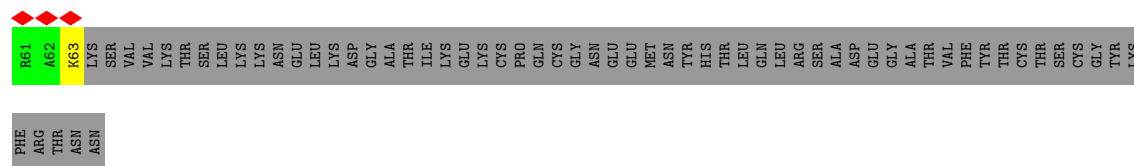


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

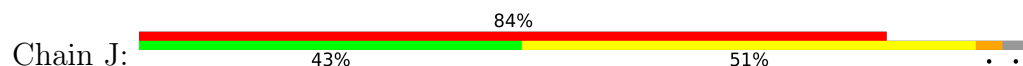


• Molecule 8: DNA-directed RNA polymerase I subunit RPA12

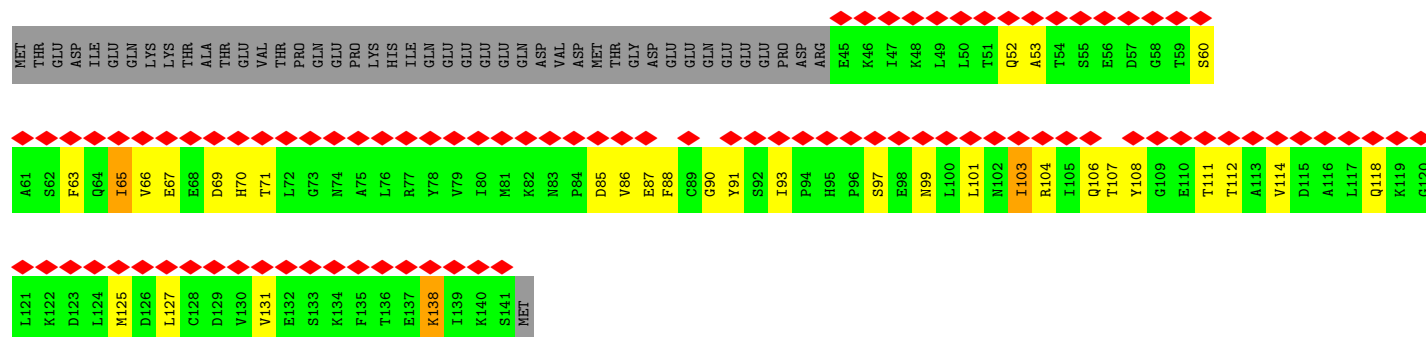




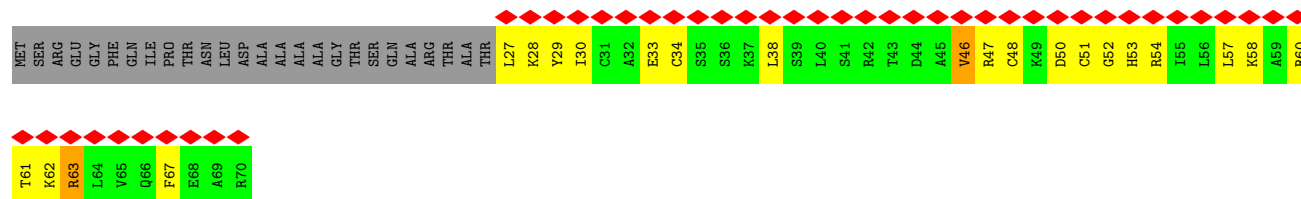
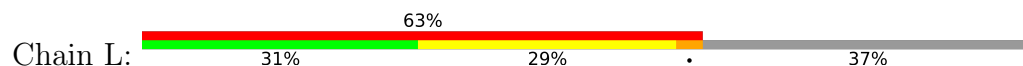
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5



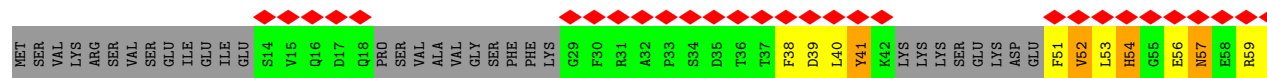
- Molecule 10: DNA-directed RNA polymerases I and III subunit RPAC2

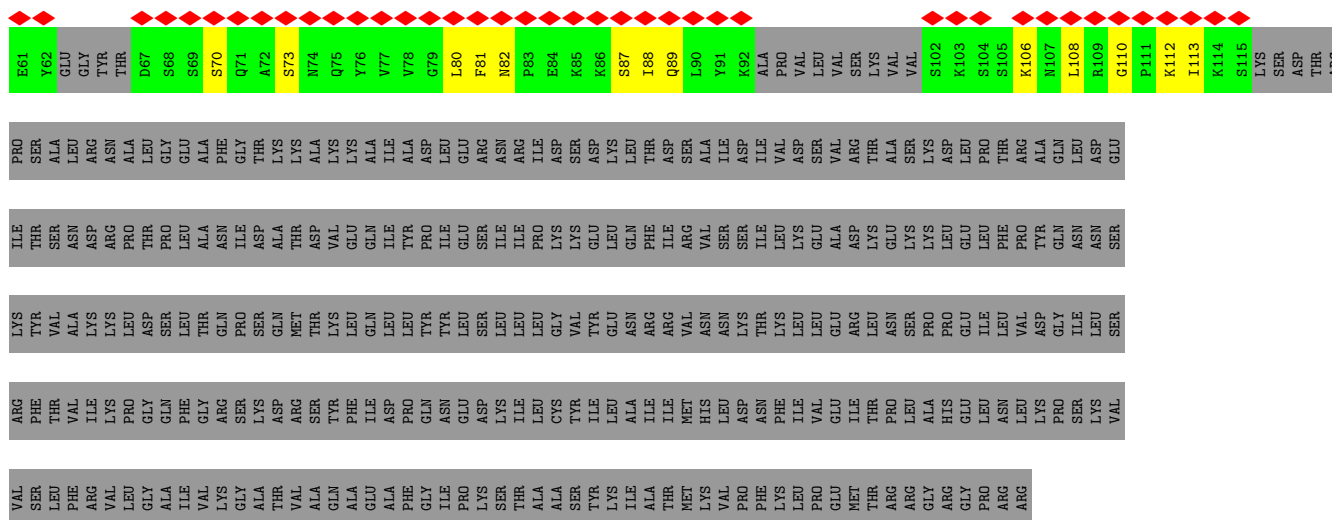


- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

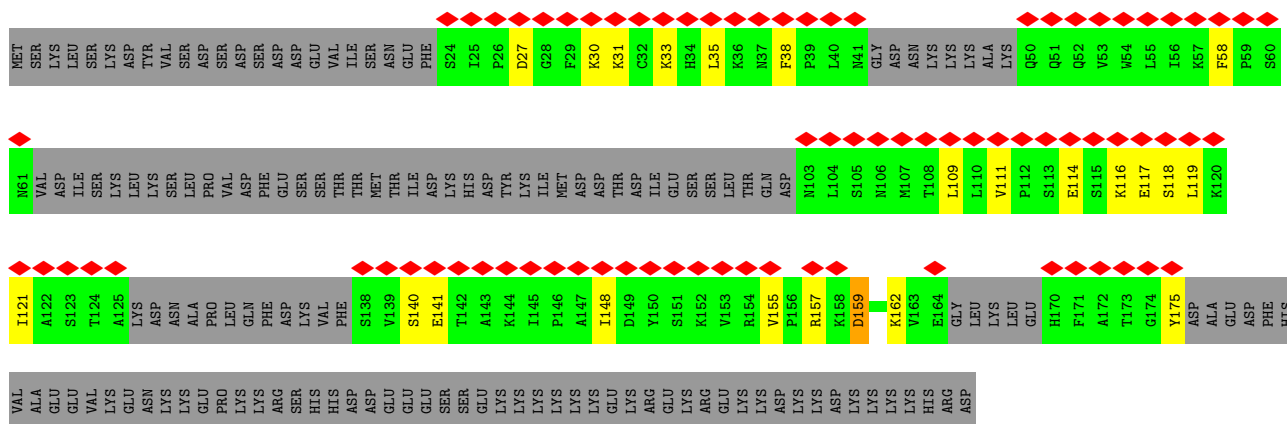


- Molecule 12: DNA-directed RNA polymerase I subunit RPA49

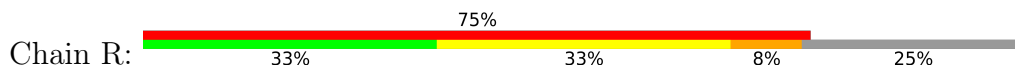




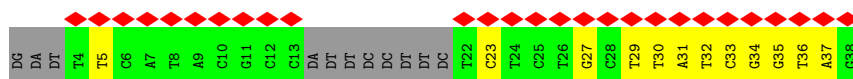
- Molecule 13: DNA-directed RNA polymerase I subunit RPA34



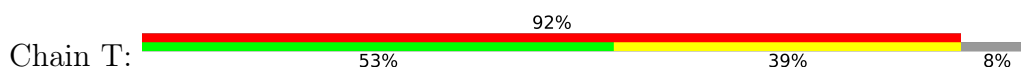
- Molecule 14: RNA



- 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 (\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 (\AA)	1.047, 1.047, 1.047	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, 3DR

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 [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	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%)	26	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	985/1053 (94%)	927 (94%)	58 (6%)	16	44
3	C	268/296 (90%)	252 (94%)	16 (6%)	16	43
4	E	166/197 (84%)	154 (93%)	12 (7%)	12	37
5	F	91/137 (66%)	86 (94%)	5 (6%)	18	46
6	G	55/291 (19%)	48 (87%)	7 (13%)	3	18
7	H	115/128 (90%)	110 (96%)	5 (4%)	25	54
8	I	50/110 (46%)	42 (84%)	8 (16%)	2	12
9	J	63/65 (97%)	59 (94%)	4 (6%)	15	42
10	K	87/130 (67%)	83 (95%)	4 (5%)	23	52
11	L	39/57 (68%)	36 (92%)	3 (8%)	10	34
12	M	65/371 (18%)	61 (94%)	4 (6%)	15	42
13	N	79/220 (36%)	73 (92%)	6 (8%)	11	35
All	All	3096/4520 (68%)	2922 (94%)	174 (6%)	20	45

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 [i](#)

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	1.53	1 (12%)	9,14,17	1.69	2 (22%)

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'	2.48	1.58	1.51

All (2) 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
16	T	17	3DR	C2'-C3'-C4'	2.93	108.82	102.75

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.

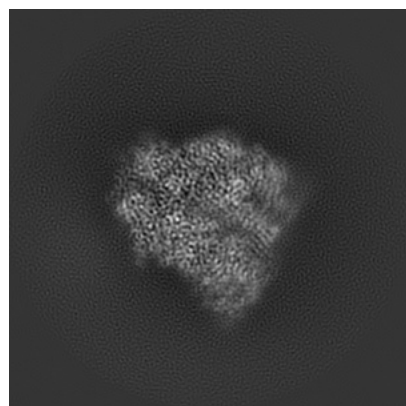
6 Map visualisation [i](#)

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.

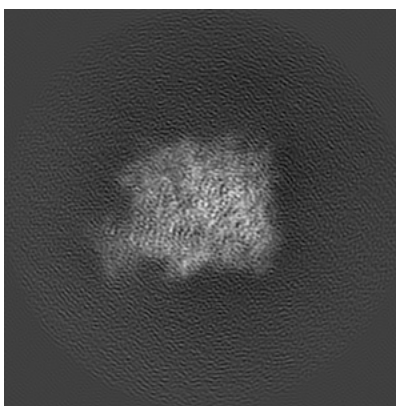
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

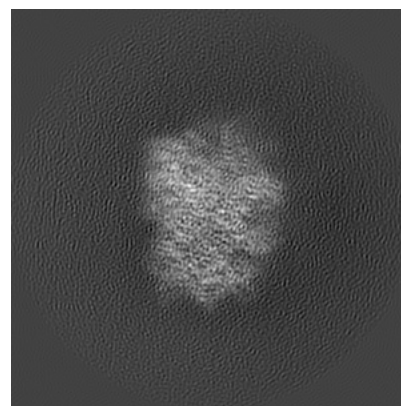
6.1.1 Primary map



X

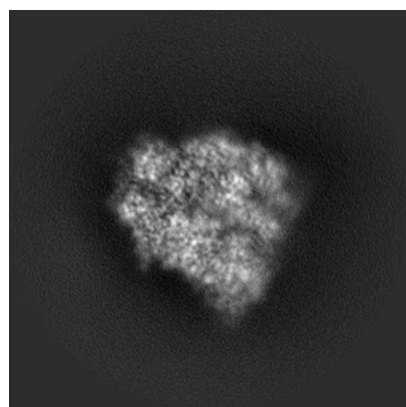


Y

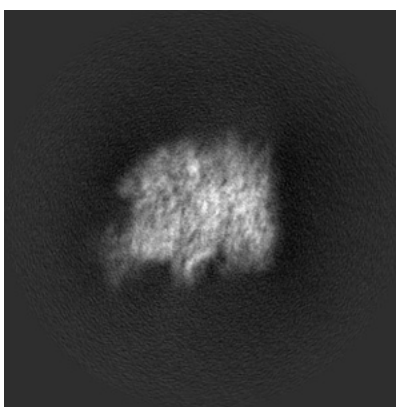


Z

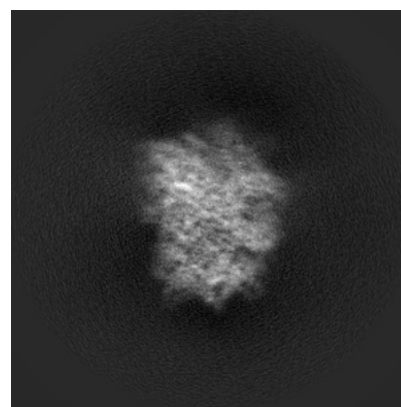
6.1.2 Raw map



X



Y

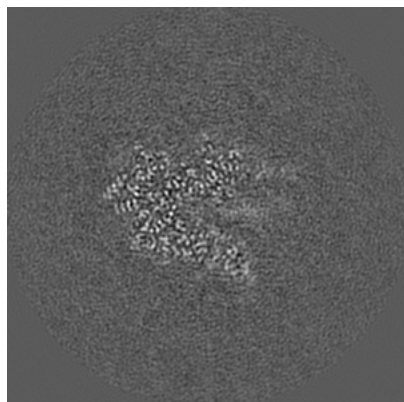


Z

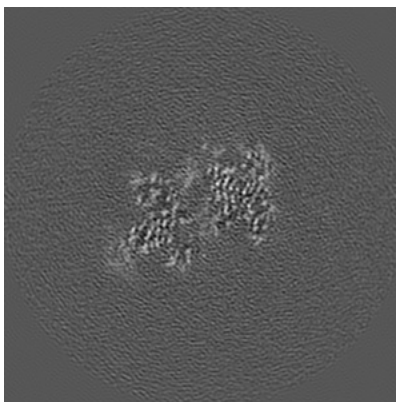
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

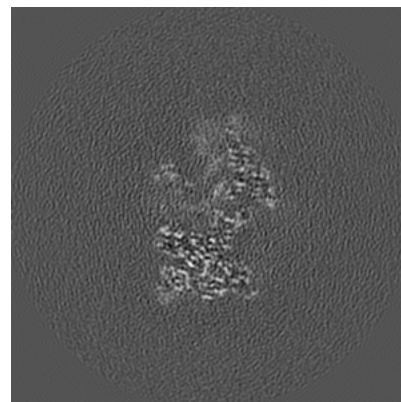
6.2.1 Primary map



X Index: 144

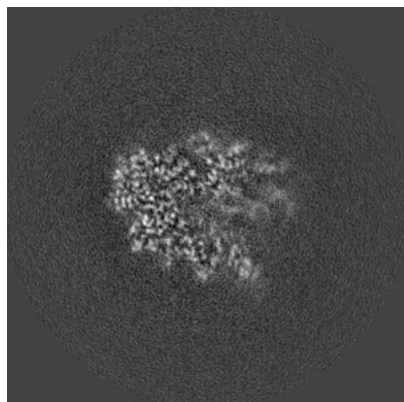


Y Index: 144

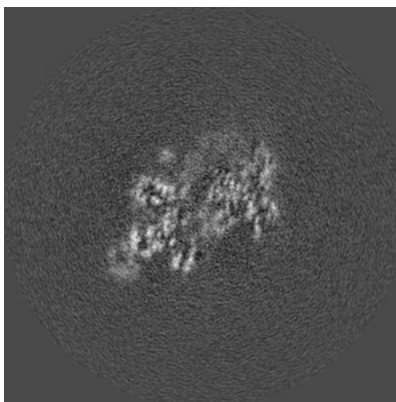


Z Index: 144

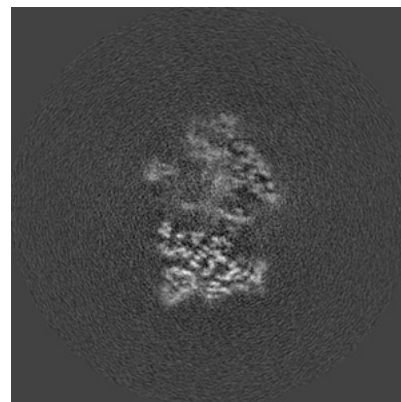
6.2.2 Raw map



X Index: 144



Y Index: 144

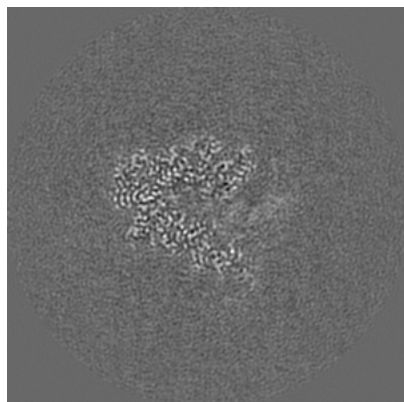


Z Index: 144

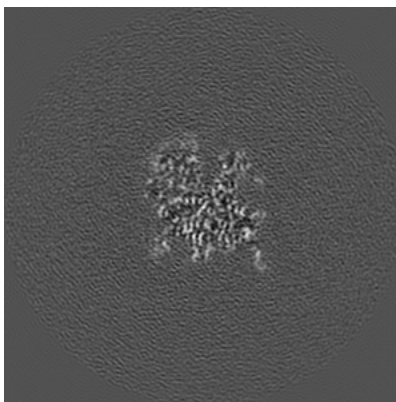
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

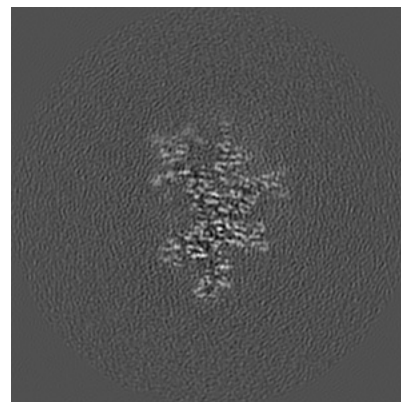
6.3.1 Primary map



X Index: 139

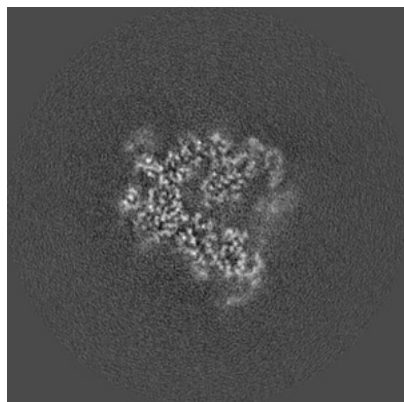


Y Index: 120

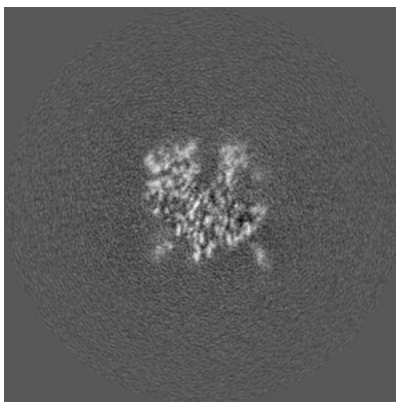


Z Index: 162

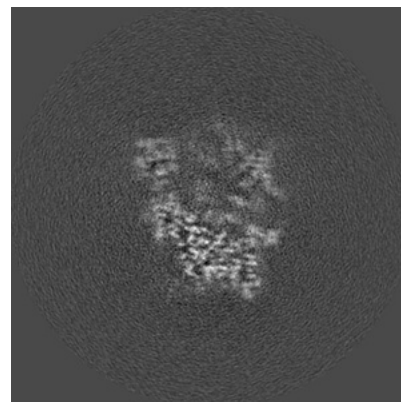
6.3.2 Raw map



X Index: 131



Y Index: 119

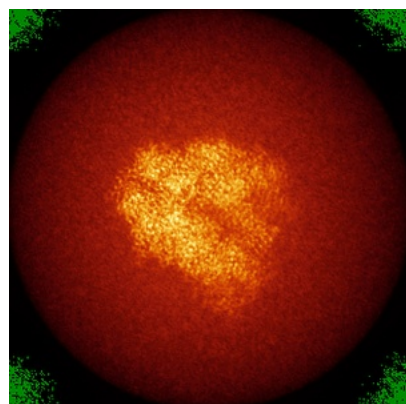


Z Index: 135

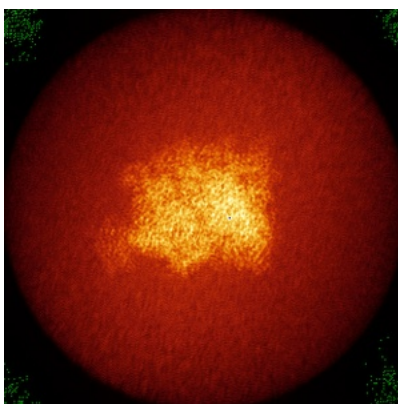
The images above show the largest variance slices of the map in three orthogonal directions.

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

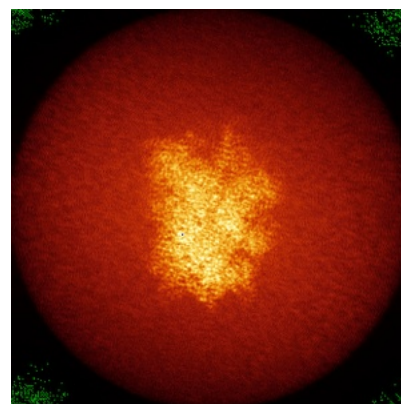
6.4.1 Primary map



X

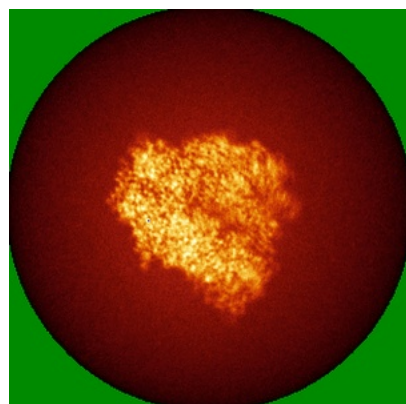


Y

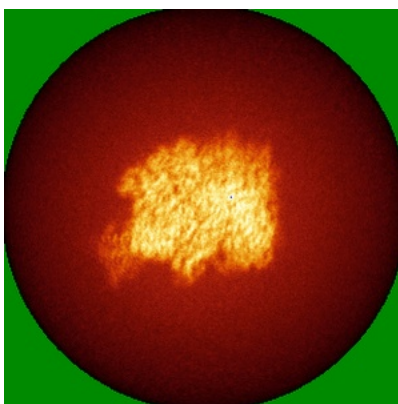


Z

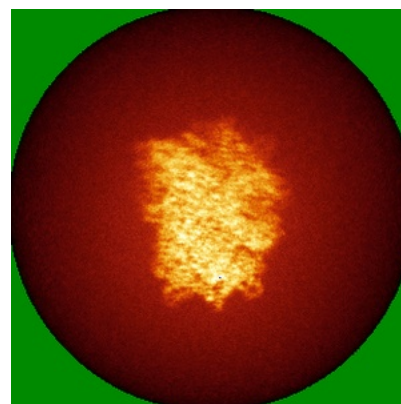
6.4.2 Raw map



X



Y

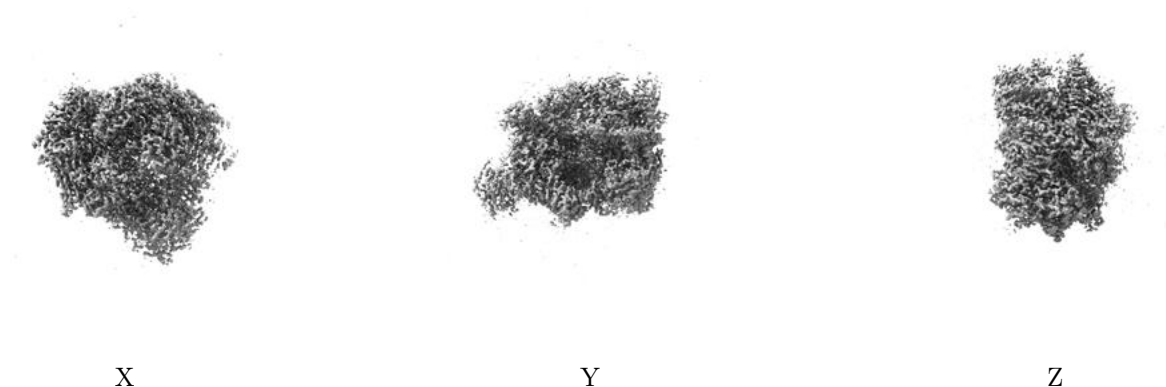


Z

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.

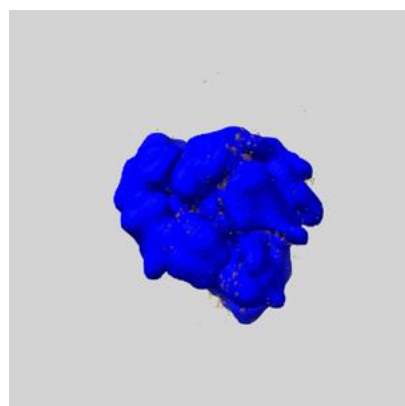
6.6 Mask visualisation [i](#)

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

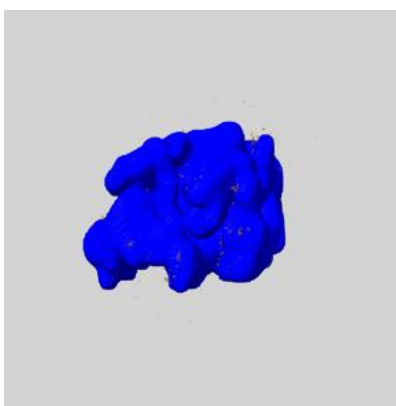
A mask typically either:

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

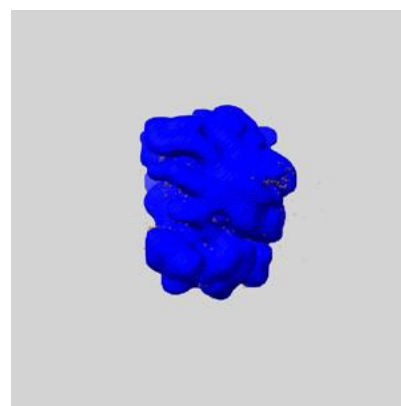
6.6.1 emd_50972_msk_1.map [i](#)



X



Y

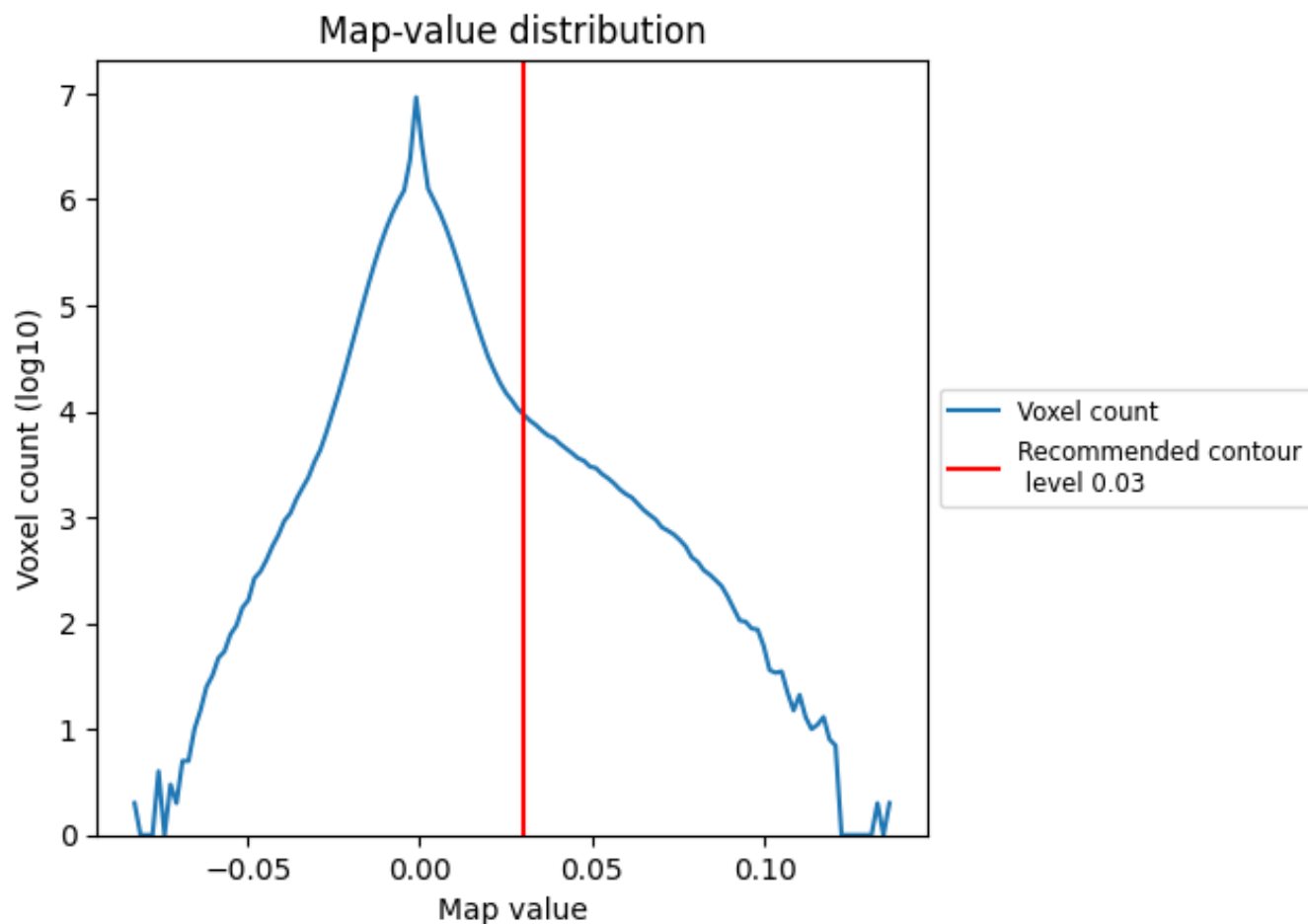


Z

7 Map analysis [i](#)

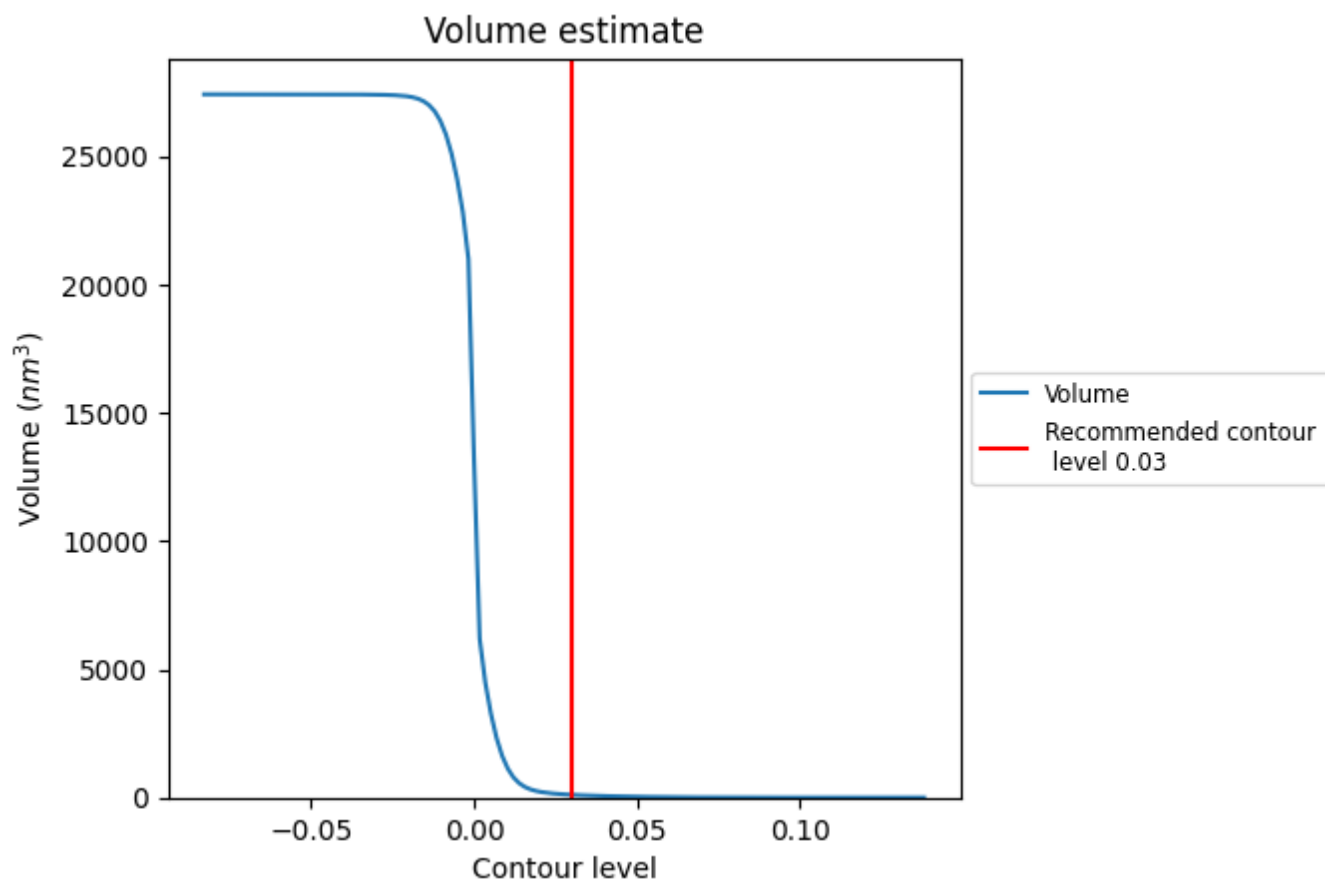
This section contains the results of statistical analysis of the map.

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.

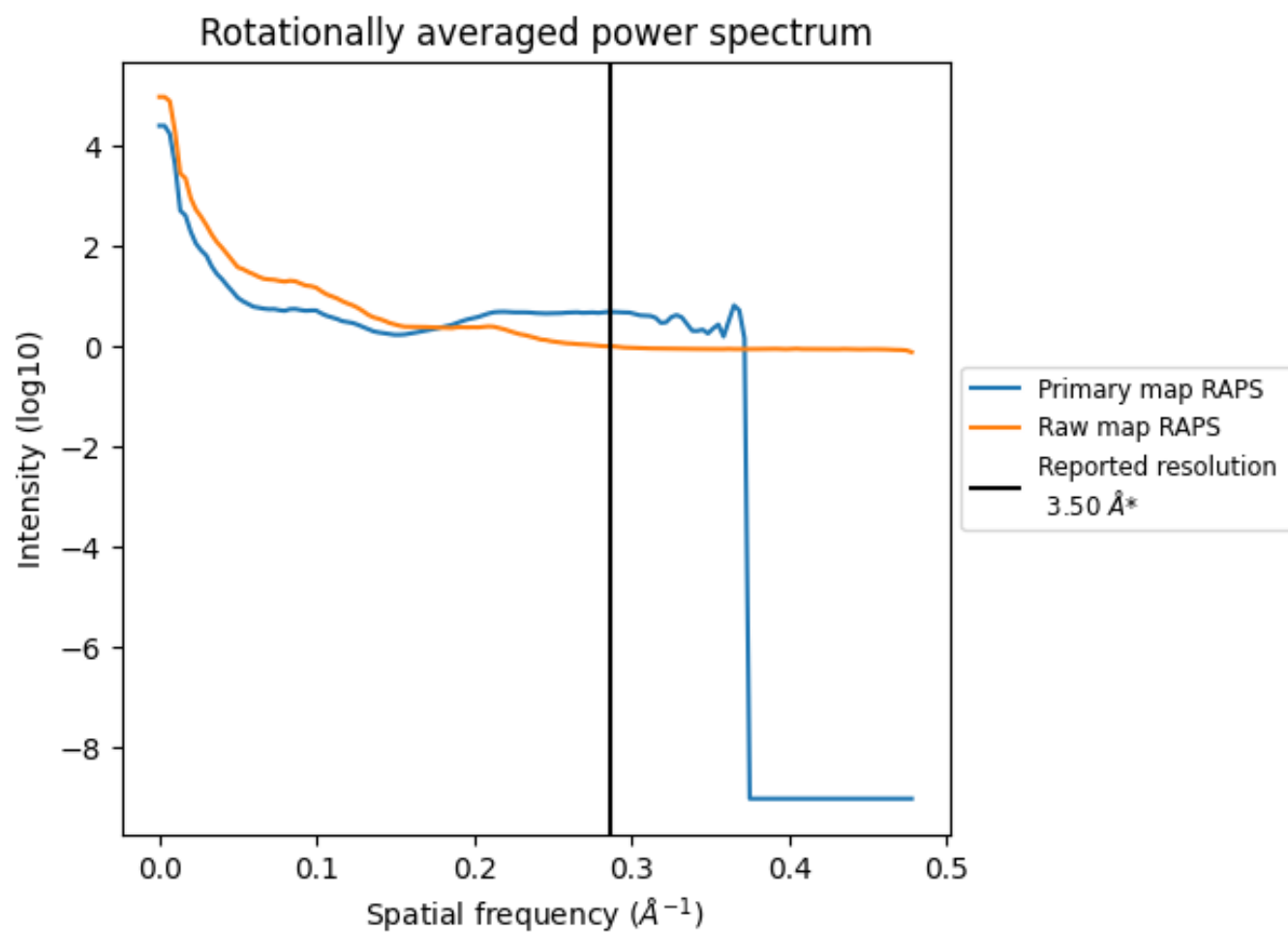
7.2 Volume estimate [i](#)



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 ⓘ

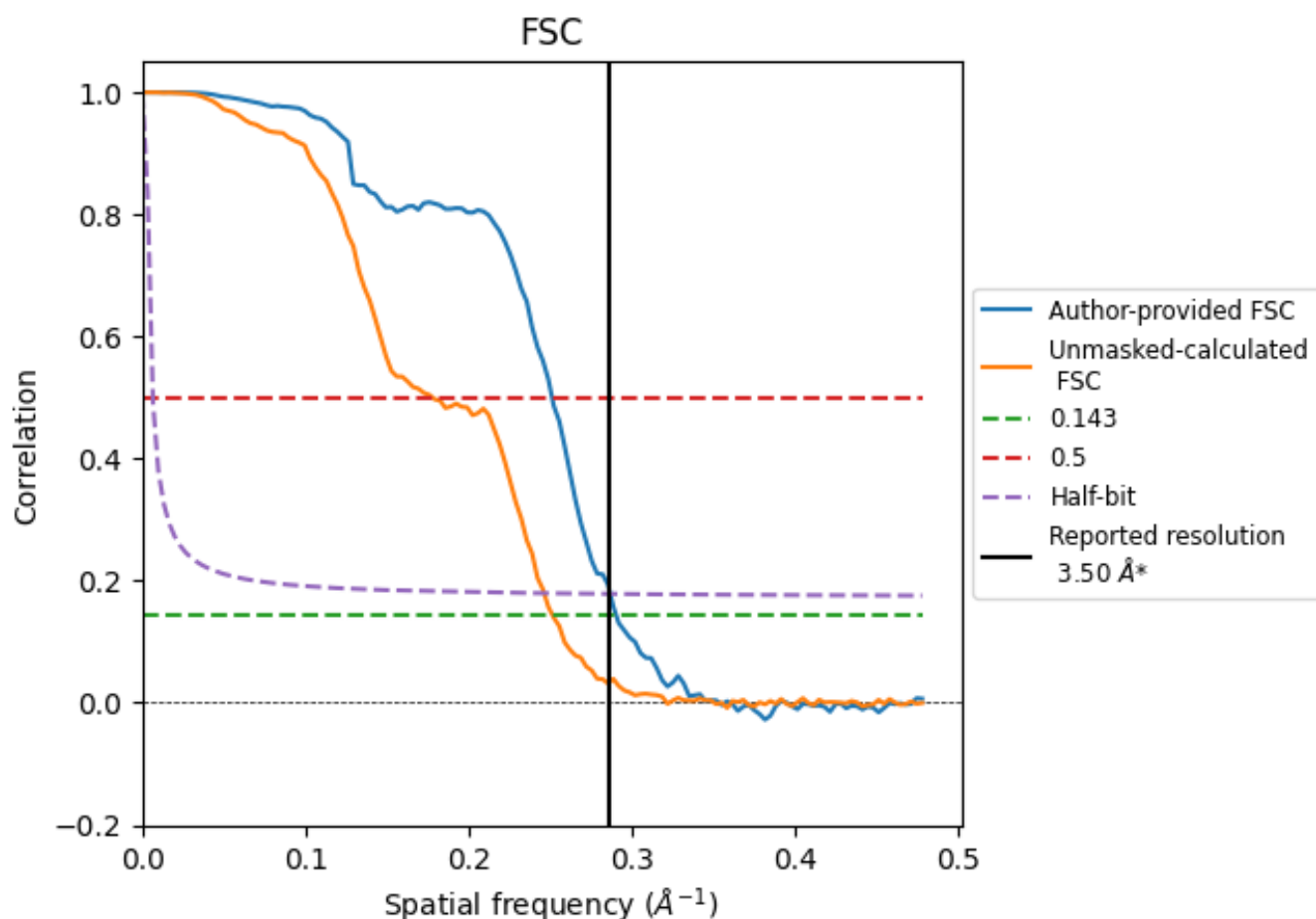


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

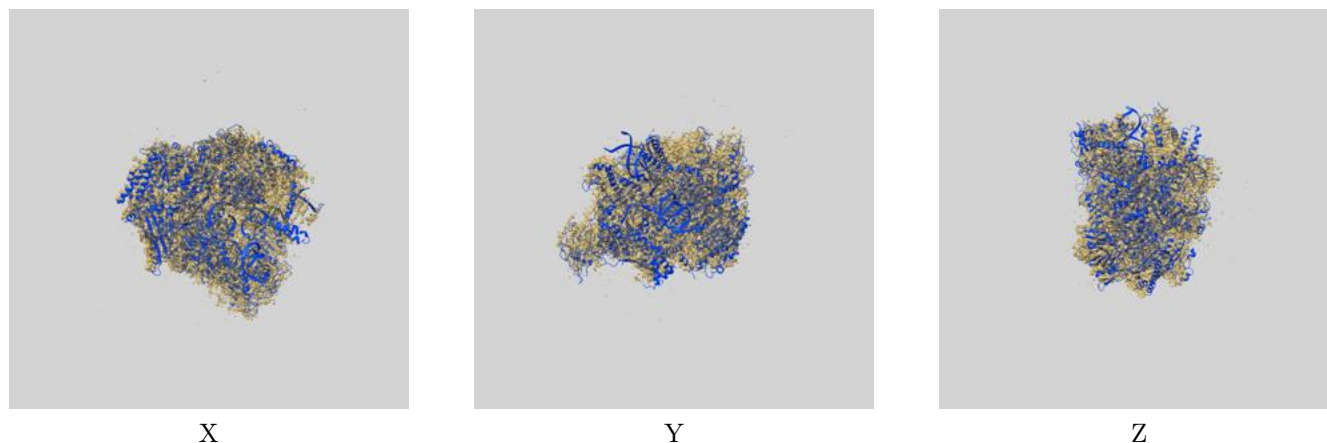
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.98	3.49
Unmasked-calculated*	3.98	5.62	4.06

*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](#)

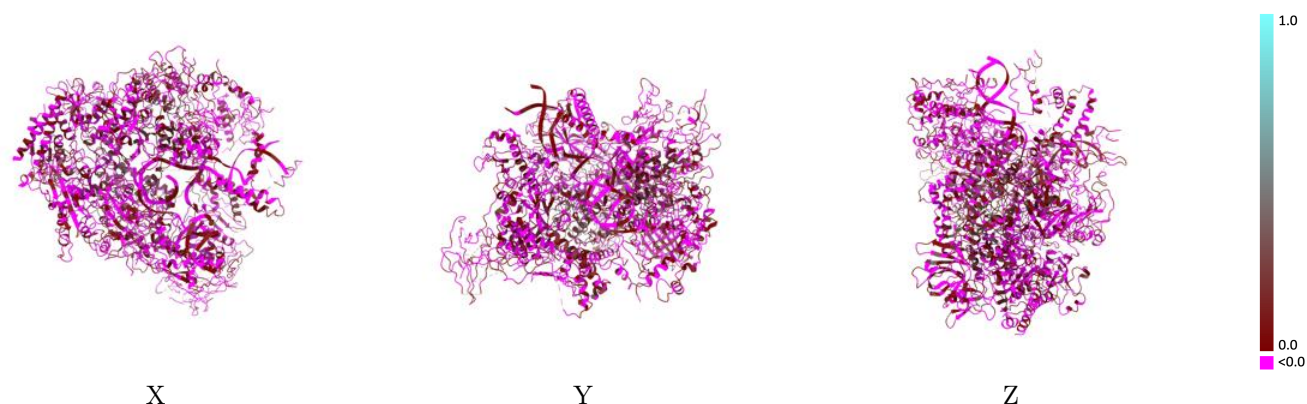
This section contains information regarding the fit between EMDB map EMD-50972 and PDB model 9G2C. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



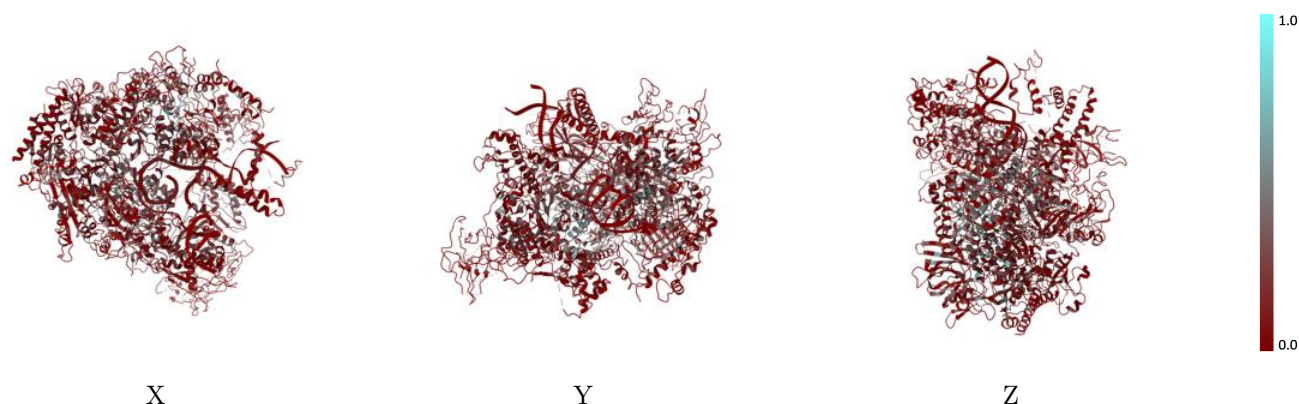
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



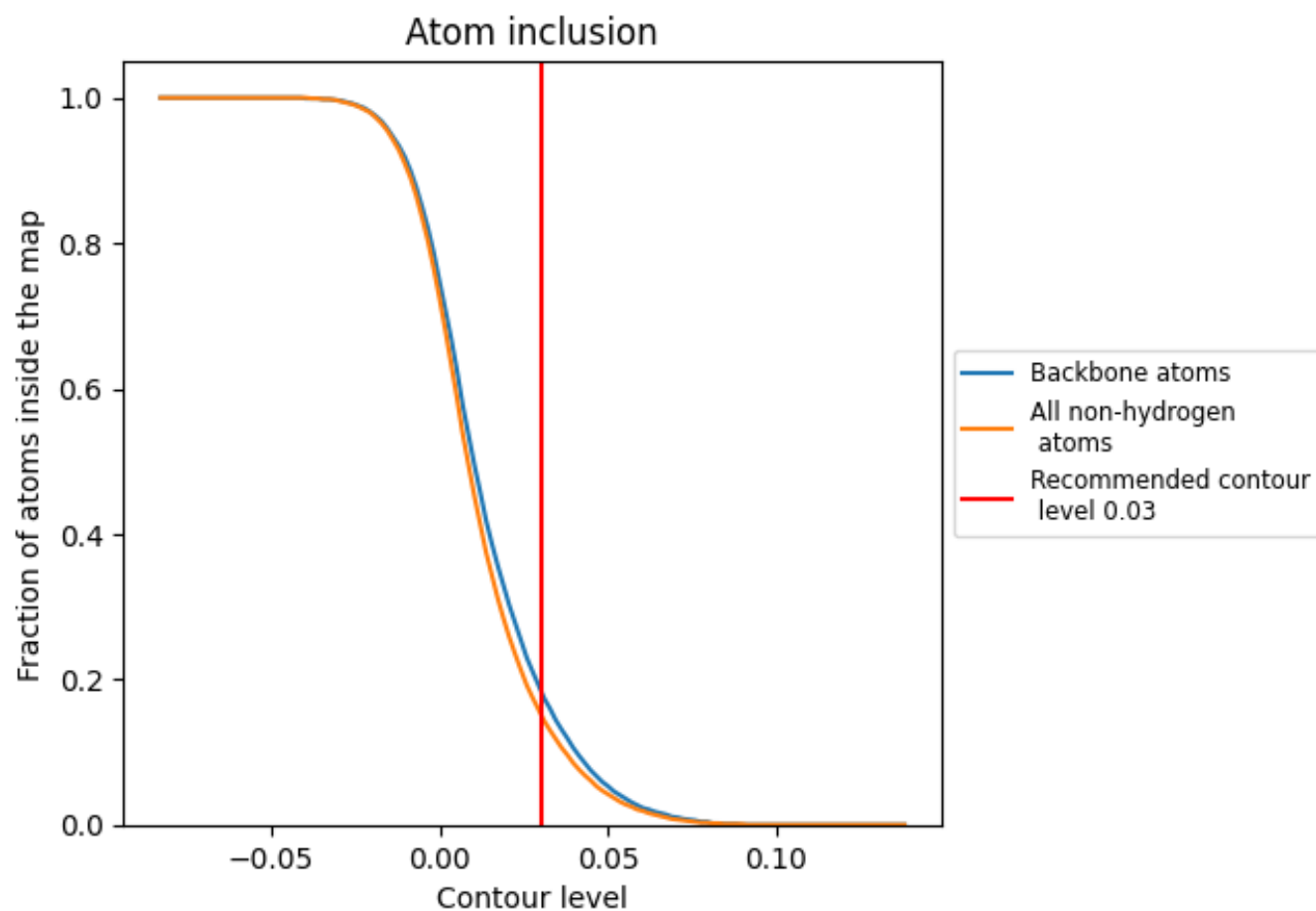
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

