



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2022 – 04:57 PM EDT

PDB ID : 5W65
EMDB ID : EMD-8775
Title : RNA polymerase I Initial Transcribing Complex State 2
Authors : Han, Y.; He, Y.
Deposited on : 2017-06-16
Resolution : 4.30 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:

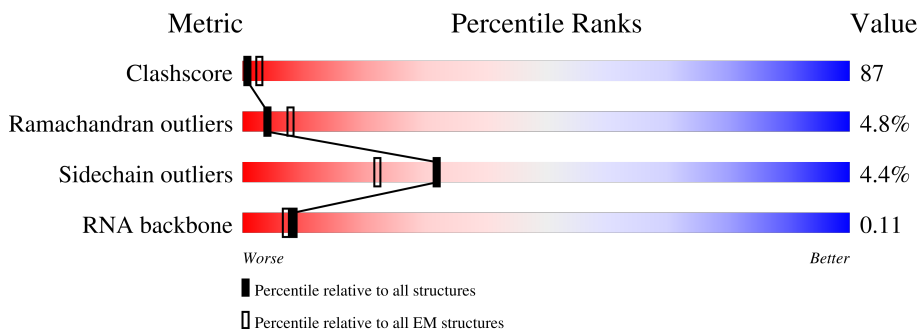
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

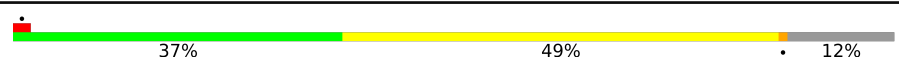




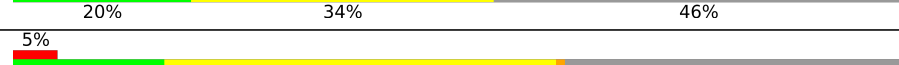
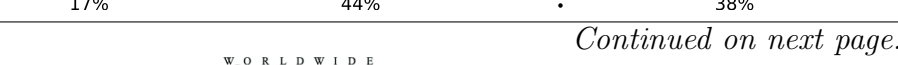
The reported resolution of this entry is 4.30 Å.

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.





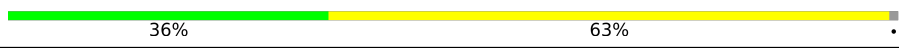
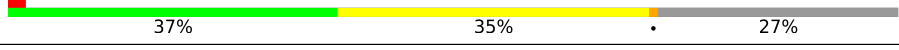
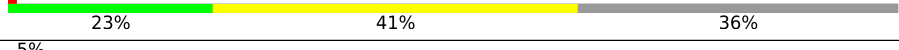


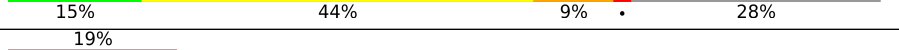
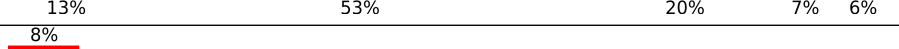
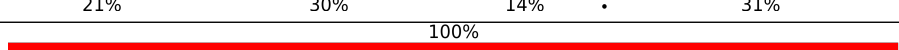

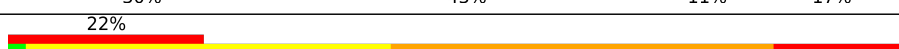
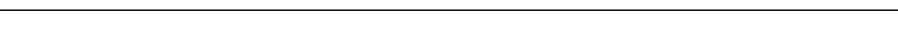
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	
6	F	155	
7	G	326	

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Mol	Chain	Length	Quality of chain
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	ZN	A	1701	-	-	X	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 47308 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
			Total	C	N	O	S		
1	A	1461	11542	7292	2004	2184	62	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	306	2431	1544	417	462	8	0	0

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

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1759	1116	310	321	12	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	670	428	114	125	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	133	1070	676	181	209	4	0	0

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

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	69	569	362	101	100	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	103	810	506	132	167	5	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	45	358	221	71	62	4	0	0

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

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

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

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

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

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

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	3	UNK	HIS	SEE REMARK 999	UNP P32786
O	4	UNK	PHE	SEE REMARK 999	UNP P32786
O	5	UNK	PHE	SEE REMARK 999	UNP P32786
O	6	UNK	LYS	SEE REMARK 999	UNP P32786
O	7	UNK	LYS	SEE REMARK 999	UNP P32786
O	8	UNK	VAL	SEE REMARK 999	UNP P32786
O	9	UNK	ASP	SEE REMARK 999	UNP P32786
O	10	UNK	VAL	SEE REMARK 999	UNP P32786
O	11	UNK	GLY	SEE REMARK 999	UNP P32786
O	12	UNK	ASN	SEE REMARK 999	UNP P32786
O	13	UNK	ASP	SEE REMARK 999	UNP P32786
O	14	UNK	SER	SEE REMARK 999	UNP P32786
O	15	UNK	MET	SEE REMARK 999	UNP P32786
O	16	UNK	PHE	SEE REMARK 999	UNP P32786
O	17	UNK	GLY	SEE REMARK 999	UNP P32786
O	18	UNK	VAL	SEE REMARK 999	UNP P32786
O	19	UNK	ASN	SEE REMARK 999	UNP P32786
O	20	UNK	CYS	SEE REMARK 999	UNP P32786
O	21	UNK	ASP	SEE REMARK 999	UNP P32786
O	22	UNK	THR	SEE REMARK 999	UNP P32786
O	23	UNK	PRO	SEE REMARK 999	UNP P32786
O	24	UNK	VAL	SEE REMARK 999	UNP P32786
O	25	UNK	SER	SEE REMARK 999	UNP P32786
O	26	UNK	PHE	SEE REMARK 999	UNP P32786
O	27	UNK	GLN	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

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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
			Total	C	N	O	S		
16	P	481	3978	2553	681	722	22	0	0

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

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

- Molecule 18 is a RNA chain called RNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	S	45	935	447	174	270	44	0	0

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

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

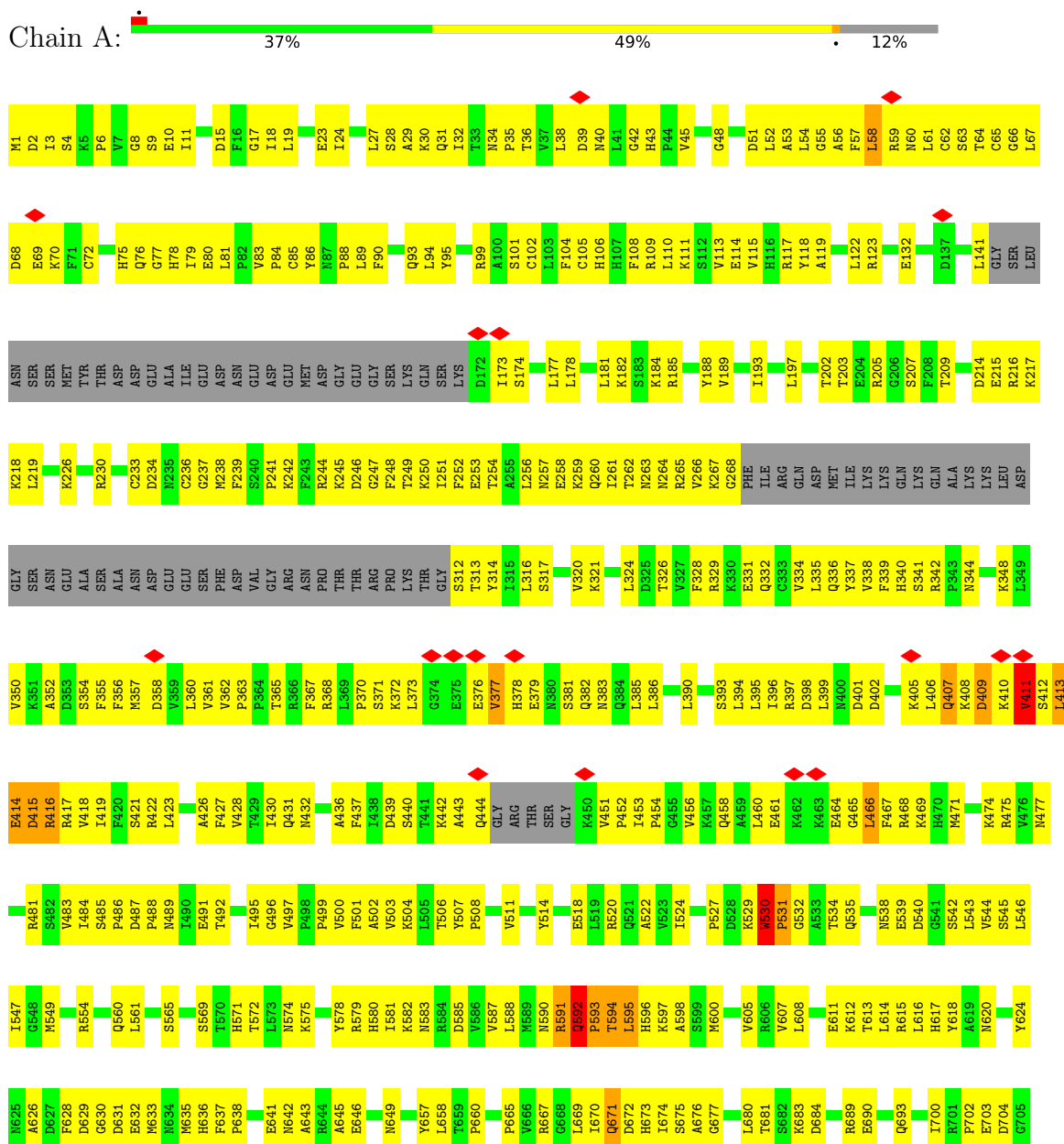
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

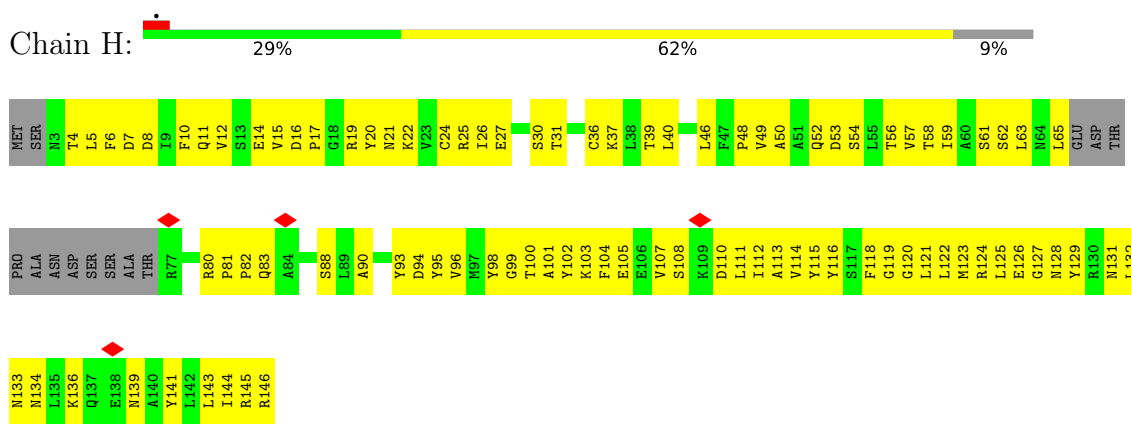
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190



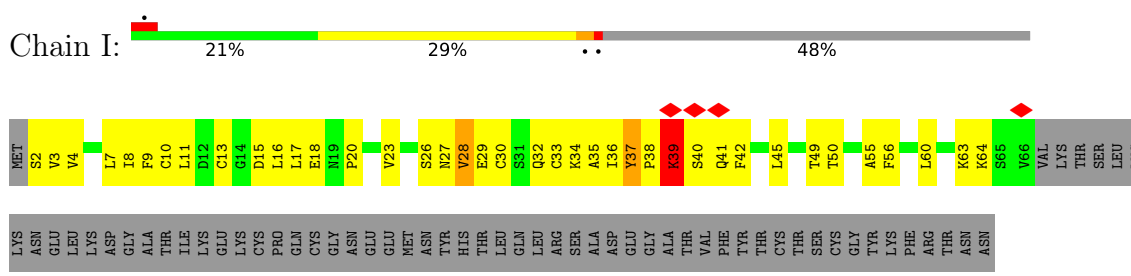
H706	H707	H708	K711	H712	P717	T718	I719	I720	K721	H722	H723	H724	L725	H726	H727	H728	K729	Q730	I731	I732	T733	T734	V735	N738	P741	P742	D743	G746	I747	N748	N749	K752	N753	K754	I755	K756	N757	K762	G763	E766	N767	F771	K772	D773	G774	A775	L776	I780	L781																																										
D782	K783	S784	Q785	Y786	S789	K790	Y791	G792	H793	H794	H795	S796	H799	V800	Y801	V805	L813	F817	I731	T732	T733	T734	H819	Y820	I821	T824	A825	F826	T827	C828	G829	M830	N831	D832	W842	K843	T844	D845	L846	L847	K848	T853	G854	R855	E856	A857	G948	Q949	Q950	T1024	A951	L952	E953	K866	D867	T868																																			
D872	P873	E874	R878	L879	I882	R883	R884	D885	H886	H887	K888	L892	D893	Y801	V805	V805	V908	S909	G984	K910	C911	K912	P913	D914	G915	T916	M917	K918	K919	F920	P921	C922	D831	N923	S824	M925	Q926	A927	M928	A929	L930	K934	M944	C945	L946	L947	G948	Q949	Q950	A951	L952	E953	K866	D867	T868																																				
Y957	P958	Y959	Y960	K964	T965	L966	P967	S968	F969	E973	F974	D975	A978	G979	G980	H981	Y982	G983	G984	R985	S988	G989	Q993	E994	T916	Y995	Y996	F997	H998	C999	M1000	R1003	L1006	I1007	M1081	M928	A929	L930	K934	M944	C945	L946	L947	G948	Q949	Q950	A951	L952	E953	K866	D867	T868																																							
V1030	H1031	V1032	S1033	Y1034	D1035	I1038	R1039	D1040	A1041	L1045	V1046	Q1047	F1048	M1049	Y1050	G1051	G1052	D1053	I1055	A1054	D1056	I1057	E1060	S1061	H1062	E994	F1066	L1070	C999	M1000	R1003	L1006	I1007	M1081	M928	A929	L930	K934	M944	C945	L946	L947	G948	Q949	Q950	A951	L952	E953	K866	D867	T868																																								
K1103	Y1104	R1105	K1106	S1109	LYS	GLU	P1112	H1113	Y1114	K1115	Q1116	S1117	V1118	K1119	Y1120	D1121	V1123	L1124	Y1127	N1128	P1129	A1130	K1131	Y1132	L1133	G1134	S1135	V1136	S1137	E1138	N1139	Q1141	L1144	F1147	L1148	L1154	F1155	K1156	S1157	S1158	D1159	G1160	V1161	M1162	E1163	K1164	K1165	F1166	R1167	Q1171	L1172																																								
K1173	Y1174	M1175	R1176	S1177	L1178	I1179	N1180	E1183	A1184	V1185	G1186	I1187	I1188	A1189	S1190	G1194	T1198	Q1199	M1200	THR	LEU	ASN	THR	PHE	HIS	PHE	ALA	GLY	GLY	HIS	GLY	ALA	N1214	V1215	T1216	L1217	G1218	P1220	R1221	L1222	R1223	E1224	I1225	V1226	M1227	T1228	A1229	I1233	K1234	E1305	K1164	P1236	L1240	P1241																																					
I1242	W1243	V1246	F1254	C1255	K1256	L1257	S1258	S1259	K1260	V1261	L1262	S1263	A1264	V1265	V1266	I1267	D1268	K1269	V1270	I1271	V1272	T1276	GLY	THR	SER	ASN	THR	ALA	GLY	GLY	ASN	A1286	A1287	R1288	S1289	Y1290	V1291	I1292	H1293	M1294	L1295	F1296	F1297	D1298	N1299	M1300	E1301	Y1302	S1303	I1304	E1305	V1306	D1307	V1308	K1310																																				
E1311	E1312	L1313	Q1314	M1315	L1316	I1317	S1318	M1319	Q1320	F1321	I1322	H1323	E1326	A1327	A1328	E1332	K1335	Q1336	K1337	ARG	THR	THR	GLY	PRO	ASP	ASP	ILE	GLY	VAL	ALA	VAL	PRO	ARG	LEU	GLN	THR	THR	ASP	VAL	VAL	ASN	ALA	ASN	SER	SER	SER	ASN	VAL	VAL	ASP	ASP	ASP	VAL	ASP	VAL	GLN	THR																																		
HIS	LYS	LYS	THR	LYS	GLN	ALA	VAL	SER	TYR	ASP	GLU	PRO	ASP	GLU	ASP	THR	MET	ARG	GLU	ALA	GLU	LYS	SER	THR	PRO	ASP	GLU	ILE	VAL	VAL	PRO	ARG	LYS	GLN	THR	THR	ASP	VAL	VAL	ASN	ALA	ASN	SER	SER	SER	ASN	VAL	VAL	ASP	ASP	ASP	VAL	GLN	THR																																					
ALA	ASN	ASN	M1438	M1439	M1440	Q1443	R1444	T1445	Q1447	I1451	H1454	R1455	F1456	I1457	T1458	K1459	Y1460	M1461	F1462	D1463	D1464	E1465	S1466	G1467	K1468	L1469	C1470	E1471	F1472	K1473	L1474	E1475	L1476	A1477	D1478	D1479	T1480	E1481	K1482	L1483	L1484	M1485	V1486	N1487	I1488	V1489	E1490	E1491	R1494	L1495	S1496	L1497	I1498	R1499	Q1500																																				
I1501	R1506	C1507	H1508	H1509	P1510	M1514	G1515	K1516	R1517	V1518	L1519	V1520	T1521	E1522	G1523	V1524	Q1527	A1528	H1529	W1530	D1531	Q1532	E1533	I1536	D1537	I1541	D1545	V1549	E1556	R1559	E1565	M1568	Y1569	F1570	S1571	R1572	Y1573	R1580	D1583	L1584	D1587	R1591	Y1595	L1596	F1598	M1599	R1600	R1601	G1602	M1603	E1604	T1605	S1609	F1610	M1613	S1614	Y1615	E1616	F1617	T1618	C1619	L1622	T1623	L1627	D1628	N1629	E1630	R1631	E1632	Q1633	L1634	D1635	A1639	R1640	I1641	V1642	V1643	G1644	K1645	L1646	N1647	M1648	V1649	F1654	D1655	V1656	L1657	A1658	K1659	A1663	ALA

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

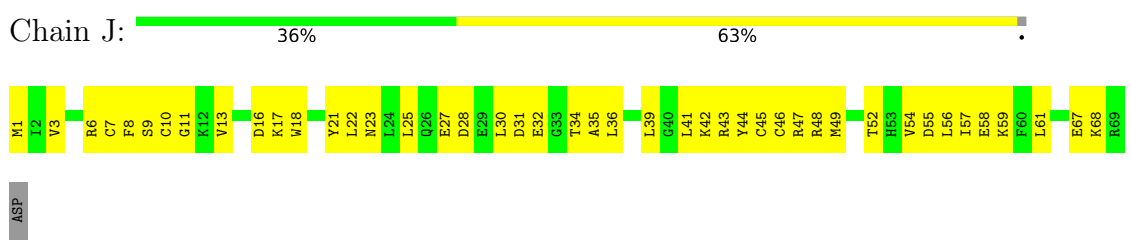




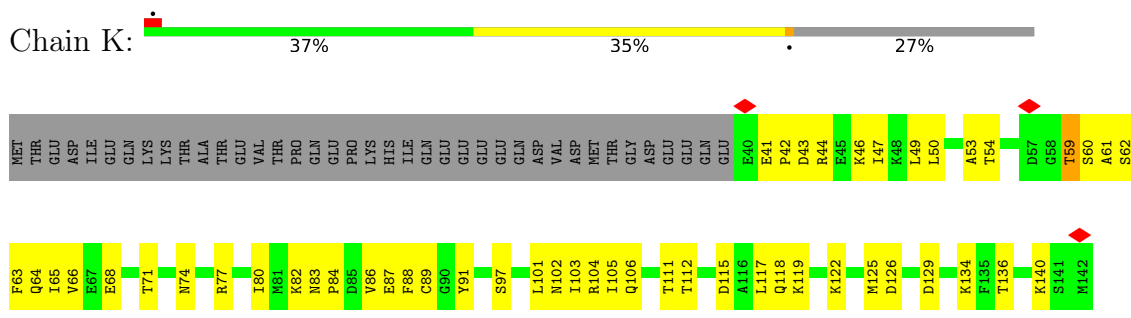
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12



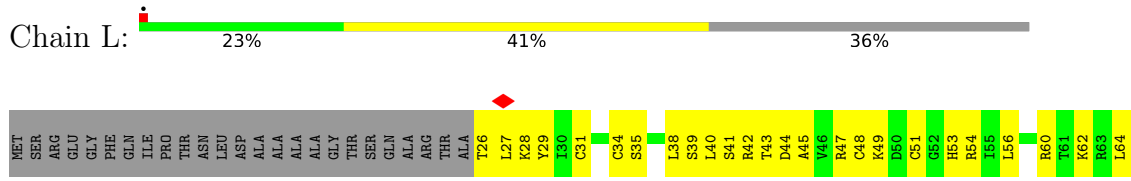
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

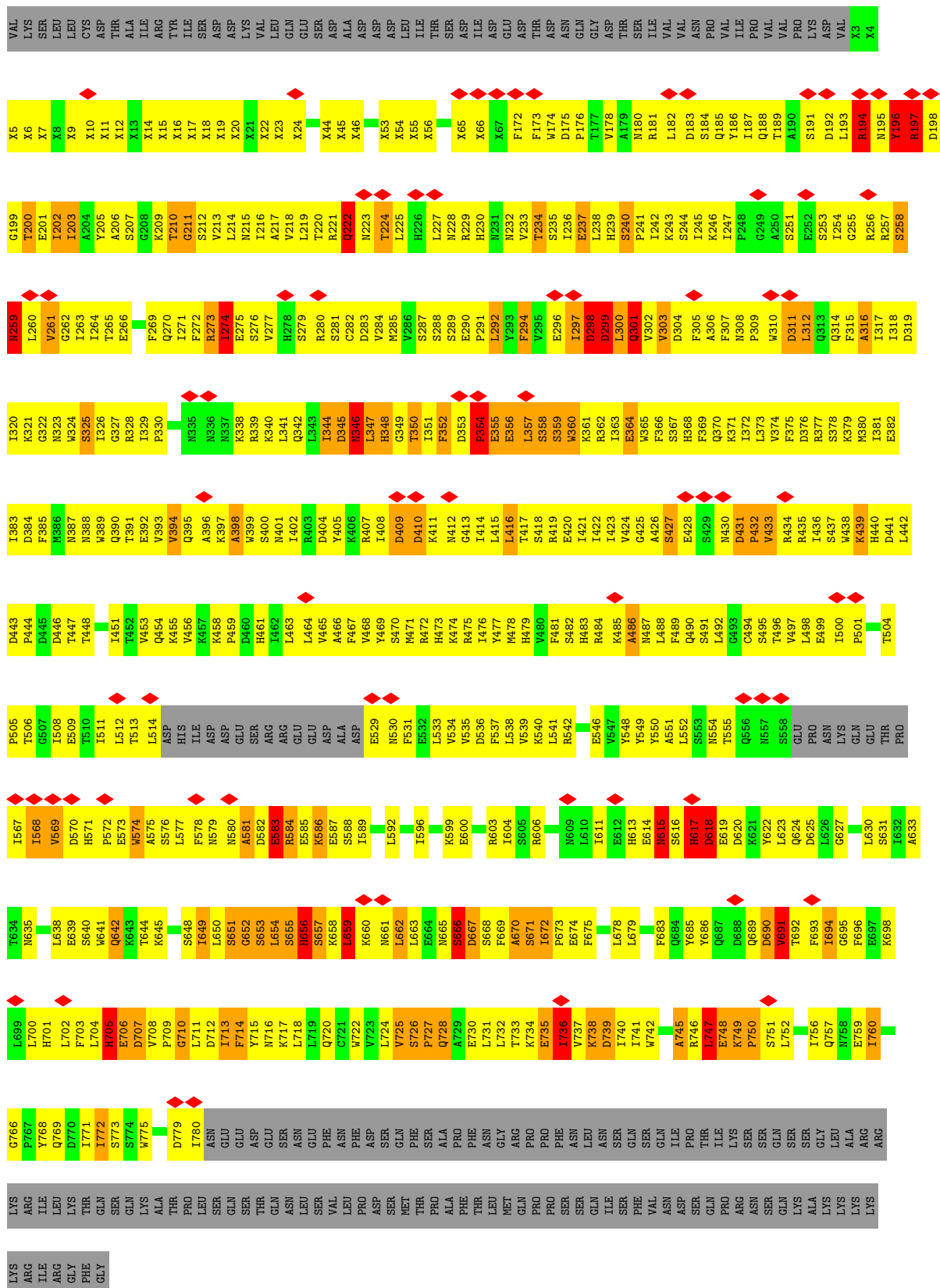


• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

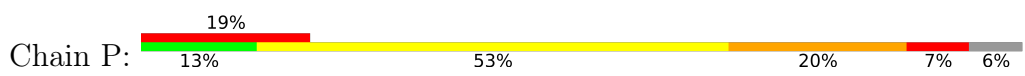


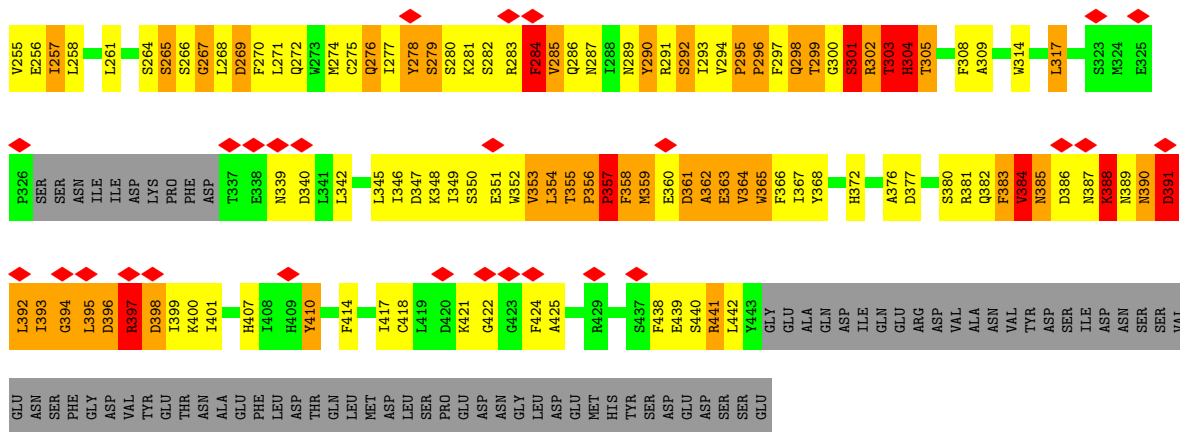
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4





● Molecule 16: RNA polymerase I-specific transcription initiation factor RRN7





• Molecule 18: RNA



• 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	38340	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	0.262	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	249.59999, 249.59999, 249.59999	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3, 1.3, 1.3	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/11752	0.59	1/15870 (0.0%)
2	B	0.52	1/9556 (0.0%)	0.66	4/12916 (0.0%)
3	C	0.43	0/2483	0.60	0/3366
4	D	0.32	0/473	0.51	0/641
5	E	0.37	0/1795	0.53	0/2416
6	F	0.42	0/682	0.60	0/922
7	G	0.34	0/1630	0.57	0/2216
8	H	0.41	0/1088	0.57	0/1474
9	I	0.37	0/485	0.72	2/657 (0.3%)
10	J	0.50	0/578	0.69	0/775
11	K	0.41	0/821	0.56	0/1108
12	L	0.38	0/360	0.58	0/478
13	M	0.33	0/857	0.60	1/1151 (0.1%)
14	N	0.33	0/1279	0.62	0/1724
15	O	0.57	2/4902 (0.0%)	1.07	42/6641 (0.6%)
16	P	0.45	3/4068 (0.1%)	1.17	54/5491 (1.0%)
17	Q	0.63	1/2990 (0.0%)	1.15	22/4030 (0.5%)
18	R	1.60	0/142	2.59	18/220 (8.2%)
19	S	1.78	1/1050 (0.1%)	2.62	101/1621 (6.2%)
20	T	1.69	2/1206 (0.2%)	2.42	101/1855 (5.4%)
All	All	0.60	10/48197 (0.0%)	0.96	346/65572 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
18	R	0	2
19	S	0	21

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	T	0	27
All	All	0	51

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	PRO	N-CD	9.56	1.61	1.47
16	P	263	PRO	N-CD	6.45	1.56	1.47
20	T	1	DT	C4'-O4'	-6.03	1.39	1.45
16	P	199	LEU	CA-C	5.77	1.68	1.52
16	P	191	PRO	N-CD	5.61	1.55	1.47

The worst 5 of 346 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	145	SER	N-CA-CB	16.78	135.67	110.50
15	O	346	ASN	N-CA-CB	-15.27	83.11	110.60
2	B	77	LYS	C-N-CD	14.74	159.35	128.40
16	P	49	ASN	N-CA-C	-12.63	76.90	111.00
19	S	2	DA	N1-C6-N6	-11.27	111.84	118.60

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	LEU	Mainchain
18	R	1	A	Sidechain
18	R	6	A	Sidechain
19	S	2	DA	Sidechain
19	S	4	DG	Sidechain

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	11631	1305	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9351	0	9242	1164	0
3	C	2431	0	2418	234	0
4	D	467	0	468	61	0
5	E	1759	0	1788	208	0
6	F	670	0	690	81	0
7	G	1592	0	1600	283	0
8	H	1070	0	1045	142	0
9	I	479	0	480	102	0
10	J	569	0	585	56	0
11	K	810	0	801	71	0
12	L	358	0	381	34	0
13	M	841	0	837	192	0
14	N	1254	0	1266	235	0
15	O	5063	0	4803	2158	0
16	P	3978	0	3983	2055	0
17	Q	2923	0	2968	1061	0
18	R	127	0	67	15	0
19	S	935	0	513	69	0
20	T	1082	0	613	78	0
21	A	2	0	0	2	0
21	B	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
21	P	1	0	0	1	0
All	All	47308	0	46179	8106	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 87.

The worst 5 of 8106 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)
16:P:417:PHE:CZ	17:Q:270:PHE:CD2	1.76	1.70
17:Q:356:PRO:CG	17:Q:357:PRO:HD3	1.21	1.68
15:O:421:ILE:HD11	17:Q:138:PHE:CE2	1.29	1.67
15:O:702:LEU:HD21	16:P:125:PHE:CE2	1.14	1.66
15:O:369:PHE:CD2	15:O:432:PRO:HG3	1.32	1.65

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	1445/1664 (87%)	1340 (93%)	82 (6%)	23 (2%)	9	45
2	B	1172/1203 (97%)	1078 (92%)	71 (6%)	23 (2%)	7	40
3	C	304/335 (91%)	286 (94%)	13 (4%)	5 (2%)	9	45
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	203 (95%)	7 (3%)	3 (1%)	11	47
6	F	81/155 (52%)	73 (90%)	7 (9%)	1 (1%)	13	50
7	G	197/326 (60%)	182 (92%)	12 (6%)	3 (2%)	10	46
8	H	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
9	I	63/125 (50%)	55 (87%)	6 (10%)	2 (3%)	4	30
10	J	67/70 (96%)	60 (90%)	6 (9%)	1 (2%)	10	46
11	K	101/142 (71%)	94 (93%)	7 (7%)	0	100	100
12	L	43/70 (61%)	38 (88%)	4 (9%)	1 (2%)	6	37
13	M	104/415 (25%)	97 (93%)	5 (5%)	2 (2%)	8	41
14	N	156/233 (67%)	129 (83%)	21 (14%)	6 (4%)	3	27
15	O	581/894 (65%)	408 (70%)	111 (19%)	62 (11%)	0	8
16	P	473/514 (92%)	320 (68%)	74 (16%)	79 (17%)	0	3
17	Q	343/507 (68%)	234 (68%)	56 (16%)	53 (16%)	0	3
All	All	5527/7151 (77%)	4772 (86%)	491 (9%)	264 (5%)	4	23

5 of 264 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	LYS
1	A	411	VAL
1	A	416	ARG
1	A	530	TRP
1	A	592	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1292/1465 (88%)	1277 (99%)	15 (1%)	71	84
2	B	1030/1053 (98%)	1009 (98%)	21 (2%)	55	73
3	C	270/296 (91%)	269 (100%)	1 (0%)	91	94
4	D	56/116 (48%)	56 (100%)	0	100	100
5	E	197/197 (100%)	196 (100%)	1 (0%)	88	93
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	179/291 (62%)	175 (98%)	4 (2%)	52	71
8	H	117/128 (91%)	116 (99%)	1 (1%)	78	88
9	I	57/110 (52%)	57 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	93/130 (72%)	92 (99%)	1 (1%)	73	85
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	96/371 (26%)	92 (96%)	4 (4%)	30	55
14	N	146/220 (66%)	143 (98%)	3 (2%)	53	72
15	O	545/778 (70%)	496 (91%)	49 (9%)	9	33
16	P	445/476 (94%)	379 (85%)	66 (15%)	3	17
17	Q	331/474 (70%)	276 (83%)	55 (17%)	2	14
All	All	5031/6364 (79%)	4810 (96%)	221 (4%)	32	54

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	P	180	ASP
16	P	389	GLN
17	Q	398	ASP
17	Q	276	GLN
16	P	223	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106

such sidechains are listed below:

Mol	Chain	Res	Type
7	G	20	HIS
14	N	103	ASN
17	Q	212	HIS
7	G	36	ASN
7	G	126	GLN

5.3.3 RNA [i](#)

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	O	2

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
1	O	28:UNK	C	41:UNK	N	6.55

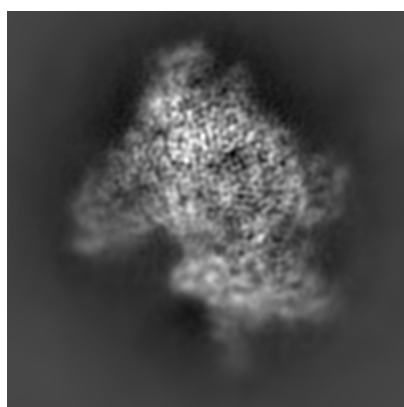
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8775. These allow visual inspection of the internal detail of the map and identification of artifacts.

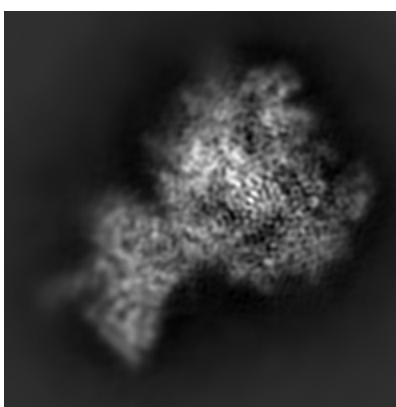
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

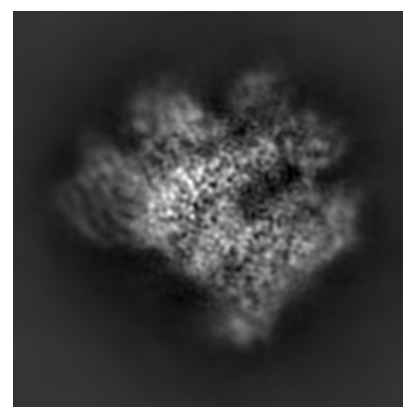
6.1.1 Primary map



X



Y

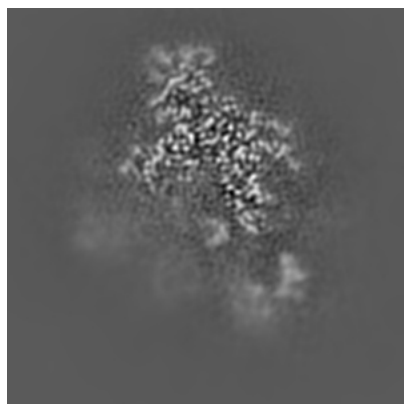


Z

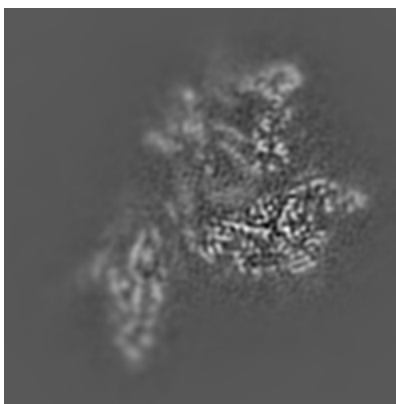
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

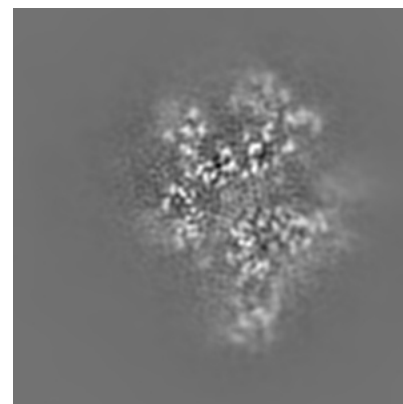
6.2.1 Primary map



X Index: 96



Y Index: 96

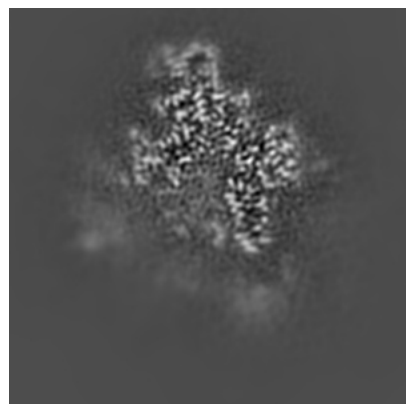


Z Index: 96

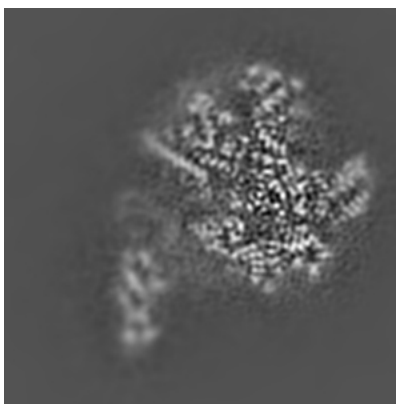
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

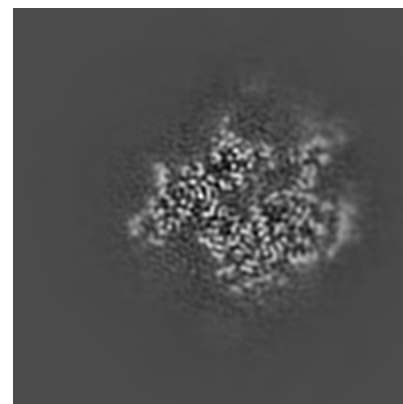
6.3.1 Primary map



X Index: 100



Y Index: 87



Z Index: 127

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

6.4 Orthogonal surface views [i](#)

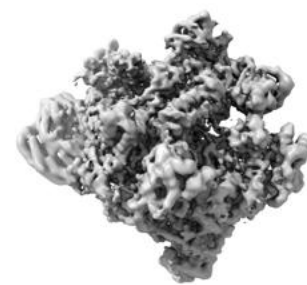
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

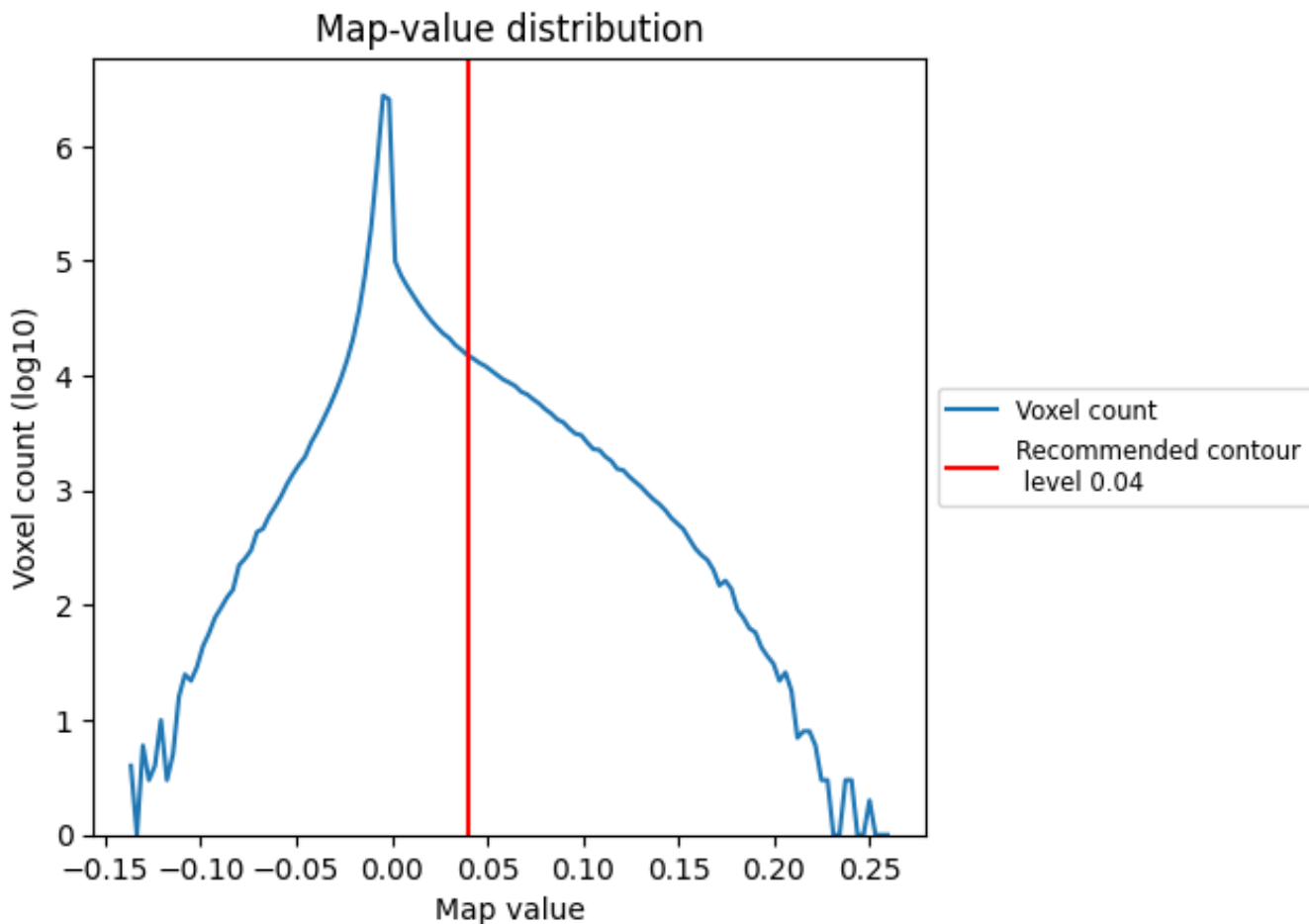
6.5 Mask visualisation

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

7 Map analysis [i](#)

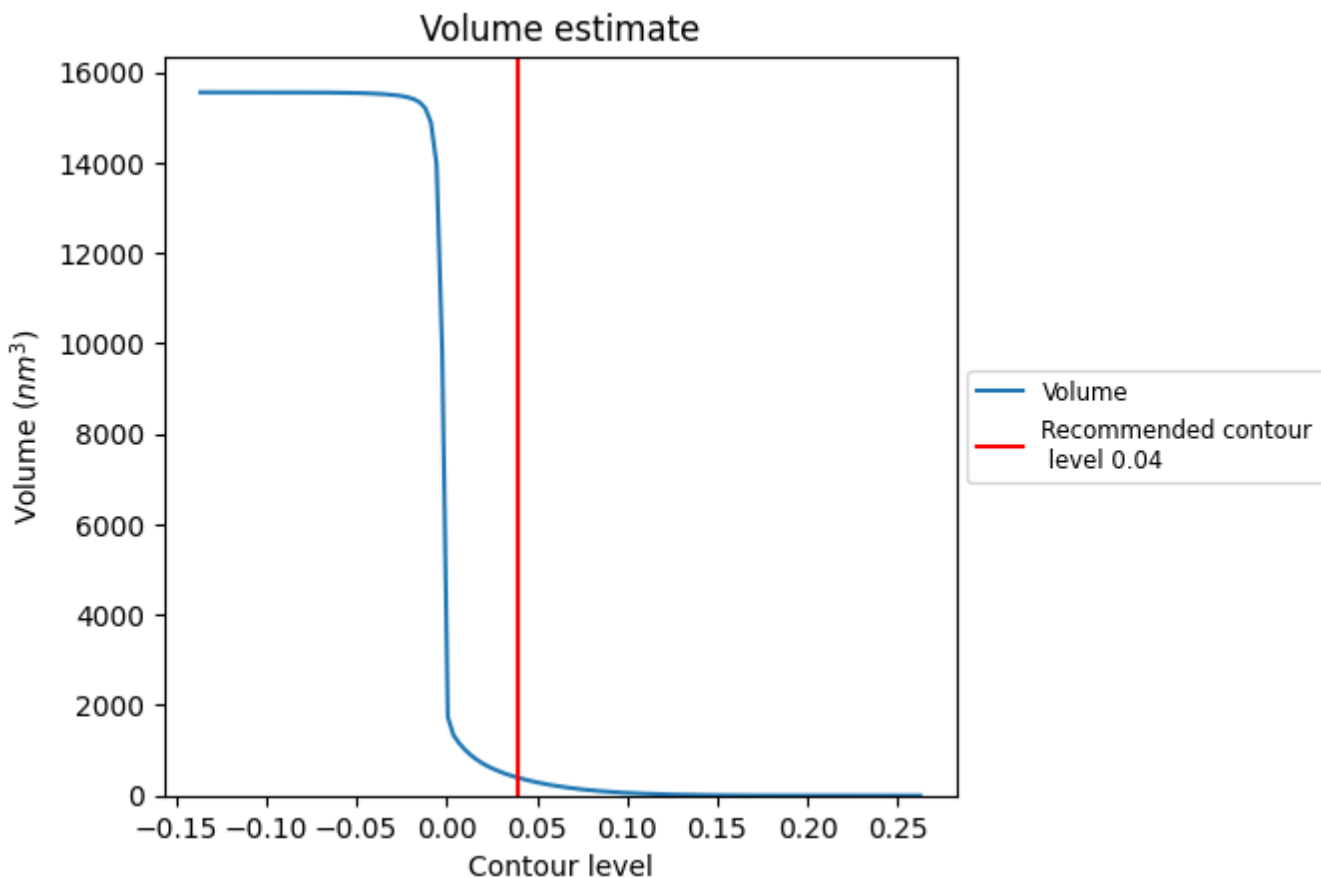
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

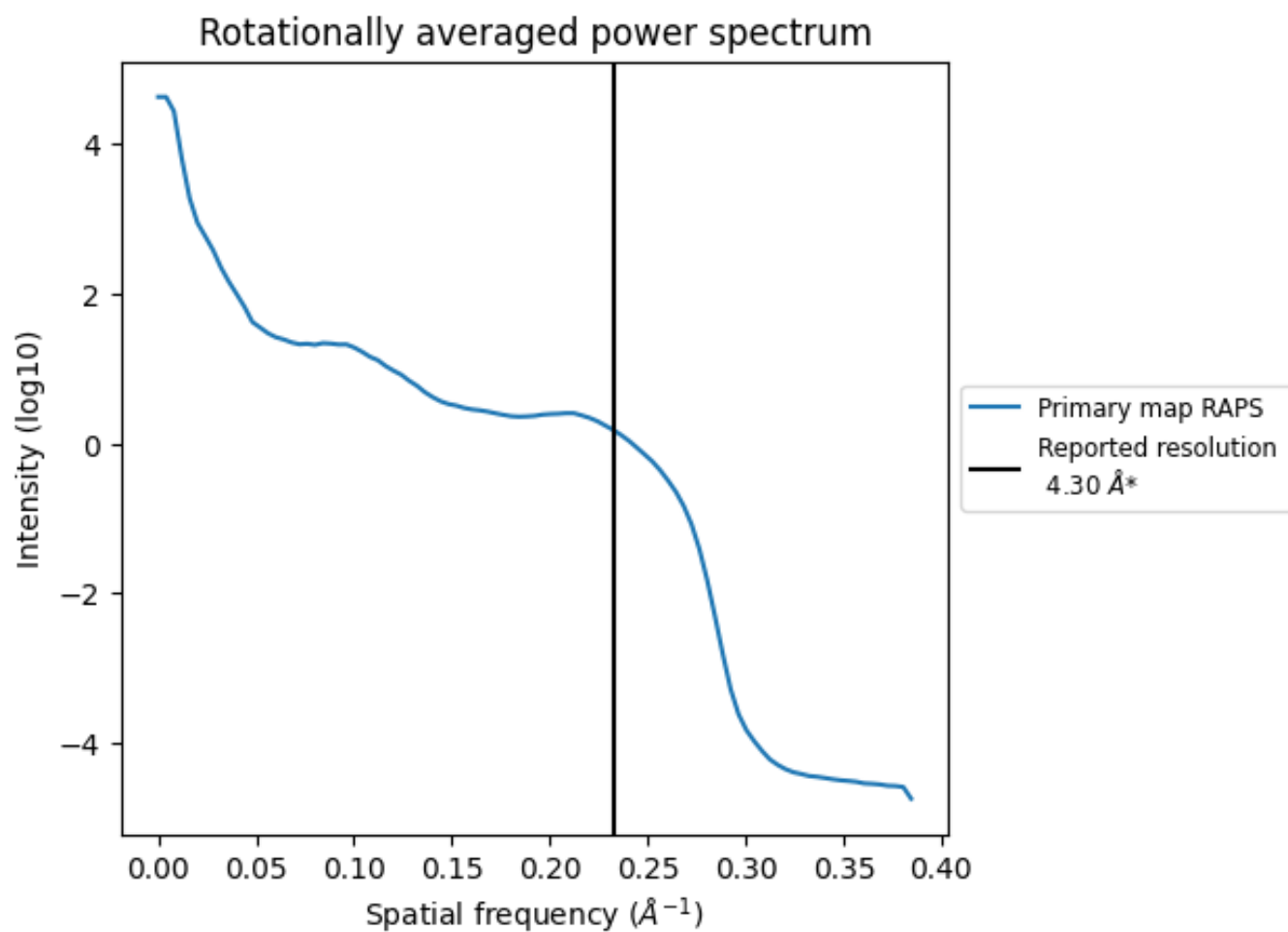
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 390 nm³; this corresponds to an approximate mass of 352 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

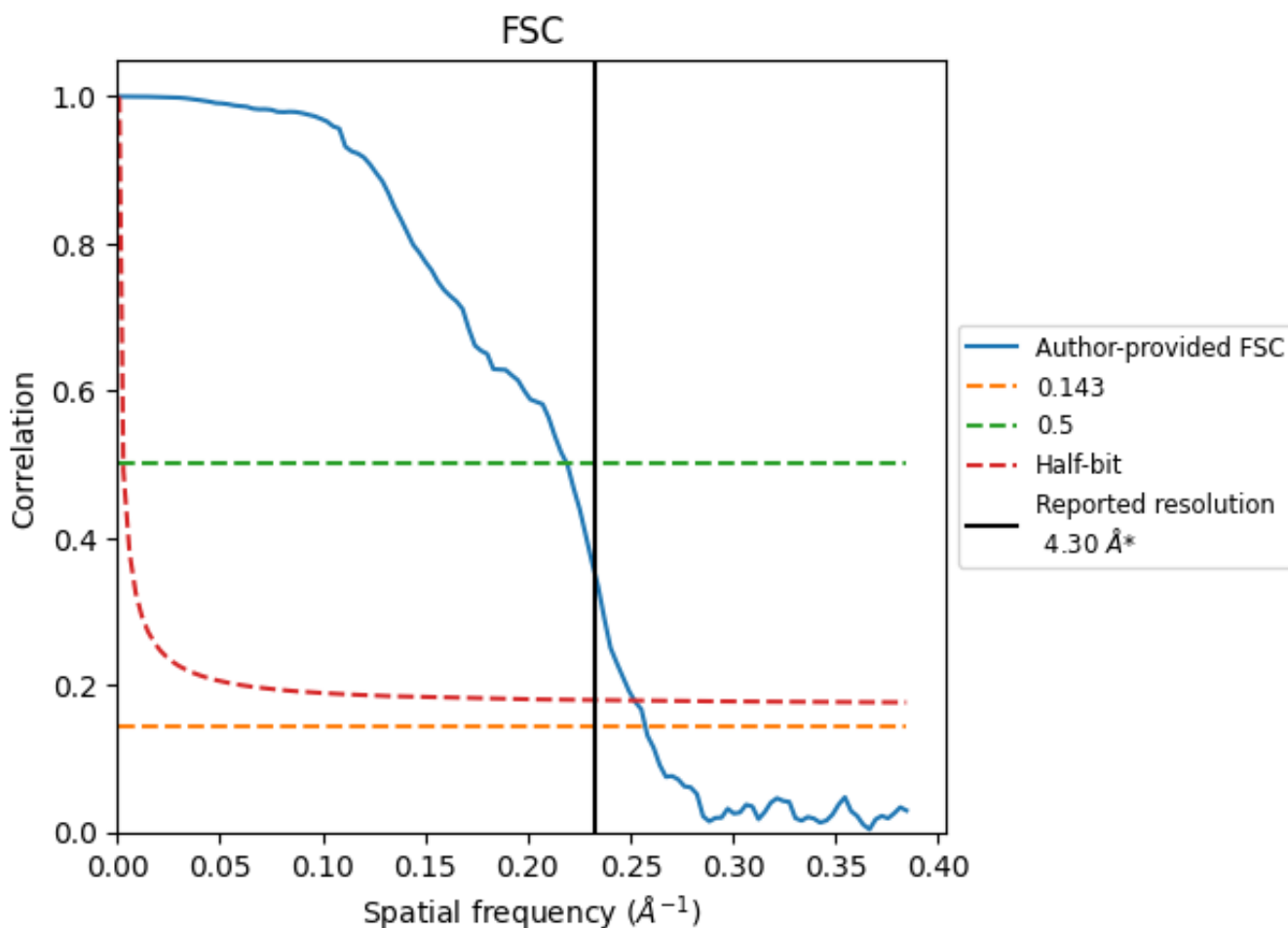


*Reported resolution corresponds to spatial frequency of 0.233\AA^{-1}

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

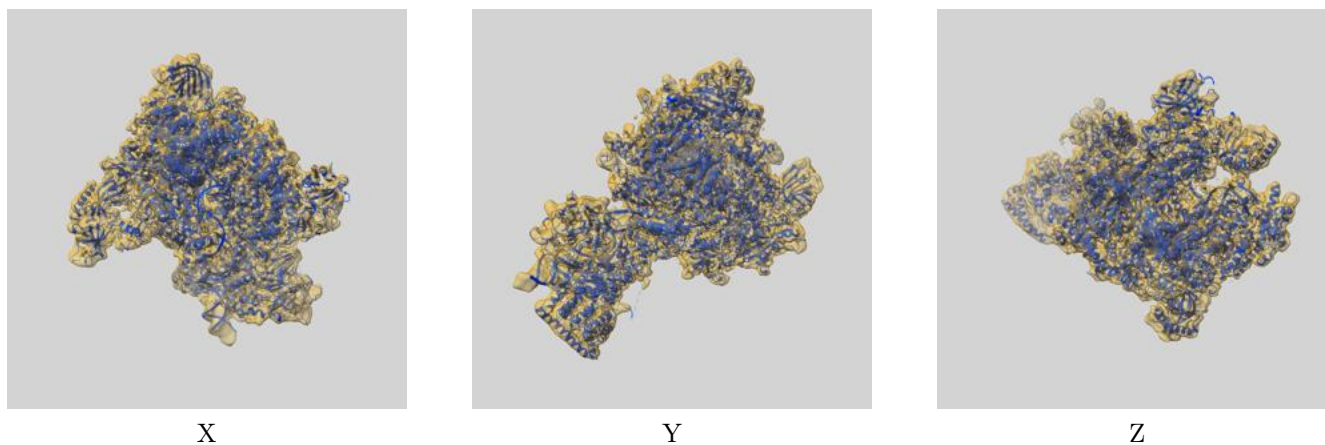
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	3.89	4.56	3.97
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

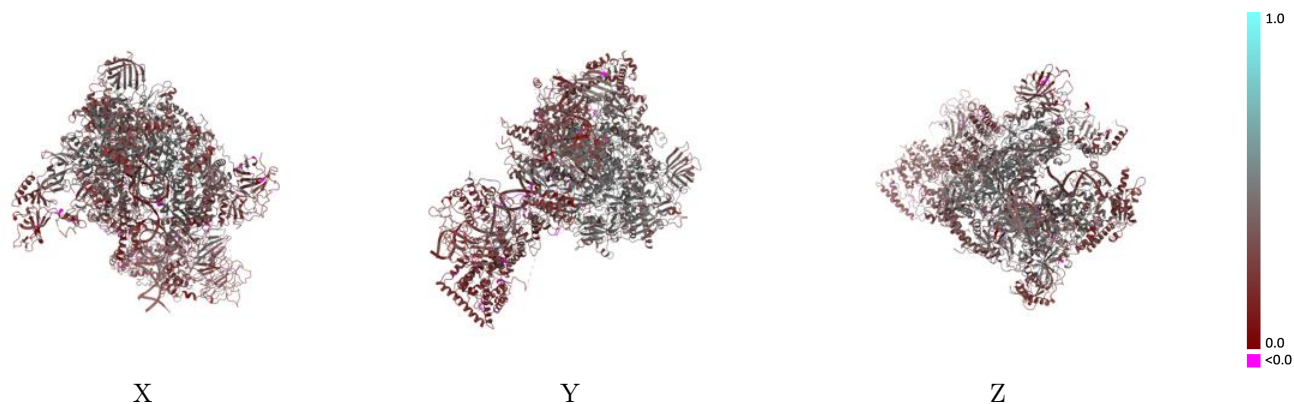
This section contains information regarding the fit between EMDB map EMD-8775 and PDB model 5W65. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



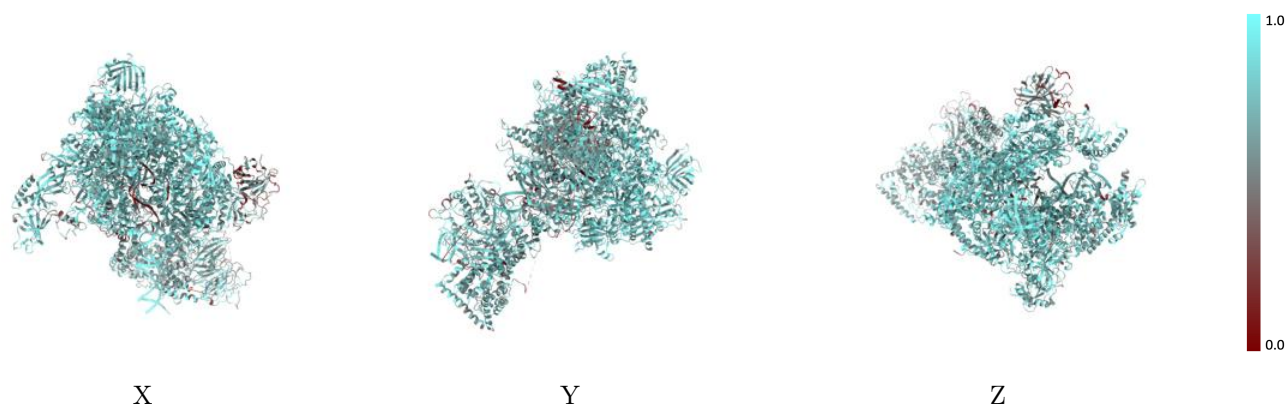
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



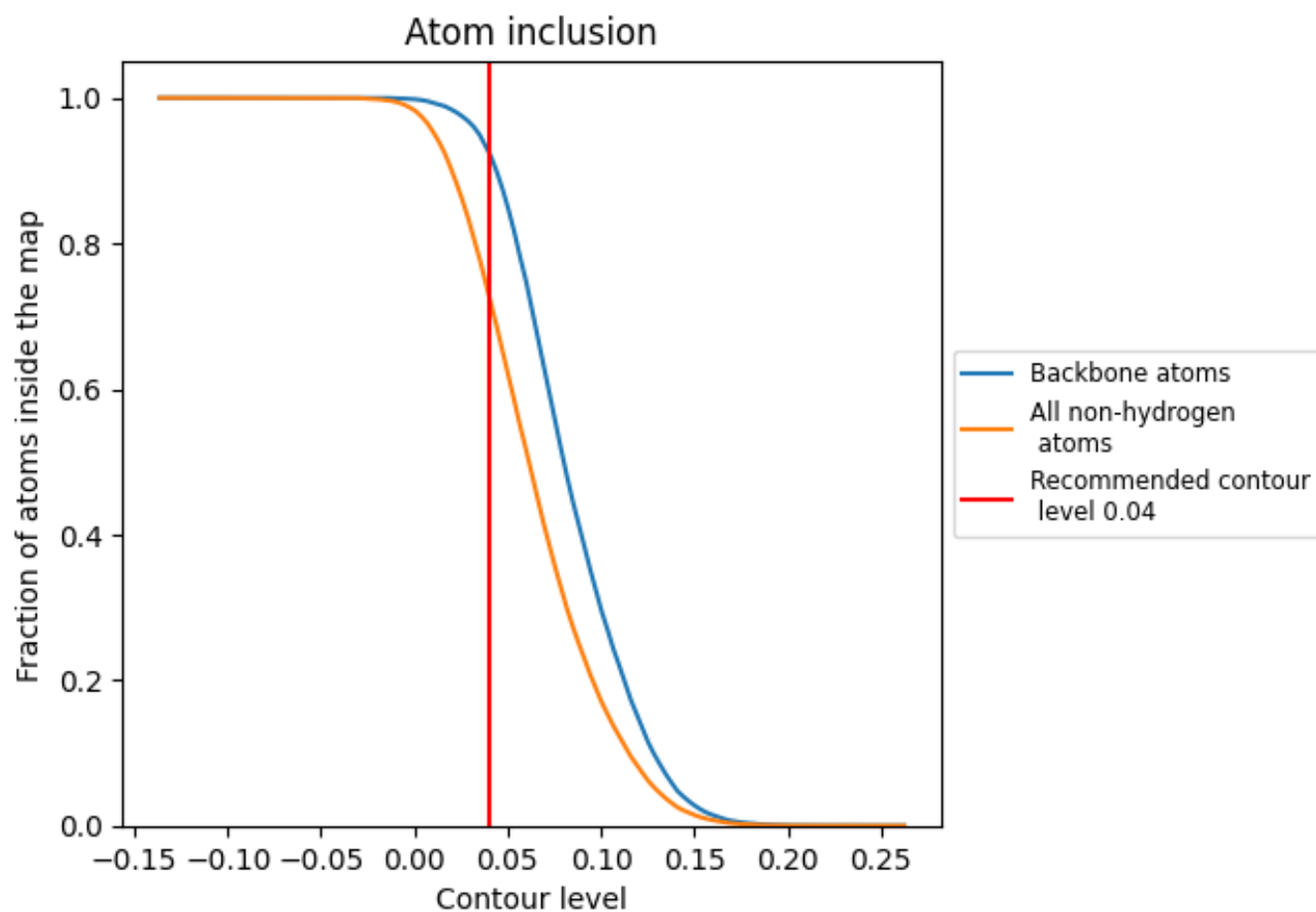
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.04).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 73% 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	 0.7279	 0.3360
A	 0.7789	 0.3860
B	 0.7959	 0.4230
C	 0.8228	 0.4070
D	 0.6868	 0.2640
E	 0.7657	 0.3280
F	 0.8206	 0.4130
G	 0.7172	 0.2790
H	 0.7946	 0.3690
I	 0.7002	 0.3270
J	 0.8442	 0.4450
K	 0.7703	 0.3980
L	 0.8092	 0.4350
M	 0.5361	 0.2680
N	 0.4703	 0.2770
O	 0.6655	 0.2350
P	 0.5810	 0.1930
Q	 0.6560	 0.2550
R	 0.1181	 0.1490
S	 0.7561	 0.2550
T	 0.6543	 0.2290

