



## wwPDB EM Validation Summary Report ⓘ

May 26, 2025 – 06:05 AM EDT

PDB ID : 6EEC / pdb\_00006eec  
EMDB ID : EMD-9041  
Title : Mycobacterium tuberculosis RNAP promoter unwinding intermediate complex  
with RbpA/CarD and AP3 promoter captured by Coralopyronin  
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.  
Deposited on : 2018-08-13  
Resolution : 3.55 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](mailto: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 : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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

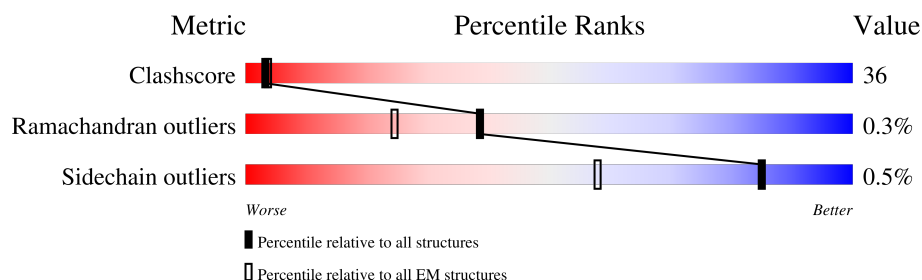
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.55 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

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  $\geq 3$ , 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	347	
1	B	347	
2	C	1179	
3	D	1326	
4	E	110	
5	F	531	
6	J	111	
7	O	90	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
8	P	90	 12% 58% 30%
9	M	162	 43% 55% ..

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29936 atoms, of which 40 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 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1759	1112	298	346	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8593	5381	1507	1666	39		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1266	Total	C	N	O	S	0	0
			9873	6184	1794	1853	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A5U053
D	0	ALA	-	expression tag	UNP A5U053

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A5U053
D	1318	HIS	-	expression tag	UNP A5U053
D	1319	HIS	-	expression tag	UNP A5U053
D	1320	HIS	-	expression tag	UNP A5U053
D	1321	HIS	-	expression tag	UNP A5U053
D	1322	HIS	-	expression tag	UNP A5U053
D	1323	HIS	-	expression tag	UNP A5U053
D	1324	HIS	-	expression tag	UNP A5U053

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	319	Total	C	N	O	S	0	0
			2518	1571	456	482	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P9WGI0
F	-1	PRO	-	expression tag	UNP P9WGI0
F	0	HIS	-	expression tag	UNP P9WGI0

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	108	Total	C	N	O	S	0	0
			881	543	168	167	3		

- Molecule 7 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	65	Total	C	N	O	P	0	0
			1336	633	243	395	65		

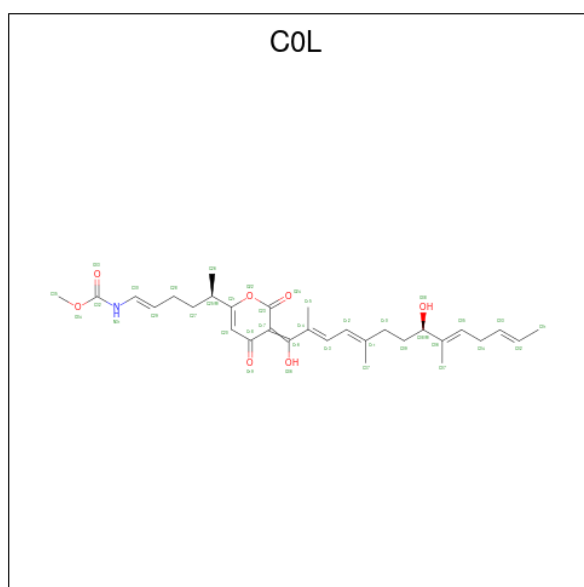
- Molecule 8 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	63	Total	C	N	O	P	0	0
			1289	610	242	374	63		

- Molecule 9 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

- Molecule 10 is methyl [(1E,5R)-5-[(3E)-3-[(2E,4E,8R,9E,12E)-1,8-dihydroxy-2,5,9-trimethyltetradeca-2,4,9,12-tetraen-1-ylidene]-2,4-dioxo-3,4-dihydro-2H-pyran-6-yl]hex-1-en-1-yl]carbamate (CCD ID: C0L) (formula: C<sub>30</sub>H<sub>41</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	H	N	O	0
			78	30	40	1	7	

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	D	1	Total	Mg	0
			1	1	



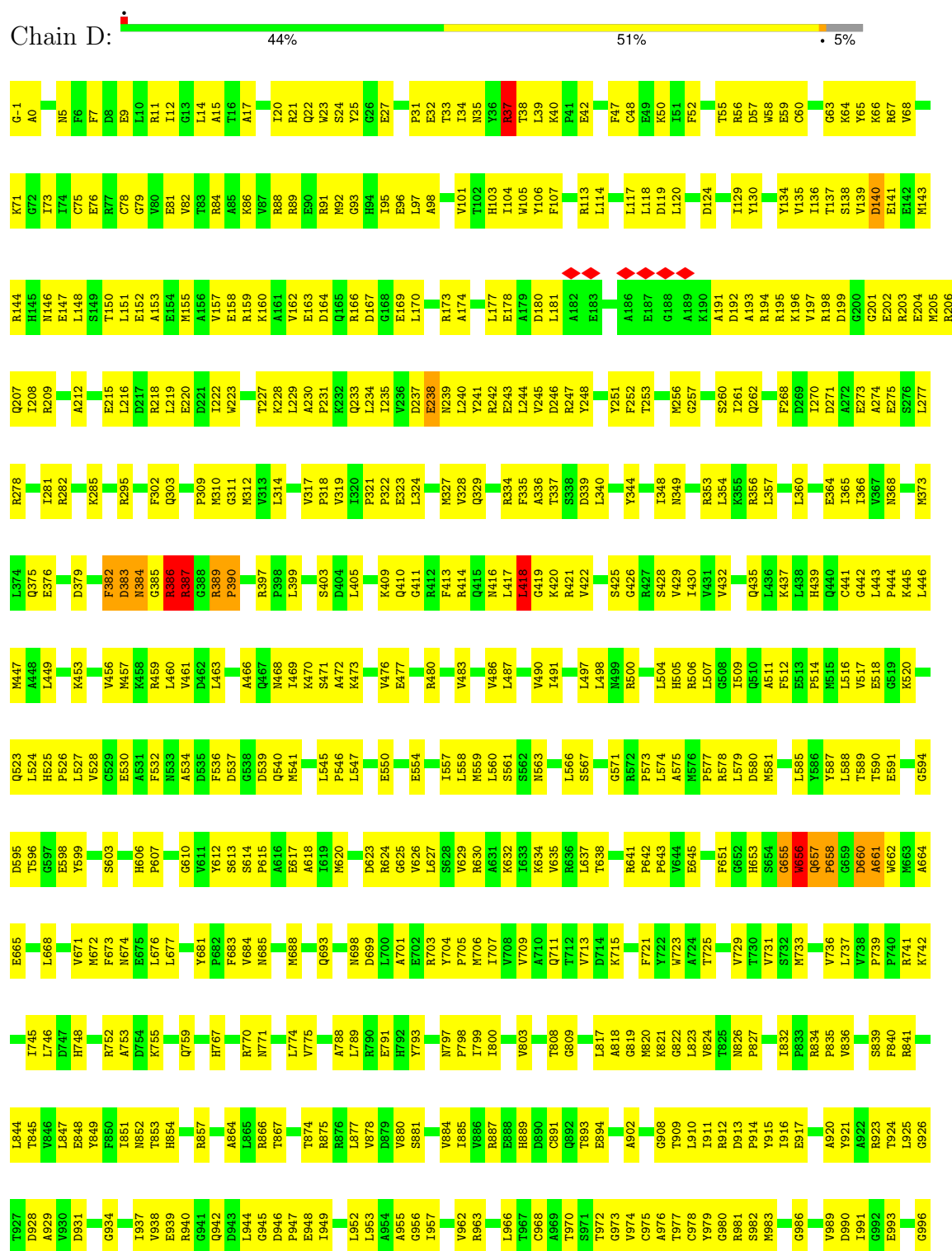


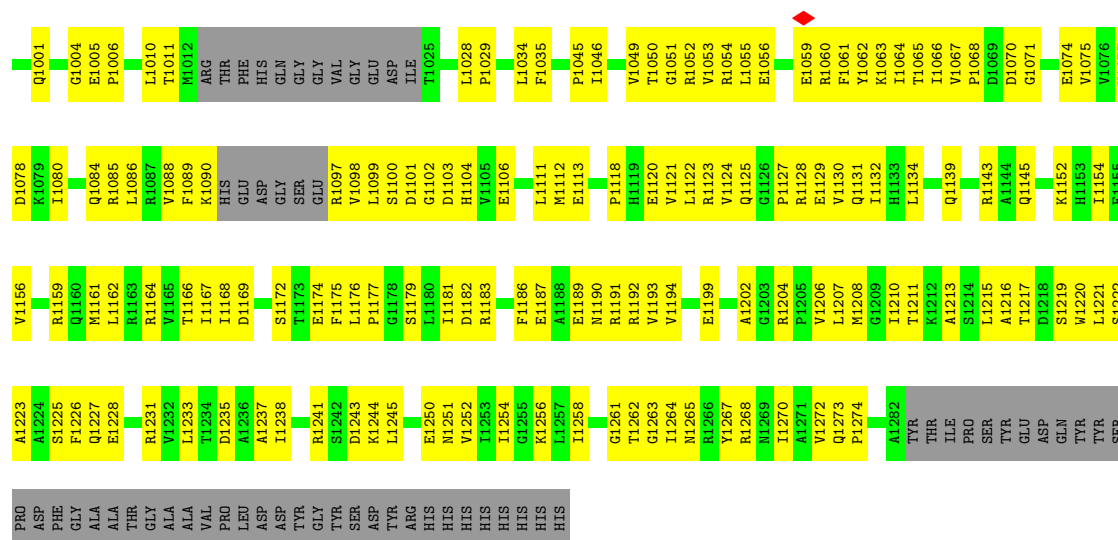
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:  44% 49% 6%

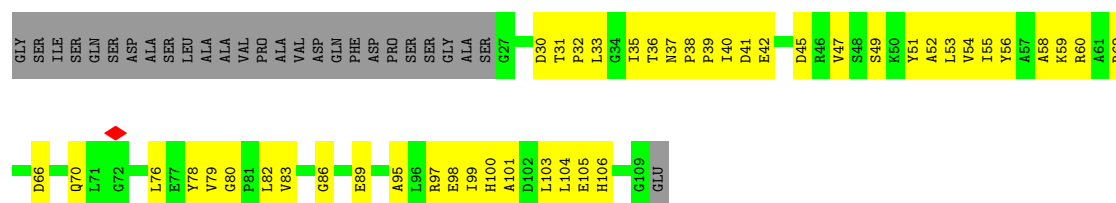
MET	ALA	ASP	SER	ARG	GLN	SER	LYS	THR	ALA	ALA	SER	PRO	SER	PRO	ASN	N30	R38	F41	A42	K43	E46	V50	G52	L53	L54	D55	S60	F61	E62	W63	L64	T65	P68	R69	W70	R71	E72	S73	E76	R77	L86	L90					
	S94	P95	I96	E97	D98		G101	S102	M103	S104	L105	S106	F107			C122	D126	M127	T128	Y129	A130	A131	P132	L133	F134	V135	E138	F139	I140	N141	N142	N143	T144	G145	E146	I147	K148	Q150	T151	V152	F153	M154	F157	P158	M159	M160	K163
	G164	T235	E297	I389	L463	D534	M611	A703	S777	B865	G933	V946	W955	A956	L959	P960	D1039	K1040	I1041	H1042	A1043	Q1063	R1067	E1070	W1074	A1075	M1076	Q1077	A1078	Y1079	D1080	A1081	A1082	G1006	T1084	E1087	L1088	I1091	K1092	S1093	D1094						
	T235	E297	I389	L463	D534	M611	A703	S777	B865	G933	V946	W955	A956	L959	P960	D1039	K1040	I1041	H1042	A1043	Q1063	R1067	E1070	W1074	A1075	M1076	Q1077	A1078	Y1079	D1080	A1081	A1082	G1006	T1084	E1087	L1088	I1091	K1092	S1093	D1094							
	T236	E298	I390	L464	D535	M612	A704	S778	B866	G934	V947	W956	A957	L960	P961	D1040	K1041	I1042	H1043	A1044	Q1064	R1068	E1071	W1075	A1076	M1077	Q1078	A1079	Y1080	D1081	A1083	G1007	T1085	E1088	L1089	I1092	K1093	S1094	D1095								
	T237	E299	I391	L465	D536	M613	A705	S779	B867	G935	V948	W957	A958	L961	P962	D1041	K1042	I1043	H1044	A1045	Q1065	R1069	E1072	W1076	A1077	M1078	Q1079	A1080	Y1081	D1082	A1084	G1008	T1086	E1089	L1090	I1093	K1094	S1095	D1096								
	T238	E300	I392	L466	D537	M614	A706	S780	B868	G936	V949	W958	A959	L962	P963	D1042	K1043	I1044	H1045	A1046	Q1066	R1070	E1073	W1077	A1078	M1079	Q1080	A1081	Y1082	D1083	A1085	G1009	T1087	E1090	L1091	I1094	K1095	S1096	D1097								
	T239	E301	I393	L467	D538	M615	A707	S781	B869	G937	V950	W959	A960	L963	P964	D1043	K1044	I1045	H1046	A1047	Q1067	R1071	E1074	W1078	A1079	M1080	Q1081	A1082	Y1083	D1084	A1086	G1010	T1088	E1091	L1092	I1095	K1096	S1097	D1098								
	T240	E302	I394	L468	D539	M616	A708	S782	B870	G938	V951	W960	A961	L964	P965	D1044	K1045	I1046	H1047	A1048	Q1068	R1072	E1075	W1079	A1080	M1081	Q1082	A1083	Y1084	D1085	A1087	G1011	T1089	E1092	L1093	I1096	K1097	S1098	D1099								
	T241	E303	I395	L469	D540	M617	A709	S783	B871	G939	V952	W961	A962	L965	P966	D1045	K1046	I1047	H1048	A1049	Q1069	R1073	E1076	W1080	A1081	M1082	Q1083	A1084	Y1085	D1086	A1088	G1012	T1090	E1093	L1094	I1097	K1098	S1099	D1100								
	T242	E304	I396	L470	D541	M618	A710	S784	B872	G940	V953	W962	A963	L966	P967	D1046	K1047	I1048	H1049	A1050	Q1070	R1074	E1077	W1081	A1082	M1083	Q1084	A1085	Y1086	D1087	A1089	G1013	T1091	E1094	L1095	I1098	K1099	S1100	D1101								
	T243	E305	I397	L471	D542	M619	A711	S785	B873	G941	V954	W963	A964	L967	P968	D1047	K1048	I1049	H1050	A1051	Q1071	R1075	E1078	W1082	A1083	M1084	Q1085	A1086	Y1087	D1088	A1090	G1014	T1092	E1095	L1096	I1100	K1101	S1101	D1102								
	T244	E306	I398	L472	D543	M620	A712	S786	B874	G942	V955	W964	A965	L968	P969	D1048	K1049	I1050	H1051	A1052	Q1072	R1076	E1079	W1083	A1084	M1085	Q1086	A1087	Y1088	D1089	A1091	G1015	T1093	E1096	L1097	I1101	K1102	S1102	D1103								
	T245	E307	I399	L473	D544	M621	A713	S787	B875	G943	V956	W965	A966	L969	P970	D1049	K1050	I1051	H1052	A1053	Q1073	R1077	E1080	W1084	A1085	M1086	Q1087	A1088	Y1089	D1090	A1092	G1016	T1094	E1097	L1098	I1102	K1103	S1103	D1104								
	T246	E308	I400	L474	D545	M622	A714	S788	B876	G944	V957	W966	A967	L970	P971	D1050	K1051	I1052	H1053	A1054	Q1074	R1078	E1081	W1085	A1086	M1087	Q1088	A1089	Y1090	D1091	A1093	G1017	T1095	E1098	L1099	I1103	K1104	S1104	D1105								
	T247	E309	I401	L475	D546	M623	A715	S789	B877	G945	V958	W967	A968	L971	P972	D1051	K1052	I1053	H1054	A1055	Q1075	R1079	E1082	W1086	A1087	M1088	Q1089	A1090	Y1091	D1092	A1094	G1018	T1096	E1099	L1100	I1104	K1105	S1105	D1106								
	T248	E310	I402	L476	D547	M624	A716	S790	B878	G946	V959	W968	A969	L972	P973	D1052	K1053	I1054	H1055	A1056	Q1076	R1080	E1083	W1087	A1088	M1089	Q1090	A1091	Y1092	D1093	A1095	G1019	T1097	E1100	L1101	I1105	K1106	S1106	D1107								
	T249	E311	I403	L477	D548	M625	A717	S791	B879	G947	V960	W969	A970	L973	P974	D1053	K1054	I1055	H1056	A1057	Q1077	R1081	E1084	W1088	A1089	M1090	Q1091	A1092	Y1093	D1094	A1096	G1020	T1098	E1101	L1102	I1106	K1107	S1107	D1108								
	T250	E312	I404	L478	D549	M626	A718	S792	B880	G948	V961	W970	A971	L974	P975	D1054	K1055	I1056	H1057	A1058	Q1078	R1082	E1085	W1089	A1090	M1091	Q1092	A1093	Y1094	D1095	A1097	G1021	T1099	E1102	L1103	I1107	K1108	S1108	D1109								
	T251	E313	I405	L479	D550	M627	A719	S793	B881	G949	V962	W971	A972	L975	P976	D1055	K1056	I1057	H1058	A1059	Q1079	R1083	E1086	W1090	A1091	M1092	Q1093	A1094	Y1095	D1096	A1098	G1022	T1100	E1103	L1104	I1108	K1109	S1109	D1110								
	T252	E314	I406	L480	D551	M628	A720	S794	B882	G950	V963	W972	A973	L976	P977	D1056	K1057	I1058	H1059	A1060	Q1080	R1084	E1087	W1091	A1092	M1093	Q1094	A1095	Y1096	D1097	A1099	G1023	T1101	E1104	L1105	I1109	K1110	S1110	D1111								
	T253	E315	I407	L481	D552	M629	A721	S795	B883	G951	V964	W973	A974	L977	P978	D1057	K1058	I1059	H1060	A1061	Q1081	R1085	E1088	W1092	A1093	M1094	Q1095	A1096	Y1097	D1098	A1100	G1024	T1102	E1105	L1106	I1110	K1111	S1111	D1112								
	T254	E316	I408	L482	D553	M630	A722	S796	B884	G952	V965	W974	A975	L978	P979	D1058	K1059	I1060	H1061	A1062	Q1082	R1086	E1089	W1093	A1094	M1095	Q1096	A1097	Y1098	D1099	A1101	G1025	T1103	E1106	L1107	I1111	K1112	S1112	D1113								
	T255	E317	I409	L483	D554	M631	A723	S797	B885	G953	V966	W975	A976	L979	P980	D1059	K1060	I1061	H1062	A1063	Q1083	R1087	E1090	W1094	A1095	M1096	Q1097	A1098	Y1099	D1100	A1102	G1026	T1104	E1107	L1108	I1112	K1113	S1113	D1114								
	T256	E318	I410	L484	D555	M632	A724	S798	B886	G954	V967	W976	A977	L980	P981	D1060	K1061	I1062	H1063	A1064	Q1084	R1088	E1091	W1095	A1096	M1097	Q1098	A1099	Y1100	D1101	A1103	G1027	T1105	E1108	L1109	I1113	K1114	S1114	D1115								
	T257	E319	I411	L485	D556	M633	A725	S799	B887	G955	V968	W977	A978	L981	P982	D1061	K1062	I1063	H1064	A1065	Q1085	R1089	E1092	W1096	A1097	M1098	Q1099	A1100	Y1101	D1102	A1104	G1028	T1106	E1109	L1110	I1114	K1115	S1115	D1116								
	T258	E320	I412	L486	D557	M634	A726	S800	B888	G956	V969	W978	A979	L982	P983	D1062	K1063	I1064	H1065	A1066	Q1086	R1090	E1093	W1097	A1098	M1099	Q1100	A1101	Y1102	D1103	A1105	G1029	T1107	E1110	L1111	I1115	K1116	S1116	D1117								
	T259	E321	I413	L487	D558	M635	A727	S801	B889	G957	V970	W979	A980	L983	P984	D1063	K1064	I1065	H1066	A1067	Q1087	R1091	E1094	W1098	A1099	M1100	Q1101	A1102	Y1103	D1104	A1106	G1030	T1108	E1111	L1112	I1116	K1117	S1117	D1118								
	T260	E322	I414	L488	D559	M636	A728	S802	B890	G958	V971	W980	A981	L984	P985	D1064	K1065	I1066	H1067	A1068	Q1088	R1092	E1095	W1099	A1100	M1101	Q1102	A1103	Y1104	D1105	A1107	G1031	T1109	E1112	L1113	I1117	K1118	S1118	D1119								
	T261	E323	I415	L489	D560	M637	A729	S803	B891	G959	V972	W981	A982	L985	P986	D1065	K1066	I1067	H1068	A1069	Q1089	R1093	E1096	W1100	A1101	M1102	Q1103	A1104	Y1105	D1106	A1108	G1032	T1110	E1113	L1114	I1118	K1119	S1119	D1120								
	T262	E324	I416	L490	D561	M638	A730	S804	B892	G960	V973	W982	A983	L986	P987	D1066	K1067	I1068	H1069	A1070	Q1090	R1094	E1097	W1101	A1102	M1103	Q1104	A1105	Y1106	D1107	A1109	G1033	T1111	E1114	L1115	I1119	K1120	S1120	D1121								
	T263	E325	I417	L491	D562	M639	A731	S805	B893	G961	V974	W983	A984	L987	P988	D1067	K1068	I1069	H1070	A1071	Q1091	R1095	E1098	W1102	A1103	M1104	Q1105	A1106	Y1107	D1108	A1110	G1034	T1112	E1115	L1116	I1120	K1121	S1121	D1122								
	T264	E326	I418	L492	D563	M640	A732	S806	B894	G962	V975	W984	A985	L988	P989	D1068	K1069	I1070	H1071	A1072	Q1092	R1096	E1099	W1103	A1104	M1105	Q1106	A1107	Y1108	D1109	A1111	G1035	T1113	E1116	L1117	I1121	K1122	S1122	D1123								
	T265	E327	I419	L493	D564	M641	A733	S807	B895	G963	V976	W985	A986	L989	P990	D1069	K1070	I1071	H1072	A1073	Q1093	R1097	E1100	W1104	A1105	M1106	Q1107	A1108	Y1109	D1110	A1112	G1036	T1114	E1117	L1118	I1122	K1123	S1123	D1124								
	T266	E328	I420	L494	D565	M642	A734	S808	B896	G964	V977	W986	A987	L990	P991	D1070	K1071	I1072	H1073	A1074	Q1094	R1098	E1101	W1105	A1106	M1107	Q1108	A1109	Y1110	D1111	A1113	G1037	T1115	E1118	L1119	I1123	K1124	S1124	D1125								
	T267	E329	I421	L495	D566	M643	A735	S809	B897	G965	V978	W987	A988	L991	P992	D1071	K1072	I1073	H1074	A1075	Q10																										

- Molecule 3: DNA-directed RNA polymerase subunit beta'

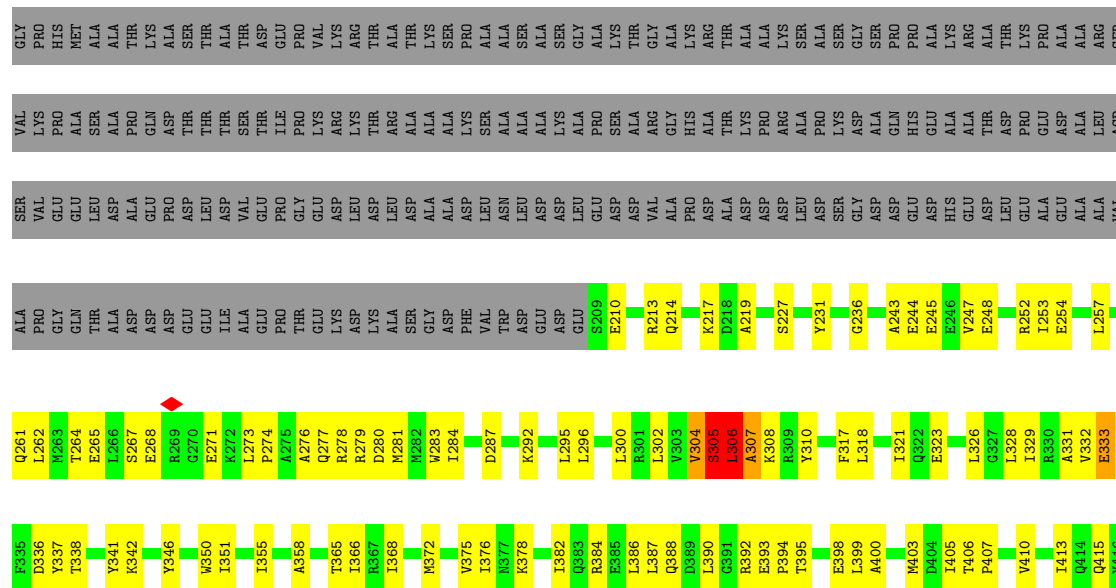


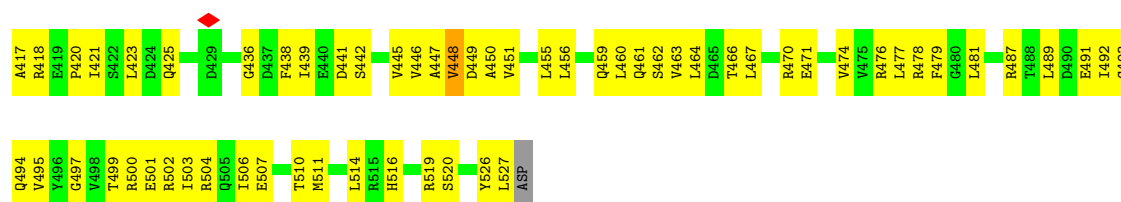


• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor SigA

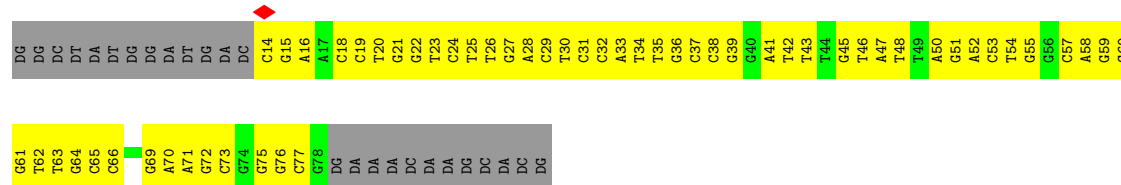
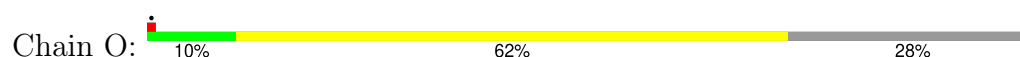




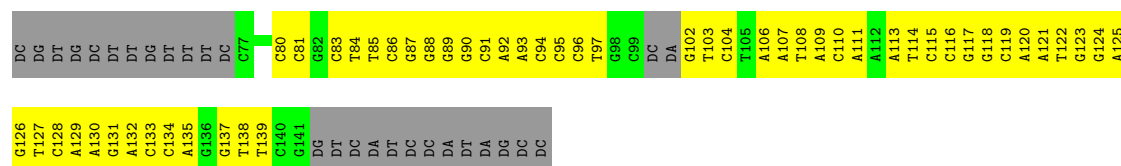
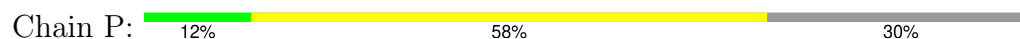
• Molecule 6: RNA polymerase-binding protein RbpA



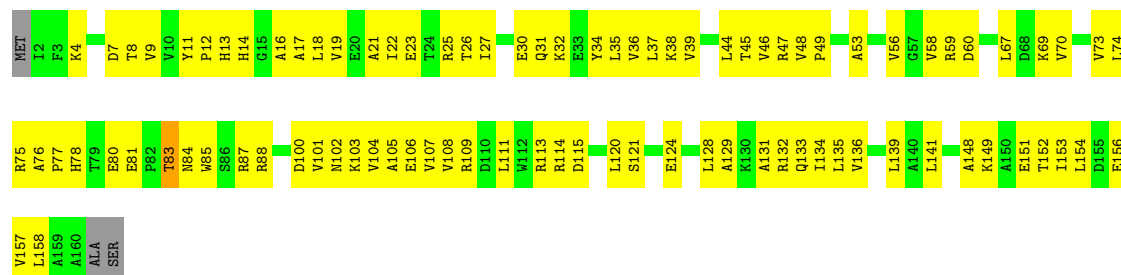
• Molecule 7: DNA (65-MER)



• Molecule 8: DNA (63-MER)



• Molecule 9: RNA polymerase-binding transcription factor CarD



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	69.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.111	Depositor
Minimum map value	-1.642	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	325.0, 325.0, 325.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, C0L, MG

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	0/1742	0.55	0/2370
1	B	0.39	0/1786	0.54	0/2435
2	C	0.57	7/8751 (0.1%)	0.67	13/11869 (0.1%)
3	D	0.63	24/10037 (0.2%)	0.65	16/13570 (0.1%)
4	E	0.37	0/662	0.51	0/901
5	F	0.55	6/2549 (0.2%)	0.63	3/3438 (0.1%)
6	J	0.32	0/897	0.62	2/1210 (0.2%)
7	O	0.35	0/1497	0.46	0/2310
8	P	0.32	0/1445	0.42	0/2224
9	M	0.29	0/1257	0.49	0/1700
All	All	0.54	37/30623 (0.1%)	0.61	34/42027 (0.1%)

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	656	TRP	CA-C	-8.86	1.41	1.52
3	D	389	ARG	CA-C	-8.74	1.43	1.52
3	D	661	ALA	CA-C	-8.66	1.41	1.52
5	F	305	SER	CA-C	-8.57	1.41	1.52
3	D	387	ARG	CA-C	-8.35	1.42	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	306	LEU	CA-C-N	-10.51	103.71	120.63
5	F	306	LEU	C-N-CA	-10.51	103.71	120.63
2	C	307	ASP	N-CA-C	8.87	122.75	110.06
2	C	288	THR	N-CA-C	-8.46	93.21	108.02
2	C	281	LEU	N-CA-C	-8.40	102.21	111.36

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	1716	0	1756	120	0
1	B	1759	0	1783	146	0
2	C	8593	0	8517	721	0
3	D	9873	0	9938	772	0
4	E	649	0	645	55	0
5	F	2518	0	2540	186	0
6	J	881	0	861	63	0
7	O	1336	0	732	119	0
8	P	1289	0	706	88	0
9	M	1241	0	1259	111	0
10	C	38	40	0	1	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
All	All	29896	40	28737	2135	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 36.

The worst 5 of 2135 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)
2:C:281:LEU:CD2	2:C:295:LEU:HD21	1.62	1.30
2:C:271:ASP:O	2:C:275:LEU:HD12	1.25	1.27
2:C:1067:ARG:CZ	3:D:418:LEU:CD2	2.13	1.25
2:C:278:TYR:CE1	2:C:292:ALA:HB2	1.73	1.23
2:C:1067:ARG:NH1	3:D:418:LEU:CD2	2.04	1.21

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	223/347 (64%)	197 (88%)	26 (12%)	0	100	100
1	B	235/347 (68%)	194 (83%)	41 (17%)	0	100	100
2	C	1109/1179 (94%)	937 (84%)	168 (15%)	4 (0%)	30	62
3	D	1260/1326 (95%)	1141 (91%)	115 (9%)	4 (0%)	37	67
4	E	81/110 (74%)	76 (94%)	5 (6%)	0	100	100
5	F	317/531 (60%)	296 (93%)	20 (6%)	1 (0%)	37	67
6	J	106/111 (96%)	87 (82%)	19 (18%)	0	100	100
9	M	157/162 (97%)	144 (92%)	12 (8%)	1 (1%)	22	56
All	All	3488/4113 (85%)	3072 (88%)	406 (12%)	10 (0%)	38	67

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	418	LEU
3	D	658	PRO
2	C	274	LEU
3	D	653	HIS
2	C	53	LEU

### 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	194/297 (65%)	194 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	194/297 (65%)	194 (100%)	0	100	100
2	C	935/997 (94%)	927 (99%)	8 (1%)	75	87
3	D	1042/1103 (94%)	1036 (99%)	6 (1%)	84	92
4	E	69/89 (78%)	69 (100%)	0	100	100
5	F	264/429 (62%)	262 (99%)	2 (1%)	79	89
6	J	93/97 (96%)	93 (100%)	0	100	100
9	M	129/131 (98%)	129 (100%)	0	100	100
All	All	2920/3440 (85%)	2904 (100%)	16 (0%)	85	93

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	305	SER
3	D	656	TRP
3	D	37	ARG
3	D	418	LEU
2	C	466	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	657	GLN
3	D	797	ASN
9	M	102	ASN
3	D	674	ASN
3	D	748	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
10	C0L	C	1201	-	37,38,38	2.65	13 (35%)	37,49,49	2.80	12 (32%)

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
10	C0L	C	1201	-	-	20/38/57/57	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	C0L	O24-C23	8.85	1.39	1.21
10	C	1201	C0L	O19-C18	5.65	1.39	1.24
10	C	1201	C0L	C17-C16	4.82	1.50	1.39
10	C	1201	C0L	O36-C16	-4.54	1.18	1.33
10	C	1201	C0L	C17-C18	-4.20	1.35	1.45

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	C0L	O34-C32-N31	9.68	120.28	109.15
10	C	1201	C0L	C35-O34-C32	-6.27	108.38	115.63
10	C	1201	C0L	O22-C21-C25	5.53	116.21	111.35
10	C	1201	C0L	O36-C16-C17	4.94	128.90	120.03

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	C0L	C23-C17-C18	4.42	121.98	119.41

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

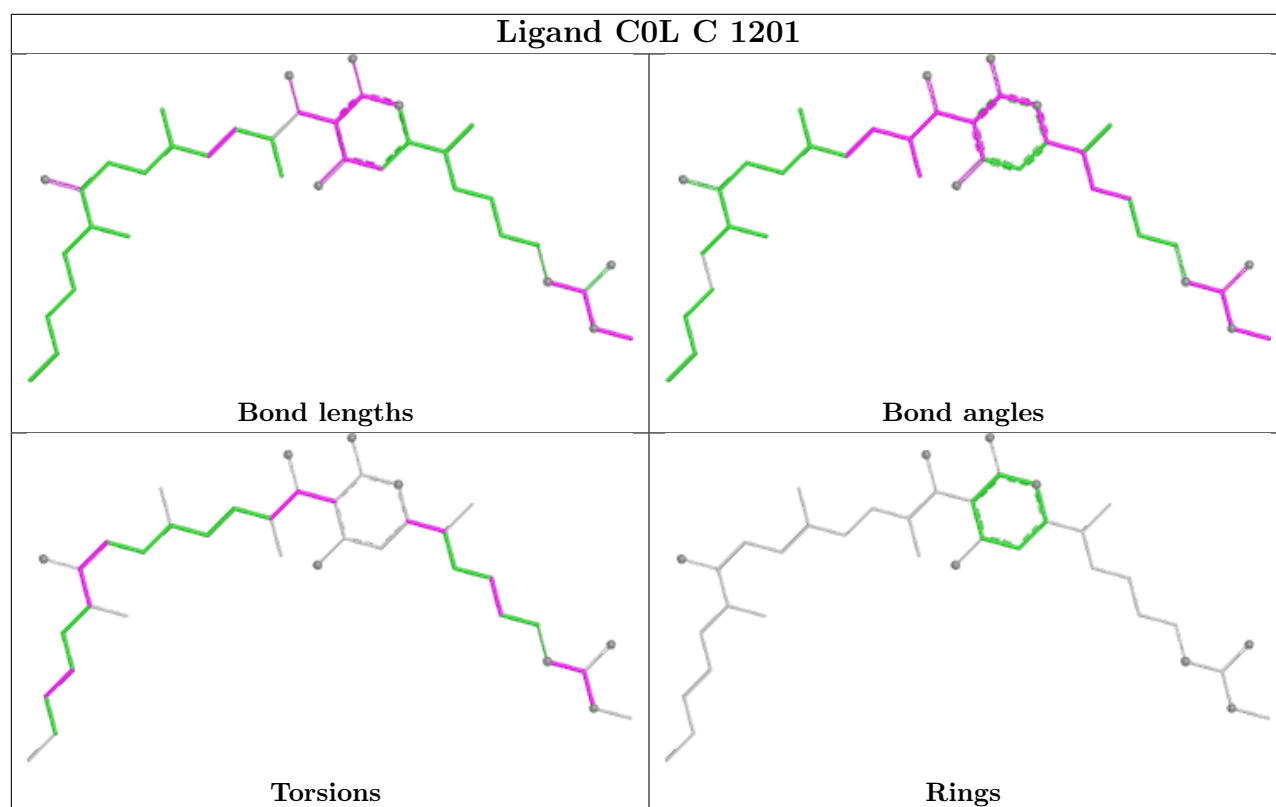
Mol	Chain	Res	Type	Atoms
10	C	1201	C0L	C13-C14-C16-O36
10	C	1201	C0L	C15-C14-C16-O36
10	C	1201	C0L	C14-C16-C17-C18
10	C	1201	C0L	C14-C16-C17-C23
10	C	1201	C0L	O36-C16-C17-C18

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	C0L	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

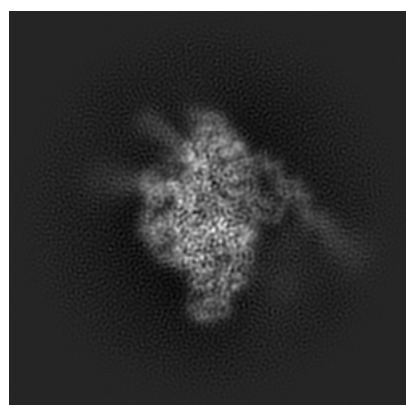
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9041. These allow visual inspection of the internal detail of the map and identification of artifacts.

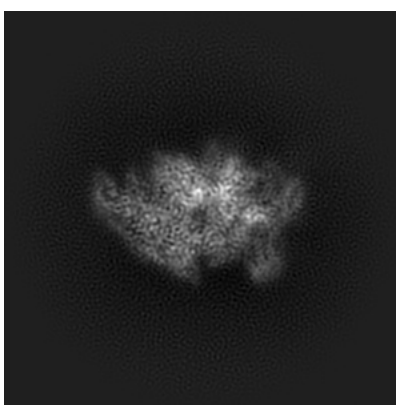
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

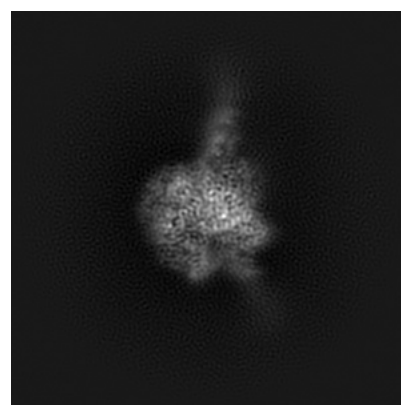
#### 6.1.1 Primary map



X



Y

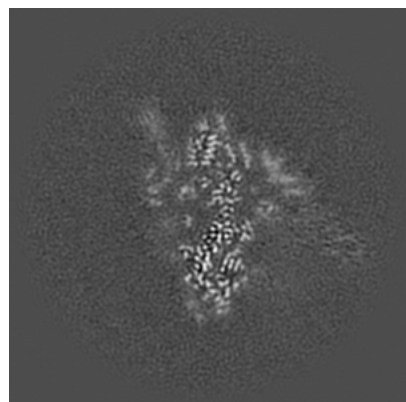


Z

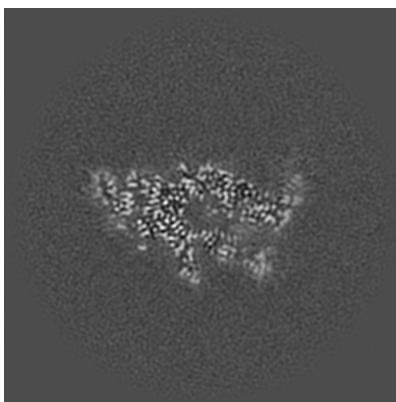
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

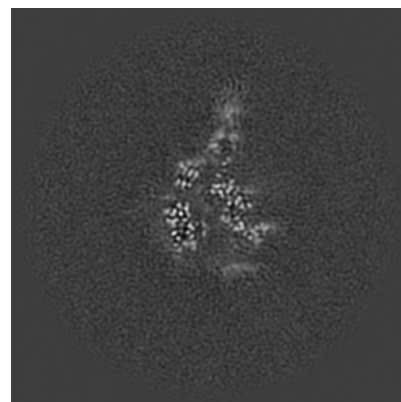
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

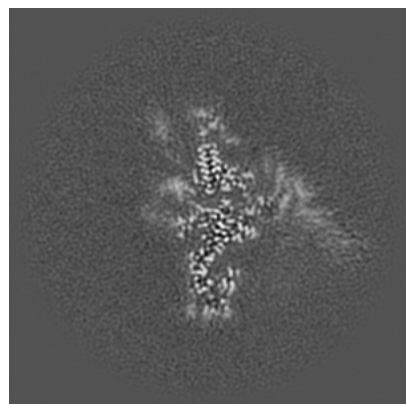


Z Index: 125

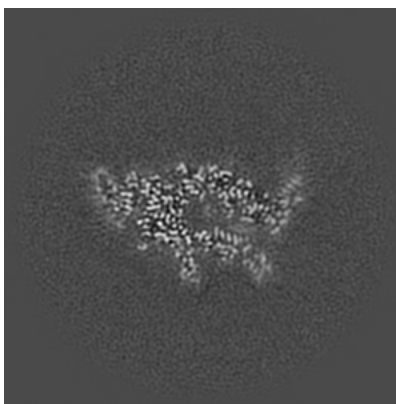
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

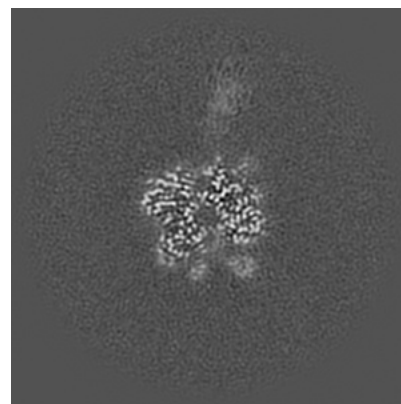
### 6.3.1 Primary map



X Index: 132



Y Index: 124

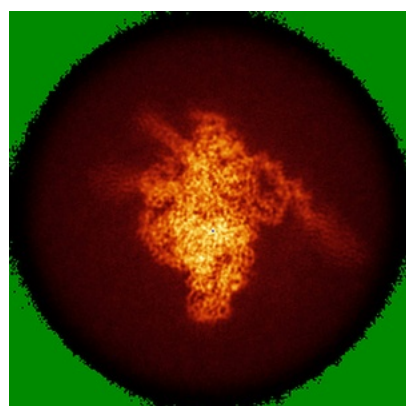


Z Index: 113

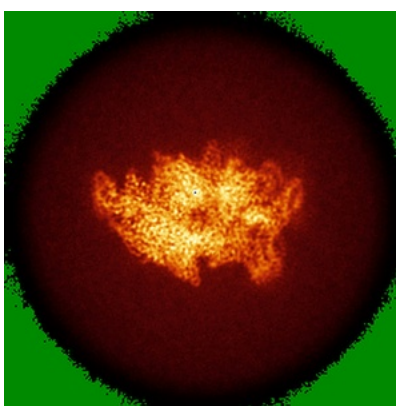
The images above show the largest variance slices of the map in three orthogonal directions.

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

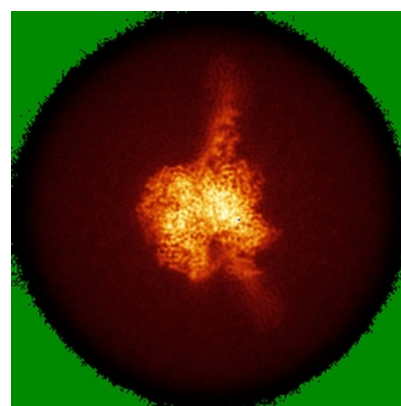
### 6.4.1 Primary map



X



Y

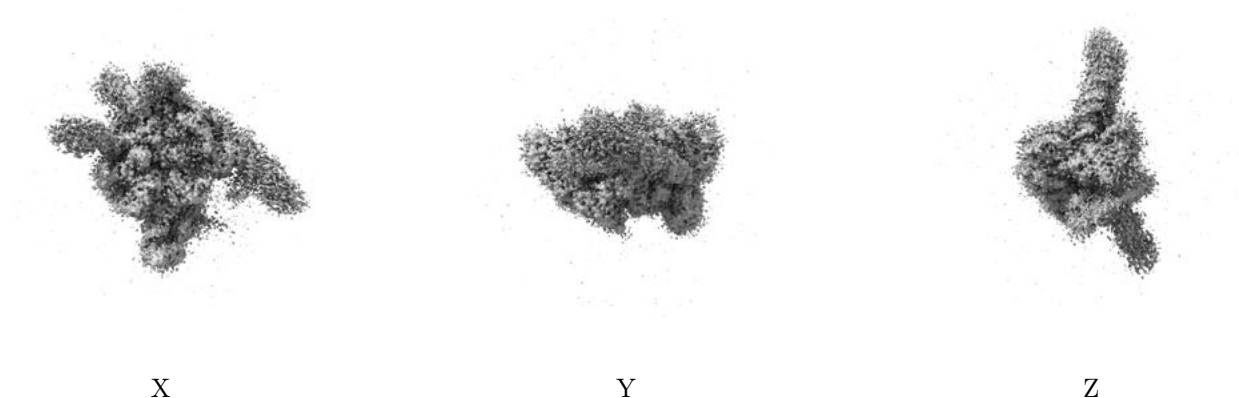


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

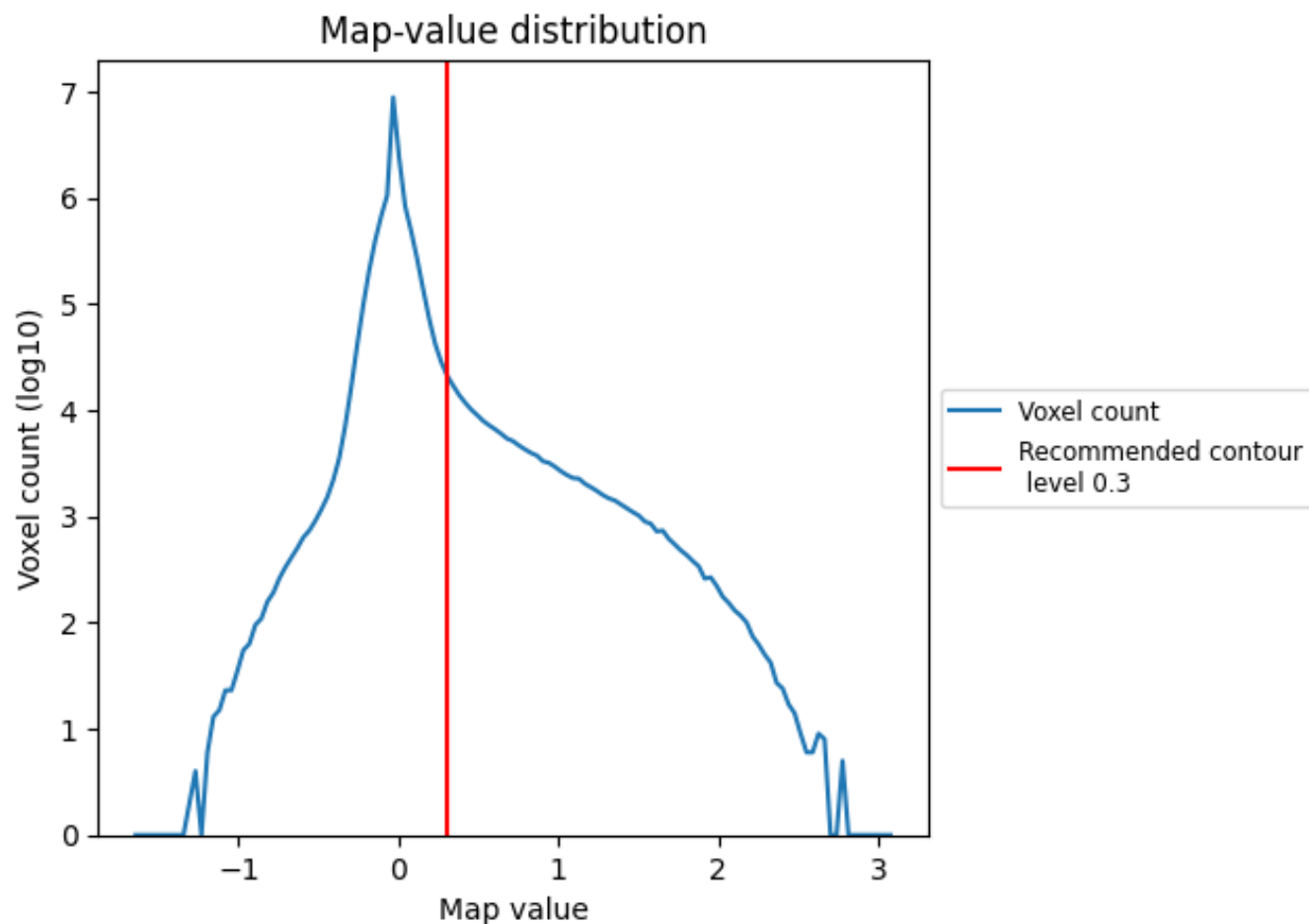
## 6.6 Mask visualisation [i](#)

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.

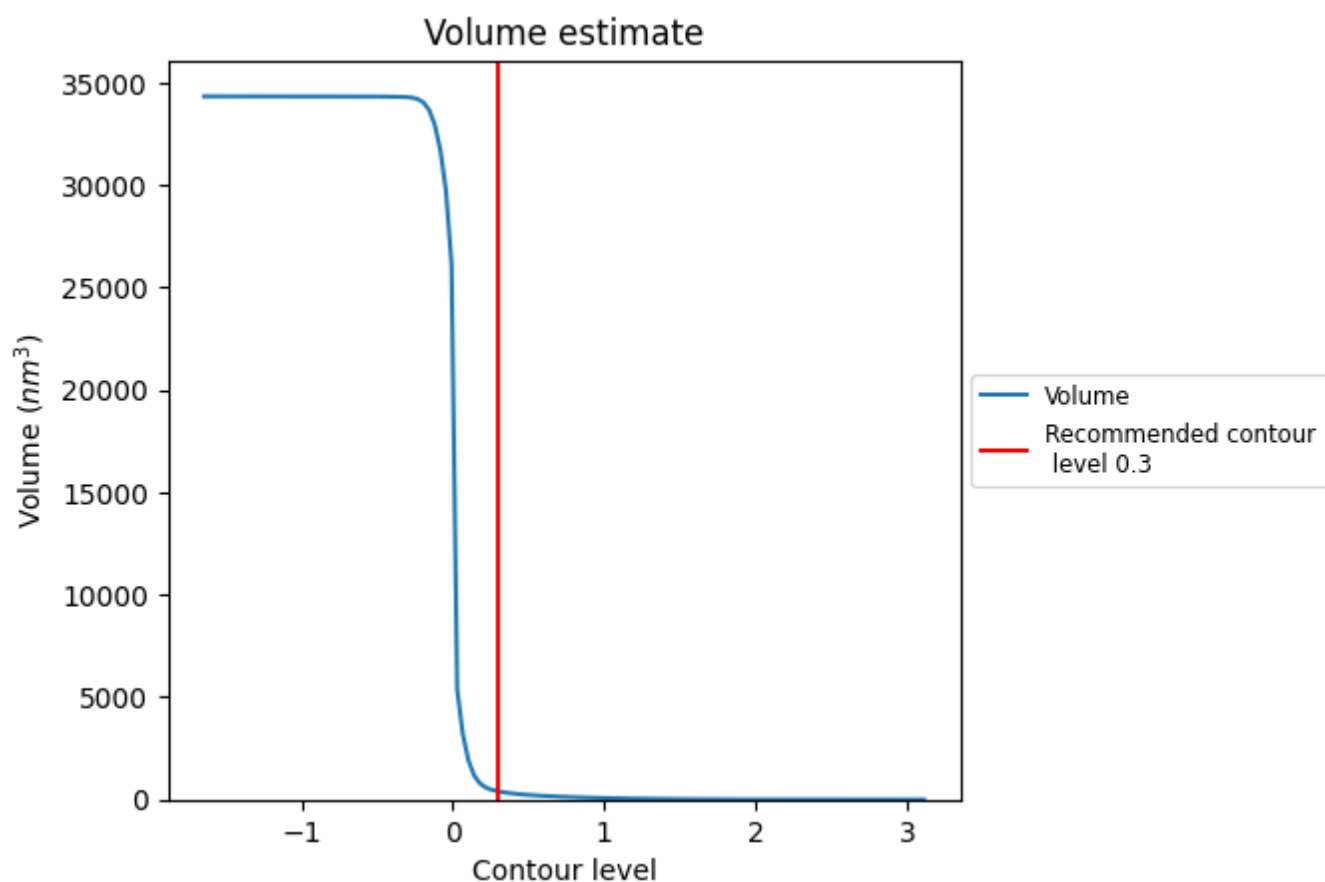
### 7.1 Map-value distribution [i](#)



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.



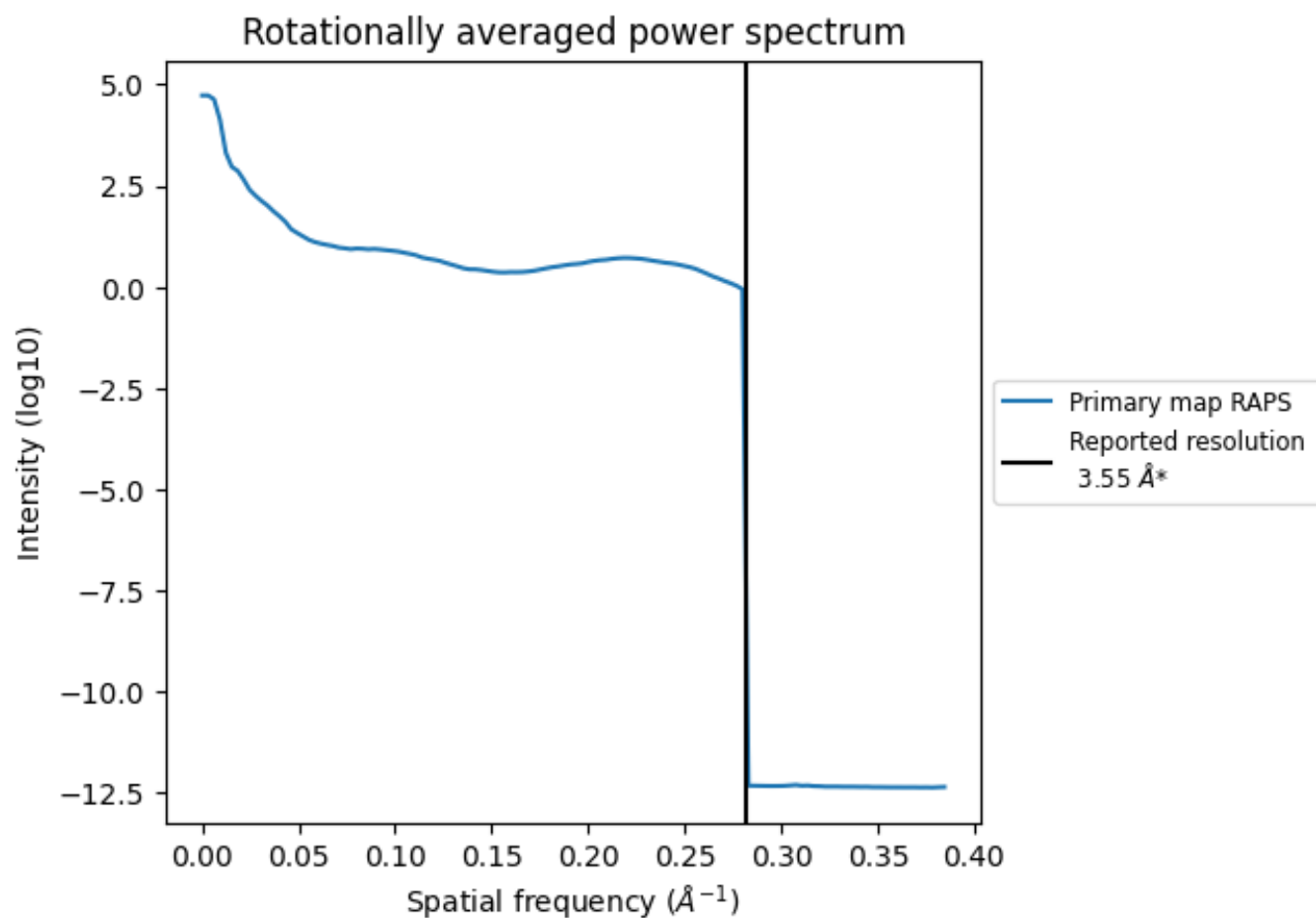
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm<sup>3</sup>; this corresponds to an approximate mass of 362 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 0.282 Å<sup>-1</sup>

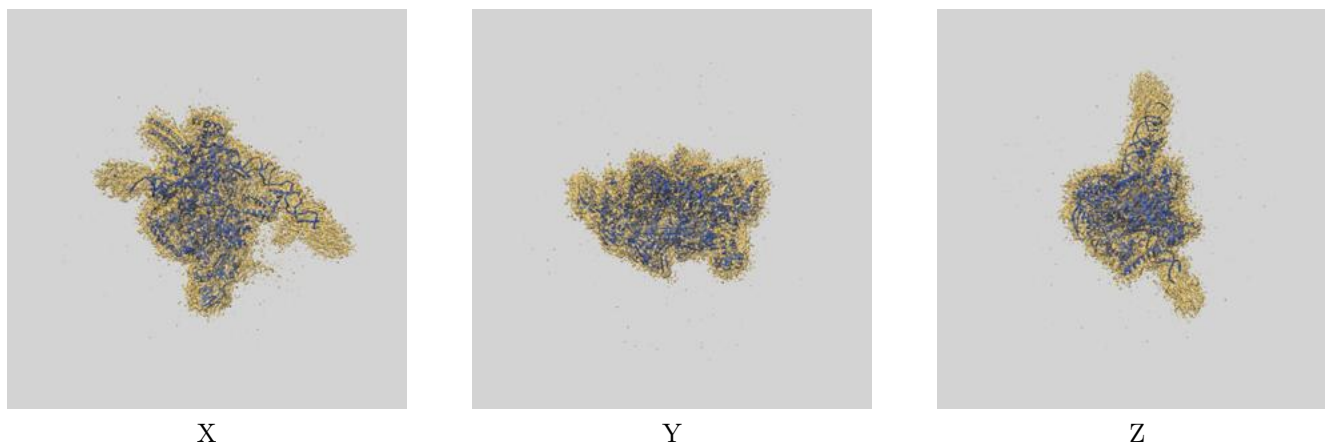
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9041 and PDB model 6EEC. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



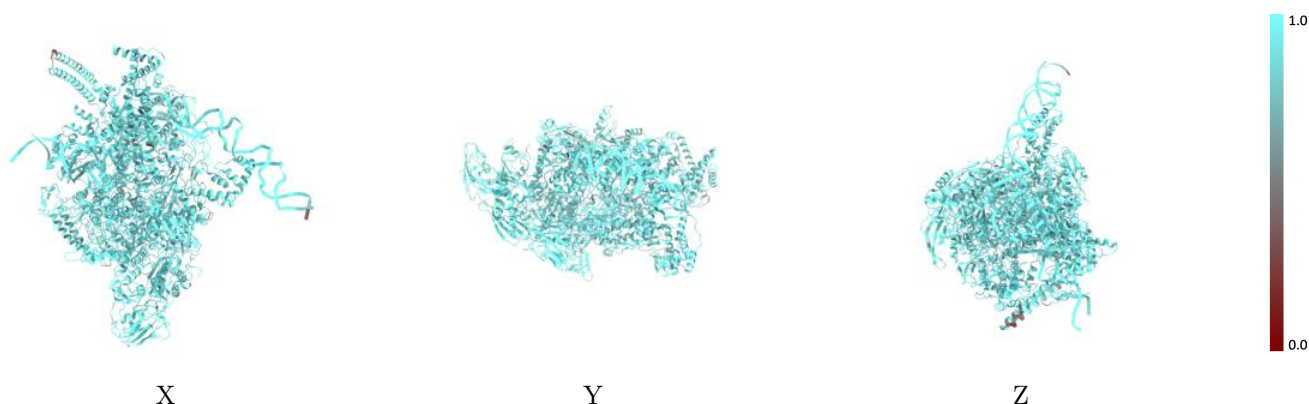
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



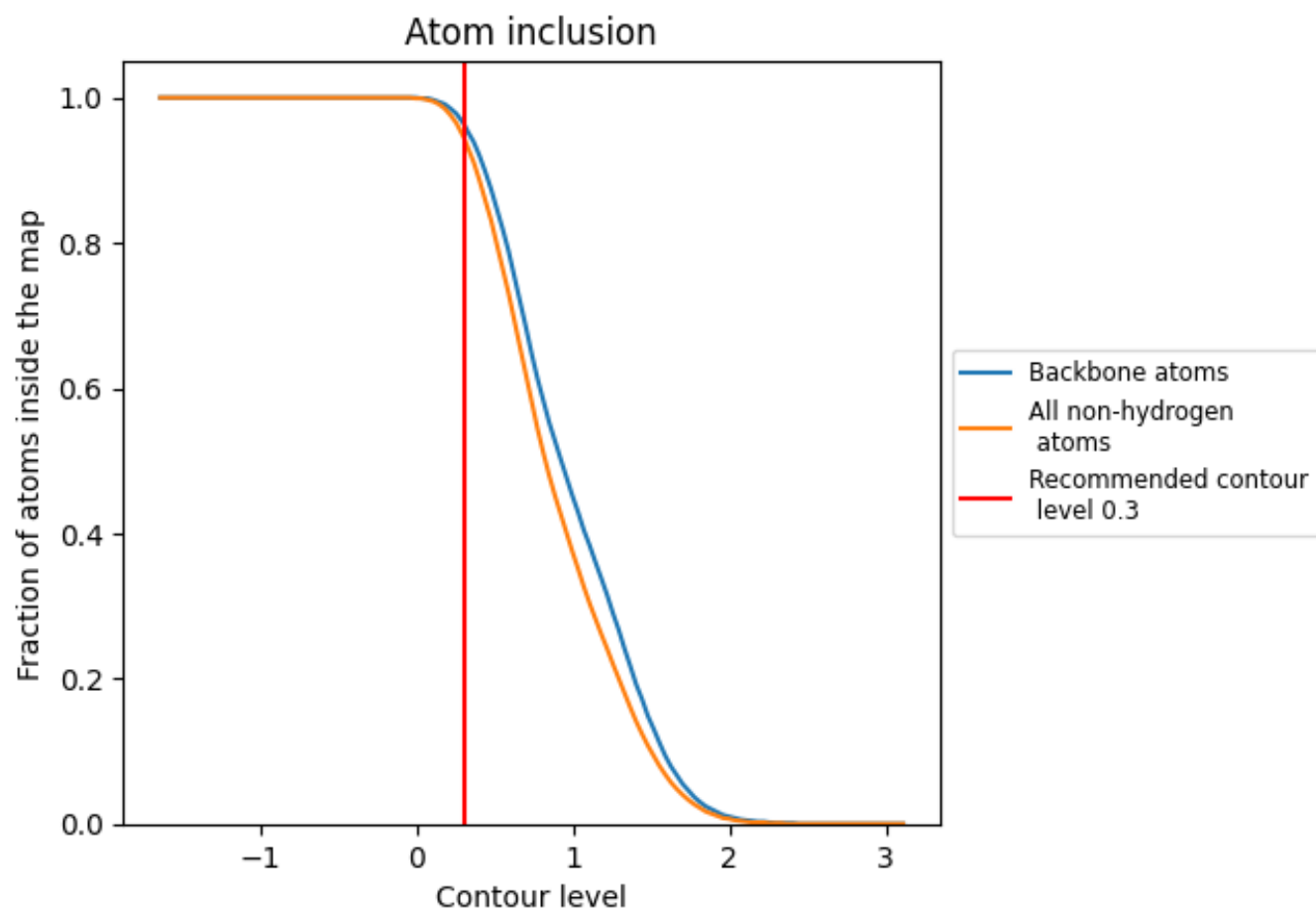
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9450	<div></div> 0.4480
A	<div></div> 0.9670	<div></div> 0.4860
B	<div></div> 0.9500	<div></div> 0.4650
C	<div></div> 0.9520	<div></div> 0.4860
D	<div></div> 0.9440	<div></div> 0.4640
E	<div></div> 0.9020	<div></div> 0.4470
F	<div></div> 0.9310	<div></div> 0.4170
J	<div></div> 0.9390	<div></div> 0.4170
M	<div></div> 0.9160	<div></div> 0.3740
O	<div></div> 0.9510	<div></div> 0.3070
P	<div></div> 0.9660	<div></div> 0.3020

