



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 08:46 AM EST

PDB ID : 6CNF
EMDB ID : EMD-7533
Title : Yeast RNA polymerase III elongation complex
Authors : Han, Y.; He, Y.
Deposited on : 2018-03-08
Resolution : 4.50 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:

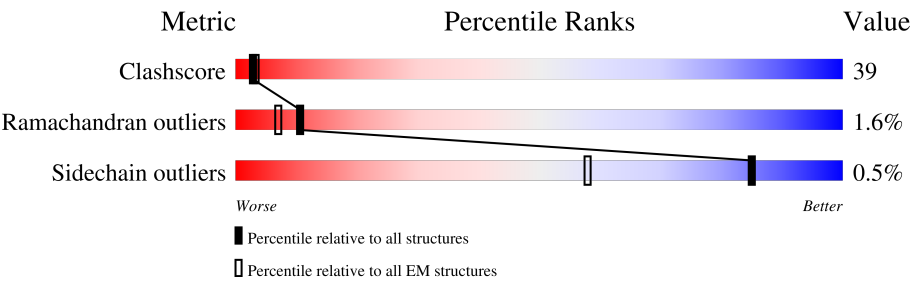
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 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

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	1460	<div><div>39%</div><div>57%</div><div>..</div></div>
2	B	1149	<div><div>37%</div><div>58%</div><div>..</div></div>
3	C	335	<div><div>41%</div><div>57%</div><div>.</div></div>
4	D	161	<div><div>30%</div><div>43%</div><div>26%</div></div>
5	E	215	<div><div>43%</div><div>57%</div></div>
6	F	155	<div><div>24%</div><div>28%</div><div>46%</div></div>
7	G	212	<div><div>6%</div><div>27%</div><div>57%</div><div>13%</div></div>
8	H	146	<div><div>36%</div><div>59%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	R	736	
19	S	594	
20	X	79	
21	Y	79	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 47675 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1428	Total	C	N	O	S	0	0
			11159	7029	1972	2099	59		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	184	Total	C	N	O	S	0	0
			1484	972	239	267	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	277	Total	C	N	O	S	0	0
			2242	1438	368	425	11		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	54	Total	C	N	O	0	0
			368	238	64	66		

- Molecule 18 is a protein called Transcription factor IIIB 70 kDa subunit,TATA-box-binding protein,Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	522	Total	C	N	O	S	0	0
			4131	2621	733	757	20		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	383	ALA	-	linker	UNP P29056
R	384	MET	-	linker	UNP P29056
R	385	PRO	-	linker	UNP P29056
R	386	TRP	-	linker	UNP P29056
R	567	GLY	-	linker	UNP P13393
R	568	SER	-	linker	UNP P13393
R	569	GLY	-	linker	UNP P13393
R	570	SER	-	linker	UNP P13393
R	571	GLY	-	linker	UNP P13393

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Chain	Residue	Modelled	Actual	Comment	Reference
R	572	SER	-	linker	UNP P13393
R	573	GLY	-	linker	UNP P13393
R	574	SER	-	linker	UNP P13393
R	575	GLY	-	linker	UNP P13393
R	576	SER	-	linker	UNP P13393
R	577	GLY	-	linker	UNP P13393
R	578	SER	CYS	engineered mutation	UNP P29056

- Molecule 19 is a protein called Transcription factor TFIIB component B'',Transcription factor TFIIB component B'',Transcription factor TFIIB component B'',Transcription factor TFIIB component B'',Transcription factor TFIIB component B''.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	217	Total	C	N	O	S	0	0
			1649	1035	286	321	7		

- Molecule 20 is a DNA chain called DNA (79-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	47	Total	C	N	O	P	0	0
			959	463	164	286	46		

- Molecule 21 is a DNA chain called DNA (79-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	57	Total	C	N	O	P	0	0
			1169	560	220	333	56		

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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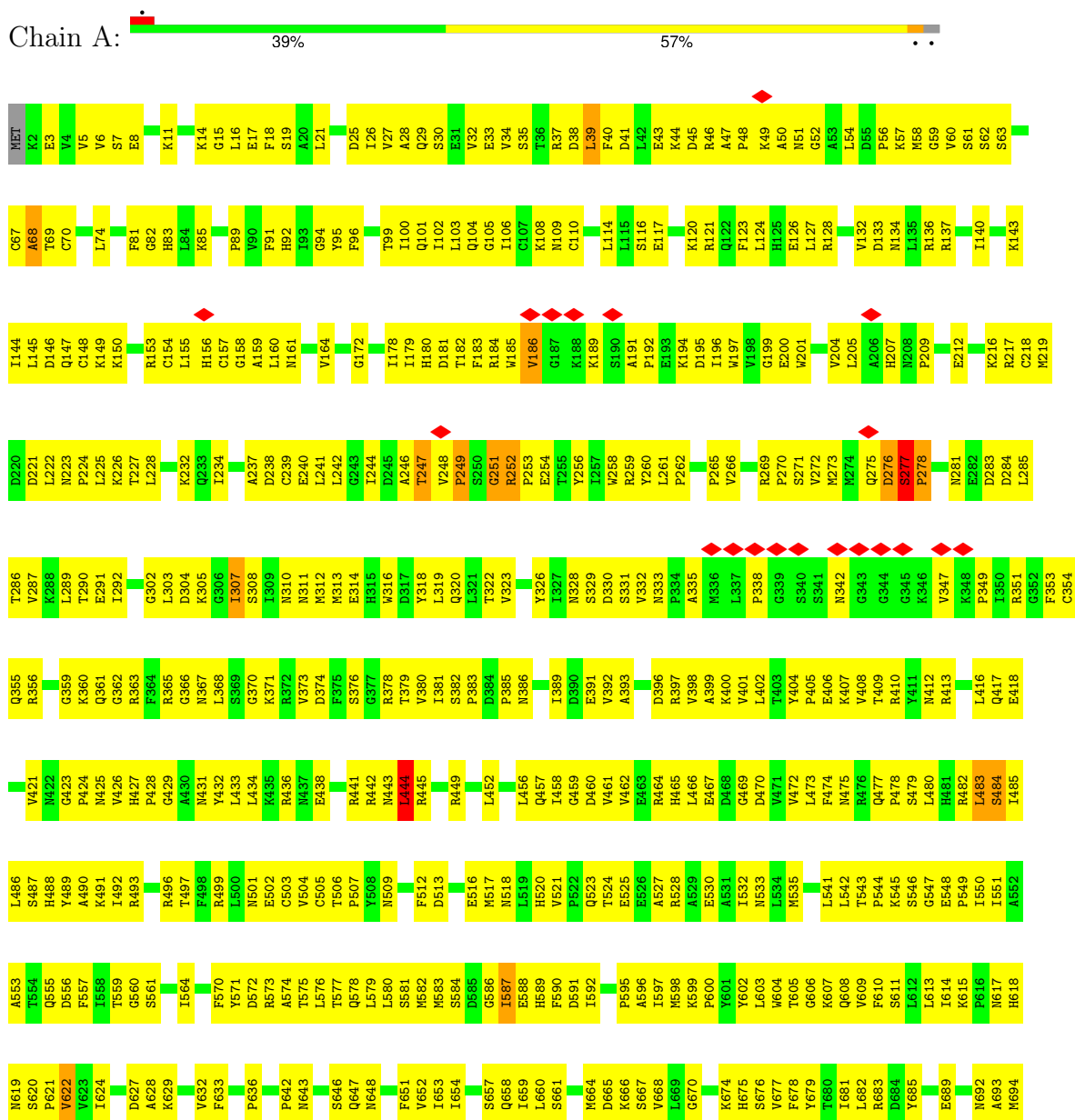
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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	R	1	1	1	0

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 III subunit RPC1

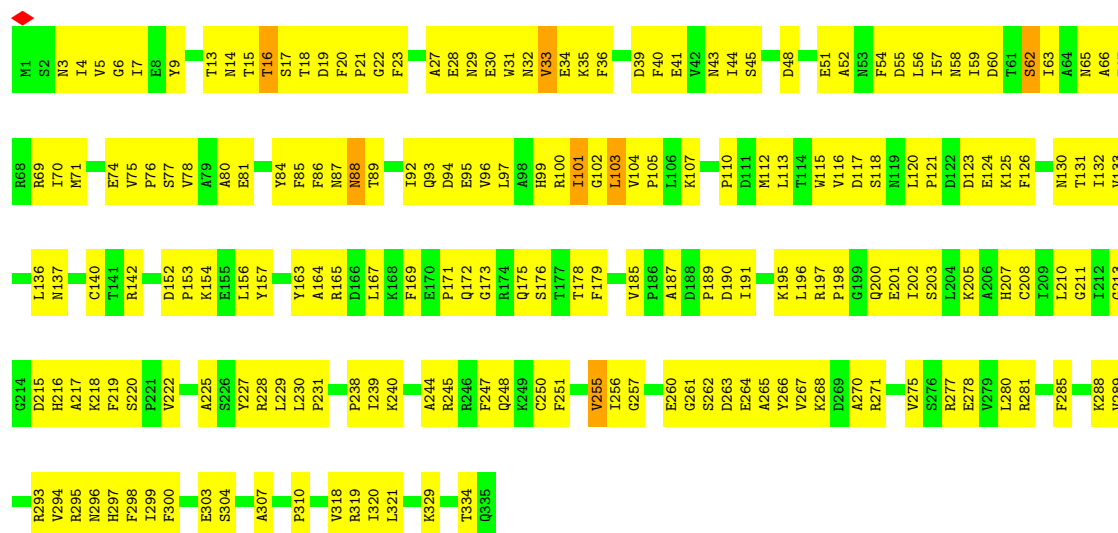


R1067	D1068	C1069	V1070	Y1073	S1076	L1077	L1078	L1079	E1011	C1012	L1013	I1017	F1018	F1019	I1022	Y1023	Y1024	Q1025	L1026	L1027	L1028	H1029	M1030	V1031	L1032	D1033	M1034	K1035	C1107	T1108	T1109	K1110	K1111	S1112	A1113	E1114	N1115	I1116	I1117	T1120	Y1123	K1126	L1127	L1128	F1129	E1130	L1131	L1132	L1133	S1134	M1135	I1137			
P848	T849	N850	S851	P855	N858	N859	V860	N861	N861	V862	Q863	T864	Q865	V866	R867	P868	P869	P870	E871	I872	Y873	E877	P878	S879	H880	R881	D882	Q883	M886	S887	N891	D892	Q893	A894	L895	I896	R901	Q902	N903	R904	R905	G909	D910	K911	F912	S913	S914	I915	H916	G917	R919	G920			
V921	C922	G923	I924	V925	V926	K927	Q928	E929	D930	M931	P932	F933	N934	D935	I938	V939	P940	D941	I942	P946	H947	P950	S951	R952	M953	T954	V955	G956	K957	L960	L961	G967	V968	L969	N970	G971	E974	Y975	G976	G981	D986	M987	G988	K989	S990	L991	L992	V993	L994	M995	Q994				
K1001	D1002	M1003	L1004	Y1005	S1006	L1007	I1008	T1009	G1010	E1011	C1012	L1013	I1017	F1018	F1019	I1022	Y1023	Y1024	Q1025	L1026	L1027	L1028	H1029	M1030	V1031	L1032	D1033	M1034	K1035	C1107	T1108	T1109	K1110	K1111	S1112	A1113	E1114	N1115	I1116	I1117	Q1049	P1050	R1054	S1055	L1056	D1057	G1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	E1066
S763	G764	Y765	D766	I767	E768	D769	A770	L771	V772	L773	N774	K775	S776	S777	I778	D779	R780	G781	F782	E786	I787	R788	R789	K790	L795	K796	R797	Y798	A799	N800	H801	Q803	D804	R810	V811	D816	P817	I818	H821	Q822	S823	L824	G825	E831	V832	I841	R842	I843	N844	V847					
P848	T849	N850	S851	P855	N858	N859	V860	N861	N861	V862	Q863	T864	Q865	V866	R867	P868	P869	P870	E871	I872	Y873	E877	P878	S879	H880	R881	D882	Q883	M886	S887	N891	D892	Q893	A894	L895	I896	R901	Q902	N903	R904	R905	G909	D910	K911	F912	S913	S914	I915	H916	G917	R919	G920			
V921	C922	G923	I924	V925	V926	K927	Q928	E929	D930	M931	P932	F933	N934	D935	I938	V939	P940	D941	I942	P946	H947	P950	S951	R952	M953	T954	V955	G956	K957	L960	L961	G967	V968	L969	N970	G971	E974	Y975	G976	G981	D986	M987	G988	K989	S990	L991	L992	V993	L994	M995	Q994				
K1001	D1002	M1003	L1004	Y1005	S1006	L1007	I1008	T1009	G1010	E1011	C1012	L1013	I1017	F1018	F1019	I1022	Y1023	Y1024	Q1025	L1026	L1027	L1028	H1029	M1030	V1031	L1032	D1033	M1034	K1035	C1107	T1108	T1109	K1110	K1111	S1112	A1113	E1114	N1115	I1116	I1117	Q1049	P1050	R1054	S1055	L1056	D1057	G1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	E1066
D63	S64	F65	M66	Y67	F68	D72	I76	I77	I78	I79	Q81	L82	I83	L84	S85	D86	V87	D88	P89	E90	F91	Y92	L93	K94	Y95	V96	D97	I98	R99	V100	A101	G101	K102	S107	T108	K109	D110	Y111	L112	H116	D122	M123	Y125	S126	A127	P128	I129	Y130	V131	D132	I133	E134	Y135	T136	R137
G138	R139	N140	I141	I142	M143	H144	K145	D146	E148	V149	G150	R151	M152	P153	S154	M155	L156	R157	S158	Y159	N159	Y164	D165	A166	D167	T168	S169	K170	M171	A172	K173	L174	N175	E176	C177	P178	L179	Y184	F185	I186	V187	M188	G189	T190	K192	V193	I194	Q197	E198	S201	K202	N203	E204	T205	
I206	V207	E208	A209	D210	E211	K212	K213	G214	I215	V216	Q217	V220	T221	S222	S223	T224	H225	E226	R227	K228	S229	Y232	V233	I234	T235	D236	N237	G238	K239	I240	Y241	L242	K243	H244	N245	S246	I247	A248	E249	I251	P252	I253	A254	I255	V256	L257	K258	A259	L263	S264	D265	L266	E267	I268	
L271	G274	S277	S278	E279	Y280	D281	I282	F283	A284	V285	N286	L287	P288	E289	K292	T295	Y296	T297	Q298	Q299	Q300	A301	L302	E303	G306	A307	K308	V309	R313	R314	Q315	K316	L317	T318	I319	L320	Q321	E322	I324	E325	A326	I327	A328	T329	I332	A333	V337	E338	A339	L340					
D341	F342	R343	E344	K345	A346	L347	Y348	M351	M352	F283	A284	V285	N286	L287	P288	E289	K292	T295	Y296	T297	Q298	Q299	Q300	A301	L302	E303	G306	A307	K308	V309	R313	R314	Q315	K316	L317	T318	I319	L320	Q321	E322	I324	E325	A326	I327	A328	T329	I332	A333	V337	E338	A339	L340			
M411	A413	M414	E415	Y416	D417	A418	L419	L420	S421	I422	H425	S426	M427	M428	I429	T430	M434	R435	S438	T439	M442	M449	E450	R451	V454	T455	H456	V457	L458	S459	R460	L461	Y463	I464	S465	M469	R472	I473	Q476	E478	K479	S480	R481	S484	G485	P486									
R487	A488	L489	Q490	Q493	F494	G495	M496	L497	C498	T499	A500	E501	T502	P503	E504	G509	L510	V511	L514	A515	N516	T518	H519	I520	T521	T522	S523	D524	E525	E526	P528	I529	K530	K531	L532	C533	Y534	V535	L536	G537	V538	E539	D540	I541	T544	D545	S546	L549	N552	Y553	G554				
V555	Y556	N557	S558	T560	L561	I562	G563	S564	I565	F566	P567	P568	F571	Q574	F575	R576	H577	L578	R579	R580	K583	V584	S585	E586	F587	I588	S589	I590	Y591	S592	N593	Q596	M597	A598	V599	H600	I601	A602	T603	G606	R607	I608	C609	P611	L612	I613	G614	V615	S616	Q619	S620				
R621	V622	G623	D624	I625	H626	L627	R628	K629	L630	L631	L635	D636	F637	D638	D639	F640	L643	G644	L645	V646	E647	Y648	L649	D650	V651	N652	E653	F654	N655	Y658	I659	A660	V667	P668	S669	M670	T671	H672	L673	E674	I675	E676	I680	L681	G682	A683	V684	G685	G686	L687	I688	P689	Y690	P691	
H692	H693	N694	Q695	S696	H697	R698	N699	Q702	A709	I710	L711	I712	A714	R715	N716	Q717	R720	I721	D722	T723	L724	L725	Y726	D727	M728	R729	E730	Y731	Q732	P733	T734	M735	V736	K737	T738	K739	T740	I741	E742	L743	Y746	D747	P750	Q753	N754	T755	V756	T757	A758	V759	S761	Y762			
S763	G764	Y765	D766	I767	E768	D769	A770	L771	V772	L773	N774	K775	S776	S777	I778	D779	R780	G781	F782	E786	I787	R788	R789	K790	L795	K796	R797	Y798	A799	N800	H801	Q803	D804	R810	V811	D816	P817	I818	H821	Q822	S823	L824	G825	E831	V832	I841	R842	I843	N844	V847					
P848	T849	N850	S851	P855	N858	N859	V860	N861	N861	V862	Q863	T864	Q865	V866	R867	P868	P869	P870	E871	I872	Y873	E877	P878	S879	H880	R881	D882	Q883	M886	S887	N891	D892	Q893	A894	L895	I896	R901	Q902	N903	R904	R905	G909	D910	K911	F912	S913	S914	I915	H916	G917	R919	G920			
V921	C922	G923	I924	V925	V926	K927	Q928	E929	D930	M931	P932	F933	N934	D935	I938	V939	P940	D941	I942	P946	H947	P950	S951	R952	M953	T954	V955	G956	K957	L960	L961	G967	V968	L969	N970	G971	E974	Y975	G976	G981	D986	M987	G988	K989	S990	L991	L992	V993	L994	M995	Q994				
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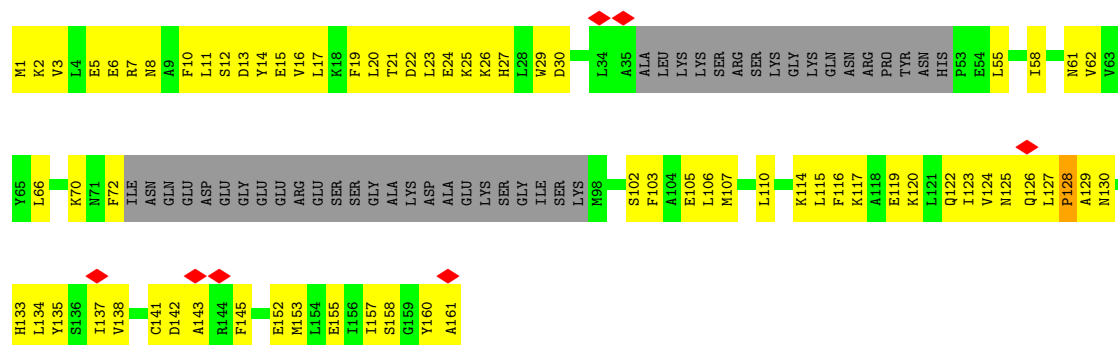
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 41% 57%



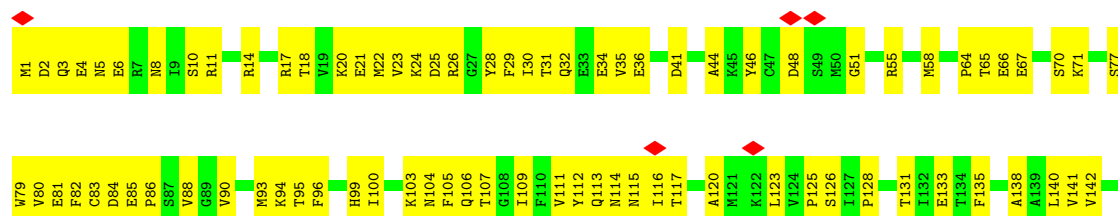
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D: 30% 43% 26%



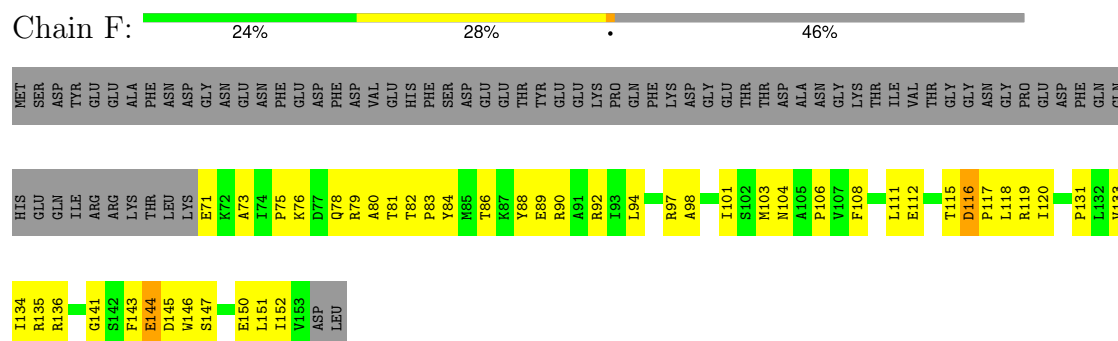
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 43% 57%

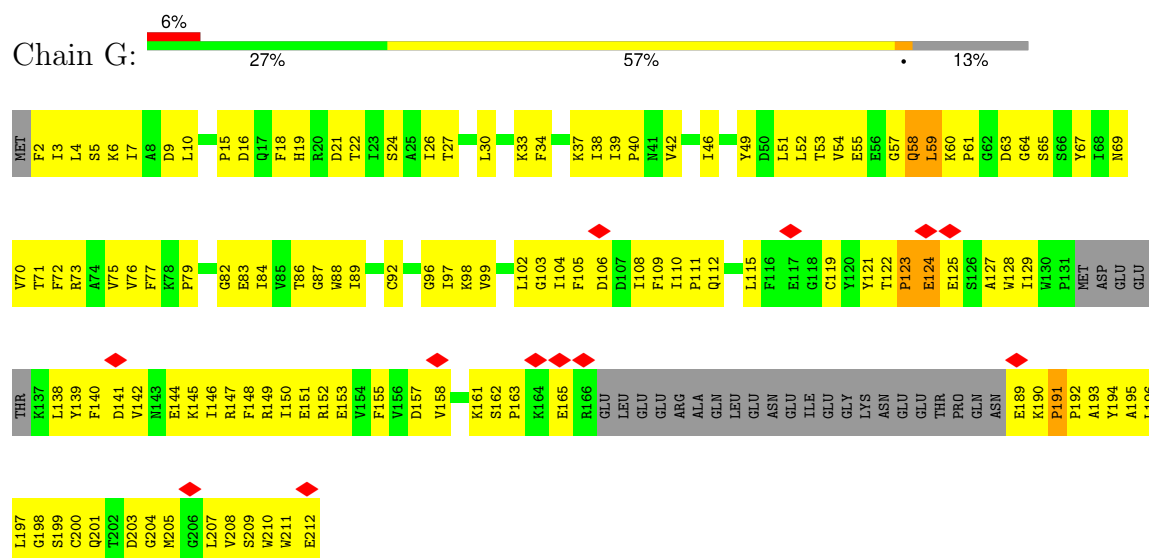




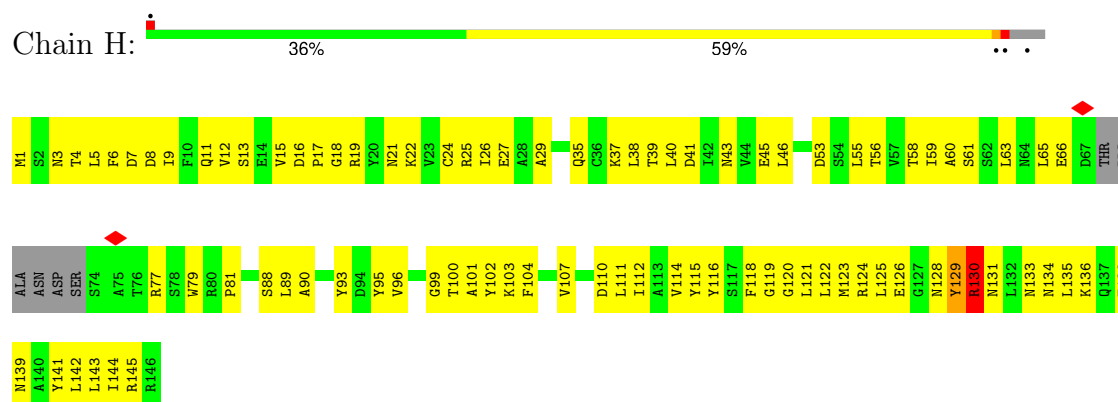
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



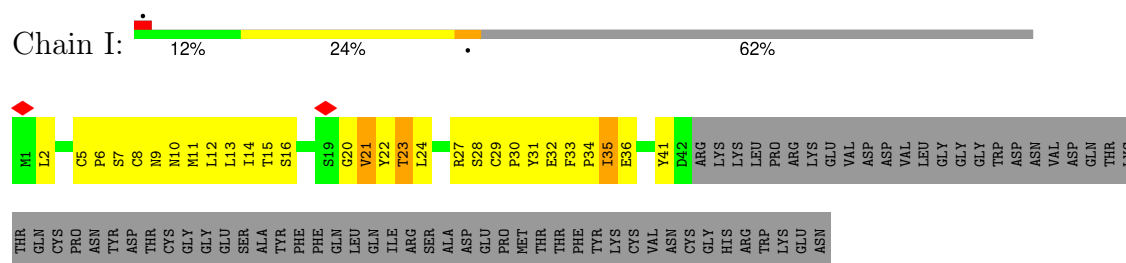
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



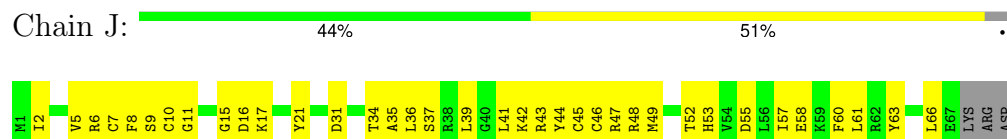
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



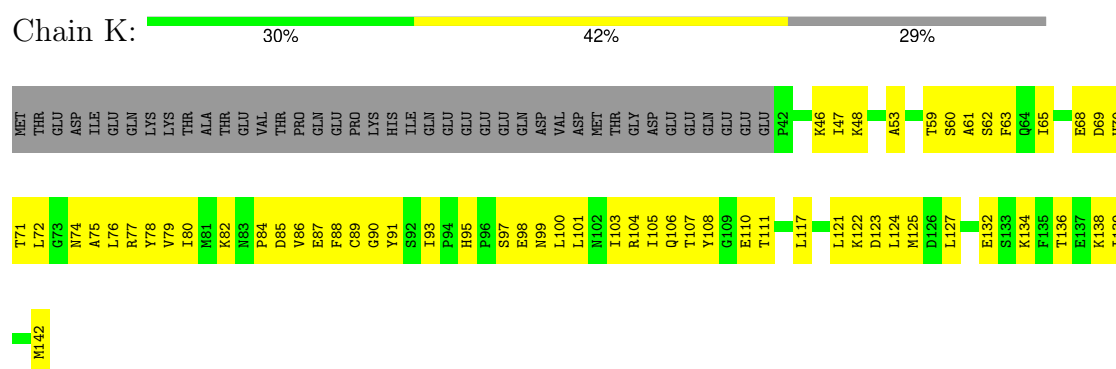
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



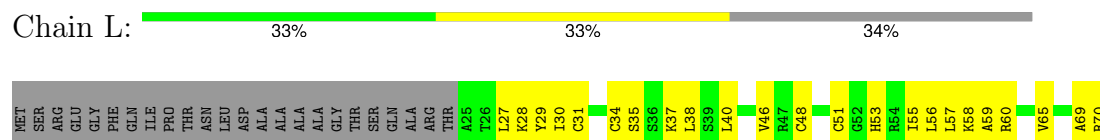
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



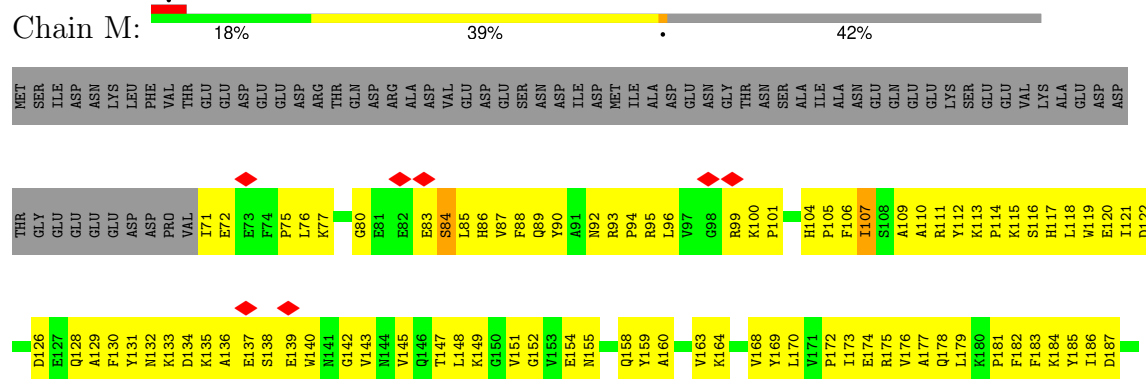
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



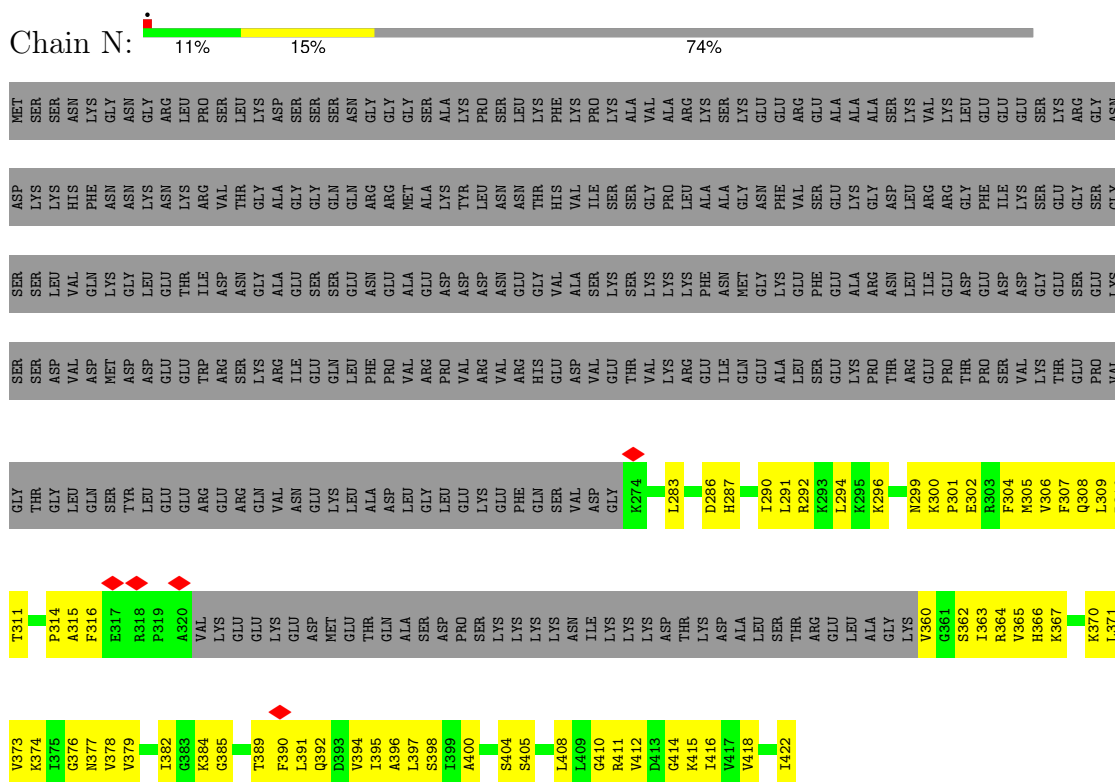
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



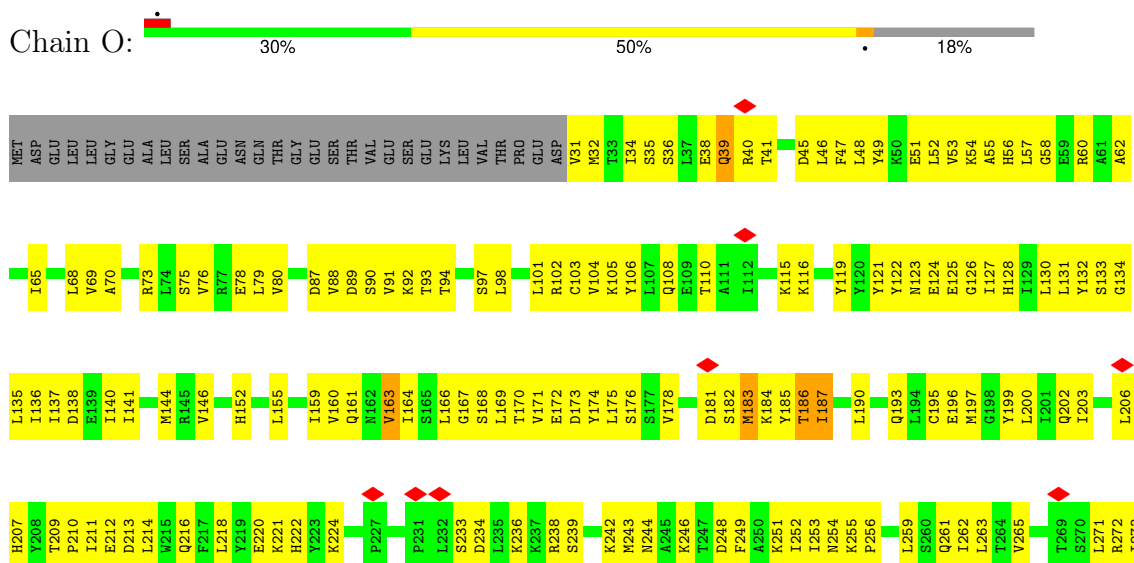
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5



- Molecule 14: DNA-directed RNA polymerase III subunit RPC4



- Molecule 15: DNA-directed RNA polymerase III subunit RPC3









A64
C65
T66
A67
A68
T69
A70
T71
A72
T73
G74
T75
T76
G77
A78
A79

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47141	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	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.9	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	0.197	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (\AA)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.18, 1.18, 1.18	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	0.36	0/11358	0.61	0/15345
2	B	0.37	0/8943	0.62	0/12068
3	C	0.35	0/2711	0.60	0/3676
4	D	0.27	0/991	0.52	0/1328
5	E	0.32	0/1795	0.55	0/2416
6	F	0.34	0/683	0.56	0/923
7	G	0.30	0/1523	0.53	0/2066
8	H	0.33	0/1138	0.59	0/1540
9	I	0.35	0/328	0.69	0/445
10	J	0.44	0/558	0.57	0/750
11	K	0.35	0/803	0.57	0/1083
12	L	0.33	0/365	0.62	0/485
13	M	0.31	0/1369	0.58	0/1851
14	N	0.28	0/855	0.61	0/1149
15	O	0.33	0/4394	0.62	0/5928
16	P	0.29	0/2282	0.55	1/3075 (0.0%)
17	Q	0.35	0/281	0.50	0/381
18	R	0.31	1/4200 (0.0%)	0.49	0/5659
19	S	0.29	0/1464	0.52	0/1971
20	X	0.66	0/1072	1.09	1/1651 (0.1%)
21	Y	0.62	0/1313	0.98	1/2022 (0.0%)
All	All	0.36	1/48426 (0.0%)	0.62	3/65812 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	173	LEU	C-N	8.59	1.50	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	X	63	DC	O4'-C4'-C3'	-7.84	101.29	106.00
16	P	152	SER	N-CA-CB	5.95	119.42	110.50
21	Y	61	DA	O4'-C4'-C3'	-5.12	102.45	104.50

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	11159	0	11285	1008	0
2	B	8788	0	8901	770	0
3	C	2655	0	2628	218	0
4	D	977	0	983	91	0
5	E	1759	0	1788	113	0
6	F	671	0	692	53	0
7	G	1484	0	1485	140	0
8	H	1120	0	1089	92	0
9	I	321	0	303	41	0
10	J	549	0	559	50	0
11	K	792	0	790	78	0
12	L	363	0	387	26	0
13	M	1338	0	1307	142	0
14	N	845	0	891	77	0
15	O	4329	0	4497	448	0
16	P	2242	0	2265	234	0
17	Q	368	0	308	27	0
18	R	4131	0	4230	269	0
19	S	1649	0	1455	111	0
20	X	959	0	539	59	0
21	Y	1169	0	645	66	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	47675	0	47027	3654	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 39.

The worst 5 of 3654 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)
1:A:484:SER:HB2	2:B:1069:CYS:SG	1.40	1.58
15:O:330:LEU:CD1	15:O:331:THR:HG23	1.27	1.58
15:O:330:LEU:CD1	15:O:331:THR:H	1.20	1.54
1:A:1145:LEU:CD1	1:A:1146:VAL:H	1.20	1.52
2:B:590:ILE:HA	2:B:601:ILE:CD1	1.45	1.45

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1422/1460 (97%)	1106 (78%)	292 (20%)	24 (2%)	7	36
2	B	1112/1149 (97%)	901 (81%)	194 (17%)	17 (2%)	8	39
3	C	333/335 (99%)	282 (85%)	44 (13%)	7 (2%)	5	30
4	D	113/161 (70%)	87 (77%)	24 (21%)	2 (2%)	7	34
5	E	213/215 (99%)	182 (85%)	29 (14%)	2 (1%)	14	51
6	F	81/155 (52%)	66 (82%)	13 (16%)	2 (2%)	4	27
7	G	178/212 (84%)	145 (82%)	30 (17%)	3 (2%)	7	36
8	H	136/146 (93%)	112 (82%)	23 (17%)	1 (1%)	19	56
9	I	40/110 (36%)	30 (75%)	7 (18%)	3 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	65/70 (93%)	54 (83%)	11 (17%)	0	100	100
11	K	99/142 (70%)	77 (78%)	22 (22%)	0	100	100
12	L	44/70 (63%)	33 (75%)	11 (25%)	0	100	100
13	M	160/282 (57%)	127 (79%)	31 (19%)	2 (1%)	10	42
14	N	106/422 (25%)	82 (77%)	24 (23%)	0	100	100
15	O	533/654 (82%)	401 (75%)	116 (22%)	16 (3%)	3	23
16	P	271/317 (86%)	219 (81%)	47 (17%)	5 (2%)	7	34
17	Q	33/251 (13%)	28 (85%)	5 (15%)	0	100	100
18	R	514/736 (70%)	439 (85%)	72 (14%)	3 (1%)	22	60
19	S	172/594 (29%)	157 (91%)	14 (8%)	1 (1%)	22	60
All	All	5625/7481 (75%)	4528 (80%)	1009 (18%)	88 (2%)	10	37

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	PRO
1	A	252	ARG
1	A	587	ILE
1	A	837	LYS
1	A	1033	GLU

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	1232/1257 (98%)	1222 (99%)	10 (1%)	79	84
2	B	975/1006 (97%)	970 (100%)	5 (0%)	86	89
3	C	296/296 (100%)	295 (100%)	1 (0%)	91	91
4	D	110/145 (76%)	110 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	164/190 (86%)	162 (99%)	2 (1%)	67	79
8	H	123/128 (96%)	121 (98%)	2 (2%)	58	74
9	I	38/98 (39%)	38 (100%)	0	100	100
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	142/249 (57%)	142 (100%)	0	100	100
14	N	92/360 (26%)	92 (100%)	0	100	100
15	O	495/593 (84%)	491 (99%)	4 (1%)	79	84
16	P	255/285 (90%)	252 (99%)	3 (1%)	67	79
17	Q	31/195 (16%)	31 (100%)	0	100	100
18	R	450/623 (72%)	450 (100%)	0	100	100
19	S	157/494 (32%)	157 (100%)	0	100	100
All	All	5023/6505 (77%)	4996 (100%)	27 (0%)	85	89

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	863	GLN
7	G	59	LEU
16	P	203	LYS
7	G	58	GLN
8	H	129	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	133	ASN
15	O	222	HIS
13	M	86	HIS
14	N	377	ASN
15	O	584	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	S	1
17	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	319:UNK	C	360:THR	N	39.73
1	Q	70:PHE	C	1070:UNK	N	13.87

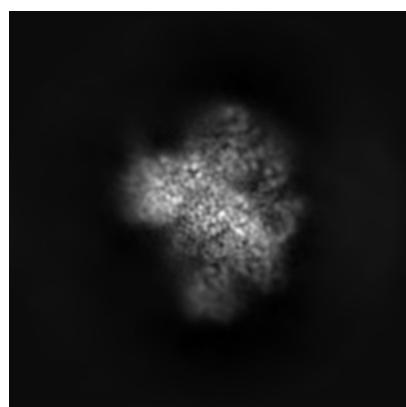
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7533. These allow visual inspection of the internal detail of the map and identification of artifacts.

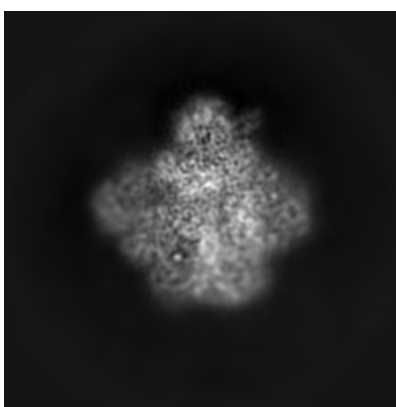
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

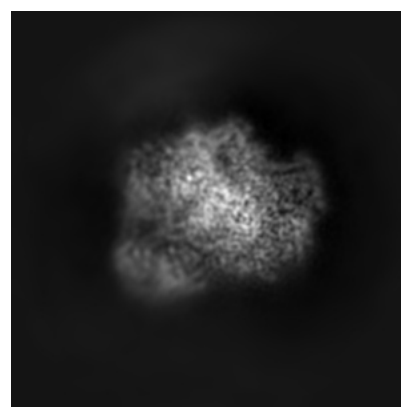
6.1.1 Primary map



X



Y

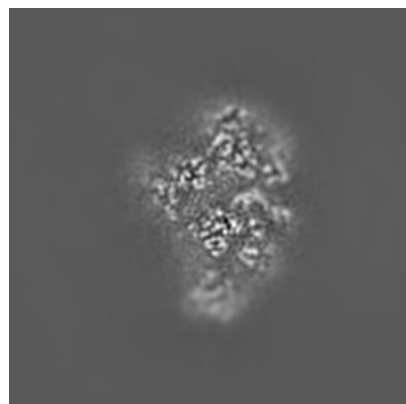


Z

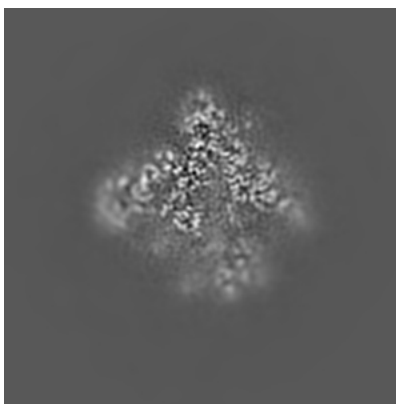
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

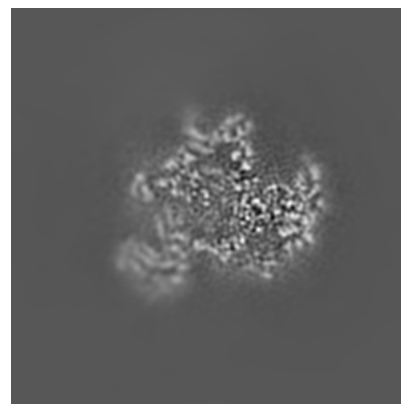
6.2.1 Primary map



X Index: 144



Y Index: 144

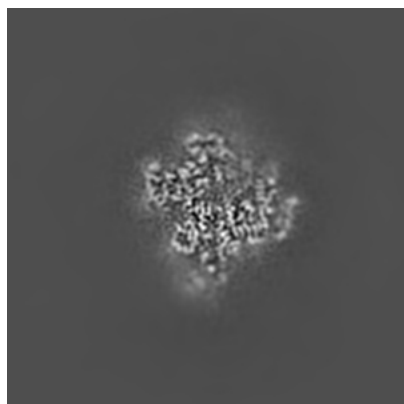


Z Index: 144

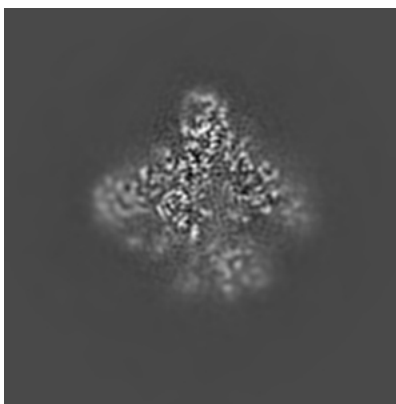
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

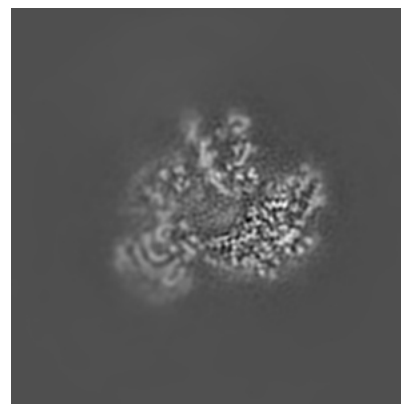
6.3.1 Primary map



X Index: 169



Y Index: 147

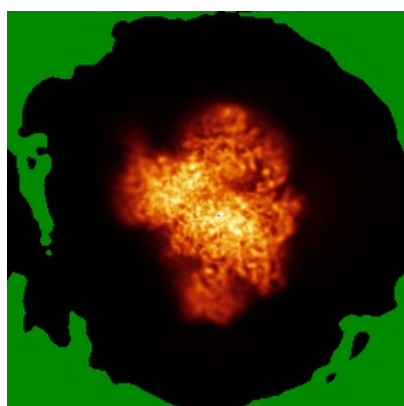


Z Index: 150

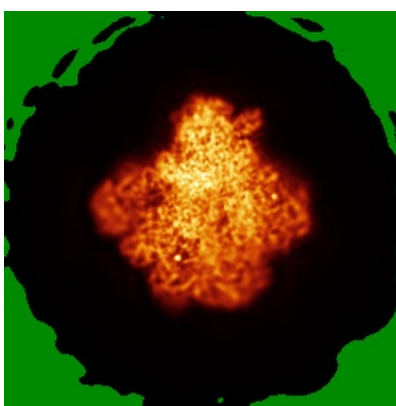
The images above show the largest variance slices of the map in three orthogonal directions.

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

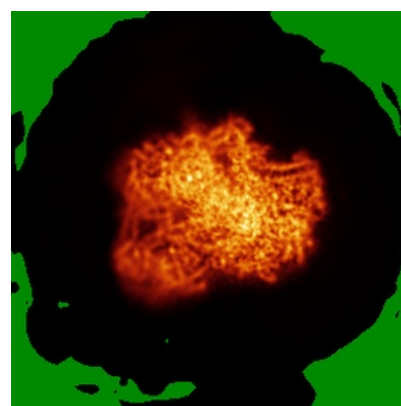
6.4.1 Primary map



X



Y

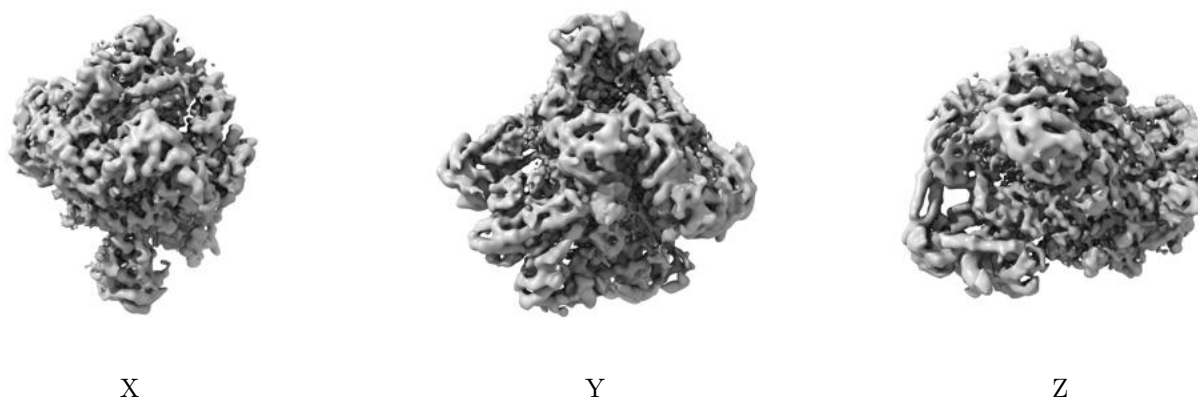


Z

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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

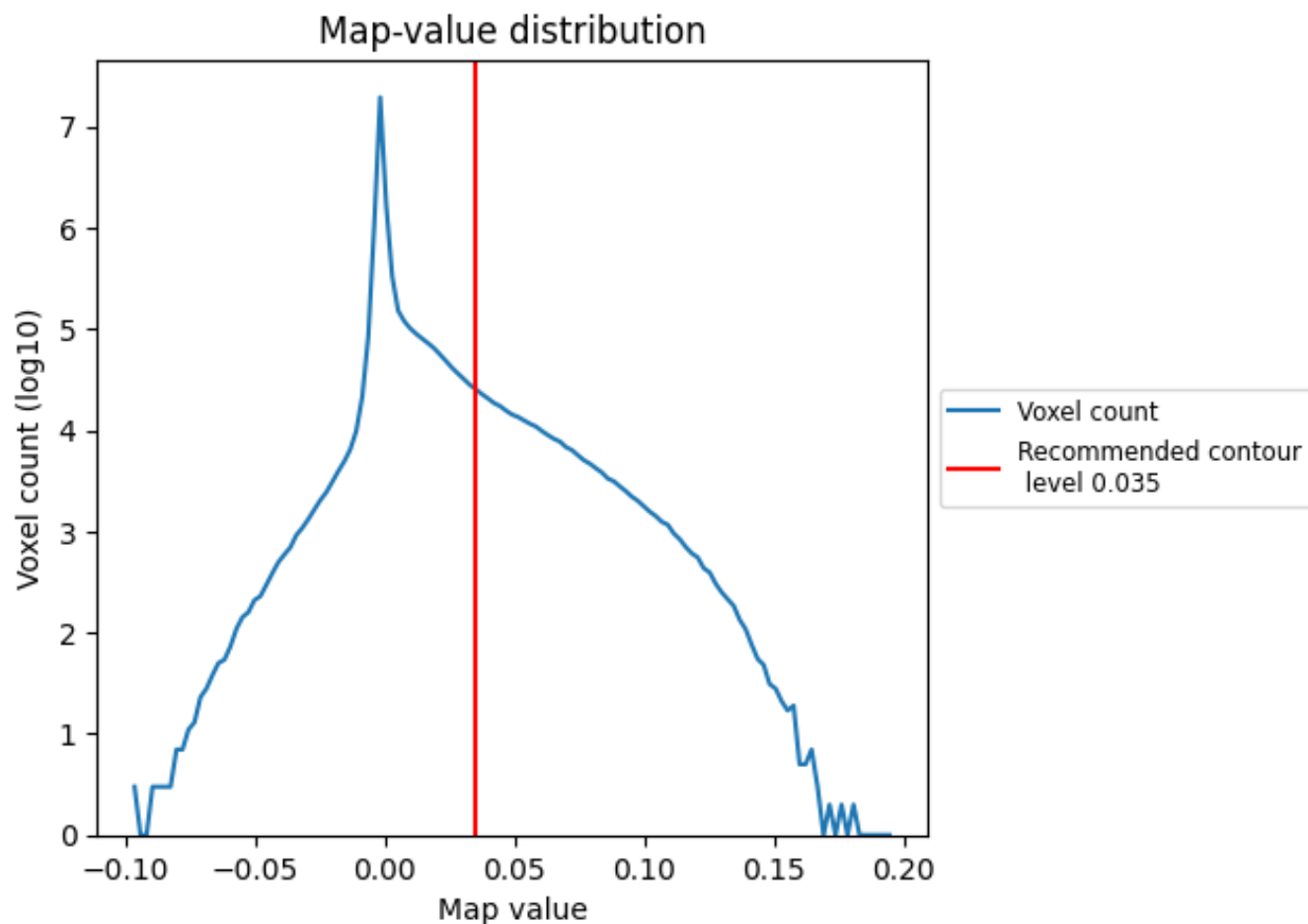
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

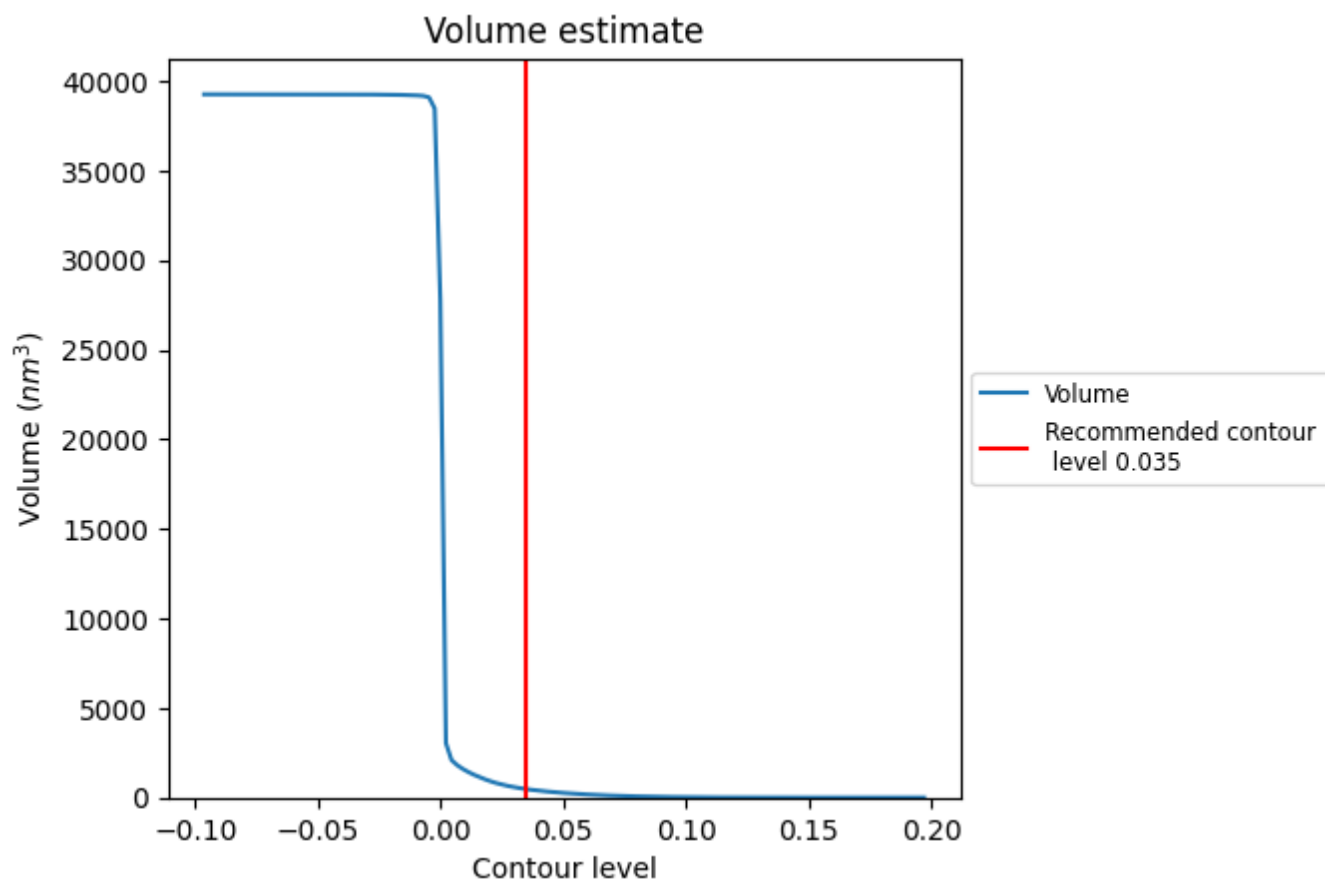
This section contains the results of statistical analysis of the map.

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.

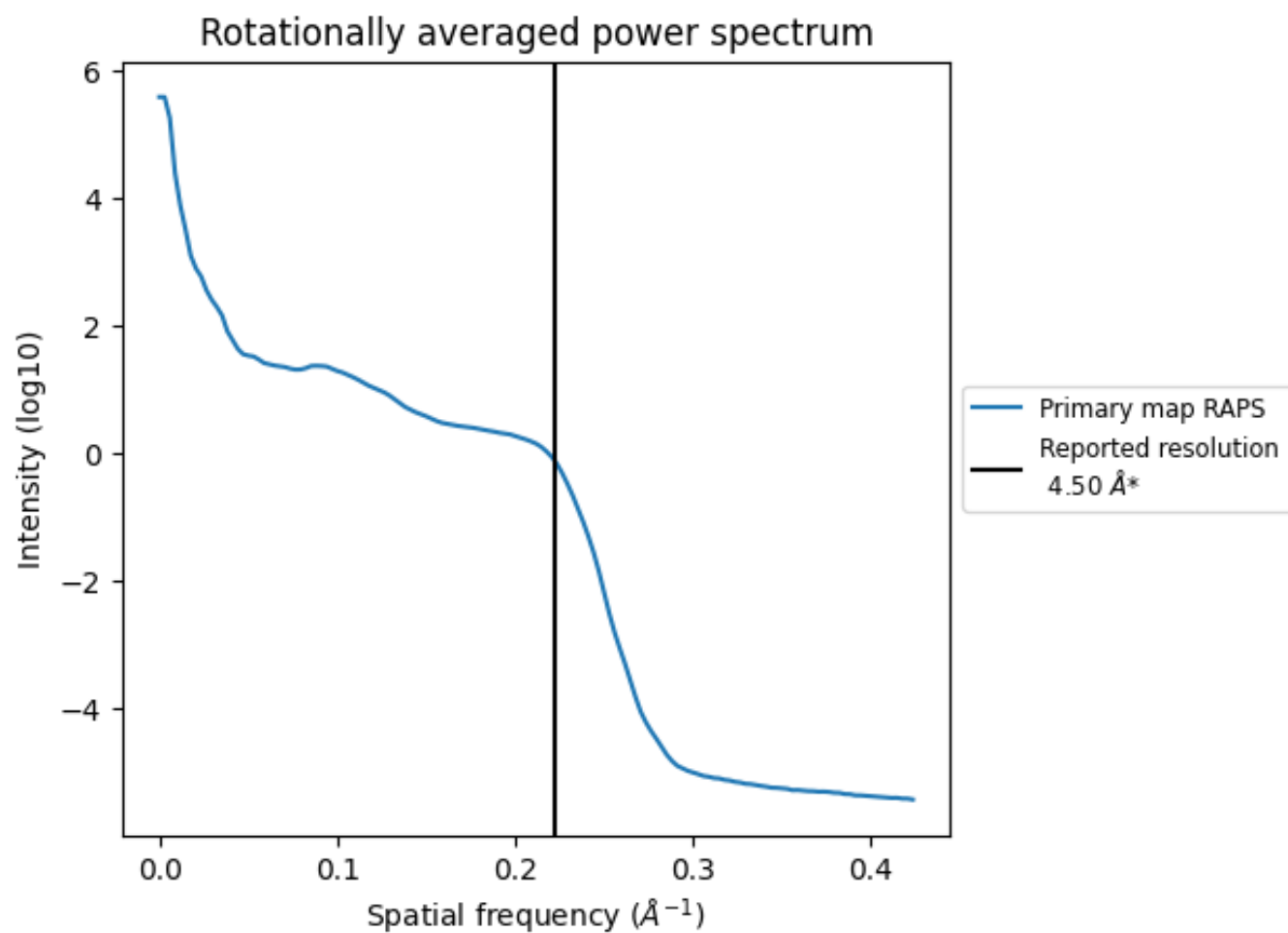
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 470 nm³; this corresponds to an approximate mass of 424 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 ⓘ

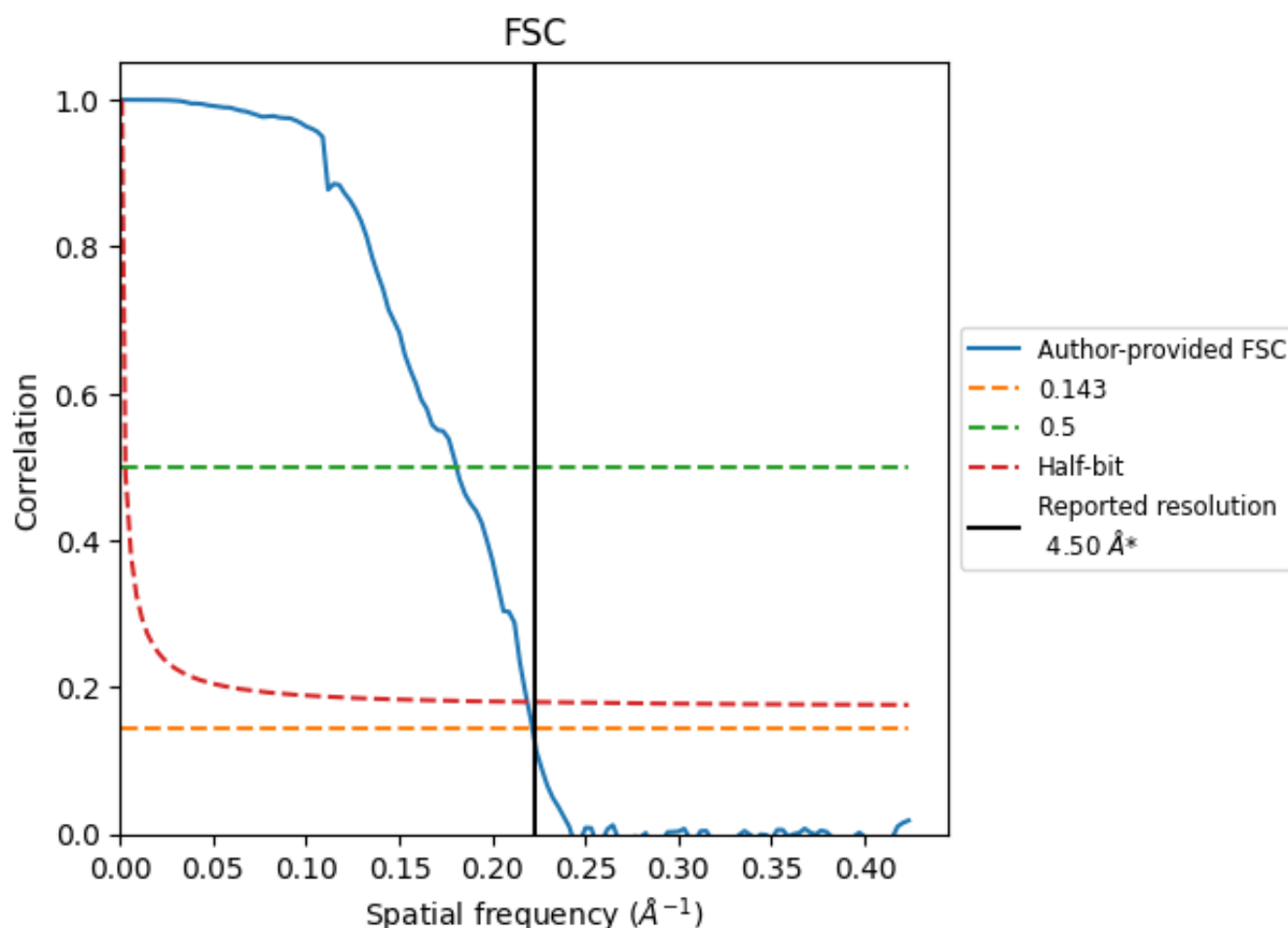


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

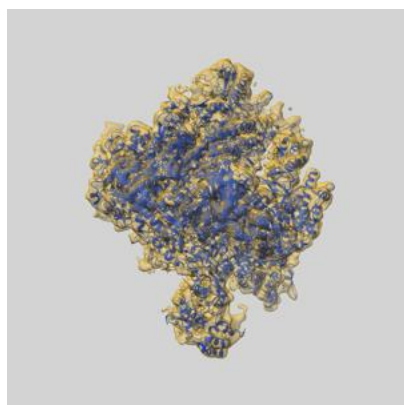
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.51	5.53	4.57
Unmasked-calculated*	-	-	-

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

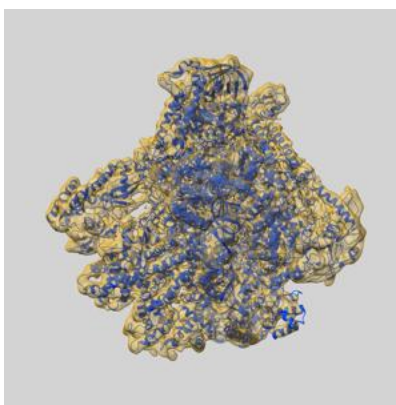
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7533 and PDB model 6CNF. Per-residue inclusion information can be found in section [3](#) on page [9](#).

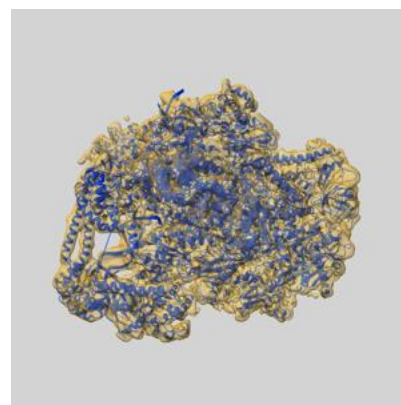
9.1 Map-model overlay [i](#)



X



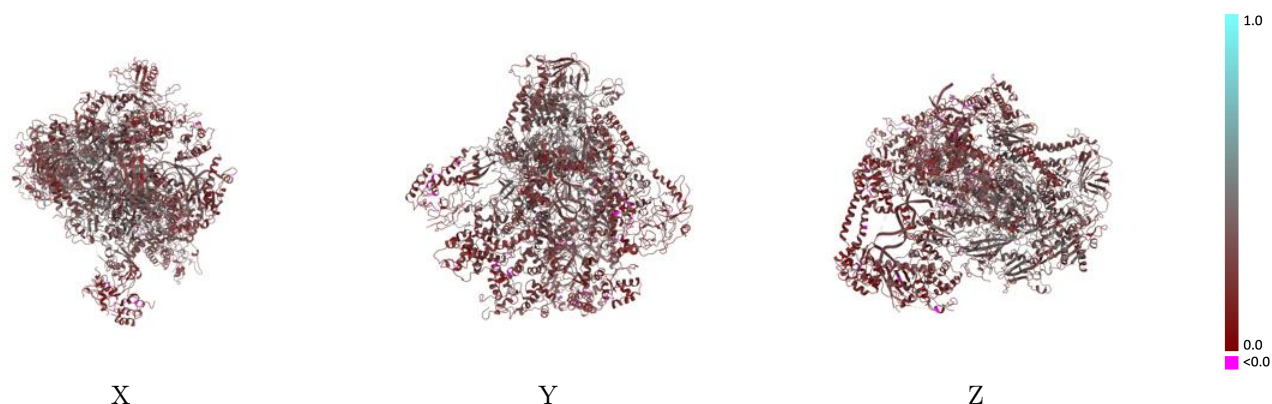
Y



Z

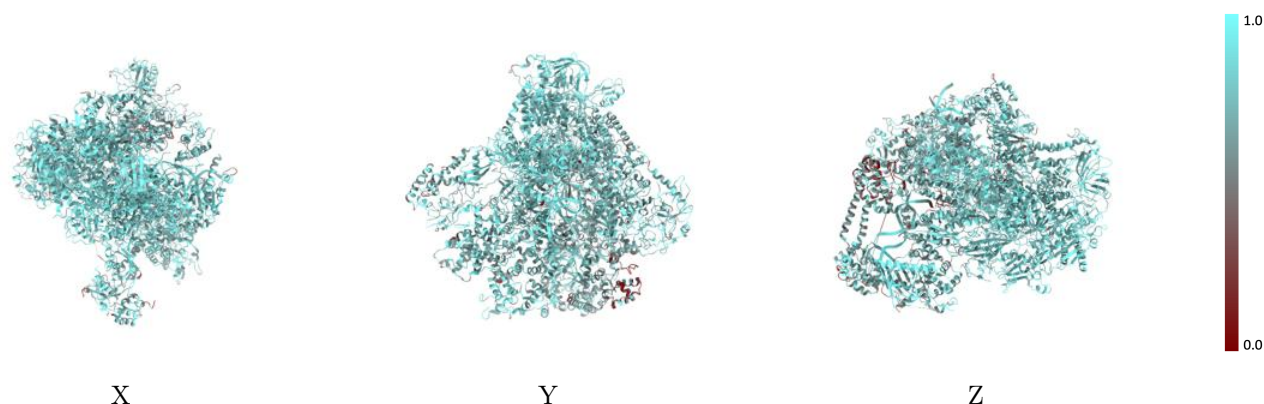
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



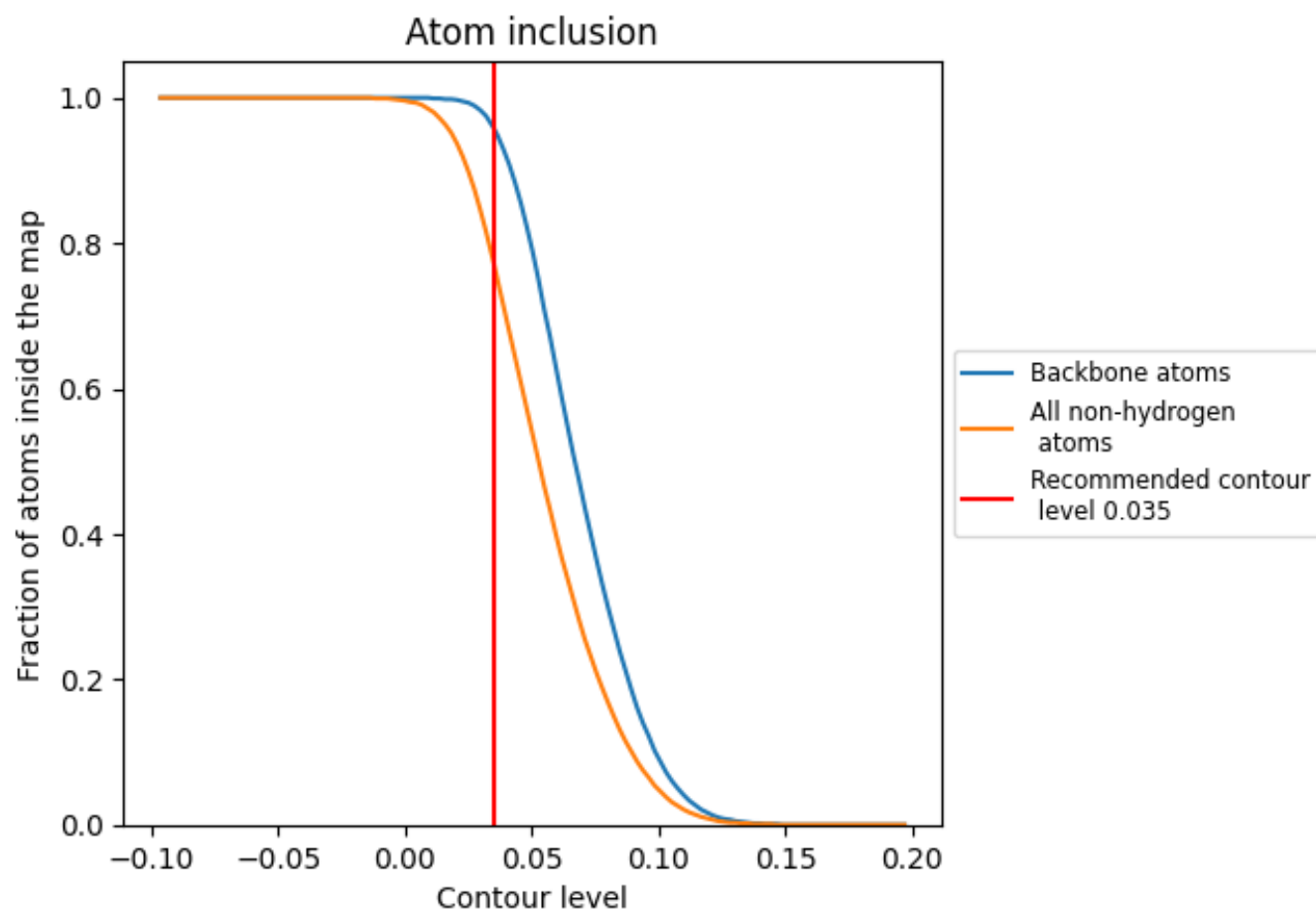
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 77% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.2950
A	 0.7880	 0.3320
B	 0.7870	 0.3390
C	 0.8500	 0.3350
D	 0.7270	 0.1820
E	 0.7870	 0.2910
F	 0.8640	 0.3640
G	 0.7800	 0.2340
H	 0.8340	 0.3170
I	 0.7760	 0.2400
J	 0.8410	 0.3440
K	 0.8290	 0.3360
L	 0.8380	 0.3490
M	 0.7080	 0.2280
N	 0.7530	 0.2430
O	 0.7260	 0.2560
P	 0.6670	 0.2290
Q	 0.8790	 0.3320
R	 0.7000	 0.2270
S	 0.6270	 0.2160
X	 0.9200	 0.2960
Y	 0.8920	 0.3150

